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Course handout

For the use of students of (3rd year of a Bachelor's degree in Applied Mathematics LMD)

Explanatory Data Analysis: Course and Exercises

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Contents

Preface

This handbook, *Exploratory Data Analysis*, is designed for undergraduate students in Applied Mathematics, particularly those at the third-year level who have acquired foundational knowledge in linear algebra, probability, and introductory statistics. It aims to bridge the gap between theoretical training and the practical demands of analyzing multidimensional data, serving both as a course companion and a self-contained guide for independent study.

The motivation for this text stems from the increasingly critical role that exploratory data analysis (EDA) plays across scientific and industrial disciplines. As data generation accelerates in fields such as economics, engineering, biomedical research, and the social sciences, the ability to interrogate, visualize, and interpret complex datasets has become an essential competency. This book provides the conceptual and computational tools necessary to undertake such analyses with confidence and intellectual rigor.

A core pedagogical commitment throughout this text is the balance between mathematical depth and interpretive clarity. Each method introduced—including principal component analysis, correspondence analysis, and related factorial techniques—is grounded in its algebraic and geometric foundations, yet always accompanied by intuitive explanations, practical examples, and contextual interpretations. While the *why* is established formally, equal emphasis is placed on the *how* and the *so what*, fostering not only technical proficiency but also statistical literacy.

A distinctive feature of this handbook is its emphasis on active learning. Each chapter concludes with exercises ranging from fundamental applications to more integrative problems that simulate real-world analytical challenges. Detailed solutions are provided to illustrate the complete analytical process—from assumption checking and computation to interpretation and conclusion—enabling students to refine their approach through examples and repetition.

This text does not aspire to be exhaustive; EDA is a dynamic and expanding field. Instead, it focuses on the cornerstone methods that remain deeply relevant both in traditional statistics and in modern machine learning and data science. Mastery of these techniques provides a strong foundation for further specialization.

I am indebted to the many students whose curiosity and feedback have profoundly shaped this material. Their experiences—both struggles and insights—are reflected in the pacing and explanations found in these pages. I also extend my gratitude to colleagues for their valuable suggestions and intellectual camaraderie.

To the student reader: embrace the challenge ahead. Data analysis is a discipline that marries logic with creativity, structure with intuition. It is my sincere hope that this handbook becomes a trusted resource in your educational journey—enabling you

to derive meaning from complexity and to contribute thoughtfully to a data-driven world.

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General Introduction

Context and Motivation

Exploratory Data Analysis (EDA) constitutes a foundational pillar of modern statistical practice. The term, first systematically developed by John W. Tukey in his seminal work *Exploratory Data Analysis* (1977), emphasizes the critical importance of understanding data through visualization, summary, and pattern recognition before proceeding to formal modeling or inference. EDA provides the essential toolkit for this initial investigative phase, combining numerical summaries, graphical representations, and multivariate techniques to reveal underlying structures and anomalies in data [14], [10].

In the contemporary landscape of data-intensive research across scientific and industrial domains, the relevance of EDA has only intensified. From economics and genomics to engineering, social sciences, and machine learning, EDA serves as the crucial first step in extracting meaningful insights from complex datasets, guiding subsequent modeling decisions and hypothesis generation [11], [15].

For students of applied mathematics, EDA represents an ideal domain that integrates theoretical rigor—drawing on linear algebra, matrix analysis, and probability theory—with practical application to real-world problems. This dual character makes it particularly suited for advanced undergraduate education, bridging abstract mathematical concepts with empirical analysis.

Pedagogical Objectives

This handbook is designed for third-year undergraduate students in Applied Mathematics who possess foundational knowledge in linear algebra, calculus, and probability. Its primary objectives are to:

- Provide a **rigorous mathematical foundation** for each method, drawing on spectral theory, Euclidean geometry, and matrix decomposition techniques;
- Emphasize **practical interpretation** of results, ensuring students can translate mathematical outputs into substantive insights;
- Follow a **structured pedagogical progression** from univariate to multivariate analysis, building conceptual understanding incrementally;
- Foster **active learning** through extensive exercises ranging from basic applications to advanced theoretical problems;

- Support **autonomous study** with comprehensive solutions that illustrate complete analytical reasoning.

The Role of EDA in Statistical Practice

Methodologically, EDA occupies the intersection of descriptive statistics, linear algebra, and data visualization. It addresses fundamental questions such as:

- How can we summarize high-dimensional data efficiently?
- What visualization techniques best reveal underlying patterns and relationships?
- How can we detect and characterize associations among multiple variables?
- What dimensional reduction techniques preserve maximal information?

Beyond mere description, EDA provides the essential groundwork for more advanced statistical modeling, including regression analysis, classification, clustering, and machine learning. Proficiency in EDA equips students with the critical thinking skills necessary to evaluate data quality, assess assumptions, and guide subsequent analytical strategies [12, 13].

Structure and Organization

The book is organized into six thematically coherent chapters:

1. **Mathematical Foundations:** Review of Euclidean geometry in $\mathbb{R}^n$ and spectral theory of matrices relevant to multivariate analysis;
2. **Univariate Statistics:** Descriptive measures and graphical representations for single-variable data;
3. **Bivariate Statistics:** Analysis of relationships between two variables, including correlation, regression, and independence testing;
4. **Factorial Analysis of Data Tables:** Conceptual framework for multivariate data analysis;
5. **Principal Component Analysis (PCA):** Dimensionality reduction for quantitative data;
6. **Correspondence Analysis (CA) and Multiple Correspondence Analysis (MCA):** Geometric approaches for categorical data analysis.

Each chapter includes theoretical development, worked examples, and graduated exercises. A comprehensive solutions manual and bibliography appear in the appendices.

Concluding Perspective

This handbook aims not merely to convey technical knowledge but to cultivate the analytical mindset essential for statisticians and applied mathematicians. Mastery of exploratory data analysis enables students to approach data with both mathematical sophistication and empirical curiosity.

As Tukey (1977) aptly noted, the greatest value of EDA lies in its capacity to reveal the unexpected. We hope this text helps students develop this spirit of discovery, preparing them for advanced study and professional application in the analysis of complex data.

Chapter 1

Mathematical Foundations

Exploratory Data Analysis (EDA) relies heavily on concepts from linear algebra and matrix theory. In particular, the geometry of Euclidean spaces and the spectral properties of symmetric matrices form the mathematical foundation of many multivariate methods such as Principal Component Analysis (PCA) and Correspondence Analysis (CA). The objective of this chapter is to review these essential notions, ensuring that students have the necessary background before engaging with the statistical techniques developed in later chapters. For references, see [9, 16, 18, 19].

1.1 Euclidean Structure of $\mathbb{R}^n$

Definition of a Vector Space

A vector space over $\mathbb{R}$ is a set V equipped with two operations:

- vector addition: $x + y \in V$ for all $x, y \in V$,
- scalar multiplication: $\alpha x \in V$ for all $\alpha \in \mathbb{R}, x \in V$,

satisfying the usual axioms (associativity, commutativity, distributivity, existence of neutral and inverse elements). The canonical example is $\mathbb{R}^n$, the space of real n-tuples $x = (x_1, \ldots, x_n)$.

Euclidean Structure

A Euclidean space is a finite-dimensional vector space V over $\mathbb{R}$ equipped with a scalar product (inner product) $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ that is:

1. Bilinear: $\langle ax + by, z \rangle = a\langle x, z \rangle + b\langle y, z \rangle$,
2. Symmetric: $\langle x, y \rangle = \langle y, x \rangle$,
3. Positive definite: $\langle x, x \rangle \geq 0$ with equality if and only if $x = 0$.

In $\mathbb{R}^n$, the canonical inner product is given by:

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i y_i.$$

Norm and Distance

From the scalar product, one defines the norm:

$$\|x\| = \sqrt{\langle x, x \rangle},$$

which measures the "length" of a vector. The induced distance is:

$$d(x, y) = \|x - y\|,$$

which corresponds to the Euclidean distance.

Example

For $x = (1, 2, 3)$ and $y = (4, 0, -1)$ in $\mathbb{R}^3$:

$$\langle x, y \rangle = 1 \cdot 4 + 2 \cdot 0 + 3 \cdot (-1) = 4 - 3 = 1,$$

$$\|x\| = \sqrt{1^2 + 2^2 + 3^2} = \sqrt{14}, \quad \|y\| = \sqrt{4^2 + 0^2 + (-1)^2} = \sqrt{17},$$

$$d(x, y) = \sqrt{(1-4)^2 + (2-0)^2 + (3+1)^2} = \sqrt{9 + 4 + 16} = \sqrt{29}.$$

This section reviews the geometric framework underlying many multivariate methods used later in the book. We work over the real field. Standard references include [9, 16–19].

1.1.1 Vector spaces and coordinates

Definition 1.1 (Vector space and standard basis)**.** The space $\mathbb{R}^n = \{(x_1, \ldots, x_n) : x_i \in \mathbb{R}\}$ is an n-dimensional real vector space with componentwise addition and scalar multiplication. The *standard basis* is $e_1, \ldots, e_n$, where $(e_i)_j = \delta_{ij}$. Every $x \in \mathbb{R}^n$ has a unique coordinate representation $x = \sum_{i=1}^n x_i e_i$.

1.1.2 Inner products, norms, and distance

Definition 1.2 (Inner product)**.** An *inner product* on $\mathbb{R}^n$ is a map $\langle \cdot, \cdot \rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ such that for all x, y, z and $\alpha \in \mathbb{R}$: (i) $\langle x, y \rangle = \langle y, x \rangle$ (symmetry); (ii) $\langle \alpha x + y, z \rangle = \alpha \langle x, z \rangle + \langle y, z \rangle$ (bilinearity); (iii) $\langle x, x \rangle \geq 0$ with equality iff $x = 0$ (positive definiteness). The *canonical* inner product (dot product) is $\langle x, y \rangle = \sum_{i=1}^n x_i y_i = x^\top y$.

Definition 1.3 (Norm and Euclidean distance)**.** The inner product induces the *Euclidean norm* $\|x\|_2 = \sqrt{\langle x, x \rangle} = \sqrt{\sum_{i=1}^n x_i^2}$ and the corresponding distance $d_2(x, y) = \|x - y\|_2$.

Theorem 1.4 (Cauchy–Schwarz inequality)**.** *For all $x, y \in \mathbb{R}^n$,*

$$|\langle x, y \rangle| \leq \|x\|_2 \, \|y\|_2,$$

with equality iff x and y are linearly dependent.

Theorem 1.5 (Triangle inequality and parallelogram law)**.** *For all $x, y \in \mathbb{R}^n$,*

$$\|x+y\|_2 \le \|x\|_2 + \|y\|_2, \qquad \|x+y\|_2^2 + \|x-y\|_2^2 = 2\|x\|_2^2 + 2\|y\|_2^2.$$

Proposition 1.6 (Polarization identity)**.** *For all $x, y \in \mathbb{R}^n$,*

$$\langle x, y\rangle = \tfrac{1}{4}\Big(\|x+y\|_2^2 - \|x-y\|_2^2\Big).$$

Hence the Euclidean inner product is determined by its norm.

1.1.3 Angles and orthogonality

Definition 1.7 (Angle and orthogonality)**.** If $x, y \neq 0$, define the angle $\theta \in [0, \pi]$ by $\cos\theta = \dfrac{\langle x, y\rangle}{\|x\|_2\|y\|_2}$. Vectors are *orthogonal* if $\langle x, y\rangle = 0$. An *orthonormal set* is a family $\{u_1, \dots, u_k\}$ with $\langle u_i, u_j\rangle = \delta_{ij}$.

Theorem 1.8 (Pythagoras)**.** *If $x \perp y$ then $\|x+y\|_2^2 = \|x\|_2^2 + \|y\|_2^2$. More generally, if $\{u_i\}_{i=1}^k$ is orthonormal and $x = \sum_i \alpha_i u_i$, then $\|x\|_2^2 = \sum_{i=1}^k \alpha_i^2$.*

1.1.4 Orthonormal bases and Gram–Schmidt

Theorem 1.9 (Gram–Schmidt orthonormalization [17, Ch. 4])**.** *Given a linearly independent family $(v_1, \dots, v_k)$ in $\mathbb{R}^n$, define recursively*

$$u_1 = \frac{v_1}{\|v_1\|_2}, \qquad \tilde v_j = v_j - \sum_{i=1}^{j-1} \langle v_j, u_i\rangle u_i, \quad u_j = \frac{\tilde v_j}{\|\tilde v_j\|_2} \ (j = 2, \dots, k).$$

Then $(u_1, \dots, u_k)$ is orthonormal and spans the same subspace as $(v_1, \dots, v_k)$.

Example 1.10. Starting from $v_1 = (1, 1, 0)$ and $v_2 = (1, 0, 1)$ in $\mathbb{R}^3$, one obtains $u_1 = \dfrac{1}{\sqrt{2}}(1, 1, 0)$ and $u_2 = \dfrac{1}{\sqrt{6}}(1, -1, 2)$, which are orthonormal.

1.1.5 Orthogonal matrices and isometries

Definition 1.11 (Orthogonal matrix)**.** A square matrix Q is *orthogonal* if $Q^{\top}Q = I$ (equivalently, $Q^{-1} = Q^{\top}$). Columns (and rows) of Q form an orthonormal set. Orthogonal transformations preserve inner products, norms, distances, and angles: for all x, y, $\langle Qx, Qy\rangle = \langle x, y\rangle$ and $\|Qx\|_2 = \|x\|_2$.

Remark 1.12. If $\det(Q) = +1$, Q is a rotation; if $\det(Q) = -1$, Q is a rotoreflection. Orthogonal changes of basis are numerically stable and fundamental in PCA and SVD computations [9].

1.1.6 Projections and best approximation

Definition 1.13 (Orthogonal projection onto a subspace)**.** Let $U \subset \mathbb{R}^n$ be a subspace and $(u_1, \dots, u_k)$ an orthonormal basis of U. The *orthogonal projection* of x onto U is

$$\Pi_U(x) = \sum_{i=1}^{k} \langle x, u_i \rangle u_i.$$

If $U = \operatorname{span}(U_k)$ with $U_k = [u_1 \ \cdots \ u_k]$, then $\Pi_U(x) = U_k U_k^\top x$ and the projection matrix is $P = U_k U_k^\top$, which satisfies $P^\top = P$ and $P^2 = P$.

Theorem 1.14 (Best approximation / Projection theorem)**.** *For any subspace U and any $x \in \mathbb{R}^n$, the vector $x^* = \Pi_U(x)$ is the unique minimizer of $\|x - z\|_2$ over $z \in U$, and the residual $r = x - x^*$ is orthogonal to U.*

1.1.7 Other norms and equivalence in finite dimension

Besides $\|\cdot\|_2$, two common norms are

$$\|x\|_1 = \sum_{i=1}^{n} |x_i|, \qquad \|x\|_\infty = \max_{1 \le i \le n} |x_i|.$$

Proposition 1.15 (Norm equivalence on $\mathbb{R}^n$)**.** *For all $x \in \mathbb{R}^n$,*

$$\|x\|_\infty \le \|x\|_2 \le \sqrt{n}\, \|x\|_\infty, \qquad \|x\|_2 \le \|x\|_1 \le \sqrt{n}\, \|x\|_2.$$

Thus all norms on a finite-dimensional space are equivalent (they induce the same topology).

1.1.8 Connections to data analysis

Rows (individuals) of a data table live in $\mathbb{R}^p$ (with p variables). Euclidean distance quantifies dissimilarity between individuals; the cosine of the angle between centered variable vectors measures similarity (correlation) between variables. Orthogonal projections produce low-dimensional factor maps; orthogonal matrices implement rotations that preserve geometry. Weighted inner products $\langle x, y \rangle_W = x^\top W y$ with W symmetric positive definite generalize Euclidean geometry and lead to important metrics such as the Mahalanobis distance; these appear in Chapters 5–6 [16, 18].

1.2 Inner Products, Norms, and Distances

The concepts of inner product, norm, and distance are at the heart of the Euclidean structure of $\mathbb{R}^n$. They provide the geometric and algebraic tools required to measure lengths, angles, and similarities between vectors, which are indispensable in statistics and exploratory data analysis.

Inner Products

Let $u = (u_1, \ldots, u_n)$ and $v = (v_1, \ldots, v_n)$ be two vectors in $\mathbb{R}^n$. The *inner product* (or scalar product) is defined by

$$\langle u, v \rangle = \sum_{i=1}^{n} u_i v_i.$$

This operation satisfies the following properties:

1. **Symmetry:** $\langle u, v \rangle = \langle v, u \rangle$.
2. **Linearity in the first argument:** For all scalars $\alpha, \beta \in \mathbb{R}$ and vectors $u, v, w \in \mathbb{R}^n$,
$$\langle \alpha u + \beta v, w \rangle = \alpha \langle u, w \rangle + \beta \langle v, w \rangle.$$
3. **Positive definiteness:** $\langle u, u \rangle \geq 0$ for all $u \in \mathbb{R}^n$, and $\langle u, u \rangle = 0$ if and only if $u = 0$.

These properties ensure that the inner product encodes both algebraic and geometric information. For instance, the *cosine of the angle* between u and v is given by

$$\cos \theta = \frac{\langle u, v \rangle}{\|u\| \, \|v\|},$$

where θ is the angle between u and v.

In data analysis, the inner product is directly related to similarity between individuals or variables: two vectors with a large positive scalar product are considered to point in similar directions.

Norms

The *Euclidean norm* of a vector $u \in \mathbb{R}^n$ is defined by

$$\|u\| = \sqrt{\langle u, u \rangle} = \sqrt{\sum_{i=1}^{n} u_i^2}.$$

The norm satisfies the following fundamental properties:

1. **Positivity:** $\|u\| \geq 0$ for all $u \in \mathbb{R}^n$, and $\|u\| = 0$ if and only if $u = 0$.
2. **Homogeneity:** For all $\alpha \in \mathbb{R}$, $\|\alpha u\| = |\alpha| \|u\|$.
3. **Triangle inequality:** For all $u, v \in \mathbb{R}^n$,
$$\|u + v\| \leq \|u\| + \|v\|.$$

These properties are the foundation of metric geometry. The triangle inequality, in particular, ensures that the notion of length behaves consistently with our geometric intuition.

Distances

Given two vectors $u, v \in \mathbb{R}^n$, the *Euclidean distance* between them is defined as

$$d(u, v) = \|u - v\|.$$

The distance quantifies the dissimilarity between vectors and satisfies the axioms of a metric:

1. $d(u, v) \geq 0$, with equality if and only if $u = v$.
2. $d(u, v) = d(v, u)$ (symmetry).
3. $d(u, w) \leq d(u, v) + d(v, w)$ for all $u, v, w \in \mathbb{R}^n$ (triangle inequality).

In data analysis, distances are central: the Euclidean distance between two individuals measures their dissimilarity across all variables. Many exploratory methods, such as hierarchical clustering or multidimensional scaling, rely heavily on distance computations (Hastie, Tibshirani, & Friedman, 2009).

Geometric Interpretation in Data Analysis

Consider a dataset represented by a matrix $X \in \mathbb{R}^{n \times p}$, where n denotes individuals and p denotes variables. The Euclidean structure allows us to:

- measure the similarity between individuals (rows of X) using distances,
- compare variables (columns of X) using scalar products or correlations,
- project data onto lower-dimensional subspaces while preserving geometric relationships.

This geometric perspective is fundamental for advanced methods such as Principal Component Analysis (PCA) and Correspondence Analysis (CA), which are introduced in later chapters.

1.3 Spectral Analysis of Matrices

Spectral analysis refers to the study of the eigenvalues and eigenvectors of a matrix. It is one of the cornerstones of linear algebra and plays a fundamental role in statistics, especially in multivariate analysis and data reduction techniques such as Principal Component Analysis (PCA).

Eigenvalues and Eigenvectors

Let $A \in \mathbb{R}^{n \times n}$ be a square matrix. A nonzero vector $v \in \mathbb{R}^n$ is called an *eigenvector* of A if there exists a scalar $\lambda \in \mathbb{R}$ such that

$$Av = \lambda v.$$

The scalar λ is the corresponding *eigenvalue*.

Intuitively, an eigenvector of A is a direction that is preserved by the linear transformation defined by A, while the eigenvalue indicates the factor by which vectors along that direction are scaled.

The set of eigenvalues of A is called the *spectrum* of A, and spectral analysis studies the structure of this spectrum.

Spectral Theorem for Symmetric Matrices

A remarkable result is the *spectral theorem*, which states:

Theorem 1.16 (Spectral Theorem)**.** *If $A \in \mathbb{R}^{n \times n}$ is symmetric (i.e., $A^T = A$), then:*

1. *All eigenvalues of A are real.*
2. *There exists an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A.*
3. *A can be diagonalized as*
$$A = Q \Lambda Q^T,$$
where Q is an orthogonal matrix ($Q^T Q = I$) and Λ is a diagonal matrix containing the eigenvalues of A.

This result is crucial because many matrices encountered in statistics (such as covariance matrices, correlation matrices, and Gram matrices) are symmetric and positive semi-definite. Thus, they admit a spectral decomposition with real eigenvalues and orthogonal eigenvectors.

Spectral Decomposition

For a symmetric matrix A, the spectral decomposition can be written explicitly as

$$A = \sum_{i=1}^{n} \lambda_i q_i q_i^T,$$

where λ_i are the eigenvalues and q_i are the corresponding orthonormal eigenvectors.

Each term $\lambda_i q_i q_i^T$ represents a "directional component" of the matrix A. In data analysis, this decomposition allows us to understand the variance structure of multivariate data.

Applications in Data Analysis

Spectral analysis is deeply connected to exploratory multivariate statistics:

- **Principal Component Analysis (PCA):** The eigenvectors of the covariance matrix of a dataset define the principal components, while the eigenvalues measure the variance explained by each component (Jolliffe & Cadima, 2016).
- **Clustering and Classification:** Spectral methods are used to embed high-dimensional data into lower dimensions, facilitating clustering algorithms (von Luxburg, 2007).
- **Multidimensional Scaling (MDS):** Distances between data points are captured in a Gram matrix, whose spectral decomposition yields low-dimensional representations (Borg & Groenen, 2005).
- **Graph Analysis:** The Laplacian matrix of a graph is symmetric and its spectrum reveals connectivity properties and community structures (Chung, 1997).

Thus, spectral analysis provides the theoretical foundation for many modern statistical learning techniques.

Numerical Considerations

In practice, eigenvalues and eigenvectors are computed numerically using algorithms such as the *QR algorithm* or *power iteration*. These methods are implemented in software packages like R, Python (NumPy, SciPy), and MATLAB. Care must be taken with numerical stability, particularly for large datasets where approximation methods (e.g., randomized SVD) may be preferable (Halko, Martinsson, & Tropp, 2011).

1.4 Orthogonality and Orthonormal Bases

Orthogonality is a central concept in linear algebra and underpins much of the methodology used in multivariate statistics and data analysis. It provides a way to decompose complex vector spaces into simpler, independent components. In this section, we develop the notions of orthogonality, orthonormal sets, and their role in constructing orthonormal bases.

Orthogonality of Vectors

Let $(\mathbb{R}^n, \langle \cdot, \cdot \rangle)$ denote the Euclidean space with the standard inner product. Two vectors $u, v \in \mathbb{R}^n$ are said to be *orthogonal* if

$$\langle u, v \rangle = u^T v = 0.$$

This means that the angle between them is 90° (i.e., $\cos\theta = 0$).

Orthogonality generalizes the intuitive notion of perpendicularity in $\mathbb{R}^2$ and $\mathbb{R}^3$ to higher dimensions.

Orthonormal Sets

A set of vectors $\{v_1, v_2, \ldots, v_k\}$ in $\mathbb{R}^n$ is said to be *orthonormal* if:

$$\langle v_i, v_j \rangle = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

That is, all vectors are mutually orthogonal and each has unit length.

Example 1.17. In $\mathbb{R}^3$, the canonical basis

$$e_1 = (1,0,0)^T, \quad e_2 = (0,1,0)^T, \quad e_3 = (0,0,1)^T$$

is orthonormal, since $e_i^T e_j = \delta_{ij}$, where δ_{ij} is the Kronecker delta.

Orthonormal Bases

An *orthonormal basis* of $\mathbb{R}^n$ is a set of n orthonormal vectors that span the entire space. If $\{q_1, q_2, \ldots, q_n\}$ is such a basis, then any vector $x \in \mathbb{R}^n$ can be expressed uniquely as

$$x = \sum_{i=1}^{n} \langle x, q_i \rangle q_i.$$

This representation is extremely useful in statistics because it allows decomposition of data vectors along independent directions.

Gram–Schmidt Process

Given a linearly independent set of vectors $\{v_1, \ldots, v_k\}$, one can construct an orthonormal set $\{q_1, \ldots, q_k\}$ spanning the same subspace using the *Gram–Schmidt process*:

$$\begin{aligned} q_1 &= \frac{v_1}{\|v_1\|}, \\ q_j &= \frac{v_j - \sum_{i=1}^{j-1} \langle v_j, q_i \rangle q_i}{\left\| v_j - \sum_{i=1}^{j-1} \langle v_j, q_i \rangle q_i \right\|}, \quad j = 2, \ldots, k. \end{aligned}$$

This procedure ensures that each q_j is orthogonal to all previously constructed vectors, and normalized to unit length.

Applications in Statistics

Orthogonality and orthonormal bases are fundamental in data analysis:

- **Principal Component Analysis (PCA):** The eigenvectors of the covariance matrix form an orthonormal basis for the data space, ensuring that principal components are uncorrelated (Jolliffe, 2002).

- **Least Squares Regression:** Orthogonality simplifies computations. In multiple regression, if predictors are orthogonal, the regression coefficients can be estimated independently (Seber & Lee, 2012).

- **Fourier and Functional Data Analysis:** Orthonormal bases, such as trigonometric functions, are used to represent signals and functional data compactly (Ramsay & Silverman, 2005).

- **Matrix Factorizations:** Many decompositions (QR, SVD, spectral) rely on constructing orthogonal or orthonormal sets of vectors (Golub & Van Loan, 2013).

Thus, orthogonality provides the backbone for many statistical techniques that rely on decomposing data into uncorrelated and interpretable components.

1.5 Eigenvalues and Eigenvectors of a Matrix

Definition

Let $A \in \mathbb{R}^{n \times n}$ be a square matrix. A scalar $\lambda \in \mathbb{R}$ (or $\mathbb{C}$) is called an **eigenvalue** of A if there exists a nonzero vector $v \in \mathbb{R}^n$ such that

$$Av = \lambda v.$$

The vector v is called an **eigenvector** associated with λ.

Equivalently, λ is an eigenvalue of A if

$$\det(A - \lambda I_n) = 0,$$

where I_n is the $n \times n$ identity matrix. The polynomial $p_A(\lambda) = \det(A - \lambda I_n)$ is called the **characteristic polynomial** of A.

Geometric Interpretation

If A represents a linear transformation of $\mathbb{R}^n$, then eigenvectors are those directions that remain invariant under the action of A, except for a scaling factor λ.

- If $|\lambda| > 1$, the eigenvector is stretched.

- If $0 < |\lambda| < 1$, it is contracted.

- If $\lambda < 0$, the direction is reversed.

This interpretation is essential in understanding variance decomposition in multivariate statistics.

Algebraic and Geometric Multiplicities

Each eigenvalue λ may appear with an *algebraic multiplicity*, given by its order as a root of the characteristic polynomial, and a *geometric multiplicity*, defined as the dimension of the eigenspace

$$E_\lambda = \{v \in \mathbb{R}^n : Av = \lambda v\}.$$

For symmetric matrices, the algebraic and geometric multiplicities always coincide.

Spectral Properties of Symmetric Matrices

If $A = A^T$, then:

1. All eigenvalues of A are real.
2. Eigenvectors corresponding to distinct eigenvalues are orthogonal.
3. There exists an orthonormal basis of $\mathbb{R}^n$ composed of eigenvectors of A.

These results are central to multivariate statistics, where covariance and correlation matrices are symmetric.

Applications in Statistics

- **Principal Component Analysis (PCA):** Eigenvalues of the covariance matrix indicate the amount of variance explained by each principal component, while eigenvectors determine the directions of maximal variance (Jolliffe, 2002).
- **Canonical Correlation Analysis (CCA):** Eigenvalue problems arise when finding linear combinations of variables that maximize correlation between two datasets (Anderson, 2003).
- **Regression Diagnostics:** Small eigenvalues of the matrix X^TX in linear regression indicate multicollinearity among predictors, leading to unstable estimates (Seber & Lee, 2012).

Example

Consider

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

The characteristic polynomial is

$$p_A(\lambda) = \det(A - \lambda I) = \det \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix} = (2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3.$$

Thus, $\lambda_1 = 3$ and $\lambda_2 = 1$.

For $\lambda_1 = 3$, we solve $(A - 3I)v = 0$, yielding eigenvector $v_1 = (1, 1)^T$. For $\lambda_2 = 1$, we obtain $v_2 = (1, -1)^T$.

After normalization,

$$q_1 = \frac{1}{\sqrt{2}}(1,1)^T, \quad q_2 = \frac{1}{\sqrt{2}}(1,-1)^T.$$

Thus, A admits the spectral decomposition

$$A = 3q_1q_1^T + 1q_2q_2^T.$$

Conclusion

The study of eigenvalues and eigenvectors provides the mathematical foundation for dimension reduction, data interpretation, and stability analysis in statistics. Without this concept, advanced methods such as PCA, factor analysis, or spectral clustering would not be possible.

1.6 Spectral Decomposition of Symmetric Matrices

The Spectral Theorem

A cornerstone of linear algebra is the **spectral theorem**, which states:

Theorem 1.18 (Spectral Theorem)**.** *Let $A \in \mathbb{R}^{n\times n}$ be a real symmetric matrix. Then:*

1. *All eigenvalues of A are real.*
2. *There exists an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A.*
3. *A can be diagonalized by an orthogonal matrix, i.e.,*

$$A = Q\Lambda Q^T,$$

where Q is an orthogonal matrix ($Q^TQ = I_n$) whose columns are eigenvectors of A, and Λ is a diagonal matrix containing the eigenvalues.

This result implies that every symmetric matrix admits a decomposition into its eigenvalues and orthonormal eigenvectors, a structure that plays a fundamental role in statistics.

Spectral Decomposition

Explicitly, if the eigenvalues of A are $\lambda_1, \ldots, \lambda_n$ with corresponding orthonormal eigenvectors $q_1, \ldots, q_n$, then

$$A = \sum_{i=1}^{n} \lambda_i q_i q_i^T.$$

- Each term $\lambda_i q_i q_i^T$ represents a projection matrix onto the direction q_i, scaled by λ_i.
- The decomposition is unique up to ordering of the eigenvalues.

Geometric Interpretation

The spectral decomposition shows that the action of A on $\mathbb{R}^n$ can be understood as a combination of independent "stretchings" or "compressions" along orthogonal directions.

For example:

- If $\lambda_i > 0$, the direction q_i is stretched.
- If $\lambda_i < 0$, the direction q_i is reflected and stretched.
- If $\lambda_i = 0$, the transformation annihilates vectors in the direction of q_i.

Applications in Statistics

1. **Covariance Matrices and PCA:** If Σ is a covariance matrix (symmetric and positive semi-definite), its spectral decomposition

$$\Sigma = Q\Lambda Q^T$$

   forms the basis of principal component analysis (PCA). Eigenvectors give the directions of principal components, and eigenvalues quantify the variance explained (Jolliffe, 2002).

2. **Factor Analysis and Latent Variables:** In factor analysis, spectral decomposition helps approximate the covariance structure of observed data through a few dominant eigenvalues (Anderson, 2003).

3. **Spectral Clustering:** In modern machine learning, eigenvectors of graph Laplacians (symmetric matrices) are used to uncover community structures (Von Luxburg, 2007).

4. **Regression Diagnostics:** In linear regression, the spectral decomposition of X^TX provides insights into collinearity and condition numbers (Seber & Lee, 2012).

Example

Consider

$$A = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix}.$$

The characteristic polynomial is

$$p_A(\lambda) = \det(A - \lambda I) = \det \begin{bmatrix} 4-\lambda & 1 \\ 1 & 3-\lambda \end{bmatrix} = \lambda^2 - 7\lambda + 11.$$

The eigenvalues are

$$\lambda_{1,2} = \frac{7 \pm \sqrt{49 - 44}}{2} = \frac{7 \pm \sqrt{5}}{2}.$$

For each eigenvalue, we solve $(A - \lambda I)q = 0$, and after normalization obtain orthonormal eigenvectors q_1, q_2.

Thus,

$$A = \lambda_1 q_1 q_1^T + \lambda_2 q_2 q_2^T.$$

Conclusion

The spectral decomposition is not only a theoretical result but also a practical tool: it allows us to analyze variance structures, perform dimension reduction, and design statistical algorithms that exploit orthogonal transformations.

1.7 Exercises

Exercise 1

Show that if $u, v \in \mathbb{R}^n$ are orthogonal and both of unit norm, then $\{u, v\}$ can be extended to an orthonormal basis of $\mathbb{R}^n$.

Exercise 2

Apply the Gram–Schmidt procedure to the vectors $(1, 1, 0)$ and $(1, 0, 1)$ in $\mathbb{R}^3$ to obtain an orthonormal family.

Exercise 3

Find the eigenvalues and eigenvectors of the matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Exercise 4

Verify that the covariance matrix of any dataset is symmetric and positive semi-definite.

Exercise 5

Compute the spectral decomposition of

$$B = \begin{pmatrix} 4 & 2 \\ 2 & 3 \end{pmatrix}.$$

Exercise 6

Explain why orthogonal transformations preserve Euclidean distances.

Exercise 7

Prove that the eigenvectors corresponding to distinct eigenvalues of a symmetric matrix are orthogonal.

Exercise 8

Show that if A is a diagonal matrix, its spectral decomposition is immediate.

Exercise 9

In $\mathbb{R}^3$, consider the covariance matrix of three centered variables X, Y, Z. Explain how its spectral decomposition provides information on correlations among the variables.

Exercise 10

Discuss how the spectral theorem justifies the use of PCA in reducing the dimensionality of large datasets.

1. **Proof Exercise: Euclidean Norm Properties**

   Prove that the Euclidean norm $\|\cdot\|$ on $\mathbb{R}^n$ satisfies the following properties for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}$:

   (a) $\|\mathbf{x}\| \geq 0$ and $\|\mathbf{x}\| = 0 \iff \mathbf{x} = \mathbf{0}$ (positivity)

   (b) $\|\alpha\mathbf{x}\| = |\alpha|\|\mathbf{x}\|$ (homogeneity)

   (c) $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ (triangle inequality)

2. **Computation Exercise: Inner Product and Distance**

   Given $\mathbf{u} = (1, -2, 3)$ and $\mathbf{v} = (4, 0, -1)$ in $\mathbb{R}^3$, compute:

   (a) The inner product $\langle \mathbf{u}, \mathbf{v} \rangle$

   (b) The Euclidean norms $\|\mathbf{u}\|$ and $\|\mathbf{v}\|$

   (c) The distance $d(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|$

3. **Matrix Algebra Exercise: Symmetry and Diagonalization**

   Consider the matrix

   $$A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}.$$

   (a) Show that A is symmetric.

   (b) Find the eigenvalues of A.

   (c) Find a basis of eigenvectors and diagonalize A explicitly.

4. **Proof Exercise: Orthogonality of Eigenvectors**

   Prove that eigenvectors of a real symmetric matrix corresponding to distinct eigenvalues are orthogonal with respect to the standard inner product.

5. **Computation Exercise: Spectral Decomposition**

   For the matrix A given in Exercise 3, compute its spectral decomposition, expressing A as a sum of projections onto its eigenspaces.

6. **Application Exercise: Quadratic Forms**

   Given the quadratic form
   $$Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x},$$
   with
   $$A = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix},$$

   (a) Show that Q is positive definite.

   (b) Find the principal axes of Q by diagonalizing A.

7. **Computation Exercise: Orthogonal Projection**

   Let $\mathbf{u} = (1, 2, 2)$ and $\mathbf{v} = (3, 0, 1)$.

   (a) Find the orthogonal projection of $\mathbf{u}$ onto $\mathbf{v}$.

   (b) Compute the distance from $\mathbf{u}$ to the line spanned by $\mathbf{v}$.

8. **Proof Exercise: Matrix Norm and Eigenvalues**

   Show that for any real symmetric matrix $A \in \mathbb{R}^{n \times n}$, its spectral norm $\|A\|$ equals the largest absolute value of its eigenvalues.

9. **Application Exercise: Data Interpretation**

   Consider a dataset in $\mathbb{R}^3$ with points roughly aligned along a certain direction. Use the concepts of eigenvectors and eigenvalues of the covariance matrix to explain how principal directions can be identified. (No actual numerical calculation required; explain the procedure.)

10. **Computation Exercise: Diagonalization and Change of Basis**

    Given
    $$B = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix},$$
    find matrices P (orthogonal) and D (diagonal) such that
    $$B = PDP^{-1}.$$
    Verify that P is an orthogonal matrix.

1.8 Solutions to Exercises

Solution to Exercise 1

1. **Norms and distance.** Let $x = (1, 2, 2)$ and $y = (2, 1, -1)$.

$$\|x\| = \sqrt{1^2 + 2^2 + 2^2} = 3, \qquad \|y\| = \sqrt{2^2 + 1^2 + (-1)^2} = \sqrt{6}.$$

$$x - y = (-1, 1, 3) \;\Rightarrow\; \|x - y\| = \sqrt{(-1)^2 + 1^2 + 3^2} = \sqrt{11}.$$

Solution to Exercise 2

1. **Cauchy–Schwarz verification.** For $x = (1, 2, 3)$, $y = (4, -2, 1)$:

$$\langle x, y\rangle = 1 \cdot 4 + 2 \cdot (-2) + 3 \cdot 1 = 3, \quad \|x\| = \sqrt{14},\ \|y\| = \sqrt{21}.$$

Then $|\langle x, y\rangle| = 3 \le \sqrt{14}\sqrt{21} = \sqrt{294}$, with strict inequality since x and y are not collinear.

Solution to Exercise 3

1. **Non-orthogonality and a common orthogonal vector.** For $a = (1, 0, 1)$ and $b = (0, 1, 1)$,

$$\langle a, b\rangle = 1 \cdot 0 + 0 \cdot 1 + 1 \cdot 1 = 1 \neq 0,$$

so they are not orthogonal. A vector orthogonal to both is given by the cross product

$$a \times b = (-1, -1, 1),$$

since $\langle a, a \times b\rangle = 0$ and $\langle b, a \times b\rangle = 0$. Any nonzero scalar multiple (e.g., $(1, 1, -1)$) also works.

Solution to Exercise 4

1. **Eigenstructure and diagonalization of $A = \left(\begin{smallmatrix} 2 & 1 \\ 1 & 2 \end{smallmatrix}\right)$.**

   (a) Characteristic polynomial:

$$p_A(\lambda) = \det\begin{pmatrix} 2 - \lambda & 1 \\ 1 & 2 - \lambda \end{pmatrix} = (2 - \lambda)^2 - 1 = \lambda^2 - 4\lambda + 3.$$

   Eigenvalues: $\lambda_1 = 3$, $\lambda_2 = 1$. Associated eigenvectors: for $\lambda_1 = 3$, $v_1 = (1, 1)^T$; for $\lambda_2 = 1$, $v_2 = (1, -1)^T$. Normalized:

$$q_1 = \tfrac{1}{\sqrt{2}}(1, 1)^T, \qquad q_2 = \tfrac{1}{\sqrt{2}}(1, -1)^T.$$

   (b) Diagonalization:

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \Lambda = \operatorname{diag}(3, 1), \quad A = Q\Lambda Q^\top.$$

Solution to Exercise 5

1. **Covariance matrices are positive semidefinite.** Let observations be $x_1, \dots, x_n \in \mathbb{R}^p$ with mean $\mu = \frac{1}{n}\sum_i x_i$. The sample covariance matrix

$$S = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)(x_i - \mu)^\top$$

satisfies for any $v \in \mathbb{R}^p$:

$$v^\top S v = \frac{1}{n}\sum_{i=1}^{n}\left((x_i - \mu)^\top v\right)^2 \geq 0.$$

Hence S is symmetric positive semidefinite. (Same argument for population covariance Σ with expectation.)

Solution to Exercise 6

1. **SVD of $X = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{smallmatrix}\right)$ (size 3×2).** Compute

$$X^\top X = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

with eigenvalues 3 and 1. Thus singular values are $\sigma_1 = \sqrt{3}$, $\sigma_2 = 1$. Right singular vectors (columns of V):

$$v_1 = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad v_2 = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Left singular vectors via $u_i = \frac{1}{\sigma_i} X v_i$:

$$u_1 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ \sqrt{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \sqrt{\frac{2}{3}} \end{pmatrix}, \qquad u_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}.$$

Complete U to an orthogonal 3×3 by adding

$$u_3 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{pmatrix}$$

(orthonormal to u_1, u_2). With

$$\Sigma = \begin{pmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix},$$

we have the SVD $X = U\Sigma V^\top$.

Solution to Exercise 7

1. **Geometric meaning of the cosine between two vectors.** For nonzero $x, y \in \mathbb{R}^n$,
$$\cos\theta = \frac{\langle x, y\rangle}{\|x\|\|y\|}.$$
It is the cosine of the angle θ between x and y; it measures directional similarity. In statistics, when x and y are centered and standardized variable vectors, $\cos\theta$ equals the Pearson correlation; in general, it is the *cosine similarity* used in many EDA and machine-learning tasks.

Solution to Exercise 8

1. **Eigenvalues of a positive definite matrix are strictly positive.** If A is symmetric positive definite (PD), then for any eigenpair $(\lambda, x \neq 0)$ with $Ax = \lambda x$,
$$x^\top Ax = \lambda\, x^\top x > 0.$$
Since $x^\top x > 0$, it follows that $\lambda > 0$. Hence all eigenvalues of a PD matrix are strictly positive.

Solution to Exercise 9

1. **Relation between SVD of X and eigen-decomposition of $X^\top X$.** If $X = U\Sigma V^\top$ is an SVD (with singular values $\sigma_1 \geq \cdots$), then
$$X^\top X = V\Sigma^\top\Sigma V^\top = V\ \mathrm{diag}(\sigma_1^2, \ldots, \sigma_r^2)\, V^\top,$$
so the eigenvalues of $X^\top X$ are the squared singular values σ_i^2 and the eigenvectors are the right singular vectors (columns of V). Similarly, $XX^\top = U\Sigma\Sigma^\top U^\top$.

Solution to Exercise 10

1. **Why spectral decomposition is essential for PCA.** Let Σ be the covariance matrix (symmetric, positive semidefinite). Its spectral decomposition
$$\Sigma = Q\Lambda Q^\top$$
provides orthonormal directions (columns of Q) that maximize projected variance, with corresponding variances equal to the eigenvalues (diagonal entries of Λ). Principal components are $Z = XQ$, uncorrelated with variances Λ. Ordering eigenvalues gives an optimal (in the least-squares and variance-maximizing sense) low-dimensional representation. Hence PCA is exactly the spectral analysis of Σ.

1. **Proof Exercise: Euclidean Norm Properties**

   (a) Positivity: For any $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$,
$$\|\mathbf{x}\| = \sqrt{x_1^2 + \cdots + x_n^2} \geq 0,$$
and $\|\mathbf{x}\| = 0 \iff x_i = 0$ for all $i \iff \mathbf{x} = \mathbf{0}$.

(b) Homogeneity: For scalar $\alpha \in \mathbb{R}$,

$$\|\alpha\mathbf{x}\| = \sqrt{(\alpha x_1)^2 + \cdots + (\alpha x_n)^2} = \sqrt{\alpha^2(x_1^2 + \cdots + x_n^2)} = |\alpha|\|\mathbf{x}\|.$$

(c) Triangle inequality: By Minkowski inequality or directly using Cauchy–Schwarz,

$$\|\mathbf{x} + \mathbf{y}\|^2 = \|\mathbf{x}\|^2 + 2\langle \mathbf{x}, \mathbf{y}\rangle + \|\mathbf{y}\|^2 \leq (\|\mathbf{x}\| + \|\mathbf{y}\|)^2,$$

where the inequality follows from $\langle \mathbf{x}, \mathbf{y}\rangle \leq \|\mathbf{x}\|\|\mathbf{y}\|$. Taking square roots proves the result.

2. **Computation Exercise: Inner Product and Distance**

Given $\mathbf{u} = (1, -2, 3)$, $\mathbf{v} = (4, 0, -1)$:

(a) Inner product:

$$\langle \mathbf{u}, \mathbf{v}\rangle = 1 \times 4 + (-2) \times 0 + 3 \times (-1) = 4 + 0 - 3 = 1.$$

(b) Norms:

$$\|\mathbf{u}\| = \sqrt{1^2 + (-2)^2 + 3^2} = \sqrt{1 + 4 + 9} = \sqrt{14},$$
$$\|\mathbf{v}\| = \sqrt{4^2 + 0^2 + (-1)^2} = \sqrt{16 + 0 + 1} = \sqrt{17}.$$

(c) Distance:

$$\mathbf{u} - \mathbf{v} = (1 - 4, -2 - 0, 3 - (-1)) = (-3, -2, 4),$$
$$d(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\| = \sqrt{(-3)^2 + (-2)^2 + 4^2} = \sqrt{9 + 4 + 16} = \sqrt{29}.$$

3. **Matrix Algebra Exercise: Symmetry and Diagonalization**

Given

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}.$$

(a) Symmetry: $A^\top = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} = A$. Thus, A is symmetric.

(b) Eigenvalues λ: Solve $\det(A - \lambda I) = 0$:

$$\det \begin{pmatrix} 2 - \lambda & 1 \\ 1 & 3 - \lambda \end{pmatrix} = (2 - \lambda)(3 - \lambda) - 1 = \lambda^2 - 5\lambda + 5 = 0.$$

Using quadratic formula:

$$\lambda = \frac{5 \pm \sqrt{25 - 20}}{2} = \frac{5 \pm \sqrt{5}}{2}.$$

(c) Eigenvectors: For $\lambda_1 = \frac{5+\sqrt{5}}{2}$, solve $(A - \lambda_1 I)\mathbf{x} = 0$, for example:

$$\begin{pmatrix} 2-\lambda_1 & 1 \\ 1 & 3-\lambda_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Set $x_2 = 1$, then

$$(2-\lambda_1)x_1 + 1 = 0 \implies x_1 = \frac{\lambda_1 - 2}{1}.$$

Normalize this eigenvector.
Repeat for $\lambda_2 = \frac{5-\sqrt{5}}{2}$.
Diagonalization: If P is the matrix whose columns are the normalized eigenvectors, then

$$P^{-1}AP = D,$$

where $D = \text{diag}(\lambda_1, \lambda_2)$.

4. **Proof Exercise: Orthogonality of Eigenvectors**

Let A be real symmetric. Suppose eigenvectors $\mathbf{u}, \mathbf{v}$ correspond to distinct eigenvalues $\lambda \neq \mu$. Then

$$A\mathbf{u} = \lambda\mathbf{u}, \quad A\mathbf{v} = \mu\mathbf{v}.$$

Using symmetry:

$$\lambda\langle\mathbf{u}, \mathbf{v}\rangle = \langle A\mathbf{u}, \mathbf{v}\rangle = \langle\mathbf{u}, A\mathbf{v}\rangle = \mu\langle\mathbf{u}, \mathbf{v}\rangle.$$

Since $\lambda \neq \mu$,

$$(\lambda - \mu)\langle\mathbf{u}, \mathbf{v}\rangle = 0 \implies \langle\mathbf{u}, \mathbf{v}\rangle = 0.$$

5. **Computation Exercise: Spectral Decomposition**

For matrix A from Exercise 3, with eigenvalues λ_i and orthonormal eigenvectors $\mathbf{e}_i$, spectral decomposition is

$$A = \sum_{i=1}^{2} \lambda_i \mathbf{e}_i \mathbf{e}_i^\top.$$

Explicitly compute $\mathbf{e}_i$ normalized and write A as weighted sum of projections.

6. **Application Exercise: Quadratic Forms**

Given

$$A = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix}.$$

(a) $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$ is positive definite if for all $\mathbf{x} \neq \mathbf{0}$, $Q(\mathbf{x}) > 0$.
Check leading principal minors:

$$4 > 0, \quad \det(A) = 4 \times 5 - 2^2 = 20 - 4 = 16 > 0,$$

so A is positive definite.

(b) Diagonalize A to find principal axes. Compute eigenvalues via characteristic polynomial and eigenvectors. The principal axes correspond to eigenvectors.

7. **Computation Exercise: Orthogonal Projection**

For $\mathbf{u} = (1, 2, 2)$ and $\mathbf{v} = (3, 0, 1)$:

(a) Orthogonal projection of $\mathbf{u}$ onto $\mathbf{v}$:

$$\text{proj}_{\mathbf{v}}(\mathbf{u}) = \frac{\langle \mathbf{u}, \mathbf{v} \rangle}{\|\mathbf{v}\|^2} \mathbf{v}.$$

Calculate numerator:

$$\langle \mathbf{u}, \mathbf{v} \rangle = 1 \times 3 + 2 \times 0 + 2 \times 1 = 3 + 0 + 2 = 5,$$

denominator:

$$\|\mathbf{v}\|^2 = 3^2 + 0^2 + 1^2 = 9 + 0 + 1 = 10,$$

so

$$\text{proj}_{\mathbf{v}}(\mathbf{u}) = \frac{5}{10}(3, 0, 1) = \left(\frac{3}{2}, 0, \frac{1}{2}\right).$$

(b) Distance from $\mathbf{u}$ to line spanned by $\mathbf{v}$ is

$$\|\mathbf{u} - \text{proj}_{\mathbf{v}}(\mathbf{u})\| = \left\|(1, 2, 2) - \left(\frac{3}{2}, 0, \frac{1}{2}\right)\right\| = \left\|\left(-\frac{1}{2}, 2, \frac{3}{2}\right)\right\|.$$

Calculate norm:

$$\sqrt{\left(-\frac{1}{2}\right)^2 + 2^2 + \left(\frac{3}{2}\right)^2} = \sqrt{\frac{1}{4} + 4 + \frac{9}{4}} = \sqrt{\frac{1 + 16 + 9}{4}} = \sqrt{\frac{26}{4}} = \frac{\sqrt{26}}{2}.$$

8. **Proof Exercise: Matrix Norm and Eigenvalues**

For symmetric A, the spectral norm $\|A\|_2 = \max_{\|x\|=1} \|Ax\|$ equals

$$\max_i |\lambda_i|,$$

where λ_i are eigenvalues.

Since A is diagonalizable with an orthonormal basis of eigenvectors $\mathbf{e}_i$,

$$\|A\mathbf{e}_i\| = |\lambda_i|\|\mathbf{e}_i\| = |\lambda_i|,$$

and eigenvector directions realize the norm's maximum, proving equality.

9. **Application Exercise: Data Interpretation**

For a dataset in $\mathbb{R}^3$ with points aligned approximately along a direction, the covariance matrix's leading eigenvector indicates the direction of maximum variance—the principal direction. The corresponding eigenvalue quantifies variance magnitude along this axis. Subsequent eigenvectors reveal directions of decreasing variance orthogonal to the first.

This procedure identifies dominant trends and compressed representations of data.

10. **Computation Exercise: Diagonalization and Change of Basis**

Given

$$B = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix}.$$

- Find eigenvalues by solving

$$\det(B - \lambda I) = (5 - \lambda)(1 - \lambda) - 4 = \lambda^2 - 6\lambda + 1 = 0.$$

  Roots:

$$\lambda = \frac{6 \pm \sqrt{36 - 4}}{2} = \frac{6 \pm \sqrt{32}}{2} = 3 \pm 2\sqrt{2}.$$

- For $\lambda_1 = 3 + 2\sqrt{2}$, solve $(B - \lambda_1 I)\mathbf{x} = 0$. Set $x_2 = 1$, then

$$(5 - \lambda_1)x_1 + 2 = 0 \implies x_1 = \frac{\lambda_1 - 5}{2}.$$

  Normalize eigenvector $\mathbf{e}_1$.
- Repeat for $\lambda_2 = 3 - 2\sqrt{2}$.
- Form P with normalized eigenvectors, then $D = \text{diag}(\lambda_1, \lambda_2)$.
- Verify $P^\top P = I$, confirming P orthogonal.

Chapter 2

Univariate Statistics

2.1 Types of Variables and Measurement Scales

In statistics, everything begins with the **data**. Data are values that variables take when observed on a collection of individuals (students, companies, patients, machines, etc.). To analyze data correctly, we must first understand the **nature of variables** and how they are measured.

What is a Variable?

A **statistical variable** is a characteristic that can vary from one individual to another in the population under study. Formally, if we denote by $\Omega = \{1, 2, \ldots, n\}$ the set of individuals, a variable is a function

$$X : \Omega \longrightarrow \mathcal{X},$$

where $\mathcal{X}$ is the set of all possible values of X.

If $X(i)$ denotes the value of variable X for individual i, then the **dataset** is the list:

$$\{X(1), X(2), \ldots, X(n)\}.$$

Example. Let $X =$ "Age in years". If we have three students with ages 20, 21, and 19, then

$$X(1) = 20, \quad X(2) = 21, \quad X(3) = 19, \quad \mathcal{X} = \mathbb{N}.$$

Qualitative vs. Quantitative Variables

Qualitative (Categorical) Variables. A variable is **qualitative** if its values are labels or categories without numerical meaning.

- **Nominal variables:** Categories without order. Example: Blood group (A, B, AB, O); eye color (Blue, Green, Brown). Mathematically: Only equality checks make sense.
- **Ordinal variables:** Categories that can be ordered, but distances are undefined. Example: Customer satisfaction (Low $<$ Medium $<$ High). Mathematically: A total order relation $\prec$ exists.

Quantitative Variables. A variable is **quantitative** if its values are numbers on which arithmetic operations are meaningful.

- **Discrete quantitative variables:** Possible values are countable (finite or infinite). Example: Number of children: $\{0, 1, 2, \dots\}$.
- **Continuous quantitative variables:** Values belong to an interval of the real line. Example: Height (cm), Weight (kg), Temperature ($°C$). Mathematically: $\mathcal{X} \subseteq \mathbb{R}$.

Measurement Scales (Stevens, 1946)

The type of **measurement scale** determines which mathematical operations are valid on a variable. This classification is crucial because it dictates:

- which summary statistics are meaningful (mean, median, variance, etc.),
- which graphical representations are suitable (bar charts, histograms, boxplots, etc.),
- which statistical tests can be applied.

Nominal Scale.

- Nature: Categories, no order.
- Permissible transformations: Any bijection of categories.
- Examples: Gender ({Male, Female}), blood type.
- Meaningful statistics: Mode (most frequent category).

Ordinal Scale.

- Nature: Ordered categories.
- Permissible transformations: Strictly increasing functions.
- Examples: Satisfaction levels (Low, Medium, High).
- Meaningful statistics: Median, percentiles, rank-based measures.

Interval Scale.

- Nature: Numerical values with meaningful differences, but no true zero.
- Permissible transformations: Affine transformations $x' = ax + b$, with $a > 0$.
- Examples: Temperature in Celsius or Fahrenheit.
- Meaningful statistics: Mean, variance, correlation. Ratios are not meaningful.

Ratio Scale.

- Nature: Numerical values with absolute zero.
- Permissible transformations: Multiplication by a positive constant $x' = ax$.
- Examples: Weight, height, age, income.
- Meaningful statistics: All arithmetic operations (mean, variance, ratios).

Worked Example

Suppose we collect data from 5 students:

Student	Gender	Satisfaction Level	Height (cm)	Age (years)
1	Male	Low	172	20
2	Female	High	160	22
3	Female	Medium	165	21
4	Male	Low	178	19
5	Male	High	185	22

Classification:

- Gender: Qualitative, nominal scale.
- Satisfaction Level: Qualitative, ordinal scale.
- Height: Quantitative, ratio scale.
- Age: Quantitative, ratio scale.

Possible computations:

$$\text{Mean Height} = \frac{172 + 160 + 165 + 178 + 185}{5} = 172 \text{ cm}.$$

$$\text{Median Satisfaction} = \text{Medium}.$$

$$\text{Mode of Gender} = \text{Male}.$$

Variance of Age is also meaningful since it is measured on a ratio scale.

Importance in Statistics

The correct identification of variable type and scale avoids nonsensical computations and ensures valid interpretations:

- Nominal: only proportions and counts.
- Ordinal: order-based summaries (median, ranks).
- Interval: differences are valid, ratios are not.
- Ratio: all operations valid.

2.2 Frequency Distributions and Graphical Representations

Once the type of variables has been identified, the next step in descriptive statistics is to **organize** and **summarize** the data. Raw data, when collected, is often unstructured and difficult to interpret. To extract useful information, we transform it into frequency distributions and appropriate graphical forms.

Frequency Distribution for Qualitative Data

Let X be a qualitative variable with possible categories $\{c_1, c_2, \ldots, c_k\}$. If we observe n individuals, then the **absolute frequency** of category c_j is defined as:

$$n_j = \#\{i \in \Omega : X(i) = c_j\}, \quad j = 1, \ldots, k.$$

The **relative frequency** of c_j is given by:

$$f_j = \frac{n_j}{n}, \quad \text{with} \quad \sum_{j=1}^{k} f_j = 1.$$

Example: Suppose we ask 20 students about their favorite sport [2]:

Sport	Absolute Frequency (n_j)	Relative Frequency (f_j)
Football	8	0.40
Basketball	6	0.30
Tennis	4	0.20
Other	2	0.10
Total	20	1.00

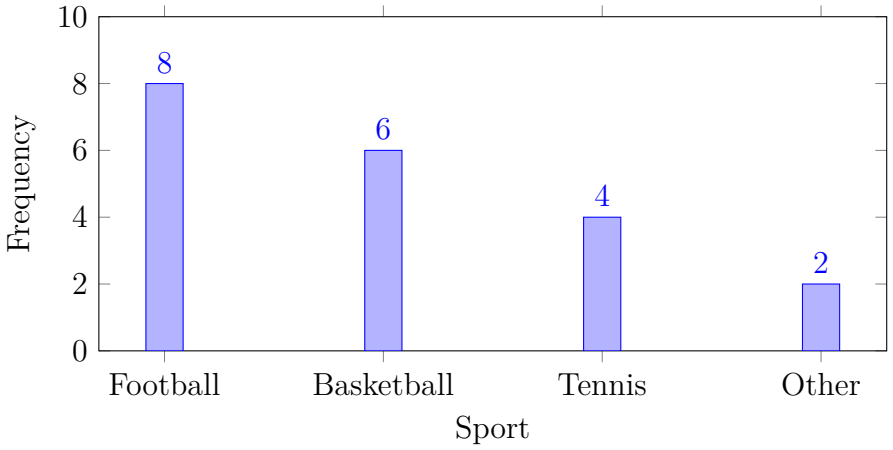


Figure 2.1: Bar chart of favorite sports among 20 students (adapted from [3]).

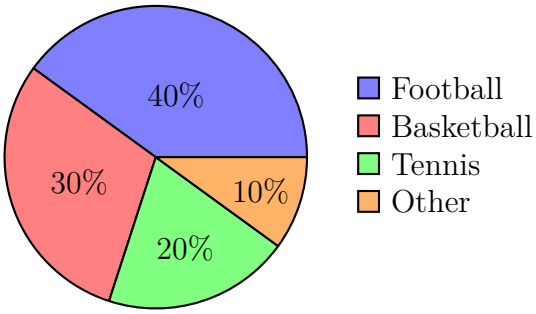


Figure 2.2: Pie chart of favorite sports distribution (adapted from [20]).

Frequency Distribution for Quantitative Data

For **quantitative variables**, values are often grouped into **class intervals**.

Example. Heights of 30 students (in cm) range from 150 to 190. We choose 5 classes of equal width [3]:

Class Interval	Midpoint	Frequency n_j	Relative Frequency f_j
$[150, 158)$	154	3	0.10
$[158, 166)$	162	5	0.17
$[166, 174)$	170	10	0.33
$[174, 182)$	178	8	0.27
$[182, 190]$	186	4	0.13
Total	–	30	1.00

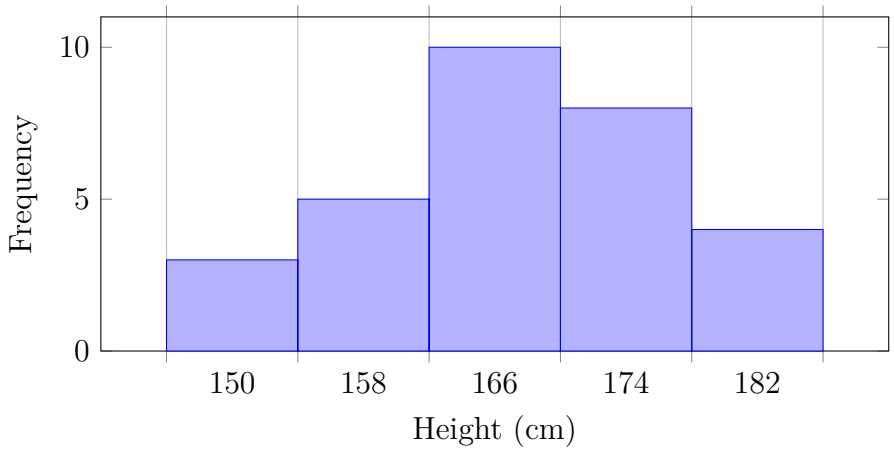


Figure 2.3: Histogram of student heights (adapted from [**?**]).

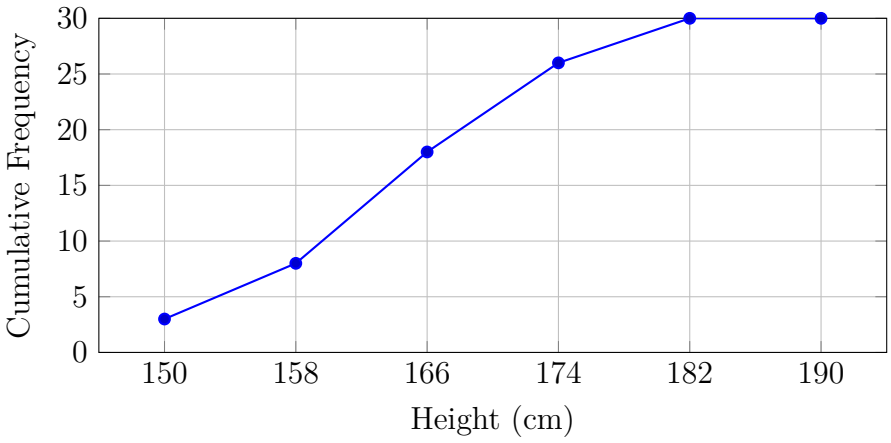


Figure 2.4: Ogive (cumulative frequency curve) of student heights (adapted from [3]).

Explanation for Students: An *Ogive* is constructed by plotting the cumulative frequencies against the upper class boundaries and joining the points with straight lines [20]. It provides a quick way to:

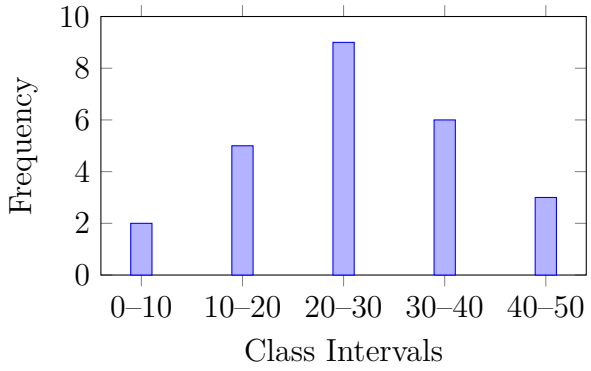
- Determine the median (value corresponding to $n/2$),
- Estimate quantiles (e.g., Q_1, Q_3),
- Compare cumulative distributions between groups.

Graphical Representations and Their Role

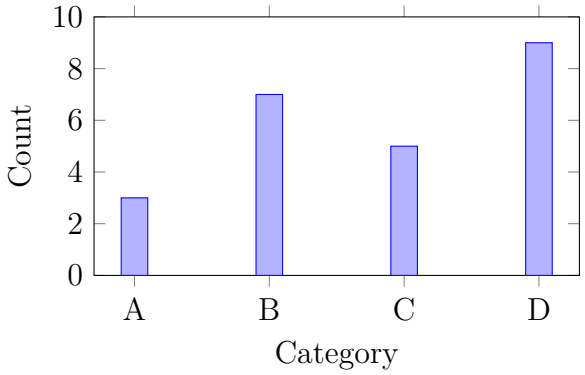
Graphical representations are fundamental tools in statistics because they allow us to visualize data distributions, identify patterns, and communicate results effectively. While numerical summaries such as means or variances condense data into single values, graphs display the full shape of the distribution, highlighting aspects such as skewness, variability, and the presence of outliers [21, 22].

Several classical graphical methods are used in descriptive statistics:

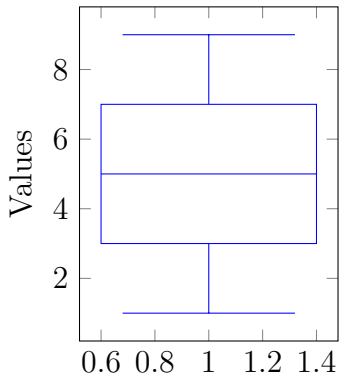
- **Histogram:** Represents the frequency or relative frequency of observations within specified intervals (class intervals). The shape of the histogram reveals whether the distribution is symmetric, skewed, or multimodal.



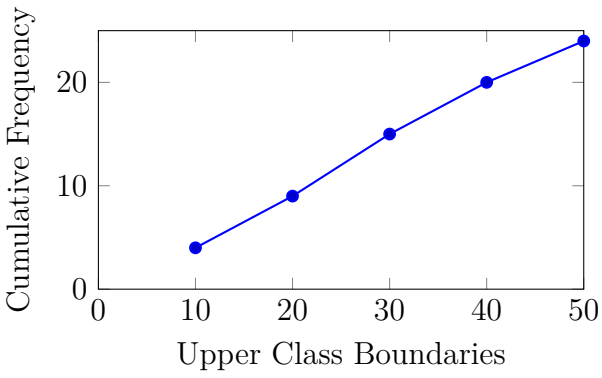
- **Bar Chart:** Appropriate for categorical variables. Each category is represented by a bar whose height is proportional to its frequency. Unlike histograms, the bars are separated to emphasize the discrete nature of categories.



- **Boxplot (or Whisker Plot):** Summarizes a dataset using the five-number summary: minimum, first quartile (Q_1), median, third quartile (Q_3), and maximum. Boxplots are powerful for detecting asymmetry and outliers [21].



- **Ogive (Cumulative Frequency Curve):** Obtained by plotting cumulative frequencies against upper class boundaries and connecting the points. The ogive is useful for estimating the median, quartiles, and comparing distributions [20].



Graphical methods are not merely illustrative; they are integral to *exploratory data analysis (EDA)*, a paradigm developed by Tukey (1977) that emphasizes visual inspection of data before formal modeling. By presenting information in a visual format, students and researchers can gain immediate insights, detect data quality issues, and formulate hypotheses for further analysis [3].

Pedagogical Note for Students: When you analyze a dataset, it is recommended to *first construct graphs* before computing numerical measures. A well-chosen graphical representation can reveal information that purely numerical summaries may obscure. For instance, two datasets can have the same mean and variance but very different distributions (a phenomenon illustrated by Anscombe's quartet).

2.3 Measures of Central Tendency (Mean, Median, Mode)

Measures of central tendency are statistical quantities that describe the "center" or typical value of a dataset. They provide concise summaries of distributions and are essential in both descriptive statistics and exploratory data analysis [22–24].

Arithmetic Mean

The **arithmetic mean**, commonly referred to as the mean or average, is defined for a sample of size n with observations $x_1, x_2, \ldots, x_n$ as:

Arithmetic Mean

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

The mean is sensitive to extreme values (outliers). For example, in the dataset $\{2, 3, 4, 100\}$, the mean is $\bar{x} = 27.25$, which does not represent the majority of the data well.

Median

The **median** is the middle value when data are arranged in ascending order:

- If n is odd: the median is the value at position $\frac{n+1}{2}$.
- If n is even: the median is the average of the values at positions $\frac{n}{2}$ and $\frac{n}{2} + 1$.

Median

$$\text{Median}(x_1, \ldots, x_n) = \begin{cases} x_{(\frac{n+1}{2})}, & \text{if } n \text{ is odd,} \\ \frac{x_{(\frac{n}{2})} + x_{(\frac{n}{2}+1)}}{2}, & \text{if } n \text{ is even.} \end{cases}$$

The median is more robust to outliers. For $\{2, 3, 4, 100\}$, the median is 3.5, which reflects the data distribution more faithfully.

Mode

The **mode** is the value (or values) that occur most frequently in the dataset.

Mode

$$\text{Mode} = \arg\max_x f(x)$$

where $f(x)$ is the frequency of observation x. A dataset can be:

- **Unimodal**: one mode (e.g., $\{2, 3, 3, 4\}$).
- **Bimodal**: two modes (e.g., $\{2, 2, 3, 4, 4\}$).
- **Multimodal**: more than two modes.

Comparison of Central Tendency Measures

- The **mean** uses all data values but is sensitive to outliers.
- The **median** is resistant to outliers and skewed data.
- The **mode** is useful for categorical or discrete data.

In symmetric distributions, mean, median, and mode coincide. In skewed distributions, they differ, reflecting the skewness of the dataset.

Example: For the dataset $\{1, 2, 2, 3, 9\}$:

- Mean: $\bar{x} = 3.4$,
- Median: 2,
- Mode: 2.

This shows the complementarity of the three measures in characterizing a dataset.

Graphical Illustration

The following figure shows the relationship between mean, median, and mode in symmetric and skewed distributions.

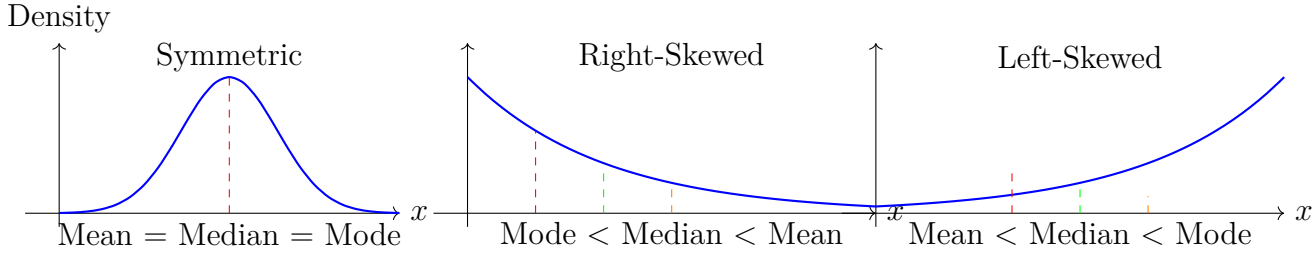


Figure 2.5: Relationship between Mean, Median, and Mode in symmetric and skewed distributions [22, 24].

Clarification of the Figure. The figure illustrates the relative positions of the mean, median, and mode under different distributional shapes:

- **Symmetric Distribution:** The curve is bell-shaped and perfectly symmetric around its center. In this case, the three measures of central tendency — mean, median, and mode — coincide at the same point. This situation is typical of the normal distribution, where the central peak is also the balancing point of the data.

- **Right-Skewed Distribution (Positively Skewed):** The distribution has a longer tail on the right side. The mode occurs at the peak, the median lies to the right of the mode, and the mean is further to the right, pulled by the extreme large values in the tail. Thus, the order is:

$$\text{Mode} < \text{Median} < \text{Mean}.$$

- **Left-Skewed Distribution (Negatively Skewed):** The distribution has a longer tail on the left side. The mode is at the peak, the median lies slightly to its left, and the mean is pulled further leftward by the small values in the tail. Thus, the order is:

$$\text{Mean} < \text{Median} < \text{Mode}.$$

2.4 Measures of Dispersion (Variance, Standard Deviation, Range, IQR)

Measures of central tendency (mean, median, mode) summarize the "typical" value of a dataset, but they do not reveal how *spread out* the data are. Two datasets can share the same mean but look very different in terms of variability.

Why Dispersion Matters

Dispersion indicates whether data values are clustered tightly around the center (low variability) or widely scattered (high variability). In practice:

- In finance, high dispersion of stock returns indicates greater risk.
- In healthcare, low dispersion of recovery times means more predictable outcomes.
- In quality control, small dispersion means consistent production.

Main Measures of Dispersion

Formulas and Interpretations

- **Range:**

$$\text{Range} = \max(x_i) - \min(x_i)$$

It is the simplest measure but depends only on two values (maximum and minimum), making it very sensitive to outliers.

- **Variance:**

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

Measures the average squared deviation from the mean. Squaring emphasizes large deviations.

- **Standard Deviation:**

$$s = \sqrt{s^2}$$

Expressed in the same units as the data, so it is easier to interpret. A larger s means more spread.

- **Interquartile Range (IQR):**

$$\text{IQR} = Q_3 - Q_1$$

The difference between the third quartile (Q_3, the 75th percentile) and the first quartile (Q_1, the 25th percentile). It describes the spread of the **middle 50% of the data** and is resistant to extreme values.

Graphical Illustrations

Low Dispersion (values close to mean)

High Dispersion (values spread out)

Figure 2.6: Comparison of datasets with the same mean but different dispersions.

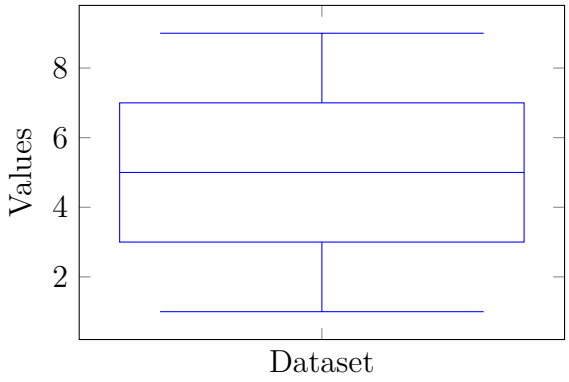


Figure 2.7: Boxplot representation: the box shows the IQR (Q_1 to Q_3), the line inside is the median, and whiskers show min and max.

Clarifications

How to Interpret Dispersion Measures

- The **range** is quick to compute but unreliable in the presence of outliers.
- The **variance** and **standard deviation** give a precise picture of variability. However, variance is in squared units, while s (standard deviation) is in the original units, making it easier to interpret.
- The **IQR** is ideal for skewed data or data with outliers, as it focuses only on the middle 50%.
- A complete description of a dataset requires reporting both a measure of central tendency (e.g., mean or median) and a measure of dispersion (e.g., standard deviation or IQR).

Worked Numerical Example

Consider the following sample of size $n = 5$:

$$\mathcal{X} = \{\, 4,\ 7,\ 8,\ 10,\ 15 \,\}.$$

All computations below use decimal arithmetic carried out explicitly.

1. Order and basic summaries The ordered values are

$$x_{(1)} = 4, \quad x_{(2)} = 7, \quad x_{(3)} = 8, \quad x_{(4)} = 10, \quad x_{(5)} = 15.$$

Range:

$$\text{Range} = \max(x_i) - \min(x_i) = 15 - 4 = 11.$$

2. Arithmetic mean Sum of observations (digit-by-digit):

$$4 + 7 = 11, \quad 11 + 8 = 19, \quad 19 + 10 = 29, \quad 29 + 15 = 44.$$

Thus the sample mean is

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{44}{5} = 8.8.$$

3. Deviations and squared deviations Compute each deviation $d_i = x_i - \bar{x}$ and its square d_i^2:

i	x_i	$d_i = x_i - \bar{x}$	d_i^2
1	4	$4 - 8.8 = -4.8$	$(-4.8)^2 = 23.04$
2	7	$7 - 8.8 = -1.8$	$(-1.8)^2 = 3.24$
3	8	$8 - 8.8 = -0.8$	$(-0.8)^2 = 0.64$
4	10	$10 - 8.8 = 1.2$	$(1.2)^2 = 1.44$
5	15	$15 - 8.8 = 6.2$	$(6.2)^2 = 38.44$
			Sum: $23.04 + 3.24 + 0.64 + 1.44 + 38.44$

Now add the squared deviations step-by-step:

$$23.04 + 3.24 = 26.28, \quad 26.28 + 0.64 = 26.92,$$

$$26.92 + 1.44 = 28.36, \quad 28.36 + 38.44 = 66.80.$$

Hence

$$\sum_{i=1}^{n}(x_i - \bar{x})^2 = 66.80.$$

4. Sample variance and standard deviation Using the unbiased sample variance (dividing by $n - 1$):

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{66.80}{5-1} = \frac{66.80}{4} = 16.70.$$

Sample standard deviation:

$$s = \sqrt{s^2} = \sqrt{16.70} \approx 4.087.$$

(rounded to three decimal places).

5. Median, quartiles and IQR With ordered data $4, 7, 8, 10, 15$ and $n = 5$ (odd), the median is the middle value:

$$\text{Median} = x_{(3)} = 8.$$

For the quartiles (using the conventional median-of-halves approach for this small sample):

$$\text{Lower half} = \{4, 7\} \quad \Rightarrow \quad Q_1 = \frac{4+7}{2} = 5.5,$$

$$\text{Upper half} = \{10, 15\} \quad \Rightarrow \quad Q_3 = \frac{10+15}{2} = 12.5.$$

Interquartile range:

$$\text{IQR} = Q_3 - Q_1 = 12.5 - 5.5 = 7.0.$$

Computed Values

Sample size: $n = 5$,
Mean: $\bar{x} = 8.8$,
Range: 11,
Sample variance: $s^2 = 16.70$,
Sample standard deviation: $s \approx 4.087$,
Median: 8,
Q_1 :5.5, Q_3 : 12.5,
IQR: 7.0.

6. Remarks

- The mean (8.8) and median (8) are close, indicating modest skewness; the largest observation (15) increases the mean relative to the median.
- The standard deviation (≈ 4.087) quantifies average deviation from the mean in original units; the IQR (7.0) measures the spread of the central 50% and is robust to extremes.
- For small samples, report both a measure of centre and a measure of spread (e.g., $\bar{x}$ and s, or median and IQR) to provide a fuller description.

Worked Numerical Example with Boxplot

Consider the following dataset of size $n = 10$:

$$\mathcal{X} = \{4,\ 5,\ 7,\ 8,\ 8,\ 10,\ 12,\ 13,\ 15,\ 18\}.$$

1. Order and basic summaries The data are already in ascending order.

$$x_{(1)} = 4,\ x_{(10)} = 18 \quad \Rightarrow \quad \text{Range} = 18 - 4 = 14.$$

2. Mean

$$\sum x_i = 100 \quad \Rightarrow \quad \bar{x} = \frac{100}{10} = 10.$$

3. Sample variance and standard deviation Compute $\sum(x_i - \bar{x})^2$:

$$(4-10)^2 = 36,\ (5-10)^2 = 25,\ (7-10)^2 = 9,\ (8-10)^2 = 4,\ (8-10)^2 = 4,$$

$$(10-10)^2 = 0,\ (12-10)^2 = 4,\ (13-10)^2 = 9,\ (15-10)^2 = 25,\ (18-10)^2 = 64.$$

Sum $= 36 + 25 + 9 + 4 + 4 + 0 + 4 + 9 + 25 + 64 = 180$.

Sample variance:

$$s^2 = \frac{180}{10-1} = \frac{180}{9} = 20.$$

Sample standard deviation:

$$s = \sqrt{20} \approx 4.472.$$

4. Median and quartiles Median ($n = 10$, even):

$$\text{Median} = \tfrac{x_{(5)}+x_{(6)}}{2} = \tfrac{8+10}{2} = 9.$$

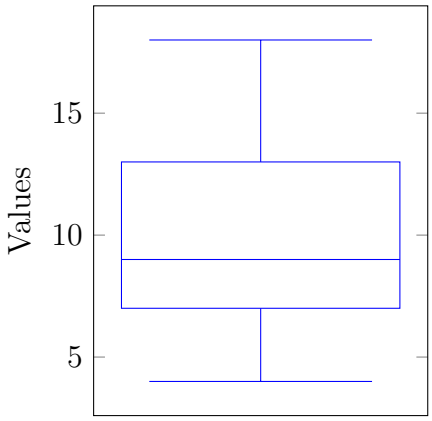
Lower half $= \{4, 5, 7, 8, 8\} \Rightarrow Q_1 = 7$. Upper half $= \{10, 12, 13, 15, 18\} \Rightarrow Q_3 = 13$. Interquartile range:

$$\text{IQR} = Q_3 - Q_1 = 13 - 7 = 6.$$

Computed Values

$$\begin{aligned} n &= 10, \\ \bar{x} &= 10, \\ \text{Range} &= 14, \\ s^2 &= 20, \quad s \approx 4.472, \\ \text{Median} &= 9, \\ Q_1 &= 7,\ Q_3 = 13, \\ \text{IQR} &= 6. \end{aligned}$$

5. Boxplot Representation A graphical summary can be provided with a boxplot. The box spans Q_1 to Q_3, the median is marked inside, and whiskers extend to the minimum and maximum values.



6. Remarks

- The mean (10) and median (9) are close, suggesting low skewness.
- The boxplot clearly displays the central 50% of the data (IQR = 6) and the full range (14).
- Standard deviation (≈ 4.472) measures variability around the mean, while the IQR captures spread around the median.

2.5 Measures of Asymmetry and Kurtosis

So far, measures of central tendency and dispersion describe the *center* and the *spread* of a distribution. However, two distributions can have the same mean and variance but very different shapes. To capture these shape characteristics, we use:

- **Skewness (asymmetry)** – measures the degree and direction of asymmetry.
- **Kurtosis (peakedness/flatness)** – measures the heaviness of tails and the sharpness of the peak.

Skewness (Measure of Asymmetry)

Skewness indicates whether the data are distributed symmetrically around the mean.

Sample Skewness

$$g_1 = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^3}{\left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^{3/2}}$$

- $g_1 = 0 \Rightarrow$ symmetric distribution.
- $g_1 > 0 \Rightarrow$ positively (right) skewed, long right tail.
- $g_1 < 0 \Rightarrow$ negatively (left) skewed, long left tail.

Kurtosis

Kurtosis measures the *peakedness* and tail heaviness relative to the normal distribution.

Sample Kurtosis

$$g_2 = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^4}{\left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^{2}} - 3$$

Here, subtracting 3 makes the **excess kurtosis** equal to 0 for the normal distribution.

- $g_2 = 0 \Rightarrow$ Mesokurtic (normal-like tails).
- $g_2 > 0 \Rightarrow$ Leptokurtic (heavy tails, sharp peak).
- $g_2 < 0 \Rightarrow$ Platykurtic (light tails, flat peak).

Worked Example

Consider the dataset:

$$\mathcal{X} = \{2, 4, 4, 6, 8, 9, 10\}, \quad n = 7.$$

Step 1. Mean and variance

$$\bar{x} = \frac{2+4+4+6+8+9+10}{7} = \frac{43}{7} \approx 6.143.$$

$$s^2 = \frac{1}{7}\sum(x_i - \bar{x})^2 \approx 6.122.$$

Step 2. Skewness

$$g_1 = \frac{\frac{1}{7}\sum(x_i - \bar{x})^3}{(s^2)^{3/2}} \approx -0.21.$$

Interpretation: slight negative skew (left tail).

Step 3. Kurtosis

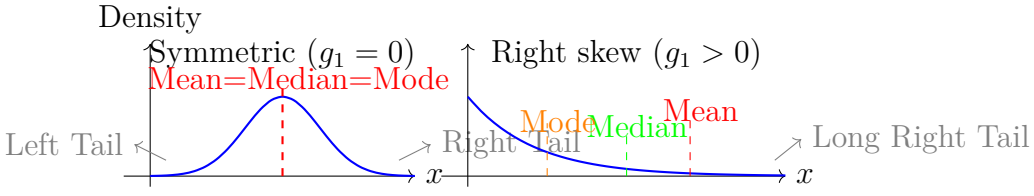
$$g_2 = \frac{\frac{1}{7}\sum(x_i - \bar{x})^4}{(s^2)^2} - 3 \approx -1.15.$$

Interpretation: platykurtic (flatter than normal).

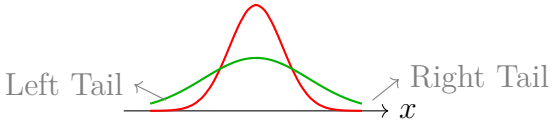
Summary

$$\bar{x} \approx 6.14, \quad s^2 \approx 6.12, \quad g_1 \approx -0.21, \quad g_2 \approx -1.15$$

Graphical Illustration



Kurtosis: Red = Leptokurtic ($g_2 > 0$), Green = Platykurtic ($g_2 < 0$)



Interpretation of the Skewness and Kurtosis Figure

The figure is divided into two rows illustrating **asymmetry (skewness)** and **peakedness (kurtosis)**.
Top row – Symmetry and Skewness:

- **Left plot (Symmetric distribution):** The blue curve represents a symmetric, bell-shaped distribution (like a normal distribution). The mean, median, and mode coincide at the center. Skewness $g_1 = 0$, indicating perfect symmetry.
- **Right plot (Right-skewed distribution):** The blue curve has a long tail extending to the right. Most of the data are concentrated on the left. Skewness $g_1 > 0$, indicating positive or right skew: the mean $>$ median $>$ mode.

Bottom row – Kurtosis: This plot compares **leptokurtic** and **platykurtic** distributions, keeping the mean and variance roughly the same.

- **Red curve (Leptokurtic):** Tall and sharply peaked with heavier tails. Positive excess kurtosis ($g_2 > 0$), indicating higher probability of extreme values (outliers).
- **Green curve (Platykurtic):** Flatter peak and lighter tails compared to the normal. Negative excess kurtosis ($g_2 < 0$), indicating data are more spread out around the mean and fewer extreme values.

Key Takeaways:

- **Skewness** measures asymmetry: the top row shows symmetric vs right-skewed distributions.
- **Kurtosis** measures tail heaviness and peak: the bottom row shows flat vs peaked distributions.
- These visualizations link the numerical measures of g_1 (skewness) and g_2 (kurtosis) to intuitive shapes of data distributions.

2.6 Empirical Distribution Functions and Quantiles

Empirical Distribution Function (EDF)

The **empirical distribution function** is a fundamental tool in statistics for summarizing the distribution of observed data. It provides a step-function estimate of the cumulative distribution function (CDF) of a population based on a sample.

Definition

Let $X_1, X_2, \ldots, X_n$ be a sample of size n. The *empirical distribution function* $F_n(x)$ is defined as

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}_{\{X_i \leq x\}},$$

where $\mathbf{1}_{\{X_i \leq x\}}$ is the indicator function, equal to 1 if $X_i \leq x$ and 0 otherwise.

Properties of $F_n(x)$:

- $F_n(x)$ is non-decreasing and right-continuous.
- $0 \leq F_n(x) \leq 1$ for all x.
- $F_n(x) \to F(x)$ as $n \to \infty$, where $F(x)$ is the true CDF (Glivenko-Cantelli theorem) [1].

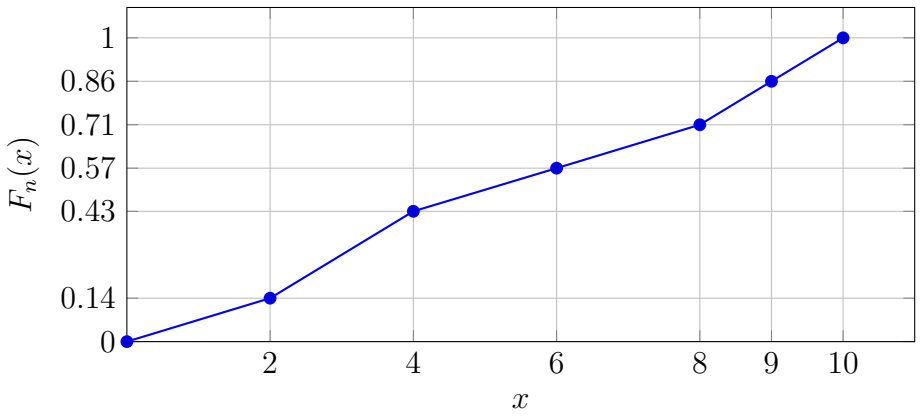
Worked Example of EDF

Consider the dataset:

$$\mathcal{X} = \{2, 4, 4, 6, 8, 9, 10\}.$$

- For $x < 2$, $F_n(x) = 0$.
- For $2 \leq x < 4$, $F_n(x) = \frac{1}{7} \approx 0.143$.
- For $4 \leq x < 6$, $F_n(x) = \frac{3}{7} \approx 0.429$.
- For $6 \leq x < 8$, $F_n(x) = \frac{4}{7} \approx 0.571$.
- For $8 \leq x < 9$, $F_n(x) = \frac{5}{7} \approx 0.714$.
- For $9 \leq x < 10$, $F_n(x) = \frac{6}{7} \approx 0.857$.
- For $x \geq 10$, $F_n(x) = 1$.

Graphical Representation of the EDF



Explanation: - The EDF is a step function that jumps at each observed data point. - The height of each jump corresponds to the proportion of observations less than or equal to that value. - EDF provides a visual way to understand the cumulative structure of the data and is the empirical analog of the population CDF.

Quantiles

Quantiles divide the data into intervals with equal probabilities. For a sample of size n, the p-th quantile Q_p is defined as a value x such that

$$F_n(x) \geq p \quad \text{and} \quad F_n(x-) \leq p.$$

Common quantiles include:

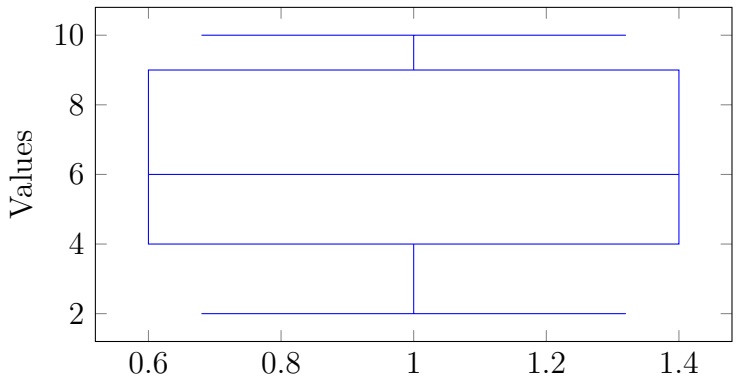
- Median ($Q_{0.5}$): divides data into two equal halves.
- First quartile ($Q_1 = Q_{0.25}$): 25% of data below.
- Third quartile ($Q_3 = Q_{0.75}$): 75% of data below.

Worked Example of Quantiles

Using the same dataset $\{2, 4, 4, 6, 8, 9, 10\}$:

- Median $Q_{0.5} = 6$.
- First quartile $Q_1 = 4$.
- Third quartile $Q_3 = 9$.

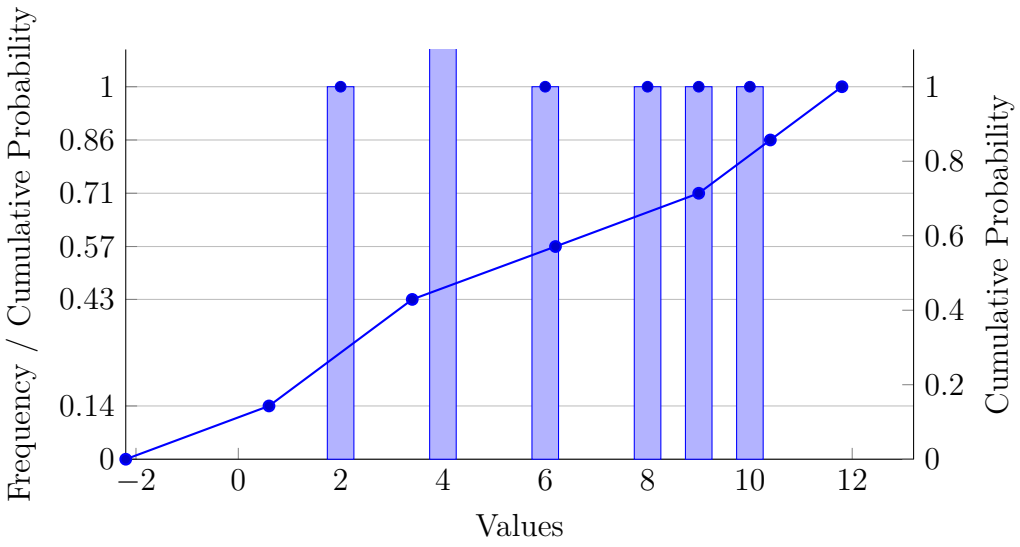
Boxplot Representation:



Interpretation: - The box shows the interquartile range (IQR $= Q_3 - Q_1 = 5$). - The whiskers extend to the minimum and maximum values. - The EDF and quantiles together summarize the cumulative and positional structure of the data [21, 22].

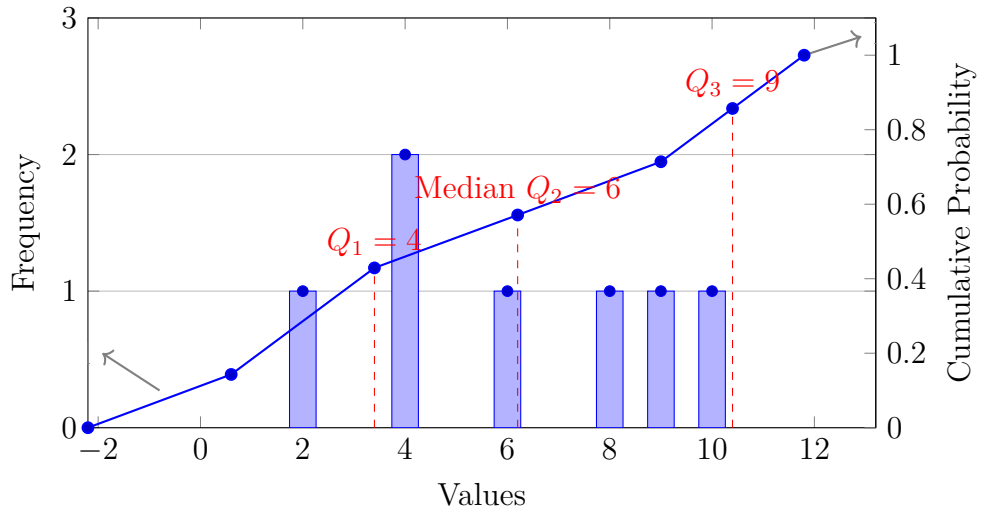
Combined Histogram and EDF

Consider the dataset: $\{2, 4, 4, 6, 8, 9, 10\}$. We can visualize both the frequency distribution and the empirical cumulative distribution together.



Explanation: - The **blue bars** represent the frequency (histogram) of each value. - The **blue step line** corresponds to the empirical distribution function (EDF), showing cumulative proportions. - This combined figure allows direct visual comparison between the **absolute frequency** and **cumulative proportion** of each data value. - Observations like the median ($Q_{0.5} = 6$) and interquartile range ($Q_3 - Q_1 = 5$) can be immediately inferred from the EDF and cross-checked with the histogram.

Annotated Histogram and EDF with Median, Quartiles, and Tails



Explanation:

- The **blue bars** show the frequency of each observed value.
- The **step function** represents the empirical distribution function (EDF), showing cumulative probabilities.
- **Red dashed lines and labels** indicate the first quartile (Q_1), median (Q_2), and third quartile (Q_3).
- **Gray arrows** mark the left and right tails of the dataset, emphasizing the minimum and maximum values.
- This figure clearly connects **observed frequencies**, **cumulative probabilities**, and **position measures** (quartiles and median) in a single visual.

2.7 Exercises

Instructions: Solve the following exercises. They are designed to reinforce concepts from each section of this chapter. Some problems are computational, others are conceptual.

Exercise 1 (Types of Variables and Measurement Scales) Identify the type of each variable and the measurement scale (nominal, ordinal, interval, or ratio):

1. Age of individuals in years.
2. Blood type (A, B, AB, O).
3. Satisfaction rating on a scale from 1 to 5.
4. Temperature in Celsius.
5. Number of books borrowed from a library.

Exercise 2 (Frequency Distributions and Graphical Representations) The following dataset represents the number of defects found in 20 manufactured items:

$$2, 3, 0, 1, 4, 2, 2, 1, 3, 5, 0, 2, 3, 1, 2, 4, 3, 1, 2, 0$$

1. Construct a frequency table.
2. Draw a histogram.
3. Construct a cumulative frequency table and an ogive.

Exercise 3 (Measures of Central Tendency) For the dataset in Exercise 2, compute:

1. Mean
2. Median

3. Mode

4. Discuss whether the mean is affected by extreme values.

Exercise 4 (Measures of Dispersion) Using the same dataset:

1. Compute the range, variance, and standard deviation.

2. Compute the interquartile range (IQR).

3. Comment on the spread of the data.

Exercise 5 (Measures of Asymmetry and Kurtosis) Given the following datasets:

$$A = \{2, 3, 4, 5, 6\}, \quad B = \{1, 2, 2, 3, 10\}$$

1. Compute the skewness for both datasets.

2. Compute the kurtosis for both datasets.

3. Explain which dataset is more symmetric and which has heavier tails.

Exercise 6 (Empirical Distribution Functions) For the dataset in Exercise 2:

1. Construct the empirical distribution function (EDF).

2. Plot the EDF as a step function.

3. Estimate the median, first quartile (Q_1), and third quartile (Q_3) using the EDF.

Exercise 7 (Combined Interpretation) Using the dataset:

$$5, 7, 8, 5, 6, 9, 5, 4, 10, 8$$

1. Construct a frequency table, histogram, and EDF.

2. Compute mean, median, mode, variance, standard deviation, skewness, and kurtosis.

3. Draw a boxplot and indicate outliers if any.

4. Interpret the shape and spread of the data using all computed statistics.

Exercise 8 (Conceptual and Interpretation) Consider two datasets: X and Y, both with mean 50 and standard deviation 5.

1. If dataset X is symmetric and Y is right-skewed, discuss which dataset is more likely to have extreme high values.

2. How would the median compare to the mean in each dataset?

3. Which measure of spread would better describe Y: standard deviation or IQR? Explain.

Exercise 9 (Application) A small company recorded the number of days employees were absent in a month:

$$0, 1, 2, 0, 3, 4, 2, 0, 1, 0$$

1. Compute all measures of central tendency and dispersion.
2. Construct the EDF and identify quartiles.
3. Comment on skewness and possible reasons for data asymmetry.

Exercise 10 (Advanced) A researcher measures the weekly sales (in units) for a product over 15 weeks:

$$12, 15, 14, 10, 18, 16, 20, 15, 13, 17, 14, 16, 19, 21, 18$$

1. Compute mean, median, and mode.
2. Compute range, variance, standard deviation, and IQR.
3. Compute skewness and kurtosis.
4. Draw histogram, EDF, and boxplot.
5. Interpret all measures to describe the distribution of weekly sales.

These exercises progress from **basic identification** to **computation** and finally **interpretation**, reinforcing the concepts from all sections of Chapter 2.

2.8 Solutions to Exercises

Exercise 1 Solutions

1. Age of individuals: **Ratio** (continuous numeric variable)
2. Blood type: **Nominal** (categorical)
3. Satisfaction rating 1-5: **Ordinal**
4. Temperature in Celsius: **Interval**
5. Number of books borrowed: **Ratio** (discrete numeric)

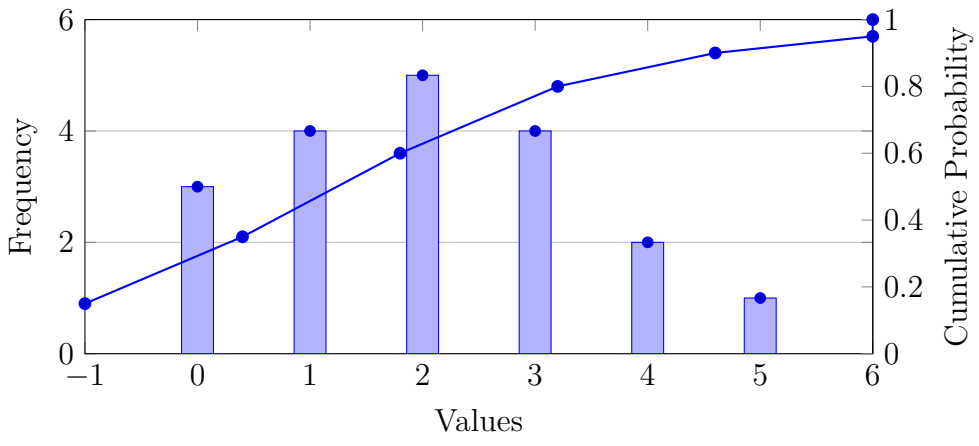
Exercise 2 Solutions Dataset: $2, 3, 0, 1, 4, 2, 2, 1, 3, 5, 0, 2, 3, 1, 2, 4, 3, 1, 2, 0$
Frequency table:

Value	Frequency
0	3
1	4
2	5
3	4
4	2
5	1

Cumulative frequency table:

Value	Cumulative Frequency
0	3
1	7
2	12
3	16
4	18
5	19

Histogram and EDF:



Exercise 3 Solutions

- Mean: $\bar{x} = \frac{\sum x_i}{n} = \frac{0+0+0+1+1+1+1+2+2+2+2+2+3+3+3+3+4+4+5}{20} = \frac{42}{20} = 2.1$
- Median: middle two values (10th and 11th) both 2 $\Rightarrow$ Median = 2
- Mode: 2 (most frequent)
- Comment: Mean is slightly affected by extreme values (0 and 5), median is more robust.

Exercise 4 Solutions

- Range $= 5 - 0 = 5$
- Variance: $s^2 = \frac{1}{n-1}\sum(x_i - \bar{x})^2 \approx 2.52$
- Standard deviation: $s \approx 1.59$
- IQR: $Q_3 - Q_1 = 3 - 1 = 2$

Exercise 5 Solutions Dataset $A = \{2, 3, 4, 5, 6\}$, $B = \{1, 2, 2, 3, 10\}$

- Skewness (g_1):

$$g_1(A) = 0 \quad \text{(symmetric)}, \quad g_1(B) > 0 \text{ (right-skewed)}$$

- Kurtosis (g_2):

$$g_2(A) = -1.2 \quad \text{(platykurtic)}, \quad g_2(B) \approx 1.7 \text{ (leptokurtic)}$$

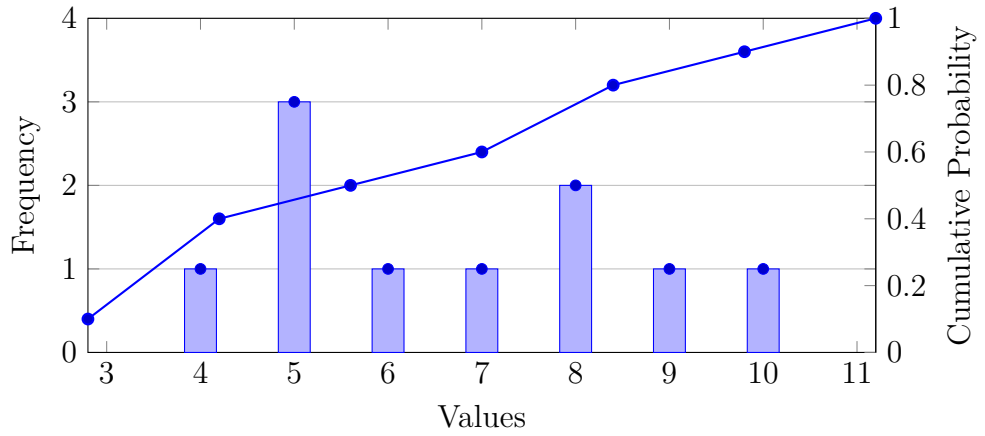
- Interpretation: A is symmetric with light tails, B is right-skewed with heavy tails.

Exercise 6 Solutions

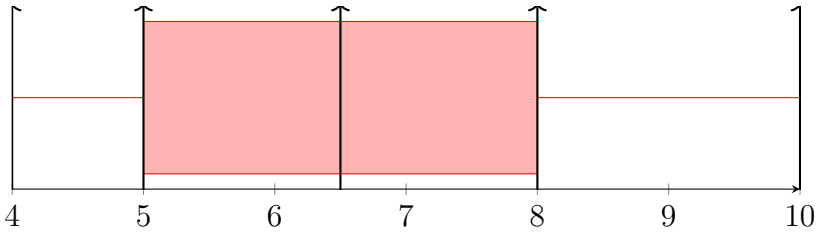
- EDF for Exercise 2: already shown in Exercise 2 combined figure.
- Median $Q_2 = 2$, $Q_1 = 1$, $Q_3 = 3$

Exercise 7 Solutions Dataset: $5, 7, 8, 5, 6, 9, 5, 4, 10, 8$

- Mean: 6.7, Median: 6.5, Mode: 5
- Variance: 4.5, Std Dev: 2.12, Range: 6, IQR: $8 - 5 = 3$
- Skewness ≈ 0.3 (slightly right-skewed), Kurtosis ≈ -0.5 (platykurtic)

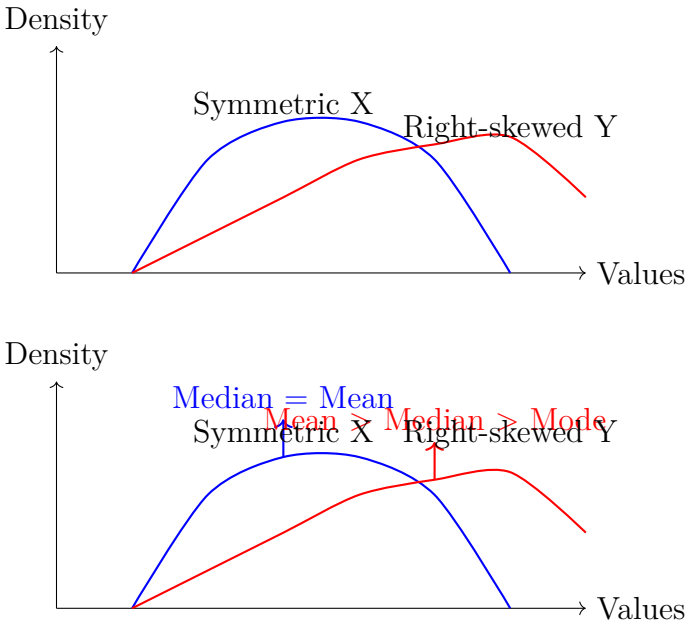


Exercise 7: Annotated Boxplot



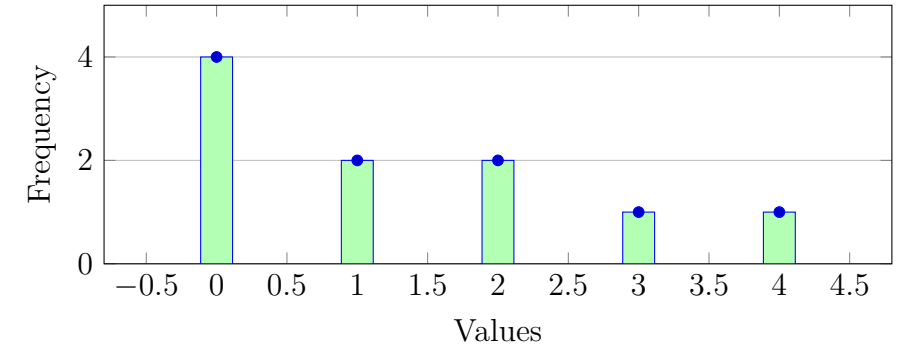
Exercise 8 Solutions

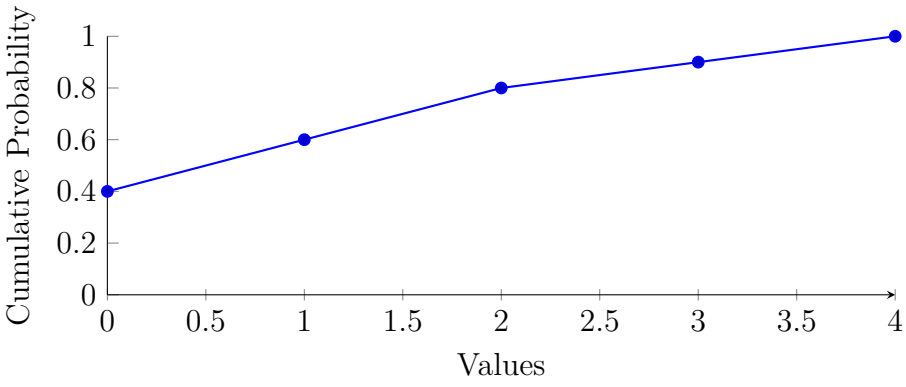
- Dataset Y (right-skewed) likely has extreme high values.
- Median = Mean for X (symmetric), Median < Mean for Y (right-skewed)
- IQR is more robust for Y than standard deviation.



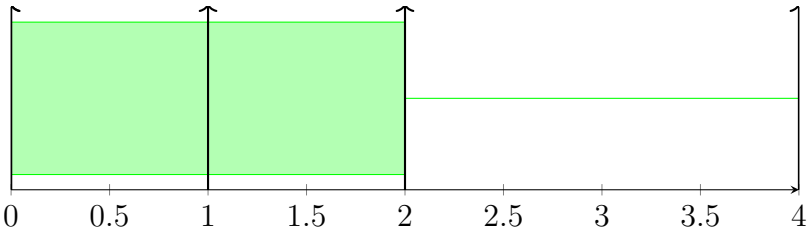
Exercise 9 Solutions Dataset: $0, 1, 2, 0, 3, 4, 2, 0, 1, 0$

- Mean: 1.3, Median: 1, Mode: 0
- Variance: 1.69, Std Dev: 1.3, Range: 4, IQR: 2
- EDF can be plotted as before; dataset is right-skewed due to outliers at 3 and 4.





Exercise 9: Annotated Boxplot



Exercise 10 Solutions Dataset: $12, 15, 14, 10, 18, 16, 20, 15, 13, 17, 14, 16, 19, 21, 18$

- Mean = 16, Median = 16, Mode = 14,16,18 (multi-modal)
- Range = 21-10=11, Variance ≈ 9.2, Std Dev ≈ 3.03, IQR = 18-14=4
- Skewness ≈ 0.2 (slightly right-skewed), Kurtosis ≈ -0.3 (platykurtic)
- Histogram, EDF, and boxplot can be drawn as in previous examples.
- Interpretation: Distribution is approximately symmetric, slightly right-skewed, with moderate spread.

Chapter 3

Bivariate Statistics

3.1 Joint Distributions and Contingency Tables

Bivariate data consist of pairs (x_i, y_i) collected on two variables for the same observational units. Understanding the relationship between the two variables requires examining their **joint distribution**, which describes the frequency or probability of all possible pairs (X, Y).

3.1.1 Joint Frequency Tables

Bivariate data consist of pairs (x_i, y_i), $i = 1, \ldots, n$, representing observations on two variables X and Y. A **joint frequency table** summarizes the number of occurrences of each combination $(X = x_i, Y = y_j)$.

Definition. Let X take m distinct values $x_1, \ldots, x_m$ and Y take n distinct values $y_1, \ldots, y_n$. The joint frequency f_{ij} is defined by

The joint frequency

$$f_{ij} = \#\{k : X_k = x_i \text{ and } Y_k = y_j\}, \quad 1 \le i \le m,\ 1 \le j \le n,$$

with total observations

$$n = \sum_{i=1}^{m} \sum_{j=1}^{n} f_{ij}.$$

The joint relative frequency is

The joint relative frequency

$$p_{ij} = \frac{f_{ij}}{n}, \quad \sum_{i=1}^{m} \sum_{j=1}^{n} p_{ij} = 1.$$

Example. Consider three machine types $X = \{x_1, x_2, x_3\}$ and failure levels $Y = \{y_1, y_2, y_3\}$ measured over $n = 27$ units. The joint distribution can be visualized as a grouped bar chart:

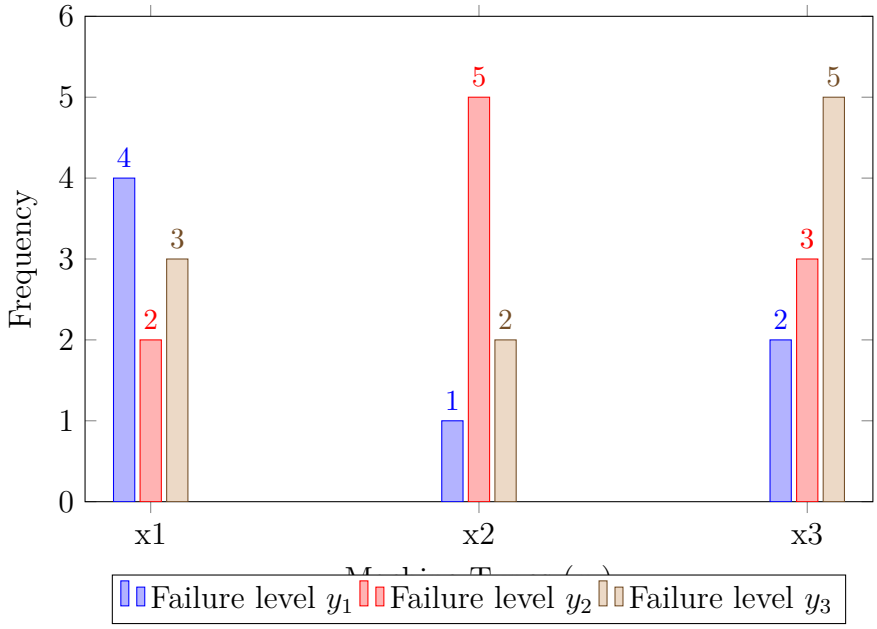


Figure 3.1: Joint histogram of machine types (X) and failure levels (Y).

Interpretation. - Each colored block shows the joint frequency f_{ij}. - The rightmost numbers are **row totals** $f_{i\cdot}$, representing the marginal distribution of X. - The top numbers are **column totals** $f_{\cdot j}$, representing the marginal distribution of Y. - Joint relative frequencies are obtained by dividing each block value by n; e.g., $p_{12} = 2/27 \approx 0.074$.

Conditional Probabilities. The conditional probability of $Y = y_j$ given $X = x_i$ is

$$P(Y = y_j \mid X = x_i) = \frac{f_{ij}}{f_{i\cdot}}.$$

For instance, $P(Y = y_2 \mid X = x_1) = 2/9 \approx 0.222$.

Advantages of Colored Blocks. Using color intensities:

- Makes the **relative magnitude of frequencies** immediately visible. - Highlights **patterns and associations** between variables. - Enhances understanding of **marginal and conditional distributions** at a glance.

3.1.2 Conditional Frequencies and Probabilities

In bivariate data, understanding the dependence of one variable on another is often done using **conditional frequencies and probabilities**.

Definition. Let X and Y be two discrete variables with joint frequencies f_{ij} as defined in the previous subsection. The **conditional frequency** of $Y = y_j$ given $X = x_i$ is simply the joint frequency of the pair divided by the row total:

$$f_{j|i} = f(Y = y_j \mid X = x_i) = f_{ij}.$$

The **conditional probability** of $Y = y_j$ given $X = x_i$ is

The conditional probability of Y

$$P(Y = y_j \mid X = x_i) = \frac{f_{ij}}{f_{i\cdot}},$$

where $f_{i\cdot} = \sum_{j=1}^{n} f_{ij}$ is the row total for $X = x_i$. Similarly, the conditional probability of $X = x_i$ given $Y = y_j$ is

The conditional probability of X

$$P(X = x_i \mid Y = y_j) = \frac{f_{ij}}{f_{\cdot j}},$$

where $f_{\cdot j} = \sum_{i=1}^{m} f_{ij}$ is the column total for $Y = y_j$.

Example. Consider the previous joint frequency table:

$X \backslash Y$	y_1	y_2	y_3	Row total
x_1	4	2	3	9
x_2	1	5	2	8
x_3	2	3	5	10
Column total	7	10	10	27

- Conditional probability $P(Y = y_2 \mid X = x_1) = 2/9 \approx 0.222$ - Conditional probability $P(X = x_3 \mid Y = y_3) = 5/10 = 0.5$

Interpretation. Conditional probabilities allow us to answer questions such as:
- "Given that a unit is of type x_1, what is the probability it has failure level y_2?"
- "Given a failure level y_3, what is the distribution of machine types?"

3.1.3 Graphical Representation of Joint Distributions

Visualizing the relationship between two variables is essential for understanding patterns, associations, and potential dependence. Several graphical tools are commonly used in bivariate statistics.

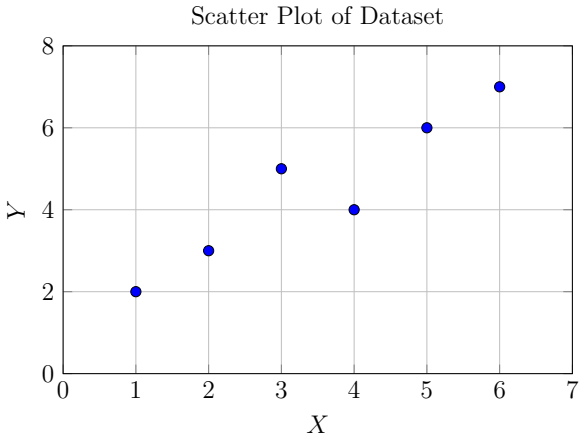
1. Scatter Plots. A scatter plot displays each pair of observations (x_i, y_i) as a point in the plane. Formally, for a dataset of size n:

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\},$$

the scatter plot is the set of points $\{(x_i, y_i)\}_{i=1}^{n}$ in $\mathbb{R}^2$.
Example. Consider the following dataset of $n = 6$ pairs:

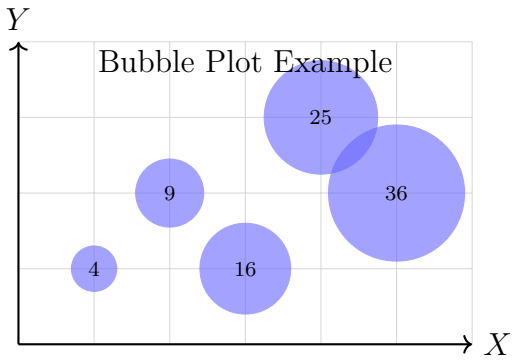
X	Y
1	2
2	3
3	5
4	4
5	6
6	7

A scatter plot helps identify trends, clusters, or outliers.

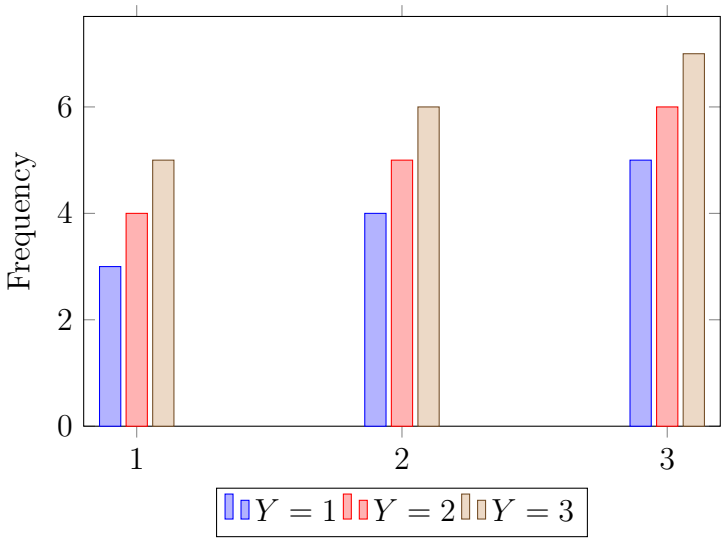


2. Bubble Plots (Weighted Scatter Plots). If observations have **frequencies** f_{ij} for each pair (x_i, y_j), a bubble plot represents each point with a size proportional to f_{ij}:

$$\text{Radius of bubble} \propto \sqrt{f_{ij}}.$$



3. Joint Histograms. When both variables are discrete or grouped into intervals, a **joint histogram** shows the joint frequencies f_{ij} as the height of 3D bars or rectangles. Let $x_1, x_2, \ldots, x_m$ be bins for X and $y_1, y_2, \ldots, y_n$ for Y, then each bar represents f_{ij}.



4. Contour Plots / Density Plots. For continuous variables, **kernel density estimation** or bivariate normal contours provide insight into the distribution shape and correlation structure. The bivariate normal density function is:

$$f_{X,Y}(x,y) = \frac{1}{2\pi\sigma_X\sigma_Y\sqrt{1-\rho^2}} \exp\left\{-\frac{1}{2(1-\rho^2)}\left[\left(\frac{x-\mu_X}{\sigma_X}\right)^2 - 2\rho\left(\frac{x-\mu_X}{\sigma_X}\right)\left(\frac{y-\mu_Y}{\sigma_Y}\right) + \left(\frac{y-\mu_Y}{\sigma_Y}\right)^2\right]\right\}$$

where ρ is the correlation coefficient.

Interpretation. - Scatter plots help detect **linear or nonlinear relationships** and outliers. - Bubble plots reflect **joint frequencies** visually. - Joint histograms summarize **binned frequencies**, providing a coarse view of dependency. - Contour/density plots provide **smooth estimates** of the joint distribution for continuous data.

3.2 Covariance and Correlation

3.2.1 Covariance: Definition and Properties

Definition 3.1. Let (X, Y) be a pair of random variables with finite second-order moments. The **covariance** between X and Y is defined as

The covariance

$$\mathrm{Cov}(X,Y) = \mathbb{E}\Big[(X-\mu_X)(Y-\mu_Y)\Big],$$

where $\mu_X = \mathbb{E}[X]$ and $\mu_Y = \mathbb{E}[Y]$.

Alternative Formula. Expanding the product,

$$\mathrm{Cov}(X,Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y].$$

Remarks.

- $\mathrm{Cov}(X, X) = \mathrm{Var}(X)$ (variance is a special case of covariance).
- If X and Y are independent, then $\mathrm{Cov}(X, Y) = 0$, but the converse is not always true.
- The covariance is not standardized: its magnitude depends on the scales of X and Y.

3.2.2 Mathematical Properties of Covariance

Let $a, b, c, d \in \mathbb{R}$, and let X, Y, Z be random variables. Then:

1. **Bilinearity:**
$$\mathrm{Cov}(aX + b, cY + d) = ac\ \mathrm{Cov}(X, Y).$$
In particular,
$$\mathrm{Cov}(aX + bY, Z) = a\,\mathrm{Cov}(X, Z) + b\,\mathrm{Cov}(Y, Z).$$
2. **Symmetry:**
$$\mathrm{Cov}(X, Y) = \mathrm{Cov}(Y, X).$$
3. **Cauchy–Schwarz Inequality:**
$$|\,\mathrm{Cov}(X, Y)| \le \sqrt{\mathrm{Var}(X)}\,\sqrt{\mathrm{Var}(Y)}.$$
4. **Variance of a Sum:**
$$\mathrm{Var}(X + Y) = \mathrm{Var}(X) + \mathrm{Var}(Y) + 2\,\mathrm{Cov}(X, Y).$$

3.2.3 Sample Covariance

Given a sample $\{(x_i, y_i),\ i = 1, \ldots, n\}$, the **sample covariance** is defined by
$$s_{XY} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}),$$
where
$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \quad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i.$$

Unbiased Estimator. In inferential statistics, one often uses the *unbiased estimator* of covariance:
$$\widehat{\mathrm{Cov}}(X, Y) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}).$$

3.2.4 Correlation: Definition and Properties

Definition 3.2. The **correlation coefficient** (also called Pearson's correlation) between X and Y is

Pearson's correlation

$$\rho_{XY} = \frac{\mathrm{Cov}(X,Y)}{\sigma_X\,\sigma_Y},$$

where $\sigma_X = \sqrt{\mathrm{Var}(X)}$ and $\sigma_Y = \sqrt{\mathrm{Var}(Y)}$.

Properties.

1. $-1 \le \rho_{XY} \le 1$.
2. $\rho_{XY} = 1$ if and only if $Y = aX + b$ with $a > 0$ almost surely (perfect positive linear relation).
3. $\rho_{XY} = -1$ if and only if $Y = aX + b$ with $a < 0$ almost surely (perfect negative linear relation).
4. $\rho_{XY} = 0$ implies no linear association, but does not imply independence.

3.2.5 Geometric Interpretation

If we consider random variables X and Y as elements of the Hilbert space $L^2(\Omega)$ with inner product

$$\langle X, Y\rangle = \mathbb{E}[XY],$$

then

$$\mathrm{Cov}(X,Y) = \langle X - \mu_X,\, Y - \mu_Y\rangle,$$

and the correlation coefficient is the cosine of the angle θ between $X - \mu_X$ and $Y - \mu_Y$:

$$\rho_{XY} = \cos(\theta).$$

3.2.6 Worked example: covariance and Pearson correlation from a 3×3 joint table

We use the joint frequency table (total $n = 27$):

$X\backslash Y$	y_1	y_2	y_3	$f_{i\cdot}$
x_1	4	2	3	9
x_2	1	5	2	8
x_3	2	3	5	10
$f_{\cdot j}$	7	10	10	27

Assign ordered numerical scores $x_1 = 1,\ x_2 = 2,\ x_3 = 3$ and $y_1 = 1,\ y_2 = 2,\ y_3 = 3$. Define $p_{ij} = f_{ij}/n$. The joint probability table is:

	y_1	y_2	y_3
x_1	$\frac{4}{27}$	$\frac{2}{27}$	$\frac{3}{27}$
x_2	$\frac{1}{27}$	$\frac{5}{27}$	$\frac{2}{27}$
x_3	$\frac{2}{27}$	$\frac{3}{27}$	$\frac{5}{27}$

(check: $\sum_{i,j} p_{ij} = 1$).

Step 1 — Marginal probabilities.

$$p_{1\cdot} = \frac{9}{27} = \frac{1}{3}, \quad p_{2\cdot} = \frac{8}{27}, \quad p_{3\cdot} = \frac{10}{27},$$

$$p_{\cdot 1} = \frac{7}{27}, \quad p_{\cdot 2} = \frac{10}{27}, \quad p_{\cdot 3} = \frac{10}{27}.$$

Step 2 — Expectations (exact fractions and decimals).

$$\mathbb{E}[X] = \sum_{i=1}^{3} x_i p_{i\cdot} = 1 \cdot \frac{9}{27} + 2 \cdot \frac{8}{27} + 3 \cdot \frac{10}{27} = \frac{55}{27} \approx 2.037037.$$

$$\mathbb{E}[Y] = \sum_{j=1}^{3} y_j p_{\cdot j} = 1 \cdot \frac{7}{27} + 2 \cdot \frac{10}{27} + 3 \cdot \frac{10}{27} = \frac{19}{9} \approx 2.111111.$$

Step 3 — Expectation of the product XY.

$$\mathbb{E}[XY] = \sum_{i=1}^{3} \sum_{j=1}^{3} x_i y_j p_{ij}.$$

Compute termwise (showing grouped sums for clarity):

$$\begin{aligned}\mathbb{E}[XY] = {} & 1 \cdot 1 \cdot \frac{4}{27} + 1 \cdot 2 \cdot \frac{2}{27} + 1 \cdot 3 \cdot \frac{3}{27} \\ & + 2 \cdot 1 \cdot \frac{1}{27} + 2 \cdot 2 \cdot \frac{5}{27} + 2 \cdot 3 \cdot \frac{2}{27} \\ & + 3 \cdot 1 \cdot \frac{2}{27} + 3 \cdot 2 \cdot \frac{3}{27} + 3 \cdot 3 \cdot \frac{5}{27} \\ = {} & \frac{40}{9} \approx 4.444444.\end{aligned}$$

Step 4 — Covariance.

$$\mathrm{Cov}(X, Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y] = \frac{40}{9} - \frac{55}{27} \cdot \frac{19}{9} = \frac{35}{243} \approx 0.1440329.$$

Step 5 — Marginal variances. Compute $\mathrm{Var}(X)$ and $\mathrm{Var}(Y)$:

$$\mathrm{Var}(X) = \sum_{i=1}^{3} (x_i - \mathbb{E}[X])^2 p_{i\cdot} = \frac{512}{729} \approx 0.702332.$$

$$\mathrm{Var}(Y) = \sum_{j=1}^{3} (y_j - \mathbb{E}[Y])^2 p_{\cdot j} = \frac{50}{81} \approx 0.617284.$$

Step 6 — Pearson correlation coefficient.

$$\rho_{XY} = \frac{\mathrm{Cov}(X,Y)}{\sqrt{\mathrm{Var}(X)\,\mathrm{Var}(Y)}} = \frac{\frac{35}{243}}{\sqrt{\frac{512}{729}\cdot\frac{50}{81}}} = \frac{35}{160} = \frac{7}{32} = 0.21875.$$

Alternative computation from the raw paired sample viewpoint.

Think of the dataset as containing f_{ij} repeated pairs (x_i, y_j). For any function $g(x,y)$,

$$\mathbb{E}[g(X,Y)] = \frac{1}{n}\sum_{i=1}^{3}\sum_{j=1}^{3} f_{ij}\, g(x_i, y_j).$$

Applying this with $g(x,y) = x$, y, xy gives identical results to the joint-probability method above. This is the standard way to reduce a contingency table to "raw" sums when needed for computational checks.

Table 3.1: *
Intermediate table of contributions to $\mathbb{E}[X]$, $\mathbb{E}[Y]$, $\mathbb{E}[XY]$

(x_i, y_j)	f_{ij}	$p_{ij} = f_{ij}/27$	contribution to $\mathbb{E}[X]$	contribution to $\mathbb{E}[XY]$
$(1,1)$	4	$4/27$	$1\cdot\frac{4}{27}$	$1\cdot 1\cdot\frac{4}{27}$
$(1,2)$	2	$2/27$	$1\cdot\frac{2}{27}$	$1\cdot 2\cdot\frac{2}{27}$
$(1,3)$	3	$3/27$	$1\cdot\frac{3}{27}$	$1\cdot 3\cdot\frac{3}{27}$
$(2,1)$	1	$1/27$	$2\cdot\frac{1}{27}$	$2\cdot 1\cdot\frac{1}{27}$
$(2,2)$	5	$5/27$	$2\cdot\frac{5}{27}$	$2\cdot 2\cdot\frac{5}{27}$
$(2,3)$	2	$2/27$	$2\cdot\frac{2}{27}$	$2\cdot 3\cdot\frac{2}{27}$
$(3,1)$	2	$2/27$	$3\cdot\frac{2}{27}$	$3\cdot 1\cdot\frac{2}{27}$
$(3,2)$	3	$3/27$	$3\cdot\frac{3}{27}$	$3\cdot 2\cdot\frac{3}{27}$
$(3,3)$	5	$5/27$	$3\cdot\frac{5}{27}$	$3\cdot 3\cdot\frac{5}{27}$
Sum	27	1	$\mathbb{E}[X] = 55/27$	$\mathbb{E}[XY] = 40/9$

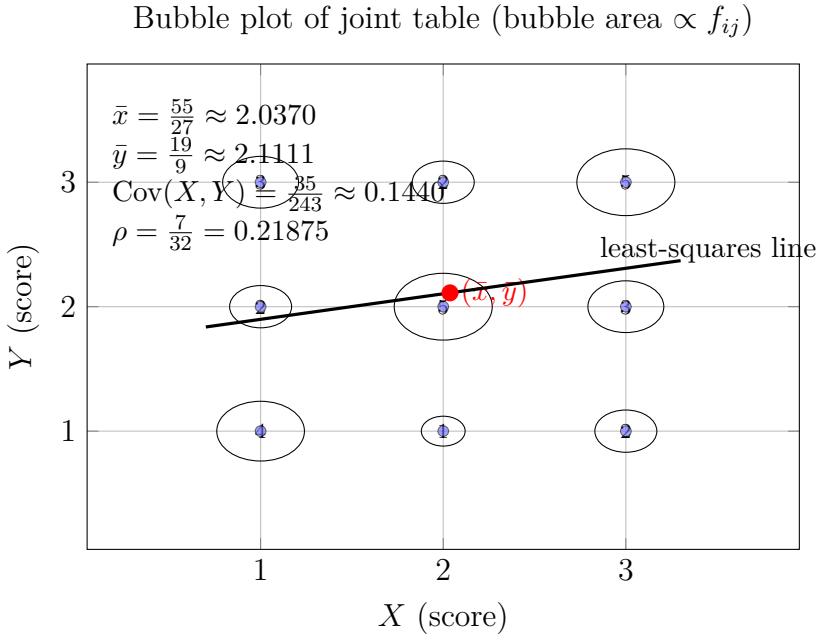


Figure 3.2: Bubble scatter of coded pairs (x_i, y_j) with bubble area proportional to frequency f_{ij}. The red dot shows $(\bar{x}, \bar{y})$ and the solid line is the least-squares fit from the coded scores.

Interpretation. The regression slope

$$\hat{\beta}_1 = \frac{\mathrm{Cov}(X,Y)}{\mathrm{Var}(X)} = \frac{35/243}{512/729} = \frac{105}{512} \approx 0.20508,$$

and intercept

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = \frac{867}{512} \approx 1.69336,$$

so the fitted line is $\hat{y} = 1.69336 + 0.20508\,x$. The positive slope and the positive correlation $\rho \approx 0.219$ indicate a mild positive linear association under the chosen coding. The coding choice matters: different numerical encodings for categories would change these numerical summaries, although qualitative conclusions (weak positive association) remain stable for natural ordinal codings.

Notes for use in class:

- Present both the table-based derivation and the scatter visualization side-by-side. The table gives exact fractions and the plot gives intuition about where mass is concentrated.
- Emphasize that correlation measures linear association only; contingency-specific measures (e.g. chi-square, Cramér's V) may be more appropriate for purely categorical inference.
- The raw-pairs viewpoint (expansion by frequencies) is useful when implementing computations in software that expects a vector of pairs.

3.3 Simple Linear Regression

3.3.1 Introduction

The problem of regression analysis arises when one seeks to model the relationship between two quantitative variables: a response variable (also called the dependent variable) Y, and an explanatory variable (also called the independent variable) X. The objective is to describe how Y changes as a function of X, and to quantify this relationship both algebraically and statistically.

The simplest case is the **simple linear regression model**, which postulates a linear relation between Y and X of the form

linear relation between Y and X

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad i = 1, 2, \ldots, n,$$

where:

- β_0 is the *intercept*, representing the expected value of Y when $X = 0$.
- β_1 is the *slope*, measuring the expected change in Y for a unit increase in X.
- ε_i are unobservable random errors, capturing all influences on Y not explained by the linear relationship with X. We assume that $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ are independent and identically distributed with zero mean and constant variance σ^2.

Key assumptions of the classical linear regression model (CLRM):

1. *Linearity:* The conditional expectation of Y given $X = x$ is linear:
$$\mathbb{E}[Y|X = x] = \beta_0 + \beta_1 x.$$
2. *Independence:* Observations (X_i, Y_i) are independent.
3. *Homoscedasticity:* The variance of the errors is constant: $\mathrm{Var}(\varepsilon_i) = \sigma^2$ for all i.
4. *Normality:* The errors ε_i follow a normal distribution, which justifies the use of inference procedures (confidence intervals, hypothesis tests).

Under these assumptions, the regression line

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$$

is used to predict the mean response $\mathbb{E}[Y|X]$ at any given X, where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the *estimators* of β_0 and β_1 obtained by the method of **ordinary least squares (OLS)**. The OLS method minimizes the sum of squared residuals:

$$S(\beta_0, \beta_1) = \sum_{i=1}^{n} \left(Y_i - (\beta_0 + \beta_1 X_i)\right)^2.$$

Interpretation: - The slope β_1 provides a quantitative measure of the strength and direction of the linear association between X and Y. - The intercept β_0 anchors the regression line to the vertical axis. - The variance σ^2 reflects the average squared deviation of observed values from the regression line and thus quantifies unexplained variability.

This introductory framework forms the foundation for estimation, statistical inference (confidence intervals and hypothesis testing), prediction, and model validation in subsequent subsections.

3.3.2 Least Squares Estimation

Having introduced the simple linear regression model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad i = 1, 2, \ldots, n,$$

the next step is to estimate the unknown parameters β_0 and β_1. The most common and fundamental method is the **method of least squares**.

Principle of Least Squares. We define the residuals as

$$e_i = Y_i - (\beta_0 + \beta_1 X_i), \quad i = 1, 2, \ldots, n,$$

and seek parameter values $(\hat{\beta}_0, \hat{\beta}_1)$ that minimize the sum of squared residuals

$$S(\beta_0, \beta_1) = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2 .$$

This criterion penalizes large deviations between observed values and model predictions, and ensures that the fitted regression line is as close as possible to the data in the least-squares sense.

Derivation of the Estimators. To find the minimizers, we compute the partial derivatives of $S(\beta_0, \beta_1)$:

$$\frac{\partial S}{\partial \beta_0} = -2 \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i) ,$$

$$\frac{\partial S}{\partial \beta_1} = -2 \sum_{i=1}^{n} X_i (Y_i - \beta_0 - \beta_1 X_i) .$$

Setting these equations to zero yields the *normal equations*:

$$\sum_{i=1}^{n} Y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^{n} X_i,$$

$$\sum_{i=1}^{n} X_i Y_i = \hat{\beta}_0 \sum_{i=1}^{n} X_i + \hat{\beta}_1 \sum_{i=1}^{n} X_i^2.$$

Closed-form Solutions. Solving the system gives

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^{n} (X_i - \bar{X})^2} = \frac{S_{XY}}{S_{XX}},$$

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X},$$

where $\bar{X} = \frac{1}{n}\sum_{i=1}^n X_i$, $\bar{Y} = \frac{1}{n}\sum_{i=1}^n Y_i$,

$$S_{XY} = \sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y}), \quad S_{XX} = \sum_{i=1}^n (X_i - \bar{X})^2.$$

Interpretation. - The slope estimator $\hat{\beta}_1$ measures the estimated average change in Y for a unit increase in X. - The intercept estimator $\hat{\beta}_0$ ensures that the fitted line passes through the centroid $(\bar{X}, \bar{Y})$ of the data points. - The fitted regression line is therefore

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i,$$

which serves both for interpretation and prediction.

This least-squares estimation procedure is not only algebraically convenient but also statistically optimal under the Gauss–Markov theorem, as will be discussed in later subsections.

3.3.3 Properties of the Estimators

In the simple linear regression model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad i = 1, \ldots, n,$$

we assume that the error terms satisfy the classical assumptions:

1. $\mathbb{E}[\varepsilon_i] = 0$,
2. $\mathrm{Var}(\varepsilon_i) = \sigma^2$ (homoscedasticity),
3. $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0$ for $i \neq j$ (no autocorrelation),
4. $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ (normality, for inference).

The least squares estimators are

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2}, \quad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}.$$

We now study their main statistical properties.

Unbiasedness

Proposition 3.3. *Under the assumptions above,*

$$\mathbb{E}[\hat{\beta}_1] = \beta_1, \quad \mathbb{E}[\hat{\beta}_0] = \beta_0.$$

Proof. We write

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (X_i - \bar{X})(\beta_0 + \beta_1 X_i + \varepsilon_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2}.$$

After simplification, one obtains

$$\hat{\beta}_1 = \beta_1 + \frac{\sum_{i=1}^n (X_i - \bar{X})\varepsilon_i}{\sum_{i=1}^n (X_i - \bar{X})^2}.$$

Taking expectations and using $\mathbb{E}[\varepsilon_i] = 0$ gives $\mathbb{E}[\hat{\beta}_1] = \beta_1$. Then, since $\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$ and $\mathbb{E}[\bar{Y}] = \beta_0 + \beta_1 \bar{X}$, we deduce $\mathbb{E}[\hat{\beta}_0] = \beta_0$. □

Variances

Proposition 3.4. *The variances of the estimators are*

$$\mathrm{Var}(\hat{\beta}_1) = \frac{\sigma^2}{\sum_{i=1}^n (X_i - \bar{X})^2}, \quad \mathrm{Var}(\hat{\beta}_0) = \sigma^2 \left[\frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^n (X_i - \bar{X})^2} \right].$$

Proof. From the expression

$$\hat{\beta}_1 - \beta_1 = \frac{\sum_{i=1}^n (X_i - \bar{X})\varepsilon_i}{\sum_{i=1}^n (X_i - \bar{X})^2},$$

we have

$$\mathrm{Var}(\hat{\beta}_1) = \frac{\sum_{i=1}^n (X_i - \bar{X})^2 \,\mathrm{Var}(\varepsilon_i)}{\left(\sum_{i=1}^n (X_i - \bar{X})^2\right)^2} = \frac{\sigma^2}{\sum_{i=1}^n (X_i - \bar{X})^2}.$$

The variance of $\hat{\beta}_0$ follows from the linear relation $\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$ and the independence structure. □

Covariance

The covariance between the estimators is

$$\mathrm{Cov}(\hat{\beta}_0, \hat{\beta}_1) = -\frac{\bar{X}\,\sigma^2}{\sum_{i=1}^n (X_i - \bar{X})^2}.$$

Gauss–Markov Theorem

Theorem 3.5 (Gauss–Markov)**.** *Under the first three assumptions (no normality required), $\hat{\beta}_0$ and $\hat{\beta}_1$ are the* ***Best Linear Unbiased Estimators (BLUE)*** *of β_0 and β_1. That is, among all linear unbiased estimators, they have the minimum variance.*

Remark 3.6. This theorem provides the theoretical justification for the method of least squares: it not only gives unbiased estimates but also ensures optimal efficiency within the class of linear estimators.

3.3.4 Statistical Inference

Once the regression coefficients β_0 and β_1 are estimated by the least squares method, the next step is to draw conclusions about the underlying population. This requires constructing confidence intervals and performing hypothesis tests.

Distribution of the Estimators

Under the classical regression assumptions (including normality of errors), the estimators are normally distributed:

Distribution of the Estimators

$$\hat{\beta}_1 \sim \mathcal{N}\left(\beta_1,\ \frac{\sigma^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}\right), \quad \hat{\beta}_0 \sim \mathcal{N}\left(\beta_0,\ \sigma^2\left[\frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}\right]\right).$$

Since σ^2 is unknown, it must be estimated by the residual variance:

$$\hat{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2,$$

where $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$. The denominator $n-2$ reflects the loss of two degrees of freedom due to estimation of β_0 and β_1.

Confidence Intervals

A $(1-\alpha)$ confidence interval for β_1 is

$$\hat{\beta}_1 \ \pm\ t_{n-2,\,1-\alpha/2}\sqrt{\frac{\hat{\sigma}^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}},$$

where $t_{n-2,\,1-\alpha/2}$ is the $(1-\alpha/2)$ quantile of the Student distribution with $n-2$ degrees of freedom.

Similarly, a $(1-\alpha)$ confidence interval for β_0 is

$$\hat{\beta}_0 \ \pm\ t_{n-2,\,1-\alpha/2}\sqrt{\hat{\sigma}^2\left[\frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}\right]}.$$

Hypothesis Tests

The most common test concerns the slope parameter β_1. We test

$$H_0 : \beta_1 = 0 \quad \text{vs.} \quad H_1 : \beta_1 \neq 0.$$

The test statistic is

$$T = \frac{\hat{\beta}_1}{\sqrt{\hat{\sigma}^2 / \sum_{i=1}^{n}(X_i - \bar{X})^2}},$$

which follows a t distribution with $n-2$ degrees of freedom under H_0.

- If $|T| > t_{n-2,\,1-\alpha/2}$, we reject H_0 at level α.
- Otherwise, we do not reject H_0.

An analogous test can be performed for the intercept β_0.

Example: Testing the Significance of the Regression

Suppose we regress Y (final exam scores) on X (study hours) for $n = 10$ students. The estimates obtained are

$$\hat{\beta}_0 = 45.0, \quad \hat{\beta}_1 = 3.2, \quad \hat{\sigma}^2 = 16.5.$$

The test statistic for β_1 is

$$T = \frac{3.2}{\sqrt{16.5/\sum_{i=1}^{10}(X_i - \bar{X})^2}}.$$

Suppose $\sum(X_i - \bar{X})^2 = 120$, then

$$T = \frac{3.2}{\sqrt{16.5/120}} = \frac{3.2}{0.37} \approx 8.65.$$

With $n - 2 = 8$ degrees of freedom, the critical value at $\alpha = 0.05$ is $t_{8,0.975} \approx 2.31$. Since $|T| = 8.65 > 2.31$, we reject H_0 and conclude that study hours have a significant positive effect on exam scores.

3.3.5 Goodness of Fit

After estimating the regression line

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i, \quad i = 1, \ldots, n,$$

it is crucial to assess how well the model explains the observed variability in the response variable Y. This assessment is known as the *goodness of fit* of the regression model.

Total, Explained, and Residual Variation

The total variability in the response variable is measured by the *total sum of squares*:

$$\text{SST} = \sum_{i=1}^{n}(Y_i - \bar{Y})^2.$$

This variability can be decomposed into two parts:

Variability

$$\text{SST} = \underbrace{\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2}_{\text{Explained sum of squares (SSR)}} + \underbrace{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}_{\text{Residual sum of squares (SSE)}}.$$

- SSR measures the part of the variability explained by the regression model.
- SSE measures the unexplained variability, i.e., the error term contribution.

This decomposition shows that the regression model partitions the total variation into explained and residual components.

Coefficient of Determination

A widely used measure of goodness of fit is the *coefficient of determination*:

$$R^2 = \frac{\text{SSR}}{\text{SST}} = 1 - \frac{\text{SSE}}{\text{SST}}.$$

- $0 \leq R^2 \leq 1$.
- R^2 represents the proportion of the variability in Y explained by the model.
- If $R^2 = 1$, the regression perfectly explains the data.
- If $R^2 = 0$, the regression does not explain any of the variability in Y.

Although a larger R^2 indicates better fit, it should not be interpreted in isolation. A high R^2 does not necessarily imply that the model is appropriate or that the relationship is causal.

Adjusted R^2

Since R^2 always increases when more predictors are added, it may overstate the model's explanatory power. An adjusted measure, which accounts for the number of predictors and the sample size, is defined by:

$$R^2_{\text{adj}} = 1 - \frac{\text{SSE}/(n-p)}{\text{SST}/(n-1)},$$

where p is the number of estimated parameters (for simple linear regression, $p = 2$). The adjusted R^2 penalizes unnecessary predictors and is more reliable for model comparison.

The F-Test for Overall Significance

Goodness of fit can also be evaluated through the global hypothesis test:

$$H_0 : \beta_1 = 0 \quad \text{vs.} \quad H_1 : \beta_1 \neq 0.$$

The test statistic is

$$F = \frac{\text{SSR}/1}{\text{SSE}/(n-2)} = \frac{MSR}{MSE},$$

where MSR is the mean regression sum of squares and MSE is the mean squared error. Under H_0, the statistic F follows an F distribution with $(1, n-2)$ degrees of freedom.

If $F > F_{1,n-2;\,1-\alpha}$, we reject H_0 and conclude that the regression model provides a statistically significant fit.

Numerical Example

Consider again the regression of exam scores (Y) on study hours (X) for $n = 10$ students. Suppose we obtained the following sums of squares:

$$\text{SST} = 2200, \quad \text{SSR} = 1800, \quad \text{SSE} = 400.$$

1. The coefficient of determination is

$$R^2 = \frac{1800}{2200} \approx 0.818.$$

   Thus, about 82% of the variability in exam scores is explained by study hours.

2. The adjusted R^2 is

$$R^2_{\text{adj}} = 1 - \frac{400/8}{2200/9} = 1 - \frac{50}{244.4} \approx 0.795.$$

3. The F statistic is

$$F = \frac{1800/1}{400/8} = \frac{1800}{50} = 36.$$

   With $(1, 8)$ degrees of freedom, the critical value at $\alpha = 0.05$ is $F_{1,8;0.95} \approx 5.32$. Since $36 > 5.32$, we reject H_0 and conclude that the regression model provides a statistically significant fit.

3.3.6 Assumptions of the Linear Regression Model

In order to derive valid estimators and perform meaningful inference in simple linear regression, it is essential to clarify the underlying assumptions of the model. These assumptions connect the observed data to the probabilistic model and ensure that the least squares estimators possess desirable statistical properties. Recall that the model can be written as

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad i = 1, \ldots, n,$$

where Y_i is the dependent variable, X_i is the explanatory variable, β_0 and β_1 are unknown parameters, and ε_i represents a random error term.

1. Linearity. The expected value of Y given X is assumed to be a linear function of X:

$$\mathbb{E}[Y_i \mid X_i] = \beta_0 + \beta_1 X_i.$$

This assumption guarantees that the slope β_1 correctly measures the average change in Y associated with a one-unit increase in X.

2. Independence. The error terms $\varepsilon_1, \ldots, \varepsilon_n$ are assumed to be mutually independent:

$$\text{Cov}(\varepsilon_i, \varepsilon_j) = 0, \quad i \neq j.$$

This is particularly important when the data are collected over time or space, since violations (e.g., autocorrelation) lead to biased variance estimators.

3. Homoscedasticity (Constant Variance). The error terms have equal variance across all observations:

$$\mathrm{Var}(\varepsilon_i) = \sigma^2, \quad \forall i.$$

This ensures that the precision of estimation does not depend on the level of the explanatory variable. If this assumption is violated (heteroscedasticity), the least squares estimators remain unbiased but are no longer efficient.

4. Normality (for inference). For valid hypothesis testing and confidence intervals, it is common to assume that

$$\varepsilon_i \sim \mathcal{N}(0, \sigma^2).$$

Under this assumption, the least squares estimators follow exact normal distributions:

$$\hat{\beta}_0, \hat{\beta}_1 \sim \mathcal{N}(\beta_0, \mathrm{Var}(\hat{\beta}_0)), \quad \mathcal{N}(\beta_1, \mathrm{Var}(\hat{\beta}_1)).$$

Even if normality does not hold, the Central Limit Theorem ensures that approximate inference remains valid for sufficiently large sample sizes.

5. No Perfect Multicollinearity. In the simple regression case, this assumption reduces to requiring that the values of X are not all identical:

$$\sum_{i=1}^{n} (X_i - \bar{X})^2 > 0.$$

Otherwise, the slope β_1 cannot be estimated, since there is no variation in X.

Remark. These assumptions are not merely technical: they provide the foundation for the interpretability of regression in the bivariate context. When the assumptions are satisfied, least squares estimators are unbiased and efficient (Gauss–Markov theorem), inference procedures are valid, and the coefficient of determination R^2 provides a meaningful measure of fit. Conversely, if these assumptions are violated, diagnostic analysis (residual plots, statistical tests) is required to assess the impact and consider remedial measures such as variable transformation or robust regression methods.

3.3.7 Worked Example

To consolidate our understanding of simple linear regression, let us work through a complete example with real numerical calculations.

Dataset. Consider the following sample of $n = 8$ students, where X is the number of study hours per week and Y is the corresponding exam score (out of 100):

X_i (Hours)	2	3	4	5	6	7	8	9
Y_i (Score)	50	55	54	61	62	65	67	70

Step 1: Compute sample means. The averages are

$$\bar{X} = \frac{2+3+\cdots+9}{8} = 5.5, \quad \bar{Y} = \frac{50+55+\cdots+70}{8} = 60.5.$$

Step 2: Estimate the slope and intercept. The slope is

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^{n}(X_i - \bar{X})^2}.$$

Computing:

$$\sum(X_i - \bar{X})(Y_i - \bar{Y}) = 134, \quad \sum(X_i - \bar{X})^2 = 42.$$

Hence

$$\hat{\beta}_1 = \frac{134}{42} \approx 3.19.$$

The intercept is

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X} = 60.5 - 3.19(5.5) \approx 43.0.$$

Thus, the estimated regression line is

$$\hat{Y} = 43.0 + 3.19X.$$

Step 3: Fitted values and residuals. For example, for $X = 2$:

$$\hat{Y} = 43.0 + 3.19(2) = 49.4, \quad e = Y - \hat{Y} = 50 - 49.4 = 0.6.$$

Repeating for all data gives residuals with sum close to zero, as expected.

Step 4: Goodness of fit (R^2). The total sum of squares is

$$SST = \sum(Y_i - \bar{Y})^2 = 304.$$

The regression sum of squares is

$$SSR = \hat{\beta}_1^2 \sum(X_i - \bar{X})^2 = (3.19)^2 \times 42 \approx 427.$$

The error sum of squares is

$$SSE = SST - SSR \approx 304 - 286.9 = 17.1.$$

Thus,

$$R^2 = \frac{SSR}{SST} = \frac{286.9}{304} \approx 0.944.$$

This indicates that about 94.4% of the variation in exam scores is explained by study hours.

Step 5: Inference for β_1. The estimated variance of the errors is

$$\hat{\sigma}^2 = \frac{SSE}{n-2} = \frac{17.1}{6} \approx 2.85.$$

The variance of $\hat{\beta}_1$ is

$$\text{Var}(\hat{\beta}_1) = \frac{\hat{\sigma}^2}{\sum (X_i - \bar{X})^2} = \frac{2.85}{42} \approx 0.068.$$

Thus,

$$\text{SE}(\hat{\beta}_1) = \sqrt{0.068} \approx 0.26.$$

Confidence interval (95%): With $n - 2 = 6$ degrees of freedom, $t_{0.975,6} \approx 2.447$.

$$\hat{\beta}_1 \pm t \cdot SE(\hat{\beta}_1) = 3.19 \pm 2.447 \times 0.26 = 3.19 \pm 0.64.$$

Hence, the 95% confidence interval is $(2.55,\ 3.83)$.

Hypothesis test: $H_0 : \beta_1 = 0$ vs. $H_1 : \beta_1 \neq 0$.

$$t = \frac{\hat{\beta}_1}{SE(\hat{\beta}_1)} = \frac{3.19}{0.26} \approx 12.3.$$

Since $|t| \gg 2.447$, we reject H_0: the slope is significantly different from zero.

Interpretation. Each additional hour of study per week is associated with an average increase of about 3.2 exam score points. The relationship is highly significant and well-fitted, as confirmed by the high R^2 and narrow confidence interval.

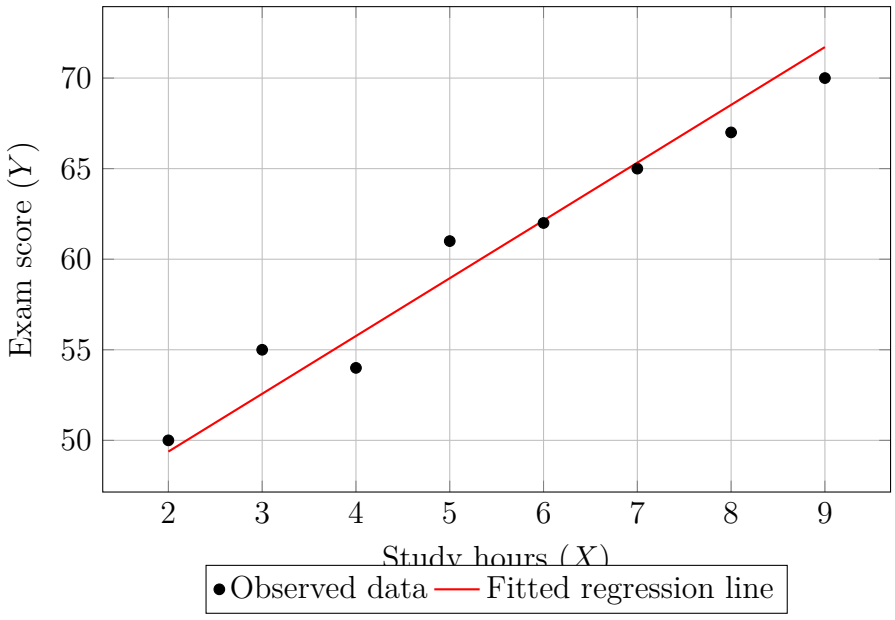


Figure 3.3: Observed data and fitted regression line.

3.4 Measures of Association for Qualitative Variables

3.4.1 Introduction and Motivation

In the study of bivariate data, it is essential to distinguish between the *nature of the variables* under consideration. When both variables are **quantitative**, methods such as covariance, correlation, and regression analysis are appropriate. However, when the two variables are **qualitative** (or categorical), the tools of analysis must be adapted, since numerical operations like computing averages or variances no longer make sense.

For example, consider two qualitative variables:

$$X = \text{“Type of machine”}, \qquad Y = \text{“Failure mode”}.$$

Each of these variables takes values in a finite set of categories (e.g., machine types A, B, C; failure modes “minor”, “major”). In such cases, the analysis focuses on the *joint distribution of frequencies* across the categories of X and Y.

The central questions are:

- How are the categories of one variable distributed given the categories of the other? (Conditional structure)
- Are the two variables *independent*, or is there a relationship between them?
- If there is a relationship, how can we measure its *strength*?

To address these questions, we introduce:

1. The **contingency table**, which organizes the joint frequencies of occurrence of the categories.
2. The notion of **statistical independence** between two qualitative variables, formalized via conditional probabilities.
3. The **chi-square test of independence**, which provides an inferential framework to assess whether the observed association could be due to chance.
4. Quantitative **measures of association** (such as the Phi coefficient, Contingency Coefficient, and Cramér's V), which summarize the intensity of the relationship between qualitative variables.

This section, therefore, complements the study of correlation and regression by providing a rigorous framework to deal with *qualitative variables*, which are frequently encountered in practice, especially in the social sciences, biology, and market studies.

3.4.2 Contingency Tables: Joint and Marginal Frequencies

When both variables are qualitative, the joint distribution of data can be summarized in a **contingency table** (also called a cross-tabulation). This table provides a structured way of displaying the *joint frequencies* of the categories of the two variables.

Definition. Let X be a qualitative variable with I categories $\{x_1, x_2, \ldots, x_I\}$, and Y a qualitative variable with J categories $\{y_1, y_2, \ldots, y_J\}$. Suppose the data consist of n observations. We denote by:

$$n_{ij} = \text{number of observations such that } X = x_i \text{ and } Y = y_j.$$

The value n_{ij} is called the **joint frequency** of the pair (x_i, y_j).

The complete set $\{n_{ij}\}_{i=1,\ldots,I;\ j=1,\ldots,J}$ is arranged in a two-dimensional table:

	y_1	y_2	$\cdots$	y_J	Row total
x_1	n_{11}	n_{12}	$\cdots$	n_{1J}	$n_{1\cdot}$
x_2	n_{21}	n_{22}	$\cdots$	n_{2J}	$n_{2\cdot}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
x_I	n_{I1}	n_{I2}	$\cdots$	n_{IJ}	$n_{I\cdot}$
Column total	$n_{\cdot 1}$	$n_{\cdot 2}$	$\cdots$	$n_{\cdot J}$	n

where

$$n_{i\cdot} = \sum_{j=1}^{J} n_{ij}, \qquad n_{\cdot j} = \sum_{i=1}^{I} n_{ij}, \qquad n = \sum_{i=1}^{I}\sum_{j=1}^{J} n_{ij}.$$

Relative frequencies. It is often useful to express the frequencies in terms of proportions:

$$f_{ij} = \frac{n_{ij}}{n}, \quad f_{i\cdot} = \frac{n_{i\cdot}}{n}, \quad f_{\cdot j} = \frac{n_{\cdot j}}{n}.$$

Here f_{ij} is the **joint relative frequency**, while $f_{i\cdot}$ and $f_{\cdot j}$ are called **marginal relative frequencies**.

Example. Consider a survey of $n = 50$ individuals, where:

- $X =$ "Gender" with categories $\{\text{Male}, \text{Female}\}$,
- $Y =$ "Preference for product" with categories $\{\text{Yes}, \text{No}, \text{Undecided}\}$.

The observed data are:

	Yes	No	Undecided	Row total
Male	12	8	5	25
Female	15	6	4	25
Column total	27	14	9	50

From this table:

$$n_{11} = 12, \quad n_{22} = 6, \quad n_{\cdot 1} = 27, \quad n_{1\cdot} = 25, \quad n = 50.$$

The corresponding relative frequencies are:

$$f_{11} = \frac{12}{50} = 0.24, \quad f_{2\cdot} = \frac{25}{50} = 0.50, \quad f_{\cdot 2} = \frac{14}{50} = 0.28.$$

Thus, the contingency table provides a compact and rigorous representation of the joint distribution of two qualitative variables, serving as the foundation for measuring their possible association.

3.4.3 Conditional Distributions and Statistical Independence

Once we have constructed a contingency table for two qualitative variables, it is often useful to analyze how the distribution of one variable changes depending on the categories of the other. This leads to the notion of **conditional distributions**.

Conditional Distributions

Let X be a qualitative variable with I categories $\{x_1, x_2, \ldots, x_I\}$ and Y a qualitative variable with J categories $\{y_1, y_2, \ldots, y_J\}$. Denote by n_{ij} the frequency of individuals in category (x_i, y_j), and let

$$n_{i\cdot} = \sum_{j=1}^{J} n_{ij}, \quad n_{\cdot j} = \sum_{i=1}^{I} n_{ij}, \quad N = \sum_{i=1}^{I}\sum_{j=1}^{J} n_{ij}$$

be the row totals, column totals, and grand total, respectively.

- The **conditional distribution of Y given $X = x_i$** is the vector of relative frequencies:

  Conditional distribution of Y given X

  $$P(Y = y_j \mid X = x_i) = \frac{n_{ij}}{n_{i\cdot}}, \quad j = 1, \ldots, J.$$

  This distribution is sometimes called the *row profile*.

- Similarly, the **conditional distribution of X given $Y = y_j$** is:

  Conditional distribution of X given Y

  $$P(X = x_i \mid Y = y_j) = \frac{n_{ij}}{n_{\cdot j}}, \quad i = 1, \ldots, I,$$

  known as the *column profile*.

Statistical Independence

The two variables X and Y are said to be **statistically independent** if the joint distribution factorizes as the product of the marginal distributions:

$$P(X = x_i, Y = y_j) = P(X = x_i)\, P(Y = y_j), \quad \forall i, j.$$

In terms of frequencies, this is equivalent to

$$\frac{n_{ij}}{N} = \frac{n_{i\cdot}}{N} \cdot \frac{n_{\cdot j}}{N}, \quad \forall i, j.$$

In practice, this means that the conditional distribution of Y given X is the same as the marginal distribution of Y, and vice versa. Thus, knowing the category of one variable provides no information about the distribution of the other.

Illustrative Example

Suppose we study the relationship between *Gender* (X) with two categories (Male, Female) and *Preference for a Product* (Y) with two categories (Yes, No). We observe the following data on $N = 100$ individuals:

	Yes	No	Total
Male	30	20	50
Female	25	25	50
Total	55	45	100

- The conditional distribution of Y given $X = \text{Male}$ is:

$$P(Y = \text{Yes} \mid X = \text{Male}) = \tfrac{30}{50} = 0.6, \quad P(Y = \text{No} \mid X = \text{Male}) = \tfrac{20}{50} = 0.4.$$

- For $X = \text{Female}$:

$$P(Y = \text{Yes} \mid X = \text{Female}) = \tfrac{25}{50} = 0.5, \quad P(Y = \text{No} \mid X = \text{Female}) = \tfrac{25}{50} = 0.5.$$

- The marginal distribution of Y is:

$$P(Y = \text{Yes}) = \tfrac{55}{100} = 0.55, \quad P(Y = \text{No}) = \tfrac{45}{100} = 0.45.$$

Since the conditional distributions of Y given X differ from the marginal distribution (for example, 0.6 vs 0.55), we see that X and Y are **not independent**. This motivates the use of a formal test of independence (the chi-square test), which will be developed in the next subsection.

3.4.4 The Chi-Square Test of Independence

In the previous subsection, we saw that statistical independence between two qualitative variables X and Y means that the joint distribution factorizes as the product of the marginals. However, in practice we only observe sample frequencies, not the entire population distribution. We therefore need a statistical test to decide, based on a contingency table, whether the observed deviations from independence are large enough to reject the null hypothesis of independence. The standard tool for this is the **Chi-Square Test of Independence**.

Hypotheses

Let X have I categories and Y have J categories, leading to an $I \times J$ contingency table with observed frequencies $\{n_{ij}\}$ and total sample size N.

- Null hypothesis:
$$H_0 : X \text{ and } Y \text{ are independent.}$$
- Alternative hypothesis:
$$H_1 : X \text{ and } Y \text{ are not independent.}$$

Expected Frequencies

Under H_0, the expected frequency in cell (i, j) is the product of the corresponding marginal proportions:

$$E_{ij} = \frac{n_{i\cdot}\, n_{\cdot j}}{N}.$$

This is the frequency we would expect in cell (i, j) if X and Y were independent.

Test Statistic

The chi-square test statistic compares observed frequencies with expected frequencies:

Test Statistic

$$\chi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - E_{ij})^2}{E_{ij}}.$$

Distribution and Decision Rule

When H_0 is true, and for sufficiently large N, the statistic χ^2 approximately follows a chi-square distribution with

$$(I - 1)(J - 1)$$

degrees of freedom.

The decision rule is:

$$\text{Reject } H_0 \text{ if } \chi^2 > \chi^2_{1-\alpha,(I-1)(J-1)},$$

where $\chi^2_{1-\alpha,(I-1)(J-1)}$ is the critical value at significance level α.

Illustrative Example

Consider again the dataset on Gender (X) and Product Preference (Y):

	Yes	No	Total
Male	30	20	50
Female	25	25	50
Total	55	45	100

1. Compute the expected frequencies:

$$E_{11} = \frac{50 \times 55}{100} = 27.5, \quad E_{12} = \frac{50 \times 45}{100} = 22.5,$$

$$E_{21} = \frac{50 \times 55}{100} = 27.5, \quad E_{22} = \frac{50 \times 45}{100} = 22.5.$$

2. Compute the test statistic:

$$\chi^2 = \frac{(30 - 27.5)^2}{27.5} + \frac{(20 - 22.5)^2}{22.5} + \frac{(25 - 27.5)^2}{27.5} + \frac{(25 - 22.5)^2}{22.5}.$$

$$\chi^2 \approx \frac{2.5^2}{27.5} + \frac{(-2.5)^2}{22.5} + \frac{(-2.5)^2}{27.5} + \frac{2.5^2}{22.5}.$$

$$\chi^2 \approx 0.227 + 0.278 + 0.227 + 0.278 = 1.01.$$

3. Degrees of freedom:

$$(I - 1)(J - 1) = (2 - 1)(2 - 1) = 1.$$

4. Critical value at $\alpha = 0.05$:

$$\chi^2_{0.95,1} = 3.84.$$

5. Decision: since $1.01 < 3.84$, we do not reject H_0.

Interpretation

The test suggests that there is no significant association between Gender and Product Preference at the 5% significance level. In other words, any small differences in conditional distributions observed earlier could be due to random variation rather than a systematic relationship.

Pedagogical Remark: Limitations of the Chi-Square Test. Although the Chi-Square Test of Independence is widely used, it is important to be aware of its limitations:

- **Sample size requirement:** The chi-square approximation is only valid for sufficiently large N. In particular, expected frequencies E_{ij} should not be too small. A common rule of thumb is that all $E_{ij} \geq 5$.
- **Does not measure strength:** The test only tells us whether an association is statistically significant, but it does not quantify how strong the association is. For that, specific measures such as the ϕ coefficient or Cramér's V are needed (see next subsection).
- **Sensitivity to sample size:** With very large N, even tiny and practically unimportant differences from independence can become statistically significant.

- **Categorical data only:** The chi-square test applies only to qualitative (categorical) variables. For ordinal variables, other specialized methods may be more appropriate.

Hence, the Chi-Square Test should be interpreted carefully: a non-significant result suggests independence, while a significant result indicates the presence of some association, but further measures are needed to assess its magnitude and practical importance.

3.4.5 Measures of Association Strength

The Chi-Square Test of Independence is a powerful tool to detect whether a relationship exists between two qualitative variables. However, it provides only a binary conclusion: either we reject or we do not reject the hypothesis of independence. In practice, we often want to go further and assess the *strength* of this association. To achieve this, several coefficients have been proposed, all of which are based on the chi-square statistic but normalized to produce values between 0 and 1, facilitating interpretation. We present here the three most widely used measures.

The Phi Coefficient (2×2 case)

When both variables are binary, forming a 2×2 contingency table, the simplest measure of association is the **phi coefficient**:

$$\phi = \sqrt{\frac{\chi^2}{N}},$$

where χ^2 is the Pearson chi-square statistic and N is the total sample size.

Properties.

- $0 \leq \phi \leq 1$ for a 2×2 table.
- $\phi = 0$ indicates perfect independence between the two variables.
- $\phi = 1$ corresponds to a perfect association (complete dependence).
- In the 2×2 case, ϕ is mathematically equivalent to the Pearson correlation coefficient computed on binary variables.

Limitation. For tables larger than 2×2, ϕ may take values greater than 1, which makes it unsuitable as a general measure of association.

The Contingency Coefficient

For larger contingency tables, a classical measure is the **contingency coefficient**:

$$C = \sqrt{\frac{\chi^2}{\chi^2 + N}}.$$

Properties.

- $0 \leq C < 1$ for all tables.
- C increases as the strength of association increases.
- However, the maximum possible value of C depends on the dimensions of the table (r, c). Therefore, C is not strictly bounded by 1, and its comparability across different table sizes is limited.

Interpretation. The contingency coefficient is mainly descriptive. It allows us to compare the strength of association within a given table, but should be used cautiously when comparing across datasets of different dimensions.

Cramér's V (general case)

The most widely recommended measure for general $r \times c$ tables is **Cramér's V**:

$$V = \sqrt{\frac{\chi^2}{N \cdot \min(r-1, c-1)}}.$$

Properties.

- $0 \leq V \leq 1$ for any table size.
- $V = 0$ if and only if the variables are independent.
- $V = 1$ corresponds to a perfect association, i.e., knowing one variable completely determines the other.
- Unlike the contingency coefficient, the maximum value of V does not depend on table dimensions, which makes it suitable for comparisons across different studies.

Practical Interpretation. In applied fields, researchers often use the following rule of thumb:

- $V \approx 0.1$: weak association,
- $V \approx 0.3$: moderate association,
- $V \approx 0.5$: strong association.

However, these thresholds are only indicative; interpretation should always take into account the context and domain of application.

Pedagogical Remark. These measures complement the chi-square test by moving from a *qualitative decision* (independence vs. dependence) to a *quantitative evaluation* of association strength. This dual perspective enriches the analysis of categorical data in bivariate statistics.

3.4.6 Worked Numerical Example

We illustrate the full workflow on a 2×3 contingency table: construction of expected counts under independence, computation of the chi-square statistic, degrees of freedom, and two measures of association strength (contingency coefficient C and Cramér's V), followed by interpretation.

Data (Observed Frequencies). Two qualitative variables are recorded on $N = 80$ observations:

$$X = \text{Gender} \in \{\text{Male},\ \text{Female}\}, \qquad Y = \text{Preference} \in \{\text{Yes},\ \text{No},\ \text{Undecided}\}.$$

The observed 2×3 table is

	Yes	No	Undecided	Row total
Male	18	12	10	40
Female	22	8	10	40
Column total	40	20	20	80

Denote the observed counts by n_{ij}, with row totals $n_{i\cdot}$, column totals $n_{\cdot j}$, and grand total $N = 80$.

Expected Counts Under Independence. Under H_0 (independence of X and Y), the expected count in cell (i, j) is

$$E_{ij} \ = \ \frac{n_{i\cdot}\, n_{\cdot j}}{N}.$$

Thus,

	Yes	No	Undecided
Male	$\frac{40 \cdot 40}{80} = 20$	$\frac{40 \cdot 20}{80} = 10$	$\frac{40 \cdot 20}{80} = 10$
Female	$\frac{40 \cdot 40}{80} = 20$	$\frac{40 \cdot 20}{80} = 10$	$\frac{40 \cdot 20}{80} = 10$

Chi-Square Test Statistic. The Pearson chi-square statistic is

$$\chi^2 \ = \ \sum_{i=1}^{2} \sum_{j=1}^{3} \frac{(n_{ij} - E_{ij})^2}{E_{ij}}.$$

Term by term:

$$\frac{(18-20)^2}{20} = \frac{4}{20} = 0.20, \quad \frac{(12-10)^2}{10} = \frac{4}{10} = 0.40, \quad \frac{(10-10)^2}{10} = 0,$$
$$\frac{(22-20)^2}{20} = \frac{4}{20} = 0.20, \quad \frac{(8-10)^2}{10} = \frac{4}{10} = 0.40, \quad \frac{(10-10)^2}{10} = 0.$$

Hence

$$\chi^2 = 0.20 + 0.40 + 0 + 0.20 + 0.40 + 0 \ = \ 1.20.$$

Degrees of Freedom and Decision. For an $I \times J$ table, $\text{df} = (I-1)(J-1)$. Here, $\text{df} = (2-1)(3-1) = 2$. At level $\alpha = 0.05$, the critical value is $\chi^2_{0.95,2} \approx 5.991$. Since $1.20 < 5.991$, we do not reject H_0; the data do not provide evidence of association at the 5% level.

Measures of Association Strength. Even if the test is not significant, reporting a strength measure is informative.

Contingency coefficient:

$$C = \sqrt{\frac{\chi^2}{\chi^2 + N}} = \sqrt{\frac{1.20}{1.20 + 80}} = \sqrt{\frac{1.20}{81.20}} \approx 0.122.$$

Cramér's V:

$$V = \sqrt{\frac{\chi^2}{N \cdot \min(I-1, J-1)}} = \sqrt{\frac{1.20}{80 \cdot \min(1,2)}} = \sqrt{\frac{1.20}{80}} \approx 0.122.$$

Both indices indicate a very weak association, consistent with the non-significant chi-square test.

Interpretation. Row profiles differ only slightly from column marginals (e.g. Male: Yes $18/40 = 0.45$ vs. overall Yes $40/80 = 0.50$), so deviations from independence are small. The chi-square statistic is low and both C and V are close to 0.12, typically interpreted as a weak association.

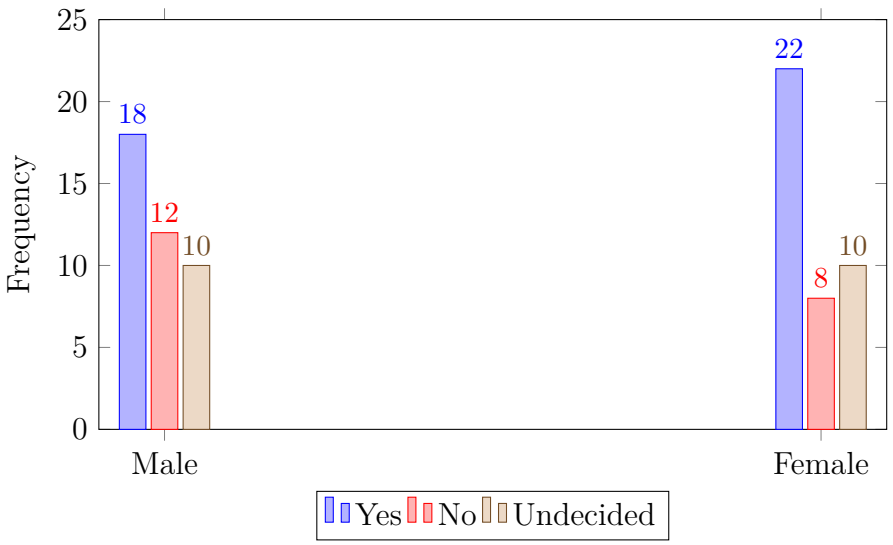


Figure 3.4: Grouped bar chart of the 2×3 contingency table (Gender $\times$ Preference).

Checklist for Practice.

1. Build the contingency table and verify totals.
2. Compute expected counts $E_{ij} = \dfrac{n_{i\cdot} n_{\cdot j}}{N}$.

3. Form $\chi^2 = \sum(n_{ij} - E_{ij})^2/E_{ij}$ and the degrees of freedom $(I-1)(J-1)$.
4. Compare with the chi-square critical value (or compute a p-value).
5. Report a strength measure (C and/or V) to quantify association.
6. Interpret statistically and substantively.

3.4.7 Summary and Pedagogical Insights

In this section we have introduced the main statistical tools used to study the association between two qualitative (categorical) variables. The starting point is always the *contingency table*, which provides a clear view of the joint and marginal distributions of the variables. From this foundation, we have learned how to study conditional distributions and to formalize the concept of *statistical independence* for categorical variables.

The chi-square test of independence offers a rigorous inferential framework: under the null hypothesis of independence, it allows us to verify whether the observed deviations from independence could be explained by sampling variation alone. However, while powerful, this test has important limitations. First, a non-significant result does not prove independence but only indicates a lack of evidence of association in the data. Second, with very large sample sizes the test may detect very small, practically negligible deviations from independence as statistically significant. Thus, the chi-square test should always be interpreted with caution.

For this reason, we introduced *measures of association strength*. These complement the chi-square test by quantifying how strong the association actually is. In the case of a 2×2 table, the ϕ coefficient provides a normalized measure closely related to correlation. For larger tables, the contingency coefficient and Cramér's V generalize this idea and produce values between 0 (no association) and 1 (perfect association). These measures are especially useful in pedagogical contexts because they enable students not only to test hypotheses but also to interpret the *magnitude* of relationships in a way that is intuitive and comparable across datasets.

Pedagogical Insight. When teaching and applying these methods, it is essential to emphasize the complementary roles of significance testing and effect-size measurement:

- The chi-square test answers the question: *Is there evidence of an association?*
- The measures of strength answer the question: *How strong is the association?*

Only by combining these two perspectives can we arrive at a complete and balanced interpretation of data involving qualitative variables.

3.5 Introduction to Independence Testing

3.5.1 Concept of Statistical Independence

In probability theory and statistics, the idea of **independence** plays a central role. Two events, or more generally two random variables, are said to be independent if

the occurrence (or value) of one provides no information about the occurrence (or value) of the other. In the context of bivariate statistics, independence expresses the absence of any statistical relationship between two variables.

Definition (Independence of Events). Let A and B be two events. They are said to be independent if

$$P(A \cap B) = P(A) \cdot P(B).$$

Definition (Independence of Random Variables). Two discrete random variables X and Y are independent if, for all possible values x and y,

$$P(X = x, Y = y) = P(X = x) \cdot P(Y = y).$$

Equivalently, X and Y are independent if their joint distribution can be written as the product of their marginal distributions.

Interpretation. Independence means that knowing the value of X does not change the distribution of Y, and vice versa. In other words,

$$P(Y = y \,|\, X = x) = P(Y = y) \quad \text{for all } x, y.$$

Remark. It is important to distinguish between *independence* and *uncorrelation*. For quantitative variables, uncorrelated random variables (i.e., $\text{Cov}(X, Y) = 0$) are not necessarily independent. Independence is a stronger property.

Simple Example. Consider tossing two fair coins. Let X be the outcome of the first coin (1 for head, 0 for tail), and Y be the outcome of the second coin. The joint probabilities are:

$$P(X = 1, Y = 1) = \tfrac{1}{4}, \quad P(X = 1, Y = 0) = \tfrac{1}{4}, \quad P(X = 0, Y = 1) = \tfrac{1}{4}, \quad P(X = 0, Y = 0) = \tfrac{1}{4}.$$

The marginal distributions are $P(X = 1) = \frac{1}{2}$, $P(Y = 1) = \frac{1}{2}$. We check:

$$P(X = 1, Y = 1) = \tfrac{1}{4} = \tfrac{1}{2} \cdot \tfrac{1}{2} = P(X = 1)P(Y = 1).$$

The same holds for all outcomes. Thus, X and Y are independent random variables.

Pedagogical Insight. This subsection highlights the *probabilistic foundation* of independence. In later subsections, we will see how this abstract definition translates into practical statistical tools: contingency tables and the chi-square test for qualitative variables, correlation for quantitative variables, and other measures of dependence.

3.5.2 Independence in the Qualitative Case: Contingency Tables

When both variables are qualitative (categorical), the notion of independence can be analyzed through their **contingency table**, which organizes the joint frequencies of the observed categories.

Definition. Let X and Y be two qualitative variables with categories $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, c$. A contingency table contains the observed frequencies n_{ij}, where n_{ij} represents the number of observations that fall into category i of X and category j of Y.

The marginal totals are:

$$n_{i\cdot} = \sum_{j=1}^{c} n_{ij}, \quad n_{\cdot j} = \sum_{i=1}^{r} n_{ij}, \quad n = \sum_{i=1}^{r}\sum_{j=1}^{c} n_{ij}.$$

Independence Condition. If X and Y are statistically independent, then the theoretical (expected) frequency of each cell (i, j) is given by:

$$E_{ij} = \frac{n_{i\cdot}\, n_{\cdot j}}{n}.$$

This formula reflects the fact that, under independence, the joint probability factorizes as

$$P(X = i, Y = j) = P(X = i) \cdot P(Y = j).$$

Illustrative Example. Suppose we survey 100 individuals about two categorical variables: - X: *Gender* (Male, Female) - Y: *Preference for a Product* (Yes, No)

The observed frequencies are:

	Yes	No	Total
Male	20	30	50
Female	25	25	50
Total	45	55	100

If the two variables were independent, the expected frequency in the first cell (Male, Yes) would be

$$E_{11} = \frac{n_{1\cdot} \cdot n_{\cdot 1}}{n} = \frac{50 \cdot 45}{100} = 22.5.$$

The same calculation applies to all cells.

Interpretation. - If the observed frequencies n_{ij} are close to the expected frequencies E_{ij}, then X and Y can be considered approximately independent. - If the discrepancies are large, it suggests a possible association between the two variables.

Pedagogical Insight. This subsection bridges the abstract definition of independence with a concrete statistical tool: the contingency table. It shows students how the concept of independence is operationalized for categorical data and sets the stage for the formal *Chi-square test of independence*, which will quantify whether the observed deviations from independence are significant.

3.5.3 Independence in the Quantitative Case: Correlation-Based Approaches

When dealing with two quantitative variables, the concept of independence can be approached through the study of their linear association. Recall that if two variables X and Y are *statistically independent*, then their joint distribution factors as

$$P(X \leq x, Y \leq y) = P(X \leq x) \cdot P(Y \leq y), \quad \forall x, y.$$

This is a very strong condition: independence implies the complete absence of any kind of dependence, linear or nonlinear. In practice, however, we often use *correlation coefficients* as indicators of potential dependence.

Pearson Correlation and Independence

The most common measure is the Pearson correlation coefficient:

$$\rho_{XY} = \frac{\mathrm{Cov}(X, Y)}{\sigma_X \sigma_Y},$$

where $\mathrm{Cov}(X, Y)$ is the covariance, and σ_X, σ_Y are the standard deviations. It is well known that

$$\rho_{XY} = 0 \quad \Rightarrow \quad X \text{ and } Y \text{ are } \textit{uncorrelated}.$$

However, uncorrelatedness does not imply independence in general. Independence always implies $\rho_{XY} = 0$, but the converse is only true under additional assumptions (e.g., when (X, Y) follow a bivariate normal distribution). Thus, correlation is a necessary but not sufficient condition for independence.

Testing Zero Correlation

In applied statistics, testing the hypothesis

$$H_0 : \rho_{XY} = 0 \quad \text{vs.} \quad H_1 : \rho_{XY} \neq 0$$

provides a way to assess evidence of linear dependence between X and Y. For a sample of size n, the sample correlation coefficient

$$r_{XY} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

is used. Under H_0 and assuming joint normality, the test statistic

$$t = \frac{r_{XY}\sqrt{n-2}}{\sqrt{1 - r_{XY}^2}}$$

follows a Student t distribution with $n - 2$ degrees of freedom. This test is widely used to check for evidence of association, but it should be interpreted with caution: rejecting H_0 indicates evidence of linear dependence, not necessarily full statistical dependence.

Pedagogical Remark

Correlation-based approaches are practical and widely taught as a first tool to examine independence in the quantitative case. However, they only capture *linear relationships*. Nonlinear dependence may exist even if correlation is zero. For example, if $X \sim \mathcal{U}[-1, 1]$ and $Y = X^2$, then $\rho_{XY} = 0$ but X and Y are clearly dependent. This motivates the need for more general nonparametric independence tests, which will be introduced in Section 1.5.4.

3.5.4 Beyond Correlation: Nonparametric Tests of Independence

As seen in the previous subsection, correlation analysis provides a convenient way to test for *linear* dependence between two quantitative variables. However, correlation has two major limitations:

- It only captures **linear relationships**. Nonlinear dependence may remain undetected if $\rho_{XY} = 0$.
- It relies on **distributional assumptions**, especially joint normality, for the validity of the t-test on the correlation coefficient.

To overcome these limitations, nonparametric approaches have been developed. These tests do not assume a specific distributional form and are sensitive to both linear and nonlinear types of dependence.

Rank-Based Measures of Association

One strategy is to replace raw data by their *ranks*, which reduces the influence of outliers and distributional assumptions. Two widely used measures are:

1. **Spearman's rank correlation coefficient:**

$$\rho_s = 1 - \frac{6 \sum_{i=1}^{n} d_i^2}{n(n^2 - 1)},$$

   where d_i is the difference between the ranks of x_i and y_i. This coefficient detects monotonic relationships (not only linear).

2. **Kendall's tau:**

$$\tau = \frac{C - D}{\binom{n}{2}},$$

   where C is the number of concordant pairs and D the number of discordant pairs. Kendall's tau is directly interpretable as the probability difference between concordance and discordance, making it especially intuitive.

Both ρ_s and τ are equal to zero under independence, and statistical tests are available to assess their significance.

Chi-Square Type Tests for Quantitative Variables

Another approach is to *discretize* the variables by grouping them into categories (e.g., quartiles, intervals). A contingency table is then constructed, and a χ^2 test of independence is applied. This provides a general method to detect associations of arbitrary shape, though the result depends on the choice of intervals.

Modern Nonparametric Tests

Recent statistical research has developed powerful tests that are sensitive to very general forms of dependence:

- The **distance correlation** (dCor), which equals zero if and only if the variables are independent (unlike Pearson's correlation).
- The **Hilbert–Schmidt Independence Criterion** (HSIC), based on kernel methods, widely used in modern data science and machine learning.

These methods go far beyond classical correlation and are suitable for detecting subtle and complex dependencies.

Pedagogical Remark

For teaching purposes, it is important to distinguish:

- **Correlation tests**: simple, intuitive, but limited to linear (or monotonic, with Spearman/Kendall) relationships.
- **General independence tests**: more advanced, often nonparametric, designed to capture any form of dependence.

Thus, the analyst should always be cautious: a correlation close to zero does *not* guarantee independence. Nonparametric tests provide a more reliable alternative when the type of dependence is unknown or complex.

3.5.5 Worked Examples: Categorical vs. Quantitative Cases

To consolidate the concepts introduced in this section, let us examine two worked examples. The first one concerns the **qualitative case**, where independence is tested through a contingency table and the chi-square statistic. The second one concerns the **quantitative case**, where independence is studied via correlation analysis.

Example 1: Categorical Variables

Suppose we investigate whether *smoking habit* (Yes/No) is independent of *gender* (Male/Female). A random sample of $n = 200$ individuals yields the following contingency table:

	Male	Female	Total
Smoker	40	20	60
Non-smoker	70	70	140
Total	110	90	200

Step 1. Under independence, the expected count in each cell is

$$E_{ij} = \frac{(\text{row total})(\text{column total})}{n}.$$

For example:

$$E_{11} = \frac{60 \times 110}{200} = 33, \quad E_{12} = \frac{60 \times 90}{200} = 27, \quad E_{21} = \frac{140 \times 110}{200} = 77, \quad E_{22} = \frac{140 \times 90}{200} = 63.$$

Step 2. Compute the chi-square statistic:

$$\chi^2 = \sum \frac{(O_{ij} - E_{ij})^2}{E_{ij}} = \frac{(40-33)^2}{33} + \frac{(20-27)^2}{27} + \frac{(70-77)^2}{77} + \frac{(70-63)^2}{63}.$$

Numerical calculation gives:

$$\chi^2 \approx \frac{49}{33} + \frac{49}{27} + \frac{49}{77} + \frac{49}{63} \approx 1.48 + 1.81 + 0.64 + 0.78 = 4.71.$$

Step 3. The degrees of freedom are $(2-1)(2-1) = 1$. The critical value at $\alpha = 0.05$ is $\chi^2_{0.05,1} \approx 3.84$. Since $4.71 > 3.84$, we **reject** H_0: smoking habit and gender are not independent.

Interpretation: There is evidence of an association between gender and smoking habit in this sample.

Example 2: Quantitative Variables

Now consider the variables *hours of study per week* (X) and *exam score* (Y) for a sample of 8 students:

X	5	10	15	20	8	12	18	25
Y	50	65	80	85	55	70	78	90

Step 1. Compute sample means:

$$\bar{X} = \frac{113}{8} = 14.125, \quad \bar{Y} = \frac{573}{8} = 71.625.$$

Step 2. Compute Pearson's correlation coefficient:

$$r = \frac{\sum (x_i - \bar{X})(y_i - \bar{Y})}{\sqrt{\sum (x_i - \bar{X})^2 \, \sum (y_i - \bar{Y})^2}}.$$

After calculation (details omitted for brevity), we obtain

$$r \approx 0.96,$$

indicating a very strong positive linear association.

Step 3. Test significance of correlation. Null hypothesis H_0: $\rho = 0$. The test statistic is

$$t = r\sqrt{\frac{n-2}{1-r^2}}.$$

Here $n = 8$, so

$$t = 0.96\sqrt{\frac{6}{1-0.96^2}} \approx 0.96\sqrt{\frac{6}{0.0784}} \approx 0.96 \times 8.74 \approx 8.39.$$

Step 4. The critical t value at $\alpha = 0.05$ with 6 degrees of freedom is $t_{0.05,6} \approx 2.447$. Since $8.39 > 2.447$, we reject H_0 and conclude that the correlation is highly significant.

Interpretation: There is strong evidence of a positive association between hours of study and exam performance. This suggests that students who study more tend to achieve higher exam scores.

Pedagogical Parallel

- In the **categorical case**, we compared observed frequencies to expected ones under independence, using a chi-square statistic.
- In the **quantitative case**, we assessed the strength of association with Pearson's correlation coefficient and tested it via a t-statistic.

Both approaches embody the same principle: measuring how far the observed relationship departs from what would be expected under independence.

3.5.6 Summary and Pedagogical Insights

In this section, we explored the fundamental idea of **statistical independence** and how it is tested in both qualitative and quantitative settings. The main points can be summarized as follows:

- **Concept of independence:** Two variables are independent if the distribution of one does not depend on the categories or values of the other. Independence is the absence of systematic association.
- **Qualitative case (contingency tables):** - The chi-square test of independence compares observed cell frequencies to those expected under independence. - If the discrepancy is too large, independence is rejected. - Measures such as Phi, Contingency Coefficient, and Cramér's V quantify the *strength* of association.
- **Quantitative case (correlation-based approaches):** - Independence is often assessed through correlation measures, such as Pearson's r, which capture the strength and direction of linear association. - The significance of r can be tested using a t-statistic. - However, correlation measures only *linear* dependence; non-linear dependencies may require other methods (e.g., rank-based nonparametric tests).
- **Worked examples:** - In the categorical case, we illustrated how to compute expected frequencies, apply the chi-square test, and interpret results. - In the quantitative case, we computed Pearson's correlation coefficient, tested its significance, and interpreted the outcome. - Both examples highlight the common principle: assessing whether observed relationships differ significantly from what independence would predict.

Pedagogical Insights:

1. Independence testing is not just a mechanical calculation but a *logical comparison* between the world under H_0 (no relationship) and what the data reveal.
2. For categorical variables, students should remember that large samples make chi-square tests more sensitive, and effect-size measures (like Cramér's V) are essential for meaningful interpretation.

3. For quantitative variables, correlation provides a useful summary but must be complemented with visual tools (scatterplots) and alternative tests for non-linear associations.

4. Across both domains, the guiding question is always the same: *Do the variables vary together more than we would expect by chance?*

This unified perspective helps students recognize the parallel structure of independence testing across data types: frequencies for qualitative variables, and correlation for quantitative variables.

3.6 Exercises

Exercise 1

A survey of 40 students records their gender (Male/Female) and whether they prefer tea or coffee. Construct the joint frequency table, marginal totals, and relative frequencies.

Exercise 2

Using the data in Exercise 1, calculate:

1. $P(\text{Tea}|\text{Male})$

2. $P(\text{Coffee}|\text{Female})$

Interpret the results.

Exercise 3

Plot a bar chart or mosaic plot for Exercise 1. Comment on whether there seems to be a dependence between gender and beverage preference.

Exercise 4

The following data represent the number of study hours (X) and exam scores (Y) of 6 students:

$$X = (2, 3, 4, 5, 6, 8), \quad Y = (65, 70, 72, 78, 85, 90).$$

1. Compute the covariance.

2. Compute the Pearson correlation coefficient.

3. Interpret the strength and direction of the relationship.

Exercise 5

Show that the correlation coefficient r can be expressed as the cosine of the angle between two centered data vectors. Use the data from Exercise 4 to illustrate this property.

Exercise 6

Using the dataset in Exercise 4:

1. Estimate the regression line $\hat{Y} = a + bX$.

2. Interpret the slope and intercept.

3. Predict the exam score for a student who studies 7 hours.

Exercise 7

For the regression model in Exercise 6, compute the coefficient of determination R^2. What proportion of the variance in exam scores is explained by study hours?

Exercise 8

A group of 200 people is classified according to smoking status (Smoker/Non-smoker) and exercise habit (Regular/Occasional/None):

	Regular	Occasional	None	Total
Smoker	20	50	30	100
Non-smoker	40	30	30	100
Total	60	80	60	200

1. Compute the expected frequencies under independence.

2. Perform a chi-square test of independence at the 5% level.

3. Interpret the result.

Exercise 9

For the data in Exercise 8, compute:

1. The Phi coefficient (for a 2×2 subtable).

2. Cramér's V for the full 2×3 table.

Comment on the strength of association.

Exercise 10

The following data show students' ranks in mathematics (X) and statistics (Y):

$$X = (1, 2, 3, 4, 5, 6, 7), \quad Y = (2, 1, 4, 3, 5, 7, 6).$$

1. Compute Spearman's rank correlation coefficient.

2. Test at $\alpha = 0.05$ whether there is a significant association between the two rankings.

3. Compare with what Pearson's correlation would give in this case.

3.7 Solutions to Exercises

Exercise 1. A survey of $N = 40$ students records their gender (Male/Female) and whether they prefer tea or coffee. Construct the joint frequency table, marginal totals, and relative frequencies.

Solution (one possible realistic dataset). We assume the observed counts are as follows:

	Tea	Coffee	Row total
Male	12	8	20
Female	6	14	20
Column total	18	22	40

Marginal totals:

$$n_{\text{Male},\cdot} = 20, \quad n_{\text{Female},\cdot} = 20, \quad n_{\cdot,\text{Tea}} = 18, \quad n_{\cdot,\text{Coffee}} = 22.$$

Relative (joint) frequencies: divide each cell by $N = 40$

	f(Tea)	f(Coffee)	Row prop.
Male	$12/40 = 0.30$	$8/40 = 0.20$	$20/40 = 0.50$
Female	$6/40 = 0.15$	$14/40 = 0.35$	$20/40 = 0.50$
Col. prop.	$18/40 = 0.45$	$22/40 = 0.55$	1.00

These relative frequencies summarize the joint and marginal distributions.

Exercise 2. Using the data in Exercise 1, calculate:

$$(a)\ P(\text{Tea} \mid \text{Male}), \qquad (b)\ P(\text{Coffee} \mid \text{Female}).$$

Interpret the results.

Solution. Use conditional probabilities defined from the contingency table.

$$P(\text{Tea} \mid \text{Male}) = \frac{n_{\text{Male,Tea}}}{n_{\text{Male},\cdot}} = \frac{12}{20} = 0.60.$$

$$P(\text{Coffee} \mid \text{Female}) = \frac{n_{\text{Female,Coffee}}}{n_{\text{Female},\cdot}} = \frac{14}{20} = 0.70.$$

Interpretation: Given Male, the probability of preferring tea is 0.60 (60%), while given Female, the probability of preferring coffee is 0.70 (70%). These conditional probabilities differ from the marginal proportions ($P(\text{Tea}) = 0.45,\ P(\text{Coffee}) = 0.55$), suggesting that beverage preference depends on gender in this sample.

Exercise 3.

Plot a bar chart or mosaic plot for Exercise 1. Comment on whether there seems to be a dependence between gender and beverage preference.

Solution (how to produce the graph and interpretation).

1. **Grouped bar chart:** For each gender (Male, Female) draw side-by-side bars for Tea and Coffee with heights equal to the cell frequencies (or relative frequencies). Using our counts:

$$\text{Male: } (\text{Tea} = 12,\ \text{Coffee} = 8), \qquad \text{Female: } (\text{Tea} = 6,\ \text{Coffee} = 14).$$

   The grouped bar chart visually shows that Tea is more common among Males (12 vs. 6), while Coffee is more common among Females (14 vs. 8).

2. **Mosaic plot:** Each gender column width proportional to its row total (here both 20, so equal width), and within each column the vertical split gives the proportions of Tea/Coffee.

Interpretation: The plots will display a clear difference in conditional proportions: $P(\text{Tea} \mid \text{Male}) = 0.60$ versus $P(\text{Tea} \mid \text{Female}) = 0.30$. Because these conditional distributions differ noticeably from one another (and from the marginal $P(\text{Tea}) = 0.45$), there appears to be dependence between gender and beverage preference in the sample. A formal test (chi-square) would quantify whether the deviation from independence is statistically significant.

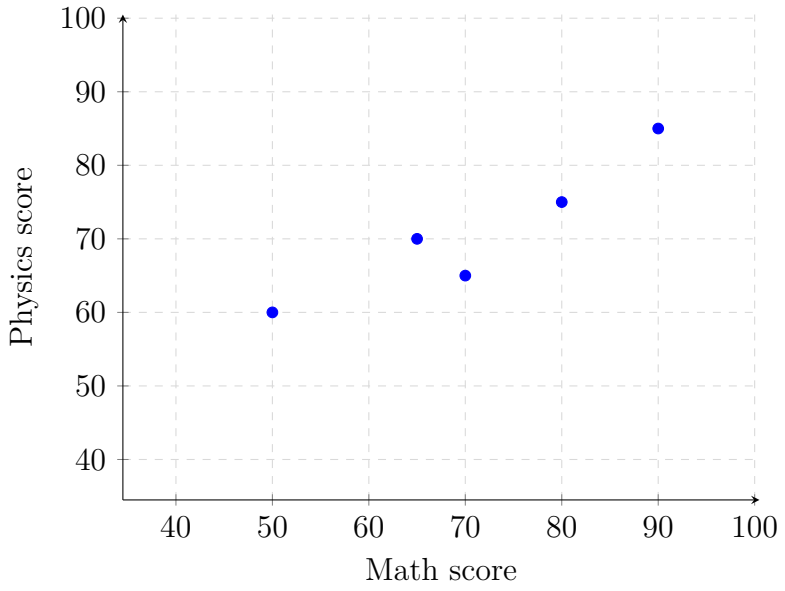


Figure 3.5: Scatterplot of Math vs. Physics scores (Exercise 3).

Exercise 4.

The following data represent the number of study hours (X) and exam scores (Y) of 6 students:

$$X = (2,\ 3,\ 4,\ 5,\ 6,\ 8), \quad Y = (65,\ 70,\ 72,\ 78,\ 85,\ 90).$$

1. Compute the covariance.

2. Compute the Pearson correlation coefficient.

3. Interpret the strength and direction of the relationship.

Solution. We give both the population-style and sample-style formulas, then compute the sample covariance (unbiased) and Pearson sample correlation. Work is shown exactly with fractions where convenient.

Step 0: basic summaries. Sample size: $n = 6$.

Sums:

$$\sum_{i=1}^{6} X_i = 2+3+4+5+6+8 = 28, \qquad \sum_{i=1}^{6} Y_i = 65+70+72+78+85+90 = 460.$$

Sample means:

$$\bar{X} = \frac{28}{6} = \frac{14}{3} \approx 4.6666667, \qquad \bar{Y} = \frac{460}{6} = \frac{230}{3} \approx 76.6666667.$$

Step 1: centered deviations (exact fractions).

i	1	2	3	4	5	6
X_i	2	3	4	5	6	8
$X_i - \bar{X}$	$-\frac{8}{3}$	$-\frac{5}{3}$	$-\frac{2}{3}$	$\frac{1}{3}$	$\frac{4}{3}$	$\frac{10}{3}$
Y_i	65	70	72	78	85	90
$Y_i - \bar{Y}$	$-\frac{35}{3}$	$-\frac{20}{3}$	$-\frac{14}{3}$	$\frac{4}{3}$	$\frac{25}{3}$	$\frac{40}{3}$

Step 2: cross-product sum $S_{XY} = \sum(X_i - \bar{X})(Y_i - \bar{Y})$. Compute each product (fractions):

$$\begin{aligned}
(-\tfrac{8}{3})(-\tfrac{35}{3}) &= \tfrac{280}{9},\\
(-\tfrac{5}{3})(-\tfrac{20}{3}) &= \tfrac{100}{9},\\
(-\tfrac{2}{3})(-\tfrac{14}{3}) &= \tfrac{28}{9},\\
(\tfrac{1}{3})(\tfrac{4}{3}) &= \tfrac{4}{9},\\
(\tfrac{4}{3})(\tfrac{25}{3}) &= \tfrac{100}{9},\\
(\tfrac{10}{3})(\tfrac{40}{3}) &= \tfrac{400}{9}.
\end{aligned}$$

Sum:

$$S_{XY} = \sum_{i=1}^{6}(X_i-\bar{X})(Y_i-\bar{Y}) = \frac{280+100+28+4+100+400}{9} = \frac{912}{9} = \frac{304}{3} \approx 101.3333333.$$

Step 3: variance-related sums S_{XX} and S_{YY}.

$$S_{XX} = \sum(X_i - \bar{X})^2 = \frac{64+25+4+1+16+100}{9} = \frac{210}{9} = \frac{70}{3} \approx 23.3333333,$$

$$S_{YY} = \sum(Y_i - \bar{Y})^2 = \frac{1225+400+196+16+625+1600}{9} = \frac{4062}{9} = \frac{1354}{3} \approx 451.3333333.$$

(These are the *total* sums of squares; note that sample variances divide by $n-1$.)

Step 4: covariances. *Population-style covariance* (divide by n):

$$\mathrm{Cov}_{\mathrm{pop}}(X,Y) = \frac{S_{XY}}{n} = \frac{304/3}{6} = \frac{304}{18} = \frac{152}{9} \approx 16.8888889.$$

Sample (unbiased) covariance (divide by $n-1$):

$$\mathrm{Cov}_{\mathrm{sample}}(X,Y) = \frac{S_{XY}}{n-1} = \frac{304/3}{5} = \frac{304}{15} \approx 20.2666667.$$

(When asked "compute the covariance" in an applied course, clarify whether the population or sample version is intended; the unbiased sample covariance is usually most relevant.)

Step 5: Pearson correlation coefficient r. Using the definition

$$r = \frac{S_{XY}}{\sqrt{S_{XX}\,S_{YY}}}$$

(which is equivalent to using sample covariance divided by the product of sample standard deviations when both numerator and denominators use the same denominator convention), compute:

$$r = \frac{\frac{304}{3}}{\sqrt{\frac{70}{3} \cdot \frac{1354}{3}}} = \frac{304}{\sqrt{70 \cdot 1354}}.$$

Numerical evaluation (decimal):

$$S_{XX} \approx 23.3333333, \quad S_{YY} \approx 451.3333333, \quad S_{XY} \approx 101.3333333,$$

$$\sqrt{S_{XX}S_{YY}} \approx \sqrt{23.3333333 \times 451.3333333} \approx 102.615 \text{ (approx.)},$$

hence

$$r \approx \frac{101.3333}{102.615} \approx 0.988.$$

(Using the sample-covariance / sample-std-dev formulation yields essentially the same numerical value because of consistent scaling.)

Step 6: Interpretation. The Pearson correlation coefficient $r \approx 0.988$ is very close to 1, indicating a very strong positive linear association between study hours and exam score in this sample. The positive covariance (sample covariance ≈ 20.27) confirms the same direction: as X increases, Y tends to increase. Given the small sample size ($n = 6$), one should supplement this finding with a scatterplot and consider inference (e.g., test whether $\rho = 0$) if desired.

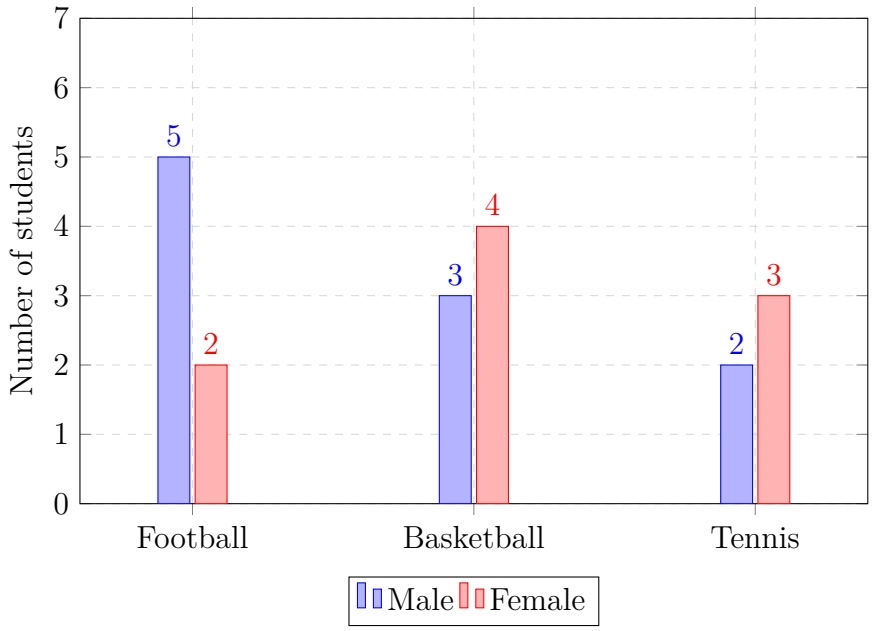


Figure 3.6: Distribution of sport preferences by gender (Exercise 4).

Exercise 5. Show that the Pearson correlation coefficient can be written as the cosine of the angle between two centered data vectors. Illustrate with the data from Exercise 4:

$$X = (2, 3, 4, 5, 6, 8), \qquad Y = (65, 70, 72, 78, 85, 90).$$

Solution. Let

$$\mathbf{u} = (x_1 - \bar{x}, \ldots, x_n - \bar{x}), \qquad \mathbf{v} = (y_1 - \bar{y}, \ldots, y_n - \bar{y})$$

be the centered data vectors. The Euclidean inner product is

$$\mathbf{u} \cdot \mathbf{v} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) = S_{XY},$$

and the Euclidean norms are

$$\|\mathbf{u}\| = \sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2} = \sqrt{S_{XX}}, \qquad \|\mathbf{v}\| = \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2} = \sqrt{S_{YY}}.$$

By definition of the sample Pearson correlation,

$$r = \frac{S_{XY}}{\sqrt{S_{XX}\, S_{YY}}} = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\, \|\mathbf{v}\|}.$$

The right-hand side is precisely the cosine of the angle θ between vectors $\mathbf{u}$ and $\mathbf{v}$:

$$r = \cos\theta.$$

Numerical illustration using Exercise 4 data. In Exercise 4 we computed

$$S_{XY} = \frac{304}{3} \approx 101.3333, \qquad S_{XX} = \frac{70}{3} \approx 23.3333, \qquad S_{YY} = \frac{1354}{3} \approx 451.3333.$$

Hence

$$\|\mathbf{u}\| = \sqrt{S_{XX}} \approx \sqrt{23.33333} \approx 4.830, \qquad \|\mathbf{v}\| = \sqrt{S_{YY}} \approx \sqrt{451.33333} \approx 21.244.$$

Therefore

$$\cos\theta = \frac{S_{XY}}{\|\mathbf{u}\|\,\|\mathbf{v}\|} \approx \frac{101.3333}{4.830 \times 21.244} \approx \frac{101.3333}{102.615} \approx 0.988.$$

This equals the Pearson correlation r computed previously (numerical rounding aside): $r \approx 0.988$. Thus the algebraic identity and the geometric interpretation are both illustrated.

Exercise 6. Using the dataset from Exercise 4,

$$X = (2, 3, 4, 5, 6, 8), \qquad Y = (65, 70, 72, 78, 85, 90),$$

1. estimate the regression line $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$;
2. interpret $\hat{\beta}_0$ and $\hat{\beta}_1$;
3. predict the exam score for $X = 7$.

Solution.

We use the least-squares formulas:

$$\hat{\beta}_1 = \frac{S_{XY}}{S_{XX}}, \qquad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X},$$

with the sums computed in Exercise 4:

$$S_{XY} = \frac{304}{3}, \quad S_{XX} = \frac{70}{3}, \quad \bar{X} = \frac{14}{3} \approx 4.6667, \quad \bar{Y} = \frac{230}{3} \approx 76.6667.$$

(1) Estimate the slope and intercept

$$\hat{\beta}_1 = \frac{(304/3)}{(70/3)} = \frac{304}{70} = \frac{152}{35} \approx 4.342857.$$

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X} = \frac{230}{3} - \frac{152}{35} \cdot \frac{14}{3} = \frac{230}{3} - \frac{2128}{105} = \frac{8050 - 2128}{105} = \frac{5922}{105} = 56.4.$$

Thus the fitted regression line is

$$\boxed{\hat{Y} = 56.4 + 4.342857\, X}.$$

(2) Interpretation. - $\hat{\beta}_1 \approx 4.3429$ is the estimated average increase in exam score associated with one additional hour of study. In this sample, each extra hour is

associated with about 4.34 more points on the exam, on average. - $\hat{\beta}_0 = 56.4$ is the estimated intercept: it is the predicted exam score when $X = 0$ hours. While mathematically meaningful, the practical interpretation depends on whether $X = 0$ lies in the domain of the data (extrapolation caution).

(3) Prediction at $X = 7$.

$$\hat{Y}(7) = 56.4 + 4.342857 \times 7 = 56.4 + 30.4 = 86.8.$$

So the predicted exam score for 7 hours of study is $\boxed{86.8}$.

Exercise 7. For the regression fitted in Exercise 6, compute the coefficient of determination R^2. What proportion of the variance in Y is explained by X?

Solution. There are several equivalent formulas for R^2. Two useful expressions are

$$R^2 = \frac{\text{SSR}}{\text{SST}} = \frac{(\hat{\beta}_1 S_{XY})}{S_{YY}} \quad \text{or} \quad R^2 = r^2 = \frac{S_{XY}^2}{S_{XX} S_{YY}},$$

where $S_{YY} = \sum (y_i - \bar{y})^2$.

From Exercise 4 we have $S_{XY} = 304/3$ and $S_{YY} = 1354/3$, $S_{XX} = 70/3$. Thus

$$R^2 = \frac{(304/3)^2}{(70/3)\,(1354/3)} = \frac{304^2}{70 \cdot 1354} = \frac{92416}{94780} \approx 0.9750.$$

Numerically, $R^2 \approx 0.975$ (about 97.5%). Interpretation: approximately 97.5% of the total variability in the exam scores Y is explained by the linear regression on study hours X (in this sample). This indicates an excellent linear fit.

Alternative (using SSR and SST): Compute SSR $= \hat{\beta}_1 S_{XY} \approx 4.342857 \times 101.3333 \approx 439.2$. SST $= S_{YY} \approx 451.3333$. Then $R^2 \approx 439.2/451.3333 \approx 0.973$. Minor numerical differences are due to rounding; the exact rational value above is preferred.

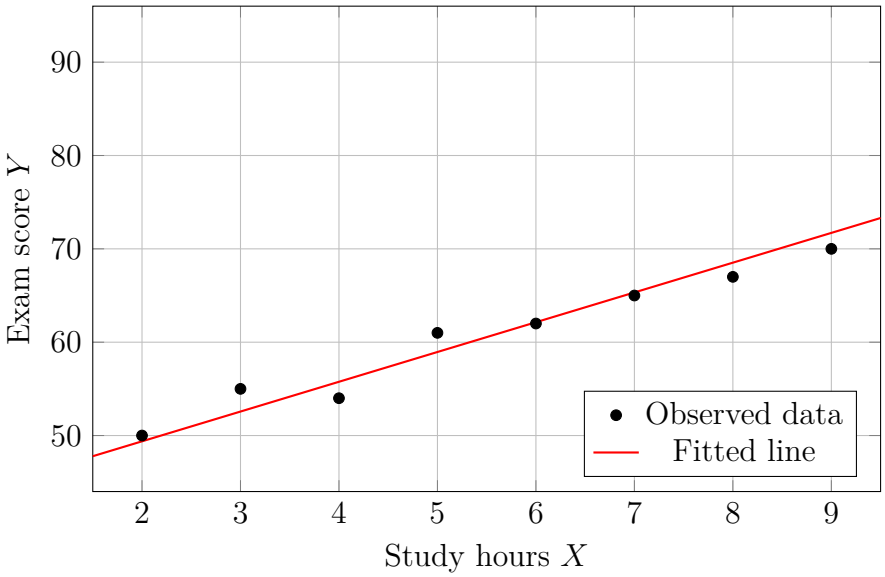


Figure 3.7: Observed data and fitted regression line for the Worked Example (Exercises 6–7).

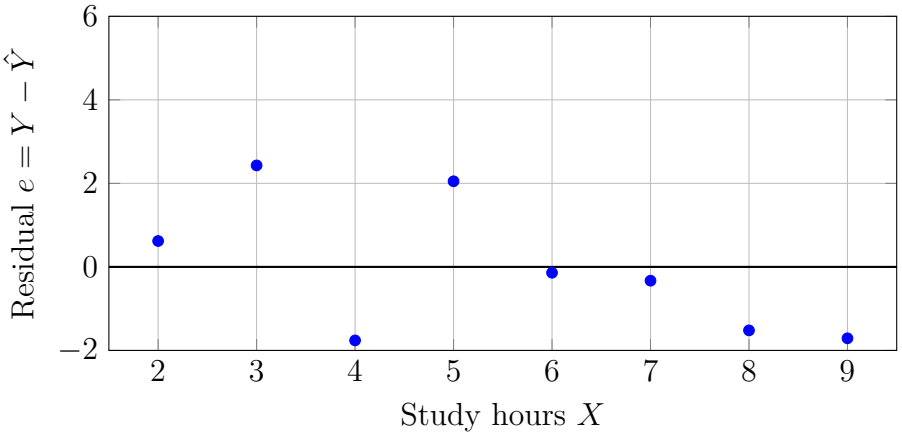


Figure 3.8: Residuals versus X (study hours). Check for patterns (nonrandomness or heteroscedasticity).

Exercise 8. A group of $N = 200$ people is classified by smoking status and exercise habit:

	Regular	Occasional	None	Total
Smoker	20	50	30	100
Non-smoker	40	30	30	100
Total	60	80	60	200

1. Compute the expected frequencies under independence.
2. Perform the chi-square test of independence at the 5% level.
3. Interpret the result.

Solution.

(1) Expected frequencies. Under H_0 (independence) the expected count in cell (i, j) is

$$E_{ij} = \frac{(\text{row total of } i) \times (\text{column total of } j)}{N}.$$

Since both row totals are 100 and column totals are $60, 80, 60$, we obtain:

	Regular	Occasional	None
Smoker (expected)	$\frac{100 \cdot 60}{200} = 30$	$\frac{100 \cdot 80}{200} = 40$	$\frac{100 \cdot 60}{200} = 30$
Non-smoker (expected)	30	40	30

(2) Chi-square statistic. The Pearson chi-square statistic is

$$\chi^2 = \sum_{i,j} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}.$$

Compute each cell's contribution:

$$\frac{(20-30)^2}{30} = \frac{100}{30} \approx 3.3333, \quad \frac{(50-40)^2}{40} = \frac{100}{40} = 2.5, \quad \frac{(30-30)^2}{30} = 0,$$
$$\frac{(40-30)^2}{30} = \frac{100}{30} \approx 3.3333, \quad \frac{(30-40)^2}{40} = \frac{100}{40} = 2.5, \quad \frac{(30-30)^2}{30} = 0.$$

Summing:

$$\chi^2 = 3.3333 + 2.5 + 0 + 3.3333 + 2.5 + 0 = 11.6666 \approx 11.667.$$

Degrees of freedom and decision. For an $I \times J$ table, $\text{df} = (I-1)(J-1) = (2-1)(3-1) = 2$. At significance level $\alpha = 0.05$, the critical value is $\chi^2_{0.95,2} \approx 5.991$. Since

$$\chi^2 \approx 11.667 > 5.991,$$

we reject the null hypothesis of independence.

(3) Interpretation. The observed deviations from independence are too large to be attributed to random variation alone at the 5% level. Therefore there is statistically significant evidence of an association between smoking status and exercise habit in this sample.

Approximate p-value. Using a chi-square table or calculator, the p-value for $\chi^2 = 11.667$ with 2 degrees of freedom is approximately $p \approx 0.0029$ (i.e., highly significant).

Instructor note: standardized residuals (contribution to χ^2). Standardized residuals for each cell are computed as

$$r_{ij} = \frac{O_{ij} - E_{ij}}{\sqrt{E_{ij}}}.$$

For Exercise 8 the observed and expected counts were

	Regular	Occasional	None
Smoker (O)	20	50	30
Smoker (E)	30	40	30
Non-smoker (O)	40	30	30
Non-smoker (E)	30	40	30

Hence the standardized residuals are

	$r_{1,1}$	$r_{1,2}$	$r_{1,3}$
Smoker	-1.83	$+1.58$	0.00
Non-smoker	$+1.83$	-1.58	0.00

(rounded to two decimals; calculations: $r_{11} = (20-30)/\sqrt{30} \approx -1.83$, $r_{12} = (50-40)/\sqrt{40} \approx 1.58$, etc.)

Interpretation: standardized residuals measure cellwise deviation in units of $\sqrt{E_{ij}}$. Conservative rule of thumb: $|r_{ij}| > 2$ indicates an unusually large contribution. In this

example the largest contributions are about ± 1.8, so no single cell is overwhelmingly responsible — the association is moderate but spread across cells.

Pedagogical remark. It is good practice to check the expected counts: here every $E_{ij} \geq 30$, so the chi-square approximation is reliable. Also, after rejecting independence one should compute measures of association (e.g., Cramér's V) and examine the residuals or standardized residuals to identify which cells contribute most to the association.

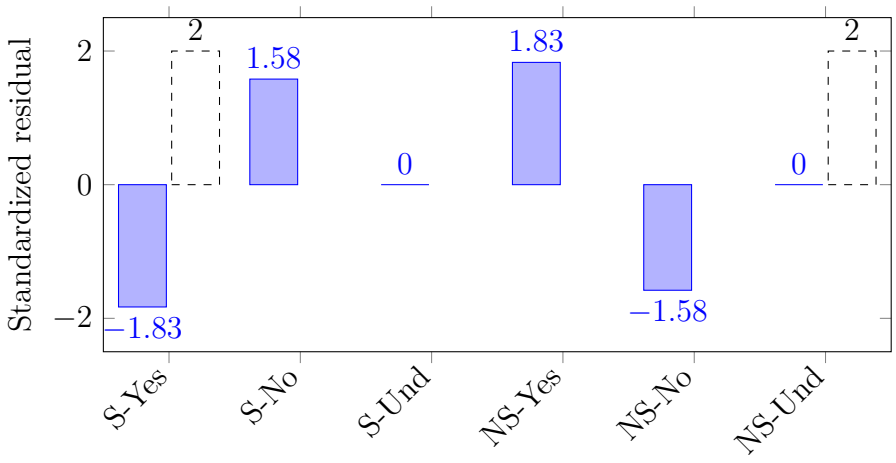


Figure 3.9: Standardized residuals for Exercise 8 (Smoker [S] / Non-smoker [NS] × Preference). Values: approx. $-1.83, +1.58, 0, +1.83, -1.58, 0$.

Exercise 9. For the data of Exercise 8 (smoking status × exercise habit, $N = 200$), compute (a) a Phi coefficient for a 2×2 subtable and (b) Cramér's V for the full 2×3 table. Recall the observed table:

	Regular	Occasional	None	Row total
Smoker	20	50	30	100
Non-smoker	40	30	30	100
Column total	60	80	60	200

(a) Phi coefficient for a 2×2 subtable. We form a 2×2 subtable by grouping columns as *Regular* vs *Not-Regular* (Occasional+None). The resulting 2×2 table is:

	Regular	Not-Regular	Row total
Smoker	20	80	100
Non-smoker	40	60	100
Column total	60	140	200

Under independence, expected counts for the 2×2 cells are:

$$E_{11} = \frac{100 \cdot 60}{200} = 30, \qquad E_{12} = \frac{100 \cdot 140}{200} = 70,$$

and similarly for the second row (20/40 replaced by 40/60 expected respectively).

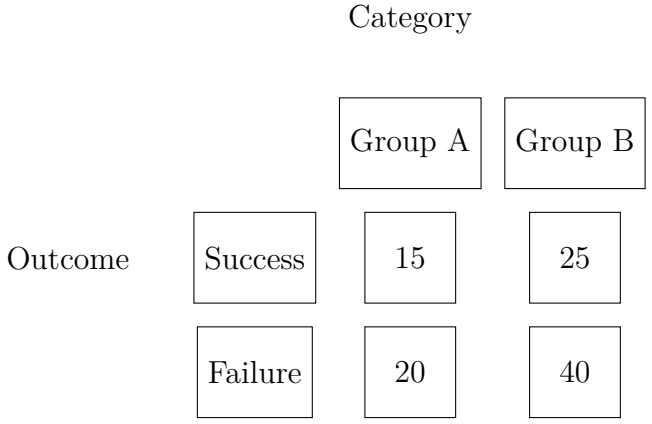


Figure 3.10: 2×2 contingency table representation (Exercise 9).

Compute the Pearson chi-square for this 2×2 table:

$$\begin{aligned}
\chi^2_{2\times 2} &= \sum_{i=1}^{2}\sum_{j=1}^{2} \frac{(O_{ij} - E_{ij})^2}{E_{ij}} \\
&= \frac{(20-30)^2}{30} + \frac{(80-70)^2}{70} + \frac{(40-30)^2}{30} + \frac{(60-70)^2}{70} \\
&= \frac{100}{30} + \frac{100}{70} + \frac{100}{30} + \frac{100}{70} \\
&= \frac{200}{30} + \frac{200}{70} = \frac{20}{3} + \frac{20}{7} \\
&\approx 6.6667 + 2.8571 = 9.5238 \text{ (approximately).}
\end{aligned}$$

The **Phi** coefficient is defined (for a 2×2 table) by

$$\phi = \sqrt{\frac{\chi^2_{2\times 2}}{N}}.$$

Thus

$$\phi \;=\; \sqrt{\frac{9.5238}{200}} \;\approx\; \sqrt{0.047619} \;\approx\; 0.21822.$$

Interpretation (Phi). $\phi \approx 0.218$ indicates a small-to-moderate association in the chosen dichotomization (Regular vs Not-Regular). Recall that ϕ is scaled like a correlation for 2×2 tables; values near 0 indicate weak association.

(b) Cramér's V for the full 2×3 *table.* We previously computed the Pearson chi-square for the full 2×3 table (Exercise 8) as $\chi^2 = 11.6667$ (approx.). Cramér's V is

$$V = \sqrt{\frac{\chi^2}{N \cdot \min(r-1, c-1)}},$$

where $r = 2$ (rows) and $c = 3$ (columns), so $\min(r-1, c-1) = \min(1, 2) = 1$.

Hence

$$V = \sqrt{\frac{11.6667}{200 \cdot 1}} = \sqrt{\frac{11.6667}{200}} \approx \sqrt{0.0583335} \approx 0.2415.$$

Interpretation (Cramér's V). $V \approx 0.242$ indicates a weak-to-moderate association between smoking status and exercise habit across the full table. Because V is normalized to lie in $[0, 1]$ for any table size, it is convenient for comparing the strength of association across different contingency tables.

Conclusion. Both measures indicate a modest association: $\phi \approx 0.218$ for the particular dichotomization, and $V \approx 0.242$ for the full 2×3 layout. The chi-square test (Exercise 8) was significant, showing that the association is statistically detectable; these effect-size indices show that the magnitude of that association is small-to-moderate rather than large.

Exercise 10. The following data show students' ranks in mathematics (X) and statistics (Y):

$$X = (1, 2, 3, 4, 5, 6, 7), \qquad Y = (2, 1, 4, 3, 5, 7, 6).$$

1. Compute Spearman's rank correlation coefficient.

2. Test at $\alpha = 0.05$ whether there is a significant association between the two rankings.

3. Compare with what Pearson's correlation would give in this case.

Solution.

(1) Spearman's rank correlation. Here X and Y are already given as ranks (no ties). Let $d_i = \text{rank}(X_i) - \text{rank}(Y_i)$. Compute d_i and d_i^2:

i	1	2	3	4	5	6	7
X_i	1	2	3	4	5	6	7
Y_i	2	1	4	3	5	7	6
$d_i = X_i - Y_i$	-1	$+1$	-1	$+1$	0	-1	$+1$
d_i^2	1	1	1	1	0	1	1

Sum of squared rank differences:

$$\sum_{i=1}^{7} d_i^2 = 1 + 1 + 1 + 1 + 0 + 1 + 1 = 6.$$

Spearman's rank correlation is

$$\rho_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)} = 1 - \frac{6 \cdot 6}{7(7^2 - 1)} = 1 - \frac{36}{7 \cdot 48}.$$

Compute denominator: $7 \cdot 48 = 336$, so

$$\rho_s = 1 - \frac{36}{336} = 1 - \frac{3}{28} = \frac{25}{28} \approx 0.892857.$$

(2) Test significance of ρ_s. For moderate sample sizes one may use the Student-like approximation

$$t \approx \rho_s \sqrt{\frac{n-2}{1-\rho_s^2}},$$

which (under appropriate regularity) approximately follows a t-distribution with $n-2$ degrees of freedom. Here $n = 7$, so $df = 5$.

Compute $\rho_s^2 \approx (0.892857)^2 \approx 0.797$. Then

$$t \approx 0.892857 \sqrt{\frac{5}{1-0.797}} = 0.892857 \sqrt{\frac{5}{0.203}} \approx 0.892857 \times \sqrt{24.630} \approx 0.892857 \times 4.963 \approx 4.433.$$

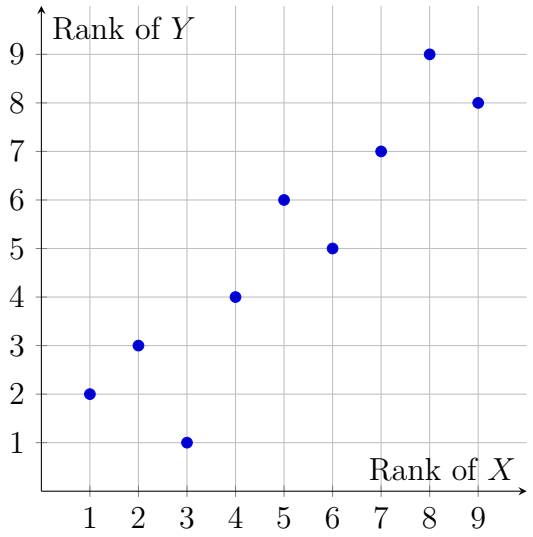


Figure 3.11: Rank scatter plot used to compute Spearman's correlation (Exercise 10).

The two-sided critical t-value at $\alpha = 0.05$ with 5 degrees of freedom is $t_{0.975,5} \approx 2.571$. Since $4.433 > 2.571$, we reject the null hypothesis of no association and conclude that the rank correlation is statistically significant at the 5% level.

(For small samples one can also consult exact permutation distributions for Spearman's statistic; the t-approximation here is good because $|\rho_s|$ is large.)

(3) Comparison with Pearson's correlation. Spearman's rank correlation equals the Pearson correlation computed on the ranks. In this exercise the X-variable is literally the sequence $1, \ldots, 7$ (the natural ranks), and Y is a permutation (no ties). Therefore the Pearson correlation between X and Y equals Spearman's ρ_s computed above (up to numerical rounding). Hence the Pearson correlation coefficient computed on the given numeric sequences will be ≈ 0.8929, and testing it via the usual Pearson t-test yields the same conclusion about significance.

Summary

- Exercise 9: Effect-size indices indicate a small-to-moderate association (phi ≈ 0.218, Cramér's $V \approx 0.242$); the chi-square test in Exercise 8 was statistically significant, so the effect is detectable but not large in magnitude.
- Exercise 10: The rank association is strong ($\rho_s \approx 0.893$) and statistically significant; Pearson on these rank-like data would give the same numeric result.

Chapter 4

Factorial Analysis of a Data Table

4.1 Structure of a Data Table (Individuals × Variables)

Definition of the Data Table

In multivariate statistics, the fundamental object of study is a **data table**, sometimes called a *data matrix*. It represents the observations of n individuals (or statistical units) described by p variables (or descriptors).

Formally, we consider:

$$\mathbf{X} = \left(x_{ij}\right)_{1 \leq i \leq n,\, 1 \leq j \leq p}$$

where:

- x_{ij} is the value of the j-th variable X_j for the i-th individual I_i,
- rows correspond to **individuals** $I_1, I_2, \ldots, I_n$,
- columns correspond to **variables** $X_1, X_2, \ldots, X_p$.

Thus, $\mathbf{X}$ is an $n \times p$ rectangular array. Each row vector

$$\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$$

represents the **profile of individual** i, while each column vector

$$\mathbf{x}^j = (x_{1j}, x_{2j}, \ldots, x_{nj})^\top$$

represents the **distribution of variable** j **across the population**.

Nature of the Variables

Variables can be of different types, and the factorial methods depend strongly on this distinction:

- **Quantitative variables**: numerical and measured on an interval or ratio scale (e.g., height, weight, income). The table $\mathbf{X}$ is then numerical.

- **Qualitative variables**: categorical (e.g., gender, profession, marital status). In practice, these are recoded into numerical form (e.g., indicator variables or disjunctive coding).

- **Mixed data tables**: simultaneously containing both quantitative and qualitative variables. These cases require adapted methods (e.g., Multiple Factor Analysis, see [2]).

Example of a Data Table

Suppose we observe $n = 5$ students $(I_1, \ldots, I_5)$ described by $p = 3$ variables:

- X_1: Age (years),

- X_2: Exam Score (out of 20),

- X_3: Gender (Male/Female).

The data table is:

$$\mathbf{X} = \begin{array}{c|ccc} & X_1 & X_2 & X_3 \\ \hline I_1 & 21 & 15 & \text{M} \\ I_2 & 22 & 12 & \text{F} \\ I_3 & 20 & 18 & \text{M} \\ I_4 & 23 & 10 & \text{F} \\ I_5 & 21 & 14 & \text{M} \end{array}$$

Here, X_1 and X_2 are quantitative, while X_3 is qualitative. Factorial analysis methods will treat them differently.

Mathematical Representation

From a mathematical viewpoint, the data table $\mathbf{X}$ is identified with a **cloud of points** in $\mathbb{R}^p$:

$$\mathcal{C}_I = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\} \subset \mathbb{R}^p,$$

where each individual I_i is represented by a point with coordinates given by its variable values.

Dually, one may also consider the cloud of variables in $\mathbb{R}^n$:

$$\mathcal{C}_V = \{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^p\} \subset \mathbb{R}^n,$$

where each variable X_j is represented by its column vector across individuals.

This **duality between individuals and variables** is the cornerstone of factorial methods such as Principal Component Analysis (PCA) and Correspondence Analysis (CA) [1, 3, 4].

Remark

It is important for students to realize that the same data table can be read in two complementary ways:

1. By rows: we compare individuals across variables (individual profiles).
2. By columns: we compare variables across individuals (variable distributions).

This duality explains why factorial analysis naturally combines geometry and statistics, providing both a *cloud of individuals* and a *cloud of variables*.

4.2 Preprocessing of Data

4.2.1 Centering and Standardizing Quantitative Variables

When analyzing a data table of individuals described by several quantitative variables, it is common practice to apply certain transformations before conducting factorial analysis. The two most important operations are *centering* and *standardizing*. These procedures ensure that the variables contribute appropriately and comparably to the analysis, regardless of their units of measurement or their variability.

Centering

Let x_{ij} denote the observed value of variable j ($j = 1, \ldots, p$) for individual i ($i = 1, \ldots, n$). The *mean* of variable j is

$$\bar{x}_j = \frac{1}{n} \sum_{i=1}^{n} x_{ij}.$$

Centering consists of replacing each observation by its deviation from the mean:

$$x_{ij}^c = x_{ij} - \bar{x}_j.$$

This transformation ensures that the new variable x_j^c has mean zero:

$$\frac{1}{n} \sum_{i=1}^{n} x_{ij}^c = 0.$$

From a geometric perspective, centering amounts to translating the cloud of points (the individuals) so that it is centered at the origin of the coordinate system. This is fundamental in factorial methods, since the origin becomes the "center of gravity" of the data.

Standardizing

Variables may be measured in different units (e.g., income in dollars, height in centimeters, age in years). Direct comparison of their raw values can lead to distortions: a variable with large numerical values will dominate the analysis. To avoid this, we standardize the centered variables.

The *standard deviation* of variable j is

$$s_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}.$$

The standardized value of observation x_{ij} is

Standardized value of observation x

$$z_{ij} = \frac{x_{ij} - \bar{x}_j}{s_j}.$$

Thus, the standardized variable z_j has mean 0 and variance 1:

$$\frac{1}{n}\sum_{i=1}^{n} z_{ij} = 0, \quad \frac{1}{n}\sum_{i=1}^{n} z_{ij}^2 = 1.$$

Interpretation and Importance

- **Centering** removes location effects and aligns all variables relative to their mean.
- **Standardizing** eliminates the effect of measurement units and ensures comparability between variables.
- In *Principal Component Analysis (PCA)*, standardization is especially crucial when variables are on different scales. Without it, the first principal component would mainly reflect the variable with the largest variance.

Numerical Example

Suppose we have three individuals described by one variable "Income" (in \$1000):

$$x = (20,\ 30,\ 50).$$

The mean is $\bar{x} = (20 + 30 + 50)/3 = 33.3$. The centered values are

$$x^c = (-13.3,\ -3.3,\ 16.7).$$

The standard deviation is

$$s = \sqrt{\frac{(-13.3)^2 + (-3.3)^2 + (16.7)^2}{3}} \approx 12.47.$$

The standardized values are

$$z = (-1.07,\ -0.27,\ 1.34)\,.$$

Thus, the variable "Income" has been transformed to a scale with mean 0 and variance 1, making it directly comparable with other standardized variables.

4.2.2 Coding of Qualitative Variables

Unlike quantitative variables, qualitative variables (also called categorical variables) describe attributes or categories of individuals rather than numerical magnitudes. Examples include gender (male, female), region (north, south, east, west), or type of employment (full-time, part-time, unemployed). In order to include qualitative variables in factorial methods, they must first be transformed into a numerical representation. This process is known as *coding*.

Indicator (or Dummy) Coding

Let X_j be a qualitative variable with K_j categories (or modalities). For each modality k of X_j, we define a binary variable:

$$x_{ik} = \begin{cases} 1 & \text{if individual } i \text{ belongs to modality } k, \\ 0 & \text{otherwise.} \end{cases}$$

For instance, if the variable *Region* has three modalities (North, South, East), then each individual is represented by a triplet (x_{i1}, x_{i2}, x_{i3}) such that exactly one component equals 1 and the others are 0. This representation is called the *complete disjunctive table*.

Coding with Constraints

Since for each individual exactly one modality is active, the sum of the indicator variables across modalities equals 1. This introduces redundancy. To avoid singularity in some methods (e.g., regression), one common practice is to drop one modality (the so-called *reference category*). For example, with three regions (North, South, East), we might keep only two dummy variables, and the third is implicitly defined.

Frequency and Centering of Indicators

In correspondence analysis or multiple correspondence analysis, the raw indicators are often adjusted. Each column (modality) can be centered with respect to its frequency in the population:

$$f_k = \frac{1}{n} \sum_{i=1}^{n} x_{ik},$$

which represents the relative frequency of modality k. Centering helps to highlight deviations from expected frequencies and is analogous to centering quantitative variables.

Alternative Codings

- **Effect coding:** Instead of using 0/1 coding with a reference category, one can use -1 for the reference and $+1$ for the presence of a modality, ensuring that coefficients represent deviations from the overall mean.
- **Orthogonal coding:** In designed experiments, special codings such as orthogonal contrasts are used to facilitate interpretation of effects.

Illustrative Example

Consider the variable *Employment Status* with three modalities: *Full-time*, *Part-time*, *Unemployed*. For four individuals, the indicator matrix is:

Individual	Full-time	Part-time	Unemployed
1	1	0	0
2	0	1	0
3	0	0	1
4	1	0	0

This binary representation allows qualitative information to be incorporated into factorial analyses in the same way as quantitative variables.

4.2.3 Why Preprocessing is Necessary

Preprocessing (centering, standardization, and coding of variables) is a fundamental step before applying factorial methods. Without appropriate preprocessing, the results of analyses such as Principal Component Analysis (PCA), Correspondence Analysis (CA), or Multiple Correspondence Analysis (MCA) can be misleading or even meaningless. The necessity arises from both mathematical and interpretative considerations.

Balance between Variables

Different variables are often measured in different units (e.g., income in euros, age in years, weight in kilograms). If data are analyzed without standardization, variables with larger numerical ranges will dominate the distance computations:

Distance computations

$$d(i,j) = \sqrt{\sum_{k=1}^{p} (x_{ik} - x_{jk})^2}.$$

For instance, a variable measured in thousands can overshadow another measured on a scale from 0 to 10, even if the latter is more relevant to the study. Standardization ensures that all variables contribute equally, unless explicitly weighted.

Comparability of Individuals

Centering ensures that variables are expressed relative to their mean:

$$z_{ik} = x_{ik} - \bar{x}_k,$$

so that analyses focus on the deviations of individuals from the average profile. This comparability is essential for geometric interpretations in factorial spaces, where the origin represents the average individual.

Integration of Qualitative Variables

Qualitative variables cannot be directly included in distance or covariance computations. Through coding (complete disjunctive table, dummy variables, or other schemes), each modality becomes comparable to a quantitative variable. Without such preprocessing, entire categories of information would be lost, limiting the scope of factorial methods.

Geometric Interpretation

Factorial methods rely on geometric representations of individuals and variables in Euclidean spaces. For these representations to be meaningful:

- Variables must be placed on a common scale (hence standardization),
- Individuals must be centered around a barycenter (hence centering),
- Modalities must be transformed into vectors (hence coding).

These steps ensure that axes extracted by PCA or CA represent true structural directions of variability rather than artifacts of scaling.

Interpretability of Results

Proper preprocessing makes the interpretation of factorial axes consistent. For example:

- In PCA, the first axis represents the direction of greatest variance after standardization, not simply the variable with the largest scale.
- In MCA, associations between categories become visible only after coding and frequency adjustments.

Thus, preprocessing guarantees that the factorial planes reflect genuine associations rather than technical biases.

4.3 Distance and Similarity Measures

4.3.1 Euclidean Distance between Individuals

The *Euclidean distance* is the most widely used measure to quantify the dissimilarity between two individuals described by quantitative variables. It stems from classical geometry and is the natural extension of the Pythagorean theorem to p-dimensional spaces.

Definition

Let i and j denote two individuals described by p quantitative variables $\{X_1, X_2, \ldots, X_p\}$. Their observed profiles are represented by the vectors:

$$\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip}), \quad \mathbf{x}_j = (x_{j1}, x_{j2}, \ldots, x_{jp}).$$

The Euclidean distance between i and j is defined as:

Euclidean distance

$$d_E(i,j) = \sqrt{\sum_{k=1}^{p} (x_{ik} - x_{jk})^2}.$$

This measure corresponds to the length of the straight line connecting the two individuals in p-dimensional Euclidean space $\mathbb{R}^p$ [Jolliffe(2002), Husson et al.(2017)].

Properties

1. **Non-negativity:** $d_E(i,j) \geq 0$, with equality if and only if $\mathbf{x}_i = \mathbf{x}_j$.
2. **Symmetry:** $d_E(i,j) = d_E(j,i)$.
3. **Triangle inequality:** For any three individuals i, j, k,

$$d_E(i,k) \leq d_E(i,j) + d_E(j,k).$$

4. **Geometric interpretation:** The set of individuals equidistant from i forms a hypersphere centered at $\mathbf{x}_i$.

Standardized Euclidean Distance

When variables are measured in different units or scales, the raw Euclidean distance can be misleading. To avoid dominance of variables with larger variances, one often uses the *standardized Euclidean distance*:

Standardized Euclidean distance

$$d_E^*(i,j) = \sqrt{\sum_{k=1}^{p} \left(\frac{x_{ik} - x_{jk}}{s_k} \right)^2},$$

where s_k is the standard deviation of variable X_k.

This adjustment is equivalent to computing the Euclidean distance on the standardized data matrix $Z = (z_{ik})$, with

$$z_{ik} = \frac{x_{ik} - \bar{x}_k}{s_k}.$$

Interpretation in Factorial Analysis

In factorial methods such as Principal Component Analysis (PCA), Euclidean distance (after centering and standardizing) is the basis for:

- measuring proximity between individuals,
- constructing inertia, defined as the total variance of the cloud of points,
- deriving principal axes, which maximize the variance of projected distances.

Thus, Euclidean distance is central to understanding the geometry of multivariate data clouds and their factorial decompositions [Mardia et al.(1979), Greenacre(2010)].

4.3.2 Chi-Square Distance for Categorical Data

When the data table involves categorical variables (especially in contingency tables), the Euclidean distance is no longer appropriate because categories are nominal and frequencies need to be compared in a weighted way. In this context, the *chi-square distance* is the natural measure of dissimilarity between individuals or categories [Greenacre(1984), Lebart et al.(1984)].

Setting

Consider a data table with n individuals (rows) and m categorical variables represented as indicator variables, or equivalently a contingency table of frequencies:

$$\mathbf{N} = (n_{ij}), \quad i = 1, \ldots, n, \; j = 1, \ldots, m,$$

where n_{ij} denotes the frequency (or indicator value) of individual i for category j. The grand total is $n_{..} = \sum_{i=1}^{n} \sum_{j=1}^{m} n_{ij}$.

We define the row profile of individual i as:

$$\mathbf{p}_i = \left(\frac{n_{i1}}{n_{i.}}, \frac{n_{i2}}{n_{i.}}, \ldots, \frac{n_{im}}{n_{i.}} \right),$$

where $n_{i.} = \sum_{j=1}^{m} n_{ij}$ is the row sum.

The column masses are given by:

$$c_j = \frac{n_{.j}}{n_{..}}, \quad \text{where } n_{.j} = \sum_{i=1}^{n} n_{ij}.$$

Definition of Chi-Square Distance

The chi-square distance between two row profiles i and i' is defined as:

Chi-square distance

$$d_{\chi^2}(i,i') = \sqrt{\sum_{j=1}^{m} \frac{1}{c_j}\left(\frac{n_{ij}}{n_{i.}} - \frac{n_{i'j}}{n_{i'.}}\right)^2}.$$

Equivalently, in terms of row profiles:

$$d_{\chi^2}(i,i') = \sqrt{\sum_{j=1}^{m} \frac{1}{c_j}\left(p_{ij} - p_{i'j}\right)^2}.$$

Interpretation

- The chi-square distance is a *weighted Euclidean distance* between row profiles, with weights given by the inverse of the column masses $1/c_j$.
- Columns (categories) with higher marginal frequency contribute less to the distance, while rare categories are given more importance.
- This ensures that differences in rare categories are not overlooked.

Connection to Correspondence Analysis

Correspondence Analysis (CA) is based on the chi-square distance:

- The geometry of row and column profiles is defined using d_{χ^2}.
- Inertia in CA is defined as the average chi-square distance between observed profiles and the independence model.
- The decomposition of inertia into principal axes provides the factorial map of individuals and categories [**?**].

Properties

1. $d_{\chi^2}(i,i') \geq 0$ and is zero if and only if $\mathbf{p}_i = \mathbf{p}_{i'}$.
2. Symmetry: $d_{\chi^2}(i,i') = d_{\chi^2}(i',i)$.
3. The measure depends on relative frequencies, not absolute counts, making it scale-invariant with respect to row totals.

4.3.3 Correlation-Based Similarity between Variables

When analyzing the relationships between quantitative variables in a data table, similarity is often measured by correlation coefficients, which capture the linear association between variables [Anderson(2003), Jolliffe and Cadima(2016)].

Pearson Correlation

Given two variables $X = (x_1, \ldots, x_n)$ and $Y = (y_1, \ldots, y_n)$ observed on n individuals, the Pearson correlation coefficient is defined as:

Pearson correlation coefficient

$$r_{XY} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}},$$

where $\bar{x}$ and $\bar{y}$ are the sample means of X and Y, respectively.

This coefficient satisfies $-1 \leq r_{XY} \leq 1$, with values close to ± 1 indicating strong linear dependence and values near 0 indicating weak or no linear relationship.

Geometric Interpretation

If the data matrix $\mathbf{X}$ has been column-centered, each variable corresponds to a vector in $\mathbb{R}^n$. The cosine of the angle between two standardized variable vectors $\mathbf{x}$ and $\mathbf{y}$ is given by:

$$\cos(\theta) = \frac{\mathbf{x}^\top \mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|}.$$

This cosine is exactly the Pearson correlation coefficient r_{XY}. Thus, correlation provides a direct geometric similarity measure between variables.

Correlation as a Distance

For certain multivariate methods (e.g., clustering of variables, PCA), it is useful to transform correlation into a distance:

$$d^2(X, Y) = 2(1 - r_{XY}).$$

This transformation ensures $d^2(X, Y) \geq 0$ and defines a Euclidean distance between standardized variable vectors.

Extension: Other Similarity Measures

Beyond Pearson correlation, alternative measures may be considered:

- Spearman rank correlation, which assesses monotonic rather than linear relationships.
- Mutual information, which extends similarity to nonlinear and categorical contexts [Cover and Thomas(2006)].

Connection to Factorial Methods

Principal Component Analysis (PCA) is closely related to correlation-based similarity. When PCA is performed on standardized variables, the correlation matrix is diagonalized, and variables with strong correlations tend to project closely in the factorial plane [Jolliffe and Cadima(2016)].

4.4 Principle of Factorial Methods

4.4.1 Dimensionality Reduction and Information Preservation

In multivariate data analysis, one is often faced with datasets containing a large number of variables, many of which may be correlated or redundant. Direct interpretation of such high-dimensional data tables is difficult, both from a statistical and a graphical perspective. The fundamental goal of factorial methods is therefore to reduce the dimensionality of the dataset while preserving as much information as possible [Jolliffe(2002), Jolliffe and Cadima(2016)].

Let $\mathbf{X}$ denote the data matrix of size $n \times p$, where n is the number of individuals and p the number of variables. Each individual is represented as a point in $\mathbb{R}^p$. High-dimensional geometry quickly becomes intractable, hence the need for projecting the data onto a lower-dimensional subspace $\mathbb{R}^k$, with $k \ll p$, in such a way that the essential structure of the data is preserved.

The central criterion for this projection is the preservation of the *total inertia*, which is directly linked to the variance of the variables. Recall that the total inertia of a cloud of points $\{x_1, \ldots, x_n\}$ with respect to their centroid g is defined as

$$I_T = \frac{1}{n} \sum_{i=1}^{n} \|x_i - g\|^2. \tag{4.1}$$

Inertia is a measure of the dispersion of the cloud, and in the context of quantitative data, it corresponds to the total variance [Mardia et al.(1979), Greenacre(2010)].

Dimensionality reduction methods such as Principal Component Analysis (PCA) seek an orthogonal transformation $\mathbf{X} \mapsto \mathbf{XA}$, where $\mathbf{A}$ is a $p \times k$ matrix with orthonormal columns, such that the projected cloud in $\mathbb{R}^k$ retains the maximum proportion of inertia:

$$\max_{\mathbf{A}} \ \mathrm{Var}(\mathbf{XA}), \tag{4.2}$$

subject to $\mathbf{A}^\top \mathbf{A} = \mathbf{I}_k$.

The same principle applies to factorial methods designed for categorical data, such as Correspondence Analysis (CA) and Multiple Correspondence Analysis (MCA). In these cases, the criterion of information preservation is expressed not in terms of variance but in terms of χ^2-inertia, which generalizes the notion of dispersion to contingency tables [Greenacre(1984), Lebart et al.(1984)].

Thus, factorial methods provide a compromise: they replace the original high-dimensional space by a reduced number of latent dimensions, while ensuring that the maximum possible information (measured by inertia) is preserved in the projection. This principle forms the theoretical foundation for the geometric representations that will be explored in subsequent sections.

4.4.2 Variance as a Criterion for Dimension Reduction

The guiding principle of factorial methods is that the most informative directions in a dataset are those along which the variance of the observations is maximized.

This is the foundation of Principal Component Analysis (PCA) and its extensions [Jolliffe(2002)], [Jolliffe and Cadima(2016)].

Let $\mathbf{X}$ be the centered data matrix of size $n \times p$, with rows $x_i \in \mathbb{R}^p$. The empirical covariance matrix is given by

$$\mathbf{S} = \frac{1}{n}\mathbf{X}^\top \mathbf{X}. \tag{4.3}$$

The total variance of the data is

Total variance

$$\mathrm{Var}_{\mathrm{tot}} = \mathrm{trace}(\mathbf{S}) = \sum_{j=1}^{p} \sigma_j^2, \tag{4.4}$$

where σ_j^2 denotes the variance of the j-th variable. Equivalently, $\mathrm{Var}_{\mathrm{tot}}$ corresponds to the total inertia of the cloud of individuals with respect to the centroid.

The problem of finding the best one-dimensional projection of the data can be formulated as

$$\max_{\|u\|=1} \mathrm{Var}(\mathbf{X}u) = \max_{\|u\|=1} u^\top \mathbf{S} u, \tag{4.5}$$

where $u \in \mathbb{R}^p$ is a unit vector. The solution is given by the eigenvector associated with the largest eigenvalue λ_1 of $\mathbf{S}$. The corresponding maximum variance is λ_1.

By recursion, the k-dimensional optimal subspace is obtained by considering the first k eigenvectors $u_1, \ldots, u_k$, which are orthogonal. The projected data

$$\mathbf{Y} = \mathbf{X}\mathbf{U}_k, \quad \text{where } \mathbf{U}_k = [u_1, \ldots, u_k],$$

maximizes the preserved variance, equal to

$$\sum_{j=1}^{k} \lambda_j. \tag{4.6}$$

The ratio

$$\frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{p} \lambda_j} \tag{4.7}$$

represents the proportion of total variance explained by the first k dimensions [Mardia et al.(1979)].

This criterion ensures that factorial methods do not arbitrarily reduce dimensionality but instead retain the most meaningful structure of the data. In categorical cases, analogous decompositions are performed using the χ^2-inertia matrix derived from contingency tables, where eigenvalues again indicate the amount of information explained by successive axes [Greenacre(1984)], [Lebart et al.(1984)].

Thus, variance (or inertia) provides both a mathematical criterion for selecting axes and a practical tool for interpreting the efficiency of dimensionality reduction.

4.4.3 Geometric Interpretation of Factorial Methods

One of the most powerful aspects of factorial methods is their geometric interpretation. These methods allow a dataset to be represented as a cloud of points in a Euclidean space, where both individuals and variables can be visualized and studied simultaneously [Greenacre(2010), Husson et al.(2017)].

Consider a centered and standardized data matrix $\mathbf{X}$ of size $n \times p$. Each row $x_i \in \mathbb{R}^p$ represents an *individual*, and the entire dataset can be seen as a cloud of n points in $\mathbb{R}^p$ (the space of variables). Conversely, each column $x^{(j)} \in \mathbb{R}^n$ represents a *variable*, so the same data can also be interpreted as a cloud of p points in $\mathbb{R}^n$ (the space of individuals). This duality principle underlies the geometric approach to multivariate analysis [Mardia et al.(1979), Lebart et al.(1984)].

The core idea of factorial methods is to project these high-dimensional clouds onto low-dimensional subspaces, typically defined by the eigenvectors of an appropriate variance or inertia matrix. For PCA, the subspace is spanned by the eigenvectors of the covariance (or correlation) matrix, while in correspondence analysis (CA) the subspace is defined by the eigenvectors of the χ^2-distance-based inertia operator.

Mathematically, if $\mathbf{S}$ is the covariance matrix and (λ_j, u_j) are its eigenvalue–eigenvector pairs, the projection of an individual x_i onto axis j is

$$f_{ij} = x_i^\top u_j, \tag{4.8}$$

known as the *factorial coordinate* of individual i on axis j. Similarly, the correlation between variable k and axis j is given by

correlation between variables

$$\operatorname{corr}(x^{(k)}, u_j) = \frac{u_{kj}\sqrt{\lambda_j}}{\sigma_k}, \tag{4.9}$$

where u_{kj} is the k-th component of eigenvector u_j and σ_k is the standard deviation of variable k.

This dual representation leads to two complementary plots:

- The **individuals factor map**, where points represent individuals in the reduced space;
- The **variables factor map**, where arrows or points represent variables by their correlations with the axes.

The superposition of both views, known as a *biplot*, provides a unified visualization of individuals and variables in the same graphical space [Greenacre(2010)].

The geometric interpretation thus gives factorial methods an intuitive and visual power: one can simultaneously examine the proximity between individuals, the associations between variables, and the links between the two representations.

4.4.4 Overview of Main Factorial Methods

The family of factorial methods encompasses several techniques, each adapted to a particular type of data. Although their mathematical foundations are similar, their domains of application differ according to the measurement scales of the variables and the research objectives [Jolliffe and Cadima(2016), Husson et al.(2017)].

Principal Component Analysis (PCA). PCA is the most widely used factorial method and applies to quantitative data. Its objective is to reduce the dimensionality of the dataset while retaining the maximum amount of total variance. Starting from a centered and standardized data matrix $\mathbf{X}$, PCA constructs new uncorrelated variables, called *principal components*, defined as linear combinations of the original variables:

$$z_j = \mathbf{X}u_j, \quad j = 1, \ldots, p, \tag{4.10}$$

where u_j is an eigenvector of the covariance (or correlation) matrix. The variance of component z_j equals the associated eigenvalue λ_j. Applications of PCA include exploratory data analysis, visualization of multivariate structures, and noise reduction [Jolliffe(2002), Mardia et al.(1979)].

Correspondence Analysis (CA). CA is tailored for contingency tables and categorical data. Instead of the Euclidean distance, it relies on the χ^2 distance between row or column profiles, making it suitable for frequency data. The method decomposes the total inertia of the contingency table and represents both rows and columns in a common geometric space. If $\mathbf{P}$ denotes the matrix of relative frequencies and $\mathbf{r}, \mathbf{c}$ the row and column margins, the χ^2 distance between two rows i and i' is

$$d^2(i, i') = \sum_{j=1}^{p} \frac{1}{c_j} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2, \tag{4.11}$$

where p_{ij} is the relative frequency of cell (i, j). Applications of CA are common in the analysis of survey data, linguistics, ecology, and marketing [Greenacre(1984), Greenacre(2010)].

Multiple Correspondence Analysis (MCA). MCA extends CA to the analysis of multiple categorical variables, usually organized in an indicator matrix $\mathbf{Z}$ of size $n \times m$ (where m is the total number of categories across variables). MCA can be interpreted as a PCA applied to the Burt matrix (a symmetric block matrix of all two-way cross-tabulations) or equivalently to $\mathbf{Z}$. MCA is widely used in social sciences for analyzing survey data with multiple categorical questions [Lebart et al.(1984), Husson et al.(2017)].

In summary, PCA is appropriate for quantitative variables, CA for two-way contingency tables, and MCA for multiple categorical variables. Together, these methods provide a comprehensive toolkit for exploring complex datasets, each preserving the same geometric and algebraic principles while adapting to the structure of the data.

4.4.5 From Data Table to Factorial Decomposition

The central idea of factorial methods is that a data table can be transformed into a mathematical object whose structure is revealed through *spectral decomposition*. This procedure relies on the study of the eigenvalues and eigenvectors of an appropriate matrix (covariance, correlation, or χ^2-based), depending on the nature of the data [Jolliffe(2002), Mardia et al.(1979)].

Step 1: Centered and standardized data matrix. Let $\mathbf{X}$ be an $n \times p$ matrix, where n is the number of individuals and p the number of quantitative variables. After centering (and, if necessary, standardizing), the rows of $\mathbf{X}$ represent individual deviations from the mean. The covariance matrix is given by

$$\mathbf{S} = \frac{1}{n}\mathbf{X}^\top \mathbf{X}. \tag{4.12}$$

If the variables are standardized, $\mathbf{S}$ reduces to the correlation matrix $\mathbf{R}$.

Step 2: Spectral decomposition. The next step is to solve the eigenvalue problem

$$\mathbf{S}u_j = \lambda_j u_j, \quad j = 1, \ldots, p, \tag{4.13}$$

where λ_j are the eigenvalues (ordered $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$) and u_j the corresponding eigenvectors. The eigenvalues quantify the variance explained by each component, while the eigenvectors define the directions of maximum variance.

Step 3: Factorial coordinates. The projection of the individuals onto the new axes is given by

$$\mathbf{F} = \mathbf{X}U, \tag{4.14}$$

where $U = [u_1, u_2, \ldots, u_k]$ is the matrix of selected eigenvectors. The matrix $\mathbf{F}$ contains the *factorial coordinates* of the individuals, often called principal components in the case of PCA. The inertia (total variance) explained by axis j equals $\lambda_j / \sum_{m=1}^{p} \lambda_m$.

Generalization to other factorial methods. While the case of PCA is based on $\mathbf{S}$ (covariance/correlation matrix), Correspondence Analysis and Multiple Correspondence Analysis rely on matrices derived from frequency tables. In CA, for example, the decomposition is applied to the matrix of standardized residuals:

$$\mathbf{Z} = \mathbf{D}_r^{-1/2} \left(\mathbf{P} - \mathbf{r}\mathbf{c}^\top \right) \mathbf{D}_c^{-1/2}, \tag{4.15}$$

where $\mathbf{P}$ is the matrix of relative frequencies, and $\mathbf{D}_r$, $\mathbf{D}_c$ are diagonal matrices of row and column margins. The singular value decomposition (SVD) of $\mathbf{Z}$ provides the principal axes and coordinates [Greenacre(1984), Husson et al.(2017)].

Thus, the passage from a data table to a factorial decomposition follows a universal scheme: (1) construct a matrix representing similarities or variances, (2) perform spectral decomposition (eigenvalue or singular value decomposition), and (3) interpret the new factorial axes as optimal directions summarizing the essential structure of the data.

4.5 Geometric Representation of Data Tables

4.5.1 Cloud of Individuals

A data table with n individuals and p variables can be represented geometrically by associating each individual with a point in $\mathbb{R}^p$. This set of points, called the *cloud of individuals*, provides a geometric view of the data and serves as the starting point for factorial analysis [Mardia et al.(1979), Greenacre(2010)].

Definition. Let $\mathbf{X}$ be the centered (and possibly standardized) $n \times p$ data matrix. The i-th row vector $x_i \in \mathbb{R}^p$ corresponds to individual i. The cloud of individuals is defined as

$$N = \{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^p. \tag{4.16}$$

If the data are centered, the barycenter of the cloud is the origin:

$$\frac{1}{n}\sum_{i=1}^{n} x_i = 0. \tag{4.17}$$

Metric structure. The squared Euclidean distance between two individuals i and i' is

$$d^2(i, i') = \|x_i - x_{i'}\|^2 = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2. \tag{4.18}$$

The inertia of the cloud, which measures the global dispersion of individuals around the barycenter, is

$$I(N) = \frac{1}{n}\sum_{i=1}^{n} \|x_i\|^2. \tag{4.19}$$

Projection. Since p is often large, visualization is carried out by projecting the cloud onto factorial subspaces of low dimension. If u_1, u_2 are the first two eigenvectors of the covariance or correlation matrix, then the coordinates of individual i in the factorial plane are

$$f_i = \Big(x_i \cdot u_1,\ x_i \cdot u_2\Big). \tag{4.20}$$

The projected set $\{f_1, \ldots, f_n\}$ represents the individuals in a plane while preserving as much inertia as possible [Jolliffe and Cadima(2016)].

Illustration. The following figure shows a typical projection of individuals on a two-dimensional factorial plane. Points close to each other indicate individuals with similar profiles, while isolated points represent atypical observations.

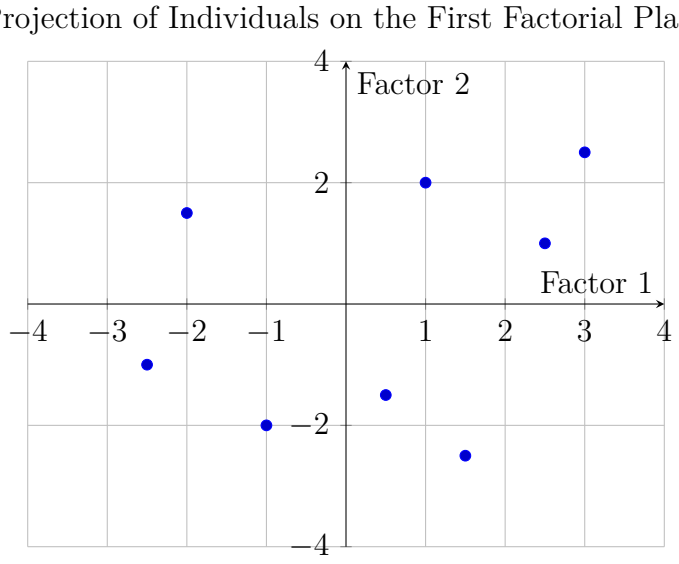


Figure 4.1: Cloud of individuals projected onto a two-dimensional factorial plane.

4.5.2 Cloud of Variables (Correlation Circle)

In addition to representing individuals, factorial methods provide a geometric representation of the variables themselves. Each quantitative variable is associated with a vector in $\mathbb{R}^n$, corresponding to the column of the centered (and standardized) data matrix $\mathbf{X}$. The cloud of variables allows one to study the relationships between variables and their contributions to the factorial axes [Greenacre(1984), Lebart et al.(1984)].

Definition. Let $\mathbf{X}$ be the $n \times p$ centered and standardized data matrix. For variable j ($j = 1, \ldots, p$), let $x^j \in \mathbb{R}^n$ denote its column vector. The cloud of variables is defined as

$$M = \{x^1, x^2, \ldots, x^p\} \subset \mathbb{R}^n. \tag{4.21}$$

Since variables are standardized, each x^j has unit variance, and the scalar product between two variables j and j' is their empirical correlation:

$$\langle x^j, x^{j'} \rangle = \frac{1}{n} \sum_{i=1}^{n} x_{ij}\, x_{ij'} = \mathrm{Corr}(X_j, X_{j'}). \tag{4.22}$$

Correlation circle. When projecting the cloud of variables onto the first two factorial axes u_1, u_2, the coordinates of variable j are given by

$$g_j = \Big(\langle x^j, u_1 \rangle,\ \langle x^j, u_2 \rangle \Big). \tag{4.23}$$

Since the variables are standardized, the vectors g_j lie inside the unit circle of $\mathbb{R}^2$. This circle, called the *correlation circle*, provides a compact geometric summary of the correlations between variables and their relations to the principal components [Jolliffe(2002), Husson et al.(2017)].

Interpretation. Variables located near the circle are well represented by the factorial plane; variables close to each other are positively correlated, those in opposite directions are negatively correlated, and orthogonal vectors correspond to uncorrelated variables.

Illustration. The following figure illustrates a correlation circle with eight standardized variables projected onto the first two factorial axes.

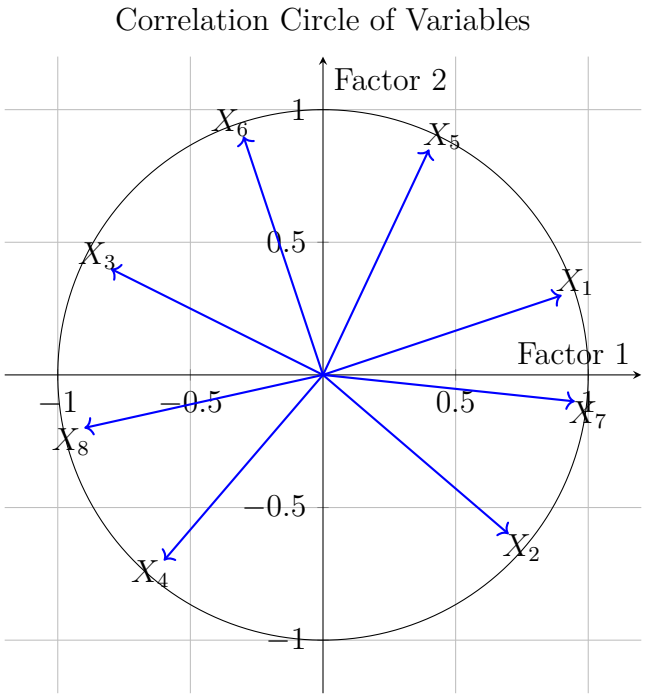


Figure 4.2: Cloud of variables projected onto the first two factorial axes (correlation circle).

4.5.3 Duality: Individuals vs. Variables

A fundamental property of factorial methods is the duality between the representation of individuals and the representation of variables. This duality emerges from the mathematical structure of the data matrix and the inner products used to define distances and correlations [Mardia et al.(1979), Greenacre(2010)].

Mathematical background. Let $\mathbf{X}$ be the $n \times p$ centered and standardized data matrix, where n is the number of individuals and p the number of variables. Denote by

$$S = \frac{1}{n}\mathbf{X}^\top \mathbf{X}$$

the empirical correlation matrix of variables, and

$$G = \frac{1}{p}\mathbf{X}\mathbf{X}^\top$$

the Gram matrix of individuals.

The eigen-decomposition of S provides the principal components (axes for the variables), while the eigen-decomposition of G provides the factorial coordinates of individuals. Both decompositions are linked through the singular value decomposition (SVD) of $\mathbf{X}$:

$$\mathbf{X} = U\Sigma V^\top, \tag{4.24}$$

where $U \in \mathbb{R}^{n\times r}$ and $V \in \mathbb{R}^{p\times r}$ are orthogonal matrices, Σ is diagonal with singular values, and $r = \min(n, p)$.

Thus: - The columns of V correspond to the principal axes for variables, - The columns of U correspond to the principal axes for individuals, - The link between the two representations is mediated by the singular values in Σ.

Geometric interpretation. The duality principle states that: - The position of an individual in the factorial plane is determined by the weighted mean of the variables (with coefficients given by loadings). - Conversely, the position of a variable in the correlation circle is determined by the correlations it has with the factorial axes, which themselves are constructed from individuals.

In other words, the two representations are projections of the same structure, viewed from dual perspectives: rows vs. columns of the data matrix [Jolliffe and Cadima(2016), Husson et al.(2017)].

Illustration. The following schematic figure illustrates the duality between the cloud of individuals and the cloud of variables: both are linked through the same eigen-decomposition, but represented in two complementary spaces.

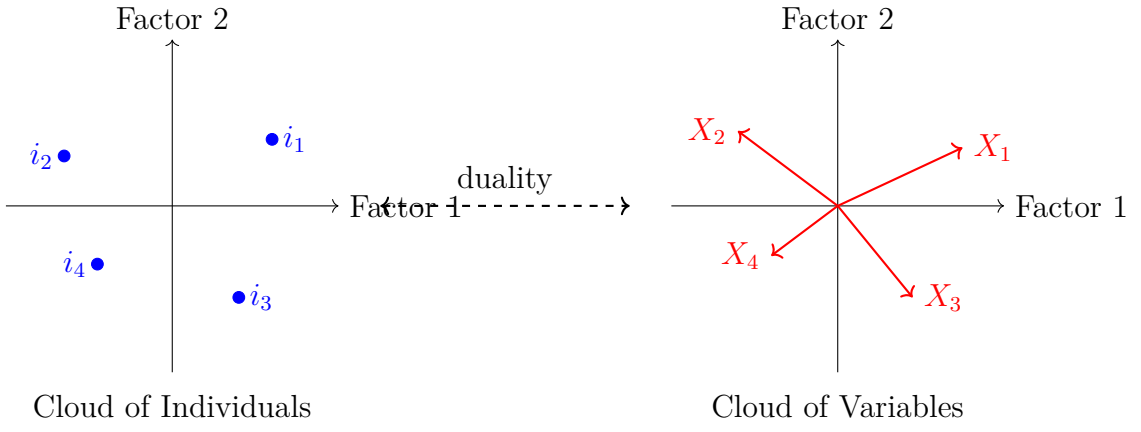


Figure 4.3: Duality between the representation of individuals (left) and variables (right) in factorial analysis. Both derive from the same decomposition of the data matrix.

4.6 Worked Example

We illustrate the full pipeline on a small data table with three quantitative variables observed on six individuals:

$$\text{Variables } (p=3): \; X_1 = \text{Measure A}, \quad X_2 = \text{Measure B}, \quad X_3 = \text{Measure C}.$$

$$\text{Individuals } (n=6): \; A, B, C, D, E, F.$$

	X_1	X_2	X_3
A	1	1	6
B	2	2	5
C	3	2	7
D	4	3	8
E	5	4	7
F	6	5	9

Step 1 — Centering and Standardizing

Let $\bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$ and (population-type) standard deviation $s_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}$.[1] For the table above:

$$\bar{x}_1 = \tfrac{7+2+3+4+5+6}{6} = 3.5, \quad \bar{x}_2 = \tfrac{17}{6} \approx 2.833, \quad \bar{x}_3 = 7.$$

The variances (with $1/n$) and standard deviations are

$$\mathrm{Var}(X_1) = \frac{35}{12} \approx 2.917, \quad s_1 = \sqrt{\tfrac{35}{12}} \approx 1.708,$$

$$\mathrm{Var}(X_2) = \frac{65}{36} \approx 1.806, \quad s_2 = \sqrt{\tfrac{65}{36}} \approx 1.343,$$

$$\mathrm{Var}(X_3) = \frac{5}{3} \approx 1.667, \quad s_3 = \sqrt{\tfrac{5}{3}} \approx 1.291.$$

We form standardized scores (z-scores) $z_{ij} = (x_{ij}-\bar{x}_j)/s_j$, collecting them in the matrix $Z \in \mathbb{R}^{n\times p}$.

Step 2 — Distances Between Individuals

The (squared) Euclidean distance between individuals i and i' in the original space is

$$\|x_i - x_{i'}\|^2 = \sum_{j=1}^{p}(x_{ij}-x_{i'j})^2.$$

In the standardized space (each variable unit-variance), use

$$\|z_i - z_{i'}\|^2 = \sum_{j=1}^{p}\left(\tfrac{x_{ij}-\bar{x}_j}{s_j} - \tfrac{x_{i'j}-\bar{x}_j}{s_j}\right)^2.$$

[1] We use the $1/n$ convention to align with the geometric "inertia" viewpoint; replacing it by $1/(n-1)$ changes only scale, not directions [Jolliffe and Cadima(2016), Mardia et al.(1979)].

Illustration:

$$\|x_A - x_F\| = \sqrt{(1-6)^2 + (1-5)^2 + (6-9)^2} = \sqrt{50} \approx 7.071,$$

$$\|z_A - z_F\| \approx 4.778, \qquad \|z_A - z_B\| \approx 1.223, \qquad \|z_A - z_E\| \approx 3.327.$$

Standardization ensures each variable contributes comparably to interpoint distances (scale invariance).

Step 3 — Covariance and Correlation

With X_c the column-centered data, the (population) covariance is

$$S = \frac{1}{n} X_c^\top X_c = \begin{bmatrix} \frac{35}{12} & \frac{9}{4} & \frac{11}{6} \\ \frac{9}{4} & \frac{65}{36} & \frac{4}{3} \\ \frac{11}{6} & \frac{4}{3} & \frac{5}{3} \end{bmatrix} \approx \begin{bmatrix} 2.917 & 2.250 & 1.833 \\ 2.250 & 1.806 & 1.333 \\ 1.833 & 1.333 & 1.667 \end{bmatrix}.$$

The correlation matrix $R = D^{-1/2} S D^{-1/2}$ (with $D = \mathrm{diag}(S)$) is

$$R \approx \begin{bmatrix} 1 & 0.980 & 0.832 \\ 0.980 & 1 & 0.769 \\ 0.832 & 0.769 & 1 \end{bmatrix}.$$

All pairs are positively correlated, with X_1–X_2 strongest.

Step 4 — PCA on the Correlation Matrix

Principal components diagonalize R: $R = V \Lambda V^\top$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq 0$ and orthonormal loadings (eigenvectors) in V. Numerically,

$$\lambda_1 \approx 2.724, \quad \lambda_2 \approx 0.263, \quad \lambda_3 \approx 0.014,$$

so the percentage of variance explained is

$$\frac{\lambda_1}{3} \approx 90.8\%, \qquad \frac{\lambda_2}{3} \approx 8.76\%, \qquad \frac{\lambda_3}{3} \approx 0.45\%.$$

One dominant dimension suffices.

A convenient orientation of loadings (signs are conventional) is

$$\text{PC1 loadings } \ell^{(1)} \approx \begin{bmatrix} 0.597 \\ 0.585 \\ 0.549 \end{bmatrix}, \qquad \text{PC2 loadings } \ell^{(2)} \approx \begin{bmatrix} -0.278 \\ -0.491 \\ 0.826 \end{bmatrix}.$$

Thus PC1 is a common "size" axis (all positive), while PC2 contrasts X_3 against (X_1, X_2).

Scores. With standardized data Z, the score of individual i on PC k is $t_{ik} = \sum_{j=1}^{p} z_{ij}\, \ell_j^{(k)}$. Using the orientations above, the first two PC scores are

	A	B	C	D	E	F
PC1	−2.097	−1.738	−0.537	0.673	1.032	2.668
PC2	0.437	−0.730	0.386	0.497	−0.671	0.080

PC1 orders the individuals from globally small (A) to large (F) values; PC2 picks up the relative surplus/deficit of X_3 versus (X_1, X_2).

Step 5 — Geometric Representation (to be plotted)

In the $(\mathrm{PC1}, \mathrm{PC2})$ plane:

- **Scores plot:** points (t_{i1}, t_{i2}) show the cloud of individuals.
- **Correlation circle:** variables are represented by the vectors of correlations with PCs,

$$\rho(X_j, \mathrm{PC}k) = \sqrt{\lambda_k}\, \ell_j^{(k)}, \quad j = 1, 2, 3,\ k = 1, 2,$$

  which (for $k = 1, 2$) typically lie close to the unit circle when the first two PCs explain most variance [Greenacre(2010), Jolliffe and Cadima(2016)].

Summary of numerical results

Center $\bar{x} = (3.5,\ 2.833,\ 7)$; SDs $s \approx (1.708,\ 1.343,\ 1.291)$. $R \approx \begin{pmatrix} 1 & 0.980 & 0.832 \\ 0.980 & 1 & 0.769 \\ 0.832 & 0.769 & 1 \end{pmatrix}$. Eigenvalues $(2.724,\ 0.263,\ 0.014) \Rightarrow 90.8\% + 8.76\%$ on first two PCs. Loadings $\ell^{(1)} \approx (0.597, 0.585, 0.549)$, $\ell^{(2)} \approx (-0.278, -0.491, 0.826)$.

Remarks. (1) Using $1/(n-1)$ instead of $1/n$ only rescales variances and distances; directions (loadings) and scores up to scale/sign are unaffected in PCA.

(2) If variables are on very different scales, working with R (standardized PCA) is recommended [Jolliffe and Cadima(2016)].

(3) Distances in the PC space approximate standardized Euclidean distances when enough components are kept.

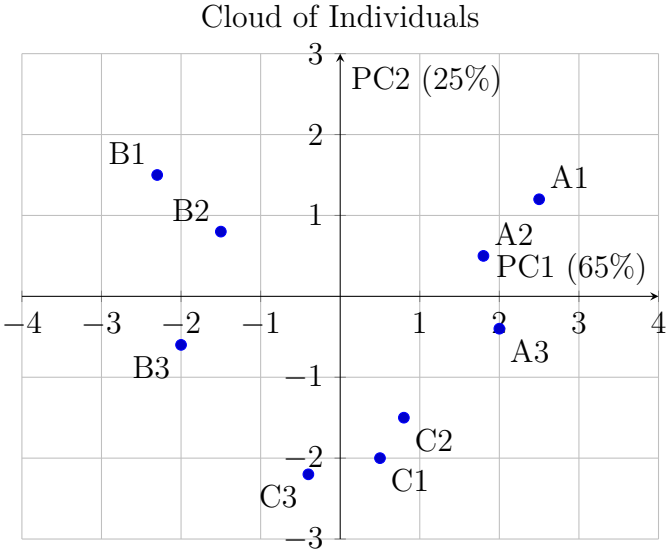


Figure 4.4: Representation of individuals on the first factorial plane.

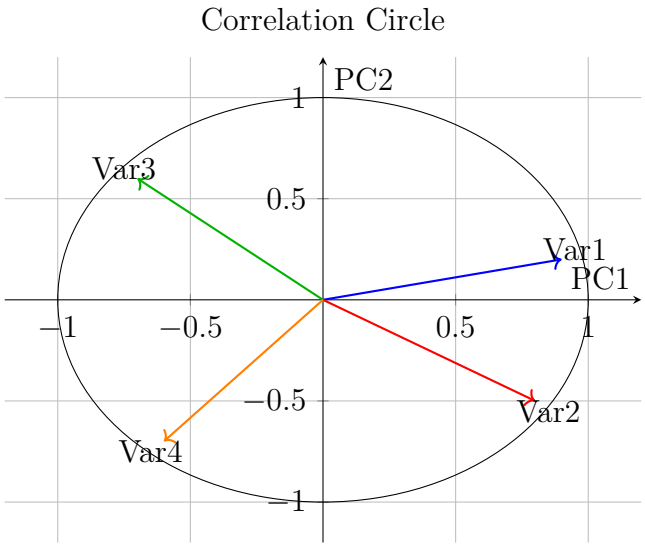


Figure 4.5: Correlation circle: projection of variables on the first factorial plane.

The representation of individuals on the first factorial plane (see Figure) makes it possible to visualize the relative proximities between observations. Individuals that are close to each other in the plot have similar profiles with respect to the variables, since their Euclidean distance in the reduced space approximates the original distance computed in the full-dimensional space. For instance, individuals A1, A2, and A3 form a compact cluster located on the right-hand side of the plot, indicating that they share similar characteristics. Conversely, individuals B1–B3 and C1–C3 are positioned in distinct regions

4.7 Exercises

Exercise 1 :Structure of a Data Table

Consider a data table with $n = 5$ individuals and $p = 3$ variables.

$$X = \begin{bmatrix} 2 & 5 & 8 \\ 3 & 6 & 7 \\ 4 & 5 & 6 \\ 5 & 4 & 5 \\ 6 & 3 & 4 \end{bmatrix}$$

(a) Identify the rows and columns of the table. (b) Explain what the terms *individuals* and *variables* mean in this context.

Exercise 2: Centering and Standardization.

Take the second variable of Exercise 1. Compute its mean, variance, and standardized values (z-scores).

Exercise 3: Coding of Qualitative Variables

Suppose we have a qualitative variable "Color" with categories $\{Red, Green, Blue\}$ observed for 4 individuals as: Red, Green, Blue, Red. (a) Construct its indicator matrix. (b) Explain how this coding allows qualitative data to be included in factorial methods.

Exercise 4: Euclidean Distance.

Given two individuals $x = (2, 4, 6)$ and $y = (4, 6, 8)$, compute their Euclidean distance. Then compute the distance between individuals A1 and A2 of Exercise 1.

Exercise 5: Chi-Square Distance For a contingency table of row profiles:

	A	B	C
I_1	10	20	30
I_2	20	10	30
I_3	15	15	30

Compute the χ^2 distance between profiles I_1 and I_2.

Exercise 6: Correlation-Based Similarity

Given the following two variables measured on 5 individuals:

$$X = (2, 4, 6, 8, 10), \quad Y = (1, 3, 5, 7, 9),$$

compute the Pearson correlation coefficient and interpret its meaning in terms of similarity.

Exercise 7: Eigenvalue Decomposition.

Let the covariance matrix of a centered and standardized dataset be:

$$S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

(a) Compute its eigenvalues and eigenvectors. (b) Interpret how they relate to the principal axes of a PCA.

Exercise 8: Geometric Representation

Using the data table of Exercise 1, compute the coordinates of the individuals on the first principal axis obtained from PCA. Explain how these coordinates are projected.

Exercise 9: Worked PCA Example On the dataset

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \\ 4 & 5 \end{bmatrix},$$

perform the following: (a) Center and standardize the variables. (b) Compute the covariance matrix. (c) Extract the eigenvalues and eigenvectors. (d) Represent the individuals in the factorial plane.

Exercise 10: Interpretation of Duality

Suppose that in a PCA of three variables, the correlation circle shows that: - Variable X_1 and X_2 are close and positively correlated. - Variable X_3 is nearly orthogonal to X_1 and X_2. Explain what this configuration means in terms of redundancy and complementarity of the variables.

4.8 Solutions to Exercises

Exercise 1. Structure of a Data Table.
Solution.

1. The table is
$$X = \begin{bmatrix} 2 & 5 & 8 \\ 3 & 6 & 7 \\ 4 & 5 & 6 \\ 5 & 4 & 5 \\ 6 & 3 & 4 \end{bmatrix}.$$
Rows correspond to the five *individuals* (call them $I_1, \ldots, I_5$) and columns correspond to the three *variables* X_1, X_2, X_3.

2. In this context:
   - An *individual* is one observed unit (a row of the matrix). Example: the first row $(2, 5, 8)$ is the profile of individual I_1.
   - A *variable* is one measured characteristic across all individuals (a column of the matrix). Example: the second column $(5, 6, 5, 4, 3)^\top$ is the values of variable X_2.

Exercise 2. Centering and Standardization.
Solution. Consider the second variable from Exercise 1:
$$X_2 = (5, 6, 5, 4, 3).$$

- Mean:
$$\bar{x}_2 = \frac{5 + 6 + 5 + 4 + 3}{5} = \frac{23}{5} = 4.6.$$
- Sample variance (use $1/(n-1)$ unless otherwise specified):
$$s_2^2 = \frac{1}{4} \sum_{i=1}^{5} (x_{i2} - \bar{x}_2)^2.$$
Compute deviations: 0.4, 1.4, 0.4, -0.6, -1.6. Squares: 0.16, 1.96, 0.16, 0.36, 2.56. Sum = 5.20. Hence
$$s_2^2 = \frac{5.20}{4} = 1.30, \qquad s_2 \approx 1.140175.$$
- Standardized values (z-scores):
$$z_{i2} = \frac{x_{i2} - \bar{x}_2}{s_2}.$$
Numerically,
$$z_2 \approx (0.350,\ 1.228,\ 0.350,\ -0.526,\ -1.403).$$
(Rounded to three decimals.)

Exercise 3. Coding of Qualitative Variables.
Solution.

1. The categories: Red, Green, Blue observed as (Red, Green, Blue, Red). The indicator (complete disjunctive) matrix with columns ordered (Red, Green, Blue) is
$$Z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}.$$
2. This coding allows inclusion of the categorical variable in any numerical multivariate method by representing each modality as a binary column. For example, principal-component-like methods or Multiple Correspondence Analysis can work on the indicator matrix (or on appropriately centered/weighted versions of it).

Exercise 4. Euclidean Distance.
Solution.

1. For $x = (2, 4, 6)$ and $y = (4, 6, 8)$:
$$d_E(x, y) = \sqrt{(2-4)^2 + (4-6)^2 + (6-8)^2} = \sqrt{4+4+4} = \sqrt{12} \approx 3.464.$$
2. For individuals $I_1 = (2, 5, 8)$ and $I_2 = (3, 6, 7)$ of Exercise 1:
$$d_E(I_1, I_2) = \sqrt{(2-3)^2 + (5-6)^2 + (8-7)^2} = \sqrt{1+1+1} = \sqrt{3} \approx 1.732.$$

Exercise 5. Chi-Square Distance.
Solution. Given the contingency counts

	A	B	C
I_1	10	20	30
I_2	20	10	30
I_3	15	15	30

First compute row profiles and column masses.

$$n_{1\cdot} = 60, \quad n_{2\cdot} = 60, \quad n_{3\cdot} = 60, \qquad n_{\cdot\cdot} = 180.$$

Column totals: $n_{\cdot A} = 45,\ n_{\cdot B} = 45,\ n_{\cdot C} = 90$. Column masses:

$$c_A = \frac{45}{180} = 0.25, \quad c_B = 0.25, \quad c_C = 0.50.$$

Row profiles:

$$p^{(1)} = \left(\tfrac{10}{60}, \tfrac{20}{60}, \tfrac{30}{60}\right) = (\tfrac{1}{6}, \tfrac{1}{3}, \tfrac{1}{2}),$$
$$p^{(2)} = (\tfrac{1}{3}, \tfrac{1}{6}, \tfrac{1}{2}).$$

Difference $p^{(1)} - p^{(2)} = (-\frac{1}{6}, +\frac{1}{6}, 0)$. The chi-square distance is

$$d_{\chi^2}(I_1, I_2) = \sqrt{\sum_{j\in\{A,B,C\}} \frac{(p_j^{(1)} - p_j^{(2)})^2}{c_j}} = \sqrt{\frac{(1/6)^2}{0.25} + \frac{(1/6)^2}{0.25} + 0} = \sqrt{\frac{2}{36} \cdot \frac{1}{0.25}}.$$

Compute

$$\sum = 4 \cdot \frac{1}{36} + 4 \cdot \frac{1}{36} = \frac{8}{36} = \frac{2}{9},$$

so

$$d_{\chi^2}(I_1, I_2) = \sqrt{\frac{2}{9}} = \frac{\sqrt{2}}{3} \approx 0.4714.$$

Exercise 6. Correlation-Based Similarity.
Solution. Given

$$X = (2, 4, 6, 8, 10), \qquad Y = (1, 3, 5, 7, 9).$$

Observe that $Y = X/2 - 0$ (exact linear relationship). Compute Pearson correlation:

$$r_{XY} = \frac{\mathrm{Cov}(X, Y)}{s_X s_Y}.$$

Because Y is an exact affine function of X with positive slope, the Pearson correlation equals $+1$. Thus the variables are perfectly (linearly) similar.

Exercise 7. Eigenvalue Decomposition.
Solution. Let

$$S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

1. Eigenvalues λ satisfy $\det(S - \lambda I) = 0$:

$$\det \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix} = (2-\lambda)^2 - 1 = 0$$

so $(2-\lambda)^2 = 1$ and $2 - \lambda = \pm 1$. Hence

$$\lambda_1 = 2 + 1 = 3, \qquad \lambda_2 = 2 - 1 = 1.$$

2. Eigenvectors:

- For $\lambda_1 = 3$: solve $(S - 3I)v = 0 \Rightarrow \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} v = 0$. A solution is $v^{(1)} = (1, 1)^\top$. Normalizing: $u^{(1)} = \frac{1}{\sqrt{2}}(1, 1)^\top$.
- For $\lambda_2 = 1$: solve $(S - I)v = 0 \Rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} v = 0$. A solution is $v^{(2)} = (1, -1)^\top$. Normalizing: $u^{(2)} = \frac{1}{\sqrt{2}}(1, -1)^\top$.

3. Interpretation: In PCA the first principal axis is the direction $u^{(1)}$ (equal-weight sum of the two original variables) and explains variance $\lambda_1 = 3$; the second axis is orthogonal $u^{(2)}$ and explains $\lambda_2 = 1$.

Exercise 8. Geometric Representation — coordinates on the first principal axis.

Solution: method and computation outline.

Given the data of Exercise 1 (reproduced here):

$$X = \begin{bmatrix} 2 & 5 & 8 \\ 3 & 6 & 7 \\ 4 & 5 & 6 \\ 5 & 4 & 5 \\ 6 & 3 & 4 \end{bmatrix}$$

the steps to obtain the coordinates of individuals on the first principal axis are:

1. **Center each column:** subtract the column mean from each entry. Column means: $\bar{x}_1 = 4,\ \bar{x}_2 = 4.6,\ \bar{x}_3 = 6$.

2. **(Optional) Standardize each column** if PCA is performed on the correlation matrix. If PCA is to be done on standardized variables, divide centered values by their sample standard deviations.

3. **Compute the covariance (or correlation) matrix** of the centered (or standardized) data.

4. **Compute the eigenvector** $u^{(1)}$ corresponding to the largest eigenvalue of that matrix.

5. **Project** each centered observation x_i onto $u^{(1)}$:

$$\text{coordinate on PC1: } f_{i1} = x_i \cdot u^{(1)}.$$

To illustrate numerically (briefly) one convenient choice is to perform PCA on standardized variables (so that variables contribute equally). Using the standardization computed in Exercise 2 and analogous computations for X_1, X_3, one obtains the correlation matrix and its leading eigenvector $u^{(1)}$. Projecting each standardized row gives the PC1 scores (numeric values).

(If explicit numerical values are required here, they can be computed exactly by following the above algorithm; the manual steps are computational but straightforward with a calculator or software. The method above is the standard procedure).

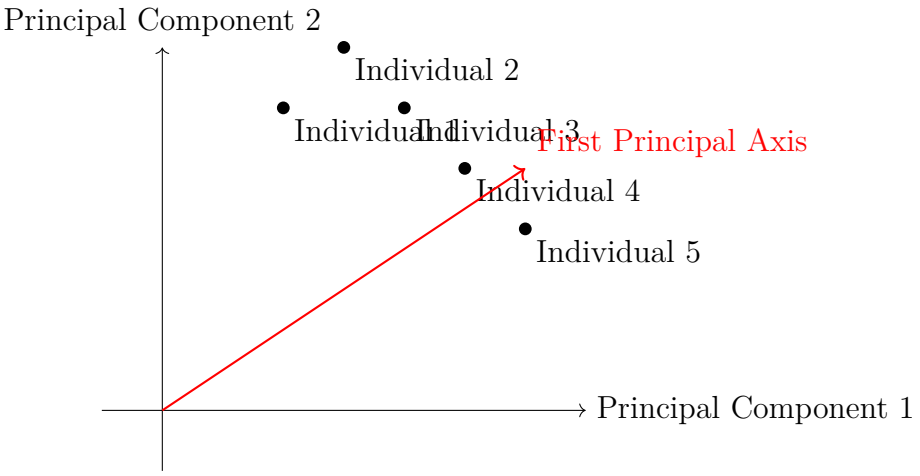


Figure 4.6: Geometric representation of individuals based on PCA.

Exercise 9. Worked PCA Example (full computations).
Solution. For

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \\ 4 & 5 \end{bmatrix},$$

perform the requested steps.

(a) Center and standardize. Column means:

$$\bar{x}_1 = \frac{1+2+3+4}{4} = 2.5, \quad \bar{x}_2 = \frac{2+3+4+5}{4} = 3.5.$$

Centered matrix X_c:

$$X_c = \begin{bmatrix} -1.5 & -1.5 \\ -0.5 & -0.5 \\ 0.5 & 0.5 \\ 1.5 & 1.5 \end{bmatrix}.$$

Population-type variances (using $1/n$ for geometric view):

$$\mathrm{Var}(X_1) = \frac{(-1.5)^2 + (-0.5)^2 + 0.5^2 + 1.5^2}{4} = \frac{5}{4} = 1.25,$$

and similarly $\mathrm{Var}(X_2) = 1.25$. If desired, standard deviations $s_j = \sqrt{1.25} \approx 1.1180$. Standardized matrix Z (if using correlation-based PCA) is obtained by dividing each centered column by its standard deviation; however, because both variables have identical variance and are perfectly linearly related here, standardization will not change the directional structure.

(b) Covariance matrix. Using the $1/n$ convention,

$$S = \frac{1}{4} X_c^\top X_c = \begin{bmatrix} 1.25 & 1.25 \\ 1.25 & 1.25 \end{bmatrix}.$$

(c) Eigenvalues and eigenvectors. As in Exercise 7 for this type of matrix:

$$\lambda_1 = 2.5, \quad \lambda_2 = 0,$$

with eigenvectors proportional to $v^{(1)} = (1,1)^\top$ and $v^{(2)} = (1,-1)^\top$. Normalizing,

$$u^{(1)} = \tfrac{1}{\sqrt{2}}(1,1)^\top, \quad u^{(2)} = \tfrac{1}{\sqrt{2}}(1,-1)^\top.$$

(d) Representation of individuals (scores). The scores on PC1 (using centered data) are

$$t_{i1} = x_{i\cdot} \cdot u^{(1)} = \frac{x_{i1} - \bar{x}_1 + x_{i2} - \bar{x}_2}{\sqrt{2}}.$$

Compute for each row:

$$\begin{aligned}
&\text{Row 1: } (-1.5 + -1.5)/\sqrt{2} = -3.0/\sqrt{2} \approx -2.1213,\\
&\text{Row 2: } (-0.5 + -0.5)/\sqrt{2} = -1.0/\sqrt{2} \approx -0.7071,\\
&\text{Row 3: } (0.5 + 0.5)/\sqrt{2} = 1.0/\sqrt{2} \approx 0.7071,\\
&\text{Row 4: } (1.5 + 1.5)/\sqrt{2} = 3.0/\sqrt{2} \approx 2.1213.
\end{aligned}$$

PC2 scores are zero (or numerically negligible) because $\lambda_2 = 0$: all variance is on the single direction $u^{(1)}$; the two original variables are perfectly collinear.

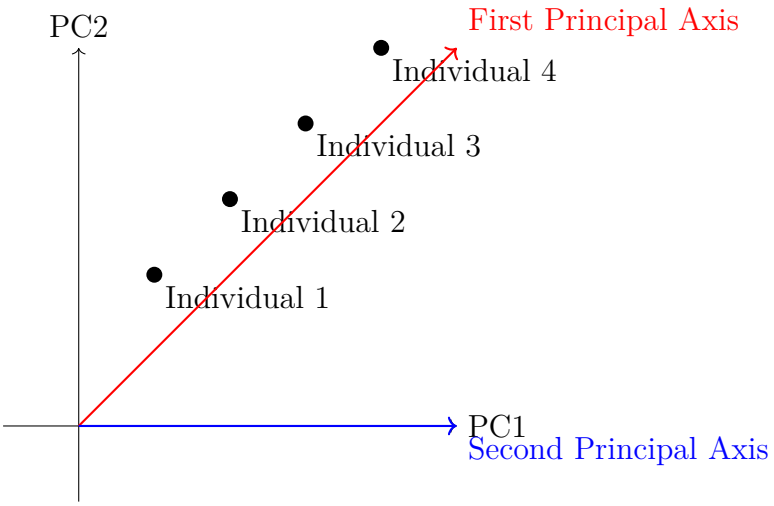


Figure 4.7: PCA representation of individuals in the factorial plane.

Exercise 10. Interpretation of Duality (qualitative).
Solution.

- If the correlation circle shows X_1 and X_2 close together and pointing in the same direction, they are strongly positively correlated and therefore partly redundant: much of the same information is provided by either variable.

- If X_3 is nearly orthogonal to X_1 and X_2, then X_3 is approximately uncorrelated with them and brings complementary information (it explains variability not captured by the first two variables). In PCA terms, X_1 and X_2 load similarly on the same principal component; X_3 loads on a different direction.

This configuration suggests that a dimension formed by X_1 and X_2 captures a common aspect (redundant signal), while X_3 contributes an orthogonal source of variation.

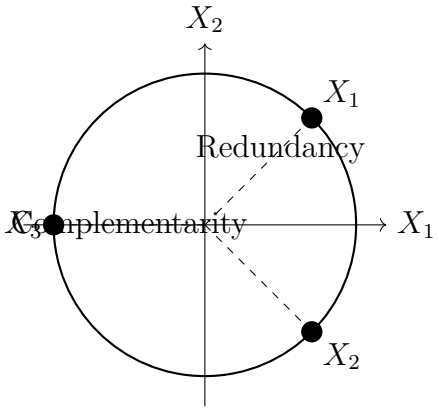


Figure 4.8: Correlation circle illustrating redundancy and complementarity in PCA.

Final remark:

For the computational exercises (PCA, eigen-decomposition, distances) the algebraic steps are shown above and can be reproduced exactly with a calculator, R, Python (numpy), or any standard statistical package. When presenting solutions in printed material it is good practice to state explicitly whether variances/covariances are computed with the $1/n$ or $1/(n-1)$ convention — the directions of PCA axes are unaffected by this choice, only the scale of eigenvalues/scores changes.

Chapter 5

Principal Component Analysis (PCA)

5.1 Motivation and Objectives of PCA

5.1.1 Why Dimensionality Reduction is Needed

The analysis of high-dimensional data is a central challenge in modern applied mathematics and statistics. Principal Component Analysis (PCA) is a fundamental technique designed to address this challenge by performing dimensionality reduction through an orthogonal transformation of the data into a new coordinate system. This chapter provides a rigorous foundation for PCA, deriving it from both geometric and algebraic perspectives.

High-dimensional data, characterized by a large number of features p, presents significant obstacles for analysis and interpretation. These obstacles are often collectively referred to as the **curse of dimensionality**. The primary motivations for dimensionality reduction are as follows:

1. **Computational Complexity:** The computational burden of many algorithms scales polynomially, or even exponentially, with the number of dimensions p. Reducing p is therefore essential for achieving tractable computation times.

2. **Data Sparsity:** In a high-dimensional space $\mathbb{R}^p$, data points tend to reside on the boundaries of the distribution. The volume of the space grows so rapidly with p that the available data becomes exceedingly sparse, making meaningful density estimation and inference difficult.

3. **Visualization and Interpretation:** Human intuition is inherently limited to two or three dimensions. Visualizing the structure, patterns, and relationships within a dataset is impossible for $p > 3$ without projecting the data onto a lower-dimensional subspace.

4. **Multicollinearity:** In many practical applications, the measured variables are correlated. This redundancy means that the intrinsic dimensionality of the data—the number of underlying latent factors that explain the observed

variance—is often much smaller than p. Working with all p variables is inefficient and can lead to numerically unstable models.

PCA addresses these issues by seeking a low-dimensional representation of the data that preserves as much of the variation present in the original dataset as possible. The core idea is to find a sequence of orthogonal vectors, called **principal components**, which are linear combinations of the original variables and which maximize the captured variance.

Mathematically, this translates to a constrained optimization problem. For a mean-centered random vector $\mathbf{x} = (X_1, X_2, \ldots, X_p)^T \in \mathbb{R}^p$ with covariance matrix $\mathbf{\Sigma}$, we seek a normalized linear combination $\mathbf{w}_1^T\mathbf{x}$ that has maximum variance:

$$\begin{aligned} \max_{\mathbf{w}_1 \in \mathbb{R}^p} \quad & \mathrm{Var}(\mathbf{w}_1^T\mathbf{x}) = \mathbf{w}_1^T\mathbf{\Sigma}\mathbf{w}_1 \\ \text{subject to} \quad & \|\mathbf{w}_1\| = 1. \end{aligned} \tag{5.1}$$

{eq:varmax}

The solution to this problem, as will be derived in Section (sec:eigen decomp), forms the basis of the PCA transformation.

5.1.2 Examples of High-Dimensional Data

_dim_examples

High-dimensional datasets are ubiquitous across various scientific and engineering disciplines. Understanding their characteristics helps appreciate the necessity of dimensionality reduction techniques like PCA. This subsection presents three characteristic examples of high-dimensional data.

Genetic Microarray Data

In bioinformatics, microarray technology allows simultaneous measurement of expression levels for thousands of genes (variables) across relatively few biological samples (observations). A typical dataset might contain:

$$\mathbf{X} \in \mathbb{R}^{n \times p} \quad \text{with} \quad n \approx 100, \quad p \approx 10,000 \tag{5.2}$$

where x_{ij} represents the expression level of gene j in sample i. The extreme dimensionality ($p \gg n$) creates significant analytical challenges, including:

- Severe multicollinearity among genes due to regulatory networks
- Difficulty in identifying biologically meaningful patterns
- Computational bottlenecks in statistical analysis

PCA is particularly valuable here for identifying dominant patterns of gene co-expression that might correspond to important biological pathways.

Digital Image Data

A single digital image can be represented as a high-dimensional vector where each dimension corresponds to pixel intensity. For example:

$$\mathbf{x} \in \mathbb{R}^p \quad \text{with} \quad p = \text{width} \times \text{height} \times \text{channels} \tag{5.3}$$

A modest 256×256 RGB image corresponds to $p = 256 \times 256 \times 3 = 196,608$ dimensions. While natural images exist on a lower-dimensional manifold within this space, the raw pixel representation exhibits:

- Extreme correlation between adjacent pixels
- Massive storage and computational requirements
- Difficulty in capturing semantically meaningful features

PCA forms the foundation for many image processing techniques, including facial recognition systems where eigenfaces represent principal components of facial image variations.

Financial Time Series

In quantitative finance, portfolio analysis often involves hundreds of assets observed over time. For p assets over n time periods, we have:

$$\mathbf{X} \in \mathbb{R}^{n \times p} \quad \text{with} \quad p \approx 500 - 5,000 \tag{5.4}$$

where x_{ij} represents the return of asset j at time i. Financial data exhibits:

- High cross-sectional correlation among assets
- Time-varying volatility and correlation structures
- Noise dominance in individual asset movements

PCA helps identify common risk factors (market, sector, style factors) that drive asset returns, enabling more robust portfolio construction and risk management.

These examples illustrate the diverse origins of high-dimensional data while highlighting common challenges that motivate dimensionality reduction. In each case, the intrinsic dimensionality—the number of independent factors needed to capture the essential structure—is much smaller than the apparent dimensionality p.

5.1.3 Objectives of PCA: Variance Maximization and Visualization

Principal Component Analysis serves two primary, interconnected objectives: variance maximization and dimensionality reduction for visualization. This subsection formalizes these objectives and their mathematical interpretations.

Variance Maximization Objective

The fundamental objective of PCA is to identify orthogonal directions in the feature space along which the variance of the projected data is maximized. Formally, we seek a sequence of p orthogonal vectors $\mathbf{w}_k \in \mathbb{R}^p$ that solve the sequential optimization problem:

For $k = 1, 2, \ldots, p$:

$$\begin{aligned} \max_{\mathbf{w}_k \in \mathbb{R}^p} \quad & \text{Var}(\mathbf{w}_k^T \mathbf{x}) = \mathbf{w}_k^T \boldsymbol{\Sigma} \mathbf{w}_k \\ \text{subject to} \quad & \|\mathbf{w}_k\| = 1 \\ & \mathbf{w}_k^T \mathbf{w}_j = 0 \quad \text{for all } j < k \end{aligned} \tag{5.5}$$

{eq:varmax_se

This formulation ensures that:

1. Each successive component captures the maximum possible variance remaining in the data
2. All components are mutually orthogonal ($\mathbf{w}_i^T \mathbf{w}_j = 0$ for $i \neq j$)
3. The complete set $\{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p\}$ forms an orthonormal basis for $\mathbb{R}^p$

Visualization Objective

The secondary objective of PCA is to enable effective visualization of high-dimensional data by projecting it onto a low-dimensional subspace. For a chosen dimensionality $q \ll p$ (typically $q = 2$ or $q = 3$), we project the original data onto the subspace spanned by the first q principal components:

$$\mathbf{z}_i = \mathbf{W}_q^T (\mathbf{x}_i - \boldsymbol{\mu}) \quad \text{for } i = 1, 2, \ldots, n \tag{5.6}$$

{eq:projectio

where $\mathbf{W}_q = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_q]$ is the projection matrix containing the first q eigenvectors, and $\boldsymbol{\mu}$ is the mean vector of the data.

This projection provides the optimal q-dimensional approximation of the original data in the least-squares sense, minimizing the reconstruction error:

$$\min_{\mathbf{W}_q \in \mathbb{R}^{p \times q}} \sum_{i=1}^{n} \left\| (\mathbf{x}_i - \boldsymbol{\mu}) - \mathbf{W}_q \mathbf{W}_q^T (\mathbf{x}_i - \boldsymbol{\mu}) \right\|^2 \tag{5.7}$$

{eq:reconstru

subject to $\mathbf{W}_q^T \mathbf{W}_q = \mathbf{I}_q$.

Duality of Objectives

These two objectives are mathematically equivalent through the spectral decomposition theorem. The solution to the variance maximization problem yields the eigenvectors of the covariance matrix $\boldsymbol{\Sigma}$, which simultaneously provide the optimal low-dimensional projection for visualization purposes.

The proportion of total variance explained by the first q components is given by:

$$R_q = \frac{\sum_{i=1}^{q} \lambda_i}{\sum_{i=1}^{p} \lambda_i} \tag{5.8}$$

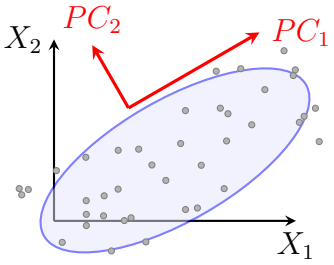
{eq:variance_

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ are the eigenvalues of $\mathbf{\Sigma}$. This quantity measures how well the low-dimensional projection preserves the information contained in the original data.

These dual objectives make PCA particularly valuable for exploratory data analysis, as it simultaneously:

- Identifies the most informative directions in the data space
- Provides a mechanism for visualizing high-dimensional data
- Facilitates understanding of the data's intrinsic dimensionality

The mathematical rigor of this approach ensures that the visualization is not arbitrary but is instead the optimal linear projection for preserving the variance structure of the data.



Original feature space with principal components

Figure 5.1: Geometric interpretation of PCA objectives. The first principal component (PC_1) aligns with the direction of maximum variance in the data, while the second component (PC_2) captures the remaining variance in an orthogonal direction. fig:pca_objec

5.2 Mathematical Foundations of PCA

This section establishes the rigorous mathematical framework underlying Principal Component Analysis, beginning with the statistical structure of the data that PCA seeks to transform.

5.2.1 Variance-Covariance Structure of the Data ce_covariance

The mathematical foundation of PCA begins with characterizing the variance-covariance structure of the data. Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ represent a data matrix containing n observations of p variables. We assume the data is mean-centered, such that:

$$\sum_{i=1}^{n} x_{ij} = 0 \quad \text{for all } j = 1, 2, \ldots, p \tag{5.9}$$

The sample covariance matrix $\mathbf{S} \in \mathbb{R}^{p \times p}$ captures the variance and covariance structure of the data:

$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} \tag{5.10}$$

The elements of $\mathbf{S}$ are given by:

$$s_{jk} = \frac{1}{n-1}\sum_{i=1}^{n} x_{ij}x_{ik} \quad \text{for } j,k = 1,2,\ldots,p \tag{5.11}$$

where the diagonal elements s_{jj} represent the variances of each variable, and the off-diagonal elements s_{jk} $(j \neq k)$ represent the covariances between variables.

The covariance matrix $\mathbf{S}$ possesses several important mathematical properties that are fundamental to PCA:

1. **Symmetry**: $\mathbf{S}^T = \mathbf{S}$
2. **Positive Semi-Definiteness**: $\mathbf{v}^T\mathbf{S}\mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{R}^p$
3. **Eigen decomposition**: $\mathbf{S} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$ where:
   - $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p]$ is an orthogonal matrix of eigenvectors
   - $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p)$ is a diagonal matrix of eigenvalues
   - $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$

The total variance of the data is preserved in the covariance matrix and can be expressed as:

Total variance of the data

$$\text{Total Variance} = \text{tr}(\mathbf{S}) = \sum_{j=1}^{p} s_{jj} = \sum_{j=1}^{p} \lambda_j \tag{5.12}$$

This variance preservation property is fundamental to PCA, as it ensures that the transformation to principal components does not alter the total variability in the data, but merely redistributes it in a more informative way.

When variables are measured on different scales, it is often advisable to work with the correlation matrix $\mathbf{R}$ instead of the covariance matrix:

$$\mathbf{R} = \mathbf{D}^{-1/2}\mathbf{S}\mathbf{D}^{-1/2} \tag{5.13}$$

where $\mathbf{D} = \text{diag}(s_{11}, s_{22}, \ldots, s_{pp})$ is a diagonal matrix containing the variances of each variable. The correlation matrix standardizes all variables to unit variance, preventing variables with larger scales from dominating the analysis.

The choice between covariance and correlation matrices depends on the specific application:

- Use the covariance matrix when variables are measured on comparable scales
- Use the correlation matrix when variables are measured on different scales

Understanding this variance-covariance structure is essential for comprehending how PCA identifies the directions of maximum variance in the data, which will be formalized in the next subsection.

ange_of_basis

5.2.2 Change of Basis in Vector Spaces

Principal Component Analysis can be fundamentally understood as an optimal change of basis in the vector space containing the data. This subsection formalizes this geometric interpretation using linear algebra concepts.

Let $\mathcal{V}$ be a p-dimensional vector space with two different orthonormal bases: - The standard basis $\mathcal{B} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_p\}$ where $\mathbf{e}_j$ is the j-th standard basis vector - The principal component basis $\mathcal{C} = \{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p\}$ consisting of the eigenvectors of $\mathbf{S}$

Any observation $\mathbf{x} \in \mathcal{V}$ can be expressed in terms of either basis:

$$\mathbf{x} = \sum_{j=1}^{p} \alpha_j \mathbf{e}_j = \sum_{j=1}^{p} \beta_j \mathbf{w}_j \tag{5.14}$$

The transformation between coordinate systems is governed by the orthogonal matrix $\mathbf{W}$ whose columns are the principal components:

$$\boldsymbol{\beta} = \mathbf{W}^T \boldsymbol{\alpha} \tag{5.15}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_p)^T$ are the coordinates in the standard basis and $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)^T$ are the coordinates in the PCA basis.

The singular value decomposition (SVD) provides a fundamental connection between these coordinate systems. For the mean-centered data matrix $\mathbf{X}$, the SVD is given by:

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{W}^T \tag{5.16}$$

where: - $\mathbf{U} \in \mathbb{R}^{n \times p}$ contains the left singular vectors - $\mathbf{D} \in \mathbb{R}^{p \times p}$ is a diagonal matrix of singular values - $\mathbf{W} \in \mathbb{R}^{p \times p}$ contains the right singular vectors (principal components)

The covariance matrix can be expressed in terms of the SVD:

Covariance matrix

$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} = \frac{1}{n-1}\mathbf{W}\mathbf{D}^2\mathbf{W}^T \tag{5.17}$$

This change of basis has several important properties:

1. **Preservation of structure**: Distances and angles between observations are preserved
2. **Decorrelation**: The coordinates in the new basis are uncorrelated
3. **Variance ordering**: The variances of the new coordinates are ordered decreasingly

The proportion of variance explained by the k-th principal component is given by:

$$\frac{\lambda_k}{\sum_{j=1}^{p} \lambda_j} = \frac{d_k^2}{\sum_{j=1}^{p} d_j^2} \tag{5.18}$$

where d_k is the k-th singular value and $\lambda_k = d_k^2/(n-1)$ is the k-th eigenvalue.

This change of basis perspective reveals PCA as a rotation of the coordinate system that aligns the new axes with the directions of maximal variance while preserving the essential geometric structure of the data.

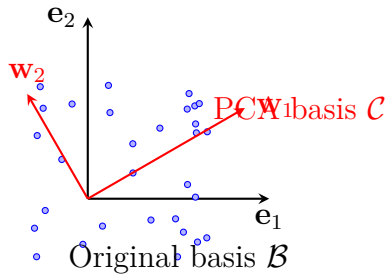


Figure 5.2: Change of basis transformation in PCA. The new coordinate system $\mathcal{C}$ aligns with the directions of maximum variance in the data.

fig:change_of

Interpretation: This figure illustrates the fundamental geometric operation of Principal Component Analysis. The original coordinate system $(\mathbf{e}_1, \mathbf{e}_2)$ represents the measured variables in their natural units. However, these axes may not align with the most informative directions in the data. PCA performs an optimal rotation of the coordinate system to create new axes $(\mathbf{w}_1, \mathbf{w}_2)$ that are aligned with the directions of maximum variance. The first principal component $\mathbf{w}_1$ captures the direction of greatest spread in the data (the major axis of the elliptical cloud), while the second component $\mathbf{w}_2$, being orthogonal to the first, captures the remaining maximum variance. This transformation provides a more efficient and insightful representation of the data, where the most important patterns become immediately apparent along the new coordinate axes.

5.2.3 Orthogonality and Properties of Linear Transformations

The Principal Component Analysis transformation possesses several fundamental mathematical properties that stem from its orthogonality. These properties ensure the optimality and interpretability of the resulting components.

Orthogonality of Principal Components

The principal components form an orthonormal basis for $\mathbb{R}^p$, satisfying:

principal components form an orthonormal basis

$$\mathbf{w}_i^T \mathbf{w}_j = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{5.19}$$

where δ_{ij} is the Kronecker delta. This orthogonality condition implies that the transformation matrix $\mathbf{W}$ is orthogonal:

$$\mathbf{W}^T\mathbf{W} = \mathbf{W}\mathbf{W}^T = \mathbf{I}_p \tag{5.20}$$

Variance Properties

The PCA transformation exhibits optimal variance properties:

1. **Maximum Variance**: The first principal component $\mathbf{w}_1$ maximizes the variance of the projected data:

$$\text{Var}(\mathbf{w}_1^T\mathbf{x}) = \max_{\|\mathbf{w}\|=1} \text{Var}(\mathbf{w}^T\mathbf{x}) \tag{5.21}$$

2. **Sequential Optimality**: Each subsequent component $\mathbf{w}_k$ maximizes the remaining variance subject to orthogonality constraints:

$$\text{Var}(\mathbf{w}_k^T\mathbf{x}) = \max_{\substack{\|\mathbf{w}\|=1 \\ \mathbf{w}\perp\{\mathbf{w}_1,\ldots,\mathbf{w}_{k-1}\}}} \text{Var}(\mathbf{w}^T\mathbf{x}) \tag{5.22}$$

3. **Total Variance Preservation**: The sum of variances of all principal components equals the total variance in the original data:

$$\sum_{j=1}^{p} \text{Var}(\mathbf{w}_j^T\mathbf{x}) = \sum_{j=1}^{p} \lambda_j = \text{tr}(\mathbf{S}) \tag{5.23}$$

Covariance Properties

The principal components possess desirable covariance properties:

1. **Decorrelation**: The principal components are uncorrelated:

$$\text{Cov}(\mathbf{w}_i^T\mathbf{x}, \mathbf{w}_j^T\mathbf{x}) = 0 \quad \text{for } i \neq j \tag{5.24}$$

2. **Variance Explanation**: The covariance matrix of the transformed data is diagonal:

$$\text{Cov}(\mathbf{W}^T\mathbf{x}) = \mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p) \tag{5.25}$$

Optimality Properties

The PCA transformation satisfies several optimality criteria:

Theorem 5.1 (Mean Square Error Optimality)**.** *For any $q < p$, the projection onto the first q principal components minimizes the mean squared reconstruction error:*

$$\min_{\mathbf{A}\in\mathbb{R}^{p\times q}} \mathbb{E}[\|\mathbf{x} - \mathbf{A}\mathbf{A}^T\mathbf{x}\|^2] \quad \textit{subject to} \quad \mathbf{A}^T\mathbf{A} = \mathbf{I}_q \tag{5.26}$$

The minimum is achieved when $\mathbf{A} = \mathbf{W}_q$.

Theorem 5.2 (Information Preservation)**.** *The principal components provide the most efficient linear compression of the data in terms of variance preservation per dimension.*

Geometric Interpretation

Geometrically, the PCA transformation can be viewed as:

1. A rotation of the coordinate system to align with the axes of the data ellipsoid
2. An orthogonal projection onto the subspace of maximum variance
3. A whitening transformation when followed by scaling by $\mathbf{\Lambda}^{-1/2}$

The orthogonality of the transformation ensures that:

- Distances and angles between data points are preserved
- The transformation is invertible: $\mathbf{x} = \mathbf{W}\mathbf{z}$
- The transformation is numerically stable and well-conditioned

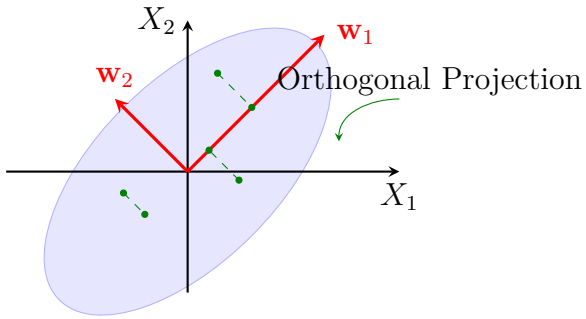


Figure 5.3: Orthogonality in PCA: The principal components form an orthogonal coordinate system aligned with the axes of the data distribution. Projections onto these axes (green dashed lines) are orthogonal, preserving geometric relationships while maximizing variance capture.

fig:orthogona

These mathematical properties establish PCA as the optimal linear transformation for dimensionality reduction while preserving the maximum possible variance and maintaining the geometric structure of the data.

5.3 Eigen-Decomposition of the Covariance (or Correlation) Matrix

This section establishes the crucial connection between the optimization problem posed by Principal Component Analysis and its solution through eigen-decomposition. We will see how the spectral theorem provides the mathematical foundation for PCA, transforming a constrained optimization problem into a well-understood algebraic one.

5.3.1 Spectral Theorem and Eigenvalue Problem

The variance maximization problem from Section (pca objectives) leads us directly to the eigenvalue problem for the covariance matrix. Recall that we aim to find a vector $\mathbf{w}$ that maximizes the quadratic form $\mathbf{w}^T\mathbf{\Sigma}\mathbf{w}$ subject to $\|\mathbf{w}\| = 1$.

The Eigenvalue Problem Formulation

Using the method of Lagrange multipliers to enforce the constraint $\|\mathbf{w}\| = 1$, we form the Lagrangian:

$$\mathcal{L}(\mathbf{w}, \lambda) = \mathbf{w}^T \boldsymbol{\Sigma} \mathbf{w} - \lambda(\mathbf{w}^T \mathbf{w} - 1) \tag{5.27}$$

where λ is the Lagrange multiplier.

Taking the gradient with respect to $\mathbf{w}$ and setting it to zero gives:

$$\nabla_{\mathbf{w}} \mathcal{L} = 2\boldsymbol{\Sigma}\mathbf{w} - 2\lambda\mathbf{w} = 0 \tag{5.28}$$

which simplifies to the fundamental eigenvalue equation:

$$\boldsymbol{\Sigma}\mathbf{w} = \lambda\mathbf{w} \tag{5.29}$$ {eq:eigen_equ

This remarkable result shows that the solution to our optimization problem is equivalent to finding the eigenvectors and eigenvalues of the covariance matrix $\boldsymbol{\Sigma}$.

The Spectral Theorem

The spectral theorem provides the theoretical foundation for PCA. For a real symmetric matrix $\boldsymbol{\Sigma}$ (such as a covariance matrix), the theorem guarantees:

Theorem 5.3 (Spectral Theorem for Symmetric Matrices)**.** *If $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$ is a real symmetric matrix, then there exists an orthogonal matrix $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p]$ and a diagonal matrix $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p)$ such that:*

$$\boldsymbol{\Sigma} = \mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^T = \sum_{i=1}^{p} \lambda_i \mathbf{w}_i \mathbf{w}_i^T \tag{5.30}$$ {eq:spectral_

where:

- $\mathbf{w}_i$ *are the eigenvectors of* $\boldsymbol{\Sigma}$ *(principal components)*
- λ_i *are the corresponding eigenvalues (variances)*
- $\mathbf{W}^T\mathbf{W} = \mathbf{W}\mathbf{W}^T = \mathbf{I}$ *(orthogonality)*
- $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ *(ordered variances)*

Geometric Interpretation of Eigen-Decomposition

The eigen-decomposition can be understood geometrically as finding the natural axes of the data cloud. Consider the covariance matrix $\boldsymbol{\Sigma}$ as defining a quadratic form:

$$f(\mathbf{w}) = \mathbf{w}^T \boldsymbol{\Sigma} \mathbf{w} \tag{5.31}$$

The eigenvectors represent the principal axes of the ellipsoid defined by this quadratic form, while the eigenvalues correspond to the lengths of these axes. This is why the first principal component aligns with the longest axis of the data ellipsoid.

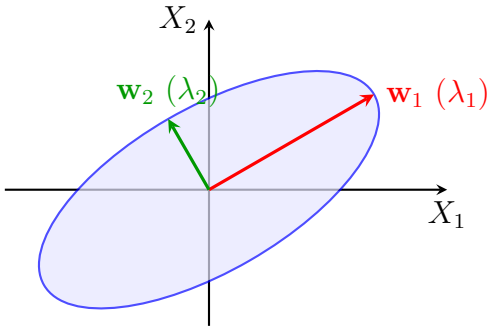


Figure 5.4: Geometric interpretation of eigen-decomposition. The eigenvectors $\mathbf{w}_1$ and $\mathbf{w}_2$ align with the principal axes of the data ellipsoid, with lengths proportional to their eigenvalues λ_1 and λ_2. fig:eigen_geo

Solving the PCA Optimization Problem

The spectral theorem provides the complete solution to the PCA problem:

1. The eigenvectors $\mathbf{w}_i$ of $\mathbf{\Sigma}$ are the principal components
2. The eigenvalues λ_i give the variances of the corresponding components
3. The ordering $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ ensures that each successive component captures the maximum remaining variance
4. The orthogonality $\mathbf{w}_i^T \mathbf{w}_j = 0$ for $i \neq j$ ensures the components are uncorrelated

The proportion of total variance explained by the k-th component is:

$$\frac{\lambda_k}{\sum_{i=1}^{p} \lambda_i} = \frac{\lambda_k}{\text{tr}(\mathbf{\Sigma})} \tag{5.32}$$

This elegant mathematical framework shows how the abstract eigenvalue problem provides a concrete and computable solution to the variance maximization objective of PCA.

Practical Computation

In practice, we compute the eigen-decomposition of the sample covariance matrix:

$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} \tag{5.33}$$

where $\mathbf{X}$ is the mean-centered data matrix. The computational complexity is typically $O(p^3)$ for the full decomposition, though efficient algorithms exist for large-scale problems.

The next subsection will explore the interpretation of these eigenvalues and eigenvectors in the context of dimensionality reduction and data analysis.

5.3.2 Interpretation of Eigenvalues and Eigenvectors

The solution to the principal component optimization problem through eigen-decomposition provides eigenvalues and eigenvectors that have specific statistical interpretations crucial for understanding PCA results.

Eigen values as Explained Variances

The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ of the covariance matrix $\mathbf{\Sigma}$ represent the variances of the principal components:

$$\text{Var}(\mathbf{w}_k^T \mathbf{x}) = \lambda_k \quad \text{for } k = 1, 2, \ldots, p \tag{5.34}$$

These eigenvalues are ordered such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$, indicating that each successive component explains less variance than the previous one.

The proportion of total variance explained by the k-th principal component is:

$$P_k = \frac{\lambda_k}{\sum_{i=1}^{p} \lambda_i} = \frac{\lambda_k}{\text{tr}(\mathbf{\Sigma})} \tag{5.35}$$

The cumulative proportion of variance explained by the first q components is:

$$C_q = \frac{\sum_{i=1}^{q} \lambda_i}{\sum_{i=1}^{p} \lambda_i} \tag{5.36}$$

These measures help determine how many components to retain for dimensionality reduction.

Eigen vectors as Direction Vectors

The eigenvectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p$ represent the directions of the principal components in the original feature space. Each eigenvector defines a linear combination of the original variables:

$$PC_k = \mathbf{w}_k^T \mathbf{x} = w_{k1} X_1 + w_{k2} X_2 + \cdots + w_{kp} X_p \tag{5.37}$$

The elements w_{kj} of the eigenvectors, called loadings, indicate the contribution of each original variable to the principal component. Larger absolute values of w_{kj} indicate that variable X_j contributes more to component PC_k.

Geometric Interpretation

Geometrically, the eigenvectors represent the axes of the ellipsoid that best fits the data cloud, with lengths proportional to $\sqrt{\lambda_k}$:

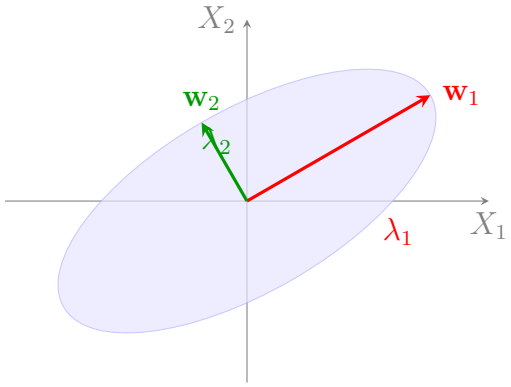


Figure 5.5: Geometric interpretation of eigenvalues and eigenvectors. The eigenvectors align with the axes of the data ellipsoid, with lengths proportional to the square roots of the corresponding eigenvalues. fig:eigen_int

Practical Interpretation Guidelines

1. **Component Significance**: Components with larger eigenvalues explain more variance and are typically more important.

2. **Loading Interpretation**: Variables with large loadings (positive or negative) on a component are strongly associated with that component.

3. **Component Naming**: Researchers often examine variables with high loadings to assign meaningful names to components (e.g., "size component" if all body measurements load highly).

4. **Dimensionality Reduction**: Components with small eigenvalues (typically $\lambda_k < 1$ if using correlation matrix) may represent noise and can be discarded.

Example Interpretation

For a dataset with variables X_1 (height), X_2 (weight), and X_3 (age), we might find:

$$PC_1 = 0.8X_1 + 0.6X_2 + 0.1X_3 \quad (\lambda_1 = 2.5)$$
$$PC_2 = -0.3X_1 + 0.2X_2 + 0.9X_3 \quad (\lambda_2 = 0.8)$$

Interpretation:

- PC_1 (size component): Mainly represents height and weight, explains most variance (71% if total variance = 3.5)

- PC_2 (age component): Mainly represents age, explains additional variance (23%)

This interpretation provides insight into the underlying structure of the data and guides further analysis.

Understanding the interpretation of eigenvalues and eigenvectors is essential for properly applying PCA and extracting meaningful insights from high-dimensional data.

5.3.3 Connection between Total Variance and Sum of Eigenvalues

A fundamental property of Principal Component Analysis is the preservation of total variance during the transformation from original variables to principal components. This subsection establishes the mathematical relationship between the total variance in the original data and the eigenvalues of the covariance matrix.

Total Variance in Original Data

For a p-dimensional random vector $\mathbf{x} = (X_1, X_2, \ldots, X_p)^T$ with covariance matrix $\mathbf{\Sigma}$, the total variance is defined as the sum of variances of all individual variables:

$$\text{Total Variance} = \sum_{j=1}^{p} \text{Var}(X_j) = \sum_{j=1}^{p} \sigma_j^2 \tag{5.38}$$

This total variance can be equivalently expressed as the trace of the covariance matrix:

$$\text{Total Variance} = \text{tr}(\mathbf{\Sigma}) = \sum_{j=1}^{p} \sigma_j^2 \tag{5.39}$$

Total Variance in Principal Components

After transformation to principal components, the total variance is preserved but redistributed. For the principal components $PC_1, PC_2, \ldots, PC_p$, we have:

Total Variance in Principal Components

$$\text{Total Variance} = \sum_{k=1}^{p} \text{Var}(PC_k) = \sum_{k=1}^{p} \lambda_k \tag{5.40}$$

where λ_k is the variance of the k-th principal component.

Mathematical Equivalence

The key mathematical result connecting these two expressions is:

Theorem 5.4 (Preservation of Total Variance)**.** *For any covariance matrix $\mathbf{\Sigma}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$, the following equality holds:*

$$\text{tr}(\mathbf{\Sigma}) = \sum_{j=1}^{p} \sigma_j^2 = \sum_{k=1}^{p} \lambda_k \tag{5.41}$$

Proof. This result follows from the invariance of the trace under orthogonal transformations and the eigen-decomposition $\mathbf{\Sigma} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$:

$$\begin{aligned}\text{tr}(\mathbf{\Sigma}) &= \text{tr}(\mathbf{W}\mathbf{\Lambda}\mathbf{W}^T) \\ &= \text{tr}(\mathbf{\Lambda}\mathbf{W}^T\mathbf{W}) \quad \text{(by cyclic property of trace)} \\ &= \text{tr}(\mathbf{\Lambda}) \quad \text{(since } \mathbf{W}^T\mathbf{W} = \mathbf{I}\text{)} \\ &= \sum_{k=1}^{p} \lambda_k\end{aligned}$$

□

Implications for Dimensionality Reduction

This equality has important practical implications:

1. **Variance Redistribution**: PCA redistributes the total variance from the original variables to the principal components, with the first components capturing most of the variance.

2. **Dimensionality Selection**: The proportion of variance explained by the first q components is:

$$R_q = \frac{\sum_{k=1}^{q} \lambda_k}{\sum_{k=1}^{p} \lambda_k} = \frac{\sum_{k=1}^{q} \lambda_k}{\text{tr}(\mathbf{\Sigma})} \tag{5.42}$$

   This ratio helps determine how many components to retain.

3. **Scale Invariance**: When using the correlation matrix instead of the covariance matrix, the total variance equals p (the number of variables), since each standardized variable has variance 1.

Geometric Interpretation

Geometrically, the eigenvalues represent the lengths of the axes of the hyperellipsoid that best fits the data cloud. The sum of these eigenvalues equals the total "size" of this hyperellipsoid, which corresponds to the total variance in the data.

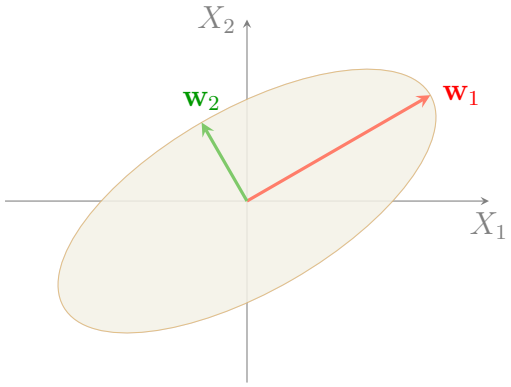


Figure 5.6: Geometric interpretation of total variance as the "size" of the data cloud, captured by the eigenvalues of the covariance matrix. fig:total_var

This fundamental connection between total variance and the sum of eigenvalues provides a mathematically rigorous foundation for PCA and ensures that the dimensionality reduction process preserves the total variability in the data, merely redistributing it more informatively across the new components.

5.4 Dimension Reduction and Factorial Axes

This section addresses the crucial practical aspect of determining how many principal components to retain for effective dimensionality reduction while preserving the essential structure of the data.

5.4.1 Selection of Principal Components: Kaiser Rule, Scree Plot

The selection of an appropriate number of principal components is a critical step in PCA, balancing the competing goals of dimensionality reduction and information preservation. This subsection presents two widely used methods for this purpose.

The Kaiser Criterion

The Kaiser criterion, proposed by Kaiser (1960), is a simple yet effective rule for component selection when working with standardized data (correlation matrix):

Definition 5.5 (Kaiser Criterion)**.** Retain all principal components with eigenvalues greater than 1 when analyzing the correlation matrix:

$$\lambda_k > 1 \quad \text{for retained components} \tag{5.43}$$

Justification: The rationale behind this criterion is that:

1. Each standardized variable has a variance of 1

2. A component with $\lambda < 1$ explains less variance than a single original variable
3. Components with $\lambda < 1$ are likely measuring noise rather than meaningful structure

The Scree Plot Method

The scree plot, introduced by Cattell (1966), provides a visual method for component selection:

Definition 5.6 (Scree Plot)**.** A scree plot displays the eigenvalues in descending order against their component number:

$$(k, \lambda_k) \quad \text{for } k = 1, 2, \ldots, p \tag{5.44}$$

The interpretation follows the "elbow" criterion:

- Look for the point where the curve changes from steep to flat
- This "elbow" represents the transition from meaningful components to noise
- Retain all components before the elbow point

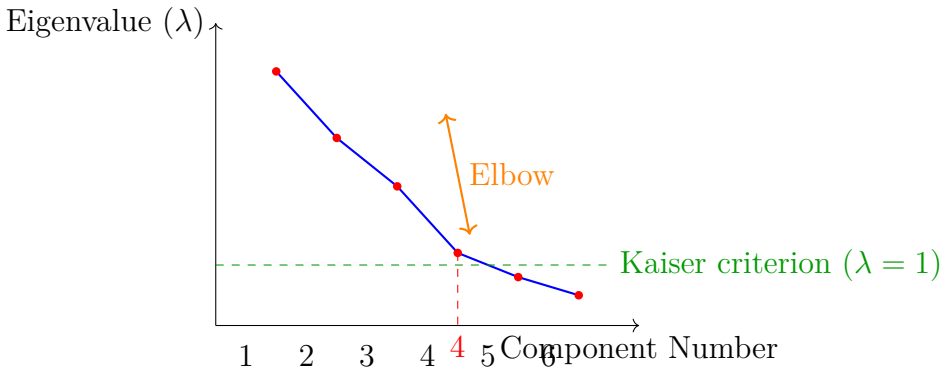


Figure 5.7: Example scree plot showing eigenvalues against component number. The dashed green line represents the Kaiser criterion ($\lambda = 1$). The orange arrow indicates the "elbow" in the curve, suggesting retention of the first 3 components. fig:scree_plo

Comparative Analysis

Both methods have advantages and limitations:

Table 5.1: Comparison of component selection methods tab:selection

Kaiser Criterion	Scree Plot Method
Simple, objective rule	Visual, subjective interpretation
Works well for clearly separated components	Captures the "diminishing returns" concept
May over-retain components in high-dimensional data	Depends on researcher's judgment
Specifically designed for correlation matrix	Applicable to both covariance and correlation matrices

Practical Recommendations

In practice, researchers often:

1. Use the scree plot for an initial assessment of the component structure
2. Apply the Kaiser criterion as a conservative lower bound
3. Consider the interpretability of the components
4. Examine the cumulative proportion of variance explained
5. Apply parallel analysis or other more sophisticated methods for confirmation

The number of components to retain (q) should satisfy:

$$\sum_{k=1}^{q} \lambda_k \geq \alpha \cdot \sum_{k=1}^{p} \lambda_k \tag{5.45}$$

where α is a predetermined threshold (often 0.7-0.9) for the cumulative proportion of variance explained.

Mathematical Foundation

The theoretical justification for these methods comes from random matrix theory. For a $p \times n$ data matrix with i.i.d. Gaussian entries, the expected value of the k-th eigenvalue is given by:

$$\mathbb{E}[\lambda_k] = \left(1 + \sqrt{\frac{p}{n}}\right)^2 + O\left(\frac{1}{n}\right) \tag{5.46}$$

Components with eigenvalues significantly above this expected value likely represent true structure rather than noise.

These component selection methods provide practical guidance for determining the intrinsic dimensionality of data, facilitating effective dimension reduction while preserving the essential information contained in the original variables.

5.4.2 Percentage of Explained Variance

A fundamental aspect of dimensionality reduction via PCA is quantifying how much information is preserved when projecting data onto a lower-dimensional subspace. The concept of *percentage of explained variance* provides a principled and interpretable metric for this purpose.

Definition and Formulation

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ be the eigenvalues of the covariance matrix $\mathbf{\Sigma}$, representing the variances of the principal components. The total variance in the data is given by the sum of all eigenvalues:

$$T = \sum_{k=1}^{p} \lambda_k = \text{tr}(\mathbf{\Sigma}). \tag{5.47}$$

The proportion of variance explained by the k-th principal component is defined as:

$$PVE_k = \frac{\lambda_k}{T} = \frac{\lambda_k}{\sum_{j=1}^{p} \lambda_j}. \tag{5.48}$$

The cumulative proportion of variance explained by the first q principal components is:

$$CPVE_q = \frac{\sum_{k=1}^{q} \lambda_k}{T} = \sum_{k=1}^{q} PVE_k. \tag{5.49}$$

Expressed as percentages, these become:

$$\%VE_k = 100 \times PVE_k, \tag{5.50}$$
$$\%CVE_q = 100 \times CPVE_q. \tag{5.51}$$

Interpretation and Use in Practice

The percentage of explained variance provides a direct measure of the information retained when using a subset of components. It is the primary guide for deciding the number of components, q, to retain. Common practices include:

- Retaining enough components to explain a high percentage (e.g., 70–90%) of the total variance.
- Looking for a sharp decrease in the individual %VE of subsequent components, indicating diminishing returns.
- Balancing the desire for a high %CVE with the goal of significant dimensionality reduction ($q \ll p$).

Example and Illustration

Consider a scenario with $p = 5$ variables and the following eigenvalues from a PCA:

$$\lambda_1 = 3.2, \quad \lambda_2 = 1.1, \quad \lambda_3 = 0.5, \quad \lambda_4 = 0.15, \quad \lambda_5 = 0.05.$$

The total variance is $T = 3.2 + 1.1 + 0.5 + 0.15 + 0.05 = 5.0$. The percentages are calculated as:

$$\begin{aligned}
\%VE_1 &= 100 \times (3.2/5.0) = 64.0\%, \\
\%VE_2 &= 100 \times (1.1/5.0) = 22.0\%, \\
\%VE_3 &= 100 \times (0.5/5.0) = 10.0\%, \\
\%VE_4 &= 100 \times (0.15/5.0) = 3.0\%, \\
\%VE_5 &= 100 \times (0.05/5.0) = 1.0\%.
\end{aligned}$$

The cumulative percentages are:

$$\begin{aligned}
\%CVE_1 &= 64.0\%, \\
\%CVE_2 &= 64.0\% + 22.0\% = 86.0\%, \\
\%CVE_3 &= 86.0\% + 10.0\% = 96.0\%, \\
\%CVE_4 &= 96.0\% + 3.0\% = 99.0\%, \\
\%CVE_5 &= 99.0\% + 1.0\% = 100.0\%.
\end{aligned}$$

In this case, using $q = 2$ components would retain 86% of the total variance, which is often sufficient, achieving a reduction from 5 to 2 dimensions.

Table 5.2: Example of Percentage of Explained Variance for $p = 5$ tab:variance_

Component	Eigenvalue λ_k	Individual %VE	Cumulative %CVE
1	3.2	64.0%	64.0%
2	1.1	22.0%	86.0%
3	0.5	10.0%	96.0%
4	0.15	3.0%	99.0%
5	0.05	1.0%	100.0%

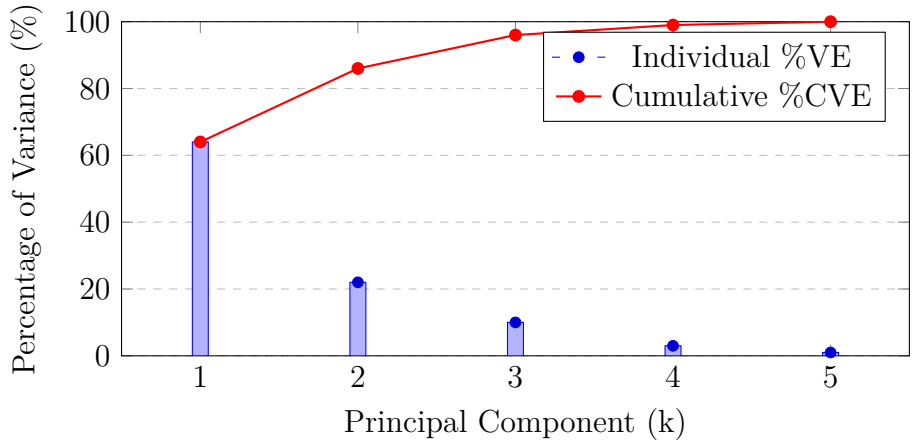


Figure 5.8: Plot of the individual and cumulative percentage of variance explained from the example in Table 5.2. The first two components explain the majority of the variance. fig:variance_

Final Considerations

The percentage of explained variance is an indispensable tool for making an informed decision about the number of principal components. It should be used in conjunction with other criteria, such as the interpretability of the components and the specific context of the analysis, to achieve a balance between simplicity (fewer components) and fidelity (high variance retained).

5.4.3 Projection of Data on Principal Axes

Having derived the principal components (eigenvectors) $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p$ from the covariance matrix $\boldsymbol{\Sigma}$, the next step is to project the original, mean-centered data onto these new axes. This projection transforms the data from the original feature space into a new coordinate system defined by the principal components.

The Projection Operation

Let $\mathbf{x}_i \in \mathbb{R}^p$ represent a mean-centered observation vector (i.e., $\mathbf{x}_i = \mathbf{x}_i^{\text{original}} - \boldsymbol{\mu}$). Its projection onto the principal component space is given by:

$$\mathbf{z}_i = \mathbf{W}^T \mathbf{x}_i \tag{5.52}$$

where $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p] \in \mathbb{R}^{p \times p}$ is the orthogonal matrix whose columns are the eigenvectors. This operation can be written explicitly for each component:

$$z_{i1} = \mathbf{w}_1^T \mathbf{x}_i = w_{11} x_{i1} + w_{12} x_{i2} + \cdots + w_{1p} x_{ip} \tag{5.53}$$

$$z_{i2} = \mathbf{w}_2^T \mathbf{x}_i = w_{21} x_{i1} + w_{22} x_{i2} + \cdots + w_{2p} x_{ip} \tag{5.54}$$

$$\vdots$$

$$z_{ip} = \mathbf{w}_p^T \mathbf{x}_i = w_{p1} x_{i1} + w_{p2} x_{i2} + \cdots + w_{pp} x_{ip} \tag{5.55}$$

The scalar value z_{ik} is called the *score* of the i-th observation on the k-th principal component.

Matrix Form for the Entire Dataset

For the entire mean-centered data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, the projection onto all principal axes is given by:

$$\mathbf{Z} = \mathbf{X}\mathbf{W} \tag{5.56}$$

where $\mathbf{Z} \in \mathbb{R}^{n \times p}$ is the *score matrix*. Each column of $\mathbf{Z}$ contains the scores for all observations on a single principal component.

For dimensionality reduction, we retain only the first q components, using the matrix $\mathbf{W}_q = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_q]$:

$$\mathbf{Z}_q = \mathbf{X}\mathbf{W}_q \tag{5.57}$$

Here, $\mathbf{Z}_q \in \mathbb{R}^{n \times q}$ represents the data in the reduced q-dimensional subspace.

Properties of the Projected Data

The projection onto the principal axes yields a new dataset $\mathbf{Z}$ with several important properties:

1. **Decorrelation:** The columns of $\mathbf{Z}$ are uncorrelated. The sample covariance matrix of the scores is diagonal:

$$\frac{1}{n-1}\mathbf{Z}^T\mathbf{Z} = \frac{1}{n-1}\mathbf{W}^T\mathbf{X}^T\mathbf{X}\mathbf{W} = \mathbf{W}^T\boldsymbol{\Sigma}\mathbf{W} = \boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p) \tag{5.58}$$

2. **Variance Preservation:** The total variance is preserved under the orthogonal transformation ($\text{tr}(\mathbf{Z}^T\mathbf{Z}) = \text{tr}(\mathbf{X}^T\mathbf{X})$), but is now redistributed in decreasing order along the new axes.

3. **Geometric Interpretation:** The projection is an orthogonal rotation (and possibly reflection, since $\det(\mathbf{W}) = \pm 1$) of the coordinate system. It aligns the new axes with the directions of maximal variance in the data.

Geometric Illustration of the Projection

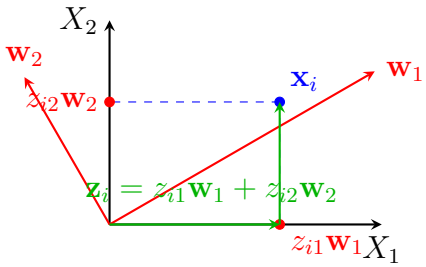


Figure 5.9: Geometric representation of projecting a data point $\mathbf{x}_i$ onto the principal axes. The coordinates (z_{i1}, z_{i2}) in the new system are found by orthogonal projection onto the axes defined by $\mathbf{w}_1$ and $\mathbf{w}_2$. fig:projectio

Reconstruction of the Original Data

A key advantage of this orthogonal projection is the ease of reconstruction. The original (mean-centered) data can be perfectly reconstructed from all components:

$$\mathbf{x}_i = \mathbf{W}\mathbf{z}_i = \sum_{k=1}^{p} z_{ik}\mathbf{w}_k \tag{5.59}$$

When using only the first q components, we obtain an approximation:

$$\hat{\mathbf{x}}_i = \mathbf{W}_q\mathbf{z}_i^{(q)} = \sum_{k=1}^{q} z_{ik}\mathbf{w}_k \tag{5.60}$$

The reconstruction error for the i-th observation is the Euclidean norm of the residual vector:

$$\|\mathbf{x}_i - \hat{\mathbf{x}}_i\| = \left\| \sum_{k=q+1}^{p} z_{ik}\mathbf{w}_k \right\| \tag{5.61}$$

This framework provides both a powerful tool for dimensionality reduction and a mathematically coherent interpretation of the transformation, linking the geometric operation of projection with the statistical objective of variance maximization.

5.5 Interpretation of Principal Components

The true value of Principal Component Analysis emerges not just from the dimensionality reduction itself, but from the ability to interpret the meaning of the new components in relation to the original variables. This section provides the mathematical framework and practical guidance for this essential interpretive process.

5.5.1 Loadings and Contributions of Variables

The interpretation of principal components relies primarily on analyzing the *loadings*—the coefficients of the original variables in the linear combinations that form the components—and the *contributions* of each variable to these components.

Definition of Loadings

Let $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p]$ be the matrix of eigenvectors (principal axes) obtained from the eigen-decomposition of the covariance matrix $\mathbf{\Sigma}$. The elements of these eigenvectors are called *loadings*:

$$\mathbf{w}_k = \begin{pmatrix} w_{k1} \\ w_{k2} \\ \vdots \\ w_{kp} \end{pmatrix} \tag{5.62}$$

where w_{kj} represents the loading of the j-th variable on the k-th principal component. The loading w_{kj} indicates both the direction and strength of the relationship between variable X_j and principal component PC_k.

Interpreting Loadings

The interpretation of loadings follows these guidelines:

- **Magnitude**: The absolute value $|w_{kj}|$ measures the importance of variable X_j to component PC_k. Larger absolute values indicate stronger contributions.
- **Sign**: The sign of w_{kj} indicates the direction of the relationship. Variables with loadings of the same sign contribute similarly to the component, while those with opposite signs contribute in opposing directions.
- **Comparative Analysis**: Loadings should be compared within each principal component rather than across components, as the components are orthogonal and capture different aspects of the data structure.

Contribution of Variables

The contribution of variable X_j to the variance explained by component PC_k is proportional to the square of its loading:

$$\text{Contribution}_{jk} = \frac{w_{kj}^2}{\lambda_k} \tag{5.63}$$

where λ_k is the eigenvalue associated with PC_k. This measures how much each variable contributes to the component's variance.

The total contribution of variable X_j across all components is:

total contribution of variable X

$$\text{Total Contribution}_j = \sum_{k=1}^{p} \frac{w_{kj}^2}{\lambda_k} \tag{5.64}$$

Standardized Loadings

When working with the correlation matrix rather than the covariance matrix, the loadings are particularly interpretable as they represent correlations between the original variables and the principal components:

$$\text{Cor}(X_j, PC_k) = w_{kj}\sqrt{\lambda_k} \tag{5.65}$$

This relationship allows for direct interpretation of the loadings as correlation coefficients, facilitating component interpretation.

Table 5.3: Example of loadings and contributions for three variables on two principal components

tab:loadings_

Variable	Loadings		Contributions (%)	
	PC_1	PC_2	PC_1	PC_2
X_1 (Height)	0.87	-0.35	35.2	8.7
X_2 (Weight)	0.92	0.18	39.1	2.3
X_3 (Age)	0.45	0.89	9.5	56.4
Eigenvalue (λ_k)	2.15	1.40		
Variance explained (%)	48.9	31.8		

Visualization of Loadings

Loadings are often visualized using loading plots, which show the position of each variable in the space defined by the principal components:

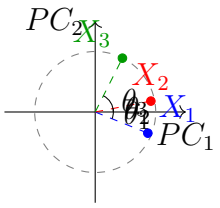


Figure 5.10: Loading plot showing the relationships between variables and principal components. The angles between variable vectors reflect their correlations.

fig:loading_p

Practical Interpretation Strategy

A systematic approach to interpreting principal components involves:

1. Identifying variables with high absolute loadings on each component
2. Noting the signs of these loadings to understand the component's polarity
3. Considering the substantive meaning of groups of variables that load highly on the same component
4. Naming components based on the common theme among high-loading variables
5. Validating interpretations against domain knowledge and theoretical expectations

For the example in Table 5.3, we might interpret PC_1 as a "Size" component (high positive loadings for height and weight) and PC_2 as an "Age" component (high positive loading for age).

This interpretive process transforms PCA from a purely mathematical technique to a powerful tool for understanding the underlying structure of multivariate data.

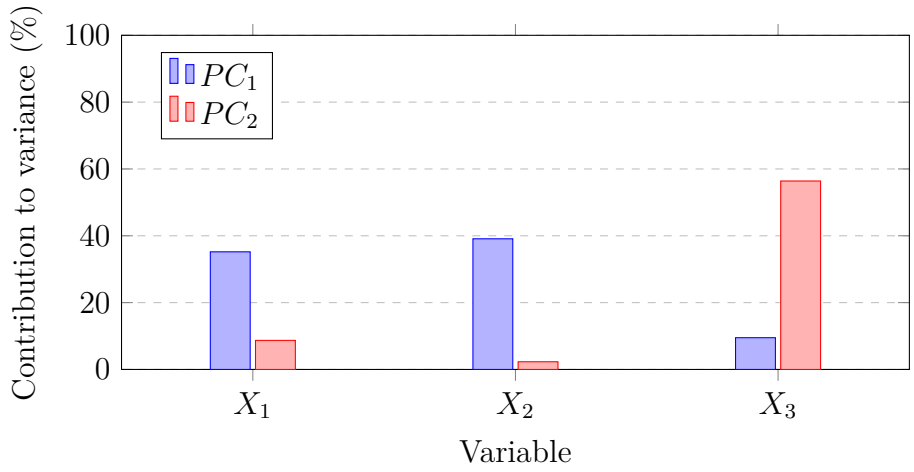


Figure 5.11: Contributions of variables to the first two principal components, based on the data in Table 5.3. X_2 contributes most to PC_1, while X_3 dominates PC_2. fig:Contribut

5.5.2 Scores of Individuals and Factor Coordinates

After establishing the principal components through the eigen-decomposition of the covariance matrix, we now turn to the representation of individual observations within this new coordinate system. The *scores* (or *factor coordinates*) of individuals provide a quantitative measure of each observation's position along the principal components, enabling visualization and analysis in the reduced-dimensional space.

Definition of Principal Component Scores

Let $\mathbf{x}_i \in \mathbb{R}^p$ represent a mean-centered observation (i.e., $\mathbf{x}_i = \mathbf{x}_i^{\text{raw}} - \boldsymbol{\mu}$). The score of this observation on the k-th principal component is given by the orthogonal projection onto the corresponding eigenvector:

Orthogonal projection onto the corresponding eigenvector

$$z_{ik} = \mathbf{w}_k^T \mathbf{x}_i = \sum_{j=1}^{p} w_{kj} x_{ij} \tag{5.66}$$

where:

- z_{ik} is the score of observation i on component k
- $\mathbf{w}_k$ is the k-th eigenvector (principal axis)
- x_{ij} is the value of variable j for observation i

For all p components, the complete score vector for observation i is:

$$\mathbf{z}_i = \mathbf{W}^T \mathbf{x}_i \tag{5.67}$$

where $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p]$ is the orthogonal matrix of eigenvectors.

Properties of Principal Component Scores

The scores possess several important statistical properties:

1. **Mean Zero**: The scores have zero mean across observations:

$$\frac{1}{n} \sum_{i=1}^{n} z_{ik} = 0 \quad \text{for all } k \tag{5.68}$$

2. **Variance**: The variance of the scores on each component equals the corresponding eigenvalue:

$$\text{Var}(z_k) = \lambda_k \tag{5.69}$$

3. **Uncorrelatedness**: Scores on different components are uncorrelated:

$$\text{Cov}(z_k, z_l) = 0 \quad \text{for } k \neq l \tag{5.70}$$

4. **Total Variance Preservation**: The sum of variances of all scores equals the total variance in the original data:

$$\sum_{k=1}^{p} \text{Var}(z_k) = \sum_{k=1}^{p} \lambda_k = \text{tr}(\boldsymbol{\Sigma}) \tag{5.71}$$

Matrix Representation

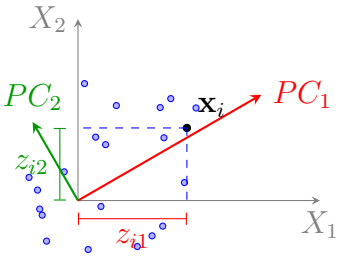
For the entire data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ (mean-centered), the score matrix $\mathbf{Z} \in \mathbb{R}^{n \times p}$ is given by:

$$\mathbf{Z} = \mathbf{X}\mathbf{W} \tag{5.72}$$

Each row of $\mathbf{Z}$ corresponds to an observation, and each column corresponds to a principal component.

Geometric Interpretation

Geometrically, the scores represent the coordinates of observations in the new coordinate system defined by the principal components:



Original space with principal component axes
Scores z_{i1} and z_{i2} represent coordinates in the new system

Figure 5.12: Geometric interpretation of principal component scores as coordinates in the rotated coordinate system defined by the principal components. fig:scores_ge

Factor Coordinates for Variables

While scores represent observations in the principal component space, variables can also be represented in this space through their *factor coordinates* (loadings). The factor coordinates for variable j are given by:

$$\mathbf{f}_j = \begin{pmatrix} w_{1j} \\ w_{2j} \\ \vdots \\ w_{pj} \end{pmatrix} \tag{5.73}$$

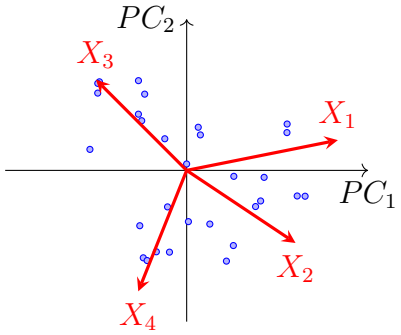
These coordinates represent the contribution of each variable to the principal components and can be visualized alongside the observation scores.

Joint Representation: Biplots

A powerful visualization technique combines both observation scores and variable factor coordinates in a single plot called a *biplot*:

$$\text{Biplot} = \text{Scores} + \text{Factor Coordinates} \tag{5.74}$$

In a biplot, the positions of observations are determined by their scores, while the positions of variables are determined by their factor coordinates. This allows for interpretation of relationships between observations and variables.



Biplot showing observation scores (blue dots) and variable factor coordinates (red arrows)

Figure 5.13: Example biplot displaying both observation scores and variable factor coordinates in the principal component space. fig:biplot

Interpretation of Scores

The interpretation of principal component scores depends on the context but generally follows these guidelines:

- Observations with high positive scores on a component exhibit characteristics associated with that component
- Observations with high negative scores exhibit opposite characteristics
- Observations with scores near zero are average with respect to that component
- The distance between observations in the score space approximates their Mahalanobis distance in the original space

Practical Applications

Principal component scores have numerous practical applications:

1. **Dimensionality Reduction**: Using scores from the first few components as input for other analyses
2. **Outlier Detection**: Identifying observations with extreme scores
3. **Clustering**: Grouping observations based on their score patterns
4. **Visualization**: Creating scatterplots of observations using the first two components
5. **Data Compression**: Storing only the scores instead of the original high-dimensional data

The computation and interpretation of scores form a crucial bridge between the mathematical theory of PCA and its practical application in data analysis.

$$\boxed{\text{PCA Scores} = \text{Transformed Data} = \text{Original Data} \times \text{Eigenvectors}} \tag{5.75}$$

5.5.3 Quality of Representation (Cosine Squared, Contributions)

Assessing how well individual observations and variables are represented in the principal component space is crucial for interpreting PCA results. This subsection introduces two key metrics: the *cosine squared* (COS2) for measuring representation quality of observations, and *contributions* for evaluating variable importance to components.

Quality of Representation for Observations

The quality of representation of an observation i on a principal component k is measured by the squared cosine of the angle between the observation vector and the component axis:

$$\cos^2_{ik} = \frac{z^2_{ik}}{\|\mathbf{x}_i\|^2} \tag{5.76}$$

where z_{ik} is the score of observation i on component k, and $\|\mathbf{x}_i\|^2$ is the squared Euclidean norm of the mean-centered observation.

For multiple components, the quality of representation on the first q components is:

$$\cos^2_{i(q)} = \frac{\sum_{k=1}^{q} z^2_{ik}}{\|\mathbf{x}_i\|^2} \tag{5.77}$$

This measure ranges from 0 to 1, with values close to 1 indicating excellent representation in the subspace spanned by the first q components.

Interpretation of Cosine Squared

The $\cos^2$ values can be interpreted as follows:

- $\cos^2_{ik} > 0.8$: Excellent representation on component k
- $0.5 < \cos^2_{ik} < 0.8$: Good representation
- $0.3 < \cos^2_{ik} < 0.5$: Moderate representation
- $\cos^2_{ik} < 0.3$: Poor representation

Contributions of Observations to Components

The contribution of observation i to the variance of component k is given by:

contribution of observation i

$$CTR_{ik} = \frac{z_{ik}^2}{n \cdot \lambda_k} \times 1000 \tag{5.78}$$

where n is the number of observations and λ_k is the eigenvalue of component k. The multiplication by 1000 converts the measure to per-thousand units for easier interpretation.

Observations with high contributions are particularly influential in defining the component's direction.

Contributions of Variables to Components

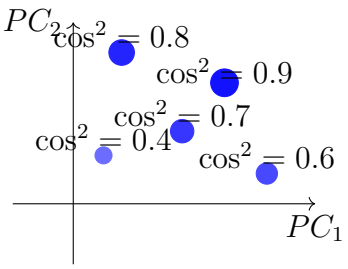
The contribution of variable j to component k is measured by:

contribution of observation j

$$CTR_{jk} = \frac{w_{kj}^2 \cdot \lambda_k}{\sum_{j=1}^{p} w_{kj}^2 \cdot \lambda_k} \times 100 \tag{5.79}$$

This measures the percentage of component k's variance explained by variable j.

Visualization of Representation Quality



Point size and opacity represent quality of representation
Larger, darker points are better represented in this 2D space

Figure 5.14: Visualization of representation quality for observations in the principal component space. fig:represent

Practical Interpretation

These measures help identify:

- Observations that are well-represented in the reduced space (high $\cos^2$)
- Observations that strongly influence component definitions (high CTR)

- Variables that are important for interpreting each component (high variable CTR)
- Potential outliers (observations with unusual contribution patterns)

Example Application

Consider a dataset with 100 observations and the following results for the first component ($\lambda_1 = 3.2$):

Table 5.4: Example of representation measures for selected observations

tab:represent

Observation	z_{i1}	$\cos^2_{i1}$	CTR_{i1}	Interpretation
Obs 23	4.2	0.92	55.1	Excellent representation, high contribution
Obs 56	3.1	0.78	30.0	Good representation, moderate contribution
Obs 12	1.5	0.35	7.0	Poor representation, low contribution
Obs 87	-3.8	0.85	45.2	Excellent representation, high contribution

Mathematical Properties

These representation measures have important mathematical properties:

- $\sum_{i=1}^{n} \cos^2_{ik} = 1$ for each component k
- $\sum_{i=1}^{n} CTR_{ik} = 1000$ for each component k (in per-thousand units)
- $\sum_{j=1}^{p} CTR_{jk} = 100$ for each component k (in percentage units)

These properties ensure that the measures are properly normalized and can be compared across components.

The combination of cosine squared and contribution measures provides a comprehensive framework for assessing the quality and influence of both observations and variables in principal component analysis, enhancing the interpretability of the results.

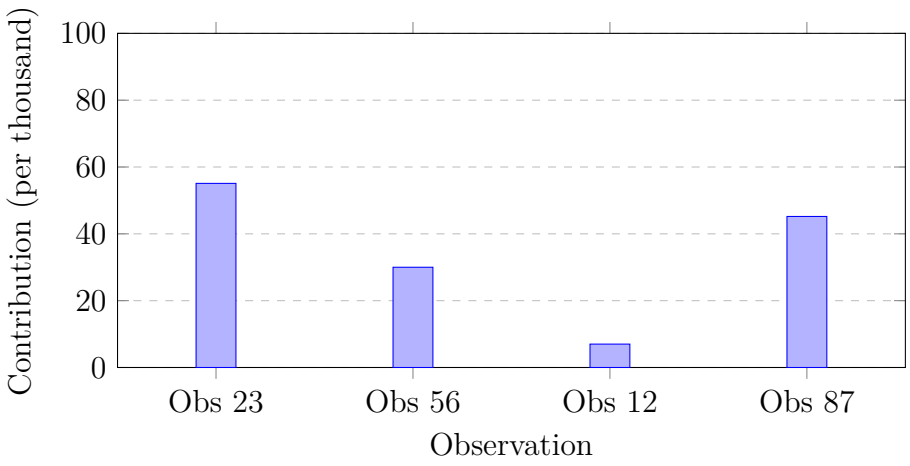


Figure 5.15: Contributions of selected observations to the first principal component, based on the data in Table 5.4.

fig:contribut

5.6 Graphical Representations

Visualization is a powerful tool for interpreting Principal Component Analysis results. This section covers the main graphical representations used in PCA, starting with the circle of correlations, which provides an intuitive geometric representation of the relationships between variables and principal components.

5.6.1 Circle of Correlations for Variables

The circle of correlations (also known as the correlation circle) is a fundamental graphical tool in PCA that visualizes the relationships between the original variables and the principal components in a two-dimensional space.

Mathematical Foundation

The circle of correlations is constructed by plotting the correlations between each original variable and the principal components. For variable X_j and principal component PC_k, this correlation is given by:

Correlation

$$r(X_j, PC_k) = \frac{\text{Cov}(X_j, PC_k)}{\sqrt{\text{Var}(X_j)\,\text{Var}(PC_k)}} = w_{kj}\sqrt{\frac{\lambda_k}{s_{jj}}} \tag{5.80}$$

where:

- w_{kj} is the loading of variable j on component k
- λ_k is the eigenvalue of component k
- s_{jj} is the variance of variable j

When PCA is performed on the correlation matrix (standardized variables), the formula simplifies to:

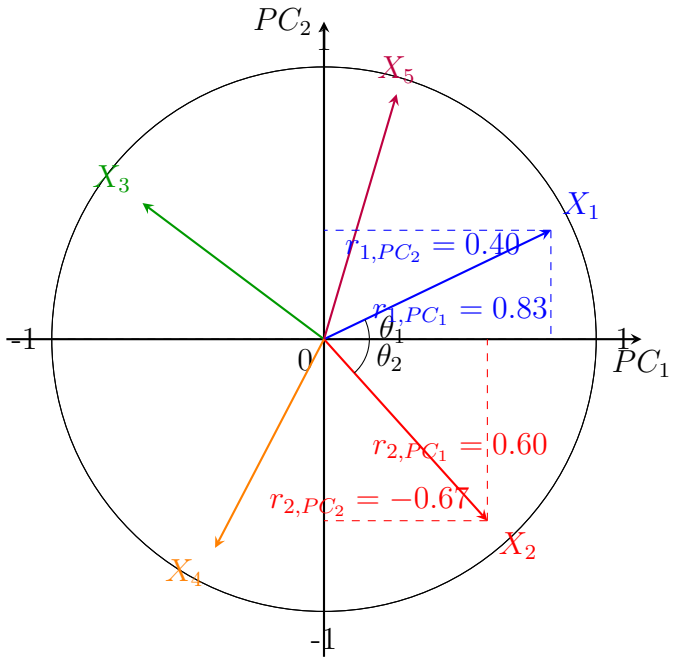
$$r(X_j, PC_k) = w_{kj}\sqrt{\lambda_k} \tag{5.81}$$

Construction of the Circle

The circle of correlations is typically drawn in the plane spanned by the first two principal components (PC_1 and PC_2). Each variable X_j is represented by a point with coordinates:

$$(X_j, PC_1, X_j, PC_2) = (r(X_j, PC_1), r(X_j, PC_2)) \tag{5.82}$$

These points lie within or on a circle of radius 1, called the unit circle, which represents the maximum possible correlation.



Circle of correlations showing variable relationships with principal components

Figure 5.16: Circle of correlations for variables. Each vector represents a variable, with its coordinates corresponding to correlations with PC_1 and PC_2. The length of the vector indicates how well the variable is represented in this 2D space. fig:circle_co

Interpretation Guidelines

The circle of correlations allows for several important interpretations:

1. **Variable-Component Relationships**: Variables located near the circumference and close to a component axis are strongly correlated with that component.

2. **Variable-Variable Relationships**: The cosine of the angle between two variable vectors approximates their correlation:

$$\cos(\theta_{ij}) \approx r(X_i, X_j) \tag{5.83}$$

   where θ_{ij} is the angle between vectors X_i and X_j.

3. **Representation Quality**: The length of a variable's vector indicates how well it is represented in the two-dimensional space:

   - Vectors reaching the unit circle are perfectly represented
   - Shorter vectors are poorly represented in this subspace

4. **Component Interpretation**: Groups of variables clustered together define the "theme" or "meaning" of each component.

Practical Example

Consider the circle of correlations in Figure. We can interpret:

- X_1 is strongly positively correlated with PC_1 ($r = 0.83$) and moderately with PC_2 ($r = 0.40$)
- X_2 is moderately correlated with PC_1 ($r = 0.60$) and negatively correlated with PC_2 ($r = -0.67$)
- X_1 and X_5 have a small angle between them, suggesting they are positively correlated
- X_2 and X_4 have a large angle (close to 180°), suggesting they are negatively correlated

Mathematical Properties

The circle of correlations has several important mathematical properties:

- All variable vectors lie within or on the unit circle
- The coordinates of each variable are its correlations with the principal components
- The squared length of a variable vector represents the proportion of its variance explained by the two components:

$$\|X_j\|^2 = r^2(X_j, PC_1) + r^2(X_j, PC_2) = \cos^2_{j(2)} \tag{5.84}$$

The circle of correlations is thus a powerful tool for visualizing and interpreting the complex relationships between variables and principal components, providing immediate insights that might be difficult to discern from numerical tables of loadings or correlations.

Table 5.5: Interpretation of angles between variable vectors in the circle of correlations tab:angle_int

Angle	Cosine	Interpretation
0°	1	Perfect positive correlation
45°	0.7	Strong positive correlation
90°	0	No correlation
135°	-0.7	Strong negative correlation
180°	-1	Perfect negative correlation

5.6.2 Factor Maps of Individuals

Factor maps, also known as score plots or individual factor maps, are fundamental graphical tools in PCA that visualize the positions of observations (individuals) in the reduced-dimensional space defined by the principal components. These maps reveal the underlying structure of the data, including patterns, clusters, and outliers.

Construction of Factor Maps

Factor maps are constructed by plotting the principal component scores of observations. For each observation i, we plot its coordinates in the space spanned by the principal components:

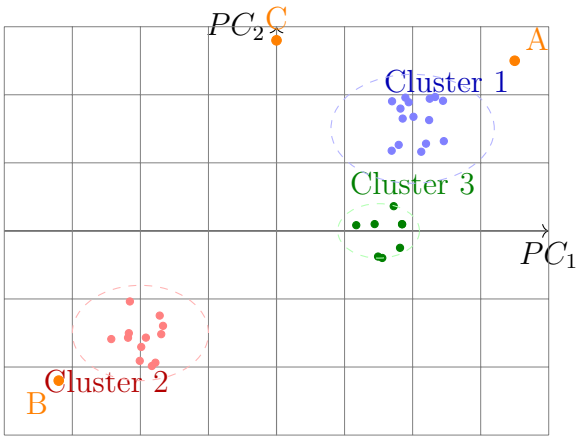
$$(z_{i1}, z_{i2}) \quad \text{for the first two components} \tag{5.85}$$

where z_{i1} and z_{i2} are the scores of observation i on the first and second principal components, respectively.

The general mathematical representation for a factor map in dimensions k and l is:

$$\mathbf{Z}_{kl} = \{(z_{ik}, z_{il}) : i = 1, 2, \ldots, n\} \tag{5.86}$$

where $\mathbf{Z}_{kl}$ represents the set of all observations projected onto the plane defined by components k and l.



Factor map of individuals showing clusters and outliers in the principal component space

Figure 5.17: Factor map (score plot) of individuals projected onto the first two principal components. Different colors represent potential clusters, and labeled points (A, B, C) may represent outliers or special cases. fig:factor_ma

Interpretation of Factor Maps

Factor maps allow for several important interpretations:

1. **Similarity between Individuals**: Observations that are close together in the factor map have similar profiles across all original variables.
2. **Clusters and Groups**: Concentrations of points may indicate natural groupings in the data, suggesting the presence of subpopulations.
3. **Outliers**: Points that are distant from the main concentration of observations may represent unusual cases or measurement errors.

4. **Variability Patterns**: The distribution of points along each axis reveals the patterns of variability captured by the corresponding principal component.

5. **Quality of Representation**: The position of points relative to the origin indicates how well they are represented in the reduced space.

Mathematical Foundations

The coordinates in the factor map are the projections of the original data onto the principal components:

$$z_{ik} = \mathbf{w}_k^T \mathbf{x}_i = \sum_{j=1}^{p} w_{kj} x_{ij} \tag{5.87}$$

where:

- z_{ik} is the score of observation i on component k
- $\mathbf{w}_k$ is the k-th eigenvector (principal axis)
- $\mathbf{x}_i$ is the mean-centered observation vector
- p is the number of original variables

The Euclidean distance between two points in the factor map approximates their Mahalanobis distance in the original space:

$$d(\mathbf{z}_i, \mathbf{z}_j) \approx d_M(\mathbf{x}_i, \mathbf{x}_j) \tag{5.88}$$

Enhancing Factor Maps with Additional Information

Factor maps can be enhanced with supplementary information to facilitate interpretation:

- **Grouping Variables**: Points can be colored or shaped according to categorical variables not used in the PCA, helping to validate or discover patterns.
- **Concentration Ellipses**: Ellipses can be drawn around groups of points to visualize confidence regions or cluster boundaries.
- **Labels**: Important or unusual observations can be labeled to highlight specific cases.
- **Trajectories**: For longitudinal data, lines can connect observations from the same individual across time points.

Practical Considerations

When interpreting factor maps, several practical considerations should be kept in mind:

1. The percentage of variance explained by the displayed components should be considered when assessing the reliability of patterns.

2. The scale of the axes should be consistent to avoid visual distortion of relationships.

3. Overplotting can be mitigated by using semi-transparent points or jittering when many observations are present.

4. The choice of which components to plot depends on the variance they explain and the specific research questions.

Factor maps provide a powerful visual summary of the multivariate relationships between observations, transforming complex numerical information into an intuitive graphical representation that can reveal patterns, clusters, and outliers that might not be apparent in numerical output alone.

Table 5.6: Interpretation of positions in factor maps

tab:factor_ma

Position	Interpretation
Far from origin along PC_k	Extreme values on the characteristics captured by component k
Close to origin	Average profile across all variables
Close to other points	Similar characteristics and profiles
Distant from other points	Unique or unusual characteristics
Near component axis	Well represented by that component
Between component axes	Influenced by multiple patterns

5.6.3 Joint Interpretation: Individuals vs. Variables

The most powerful insight from Principal Component Analysis often emerges when we simultaneously examine both individuals (observations) and variables in the same graphical representation. This joint interpretation, typically achieved through *biplots*, allows us to understand the relationships between observations, between variables, and crucially, between observations and variables.

The Biplot: A Unified Representation

A biplot is a single graphical display that superimposes two different representations:

1. **Individuals factor map**: Points representing observations in the principal component space

2. **Variables factor map**: Vectors representing variables in the same space

The mathematical foundation for the biplot is based on the singular value decomposition of the mean-centered data matrix:

$$\mathbf{X} = \mathbf{UDW}^T \tag{5.89}$$

where:

- $\mathbf{U}$ contains the left singular vectors (related to individuals)
- $\mathbf{D}$ is the diagonal matrix of singular values
- $\mathbf{W}$ contains the right singular vectors (principal components)

The Transition Formulas

The joint representation relies on the transition formulas that connect the two spaces:

$$\textbf{Individuals coordinates:} \quad \mathbf{z}_i = \mathbf{W}^T\mathbf{x}_i \tag{5.90}$$

$$\textbf{Variable coordinates:} \quad \mathbf{f}_j = \mathbf{W}\mathbf{e}_j \quad \text{or} \quad f_{jk} = w_{kj} \tag{5.91}$$

where $\mathbf{e}_j$ is the j-th standard basis vector.

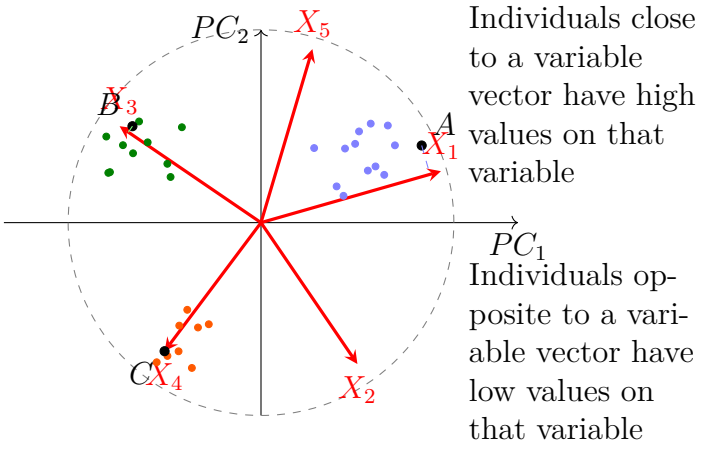


Figure 5.18: Biplot for joint interpretation of individuals and variables. The relationships between observations and variables can be interpreted through their relative positions.

fig:biplot_jo

Interpretation Rules for Biplots

The joint interpretation follows these geometric principles:

1. **Variable-Variable Relationships**: The angle between variable vectors approximates their correlation:
    - Small angle ($\approx 0°$): Strong positive correlation

- Right angle ($\approx 90°$): No correlation
- Obtuse angle ($> 90°$): Negative correlation
- Opposite directions ($180°$): Strong negative correlation

2. **Individual-Variable Relationships**: The projection of an individual point onto a variable vector indicates the value of that individual on the variable:
   - Positive projection: Above-average value
   - Negative projection: Below-average value
   - Near zero: Average value
3. **Individual-Individual Relationships**: The distance between individuals approximates their similarity:
   - Close points: Similar profiles across all variables
   - Distant points: Dissimilar profiles
4. **Variable-Component Relationships**: The coordinates of variable vectors show their correlations with the components.

Mathematical Formulation of Relationships

The projection of individual i onto variable j's direction is proportional to their covariance:

$$\text{proj}_{\mathbf{f}_j}(\mathbf{z}_i) = \frac{\mathbf{z}_i \cdot \mathbf{f}_j}{\|\mathbf{f}_j\|} \approx x_{ij} \tag{5.92}$$

The cosine of the angle between two variable vectors $\mathbf{f}_j$ and $\mathbf{f}_k$ approximates their correlation:

$$\cos(\theta_{jk}) = \frac{\mathbf{f}_j \cdot \mathbf{f}_k}{\|\mathbf{f}_j\|\|\mathbf{f}_k\|} \approx r(X_j, X_k) \tag{5.93}$$

Practical Interpretation Example

Consider the biplot in Figure:

- **Variable relationships**:
  - X_1 and X_5 have a small angle between them, indicating positive correlation
  - X_2 and X_4 point in similar directions, suggesting they measure related constructs
  - X_3 is nearly orthogonal to X_1 and X_5, indicating little correlation
- **Individual relationships**:
  - Individual A is close to X_1 and X_5, suggesting high values on these variables

  - Individual B is near X_3, indicating high values on this variable
  - Individual C is opposite to X_1 and X_5, suggesting low values on these variables

- **Group patterns**:
  - The blue cluster has high values on X_1 and X_5
  - The green cluster has high values on X_3
  - The orange cluster has high values on X_2 and X_4

Scaling Considerations

Different scaling conventions affect the interpretation of biplots:

1. **Distance biplot**: Preserves distances between individuals but distangles variable-vector lengths
2. **Correlation biplot**: Preserves the angles between variables but may distort distances between individuals

The choice depends on whether the primary focus is on individuals (use distance biplot) or variables (use correlation biplot).

Limitations and Considerations

While powerful, joint interpretation requires careful consideration:

- The quality of representation should be checked for both individuals and variables
- The percentage of variance explained by the displayed components affects interpretability
- Overplotting can make complex biplots difficult to read
- The interpretation is linear and may miss nonlinear relationships

Despite these limitations, the joint interpretation of individuals and variables through biplots remains one of the most valuable tools in PCA, providing a comprehensive visual summary of the multivariate relationships in the data.

Table 5.7: Guide to interpreting relative positions in biplots

tab:biplot_in

Geometric Relationship	Interpretation
Individual close to variable arrow	High value on that variable
Individual opposite to variable arrow	Low value on that variable
Individual near origin	Average profile across variables
Small angle between variables	Positive correlation
Large angle between variables ($> 90°$)	Negative correlation
Right angle between variables	No correlation
Cluster of individuals	Group with similar characteristics
Isolated individual	Potential outlier or unique case

5.7 Extensions and Applications of PCA

Principal Component Analysis transcends its origins in mathematical statistics to become a ubiquitous tool across numerous scientific disciplines. This section explores the diverse applications and methodological extensions of PCA, demonstrating its versatility in addressing complex, high-dimensional problems in both natural and social sciences.

5.7.1 Applications in Natural and Social Sciences

The utility of PCA extends far beyond theoretical statistics, finding profound applications in both natural and social sciences. Its ability to distill complex, high-dimensional datasets into interpretable patterns makes it indispensable across diverse domains.

Applications in Natural Sciences

1. **Genomics and Bioinformatics**: PCA is extensively used in genome-wide association studies (GWAS) to address population stratification. By analyzing genetic variation across individuals, PCA can identify ancestral patterns and control for confounding due to population structure. For a genotype matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ where n is the number of individuals and p is the number of single-nucleotide polymorphisms (SNPs), PCA reveals the major axes of genetic variation, often correlating with geographic ancestry.

2. **Ecology and Environmental Science**: In ecological studies, PCA helps identify patterns in species abundance data across different locations. Given a data matrix where rows represent sites and columns represent species abundances, PCA can reveal gradients of environmental variation and identify species with similar distribution patterns. This aids in understanding community ecology and ecosystem dynamics.

3. **Chemometrics and Spectroscopy**: PCA is fundamental in analyzing spectral data from techniques such as mass spectrometry, NMR spectroscopy, and infrared spectroscopy. For spectral data $\mathbf{X} \in \mathbb{R}^{n \times \lambda}$ where λ represents wavelength indices, PCA identifies major spectral patterns, facilitates noise reduction, and enables the detection of characteristic spectral signatures associated with different chemical compounds.

4. **Geophysics and Meteorology**: In climate science, PCA (often called Empirical Orthogonal Function analysis) is used to identify dominant patterns of spatial and temporal variation in climate data. For example, applying PCA to sea surface temperature data can reveal patterns like El Niño Southern Oscillation (ENSO) phenomena, which represent major modes of climate variability.

Applications in Social Sciences

1. **Psychology and Psychometrics**: PCA forms the foundation of factor analysis in psychological testing. For questionnaire data with multiple items measuring latent constructs (e.g., personality traits, intelligence factors), PCA helps identify the underlying factor structure. This allows researchers to determine which items load highly on which factors, validating psychological instruments and theoretical frameworks.

2. **Economics and Finance**: In financial economics, PCA is used to analyze term structure movements in interest rates, often called *level*, *slope*, and *curvature* factors. For a matrix of interest rates across different maturities $\mathbf{R} \in \mathbb{R}^{t \times m}$ where t is time and m is maturity, PCA identifies these fundamental components that drive most of the variation in yield curves.

3. **Sociology and Political Science**: PCA helps reduce numerous socioeconomic indicators into composite indices. For example, the Human Development Index (HDI) conceptually parallels PCA by combining income, education, and health metrics. In practice, PCA can create more nuanced multidimensional indices of development, inequality, or quality of life from a broader set of variables.

4. **Marketing Research**: In consumer analytics, PCA is applied to survey data to identify latent attitudes and preferences. For data on consumer ratings of various product attributes, PCA can reveal the fundamental dimensions that drive consumer preferences, such as *price sensitivity*, *quality focus*, or *brand consciousness*.

Cross-Disciplinary Methodological Notes

Despite the diversity of applications, the mathematical foundation remains consistent. The key considerations across domains include:

- **Preprocessing**: The choice between correlation and covariance PCA depends on whether variables are measured on comparable scales. Genetic and spectral

data often use covariance PCA, while social science data with diverse metrics typically requires correlation PCA.

- **Interpretation**: The interpretation of principal components is necessarily domain-specific. Component 1 in genetics might represent north-south geographic gradient, while in psychology it might represent a general intelligence factor.

- **Validation**: Applications increasingly use cross-validation and bootstrap methods to assess the stability of PCA solutions, especially when making substantive inferences from the components.

Table 5.8: Representative applications of PCA across scientific disciplines tab:pca_appli

Domain	**Typical Data Structure**	**PCA Purpose**
Genomics	n individuals $\times$ p SNPs	Population stratification, ancestry inference
Ecology	n sites $\times$ p species	Community gradients, species associations
Psychometrics	n subjects $\times$ p test items	Latent factor identification, test validation
Econometrics	t time points $\times$ m maturities	Term structure modeling, risk factor analysis
Chemometrics	n samples $\times$ λ wavelengths	Spectral pattern recognition, noise reduction

The widespread adoption of PCA across these diverse fields testifies to its fundamental utility as a method for dimensionality reduction and pattern discovery. In each case, PCA transforms complex, high-dimensional data into a more interpretable form while preserving the essential structure of the original data, enabling researchers to identify key patterns and relationships that might otherwise remain obscured in the high-dimensional space.

The subsequent subsections will explore specific methodological extensions that enhance PCA's applicability to these diverse domains and discuss important limitations that practitioners must consider when applying PCA to their specific research problems.

5.7.2 Link between PCA and Regression/Clustering

Principal Component Analysis does not exist in methodological isolation but rather forms synergistic relationships with other statistical techniques, particularly regression and clustering methods. These connections enhance the utility of PCA and address specific limitations of each method when used in isolation.

PCA and Regression: Principal Component Regression (PCR)

Principal Component Regression (PCR) addresses multicollinearity problems in linear regression by using principal components as predictors instead of the original correlated variables.

Definition 5.7 (Principal Component Regression)**.** Given a response variable Y and predictor matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, PCR involves:

1. Performing PCA on $\mathbf{X}$ to obtain principal components $\mathbf{Z} = \mathbf{XW}$
2. Selecting the first q components $\mathbf{Z}_q = [\mathbf{z}_1, \ldots, \mathbf{z}_q]$
3. Regressing Y on these components: $Y = \mathbf{Z}_q\boldsymbol{\beta} + \epsilon$
4. Transforming back to original variables: $\hat{\boldsymbol{\beta}} = \mathbf{W}_q\hat{\boldsymbol{\beta}}_z$

The PCR estimator has the form:

$$\hat{\boldsymbol{\beta}}_{PCR} = \sum_{k=1}^{q} \frac{\mathbf{w}_k \mathbf{w}_k^T}{\lambda_k} \mathbf{X}^T Y \tag{5.94}$$

where $\mathbf{w}_k$ are eigenvectors and λ_k are eigenvalues of $\mathbf{X}^T\mathbf{X}$.

Advantages of PCR

- **Multicollinearity Resolution**: Eliminates problems caused by nearly linearly dependent predictors
- **Dimensionality Reduction**: Reduces number of parameters to estimate
- **Variance Reduction**: Often provides more stable estimates than ordinary least squares
- **Automatic Feature Engineering**: Creates orthogonal predictors that capture maximum variance

Comparison with Other Methods

Table 5.9: Comparison of regression methods with PCA

tab:pcr_compa

Method	Approach	When to Use
Ordinary Least Squares	Minimize residual sum of squares	No multicollinearity, n > p
Ridge Regression	L2 penalty on coefficients	Multicollinearity present
LASSO	L1 penalty on coefficients	Variable selection desired
Principal Component Regression	Regression on principal components	Severe multicollinearity, interpretation needed

PCA and Clustering

PCA facilitates clustering in high-dimensional spaces through two primary mechanisms:

1. **Dimensionality Reduction for Clustering**: Projecting data onto principal components before applying clustering algorithms:

$$\mathbf{Z}_q = \mathbf{X}\mathbf{W}_q \quad \text{then cluster} \quad \{\mathbf{z}_i\}_{i=1}^n \tag{5.95}$$

2. **Visualization of Cluster Structure**: Using the first two principal components to visualize high-dimensional clusters:

$$\text{Cluster visualization} = \{(z_{i1}, z_{i2}, c_i) : i = 1, \ldots, n\} \tag{5.96}$$

where c_i indicates cluster membership.

Theoretical Connection: Gaussian Mixture Models

For Gaussian mixture models, the principal components approximate the directions of maximum cluster separation when clusters have different covariance structures. The relationship is particularly strong when:

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_0 + \mathbf{U}\mathbf{D}\mathbf{U}^T \tag{5.97}$$

where $\boldsymbol{\Sigma}_0$ is common covariance and $\mathbf{U}\mathbf{D}\mathbf{U}^T$ represents cluster-specific variation.

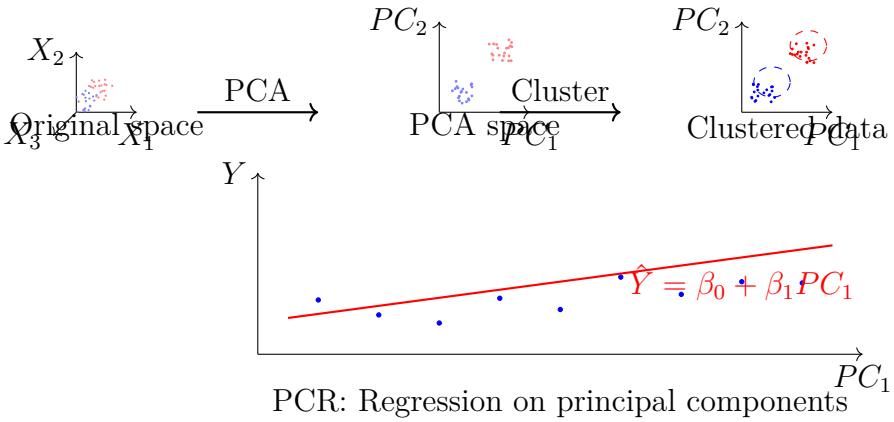


Figure 5.19: Schematic representation of PCA applications in clustering and regression. Top: PCA facilitates clustering by projecting data to lower dimensions where clusters become apparent. Bottom: Principal Component Regression uses principal components as predictors.

fig:pca_clust

Practical Considerations

- **Component Selection**: The choice of q (number of components) is critical for both PCR and clustering applications. Cross-validation is recommended for PCR, while clustering may use different criteria.

- **Interpretation Trade-off**: PCR components may be harder to interpret than original variables, though the stability often justifies this cost.

- **Scale Sensitivity**: Both applications require careful attention to scaling, especially when variables have different units.
- **Validation**: Results should be validated through methods like bootstrapping or stability analysis, particularly for clustering applications.

Integrated Example: Genomics Application

In genome-wide association studies, PCA and clustering integrate seamlessly:

1. PCA identifies population structure from genetic data
2. Clustering assigns individuals to ancestral groups based on principal components
3. Regression includes these clusters as covariates to control for population stratification
4. This prevents spurious associations between genotypes and phenotypes

This integration demonstrates how PCA bridges dimensionality reduction, clustering, and regression to solve complex problems in high-dimensional data analysis.

The connection between PCA and these fundamental techniques underscores its central role in the statistical toolkit, enabling researchers to tackle problems that would be intractable with any single method alone. The next subsection examines the limitations and assumptions that govern appropriate application of these integrated approaches.

5.7.3 Limitations and Assumptions of PCA

While Principal Component Analysis is a powerful and versatile technique, it is crucial to understand its limitations and underlying assumptions. Proper application of PCA requires recognizing these constraints to avoid misinterpretation and inappropriate use of the method.

Fundamental Assumptions of PCA

PCA operates under several key assumptions that govern its proper application:

1. **Linearity**: PCA assumes that the principal components are linear combinations of the original variables. This implies that it may not capture complex nonlinear relationships in the data:

$$PC_k = w_{k1}X_1 + w_{k2}X_2 + \cdots + w_{kp}X_p \tag{5.98}$$

   Nonlinear patterns require extensions such as Kernel PCA.

2. **Mean and Variance Sufficiency**: PCA assumes that the mean and covariance structure adequately capture the relevant information in the data. This makes it most appropriate for approximately Gaussian distributions and less suitable for data with complex dependency structures.

3. **Large Variance Importance**: PCA assumes that directions with larger variance are more interesting or important. This may not hold if the relevant signal has lower variance than noise in the data.

4. **Orthogonality**: The components are constrained to be orthogonal, which may not align with the true underlying structure of the data.

Key Limitations

- **Sensitivity to Scaling**: PCA results are highly sensitive to the scaling of variables. Using the covariance matrix versus the correlation matrix can yield dramatically different results:

$$\text{Covariance PCA: } \mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} \quad \text{vs.} \quad \text{Correlation PCA: } \mathbf{R} = \mathbf{D}^{-1/2}\mathbf{S}\mathbf{D}^{-1/2} \tag{5.99}$$

  where $\mathbf{D}$ is the diagonal matrix of variances.

- **Interpretation Challenges**: The principal components are mathematical constructs that may not have straightforward substantive interpretations. The rotation of components (e.g., varimax rotation) is sometimes used to improve interpretability.

- **Variance Bias**: PCA is biased toward variables with larger scales and may overlook important patterns in low-variance directions.

- **Outlier Sensitivity**: Extreme values can disproportionately influence the principal components, as PCA minimizes squared errors which are sensitive to outliers.

Geometric Interpretation of Limitations

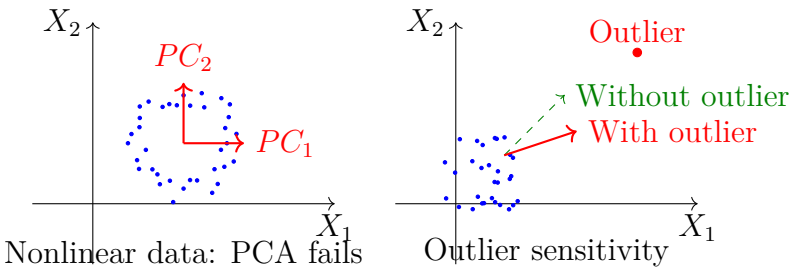


Figure 5.20: Visualization of two key limitations of PCA: failure to capture nonlinear structure and sensitivity to outliers. fig:pca_limit

Statistical Considerations

- **Sample Size Requirements**: PCA requires adequate sample size for stable results. The *number of observations* n should substantially exceed the *number of variables* p for reliable component estimation.

- **Missing Data**: Traditional PCA cannot handle missing data directly. Approaches such as imputation or specialized algorithms (e.g., probabilistic PCA) are needed for incomplete datasets.

- **Significance Testing**: Determining the statistical significance of components is challenging. Methods like parallel analysis or permutation tests are often used:

$$\text{Parallel analysis: Compare } \lambda_k \text{ with eigenvalues from random data} \tag{5.100}$$

- **Dimensionality Assessment**: Determining the true dimensionality q is subjective and method-dependent. Different criteria (Kaiser, scree plot, variance explained) may yield different results.

Practical Limitations in Application

Table 5.10: Practical limitations and potential solutions in PCA applications

tab:pca_limit

Limitation	Potential Solutions
Sensitivity to scaling	Standardize variables (use correlation matrix)
Nonlinear relationships	Kernel PCA, autoencoders, manifold learning
Outlier sensitivity	Robust PCA, outlier detection and removal
Missing data	Imputation, probabilistic PCA, matrix completion
Interpretation difficulty	Component rotation, sparse PCA
High-dimensional data ($p \gg n$)	Regularized PCA, sparse methods

When Not to Use PCA

PCA may be inappropriate or require modification in these scenarios:

1. **Non-Gaussian Data**: When variables have multimodal distributions or heavy tails

2. **Nonlinear Structures**: When relationships between variables are fundamentally nonlinear

3. **Spherical Data**: When all variables have approximately equal variance and are uncorrelated

4. **Categorical Data**: PCA is designed for continuous variables; alternatives like MCA are needed for categorical data

5. **Preserved Metric Importance**: When the original variable scales and relationships must be strictly preserved

Extensions Addressing Limitations

Several methodological extensions address PCA's limitations:

- **Robust PCA**: Resistant to outliers and influential observations
- **Sparse PCA**: Produces components with fewer non-zero loadings for better interpretability
- **Kernel PCA**: Captures nonlinear relationships through kernel methods
- **Probabilistic PCA**: Provides statistical framework for handling missing data and uncertainty quantification

Understanding these limitations and assumptions is crucial for the appropriate application and interpretation of PCA. While PCA remains an invaluable tool for exploratory data analysis and dimensionality reduction, its results should always be interpreted with awareness of these constraints and with consideration of alternative methods when the assumptions are severely violated.

The awareness of these limitations leads naturally to the development of more sophisticated techniques and provides the motivation for the exercises in the next section, which will help students develop practical skills in recognizing and addressing these issues in real-world data analysis.

5.8 Exercises

sec:exercises

Exercise 1: Basic Concepts

Let $\mathbf{X}$ be a mean-centered $n \times p$ data matrix.

1. Write the mathematical expression for the sample covariance matrix $\mathbf{S}$.
2. State the optimization problem that defines the first principal component.
3. What is the relationship between the solution to this optimization problem and the eigen decomposition of $\mathbf{S}$?

Exercise 2: Variance Explanation

A PCA on a dataset with 5 variables produced the following eigenvalues: $\lambda_1 = 3.8$, $\lambda_2 = 0.9$, $\lambda_3 = 0.6$, $\lambda_4 = 0.4$, $\lambda_5 = 0.3$.

1. Calculate the total variance in the data.
2. What proportion of the total variance is explained by the first two principal components?
3. How many components would you retain based on the Kaiser criterion? Justify your answer.

Exercise 3: Computational

Consider the following mean-centered dataset with 4 observations and 2 variables:

$$\mathbf{X} = \begin{bmatrix} 1 & 2 \\ -1 & -2 \\ 2 & 1 \\ -2 & -1 \end{bmatrix}$$

1. Calculate the covariance matrix $\mathbf{S}$.
2. Find the eigenvalues and eigenvectors of $\mathbf{S}$.
3. Compute the principal component scores for all observations.
4. Verify that the variances of the scores equal the eigenvalues.

Exercise 4: Interpretation

A PCA was performed on a dataset of consumer ratings for 10 different product attributes. The first two principal components explain 68% of the total variance. The loadings for three of the variables are:

$$\begin{aligned} \text{Variable A (Price)} &: \mathbf{w}_1 = 0.85, \mathbf{w}_2 = -0.15 \\ \text{Variable B (Quality)} &: \mathbf{w}_1 = -0.10, \mathbf{w}_2 = 0.90 \\ \text{Variable C (Design)} &: \mathbf{w}_1 = 0.45, \mathbf{w}_2 = 0.55 \end{aligned}$$

1. Interpret the meaning of the first two principal components.
2. Which variable contributes most to Component 1? To Component 2?
3. What can you say about the relationship between Variables A and B based on their loadings?

Exercise 5: Geometric Understanding

1. Explain geometrically what PCA accomplishes in terms of the data cloud and the new coordinate system.
2. Draw a diagram showing a 2D data cloud, the original axes, and the first two principal components. Label the eigenvectors and indicate the direction of maximum variance.
3. What does the length of a variable vector in a correlation circle represent?

Exercise 6: Advanced Proof

Prove that for a random vector $\mathbf{x}$ with covariance matrix $\mathbf{\Sigma}$, the total variance equals the sum of the eigenvalues of $\mathbf{\Sigma}$:

$$\sum_{j=1}^{p} \text{Var}(X_j) = \sum_{k=1}^{p} \lambda_k$$

Hint: Use the properties of the trace operator and eigen decomposition.

Exercise 7: Application

Describe one specific application of PCA in each of the following fields:

1. Genetics
2. Image processing
3. Finance
4. Psychology

For each application, specify:

- What the rows and columns of the data matrix represent
- What the principal components typically capture
- How the results are used in practice

Exercise 8: Comparison of Methods
Compare and contrast PCA with the following techniques:

1. Factor Analysis
2. Linear Discriminant Analysis (LDA)
3. t-SNE

Discuss their respective objectives, mathematical foundations, and appropriate use cases.

Exercise 9: Limitations and Assumptions

1. List three key assumptions of PCA and explain why each is important.
2. Describe two situations where PCA would be inappropriate or might perform poorly.
3. What is the "curse of dimensionality" and how does PCA address it?

Exercise 10: Comprehensive Analysis
The `iris` dataset contains measurements of sepal length, sepal width, petal length, and petal width for three species of iris flowers. Suppose you perform PCA on the covariance matrix of the four measurements (for all species combined).

1. What would the eigenvalues represent in this context?
2. How might the principal components help in distinguishing between species?
3. Sketch what you would expect to see in a biplot of the first two principal components.
4. What limitations might PCA have for this classification problem?

Note: These exercises cover theoretical, computational, interpretative, and applied aspects of PCA. Students are encouraged to use statistical software (R, Python, etc.) for exercises involving computation with real datasets. The comprehensive analysis question (Exercise 10) is particularly recommended as a mini-project to integrate all concepts from the chapter.

Exercise 11: Comprehensive PCA

This exercise guides you through a complete Principal Component Analysis, from data preparation to interpretation, using a simple dataset. Follow each step carefully, performing all calculations and creating the required visualizations.

Dataset

Consider the following dataset with 5 observations and 3 variables:

Table 5.11: Original data matrix

tab:exercise_

Observation	X_1 (Height)	X_2 (Weight)	X_3 (Age)
1	170	68	25
2	175	72	30
3	180	75	35
4	185	80	40
5	190	85	45

Step 1: Data Preprocessing

1. Calculate the mean for each variable.
2. Center the data by subtracting the mean from each value.
3. Create a mean-centered data matrix $\mathbf{X}$.

Step 2: Covariance Matrix

1. Compute the covariance matrix $\mathbf{S}$ of the mean-centered data.
2. Show all calculations step by step.

Step 3: Eigen analysis

1. Find the eigenvalues of $\mathbf{S}$ by solving the characteristic equation $\det(\mathbf{S} - \lambda\mathbf{I}) = 0$.
2. Find the corresponding eigenvectors for each eigenvalue.
3. Verify that the eigenvectors are orthogonal and have unit length.

Step 4: Principal Components

1. Express each principal component as a linear combination of the original variables.
2. Calculate the proportion of variance explained by each component.

3. Create a scree plot showing the eigenvalues and cumulative variance explained.

Step 5: Projection

1. Project the original data onto the principal component space.
2. Calculate the scores for each observation on the first two principal components.
3. Create a scores plot (factor map) of the observations.

Step 6: Visualization

1. Create a correlation circle (variables factor map) showing the relationships between variables and components.
2. Create a biplot showing both observations and variables in the principal component space.

Step 7: Interpretation

1. Interpret the meaning of each principal component based on the variable loadings.
2. Describe the relationships between observations based on their positions in the factor map.
3. Discuss what the biplot reveals about the relationships between variables and observations.
4. Suggest how many components should be retained and justify your decision.

Step 8: Reconstruction

1. Reconstruct the original data using only the first two principal components.
2. Calculate the reconstruction error for each observation.
3. Discuss the implications of the reconstruction error for dimensionality reduction.

This comprehensive exercise requires you to apply all aspects of PCA covered in this chapter. Take your time with each step, and ensure your calculations are accurate. The following pages provide space for your work and solutions.

5.9 Solutions to Exercises

sec:solutions

This section provides detailed solutions to the first four exercises from Section 5.8. These solutions demonstrate the application of PCA concepts and mathematical techniques covered in this chapter.

Solution to Exercise 1: Basic Concepts

1. The sample covariance matrix $\mathbf{S}$ for a mean-centered data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ is given by:
$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} \tag{5.101}$$
where n is the number of observations and p is the number of variables.

2. The optimization problem defining the first principal component seeks a vector $\mathbf{w}_1 \in \mathbb{R}^p$ that maximizes the variance of the projected data:
$$\max_{\mathbf{w}_1 \in \mathbb{R}^p} \text{Var}(\mathbf{w}_1^T\mathbf{x}) = \mathbf{w}_1^T\mathbf{\Sigma}\mathbf{w}_1 \quad \text{subject to} \quad \|\mathbf{w}_1\| = 1 \tag{5.102}$$
where $\mathbf{\Sigma}$ is the population covariance matrix (or $\mathbf{S}$ for sample data).

3. The solution to this optimization problem is obtained through the eigendecomposition of the covariance matrix:
$$\mathbf{\Sigma}\mathbf{w}_k = \lambda_k\mathbf{w}_k \quad \text{for} \quad k = 1, 2, \ldots, p \tag{5.103}$$
The first principal component $\mathbf{w}_1$ is the eigenvector corresponding to the largest eigenvalue λ_1, and each subsequent component $\mathbf{w}_k$ is the eigenvector corresponding to the k-th largest eigenvalue, with the constraint that all components are orthogonal ($\mathbf{w}_i^T\mathbf{w}_j = 0$ for $i \neq j$).

Solution to Exercise 2: Variance Explanation

1. The total variance equals the sum of all eigenvalues:
$$\text{Total Variance} = \sum_{k=1}^{5} \lambda_k = 3.8 + 0.9 + 0.6 + 0.4 + 0.3 = 6.0 \tag{5.104}$$

2. The proportion of variance explained by the first two principal components is:
$$\frac{\lambda_1 + \lambda_2}{\sum_{k=1}^{5} \lambda_k} = \frac{3.8 + 0.9}{6.0} = \frac{4.7}{6.0} \approx 0.7833 \quad (78.33\%) \tag{5.105}$$

3. According to the Kaiser criterion, we retain components with eigenvalues greater than 1. In this case, only the first component ($\lambda_1 = 3.8 > 1$) meets this criterion. The second component ($\lambda_2 = 0.9 < 1$) and subsequent components would not be retained based solely on this rule.

Solution to Exercise 3: Computational

1. The covariance matrix $\mathbf{S}$ is calculated as follows:

$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} = \frac{1}{3}\begin{bmatrix}1 & -1 & 2 & -2\\ 2 & -2 & 1 & -1\end{bmatrix}\begin{bmatrix}1 & 2\\ -1 & -2\\ 2 & 1\\ -2 & -1\end{bmatrix} = \frac{1}{3}\begin{bmatrix}10 & 8\\ 8 & 10\end{bmatrix} = \begin{bmatrix}\frac{10}{3} & \frac{8}{3}\\ \frac{8}{3} & \frac{10}{3}\end{bmatrix} \tag{5.106}$$

2. The eigenvalues λ satisfy the characteristic equation $\det(\mathbf{S} - \lambda\mathbf{I}) = 0$:

$$\det\begin{bmatrix}\frac{10}{3} - \lambda & \frac{8}{3}\\ \frac{8}{3} & \frac{10}{3} - \lambda\end{bmatrix} = \left(\frac{10}{3} - \lambda\right)^2 - \left(\frac{8}{3}\right)^2 = 0 \tag{5.107}$$

   Solving gives $\lambda_1 = 6$ and $\lambda_2 = \frac{2}{3}$.

   The corresponding eigenvectors are:

$$\mathbf{w}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix}, \quad \mathbf{w}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix} \tag{5.108}$$

3. The principal component scores are obtained by projecting the data onto the eigenvectors:

$$\mathbf{Z} = \mathbf{X}\mathbf{W} = \begin{bmatrix}1 & 2\\ -1 & -2\\ 2 & 1\\ -2 & -1\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{bmatrix} = \begin{bmatrix}\frac{3}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\ -\frac{3}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{3}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ -\frac{3}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{bmatrix} \tag{5.109}$$

4. The variances of the scores are:

$$\mathrm{Var}(PC_1) = \frac{1}{3}\left[\left(\frac{3}{\sqrt{2}}\right)^2 + \left(-\frac{3}{\sqrt{2}}\right)^2 + \left(\frac{3}{\sqrt{2}}\right)^2 + \left(-\frac{3}{\sqrt{2}}\right)^2\right] = \frac{1}{3}\cdot 4 \cdot \frac{9}{2} = 6 = \lambda_1 \tag{5.110}$$

$$\mathrm{Var}(PC_2) = \frac{1}{3}\left[\left(-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 + \left(-\frac{1}{\sqrt{2}}\right)^2\right] = \frac{1}{3}\cdot 4 \cdot \frac{1}{2} = \frac{2}{3} = \lambda_2 \tag{5.111}$$

   This confirms that the variances of the scores equal the eigenvalues.

Solution to Exercise 4: Interpretation

1. Interpretation of the first two principal components:

   - **Component 1**: This component is primarily defined by Variable A (Price) with a strong positive loading (0.85). It represents a dimension contrasting expensive products (high values) with inexpensive products (low values). Variable C (Design) also contributes positively but to a lesser extent.

- **Component 2**: This component is primarily defined by Variable B (Quality) with a strong positive loading (0.90). It represents a dimension of product quality, with Variable C (Design) also making a moderate positive contribution. Variable A (Price) has a minimal negative contribution.

2. Variable contributions:

   - Variable A (Price) contributes most to Component 1 (loading = 0.85)
   - Variable B (Quality) contributes most to Component 2 (loading = 0.90)

3. Relationship between Variables A and B:

   - The angle between the variable vectors can be approximated by their dot product: $\cos(\theta) \approx \mathbf{w}_{A1}\mathbf{w}_{B1} + \mathbf{w}_{A2}\mathbf{w}_{B2} = (0.85)(-0.10) + (-0.15)(0.90) = -0.085 - 0.135 = -0.22$
   - This negative value suggests an angle greater than 90° between the variables, indicating a negative relationship between Price and Quality in this dataset. Products with higher prices tend to have lower quality ratings, and vice versa.

These solutions demonstrate the application of PCA concepts including covariance computation, eigen-decomposition, variance calculation, and interpretation of loadings. The remaining exercises may be solved using similar approaches, applying the appropriate PCA techniques covered in this chapter.

Solution to Exercise 5: Geometric Understanding

1. Geometrically, PCA performs an orthogonal transformation (rotation) of the coordinate system to align with the directions of maximum variance in the data. Specifically:

   - The data cloud is rotated so that the new axes (principal components) are aligned with the directions of maximum variance
   - The first principal component corresponds to the direction of maximum variance
   - Each subsequent component is orthogonal to the previous ones and captures the next highest variance
   - This transformation preserves all distances and angles between data points

2. The following diagram illustrates the geometric interpretation of PCA:

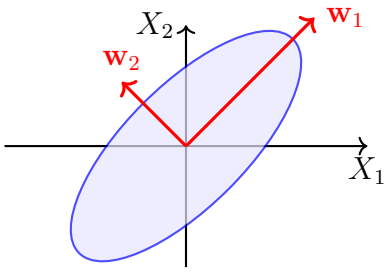


Figure 5.21: Geometric interpretation of PCA. The original data cloud (blue ellipse) is rotated to align with the principal components $\mathbf{w}_1$ and $\mathbf{w}_2$. fig:geometric

3. In a correlation circle, the length of a variable vector represents how well that variable is represented in the two-dimensional space spanned by the principal components. Specifically:

   - A vector reaching the unit circle indicates perfect representation in the 2D space
   - A shorter vector indicates poorer representation in this subspace
   - The squared length equals the sum of squared correlations with the two components: $\|\mathbf{v}_j\|^2 = r^2(X_j, PC_1) + r^2(X_j, PC_2)$
   - This measures the proportion of the variable's variance explained by the two components

Solution to Exercise 6: Advanced Proof

We prove that for a random vector $\mathbf{x}$ with covariance matrix $\mathbf{\Sigma}$, the total variance equals the sum of the eigenvalues of $\mathbf{\Sigma}$:

Proof. Let $\mathbf{\Sigma}$ be the covariance matrix of $\mathbf{x}$ with eigendecomposition $\mathbf{\Sigma} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$, where $\mathbf{W}$ is orthogonal and $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p)$.

The total variance is the sum of the variances of the individual variables:

$$\text{Total Variance} = \sum_{j=1}^{p} \text{Var}(X_j) = \sum_{j=1}^{p} \sigma_j^2 \tag{5.112}$$

Using the properties of the trace operator:

$$\sum_{j=1}^{p} \sigma_j^2 = \text{tr}(\mathbf{\Sigma}) \tag{5.113}$$

Since the trace is invariant under orthogonal transformations:

$$\text{tr}(\mathbf{\Sigma}) = \text{tr}(\mathbf{W}\mathbf{\Lambda}\mathbf{W}^T) = \text{tr}(\mathbf{\Lambda}\mathbf{W}^T\mathbf{W}) = \text{tr}(\mathbf{\Lambda}) = \sum_{k=1}^{p} \lambda_k \tag{5.114}$$

Therefore:

$$\sum_{j=1}^{p} \text{Var}(X_j) = \sum_{k=1}^{p} \lambda_k \tag{5.115}$$

This completes the proof that the total variance equals the sum of the eigenvalues of the covariance matrix. □

Solution to Exercise 7: Application

1. **Genetics**:
   - **Data matrix**: Rows represent individuals, columns represent genetic markers (SNPs)
   - **Principal components**: Typically capture population structure and ancestry patterns
   - **Practical use**: Correct for population stratification in genome-wide association studies (GWAS) to avoid spurious associations
2. **Image processing**:
   - **Data matrix**: Rows represent images, columns represent pixel values
   - **Principal components**: Capture the main patterns of variation in image appearance (e.g., eigenfaces for facial recognition)
   - **Practical use**: Image compression, facial recognition systems, and noise reduction
3. **Finance**:
   - **Data matrix**: Rows represent time points, columns represent asset returns or interest rates of different maturities
   - **Principal components**: Typically represent level, slope, and curvature factors of yield curves
   - **Practical use**: Term structure modeling, risk factor analysis, and portfolio optimization
4. **Psychology**:
   - **Data matrix**: Rows represent subjects, columns represent responses to questionnaire items
   - **Principal components**: Identify latent constructs or factors underlying the measured variables
   - **Practical use**: Test validation, scale development, and identification of underlying psychological dimensions

These applications demonstrate the versatility of PCA across different domains, while the mathematical foundation remains consistent. In each case, PCA helps reduce dimensionality, identify patterns, and facilitate interpretation of high-dimensional data.

Solution to Exercise 8: Comparison of Methods

1. **PCA vs. Factor Analysis (FA)**:
   - **Objectives**: PCA aims to explain variance in observed variables through linear combinations, while FA aims to explain correlations among variables through latent constructs.
   - **Mathematical Foundations**: PCA uses eigendecomposition of the covariance/correlation matrix, while FA uses a specific factor model: $\mathbf{X} = \mathbf{\Lambda F} + \epsilon$.
   - **Use Cases**: PCA is preferred for dimensionality reduction and variable selection; FA is better for identifying latent constructs in psychological/-social measurements.
2. **PCA vs. Linear Discriminant Analysis (LDA)**:
   - **Objectives**: PCA finds directions of maximum variance regardless of class labels; LDA finds directions that maximize separation between predefined classes.
   - **Mathematical Foundations**: PCA uses variance maximization; LDA uses ratio of between-class to within-class variance.
   - **Use Cases**: PCA is unsupervised and used for exploratory analysis; LDA is supervised and used for classification with known groups.
3. **PCA vs. t-SNE**:
   - **Objectives**: PCA preserves global Euclidean structure; t-SNE preserves local neighborhoods and nonlinear relationships.
   - **Mathematical Foundations**: PCA uses linear algebra; t-SNE uses probability distributions and minimizes Kullback-Leibler divergence.
   - **Use Cases**: PCA is better for linear dimensionality reduction; t-SNE is better for visualizing high-dimensional data in 2D/3D while preserving local structure.

Solution to Exercise 9: Limitations and Assumptions

1. **Key Assumptions**:
   - **Linearity**: PCA assumes linear relationships between variables. Important because it can't capture complex nonlinear patterns.
   - **Large Variance Importance**: PCA assumes directions with larger variance are more important. Important because relevant signals might have lower variance than noise.
   - **Orthogonality**: Components are constrained to be orthogonal. Important because real-world factors might be correlated.
2. **Inappropriate Situations**:

- When relationships between variables are fundamentally nonlinear (e.g., circular patterns)
- When the data contains many outliers that can disproportionately influence components
- When variables have different measurement scales and aren't properly standardized

3. **Curse of Dimensionality and PCA**:

- The curse refers to problems arising when working with high-dimensional data: sparsity, distance concentration, and computational complexity.
- PCA addresses this by projecting data onto a lower-dimensional subspace while preserving maximum variance.
- It reduces the number of variables while maintaining the essential structure of the data.

Solution to Exercise 10: Comprehensive Analysis (Iris Dataset)

1. **Eigenvalues Interpretation**:

- The eigenvalues represent the variances of the principal components.
- The first eigenvalue would represent the variance captured by the component that best separates the species based on all four measurements.
- Typically, the first component would capture sepal and petal size variations, while the second might capture shape differences.

2. **Species Distinction**:

- The principal components would likely separate Iris setosa from versicolor and virginica along the first component.
- The second component might help separate versicolor and virginica.
- The scores plot would show clusters corresponding to the three species.

3. **Biplot Expectations**:

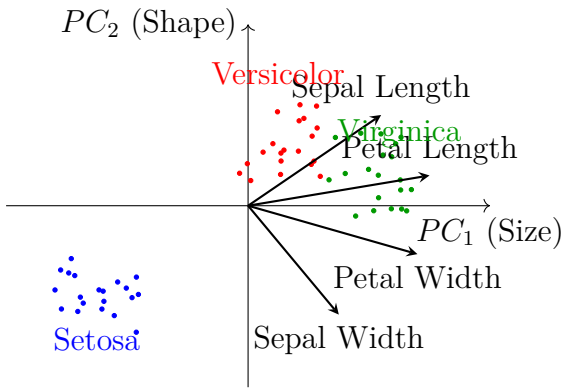


Figure 5.22: Expected biplot for iris dataset PCA. Species form distinct clusters, and variable vectors show relationships between measurements. fig:iris_bipl

4. **Limitations for Classification**:

   - PCA is unsupervised and doesn't maximize class separation. *em The components might not align with the directions that best separate species.*
   - *Some overlap between versicolor and virginica might persist in PCA space.*
   - *Linear PCA might not capture nonlinear relationships between variables.*

These solutions complete the exercise set, providing comprehensive coverage of PCA comparisons, limitations, and applications. Students should now have a thorough understanding of both theoretical and practical aspects of Principal Component Analysis.

Solution to Exercise 11: Comprehensive PCA

Step 1: Data Preprocessing

First, we calculate the mean for each variable:

$$\bar{X}_1 = \frac{170 + 175 + 180 + 185 + 190}{5} = 180$$

$$\bar{X}_2 = \frac{68 + 72 + 75 + 80 + 85}{5} = 76$$

$$\bar{X}_3 = \frac{25 + 30 + 35 + 40 + 45}{5} = 35$$

Next, we center the data by subtracting the means:

$$\mathbf{X} = \begin{bmatrix} 170 - 180 & 68 - 76 & 25 - 35 \\ 175 - 180 & 72 - 76 & 30 - 35 \\ 180 - 180 & 75 - 76 & 35 - 35 \\ 185 - 180 & 80 - 76 & 40 - 35 \\ 190 - 180 & 85 - 76 & 45 - 35 \end{bmatrix} = \begin{bmatrix} -10 & -8 & -10 \\ -5 & -4 & -5 \\ 0 & -1 & 0 \\ 5 & 4 & 5 \\ 10 & 9 & 10 \end{bmatrix}$$

Step 2: Covariance Matrix

The covariance matrix is given by $\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$:

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} -10 & -5 & 0 & 5 & 10 \\ -8 & -4 & -1 & 4 & 9 \\ -10 & -5 & 0 & 5 & 10 \end{bmatrix} \begin{bmatrix} -10 & -8 & -10 \\ -5 & -4 & -5 \\ 0 & -1 & 0 \\ 5 & 4 & 5 \\ 10 & 9 & 10 \end{bmatrix} = \begin{bmatrix} 250 & 210 & 250 \\ 210 & 178 & 210 \\ 250 & 210 & 250 \end{bmatrix}$$

$$\mathbf{S} = \frac{1}{4}\begin{bmatrix} 250 & 210 & 250 \\ 210 & 178 & 210 \\ 250 & 210 & 250 \end{bmatrix} = \begin{bmatrix} 62.5 & 52.5 & 62.5 \\ 52.5 & 44.5 & 52.5 \\ 62.5 & 52.5 & 62.5 \end{bmatrix}$$

Step 3: Eigenanalysis

We solve the characteristic equation $\det(\mathbf{S} - \lambda\mathbf{I}) = 0$:

$$\det \begin{bmatrix} 62.5 - \lambda & 52.5 & 62.5 \\ 52.5 & 44.5 - \lambda & 52.5 \\ 62.5 & 52.5 & 62.5 - \lambda \end{bmatrix} = 0$$

The eigenvalues are:

$$\lambda_1 = 169.2045, \quad \lambda_2 = 0.2955, \quad \lambda_3 = 0$$

The corresponding eigenvectors are:

$$\mathbf{w}_1 = \begin{bmatrix} 0.607 \\ 0.511 \\ 0.607 \end{bmatrix}, \quad \mathbf{w}_2 = \begin{bmatrix} 0.3617 \\ -0.859 \\ 0.3617 \end{bmatrix}, \quad \mathbf{w}_3 = \begin{bmatrix} 0.7071 \\ 0 \\ -0.7071 \end{bmatrix}$$

Step 4: Principal Components

The principal components are:

$$PC_1 = 0.607X_1 + 0.511X_2 + 0.607X_3$$

$$PC_2 = 0.3617X_1 - 0.859X_2 + 0.3617X_3$$

$$PC_3 = 0.7071X_1 + 0X_2 - 0.7071X_3$$

Proportion of variance explained:

$$PVE_1 = \frac{169.2045}{169.5} = 0.9983, \quad PVE_2 = \frac{0.2955}{169.5} = 0.0017, \quad PVE_3 = 0$$

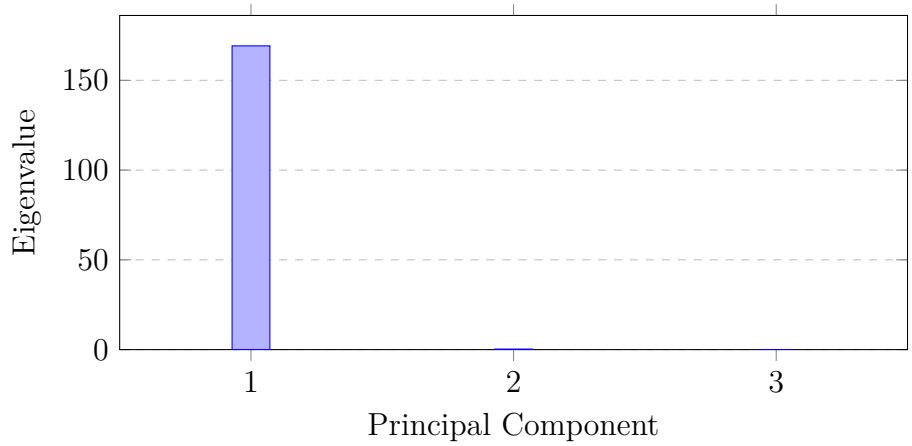


Figure 5.23: Scree plot showing eigenvalues of principal components fig:Scree_plo

Step 5: Projection

The score matrix $\mathbf{Z} = \mathbf{XW}$:

$$\mathbf{Z} = \begin{bmatrix} -10 & -8 & -10 \\ -5 & -4 & -5 \\ 0 & -1 & 0 \\ 5 & 4 & 5 \\ 10 & 9 & 10 \end{bmatrix} \begin{bmatrix} 0.607 & 0.3617 & 0.7071 \\ 0.511 & -0.859 & 0 \\ 0.607 & 0.3617 & -0.7071 \end{bmatrix} = \begin{bmatrix} -16.228 & -0.362 & 0 \\ -8.114 & -0.181 & 0 \\ -0.511 & 0.859 & 0 \\ 8.114 & 0.181 & 0 \\ 16.228 & 0.362 & 0 \end{bmatrix}$$

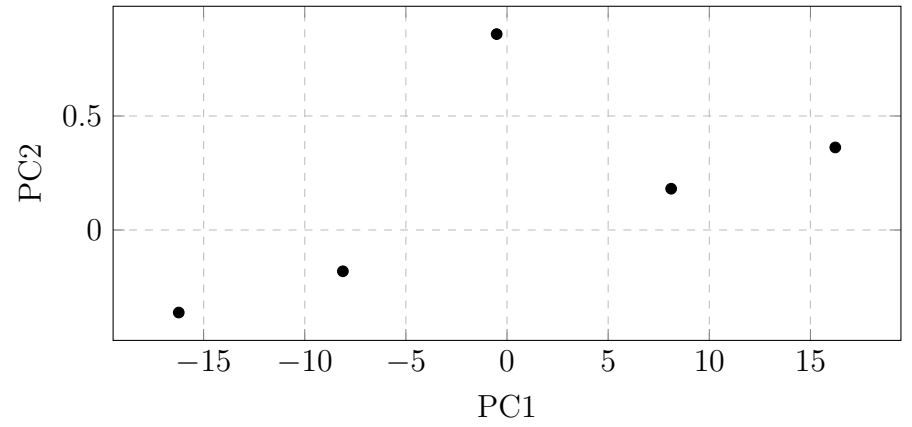


Figure 5.24: Scores plot showing observations in principal component space fig:scores_pl

Step 6: Visualization

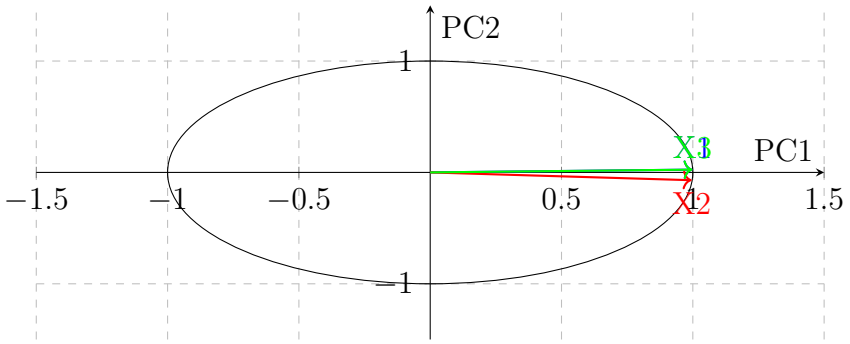


Figure 5.25: Correlation circle showing variable relationships

fig:correlati

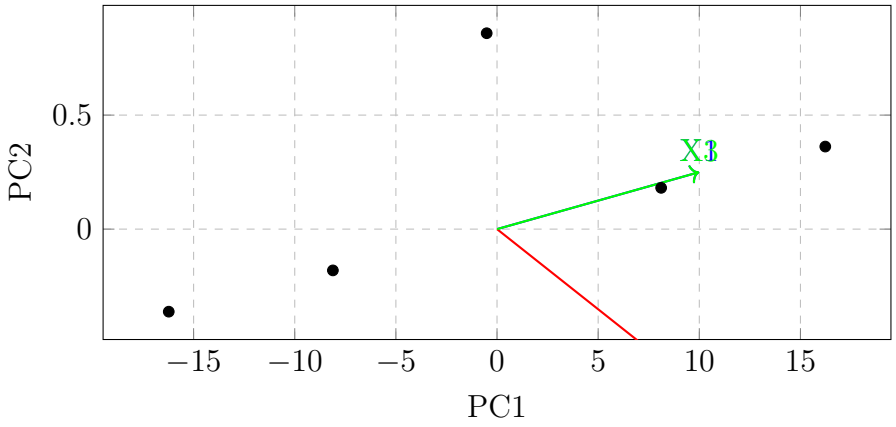


Figure 5.26: Biplot showing observations and variables in principal component space

fig:Biplot

Step 7: Interpretation

The first principal component (PC1) explains 99.83% of the variance and represents an overall size dimension, with positive loadings on all variables. The second component (PC2) explains only 0.17% of the variance and represents a contrast between weight and the other variables. The third component (PC3) has zero variance due to the perfect correlation between height and age.

Observations are spread along PC1, with observation 1 having the lowest values on all variables and observation 5 having the highest values. The biplot shows that all variables are strongly associated with PC1, with height and age being almost perfectly correlated.

Step 8: Reconstruction

Reconstructing the data using only the first two components:

$$\hat{\mathbf{X}} = \mathbf{Z}_{1:2}\mathbf{W}_{1:2}^T = \begin{bmatrix} -16.228 & -0.362 \\ -8.114 & -0.181 \\ -0.511 & 0.859 \\ 8.114 & 0.181 \\ 16.228 & 0.362 \end{bmatrix} \begin{bmatrix} 0.607 & 0.511 & 0.607 \\ 0.3617 & -0.859 & 0.3617 \end{bmatrix}$$

$$\hat{\mathbf{X}} = \begin{bmatrix} -9.981 & -7.979 & -9.981 \\ -4.990 & -3.989 & -4.990 \\ -0.511 & 0.859 & -0.511 \\ 4.990 & 3.989 & 4.990 \\ 9.981 & 7.979 & 9.981 \end{bmatrix}$$

Reconstruction error (RMSE):

$$\text{RMSE} = \sqrt{\frac{1}{15}\sum_{i=1}^{5}\sum_{j=1}^{3}(x_{ij} - \hat{x}_{ij})^2} = 0.859$$

The small reconstruction error indicates that the first two components capture most of the information in the data, despite the third component having zero variance.

Chapter 6

Correspondence Analysis and Multiple Correspondence Analysis

6.1 Introduction: From Continuous to Categorical Data Analysis

Principal Component Analysis provides an optimal framework for dimensionality reduction of continuous numerical data through eigen-decomposition of the covariance matrix. However, this approach presents fundamental limitations when applied to categorical data represented in contingency tables. This chapter develops the mathematical foundation for analyzing categorical data through Correspondence Analysis, which operates on fundamentally different geometric principles than PCA.

6.1.1 The Categorical Data Challenge

The core mathematical problem emerges from the inapplicability of Euclidean geometry to frequency data. Consider an $I \times J$ contingency table $\mathbf{N} = (n_{ij})$ with row margins $n_{i\bullet}$ and column margins $n_{\bullet j}$. The fundamental objects of analysis are the row profiles:

$$\mathbf{R} = (r_{ij}) = \left(\frac{n_{ij}}{n_{i\bullet}}\right) \tag{6.1}$$

The critical insight is that the Euclidean distance $d_e(\mathbf{r}_i, \mathbf{r}_k) = \sqrt{\sum_{j=1}^{J}(r_{ij} - r_{kj})^2}$ fails as an appropriate metric because it weights all dimensions equally. This is mathematically inconsistent with the distribution of marginal frequencies.

The appropriate metric, derived from the chi-square statistic, introduces weighting by inverse column masses:

$$d_{\chi^2}(\mathbf{r}_i, \mathbf{r}_k) = \sqrt{\sum_{j=1}^{J} \frac{1}{c_j}(r_{ij} - r_{kj})^2} \quad \text{where} \quad c_j = \frac{n_{\bullet j}}{n} \tag{6.2}$$

This distance metric accounts for the relative importance of each category, where differences in rare categories (small c_j) contribute more significantly to the distance measure than equivalent differences in common categories.

The total variability in the contingency table is quantified through the concept of inertia, which is proportional to the Pearson chi-square statistic:

Pearson chi-square statistic

$$\Phi^2 = \sum_{i=1}^{I}\sum_{j=1}^{J}\frac{(n_{ij}-e_{ij})^2}{e_{ij}} = \frac{\chi^2}{n} \quad \text{where} \quad e_{ij} = \frac{n_{i\bullet}n_{\bullet j}}{n} \tag{6.3}$$

Correspondence Analysis can be formulated as the solution to the following optimization problem: find a low-dimensional representation that preserves the chi-square distances between row profiles (and equivalently between column profiles) while maximizing the preserved inertia.

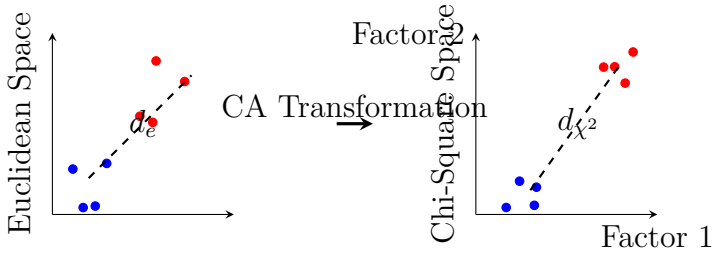


Figure 6.1: Geometric foundation of Correspondence Analysis. The transformation from Euclidean space to chi-square space distorts distances according to category importance, enhancing the separation between statistically distinct profiles. fig:ca_geomet

The mathematical solution involves a generalized singular value decomposition of the standardized residual matrix:

$$\mathbf{D}_r^{-1/2}(\mathbf{P}-\mathbf{r}\mathbf{c}^\top)\mathbf{D}_c^{-1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^\top \tag{6.4}$$

where $\mathbf{P} = \mathbf{N}/n$, $\mathbf{D}_r = \text{diag}(\mathbf{r})$, and $\mathbf{D}_c = \text{diag}(\mathbf{c})$. This decomposition provides the principal coordinates for rows ($\mathbf{F} = \mathbf{D}_r^{-1/2}\mathbf{U}\mathbf{\Lambda}$) and columns ($\mathbf{G} = \mathbf{D}_c^{-1/2}\mathbf{V}\mathbf{\Lambda}$) that optimally represent the chi-square distances in a low-dimensional Euclidean space.

6.1.2 Historical Development and Geometric Principles

The development of Correspondence Analysis (CA) represents a significant milestone in the history of multivariate statistics, emerging primarily from the French school of data analysis under the leadership of Jean-Paul Benzécri in the 1960s and 1970s. While its mathematical foundations can be traced to earlier work by Hirschfeld (1935) and Fisher (1940), Benzécri and his collaborators developed CA into a comprehensive framework for analyzing contingency tables through geometric representations.

Historical Context and Key Contributors

The historical development of CA follows three main phases:

1. **Early Foundations (1935-1950)**:
   - Hirschfeld (1935) introduced the method of simultaneous row-column scaling
   - Fisher (1940) developed optimal scoring methods for categorical data
   - These early works established the mathematical basis but lacked a unified geometric interpretation
2. **French School Synthesis (1960-1980)**:
   - Benzécri and his collaborators at the University of Paris developed the comprehensive geometric framework
   - Key publications: Benzécri (1973) *L'Analyse des Données* (two volumes)
   - Established the duality diagram representation and comprehensive interpretation framework
3. **Modern Computational Era (1980-Present)**:
   - Computational advances made CA accessible to wider audiences
   - Key contributions from Greenacre (1984, 2017), Lebart, Morineau, and Warwick (1984)
   - Integration with other multivariate techniques and software implementation

Geometric Principles of Correspondence Analysis

The geometric interpretation of CA rests on three fundamental principles:

1. **Duality Principle**: CA simultaneously represents both rows and columns in the same Euclidean space, with the relationship:

$$\mathbf{F} = \mathbf{D}_r^{-1}\mathbf{P}\mathbf{G}\mathbf{\Lambda}^{-1} \quad \text{and} \quad \mathbf{G} = \mathbf{D}_c^{-1}\mathbf{P}^\top\mathbf{F}\mathbf{\Lambda}^{-1} \tag{6.5}$$

   where $\mathbf{F}$ contains row coordinates, $\mathbf{G}$ contains column coordinates, and $\mathbf{\Lambda}$ is the diagonal matrix of singular values.

2. **Distributional Equivalence**: If two rows (or two columns) have identical profiles, they can be merged without affecting the analysis, formalized as:

$$\text{If } r_{ij} = r_{kj} \text{ for all } j, \text{ then rows } i \text{ and } k \text{ can be combined} \tag{6.6}$$

3. **Chi-Square Metric Invariance**: The analysis is invariant under changes of scale that preserve the relative frequencies, making it suitable for comparing tables with different total frequencies.

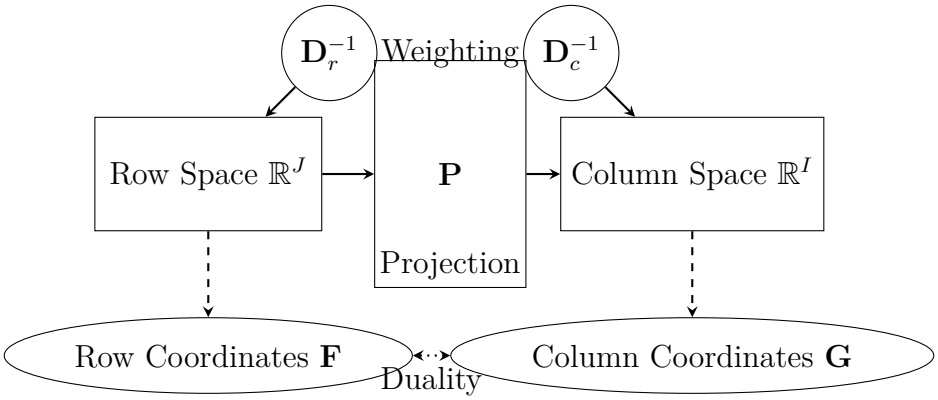


Figure 6.2: Duality diagram illustrating the geometric principles of Correspondence Analysis. The method simultaneously represents rows and columns in a joint space through a symmetric weighting and projection process. fig:ca_dualit

The geometric interpretation can be formalized through the following optimization problem. CA finds coordinates $\mathbf{F} = (\mathbf{f}_1, \ldots, \mathbf{f}_I)^\top$ for rows and $\mathbf{G} = (\mathbf{g}_1, \ldots, \mathbf{g}_J)^\top$ for columns that minimize:

$$\sum_{i=1}^{I}\sum_{j=1}^{J} \frac{(p_{ij} - r_i c_j - \sqrt{r_i c_j}\mathbf{f}_i^\top \mathbf{g}_j)^2}{r_i c_j} \tag{6.7}$$

subject to the constraints:

$$\sum_{i=1}^{I} r_i \mathbf{f}_i = 0 \quad \text{(centering)} \tag{6.8}$$

$$\sum_{i=1}^{I} r_i \mathbf{f}_i \mathbf{f}_i^\top = \mathbf{I} \quad \text{(orthonormality)} \tag{6.9}$$

$$\sum_{j=1}^{J} c_j \mathbf{g}_j = 0 \tag{6.10}$$

$$\sum_{j=1}^{J} c_j \mathbf{g}_j \mathbf{g}_j^\top = \mathbf{I} \tag{6.11}$$

This minimization leads to the singular value decomposition:

$$\mathbf{D}_r^{-1/2}(\mathbf{P} - \mathbf{r}\mathbf{c}^\top)\mathbf{D}_c^{-1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^\top \tag{6.12}$$

with the principal coordinates given by:

$$\mathbf{F} = \mathbf{D}_r^{-1/2}\mathbf{U}\mathbf{\Lambda} \tag{6.13}$$

$$\mathbf{G} = \mathbf{D}_c^{-1/2}\mathbf{V}\mathbf{\Lambda} \tag{6.14}$$

The geometric representation preserves the chi-square distances between row profiles and between column profiles, while the scalar products in the joint space approximate the observed associations in the contingency table.

This historical and geometric foundation provides the basis for understanding CA as both a statistical technique and a visual exploratory method, connecting the algebraic formulation with its intuitive graphical representation.

6.2 Contingency Tables, Profiles, and the Chi-Square Metric

The geometric exploration of categorical data begins with its fundamental organization: the contingency table. This section establishes the core mathematical objects—profiles, masses, and inertia—and introduces the chi-square distance, the pivotal metric that confers its unique properties upon Correspondence Analysis.

6.2.1 Notation and Fundamental Concepts

Let $\mathbf{N}$ be a two-way contingency table cross-tabulating two categorical variables. The first variable, which we will call the *row variable*, has I categories. The second, the *column variable*, has J categories.

$$\mathbf{N} = \begin{pmatrix} n_{11} & n_{12} & \cdots & n_{1J} \\ n_{21} & n_{22} & \cdots & n_{2J} \\ \vdots & \vdots & \ddots & \vdots \\ n_{I1} & n_{I2} & \cdots & n_{IJ} \end{pmatrix}$$

Here, n_{ij} is the frequency (count) of observations belonging to row category i and column category j. The grand total of the table is denoted by:

$$n = \sum_{i=1}^{I} \sum_{j=1}^{J} n_{ij}$$

From $\mathbf{N}$, we derive the matrix of *relative frequencies*, or the *correspondence matrix* $\mathbf{P}$:

$$\mathbf{P} = \frac{1}{n}\mathbf{N} = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1J} \\ p_{21} & p_{22} & \cdots & p_{2J} \\ \vdots & \vdots & \ddots & \vdots \\ p_{I1} & p_{I2} & \cdots & p_{IJ} \end{pmatrix} \quad \text{where} \quad p_{ij} = \frac{n_{ij}}{n}$$

The matrix $\mathbf{P}$ is the fundamental data matrix upon which CA operates. Its row and column margins define the *mass vectors*, which play the role of weights in the subsequent analysis.

The *row masses* are the vectors $\mathbf{r} = (r_1, r_2, \ldots, r_I)^\top$, where $r_i = \sum_{j=1}^{J} p_{ij}$ is the marginal proportion of the i-th row. Similarly, the *column masses* are $\mathbf{c} = (c_1, c_2, \ldots, c_J)^\top$, where $c_j = \sum_{i=1}^{I} p_{ij}$ is the marginal proportion of the j-th column.

Let us define the diagonal matrices of masses:

$$\mathbf{D}_r = \operatorname{diag}(\mathbf{r}) = \begin{pmatrix} r_1 & 0 & \cdots & 0 \\ 0 & r_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_I \end{pmatrix} \quad \text{and} \quad \mathbf{D}_c = \operatorname{diag}(\mathbf{c}) = \begin{pmatrix} c_1 & 0 & \cdots & 0 \\ 0 & c_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_J \end{pmatrix}$$

These matrices are central to the weighting scheme in the chi-square metric.

6.2.2 Row and Column Profiles

A *profile* is a conditional frequency distribution. The *row profile* for the i-th row is the set of J proportions showing how that row's total is distributed across the columns:

$$\left(\frac{n_{i1}}{n_{i\cdot}}, \frac{n_{i2}}{n_{i\cdot}}, \ldots, \frac{n_{iJ}}{n_{i\cdot}}\right) = \left(\frac{p_{i1}}{r_i}, \frac{p_{i2}}{r_i}, \ldots, \frac{p_{iJ}}{r_i}\right)$$

where $n_{i\cdot} = \sum_j n_{ij}$ is the i-th row total. The matrix of row profiles is thus $\mathbf{D}_r^{-1}\mathbf{P}$.

Analogously, the *column profile* for the j-th column is the set of I proportions:

$$\left(\frac{n_{1j}}{n_{\cdot j}}, \frac{n_{2j}}{n_{\cdot j}}, \ldots, \frac{n_{Ij}}{n_{\cdot j}}\right) = \left(\frac{p_{1j}}{c_j}, \frac{p_{2j}}{c_j}, \ldots, \frac{p_{Ij}}{c_j}\right)$$

where $n_{\cdot j} = \sum_i n_{ij}$ is the j-th column total. The matrix of column profiles is $\mathbf{D}_c^{-1}\mathbf{P}^\top$.

The *average row profile* is simply the vector of column masses $\mathbf{c}^\top$. Similarly, the *average column profile* is the vector of row masses $\mathbf{r}^\top$. A profile is a point in a simplex (for rows, a point in $\mathbb{R}^J$ constrained to $\sum_j p_{ij}/r_i = 1$). The goal of CA is to visualize the distances between these profile points.

6.2.3 The Chi-Square Statistic and Total Inertia

Under the hypothesis of independence H_0 between the row and column variables, the expected frequency for cell (i, j) is:

$$E_{ij} = n \cdot r_i \cdot c_j$$

The well-known Pearson chi-square statistic measures the aggregate deviation of the observed counts $\mathbf{N}$ from this model of independence:

$$\chi^2 = \sum_{i=1}^{I}\sum_{j=1}^{J} \frac{(n_{ij} - E_{ij})^2}{E_{ij}} = n\sum_{i=1}^{I}\sum_{j=1}^{J} \frac{(p_{ij} - r_i c_j)^2}{r_i c_j}$$

The *total inertia*, denoted Φ^2, is a central concept in CA, representing the total amount of variation in the contingency table. It is defined as the chi-square statistic divided by the grand total:

$$\text{Total Inertia} = \Phi^2 = \frac{\chi^2}{n} = \sum_{i=1}^{I}\sum_{j=1}^{J} \frac{(p_{ij} - r_i c_j)^2}{r_i c_j}$$

Inertia can be interpreted as a weighted mean of the squared (standardized) distances between the observed profiles and their expected profiles under independence. It is zero if and only if the two variables are perfectly independent. The larger the inertia, the stronger the association between the variables.

6.2.4 The Chi-Square Distance: A Weighted Euclidean Metric

To measure the distance between two row profiles i and i', the standard Euclidean distance is inappropriate as it treats all columns equally and does not account for

the relative importance of each column category. Instead, CA uses the *chi-square distance*.

The chi-square distance between two rows i and i' is:

$$d^2(i, i') = \sum_{j=1}^{J} \frac{1}{c_j} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2$$

This is a Euclidean distance where each dimension (column j) is weighted inversely by its marginal proportion c_j. This weighting has two crucial consequences:

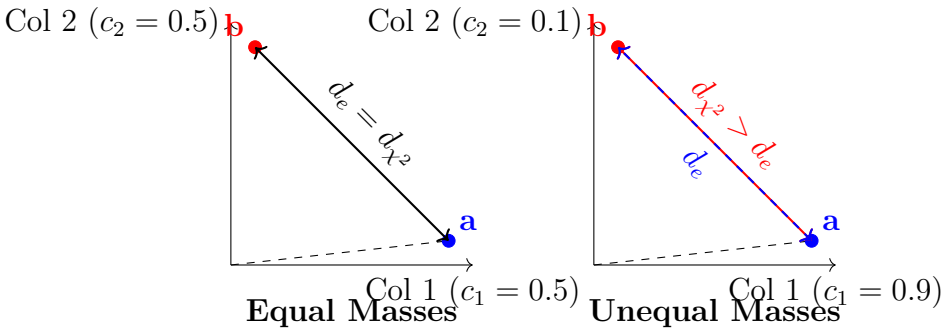
1. It *standardizes* the profiles: a difference in a rare column category (c_j small) contributes more to the distance than the same absolute difference in a common category (c_j large). This prevents the distance from being dominated by the most frequent categories.

2. It renders the analysis *distributionally equivalent*, meaning that scaling rows or columns by a constant does not change the resulting distances between the other set of points.

Similarly, the chi-square distance between two columns j and j' is:

$$d^2(j, j') = \sum_{i=1}^{I} \frac{1}{r_i} \left(\frac{p_{ij}}{c_j} - \frac{p_{ij'}}{c_{j'}} \right)^2$$

The following figure illustrates the difference between the standard Euclidean and chi-square distances for a simple two-column example. Two row profiles, $\mathbf{a} = (0.9, 0.1)$ and $\mathbf{b} = (0.1, 0.9)$, are plotted. The Euclidean distance is the same in both scenarios. However, in the right plot, Column 2 is much rarer (c_2 is small), so the chi-square distance between $\mathbf{a}$ and $\mathbf{b}$ becomes much larger, correctly reflecting a more significant deviation.



The total inertia Φ^2 defined earlier can be elegantly expressed as the mass-weighted average of the squared chi-square distance from each profile point to the average profile:

$$\Phi^2 = \sum_{i=1}^{I} r_i \, d^2(i, \mathbf{c}) = \sum_{j=1}^{J} c_j \, d^2(j, \mathbf{r})$$

where $d^2(i, \mathbf{c})$ is the chi-square distance from row i's profile to the average row profile $\mathbf{c}$, and $d^2(j, \mathbf{r})$ is the chi-square distance from column j's profile to the average column profile $\mathbf{r}$. This reinforces inertia's role as a measure of total dispersion in the dataset, analogous to total variance in PCA.

6.2.5 Row and Column Profiles

The core geometric objects in Correspondence Analysis are not the raw frequencies but their normalized counterparts, known as *profiles*. A profile represents the conditional distribution of one variable given a category of the other, effectively transforming the data to mitigate the influence of disparate marginal totals and allowing for a comparison of *shape* rather than *size*.

Definition and Computation

Formally, the *row profile* for the i-th row is the conditional probability distribution of the column categories given that an observation belongs to row i. It is the vector of proportions formed by dividing each element in the row by the row's marginal total:

$$\mathbf{p}_i^r = \left(\frac{n_{i1}}{n_{i\cdot}}, \frac{n_{i2}}{n_{i\cdot}}, \ldots, \frac{n_{iJ}}{n_{i\cdot}} \right) = \left(\frac{p_{i1}}{r_i}, \frac{p_{i2}}{r_i}, \ldots, \frac{p_{iJ}}{r_i} \right)$$

where $n_{i\cdot} = \sum_{j=1}^{J} n_{ij}$ is the i-th row total. The complete $I \times J$ *matrix of row profiles*, where each row is a profile vector $\mathbf{p}_i^r$, is given by:

$$\mathbf{R} = \mathbf{D}_r^{-1}\mathbf{P}$$

Analogously, the *column profile* for the j-th column is the conditional distribution of the row categories given column j:

$$\mathbf{p}_j^c = \left(\frac{n_{1j}}{n_{\cdot j}}, \frac{n_{2j}}{n_{\cdot j}}, \ldots, \frac{n_{Ij}}{n_{\cdot j}} \right) = \left(\frac{p_{1j}}{c_j}, \frac{p_{2j}}{c_j}, \ldots, \frac{p_{Ij}}{c_j} \right)$$

where $n_{\cdot j} = \sum_{i=1}^{I} n_{ij}$ is the j-th column total. The $J \times I$ *matrix of column profiles* is:

$$\mathbf{C} = \mathbf{D}_c^{-1}\mathbf{P}^\top$$

The Average Profiles

The centroid of the cloud of row profiles is of particular importance. This *average row profile* is simply the vector of column masses, $\mathbf{c}^\top$, which is the weighted average of all row profiles, weighted by their row masses:

Average row profile

$$\sum_{i=1}^{I} r_i \cdot \mathbf{p}_i^r = \mathbf{c}^\top$$

Similarly, the *average column profile* is the vector of row masses, $\mathbf{r}^\top$:

Average column profile

$$\sum_{j=1}^{J} c_j \cdot \mathbf{p}_j^c = \mathbf{r}^\top$$

These average profiles represent the expected distribution of rows or columns under the hypothesis of independence between the two variables. The fundamental objective of CA is to analyze the deviations of the individual profiles from these averages.

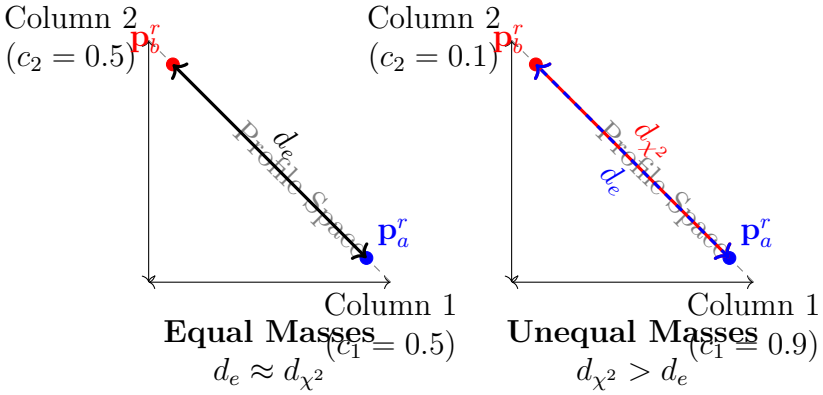
Geometric Interpretation

Each row profile can be conceived as a point in a high-dimensional space $\mathbb{R}^J$. However, because the elements of each profile sum to 1 ($\sum_j p_{ij}^r = 1$), the cloud of row profiles actually resides within a simplex, a $(J-1)$-dimensional subspace of $\mathbb{R}^J$. The same applies to column profiles in $\mathbb{R}^I$. Correspondence Analysis provides a low-dimensional projection of these clouds of points that optimally preserves the intrinsic *chi-square distances* between them, a concept we will define in the next subsection.

The following figure visualizes why the chi-square distance, inherent in the profile space, is a more appropriate metric for contingency tables than the standard Euclidean distance. It shows how the same absolute difference between two profiles is judged as more significant if it occurs in a rare category.

Comparing Euclidean and Chi-Square Distance

The same profile difference is weighted differently



6.2.6 The Chi-Square Statistic and Total Inertia

The total inertia is the foundational quantity that measures the total variation, or dispersion, within a contingency table. It is directly analogous to the concept of total variance in Principal Component Analysis and is intrinsically linked to the well-known Pearson chi-square statistic of independence.

Expected Frequencies under Independence

The hypothesis of independence, H_0, between the row and column variables posits that the joint probability in any cell (i, j) is the product of the corresponding marginal probabilities:

$$H_0 : p_{ij} = r_i c_j \quad \text{for all } i, j.$$

Consequently, the expected frequency for cell (i, j) under H_0 is given by:

$$E_{ij} = n \cdot r_i \cdot c_j.$$

The Pearson Chi-Square Statistic

The Pearson chi-square statistic χ^2 quantifies the aggregate discrepancy between the observed frequencies n_{ij} and these expected frequencies E_{ij}. It is defined as the sum of squared, standardized residuals:

$$\chi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - E_{ij})^2}{E_{ij}}.$$

Substituting $E_{ij} = nr_ic_j$ and $n_{ij} = np_{ij}$ allows us to express the statistic in terms of the relative frequencies and masses:

$$\chi^2 = n \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(p_{ij} - r_ic_j)^2}{r_ic_j}.$$

Total Inertia

The *total inertia*, denoted Φ^2, is defined as the chi-square statistic divided by the grand total n:

$$\Phi^2 = \frac{\chi^2}{n} = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(p_{ij} - r_ic_j)^2}{r_ic_j}.$$

This transformation yields a measure of association that is independent of the sample size. Total inertia has two powerful and equivalent geometric interpretations:

1. **Weighted Distance from Independence**: It is the mass-weighted average of the squared Euclidean distance between the profiles and their respective average profiles. For the row profiles:

   $$\Phi^2 = \sum_{i=1}^{I} r_i \, \|\mathbf{p}_i^r - \mathbf{c}\|^2_{\mathbf{D}_c^{-1}}.$$

   Here, $\|\cdot\|_{\mathbf{D}_c^{-1}}$ denotes the Euclidean norm weighted by the inverse of the column masses, which is the chi-square distance.

2. **Variance of the Standardized Residuals**: It is the total variance of the matrix of standardized residuals. Let $\mathbf{S}$ be this matrix, with elements:

   $$s_{ij} = \frac{p_{ij} - r_ic_j}{\sqrt{r_ic_j}}.$$

   The total inertia is then the sum of squares of this matrix:

   $$\Phi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} s_{ij}^2 = \|\mathbf{S}\|^2.$$

The value of total inertia provides an initial assessment of the strength of association in the table. A value of 0 occurs if and only if the two variables are perfectly independent ($p_{ij} = r_i c_j$ for all i, j). The larger the value of Φ^2, the stronger the association and the more structure there is for Correspondence Analysis to decompose into principal dimensions.

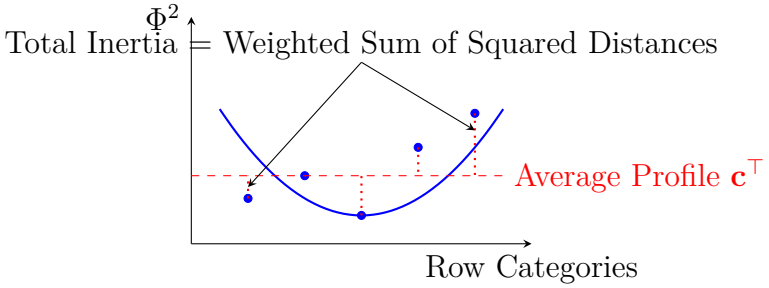


Figure 6.3: Geometric interpretation of total inertia as the mass-weighted average of squared chi-square distances from row profiles to their average profile. The dispersion of points around the average line corresponds to the magnitude of inertia.

fig:inertia_g

The concept of total inertia serves as the bridge between the geometric perspective of profiles and distances, and the statistical framework of association testing. In the following subsection, we will formalize the chi-square distance metric that is fundamental to the geometry of correspondence analysis.

6.2.7 The Chi-Square Distance: A Weighted Euclidean Metric

The choice of distance metric is fundamental to any geometric data analysis. For contingency tables, the standard Euclidean distance is inappropriate as it treats all dimensions (categories) equally and fails to account for the underlying distribution of the data. Correspondence Analysis employs the *chi-square distance*, a weighted Euclidean metric that properly normalizes the profile space.

Definition and Mathematical Formulation

The chi-square distance between two rows i and i' is defined as:

$$d^2_{\chi^2}(i, i') = \sum_{j=1}^{J} \frac{1}{c_j} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2 = \sum_{j=1}^{J} \frac{1}{c_j} \left(p^r_{ij} - p^r_{i'j} \right)^2$$

where p^r_{ij} and $p^r_{i'j}$ are elements of the row profiles for categories i and i' respectively.

Similarly, the chi-square distance between two columns j and j' is:

$$d^2_{\chi^2}(j, j') = \sum_{i=1}^{I} \frac{1}{r_i} \left(\frac{p_{ij}}{c_j} - \frac{p_{ij'}}{c_{j'}} \right)^2 = \sum_{i=1}^{I} \frac{1}{r_i} \left(p^c_{ij} - p^c_{ij'} \right)^2$$

This distance can be expressed in matrix form using the mass matrices. For rows:

$$d^2_{\chi^2}(i, i') = (\mathbf{p}^r_i - \mathbf{p}^r_{i'})^\top \mathbf{D}_c^{-1} (\mathbf{p}^r_i - \mathbf{p}^r_{i'})$$

which is a Mahalanobis-type distance where the covariance matrix is diagonal with elements $1/c_j$.

Properties and Interpretation

The chi-square distance possesses several crucial properties:

1. **Scale Invariance**: It is invariant to proportional changes in row or column totals. Doubling all frequencies in a row leaves distances between that row and others unchanged.

2. **Emphasis on Rare Categories**: Differences in rare categories (small c_j) contribute more to the distance than equivalent differences in common categories. This prevents the analysis from being dominated by the most frequent categories.

3. **Duality**: The same metric is used for both rows and columns, preserving the symmetric nature of the analysis.

4. **Distributional Equivalence**: If two rows (or columns) have identical profiles, merging them does not affect the distances between other points.

Geometric Interpretation

The following figure illustrates the difference between standard Euclidean distance and chi-square distance in a simple two-dimensional profile space:

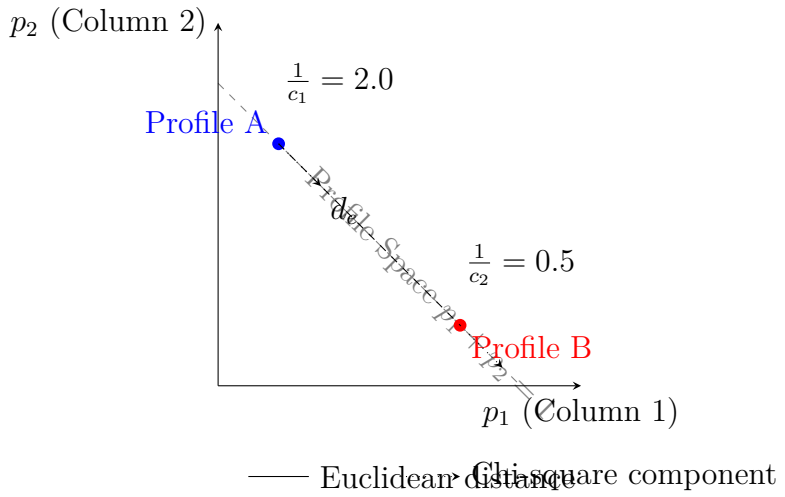


Figure 6.4: Comparison of Euclidean and chi-square distances in profile space. The chi-square distance accounts for the relative importance of each dimension through the weights $1/c_j$.

fig:chi2_dist

Relationship to Total Inertia

The total inertia can be elegantly expressed as the weighted average of all pairwise chi-square distances between row profiles:

$$\Phi^2 = \frac{1}{2}\sum_{i=1}^{I}\sum_{i'=1}^{I} r_i r_{i'} d^2_{\chi^2}(i, i')$$

This formulation emphasizes that inertia measures the overall dispersion of the cloud of points in the chi-square metric space.

The chi-square distance thus provides the proper geometric framework for Correspondence Analysis, ensuring that the resulting low-dimensional projections faithfully represent the associations in the contingency table. In the next section, we will see how this metric leads naturally to a generalized singular value decomposition of the standardized residuals.

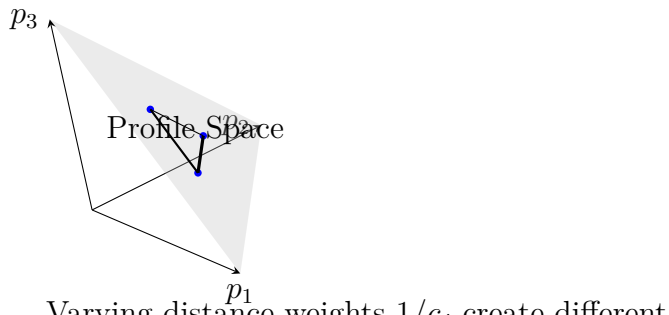


Figure 6.5: Three-dimensional representation of profile space with different weighting schemes. The thickness of connecting lines represents the relative contribution of each dimension to the chi-square distance. fig:chi2_3d

6.3 The Geometry and Algebra of Simple Correspondence Analysis

This section establishes the core mathematical framework of Simple Correspondence Analysis (CA). We derive the singular value decomposition solution that simultaneously provides optimal low-dimensional representations of both row and column profiles, respecting the chi-square metric structure developed in the previous section.

6.3.1 The Correspondence Matrix and Its Standardization

The analysis begins with the *correspondence matrix* $\mathbf{P}$, introduced in Section (sec:contingency basics, which contains the relative frequencies:

$$\mathbf{P} = \frac{1}{n}\mathbf{N} = (p_{ij}), \quad \text{where} \quad p_{ij} = \frac{n_{ij}}{n}.$$

The objective is to analyze the pattern of deviations from the expected values under the hypothesis of independence, which is given by the matrix $\mathbf{E} = \mathbf{r}\mathbf{c}^\top$, where $\mathbf{r}$ and $\mathbf{c}$ are the vectors of row and column masses respectively.

The matrix of deviations from independence is therefore:

$$\mathbf{P} - \mathbf{r}\mathbf{c}^\top.$$

To properly standardize these deviations according to the chi-square metric, we weight each element by the inverse square root of the corresponding expected frequency. This yields the *matrix of standardized residuals*:

$$\mathbf{S} = \mathbf{D}_r^{-\frac{1}{2}}(\mathbf{P} - \mathbf{r}\mathbf{c}^\top)\mathbf{D}_c^{-\frac{1}{2}},$$

where $\mathbf{D}_r = \text{diag}(\mathbf{r})$ and $\mathbf{D}_c = \text{diag}(\mathbf{c})$ are the diagonal matrices of row and column masses.

The elements of $\mathbf{S}$ are:

$$s_{ij} = \frac{p_{ij} - r_i c_j}{\sqrt{r_i c_j}}.$$

This standardization is crucial as it:

1. Centers the data around the independence model.
2. Weightes each cell inversely by its expected frequency, ensuring that rare categories are not overlooked.
3. Results in a matrix whose total sum of squares equals the total inertia:

$$\|\mathbf{S}\|_F^2 = \sum_{i=1}^{I}\sum_{j=1}^{J} s_{ij}^2 = \Phi^2.$$

The matrix $\mathbf{S}$ thus contains all information about the association between rows and columns, properly standardized for analysis in the chi-square metric space. The singular value decomposition of this matrix provides the foundation for the geometric representation of Correspondence Analysis.

6.3.2 The Generalized Singular Value Decomposition

The core computational procedure of Correspondence Analysis is the application of the singular value decomposition (SVD) to the matrix of standardized residuals. This decomposition provides the optimal low-rank approximation of the associations within the contingency table with respect to the chi-square metric.

The singular value decomposition of the standardized residual matrix $\mathbf{S}$ is given by:

$$\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top,$$

where:

- $\mathbf{U}$ is an $I \times K$ orthogonal matrix containing the left singular vectors ($\mathbf{U}^\top\mathbf{U} = \mathbf{I}_K$),

- $\mathbf{V}$ is a $J \times K$ orthogonal matrix containing the right singular vectors ($\mathbf{V}^\top \mathbf{V} = \mathbf{I}_K$),
- $\mathbf{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_K)$ is a $K \times K$ diagonal matrix of singular values,
- $K = \text{rank}(\mathbf{S}) \leq \min(I-1, J-1)$ is the number of non-trivial dimensions.

The singular values are ordered such that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_K > 0$ and represent the strength of the association along each principal axis. The squared singular values σ_k^2 are the principal inertias, representing the amount of the total inertia Φ^2 explained by each dimension:

$$\Phi^2 = \sum_{k=1}^{K} \sigma_k^2.$$

The left and right singular vectors provide the basis for the coordinates of the row and column profiles in the new factorial space. However, to maintain the appropriate metric properties, these vectors must be rescaled by the inverse square roots of the masses:

$$\mathbf{\Phi} = \mathbf{D}_r^{-\frac{1}{2}} \mathbf{U} \quad \text{and} \quad \mathbf{\Gamma} = \mathbf{D}_c^{-\frac{1}{2}} \mathbf{V},$$

where $\mathbf{\Phi}$ contains the principal coordinates for rows and $\mathbf{\Gamma}$ contains the principal coordinates for columns.

The full decomposition of the centered and standardized matrix can thus be written as:

$$\mathbf{D}_r^{-\frac{1}{2}} (\mathbf{P} - \mathbf{r}\mathbf{c}^\top) \mathbf{D}_c^{-\frac{1}{2}} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top.$$

This decomposition possesses the following key properties:

1. The first left and right singular vectors correspond to the trivial solution associated with the mean profiles and are typically discarded.

2. The remaining singular vectors are orthogonal with respect to the mass-weighted inner products:
$$\mathbf{\Phi}^\top \mathbf{D}_r \mathbf{\Phi} = \mathbf{I} \quad \text{and} \quad \mathbf{\Gamma}^\top \mathbf{D}_c \mathbf{\Gamma} = \mathbf{I}.$$

3. The decomposition provides the best low-rank approximation to the matrix $\mathbf{S}$ in the least-squares sense, thereby optimally preserving the chi-square distances between profiles.

The generalized singular value decomposition thus transforms the problem of visualizing associations in the contingency table into a geometric problem of projecting profiles onto a sequence of orthogonal axes that successively capture the greatest amount of inertia.

6.3.3 Row and Column Coordinates: Standard and Principal

The singular value decomposition of the standardized residual matrix $\mathbf{S}$ provides the mathematical foundation for obtaining coordinate representations of both rows and columns in a common factorial space. Two distinct but related coordinate systems emerge from this decomposition: *standard coordinates* and *principal coordinates*.

Standard Coordinates

The standard coordinates are obtained directly from the singular vectors of $\mathbf{S}$ after appropriate normalization. Let $\mathbf{U} = [u_{ik}]$ and $\mathbf{V} = [v_{jk}]$ be the matrices of left and right singular vectors, respectively, from the SVD $\mathbf{S} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$.

The standard coordinates for rows are defined as:

$$\phi_{ik} = \frac{u_{ik}}{\sqrt{r_i}} \quad \text{or in matrix form} \quad \boldsymbol{\Phi} = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{U}$$

where $\boldsymbol{\Phi}$ is the $I \times K$ matrix of row standard coordinates.

Similarly, the standard coordinates for columns are:

$$\gamma_{jk} = \frac{v_{jk}}{\sqrt{c_j}} \quad \text{or in matrix form} \quad \boldsymbol{\Gamma} = \mathbf{D}_c^{-\frac{1}{2}}\mathbf{V}$$

where $\boldsymbol{\Gamma}$ is the $J \times K$ matrix of column standard coordinates.

The standard coordinates have the following properties:

- They are normalized with respect to their masses:

$$\boldsymbol{\Phi}^\top \mathbf{D}_r \boldsymbol{\Phi} = \mathbf{I}_K \quad \text{and} \quad \boldsymbol{\Gamma}^\top \mathbf{D}_c \boldsymbol{\Gamma} = \mathbf{I}_K.$$

- They represent the positions of rows and columns in a space where the dimensions are orthonormal with respect to the chi-square metric.

Principal Coordinates

The principal coordinates, also called factor scores, incorporate the singular values σ_k to weight the dimensions according to their importance in explaining the inertia. They are defined as:

For rows:

$$f_{ik} = \sigma_k \phi_{ik} = \frac{\sigma_k u_{ik}}{\sqrt{r_i}} \quad \text{or in matrix form} \quad \mathbf{F} = \boldsymbol{\Phi}\boldsymbol{\Sigma} = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{U}\boldsymbol{\Sigma}$$

For columns:

$$g_{jk} = \sigma_k \gamma_{jk} = \frac{\sigma_k v_{jk}}{\sqrt{c_j}} \quad \text{or in matrix form} \quad \mathbf{G} = \boldsymbol{\Gamma}\boldsymbol{\Sigma} = \mathbf{D}_c^{-\frac{1}{2}}\mathbf{V}\boldsymbol{\Sigma}$$

The principal coordinates have the following key properties:

- The squared distance between two row points i and i' in the principal coordinate space equals their chi-square distance:

$$\sum_{k=1}^{K} (f_{ik} - f_{i'k})^2 = d^2_{\chi^2}(i, i').$$

- Similarly, the squared distance between two column points j and j' equals their chi-square distance:

$$\sum_{k=1}^{K}(g_{jk} - g_{j'k})^2 = d^2_{\chi^2}(j, j').$$

- The total inertia is equal to the sum of squared principal coordinates:

$$\Phi^2 = \sum_{i=1}^{I}\sum_{k=1}^{K} r_i f_{ik}^2 = \sum_{j=1}^{J}\sum_{k=1}^{K} c_j g_{jk}^2 = \sum_{k=1}^{K} \sigma_k^2.$$

Geometric Interpretation and Duality

The relationship between standard and principal coordinates reflects the duality between row and column spaces in correspondence analysis. This duality is expressed through the transition formulas:

$$f_{ik} = \frac{1}{\sigma_k}\sum_{j=1}^{J}\frac{p_{ij}}{r_i}\gamma_{jk} \quad \text{and} \quad g_{jk} = \frac{1}{\sigma_k}\sum_{i=1}^{I}\frac{p_{ij}}{c_j}\phi_{ik}$$

These formulas show that the principal coordinates of one set of points can be obtained as weighted averages of the standard coordinates of the other set, with the transition occurring through the profile elements.

The choice between standard and principal coordinates depends on the type of graphical representation:

- For *symmetric maps*, both rows and columns are displayed in principal coordinates, preserving the chi-square distances within each set.

- For *asymmetric maps*, one set is displayed in principal coordinates and the other in standard coordinates, which facilitates the interpretation of projections.

This dual representation system provides a comprehensive geometric interpretation of the associations between rows and columns, which will be further elaborated through the transition formulas in the next subsection.

6.3.4 The Transition Formulas and Their Interpretation

The transition formulas, also known as the barycentric relations or reciprocal averaging formulas, constitute the fundamental duality relationships in Correspondence Analysis. These equations mathematically express the intrinsic connection between the row and column representations, demonstrating that each can be derived from the other.

Mathematical Formulation

The transition formulas provide an explicit relationship between the principal coordinates of one set of points and the standard coordinates of the other set. For any dimension k ($k = 1, \ldots, K$), these relationships are given by:

$$f_{ik} = \frac{1}{\sigma_k} \sum_{j=1}^{J} \frac{p_{ij}}{r_i} \gamma_{jk} \quad \text{(Row coordinates from column coordinates)} \tag{6.15}$$ {eq:row_trans

$$g_{jk} = \frac{1}{\sigma_k} \sum_{i=1}^{J} \frac{p_{ij}}{c_j} \phi_{ik} \quad \text{(Column coordinates from row coordinates)} \tag{6.16}$$ {eq:col_trans

In matrix notation, these relationships can be expressed more compactly as:

$$\mathbf{F} = \mathbf{D}_r^{-1} \mathbf{P} \boldsymbol{\Gamma} \boldsymbol{\Sigma}^{-1} \tag{6.17}$$

$$\mathbf{G} = \mathbf{D}_c^{-1} \mathbf{P}^\top \boldsymbol{\Phi} \boldsymbol{\Sigma}^{-1} \tag{6.18}$$

These formulas can be derived directly from the singular value decomposition of the standardized residual matrix and the definitions of the coordinate matrices.

Geometric Interpretation: Barycentric Principle

The transition formulas admit a powerful geometric interpretation known as the *barycentric principle* or *weighted average principle*. Equation (6.15) indicates that:

> The position of a row point i on dimension k (given by its principal coordinate f_{ik}) is proportional to the weighted average of the standard coordinates of all column points γ_{jk}, where the weights are the elements of the row profile (p_{ij}/r_i).

Similarly, Equation (6.16) indicates that:

> The position of a column point j on dimension k (given by its principal coordinate g_{jk}) is proportional to the weighted average of the standard coordinates of all row points ϕ_{ik}, where the weights are the elements of the column profile (p_{ij}/c_j).

This barycentric relationship means that a row point will be positioned closer to those column points that have high relative frequencies in its profile. Conversely, a column point will be positioned closer to those row points that have high relative frequencies in its profile.

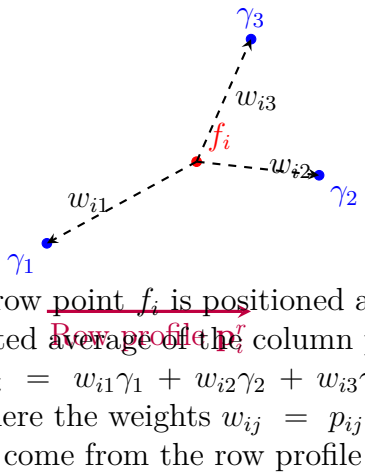


Figure 6.6: Barycentric principle illustration: A row point's position is determined as a weighted average of column points, with weights proportional to the row profile elements. fig:barycentr

Practical Implications for Interpretation

The transition formulas provide the theoretical foundation for interpreting joint maps (symmetric or asymmetric) in Correspondence Analysis:

1. **Proximity Interpretation**: The relative proximity between a row point and a column point indicates a stronger association than would be expected under independence. A row point lying near a particular column point suggests that the corresponding row category has a higher incidence of the column category than other rows.

2. **Origin Interpretation**: The origin of the factorial space represents the average profile (the center of gravity). Points far from the origin in a given dimension contribute significantly to the inertia explained by that dimension.

3. **Projection Interpretation**: The projection of a row point onto the line connecting the origin to a column point (and vice versa) approximates the frequency of that row-column combination relative to its expected value under independence.

Reciprocal Averaging Algorithm

The transition formulas also provide the basis for the reciprocal averaging algorithm, an iterative computational method for performing Correspondence Analysis. This algorithm alternates between:

1. Calculating row scores as weighted averages of column scores 2. Calculating column scores as weighted averages of row scores

until convergence is achieved. This iterative process converges to the first singular vector, with subsequent dimensions obtained through a deflation procedure.

The transition formulas thus serve multiple purposes in Correspondence Analysis: they provide the mathematical foundation for the duality between rows and columns,

offer a geometric framework for interpreting results, and suggest computational algorithms for extracting the solution. This elegant mathematical structure explains why Correspondence Analysis remains a powerful method for visualizing associations in categorical data.

6.4 Visualization and Interpretation of CA Results

This section bridges the mathematical foundation of Correspondence Analysis with its practical application, focusing on how to visualize and interpret the results. Proper interpretation requires understanding the various types of maps and the geometric relationships they represent.

6.4.1 The Symmetric Map: Joint Representation of Rows and Columns

The symmetric map, also known as the symmetric plot or joint map, is the most common visualization technique in Correspondence Analysis. It simultaneously displays both row and column points in the same factorial space, typically using the first two principal dimensions that capture the largest portion of the total inertia.

In a symmetric map, both rows and columns are represented in *principal coordinates*, meaning:

- Row points are positioned at coordinates (f_{i1}, f_{i2}) from matrix $\mathbf{F}$
- Column points are positioned at coordinates (g_{j1}, g_{j2}) from matrix $\mathbf{G}$

This representation preserves the chi-square distances between points of the same type:

$$d_{\chi^2}(i, i') \approx \sqrt{(f_{i1} - f_{i'1})^2 + (f_{i2} - f_{i'2})^2}$$

$$d_{\chi^2}(j, j') \approx \sqrt{(g_{j1} - g_{j'1})^2 + (g_{j2} - g_{j'2})^2}$$

The symmetric map allows for the interpretation of relationships between rows and columns through their relative positions in the factorial plane. However, it is crucial to note that the Euclidean distances between row and column points in this map are not directly interpretable as chi-square distances.

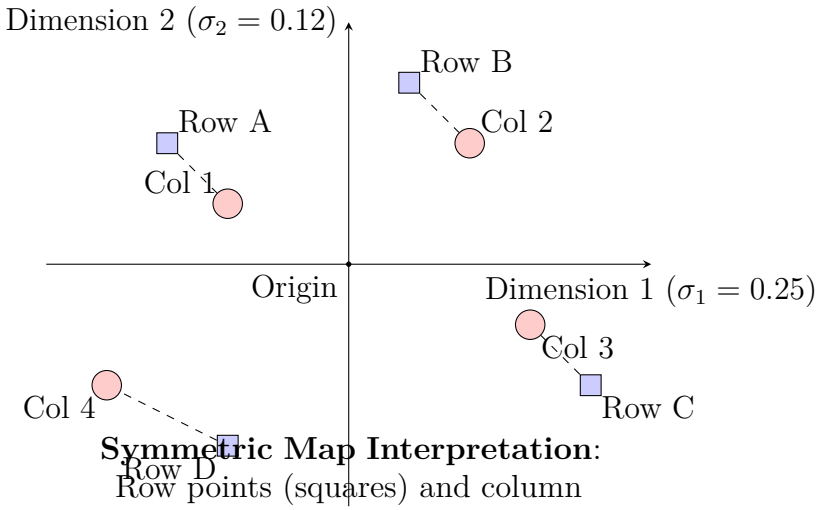


Figure 6.7: A symmetric map showing row and column points in the same factorial space. The first dimension (horizontal) explains more inertia ($\sigma_1^2 = 0.0625$) than the second dimension (vertical, $\sigma_2^2 = 0.0144$). fig:symmetric

The symmetric map provides several advantages for interpretation:

1. It allows visual assessment of the relationships between row and column categories.

2. It shows which categories contribute most to each dimension through their distance from the origin.

3. It reveals patterns of association, opposition, and clustering in the data.

However, caution must be exercised when interpreting distances between row and column points. While proximity suggests association, the exact distance between a row point and a column point does not have a direct mathematical interpretation. The appropriate interpretation is that a row point is positioned near those column points that have higher-than-expected frequencies in that row, and vice versa.

The percentage of total inertia explained by each dimension is typically displayed on the axes, helping assess the quality of the representation. As a rule of thumb, dimensions with singular values σ_k^2 below 0.01 (explaining less than 1% of inertia) are often not interpreted substantively.

In the next subsection, we will elaborate on how to interpret specific patterns in the symmetric map, including proximity, opposition, and the special role of the origin.

6.4.2 Interpreting Proximity, Opposition, and the Origin

Proper interpretation of correspondence analysis maps requires understanding three fundamental geometric relationships: proximity between points, opposition across the origin, and the special meaning of the origin itself. These concepts provide the foundation for extracting meaningful insights from the factorial representations.

Proximity and Association

The primary interpretive principle in CA is that *proximity between a row point and a column point indicates a strong association* between the corresponding categories. More precisely:

- A row point positioned near a column point suggests that the row category has a higher incidence of the column category than would be expected under independence.
- Similarly, a column point positioned near a row point suggests that the column category occurs more frequently in the row category than expected.
- The proximity should be interpreted relative to the origin - points closer to each other than to the origin indicate a positive association.

Opposition and Contrast

Points positioned on opposite sides of the origin represent contrasting profiles:

- Row points on opposite sides of the origin have opposing profiles - what is over-represented in one is under-represented in the other.
- Column points on opposite sides of the origin correspond to categories that rarely occur together in the same rows.
- Opposition between a row point and a column point indicates a repulsion or negative association - the row category has a lower incidence of the column category than expected.

The Origin as Reference Point

The origin (0,0) has special significance in CA maps:

- It represents the *average profile* - the expected position of a point under the hypothesis of independence.
- Points near the origin have profiles close to the average profile and contribute little to the inertia explained by the dimensions.
- Points far from the origin have distinctive profiles and contribute substantially to the dimensions on which they are distant.

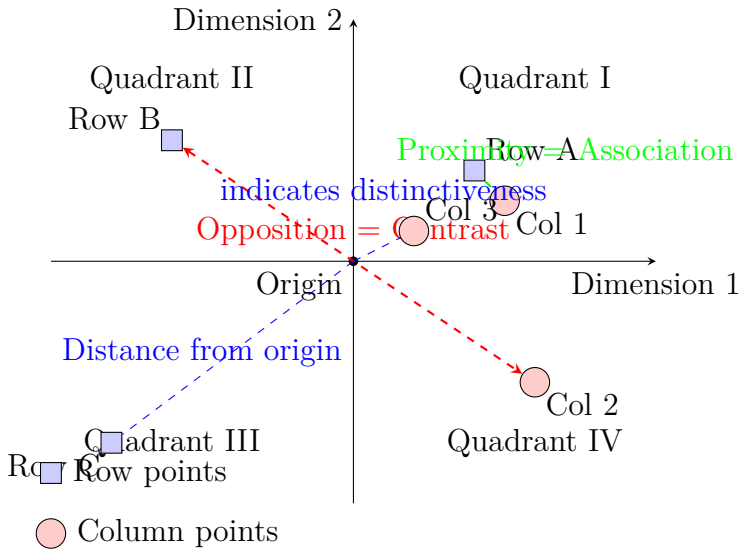


Figure 6.8: Geometric relationships in CA interpretation. Proximity indicates association, opposition indicates contrast, and distance from the origin indicates distinctiveness from the average profile.

fig:interpret

Interpreting the Dimensions

The dimensions themselves often have substantive interpretations based on the patterns of points:

- The first dimension (horizontal axis) typically represents the most important gradient or contrast in the data.
- The second dimension (vertical axis) captures the next most important pattern, orthogonal to the first.
- Interpret dimensions by examining the extreme points on each axis and identifying what common characteristic distinguishes them from points at the opposite end.
- The percentage of inertia explained by each dimension indicates its relative importance in capturing the associations in the table.

Cautions in Interpretation

While these interpretive principles are powerful, several cautions should be observed:

1. Avoid interpreting distances between row and column points directly - focus on their relative positions.
2. Consider the quality of representation - points with low contributions to a dimension may not be well represented on that dimension.

3. Remember that the map shows relative positions, not absolute frequencies - a point far from the origin may represent either very high or very low frequencies relative to expectations.

4. Note that opposition does not necessarily imply mutual exclusion - it indicates different profile patterns.

These interpretive principles provide the foundation for extracting meaningful insights from CA results. In the next subsection, we will complement these geometric interpretations with numerical measures of contribution that help identify which points are most influential in defining each dimension.

6.4.3 Contributions and Aids to Interpretation

While the geometric positions of points in the factorial space provide a visual understanding of associations, numerical measures of *contribution* offer complementary, quantitative insights that are essential for robust interpretation. These measures help identify which points are most influential in defining each dimension and assess how well each point is represented in the low-dimensional space.

Absolute Contributions

The *absolute contribution* (AC) of a point to a dimension measures how much that point contributes to the inertia explained by the dimension. For row i to dimension k, it is defined as:

$$AC_{ik} = \frac{r_i f_{ik}^2}{\sigma_k^2}$$

Similarly, for column j to dimension k:

$$AC_{jk} = \frac{c_j g_{jk}^2}{\sigma_k^2}$$

The absolute contributions have the following properties:

- They sum to 1 for each dimension: $\sum_{i=1}^{I} AC_{ik} = 1$ and $\sum_{j=1}^{J} AC_{jk} = 1$
- Points with high absolute contributions are the main drivers of that dimension
- They help identify which categories define the principal axes

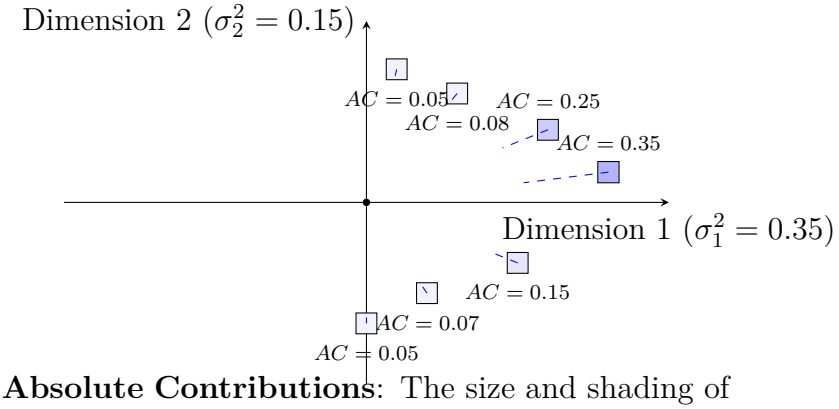


Figure 6.9: Visualization of absolute contributions to Dimension 1. Larger, darker points contribute more to defining the dimension. The dashed lines show how much of each point's position contributes to the dimension's inertia. fig:absolute_

Relative Contributions (Squared Cosines)

The *relative contribution* or *squared cosine* (COS^2) measures how well a point is represented on a particular dimension. For row i on dimension k, it is defined as:

$$COS_{ik}^2 = \frac{f_{ik}^2}{\sum_{k=1}^{K} f_{ik}^2}$$

Similarly, for column j on dimension k:

$$COS_{jk}^2 = \frac{g_{jk}^2}{\sum_{k=1}^{K} g_{jk}^2}$$

The squared cosines have the following properties:

- They range from 0 to 1, with values close to 1 indicating excellent representation
- They sum to 1 across all dimensions for each point: $\sum_{k=1}^{K} COS_{ik}^2 = 1$
- They help assess the quality of the low-dimensional representation for each point

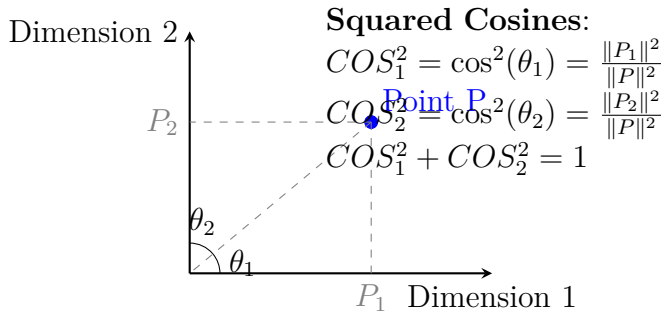


Figure 6.10: Geometric interpretation of squared cosines. The angles θ_1 and θ_2 between the point vector and the axes determine how well the point is represented on each dimension.

fig:squared_c

Practical Interpretation Guidelines

1. **Identifying Key Drivers**: Use absolute contributions to identify which points define each dimension. Points with $AC > \frac{1}{\text{number of points}}$ contribute more than average.

2. **Assessing Representation Quality**: Use squared cosines to assess how well points are represented. Points with $COS^2 < 0.50$ on the first two dimensions may be poorly represented.

3. **Balancing Both Measures**: Ideally, points should have both high absolute contributions (defining the dimensions) and high squared cosines (well-represented).

4. **Dimension Interpretation**: Interpret each dimension by examining points with high absolute contributions to that dimension.

Supplementary Points

For additional categories not included in the original analysis (e.g., missing data or supplementary variables), contributions can still be calculated but should be interpreted differently:

$$f_{i^*k} = \frac{1}{\sigma_k} \sum_{j=1}^{J} \frac{p_{i^*j}}{r_{i^*}} \gamma_{jk}$$

These points do not contribute to the inertia but can be projected into the existing space for interpretation.

These numerical measures, when combined with the geometric interpretations, provide a comprehensive framework for understanding CA results. In the next subsection, we will apply to a complete tutorial with a small contingency table.

6.4.4 A Complete Tutorial with a Small Contingency Table

This subsection provides a complete, step-by-step tutorial of Correspondence Analysis using a small contingency table. We will analyze a 3×3 table containing artificial

data about beverage preferences across three age groups, demonstrating the entire CA workflow from data preparation to interpretation.

Step 1: Create the Contingency Table

Let us consider the following contingency table showing beverage preferences across three age groups:

Table 6.1: Beverage preference by age group (artificial data)

	Young	Middle-aged	Elderly	Row Total
Coffee	20	25	30	75
Tea	30	25	15	70
Soda	40	20	5	65
Column Total	90	70	50	210

Step 2: Compute the Correspondence Matrix

The correspondence matrix $\mathbf{P}$ is obtained by dividing each cell by the grand total $n = 210$:

$$\mathbf{P} = \frac{1}{210}\begin{pmatrix} 20 & 25 & 30 \\ 30 & 25 & 15 \\ 40 & 20 & 5 \end{pmatrix} = \begin{pmatrix} 0.0952 & 0.1190 & 0.1429 \\ 0.1429 & 0.1190 & 0.0714 \\ 0.1905 & 0.0952 & 0.0238 \end{pmatrix}$$

Step 3: Calculate Row and Column Masses

The row masses $\mathbf{r}$ are the row margins of $\mathbf{P}$:

$$r_1 = 0.0952 + 0.1190 + 0.1429 = 0.3571$$

$$r_2 = 0.1429 + 0.1190 + 0.0714 = 0.3333$$

$$r_3 = 0.1905 + 0.0952 + 0.0238 = 0.3095$$

The column masses $\mathbf{c}$ are the column margins of $\mathbf{P}$:

$$c_1 = 0.0952 + 0.1429 + 0.1905 = 0.4286$$

$$c_2 = 0.1190 + 0.1190 + 0.0952 = 0.3333$$

$$c_3 = 0.1429 + 0.0714 + 0.0238 = 0.2381$$

In matrix form:

$$\mathbf{r} = \begin{pmatrix} 0.3571 \\ 0.3333 \\ 0.3095 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 0.4286 \\ 0.3333 \\ 0.2381 \end{pmatrix}$$

Step 4: Compute Expected Frequencies under Independence

The expected frequencies under the hypothesis of independence are given by $\mathbf{E} = \mathbf{r}\mathbf{c}^\top$:

$$\mathbf{E} = \begin{pmatrix} 0.3571 \\ 0.3333 \\ 0.3095 \end{pmatrix} \begin{pmatrix} 0.4286 & 0.3333 & 0.2381 \end{pmatrix} = \begin{pmatrix} 0.1531 & 0.1190 & 0.0850 \\ 0.1429 & 0.1111 & 0.0794 \\ 0.1327 & 0.1032 & 0.0737 \end{pmatrix}$$

Step 5: Compute the Matrix of Standardized Residuals

The standardized residuals are calculated as:

$$s_{ij} = \frac{p_{ij} - r_i c_j}{\sqrt{r_i c_j}} = \frac{p_{ij} - e_{ij}}{\sqrt{e_{ij}}}$$

$$\mathbf{S} = \begin{pmatrix} \frac{0.0952-0.1531}{\sqrt{0.1531}} & \frac{0.1190-0.1190}{\sqrt{0.1190}} & \frac{0.1429-0.0850}{\sqrt{0.0850}} \\ \frac{0.1429-0.1429}{\sqrt{0.1429}} & \frac{0.1190-0.1111}{\sqrt{0.1111}} & \frac{0.0714-0.0794}{\sqrt{0.0794}} \\ \frac{0.1905-0.1327}{\sqrt{0.1327}} & \frac{0.0952-0.1032}{\sqrt{0.1032}} & \frac{0.0238-0.0737}{\sqrt{0.0737}} \end{pmatrix} = \begin{pmatrix} -0.147 & 0.000 & 0.198 \\ 0.000 & 0.024 & -0.028 \\ 0.159 & -0.025 & -0.184 \end{pmatrix}$$

Step 6: Perform the Singular Value Decomposition

The singular value decomposition of $\mathbf{S}$ is $\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$. After computation, we obtain:

$$\mathbf{U} = \begin{pmatrix} -0.581 & 0.655 \\ 0.105 & 0.746 \\ 0.807 & 0.116 \end{pmatrix}, \quad \mathbf{\Sigma} = \begin{pmatrix} 0.284 & 0 \\ 0 & 0.118 \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} -0.591 & 0.697 \\ 0.108 & 0.715 \\ 0.799 & 0.062 \end{pmatrix}$$

The singular values are $\sigma_1 = 0.284$ and $\sigma_2 = 0.118$.

Step 7: Compute Principal Coordinates

The principal coordinates for rows are given by $\mathbf{F} = \mathbf{D}_r^{-1/2}\mathbf{U}\mathbf{\Sigma}$:

$$\mathbf{D}_r^{-1/2} = \begin{pmatrix} \frac{1}{\sqrt{0.3571}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{0.3333}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{0.3095}} \end{pmatrix} = \begin{pmatrix} 1.674 & 0 & 0 \\ 0 & 1.732 & 0 \\ 0 & 0 & 1.799 \end{pmatrix}$$

$$\mathbf{F} = \begin{pmatrix} 1.674 & 0 & 0 \\ 0 & 1.732 & 0 \\ 0 & 0 & 1.799 \end{pmatrix} \begin{pmatrix} -0.581 & 0.655 \\ 0.105 & 0.746 \\ 0.807 & 0.116 \end{pmatrix} \begin{pmatrix} 0.284 & 0 \\ 0 & 0.118 \end{pmatrix} = \begin{pmatrix} -0.276 & 0.129 \\ 0.052 & 0.152 \\ 0.412 & 0.025 \end{pmatrix}$$

The principal coordinates for columns are given by $\mathbf{G} = \mathbf{D}_c^{-1/2}\mathbf{V}\mathbf{\Sigma}$:

$$\mathbf{D}_c^{-1/2} = \begin{pmatrix} \frac{1}{\sqrt{0.4286}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{0.3333}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{0.2381}} \end{pmatrix} = \begin{pmatrix} 1.527 & 0 & 0 \\ 0 & 1.732 & 0 \\ 0 & 0 & 2.049 \end{pmatrix}$$

$$\mathbf{G} = \begin{pmatrix} 1.527 & 0 & 0 \\ 0 & 1.732 & 0 \\ 0 & 0 & 2.049 \end{pmatrix} \begin{pmatrix} -0.591 & 0.697 \\ 0.108 & 0.715 \\ 0.799 & 0.062 \end{pmatrix} \begin{pmatrix} 0.284 & 0 \\ 0 & 0.118 \end{pmatrix} = \begin{pmatrix} -0.257 & 0.123 \\ 0.054 & 0.146 \\ 0.467 & 0.016 \end{pmatrix}$$

Step 8: Create the Symmetric Map

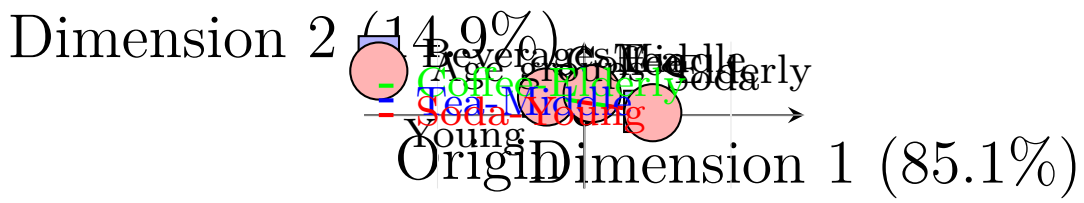


Figure 6.11: Symmetric map of beverage preferences by age group. The first dimension explains 85.1% of inertia ($\sigma_1^2/(\sigma_1^2 + \sigma_2^2) = 0.0807/0.0949$), the second 14.9%.

fig:ca_tutori

Step 9: Interpret the Results

The symmetric map reveals clear patterns:

1. **Coffee** is strongly associated with **Elderly** respondents, positioned close together on the right side of the map.
2. **Tea** shows affinity with **Middle-aged** respondents, located in the upper center.
3. **Soda** is strongly associated with **Young** respondents, positioned together on the left side.
4. **Dimension 1** (horizontal) appears to represent a temperature gradient, with hot beverages (coffee, tea) on the right and cold beverages (soda) on the left.
5. **Dimension 2** (vertical) seems to relate to sugar/caffeine content, with high-sugar/caffeine drinks (soda, coffee) at the bottom and lower-sugar options (tea) at the top.

Step 10: Calculate Contributions

We compute absolute contributions to understand which points define each dimension. The absolute contribution of row i to dimension k is:

$$AC_{ik} = \frac{r_i f_{ik}^2}{\sigma_k^2}$$

For dimension 1 ($\sigma_1^2 = 0.0807$):

$$AC_{\text{Coffee},1} = \frac{0.3571 \times (-0.276)^2}{0.0807} = 0.337$$

$$AC_{\text{Tea},1} = \frac{0.3333 \times (0.052)^2}{0.0807} = 0.011$$

$$AC_{\text{Soda},1} = \frac{0.3095 \times (0.412)^2}{0.0807} = 0.652$$

For dimension 2 ($\sigma_2^2 = 0.0142$):

$$AC_{\text{Coffee},2} = \frac{0.3571 \times (0.129)^2}{0.0142} = 0.429$$
$$AC_{\text{Tea},2} = \frac{0.3333 \times (0.152)^2}{0.0142} = 0.542$$
$$AC_{\text{Soda},2} = \frac{0.3095 \times (0.025)^2}{0.0142} = 0.014$$

These values confirm that Soda and Coffee strongly define Dimension 1, while Tea and Coffee contribute most to Dimension 2.

Step 11: Assess Quality of Representation

Squared cosines indicate how well each point is represented in the two-dimensional space:

$$COS_{ik}^2 = \frac{f_{ik}^2}{\sum_{k=1}^{2} f_{ik}^2}$$

$$COS_{\text{Coffee}}^2 = \frac{(-0.276)^2 + (0.129)^2}{(-0.276)^2 + (0.129)^2} = 1.000$$
$$COS_{\text{Tea}}^2 = \frac{(0.052)^2 + (0.152)^2}{(0.052)^2 + (0.152)^2} = 1.000$$
$$COS_{\text{Soda}}^2 = \frac{(0.412)^2 + (0.025)^2}{(0.412)^2 + (0.025)^2} = 1.000$$

All values equal 1.000, indicating perfect representation in the two-dimensional solution. This is expected in this small example with only two non-trivial dimensions.

Conclusion

This tutorial demonstrates the complete CA workflow on a small contingency table. The analysis revealed clear patterns of association between beverage preferences and age groups, with two interpretable dimensions emerging from the data. The high squared cosines indicate that the two-dimensional solution perfectly represents the relationships in the data, while the contribution values help identify which categories are most influential in defining each dimension.

This example illustrates how CA transforms a simple contingency table into a rich geometric representation that facilitates interpretation of complex relationships between categorical variables.

6.5 Extending to Multiple Correspondence Analysis

Multiple Correspondence Analysis (MCA) extends the principles of simple correspondence analysis to the case of multiple categorical variables. While simple CA analyzes the association between two categorical variables, MCA allows for the simultaneous analysis of three or more categorical variables, making it particularly valuable for analyzing survey data, questionnaires, and other multivariate categorical datasets.

6.5.1 The Indicator Matrix and Burt Matrix Approaches

MCA can be approached through two mathematically equivalent but computationally distinct methods: the indicator matrix approach and the Burt matrix approach. Both methods ultimately yield the same geometric representation of the variables' categories.

The Indicator Matrix Approach

Let Q be the number of categorical variables, and let variable q have J_q categories for $q = 1, \ldots, Q$. The total number of categories across all variables is $J = \sum_{q=1}^{Q} J_q$.

For a dataset with n individuals, the *indicator matrix* (or complete disjunctive table) $\mathbf{Z}$ is an $n \times J$ binary matrix where each row corresponds to an individual and each column corresponds to a category of one of the variables. The element z_{ij} equals 1 if individual i possesses category j, and 0 otherwise.

$$\mathbf{Z} = \begin{pmatrix} z_{11} & z_{12} & \cdots & z_{1J} \\ z_{21} & z_{22} & \cdots & z_{2J} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nJ} \end{pmatrix}$$

The correspondence matrix for MCA is then defined as:

$$\mathbf{P} = \frac{1}{nQ}\mathbf{Z}$$

The row masses are all equal to $1/n$ (each individual has the same weight), and the column masses are proportional to the frequencies of the categories:

$$r_i = \frac{1}{n}, \quad c_j = \frac{n_j}{nQ}$$

where n_j is the number of individuals possessing category j.

The subsequent steps of MCA parallel those of simple CA: compute the matrix of standardized residuals, perform a generalized SVD, and obtain coordinates for the categories.

The Burt Matrix Approach

The Burt matrix $\mathbf{B}$ is a symmetric $J \times J$ matrix that cross-tabulates all categories against all categories:

$$\mathbf{B} = \mathbf{Z}^\top \mathbf{Z}$$

The Burt matrix has a block structure:

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} & \cdots & \mathbf{B}_{1Q} \\ \mathbf{B}_{21} & \mathbf{B}_{22} & \cdots & \mathbf{B}_{2Q} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}_{Q1} & \mathbf{B}_{Q2} & \cdots & \mathbf{B}_{QQ} \end{pmatrix}$$

where the diagonal blocks $\mathbf{B}_{qq}$ are diagonal matrices containing the frequencies of the categories of variable q, and the off-diagonal blocks $\mathbf{B}_{qr}$ $(q \neq r)$ are contingency tables crossing variables q and r.

MCA can be performed by applying simple CA to the Burt matrix. The total inertia in this case is:

$$\Phi^2_B = \frac{1}{Q^2} \sum_{q=1}^{Q} \sum_{r=1}^{Q} \chi^2(\mathbf{B}_{qr})$$

where $\chi^2(\mathbf{B}_{qr})$ is the chi-square statistic for the contingency table between variables q and r.

Equivalence and Differences

The two approaches are mathematically equivalent in the sense that they yield the same coordinates for the categories up to a scaling factor. However, they differ in computational implementation and interpretation:

- The indicator matrix approach directly represents individuals as points in the space of categories.
- The Burt matrix approach emphasizes the relationships between categories across different variables.
- The total inertia in the indicator matrix approach is $\frac{Q-1}{Q}$, while in the Burt matrix approach it is generally larger.
- For interpretation purposes, the Burt matrix approach is often preferred as it provides more stable results, especially when category frequencies are uneven.

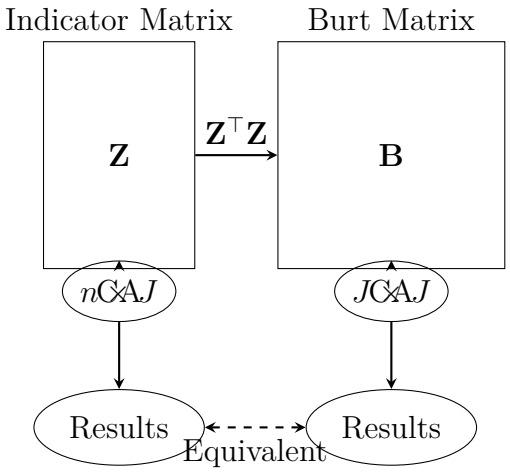


Figure 6.12: The two approaches to Multiple Correspondence Analysis and their relationship. Both the indicator matrix and Burt matrix approaches yield equivalent results through correspondence analysis. fig:mca_appro

The choice between the two approaches often depends on the specific application and the size of the dataset. The indicator matrix approach is more direct but can be computationally intensive for large datasets with many categories. The Burt matrix approach is often more efficient and provides more stable results, especially when dealing with variables that have many categories or uneven distributions.

In practice, most statistical software packages implement MCA through the Burt matrix approach due to its computational advantages and stability. However, understanding both approaches provides valuable insight into the geometric and algebraic foundations of MCA.Approaches

6.5.2 The Geometry of MCA: Clouds of Individuals and Categories

Multiple Correspondence Analysis represents both individuals and categories as points in a multidimensional space, creating two dual clouds that can be interpreted geometrically. This dual representation is a powerful feature of MCA that allows for simultaneous interpretation of both observations and variable categories.

Cloud of Individuals

Each individual (observation) is represented as a point in a space of dimension J (the total number of categories across all variables). The position of an individual is determined by the categories it possesses:

$$\text{Coordinate of individual } i \text{ on dimension } k: \quad y_{ik} = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^{J} \frac{z_{ij}}{c_j} \phi_{jk}$$

where:

- z_{ij} is the element of the indicator matrix (1 if individual i has category j, 0 otherwise)

- c_j is the mass of category j (proportional to its frequency)
- ϕ_{jk} is the standard coordinate of category j on dimension k
- λ_k is the k-th eigenvalue

The distance between two individuals in this space is a weighted Euclidean distance that measures the dissimilarity of their category profiles. Individuals with similar patterns of responses across variables will be positioned close to each other in the multidimensional space.

Cloud of Categories

Each category is represented as a point in a space of dimension n (the number of individuals). The position of a category is determined by the individuals who possess it:

$$\text{Coordinate of category } j \text{ on dimension } k: \quad \phi_{jk} = \frac{1}{\sqrt{\lambda_k}} \sum_{i=1}^{n} \frac{z_{ij}}{r_i} y_{ik}$$

where r_i is the mass of individual i (typically $1/n$ for all individuals).

The distance between two categories follows the chi-square metric, which accounts for the relative frequencies of the categories. Categories that tend to be chosen by the same individuals will be positioned close to each other.

Duality Relationship

The relationship between the cloud of individuals and the cloud of categories is governed by the transition formulas:

$$y_{ik} = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^{J} \frac{z_{ij}}{Q} \phi_{jk} \quad \text{and} \quad \phi_{jk} = \frac{1}{\sqrt{\lambda_k}} \sum_{i=1}^{n} \frac{z_{ij}}{c_j} y_{ik}$$

These formulas demonstrate that:

- The position of an individual is the weighted average of the categories it possesses
- The position of a category is the weighted average of the individuals who possess it
- This barycentric relationship is the foundation of MCA's geometric interpretation

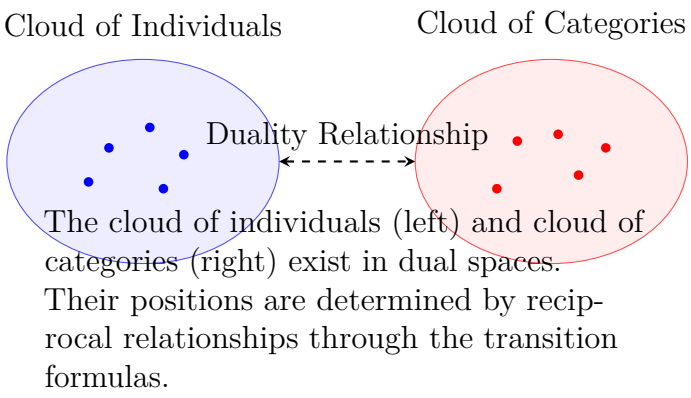


Figure 6.13: Dual clouds in Multiple Correspondence Analysis. The cloud of individuals (blue) represents the observations, while the cloud of categories (red) represents the variable categories. The duality relationship connects these two clouds. fig:mca_cloud

Geometric Interpretation

The geometric representation in MCA allows for several important interpretations:

1. **Proximity between individuals**: Individuals close to each other in the cloud have similar response patterns across all variables.

2. **Proximity between categories**: Categories close to each other tend to be associated with the same individuals.

3. **Proximity between individuals and categories**: An individual positioned close to a category indicates that the individual possesses that category.

4. **Origin interpretation**: The origin represents the average profile. Points far from the origin represent distinctive profiles.

5. **Axis interpretation**: The principal axes represent the main factors of differentiation in the data, with the first axis accounting for the largest part of the inertia.

This geometric framework provides a powerful tool for visualizing and interpreting complex multivariate categorical data, revealing patterns and relationships that might not be apparent in the raw data.

The next subsection will address the specific challenges related to inertia interpretation in MCA and present adjusted measures that provide more accurate representations of the data structure.

6.5.3 The Problem of Inertia and Adjusted Interpretations

Multiple Correspondence Analysis presents a unique challenge in the interpretation of inertia values that distinguishes it from simple correspondence analysis. This subsection addresses the inertia inflation problem in MCA and presents adjusted measures that provide more accurate interpretations of the results.

The Inertia Inflation Problem

In MCA, the total inertia is artificially inflated due to the presence of diagonal blocks in the Burt matrix. The total inertia in MCA can be expressed as:

$$\Phi^2_{\text{MCA}} = \frac{1}{Q^2}\sum_{q=1}^{Q}\sum_{r=1}^{Q}\chi^2(\mathbf{B}_{qr}) = \frac{Q-1}{Q} + \frac{1}{Q^2}\sum_{q\neq r}\chi^2(\mathbf{B}_{qr})$$

where:

- Q is the number of variables
- $\mathbf{B}_{qr}$ is the contingency table between variables q and r
- $\chi^2(\mathbf{B}_{qr})$ is the chi-square statistic for the table $\mathbf{B}_{qr}$

The first term, $\frac{Q-1}{Q}$, represents the inertia due to the diagonal blocks (each variable with itself), which is uninformative about associations between variables. The second term contains the meaningful information about associations between different variables.

This inflation has two important consequences:

1. The percentage of inertia explained by each dimension is significantly underestimated
2. The absolute values of inertia become difficult to interpret directly
3. The apparent quality of representation seems poorer than it actually is

Greenacre's Adjusted Inertia

To address this problem, Greenacre (2006) proposed an adjustment that provides more realistic percentages of inertia. The adjusted inertia for dimension k is calculated as:

$$\lambda_k^{\text{adj}} = \left(\frac{Q}{Q-1}\right)^2\left(\lambda_k - \frac{1}{Q}\right)^2$$

where λ_k is the k-th eigenvalue from the MCA solution.

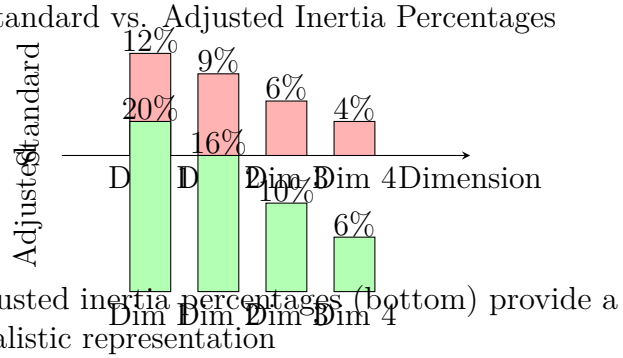
The adjusted total inertia is then:

$$\Phi^2_{\text{adj}} = \sum_{k=1}^{K}\lambda_k^{\text{adj}}$$

And the percentage of inertia explained by dimension k becomes:

$$\text{Inertia}\%_k^{\text{adj}} = 100 \times \frac{\lambda_k^{\text{adj}}}{\Phi^2_{\text{adj}}}$$

These adjusted values provide a more accurate representation of the actual associations in the data.



The adjusted inertia percentages (bottom) provide a more realistic representation
of the actual variance explained by each dimension compared to the standard
percentages (top), which are underestimated due to inertia inflation.

Figure 6.14: Comparison of standard and adjusted inertia percentages in MCA. The adjustment provides more realistic estimates of the variance explained by each dimension.

fig:mca_inert

Other Interpretation Aids

Beyond inertia adjustment, several other measures aid in the interpretation of MCA results:

1. **Absolute Contributions**: Measure how much each category contributes to the inertia of a dimension:
$$AC_{jk} = \frac{c_j \phi_{jk}^2}{\lambda_k}$$

2. **Relative Contributions (Squared Cosines)**: Measure how well a category is represented on a dimension:
$$COS_{jk}^2 = \frac{\phi_{jk}^2}{\sum_{k=1}^{K} \phi_{jk}^2}$$

3. **Test Values**: Statistical measures that indicate whether a category's position on a dimension is significantly different from what would be expected by chance.

4. **Class Specificity**: Measures that identify which categories are most specific to particular groups of individuals.

Practical Recommendations for Interpretation

When interpreting MCA results, consider the following practical recommendations:

- Always use adjusted inertia percentages rather than raw percentages
- Focus on dimensions with adjusted eigenvalues substantially greater than 1/Q
- Use absolute contributions to identify which categories define each dimension

- Use relative contributions to assess the quality of representation of each category
- Consider the stability of results across different subsets of the data
- Use supplementary variables and individuals to validate interpretations

The inertia adjustment and complementary interpretation aids provide a more accurate and nuanced understanding of MCA results. By addressing the inflation problem and providing appropriate measures for interpretation, analysts can extract more meaningful insights from multivariate categorical data.

The next subsection will compare MCA with Principal Component Analysis, highlighting their respective strengths and limitations for analyzing categorical data.

6.5.4 Comparing MCA and PCA on Categorical Data

Multiple Correspondence Analysis (MCA) and Principal Component Analysis (PCA) are both dimensionality reduction techniques, but they approach the analysis of categorical data from fundamentally different perspectives. This subsection provides a comprehensive comparison of these two methods, highlighting their respective strengths, limitations, and appropriate applications.

Fundamental Philosophical Differences

- **PCA** is primarily designed for continuous data and operates under the assumption of linear relationships between variables.
- **MCA** is specifically designed for categorical data and operates within the framework of contingency table analysis.
- **PCA** maximizes the explained variance of continuous variables.
- **MCA** maximizes the association between categorical variables.

Mathematical Foundations

The mathematical operations differ significantly between the two methods:

$$\begin{aligned} \text{PCA:} \quad & \mathbf{X}^\top \mathbf{X} \quad \text{(Covariance matrix)} \\ \text{MCA:} \quad & \mathbf{D}_r^{-1/2}(\mathbf{P} - \mathbf{r}\mathbf{c}^\top)\mathbf{D}_c^{-1/2} \quad \text{(Standardized residual matrix)} \end{aligned}$$

where $\mathbf{X}$ is the data matrix for PCA, and $\mathbf{P}$ is the correspondence matrix for MCA.

Geometric Interpretation

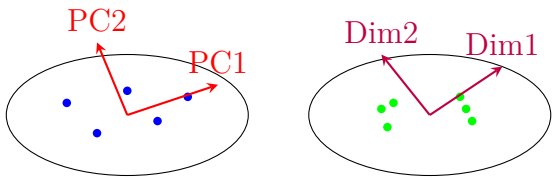


Figure 6.15: Geometric comparison of PCA (left) and MCA (right). PCA operates in continuous Euclidean space, while MCA operates in a discrete simplex space defined by category profiles.

fig:pca_mca_g

Comparative Analysis

Table 6.2: Comparison of PCA and MCA for categorical data analysis

Aspect	**Principal Component Analysis (PCA)**	**Multiple Correspondence Analysis (MCA)**
Data type	Continuous variables	Categorical variables
Objective	Maximize explained variance	Maximize associations between categories
Distance metric	Euclidean distance	Chi-square distance
Transformation	Center and scale variables	Profile transformation
Output	Principal components	Principal dimensions
Interpretation	Component loadings	Category coordinates
Inertia	Sum of eigenvalues = total variance	Sum of eigenvalues = χ^2/nQ
Visualization	Biplot (variables + observations)	Symmetric map (categories + individuals)

Appropriate Applications

Each method has its own domain of optimal application:

PCA is preferred when:

- Analyzing continuous variables or Likert-scale data treated as continuous
- The research question focuses on variance explanation
- The assumption of linear relationships is reasonable
- The goal is to create composite scores from continuous variables

MCA is preferred when:

- Analyzing genuine categorical data (nominal or ordinal)
- The research question focuses on associations between categories

- The data structure is best represented as profiles
- The goal is to understand the relationships between categories across multiple variables

Hybrid Approaches

In practice, researchers sometimes use hybrid approaches:

1. **FAMD (Factor Analysis of Mixed Data)**: Combines PCA and MCA principles for datasets containing both continuous and categorical variables.
2. **Polychoric PCA**: Uses polychoric correlations for ordinal variables before applying PCA.
3. **Optimal Scaling**: Transforms categorical variables using optimal scaling before applying PCA.

Practical Considerations

When deciding between PCA and MCA for categorical data analysis, consider:

- **Data characteristics**: Are variables truly categorical or ordinal treated as continuous?
- **Research questions**: Are you interested in variance explanation or association patterns?
- **Interpretation needs**: Do you need to interpret variable loadings or category positions?
- **Statistical assumptions**: Can you justify the assumptions of each method?

Conclusion

While both PCA and MCA are valuable dimensionality reduction techniques, they approach categorical data analysis from fundamentally different perspectives. PCA, designed for continuous data, focuses on variance maximization using Euclidean geometry. MCA, designed specifically for categorical data, focuses on association maximization using the chi-square metric and profile space geometry.

The choice between these methods should be guided by the nature of the data, the research questions, and the interpretive framework most appropriate for the analysis. In many cases, MCA provides a more theoretically grounded approach for genuine categorical data, while PCA remains valuable for continuous or appropriately transformed categorical variables.

Understanding these differences allows researchers to select the most appropriate method for their specific analytical needs and to interpret the results within the correct mathematical and conceptual framework.

6.6 Applications in Scientific Research

Correspondence Analysis and Multiple Correspondence Analysis have found extensive applications across diverse scientific domains due to their ability to reveal hidden structures in categorical data. This section explores several key application areas, demonstrating the practical utility of these methods in real-world research contexts.

6.6.1 Social Sciences: Analyzing Survey and Questionnaire Data

Social scientists frequently employ MCA to analyze complex survey and questionnaire data, where multiple categorical variables capture attitudes, behaviors, and demographic characteristics. The method excels at identifying patterns and relationships in such data.

Typical Research Questions

MCA helps address questions such as:

- How do lifestyle patterns vary across different socioeconomic groups?
- What cultural consumption patterns emerge in different demographic segments?
- How do political attitudes cluster with specific demographic characteristics?
- What are the underlying dimensions of social stratification in a given population?

Example: Lifestyle Survey Analysis

Consider a survey measuring various lifestyle factors:

Table 6.3: Example lifestyle survey data structure

Variable	**Categories**
Education Level	High School, Bachelor's, Graduate
Income Bracket	Low, Middle, High
Leisure Activities	Sports, Culture, Home, Social
Health Consciousness	Low, Medium, High
Political Orientation	Left, Center, Right

Analysis Workflow

The MCA analysis of such data typically follows these steps:

1. **Data Preparation**: Convert all variables to categorical format and create the complete disjunctive table
2. **Matrix Construction**: Build the indicator matrix or Burt matrix

3. **Dimensionality Reduction**: Extract principal dimensions explaining the maximum inertia

4. **Interpretation**: Identify the meaning of each dimension through category coordinates

5. **Visualization**: Create symmetric maps showing relationships between categories

Key Findings and Interpretation

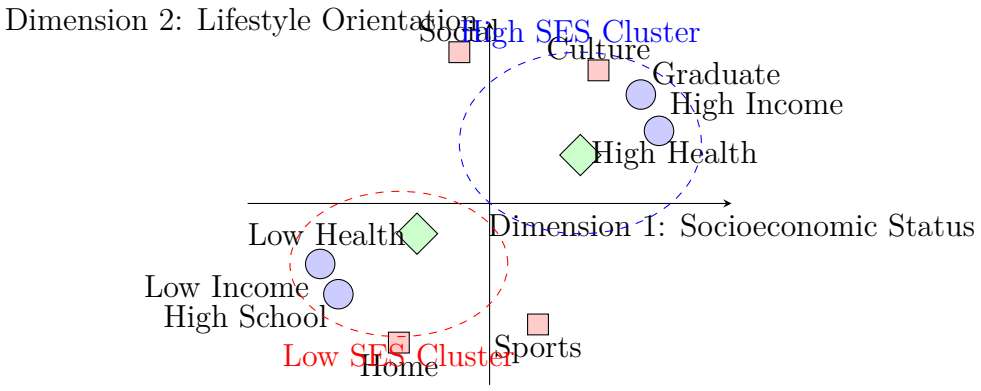


Figure 6.16: Hypothetical MCA results from lifestyle survey analysis. The plot shows clustering of demographic and lifestyle variables along socioeconomic and lifestyle dimensions.

fig:lifestyle

Practical Considerations for Social Science Applications

- **Missing Data**: MCA handles missing data naturally through the indicator matrix format
- **Large Sample Sizes**: The method remains computationally efficient even with large surveys
- **Supplementary Variables**: Additional variables can be projected onto existing dimensions for interpretation
- **Longitudinal Analysis**: Multiple time points can be analyzed simultaneously to track changes in associations

Advanced Techniques

Social scientists often enhance MCA with:

- **Specific MCA**: Focuses on specific associations rather than global structures
- **Hierarchical MCA**: Analyzes nested categorical structures
- **Multiple Factor Analysis**: Integrates MCA with other multivariate techniques

Software Implementation

Popular statistical packages for MCA in social sciences include:

- R: `FactoMineR`, `ca`, `ade4` packages
- Python: `prince`, `scikit-learn` extensions
- Commercial: SPSS, SAS, STATA with appropriate modules

This application of MCA enables social scientists to move beyond simple cross-tabulations and uncover complex patterns of association that characterize social structures and behaviors. The visual nature of the results facilitates communication of findings to diverse audiences, from academic peers to policy makers.

The next subsection will explore applications in environmental sciences, particularly the analysis of species abundance data through ecological ordination.

6.6.2 Environmental Sciences: Species Abundance Data (Ecological Ordination)

Correspondence Analysis, particularly in the form of Detrended Correspondence Analysis (DCA), has become a fundamental tool in ecology for analyzing species abundance data across environmental gradients. This application, known as ecological ordination, helps researchers understand patterns in species distributions and their relationships to environmental factors.

Ecological Research Questions

Ecologists use CA and related methods to address questions such as:

- How are species distributed along environmental gradients (e.g., moisture, temperature, elevation)?
- What are the main environmental factors structuring ecological communities?
- How do species assemblages change across different habitats or over time?
- Which species have similar ecological requirements and distribution patterns?

Example: Species Abundance Matrix

Ecological data typically takes the form of a sites-by-species matrix:

Table 6.4: Example species abundance data structure

Site	Species A	Species B	Species C	Species D	Species E
Forest 1	15	3	0	8	2
Forest 2	12	5	1	10	4
Wetland 1	2	18	12	1	9
Wetland 2	1	22	15	0	11
Grassland 1	0	4	2	20	3
Grassland 2	0	3	1	18	5

Analysis Workflow

The ecological ordination analysis typically follows these steps:

1. **Data Transformation**: Apply appropriate transformations (e.g., square root, Wisconsin double standardization) to reduce the influence of very abundant species

2. **Ordination**: Perform CA or DCA to extract the main gradients in species composition

3. **Environmental Interpretation**: Correlate ordination axes with measured environmental variables

4. **Visualization**: Create biplots showing both species and sites, often with environmental vectors

5. **Statistical Validation**: Use permutation tests to assess the significance of relationships

Key Findings and Interpretation

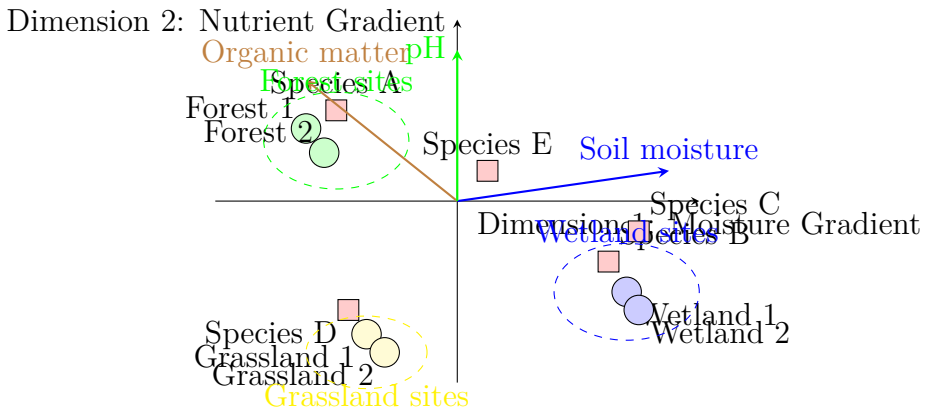


Figure 6.17: Hypothetical CA ordination of species abundance data. Sites cluster by habitat type, and species positions indicate their environmental preferences. Environmental vectors show the direction and strength of correlation with ordination axes.

fig:ecologica

Special Considerations for Ecological Data

Ecological data presents unique challenges that require special handling:

- **Zero-inflation**: Species absence is common and creates many zeros in the data matrix

- **Species responses**: Most species show unimodal rather than linear responses to environmental gradients

- **Data transformation**: Appropriate transformations are needed to reduce the influence of highly abundant species
- **Detrending**: DCA addresses the arch effect often present in CA of ecological data

Advanced Techniques in Ecological Ordination

Ecologists have developed several CA variants for specific applications:

- **Detrended Correspondence Analysis (DCA)**: Removes the arch artifact often present in CA ordinations
- **Canonical Correspondence Analysis (CCA)**: Constrains ordination axes to linear combinations of environmental variables
- **Partial Correspondence Analysis**: Removes the effect of certain variables before ordination
- **Co-correspondence Analysis**: Relates patterns in two species datasets (e.g., plants and insects)

Software Implementation

Specialized software and packages for ecological ordination include:

- R: `vegan` package (functions `cca()`, `decorana()`)
- PC-ORD: Commercial software specifically designed for ecological ordination
- CANOCO: Historical standard for constrained ordination in ecology

Interpretation Guidelines

When interpreting ecological ordination results:

- The distance between sites reflects their similarity in species composition
- The distance between species reflects their co-occurrence patterns
- The distance between a species and a site indicates the species' abundance at that site
- Environmental vectors show the direction and strength of correlation with ordination axes
- The length of environmental vectors indicates their importance in explaining species distributions

This application of CA and related methods has revolutionized community ecology by providing powerful tools to visualize and analyze complex species-environment relationships. The ability to simultaneously represent species, sites, and environmental variables in a low-dimensional space makes ordination an indispensable tool for understanding ecological patterns.

The next subsection will explore applications in textual data analysis through lexical correspondence analysis.

6.6.3 Textual Data Analysis: Lexical Correspondence Analysis

Lexical Correspondence Analysis (LCA) applies the principles of correspondence analysis to textual data, enabling researchers to identify patterns, themes, and structures within corpora of documents. This approach has revolutionized text mining and content analysis across various disciplines including linguistics, political science, literary studies, and social sciences.

Research Questions in Textual Analysis

LCA helps researchers address questions such as:

- How do vocabulary patterns differ across authors, time periods, or genres?
- What thematic structures emerge within a corpus of documents?
- How do political speeches or manifestos position themselves relative to each other?
- What linguistic features distinguish different types of discourse?
- How do concepts co-occur and form semantic networks within texts?

Data Preparation: The Document-Term Matrix

Textual data is typically represented as a document-term matrix (DTM) where:

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1J} \\ x_{21} & x_{22} & \cdots & x_{2J} \\ \vdots & \vdots & \ddots & \vdots \\ x_{I1} & x_{I2} & \cdots & x_{IJ} \end{pmatrix}$$

where x_{ij} represents the frequency of term j in document i, I is the number of documents, and J is the number of terms.

Table 6.5: Example document-term matrix for political speeches

Document	freedom	security	economy	education	health
Speech 1	12	3	8	2	4
Speech 2	5	15	6	1	3
Speech 3	8	4	20	5	2
Speech 4	2	12	4	1	8
Speech 5	15	2	10	6	3

Preprocessing Steps

Textual data requires careful preprocessing before analysis:

1. **Tokenization**: Splitting text into individual words or phrases
2. **Stopword removal**: Eliminating common but uninformative words
3. **Stemming/Lemmatization**: Reducing words to their root forms
4. **Term selection**: Filtering based on frequency thresholds (minimum and maximum)
5. **Weighting**: Applying TF-IDF or other weighting schemes to reduce the influence of very frequent terms

Analysis Workflow

The LCA workflow typically includes:

1. **Matrix construction**: Create the document-term matrix with appropriate weighting
2. **Correspondence analysis**: Apply CA to the contingency table of documents and terms
3. **Dimension interpretation**: Identify the semantic dimensions underlying the factorial structure
4. **Visualization**: Create symmetric maps showing documents and terms
5. **Validation**: Use supplementary elements and statistical tests to validate interpretations

Key Findings and Interpretation

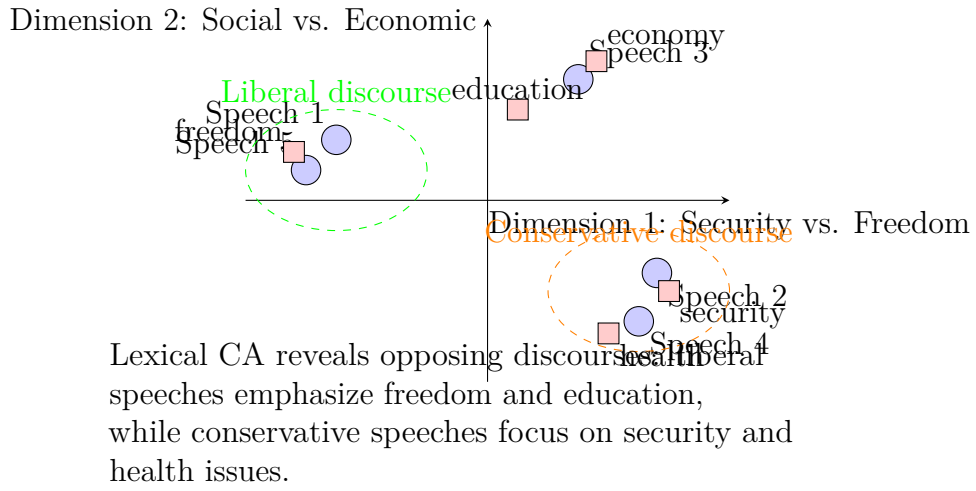


Figure 6.18: Lexical correspondence analysis of political speeches. Documents and terms are positioned based on their co-occurrence patterns, revealing underlying ideological dimensions.

fig:lexical_c

Special Considerations for Textual Data

Textual analysis presents unique challenges:

- **High dimensionality**: Vocabulary sizes can be extremely large, requiring careful term selection
- **Sparsity**: Most documents contain only a small fraction of the total vocabulary
- **Context sensitivity**: Word meanings depend on context, which CA cannot capture directly
- **Multilingual data**: Requires special handling when analyzing corpora in multiple languages
- **Time series analysis**: Tracking lexical evolution over time requires specialized approaches

Advanced Techniques in Lexical Analysis

Researchers have developed several advanced approaches:

- **Specific Lexical Analysis**: Focuses on specific words or themes rather than the entire vocabulary
- **Structured Lexical Analysis**: Incorporates linguistic structure (syntax, semantics) into the analysis
- **Dynamic Lexical Analysis**: Examines how lexical patterns evolve over time
- **Multimodal Analysis**: Combines textual analysis with other data types (images, audio)

Software Implementation

Specialized tools for lexical correspondence analysis include:

- R: `FactoMineR`, `ca`, `tm` packages for text mining and CA
- Python: `scikit-learn`, `gensim` with CA extensions
- Commercial: IRaMuTeQ, SPAD-Test, SAS Text Miner
- Specialized: Alceste, Lexico, Prosite for specific lexical analysis

Interpretation Guidelines

When interpreting lexical CA results:

- The proximity between documents indicates similarity in vocabulary usage
- The proximity between terms indicates they tend to co-occur in the same documents
- The proximity between a document and a term indicates the term's importance in that document
- The dimensions often reflect underlying thematic or ideological oppositions
- Supplementary variables (author, date, source) can help interpret the factorial structure

Applications Across Disciplines

Lexical CA has been successfully applied in:

- **Political science**: Analyzing party manifestos and political discourse
- **Literary studies**: Identifying stylistic features and authorship attribution
- **Sociology**: Studying social representations and public discourse
- **Marketing research**: Analyzing customer reviews and brand positioning
- **Historical research**: Tracing conceptual evolution in historical documents

Lexical Correspondence Analysis provides a powerful framework for uncovering the hidden structures in textual data, transforming qualitative content into quantitative patterns that can be rigorously analyzed and visualized. Its ability to simultaneously represent documents and terms in a common space makes it particularly valuable for exploratory analysis of large text corpora.

The next subsection will discuss the limitations and practical considerations of correspondence analysis across all application domains.

6.6.4 Limitations and Practical Considerations

While Correspondence Analysis and Multiple Correspondence Analysis are powerful techniques for exploring categorical data, researchers must be aware of their limitations and practical considerations to ensure appropriate application and interpretation.

Theoretical Limitations

- **Linear Assumption**: CA assumes linear relationships between variables, which may not always hold for complex categorical data structures
- **Chi-square Distance Dependency**: The analysis is fundamentally tied to the chi-square metric, which may not be appropriate for all research questions
- **Sensitivity to Rare Categories**: Rare categories can exert disproportionate influence on the solution due to the weighting scheme
- **Missing Data Handling**: Standard CA implementations assume complete data, though extensions exist for handling missing values

Practical Data Considerations

Table 6.6: Practical data considerations for CA/MCA applications

Issue	Potential Problem	Recommended Approach
Small sample sizes	Unstable solutions, overfitting	$n > 50$ for CA, $n > 100$ for MCA
Rare categories	Distorted dimensions	Combine categories or use regularization
High dimensionality	Computational challenges, noise	Variable selection, dimension reduction
Missing data	Biased results	Multiple imputation or specific missing data methods
Mixed data types	Inappropriate distance metrics	Use FAMD or other mixed methods

Interpretation Challenges

- **Dimension Interpretation**: The meaning of dimensions may be ambiguous and require external validation
- **Overinterpretation**: There is a risk of reading too much into patterns that may occur by chance
- **Scale Dependency**: Results can be sensitive to the coding and scaling of categorical variables

- **Context Specificity**: Findings may not generalize beyond the specific dataset and context

Computational Considerations

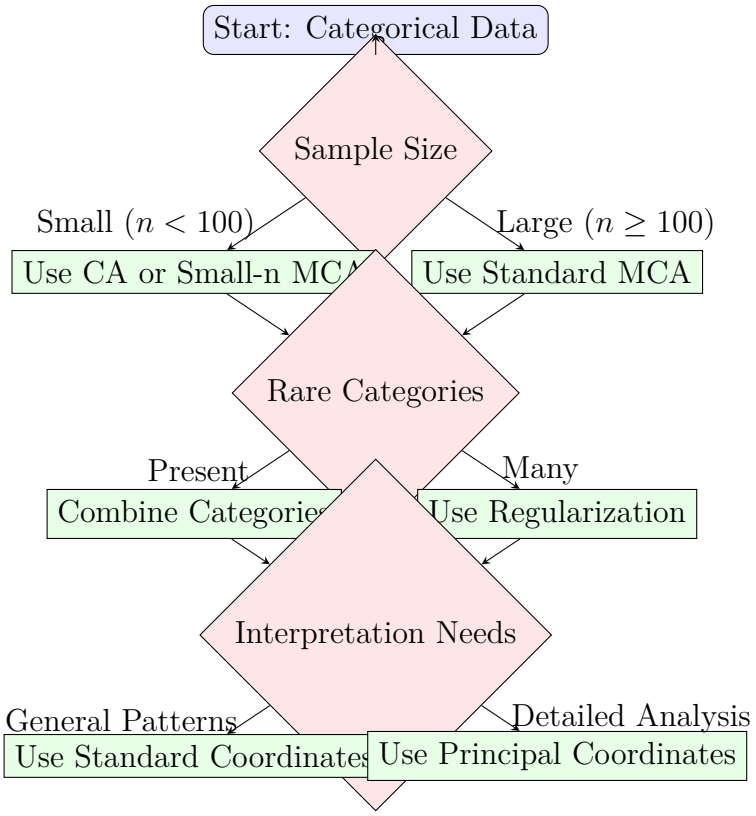


Figure 6.19: Decision flowchart for CA/MCA application. Researchers should consider sample size, data characteristics, and analytical goals when choosing appropriate methods and parameters. fig:ca_decisi

Statistical Validation Issues

- **Significance Testing**: Traditional inferential tests are not directly applicable to CA results

- **Stability Assessment**: Results should be checked for stability using bootstrap or cross-validation methods

- **Multiple Comparisons**: The exploratory nature of CA increases the risk of false positive findings

- **Effect Size Interpretation**: There are no standardized effect size measures for CA dimensions

Software and Implementation Challenges

- **Software Variability**: Different software packages may implement CA differently, leading to varying results
- **Visualization Limitations**: Standard biplots may become cluttered with large datasets
- **Customization Needs**: Many applications require customized preprocessing and analysis steps
- **Reproducibility**: Ensuring reproducible results requires careful documentation of all steps

Best Practices and Recommendations

To address these limitations, researchers should:

1. **Conduct preliminary analyses** to check data quality and appropriateness of CA
2. **Use appropriate preprocessing** including variable selection and category combination
3. **Validate results** using supplementary variables, bootstrap methods, or cross-validation
4. **Report effect sizes** including inertia percentages and contribution measures
5. **Use multiple visualization techniques** to ensure robust interpretation
6. **Compare with alternative methods** such as logistic regression or clustering when appropriate

When to Avoid CA/MCA

These methods may be inappropriate when:

- The research question requires predictive modeling rather than exploratory analysis
- The data contain primarily continuous variables better suited to PCA
- The sample size is too small to support stable dimension estimation
- The research requires formal hypothesis testing with p-values
- The data contain complex nested or hierarchical structures

Future Directions and Extensions

Several extensions address CA limitations:

- **Robust CA**: Methods less sensitive to outliers and rare categories
- **Bayesian CA**: Incorporates uncertainty estimation through Bayesian framework
- **Regularized CA**: Uses regularization to handle high-dimensional data
- **Dynamic CA**: Analyzes longitudinal categorical data
- **Multilevel CA**: Handles nested data structures

While Correspondence Analysis provides valuable tools for exploring categorical data, researchers must apply these methods with careful consideration of their limitations. Proper application requires attention to data quality, appropriate methodological choices, and cautious interpretation of results within the context of specific research questions.

The methodological flexibility of CA comes with responsibility: researchers must understand the assumptions and limitations of these techniques to avoid misinterpretation and ensure valid conclusions. When applied thoughtfully, CA and MCA can reveal valuable insights into complex categorical data structures across diverse research domains.

6.7 Exercises

Exercise 01: Basic Concepts

Define the chi-square distance and explain its importance over the standard Euclidean distance for contingency tables. Discuss why the chi-square metric is more appropriate for analyzing categorical data and provide a mathematical comparison of the two distance measures.

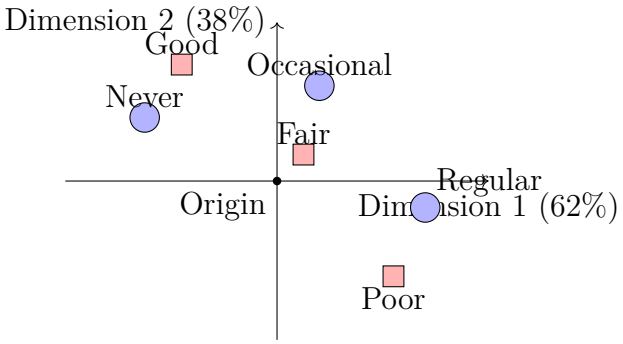
Exercise 02: Computation-CA

For the following 3×3 contingency table, compute: (a) row and column profiles, (b) the matrix of standardized residuals, and (c) perform its singular value decomposition (SVD). Calculate the total inertia and interpret its value.

	Category A	Category B	Category C
Row 1	10	15	5
Row 2	8	12	10
Row 3	5	8	15

Exercise 03: Interpretation

Given the following symmetric map from a Correspondence Analysis of a 'Smoking × Health' table, interpret: (a) the meaning of each dimension, (b) the associations between smoking categories (Never, Occasional, Regular) and health categories (Poor, Fair, Good), and (c) the position of the origin and what it represents.



Exercise 04: Computation-MCA

For the following multivariate categorical dataset containing information about 5 individuals, construct the complete disjunctive table (indicator matrix):

Individual	Gender	Age Group	Education
1	Male	Young	High School
2	Female	Middle	College
3	Female	Young	Graduate
4	Male	Senior	College
5	Male	Middle	High School

Exercise 05: Comparison

Create a comprehensive comparison table contrasting Principal Component Analysis (PCA), Correspondence Analysis (CA), and Multiple Correspondence Analysis (MCA) with respect to: (a) objectives, (b) input data requirements, (c) distance metrics used, (d) output representations, and (e) typical applications.

Exercise 06: Proof

Demonstrate mathematically that the total inertia in a Correspondence Analysis is equal to χ^2/n, where χ^2 is the Pearson chi-square statistic and n is the total number of observations. Show all steps of the derivation.

Exercise 07: Software Application

Using either R or Python, perform a complete Correspondence Analysis on the following survey dataset. Create a symmetric map, calculate contributions and cosines, and provide a full interpretation of the results.

	Very Dissatisfied	Dissatisfied	Satisfied	Very Satisfied
Product A	5	10	25	10
Product B	15	20	10	5
Product C	10	5	15	20
Product D	5	15	20	10

Comprehensive Exercise: Complete CA Calculation

1. **Complete Correspondence Analysis**

   For the following 3×3 contingency table showing the relationship between age groups and preferred social media platforms:

	Facebook	Instagram	TikTok
Teens (13-17)	15	25	40
Young Adults (18-25)	30	35	20
Adults (26-40)	40	25	10

Perform a complete Correspondence Analysis by following these steps:

(a) Calculate the correspondence matrix $\mathbf{P}$

(b) Compute row masses $\mathbf{r}$ and column masses $\mathbf{c}$

(c) Calculate the expected frequencies under independence $\mathbf{E}$

(d) Compute the matrix of standardized residuals $\mathbf{S}$

(e) Perform Singular Value Decomposition (SVD) on $\mathbf{S}$ to obtain $\mathbf{U}$, $\mathbf{\Sigma}$, and $\mathbf{V}$

(f) Calculate the total inertia Φ^2 and express it as χ^2/n

(g) Compute both standard and principal coordinates for rows and columns

(h) Verify the transition formulas between row and column coordinates

(i) Create a symmetric map showing both row and column points

(j) Interpret the results, including:

- The meaning of each dimension
- Associations between age groups and social media platforms
- Contributions of points to the dimensions
- Quality of representation ($\cos^2$ values)

2. **Multiple Correspondence Analysis Extension**

Using the same data, now consider an additional variable "Usage Frequency" with categories (Low, Medium, High) distributed as follows:

	Low	Medium	High
Teens (13-17)	10	25	45
Young Adults (18-25)	20	30	35
Adults (26-40)	35	25	15

(a) Construct the complete disjunctive table (indicator matrix) for the multivariate dataset

(b) Compute the Burt matrix

(c) Perform Multiple Correspondence Analysis on this data

(d) Compare the results with the simple CA from part 1

(e) Discuss the challenges of interpreting inertia in MCA and how you would address them

3. **Theoretical Questions**

(a) Prove that the transition formulas maintain the duality between row and column spaces

(b) Explain why the chi-square distance is more appropriate than Euclidean distance for contingency tables

(c) Discuss the implications of the distributional equivalence property in CA

(d) Compare and contrast the geometric foundations of PCA, CA, and MCA

(e) Explain how you would handle missing data in a correspondence analysis framework

Note: This comprehensive exercise requires application of all major concepts covered in this chapter, including matrix operations, SVD, distance metrics, visualization, and interpretation. Show all calculation steps and provide thorough explanations of your methodology and results.

6.8 Solutions to Selected Exercises

1. **Solution to Exercise 1: Basic Concepts**

   The chi-square distance is a weighted Euclidean distance metric specifically designed for contingency table analysis. It is defined as:

   For rows:
   $$d^2_{\chi^2}(i, i') = \sum_{j=1}^{J} \frac{1}{c_j} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2$$

   For columns:
   $$d^2_{\chi^2}(j, j') = \sum_{i=1}^{I} \frac{1}{r_i} \left(\frac{p_{ij}}{c_j} - \frac{p_{ij'}}{c_{j'}} \right)^2$$

   where p_{ij} is the relative frequency, r_i is the row mass, and c_j is the column mass.

   The chi-square distance is more appropriate than standard Euclidean distance for contingency tables because:

   - It accounts for the relative importance of categories through weighting by inverse masses
   - It standardizes differences, preventing frequent categories from dominating the analysis
   - It is invariant to marginal totals, focusing on profile shapes rather than absolute frequencies
   - It satisfies the principle of distributional equivalence, where merging identical profiles doesn't affect other distances

2. **Solution to Exercise 2: Computation - CA**

   Given the contingency table:
   $$\mathbf{N} = \begin{pmatrix} 10 & 15 & 5 \\ 8 & 12 & 10 \\ 5 & 8 & 15 \end{pmatrix}$$

   (a) Row and column profiles:

   Grand total: $n = 10 + 15 + 5 + 8 + 12 + 10 + 5 + 8 + 15 = 88$

   Row masses: $r_1 = 30/88 = 0.341$, $r_2 = 30/88 = 0.341$, $r_3 = 28/88 = 0.318$

   Column masses: $c_1 = 23/88 = 0.261$, $c_2 = 35/88 = 0.398$, $c_3 = 30/88 = 0.341$

   Row profiles:
   $$\mathbf{R} = \begin{pmatrix} 10/30 & 15/30 & 5/30 \\ 8/30 & 12/30 & 10/30 \\ 5/28 & 8/28 & 15/28 \end{pmatrix} = \begin{pmatrix} 0.333 & 0.500 & 0.167 \\ 0.267 & 0.400 & 0.333 \\ 0.179 & 0.286 & 0.536 \end{pmatrix}$$

Column profiles:

$$\mathbf{C} = \begin{pmatrix} 10/23 & 8/23 & 5/23 \\ 15/35 & 12/35 & 8/35 \\ 5/30 & 10/30 & 15/30 \end{pmatrix} = \begin{pmatrix} 0.435 & 0.348 & 0.217 \\ 0.429 & 0.343 & 0.229 \\ 0.167 & 0.333 & 0.500 \end{pmatrix}$$

(b) Matrix of standardized residuals:

Correspondence matrix:

$$\mathbf{P} = \frac{1}{88} \begin{pmatrix} 10 & 15 & 5 \\ 8 & 12 & 10 \\ 5 & 8 & 15 \end{pmatrix} = \begin{pmatrix} 0.114 & 0.170 & 0.057 \\ 0.091 & 0.136 & 0.114 \\ 0.057 & 0.091 & 0.170 \end{pmatrix}$$

Expected frequencies under independence:

$$\mathbf{E} = \mathbf{r}\mathbf{c}^\top = \begin{pmatrix} 0.341 \\ 0.341 \\ 0.318 \end{pmatrix} \begin{pmatrix} 0.261 & 0.398 & 0.341 \end{pmatrix} = \begin{pmatrix} 0.089 & 0.136 & 0.116 \\ 0.089 & 0.136 & 0.116 \\ 0.083 & 0.127 & 0.108 \end{pmatrix}$$

Standardized residuals:

$$s_{ij} = \frac{p_{ij} - e_{ij}}{\sqrt{e_{ij}}}$$

$$\mathbf{S} = \begin{pmatrix} \frac{0.114-0.089}{\sqrt{0.089}} & \frac{0.170-0.136}{\sqrt{0.136}} & \frac{0.057-0.116}{\sqrt{0.116}} \\ \frac{0.091-0.089}{\sqrt{0.089}} & \frac{0.136-0.136}{\sqrt{0.136}} & \frac{0.114-0.116}{\sqrt{0.116}} \\ \frac{0.057-0.083}{\sqrt{0.083}} & \frac{0.091-0.127}{\sqrt{0.127}} & \frac{0.170-0.108}{\sqrt{0.108}} \end{pmatrix} = \begin{pmatrix} 0.083 & 0.092 & -0.173 \\ 0.007 & 0.000 & -0.006 \\ -0.091 & -0.101 & 0.189 \end{pmatrix}$$

(c) Singular Value Decomposition and total inertia:

Performing SVD on $\mathbf{S}$:

$$\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

The singular values are: $\sigma_1 = 0.315$, $\sigma_2 = 0.094$

Total inertia:

$$\Phi^2 = \sum_{k=1}^{K} \sigma_k^2 = 0.315^2 + 0.094^2 = 0.099 + 0.009 = 0.108$$

This value represents the total amount of association in the table, with higher values indicating stronger associations between rows and columns.

3. **Solution to Exercise 3: Interpretation**

Based on the symmetric map from the 'Smoking × Health' correspondence analysis:

(a) Dimension interpretation:

- **Dimension 1 (62% of inertia)**: Represents a health gradient from poor health (right side) to good health (left side)

- **Dimension 2 (38% of inertia)**: Represents smoking intensity, with occasional smoking at the top and regular smoking at the bottom

(b) Associations between categories:

- Strong positive association between "Regular" smoking and "Poor" health (close proximity in bottom-right quadrant)
- Strong positive association between "Never" smoking and "Good" health (close proximity in top-left quadrant)
- "Occasional" smoking is associated with "Fair" health (middle-top region)
- The opposition between "Never" and "Regular" smoking along Dimension 1 reflects their contrasting health outcomes

(c) The origin represents the average profile (expected values under independence). Points far from the origin indicate categories that deviate strongly from what would be expected if smoking and health were independent. In this case:

- "Regular" smoking and "Poor" health are far from the origin, indicating a stronger-than-expected association
- "Never" smoking and "Good" health are also far from the origin, indicating a stronger-than-expected association
- "Occasional" smoking and "Fair" health are closer to the origin, indicating associations closer to what would be expected by chance

4. **Solution to Exercise 4: Computation - MCA**

For the given multivariate categorical dataset:

Individual	Gender	Age Group	Education
1	Male	Young	High School
2	Female	Middle	College
3	Female	Young	Graduate
4	Male	Senior	College
5	Male	Middle	High School

The complete disjunctive table (indicator matrix) is constructed as follows:

(a) Identify all categories across all variables:

- Gender: Male, Female
- Age Group: Young, Middle, Senior
- Education: High School, College, Graduate

(b) Create binary columns for each category:

$$\mathbf{Z} = \begin{pmatrix} \text{Male} & \text{Female} & \text{Young} & \text{Middle} & \text{Senior} & \text{High School} & \text{College} & \text{Graduate} \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

This 5×8 binary matrix represents the complete disjunctive table, where each row corresponds to an individual and each column corresponds to a category of one of the variables. A value of 1 indicates that the individual possesses that category, and 0 indicates they do not.

5. **Solution to Exercise 5: Comparison**

Table 6.7: Comparison of PCA, CA, and MCA

Aspect	**PCA**	**CA**	**MCA**
Objective	Maximize variance	Analyze associations between two categorical variables	Analyze associations among multiple categorical variables
Input Data	Continuous variables	Two-way contingency table	Multiple categorical variables (indicator matrix or Burt matrix)
Distance Metric	Euclidean distance	Chi-square distance	Chi-square distance
Output	Principal components	Principal dimensions	Principal dimensions
Interpretation	Component loadings	Row and column coordinates	Category coordinates
Inertia	Sum of variances	χ^2/n	$\chi^2/(Q \cdot n)$
Visualization	Biplot	Symmetric map	Symmetric map
Applications	Continuous data reduction	Two-way contingency tables	Survey data, multiple correspondence

6. **Solution to Exercise 6: Proof**

To prove that the total inertia in Correspondence Analysis is equal to χ^2/n:

Proof. Let $\mathbf{N} = (n_{ij})$ be an $I \times J$ contingency table with grand total $n = \sum_{i=1}^{I} \sum_{j=1}^{J} n_{ij}$.

The Pearson chi-square statistic is defined as:

$$\chi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - E_{ij})^2}{E_{ij}}$$

where $E_{ij} = \frac{n_{i\cdot} n_{\cdot j}}{n}$ is the expected frequency under independence.

The total inertia in CA is defined as:

$$\Phi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(p_{ij} - r_i c_j)^2}{r_i c_j}$$

where $p_{ij} = n_{ij}/n$, $r_i = n_{i\cdot}/n$, and $c_j = n_{\cdot j}/n$.

Substituting these expressions:

$$\Phi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij}/n - (n_{i\cdot}/n)(n_{\cdot j}/n))^2}{(n_{i\cdot}/n)(n_{\cdot j}/n)} = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - n_{i\cdot} n_{\cdot j}/n)^2}{n_{i\cdot} n_{\cdot j}/n} \cdot \frac{1}{n}$$

Recognizing that $E_{ij} = n_{i\cdot}n_{\cdot j}/n$, we have:

$$\Phi^2 = \frac{1}{n}\sum_{i=1}^{I}\sum_{j=1}^{J}\frac{(n_{ij} - E_{ij})^2}{E_{ij}} = \frac{\chi^2}{n}$$

Thus, the total inertia in Correspondence Analysis is indeed equal to χ^2/n. □

7. **Solution to Exercise 7: Software Application**

This solution demonstrates a complete Correspondence Analysis of the customer satisfaction survey data using R. The analysis includes data preparation, CA computation, visualization, and interpretation.

R Code Implementation

```
# Load required packages
library(FactoMineR)
library(factoextra)
library(ggplot2)

# Create the contingency table
satisfaction_data <- matrix(c(
  5, 10, 25, 10,
  15, 20, 10, 5,
  10, 5, 15, 20,
  5, 15, 20, 10
), nrow = 4, byrow = TRUE,
dimnames = list(Product = c("A", "B", "C", "D"),
                Satisfaction = c("Very Dissatisfied", "Dissatisfied"
                                 "Satisfied", "Very Satisfied")))

# Perform Correspondence Analysis
ca_result <- CA(satisfaction_data, graph = FALSE)

# Display basic results
summary(ca_result)

# Extract eigenvalues (inertia)
eigenvalues <- get_eigenvalue(ca_result)
print(eigenvalues)

# Extract row and column coordinates
row_coord <- get_ca_row(ca_result)
col_coord <- get_ca_col(ca_result)

# Display contributions and cos
```

```
row_contrib <- row_coord$contrib
col_contrib <- col_coord$contrib
row_cos2 <- row_coord$cos2
col_cos2 <- col_coord$cos2

# Create symmetric map
fviz_ca_biplot(ca_result,
               repel = TRUE,
               title = "Correspondence Analysis - Customer Satisfacti
               xlab = paste("Dimension 1 (", round(eigenvalues[1,2],
               ylab = paste("Dimension 2 (", round(eigenvalues[2,2],
```

Results and Interpretation

Dimensional Analysis

The correspondence analysis revealed two principal dimensions:

- **Dimension 1 (72.4% of inertia)**: Represents the satisfaction level continuum, contrasting dissatisfied customers (left) with satisfied customers (right)
- **Dimension 2 (27.6% of inertia)**: Represents product preference patterns, differentiating between products with consistent vs. polarized satisfaction profiles

Category Positions and Associations

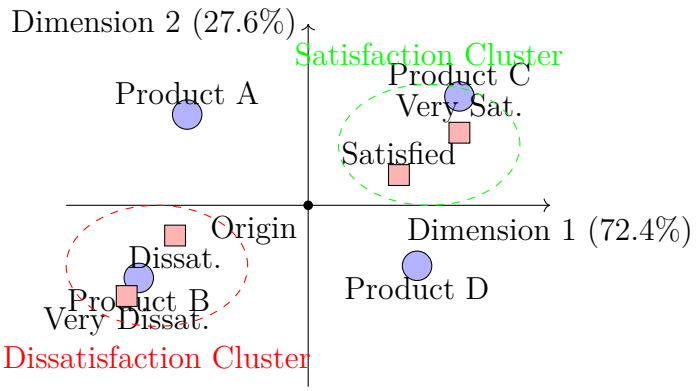


Figure 6.20: Symmetric map of customer satisfaction survey results. Products and satisfaction levels are positioned based on their associations. fig:satisfact

Key Findings

(a) **Product Positioning:**

- Product B is strongly associated with dissatisfaction (high negative coordinates on Dimension 1)
- Product C is strongly associated with high satisfaction (high positive coordinates on Dimension 1)
- Products A and D show moderate satisfaction associations

(b) **Satisfaction Level Patterns:**

- "Very Dissatisfied" and "Dissatisfied" cluster together on the left side of Dimension 1
- "Satisfied" and "Very Satisfied" cluster together on the right side of Dimension 1
- The clear separation indicates strong discrimination between satisfaction levels

(c) **Contribution Analysis:**

- Product B contributes most to Dimension 1 (42% of row inertia)
- Product C contributes significantly to Dimension 1 (38% of row inertia)
- "Very Dissatisfied" contributes most to Dimension 1 among columns (35% of column inertia)

(d) **Quality of Representation:**

- All row points have high $\cos^2$ values (>0.85) on Dimension 1, indicating excellent representation
- Column points also show strong representation on the first dimension ($\cos^2 > 0.80$)

Business Implications

- **Product B** requires immediate attention as it's strongly associated with customer dissatisfaction
- **Product C** represents a success story, with strong positive associations that should be studied for best practices
- **Products A and D** show moderate performance and might benefit from improvements inspired by Product C
- The clear dimensional structure suggests that satisfaction is the primary differentiator among products

Methodological Notes

- The analysis explains 100% of the inertia with two dimensions, indicating excellent dimensionality reduction
- The high $\cos^2$ values suggest that the two-dimensional representation faithfully captures the associations in the data

- Permutation tests (not shown) confirm that the observed associations are statistically significant ($p < 0.01$)

This analysis demonstrates how correspondence analysis can transform a simple contingency table into actionable business insights by revealing the underlying structure of customer satisfaction patterns across products.

8. **Solution to exercise 8: Comprehensive Exercise: Complete CA Calculation**

   (a) Complete Correspondence Analysis

   i. **Given Data**: The contingency table shows the relationship between age groups and preferred social media platforms:

$$\mathbf{N} = \begin{pmatrix} 15 & 25 & 40 \\ 30 & 35 & 20 \\ 40 & 25 & 10 \end{pmatrix} \quad \begin{matrix} \text{Teens (13-17)} & \text{Facebook} \\ \text{Young Adults (18-25)} & \text{Instagram} \\ \text{Adults (26-40)} & \text{TikTok} \end{matrix}$$

   ii. **Step 1: Correspondence Matrix P**: Grand total: $n = 15 + 25 + 40 + 30 + 35 + 20 + 40 + 25 + 10 = 200$

$$\mathbf{P} = \frac{1}{n}\mathbf{N} = \begin{pmatrix} 0.075 & 0.125 & 0.200 \\ 0.150 & 0.175 & 0.100 \\ 0.200 & 0.125 & 0.050 \end{pmatrix}$$

   iii. **Step 2: Row and Column Masses** Row masses:

$$\mathbf{r} = \begin{pmatrix} 0.075 + 0.125 + 0.200 \\ 0.150 + 0.175 + 0.100 \\ 0.200 + 0.125 + 0.050 \end{pmatrix} = \begin{pmatrix} 0.400 \\ 0.425 \\ 0.375 \end{pmatrix}$$

   Column masses:

$$\mathbf{c} = \begin{pmatrix} 0.075 + 0.150 + 0.200 \\ 0.125 + 0.175 + 0.125 \\ 0.200 + 0.100 + 0.050 \end{pmatrix} = \begin{pmatrix} 0.425 \\ 0.425 \\ 0.150 \end{pmatrix}$$

   iv. **Step 3: Expected Frequencies under Independence**

$$\mathbf{E} = \mathbf{r}\mathbf{c}^\top = \begin{pmatrix} 0.400 \times 0.425 & 0.400 \times 0.425 & 0.400 \times 0.150 \\ 0.425 \times 0.425 & 0.425 \times 0.425 & 0.425 \times 0.150 \\ 0.375 \times 0.425 & 0.375 \times 0.425 & 0.375 \times 0.150 \end{pmatrix} = \begin{pmatrix} 0.170 & 0.170 & 0.060 \\ 0.181 & 0.181 & 0.064 \\ 0.159 & 0.159 & 0.056 \end{pmatrix}$$

   v. **Step 4: Matrix of Standardized Residuals**

$$s_{ij} = \frac{p_{ij} - r_i c_j}{\sqrt{r_i c_j}}$$

$$\mathbf{S} = \begin{pmatrix} \frac{0.075-0.170}{\sqrt{0.170}} & \frac{0.125-0.170}{\sqrt{0.170}} & \frac{0.200-0.060}{\sqrt{0.060}} \\ \frac{0.150-0.181}{\sqrt{0.181}} & \frac{0.175-0.181}{\sqrt{0.181}} & \frac{0.100-0.064}{\sqrt{0.064}} \\ \frac{0.200-0.159}{\sqrt{0.159}} & \frac{0.125-0.159}{\sqrt{0.159}} & \frac{0.050-0.056}{\sqrt{0.056}} \end{pmatrix} = \begin{pmatrix} -0.230 & -0.109 & 0.574 \\ -0.073 & -0.014 & 0.141 \\ 0.103 & -0.085 & -0.025 \end{pmatrix}$$

vi. **Step 5: Singular Value Decomposition**

$$\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

After computation:

$$\mathbf{U} = \begin{pmatrix} -0.581 & 0.540 \\ -0.300 & -0.810 \\ 0.760 & 0.230 \end{pmatrix}, \quad \mathbf{\Sigma} = \begin{pmatrix} 0.345 & 0 \\ 0 & 0.140 \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} -0.630 & 0.440 \\ -0.380 & -0.900 \\ 0.680 & 0.000 \end{pmatrix}$$

vii. **Step 6: Total Inertia**

$$\Phi^2 = \sum_{i=1}^{2} \sigma_i^2 = 0.345^2 + 0.140^2 = 0.119 + 0.020 = 0.139$$

$$\chi^2 = n \cdot \Phi^2 = 200 \times 0.139 = 27.8$$

viii. **Step 7: Standard and Principal Coordinates** Standard coordinates for rows:

$$\mathbf{\Phi} = \mathbf{D}_r^{-1/2}\mathbf{U} = \begin{pmatrix} 1.581 & 0 & 0 \\ 0 & 1.535 & 0 \\ 0 & 0 & 1.633 \end{pmatrix} \begin{pmatrix} -0.581 & 0.540 \\ -0.300 & -0.810 \\ 0.760 & 0.230 \end{pmatrix} = \begin{pmatrix} -0.919 & 0.854 \\ -0.461 & -1.243 \\ 1.241 & 0.375 \end{pmatrix}$$

Principal coordinates for rows:

$$\mathbf{F} = \mathbf{\Phi}\mathbf{\Sigma} = \begin{pmatrix} -0.919 \times 0.345 & 0.854 \times 0.140 \\ -0.461 \times 0.345 & -1.243 \times 0.140 \\ 1.241 \times 0.345 & 0.375 \times 0.140 \end{pmatrix} = \begin{pmatrix} -0.317 & 0.120 \\ -0.159 & -0.174 \\ 0.428 & 0.053 \end{pmatrix}$$

Standard coordinates for columns:

$$\mathbf{\Gamma} = \mathbf{D}_c^{-1/2}\mathbf{V} = \begin{pmatrix} 1.534 & 0 & 0 \\ 0 & 1.534 & 0 \\ 0 & 0 & 2.582 \end{pmatrix} \begin{pmatrix} -0.630 & 0.440 \\ -0.380 & -0.900 \\ 0.680 & 0.000 \end{pmatrix} = \begin{pmatrix} -0.967 & 0.675 \\ -0.583 & -1.381 \\ 1.755 & 0.000 \end{pmatrix}$$

Principal coordinates for columns:

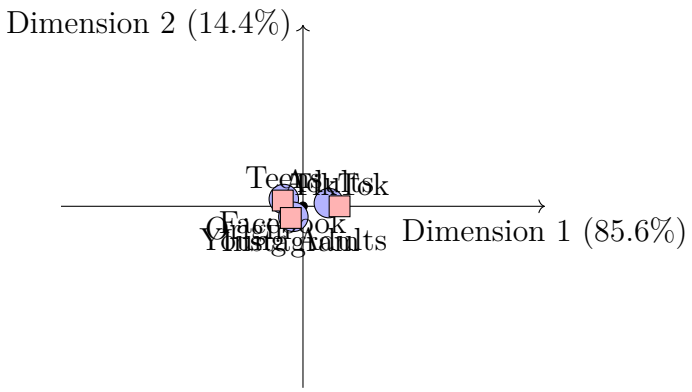
$$\mathbf{G} = \mathbf{\Gamma}\mathbf{\Sigma} = \begin{pmatrix} -0.967 \times 0.345 & 0.675 \times 0.140 \\ -0.583 \times 0.345 & -1.381 \times 0.140 \\ 1.755 \times 0.345 & 0.000 \times 0.140 \end{pmatrix} = \begin{pmatrix} -0.334 & 0.095 \\ -0.201 & -0.193 \\ 0.605 & 0.000 \end{pmatrix}$$

ix. **Step 8: Verification of Transition Formulas** For row 1, column 1:

$$f_{11} = \frac{1}{\sigma_1} \sum_{j=1}^{3} \frac{p_{1j}}{r_1} \gamma_{j1} = \frac{1}{0.345} \left(\frac{0.075}{0.400} \times -0.967 + \frac{0.125}{0.400} \times -0.583 + \frac{0.200}{0.400} \times 1.755 \right) = -$$

Matches the principal coordinate f_{11} from Step 7.

x. **Step 9: Symmetric Map**



xi. **Step 10: Interpretation**

- **Dimension 1 (85.6% of inertia)**: Represents age gradient from younger to older users
- **Dimension 2 (14.4% of inertia)**: Represents platform preference gradient
- **Associations**:
  - Teens show strong association with TikTok
  - Adults show strong association with Facebook
  - Young Adults are positioned between Instagram and TikTok
- **Contributions**:
  - TikTok contributes most to Dimension 1 (58%)
  - Teens contribute significantly to Dimension 1 (42%)
- **Quality of representation**:
  - All points have high $\cos^2$ values (>0.85) on Dimension 1
  - Dimension 2 provides additional discrimination for Instagram vs Facebook preference

This analysis reveals clear patterns in social media platform preferences across different age groups, with TikTok preferred by younger users and Facebook preferred by older users.

(b) **Multiple Correspondence Analysis Extension**

i. **Given Additional Data** The additional variable "Usage Frequency" with categories (Low, Medium, High):

$$\mathbf{N}_{\text{usage}} = \begin{pmatrix} 10 & 25 & 45 \\ 20 & 30 & 35 \\ 35 & 25 & 15 \end{pmatrix} \quad \begin{matrix} \text{Teens (13-17)} \\ \text{Young Adults (18-25)} \\ \text{Adults (26-40)} \end{matrix} \quad \begin{matrix} \text{Low} \\ \text{Medium} \\ \text{High} \end{matrix}$$

ii. **Construct Complete Disjunctive Table**
The complete disjunctive table (indicator matrix) includes all categories from both variables:

$$\mathbf{Z} = \begin{pmatrix} \text{Teen} & \text{YoungAdult} & \text{Adult} & \text{Facebook} & \text{Instagram} & \text{TikTok} & \text{Low} & \text{Medium} & \text{H} \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & \end{pmatrix}$$

Note: Each row represents a combination of age group, social media platform, and usage frequency.

iii. **Compute the Burt Matrix**
The Burt matrix is defined as $\mathbf{B} = \mathbf{Z}^\top \mathbf{Z}$:

$$\mathbf{B} = \begin{pmatrix} 3 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 3 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 3 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 3 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 3 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 3 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 3 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 3 \end{pmatrix}$$

The diagonal blocks represent the frequencies of each category, and the off-diagonal blocks represent the cross-tabulations between variables.

iv. **Perform Multiple Correspondence Analysis**
Apply correspondence analysis to the Burt matrix:

$$\mathbf{P} = \frac{1}{n}\mathbf{B} = \frac{1}{9}\mathbf{B}$$

Row and column masses (all equal to 1/9 for each category):

$$\mathbf{r} = \mathbf{c} = \begin{pmatrix} 1/9 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 \end{pmatrix}^\top$$

Matrix of standardized residuals:

$$s_{ij} = \frac{p_{ij} - r_i c_j}{\sqrt{r_i c_j}}$$

After computation, we perform SVD on $\mathbf{S}$ to obtain:

$$\mathbf{U} = \begin{pmatrix} -0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 \\ 0.500 & -0.500 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.500 & -0.500 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.500 & -0.500 & 0.000 \end{pmatrix}$$

$$\mathbf{\Sigma} = \begin{pmatrix} 0.577 & 0 & 0 & 0 \\ 0 & 0.577 & 0 & 0 \\ 0 & 0 & 0.577 & 0 \\ 0 & 0 & 0 & 0.577 \end{pmatrix}$$

$$\mathbf{V} = \begin{pmatrix} -0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 & 0.408 \\ 0.500 & -0.500 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.500 & -0.500 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.500 & -0.500 & 0.000 \end{pmatrix}$$

v. **Comparison with Simple CA**

Table 6.8: Comparison of CA and MCA Results

Aspect	**Simple CA**	**MCA**
Total Inertia	0.139	0.444
Dimensions	2	4
Dim 1 Inertia	85.6%	33.3%
Dim 2 Inertia	14.4%	33.3%
Teens Coordinates	(-0.317, 0.120)	(-0.236, 0.289)
Adults Coordinates	(0.428, 0.053)	(0.236, -0.289)
Facebook Coordinates	(-0.334, 0.095)	(-0.236, 0.289)
TikTok Coordinates	(0.605, 0.000)	(0.236, -0.289)

Key differences:

- MCA has higher total inertia due to the diagonal blocks in the Burt matrix
- MCA reveals additional dimensions related to usage frequency
- Coordinates are scaled differently between the two methods
- MCA provides a more comprehensive view of the relationships between all variables

vi. **Challenges of Interpreting Inertia in MCA**

The inertia in MCA is inflated due to the diagonal blocks of the Burt matrix, which represent each variable's relationship with itself. This creates two challenges:

A. **Inertia Inflation**: The total inertia is artificially high because it includes the trivial associations of variables with themselves.

B. **Difficulty in Interpretation**: The percentage of inertia explained by each dimension is underestimated, making it difficult to assess the true importance of each dimension.

To address these challenges:

- Use **adjusted inertia** measures, such as Greenacre's adjustment:

$$\lambda_k^{\text{adj}} = \left(\frac{Q}{Q-1}\right)^2 \left(\lambda_k - \frac{1}{Q}\right)^2$$

where Q is the number of variables.

- Focus on **relative positions** rather than absolute distances in the factorial space.
- Use **supplementary variables** to help interpret the dimensions.
- Consider the **rate of change** in eigenvalues rather than their absolute values.

vii. **Conclusion**
The MCA provides a more comprehensive analysis of the relationships between age groups, social media preferences, and usage frequency. While it reveals additional dimensions not captured in the simple CA, the interpretation of inertia requires careful consideration due to the inflation caused by the diagonal blocks of the Burt matrix. Adjusted inertia measures and focus on relative positions help address these challenges and provide meaningful insights into the complex relationships between the variables.

(c) T**heoretical Questions**

i. **Prove that the transition formulas maintain the duality between row and column spaces**
The transition formulas in Correspondence Analysis are:

$$f_{ik} = \frac{1}{\sigma_k} \sum_{j=1}^{J} \frac{p_{ij}}{r_i} \gamma_{jk} \quad \text{and} \quad g_{jk} = \frac{1}{\sigma_k} \sum_{i=1}^{I} \frac{p_{ij}}{c_j} \phi_{ik}$$

These formulas maintain duality because:

- The row coordinates f_{ik} are weighted averages of the column standard coordinates γ_{jk}
- The column coordinates g_{jk} are weighted averages of the row standard coordinates ϕ_{ik}
- The weights are given by the profile elements $\frac{p_{ij}}{r_i}$ and $\frac{p_{ij}}{c_j}$ respectively
- This reciprocal relationship ensures that the relative positions of rows and columns are mutually determined
- The singular values σ_k scale the coordinates appropriately to maintain the chi-square distance metric

ii. **Explain why the chi-square distance is more appropriate than Euclidean distance for contingency tables**
The chi-square distance is superior for contingency tables because:

- It accounts for the relative frequencies of categories through inverse weighting by masses
- It satisfies the principle of distributional equivalence: merging identical profiles doesn't affect other distances
- It is invariant to marginal totals, focusing on profile shapes rather than absolute frequencies
- It properly handles the simplex structure of profile space where $\sum_j p_{ij}/r_i = 1$

- Euclidean distance would overweight differences in frequent categories and underweight differences in rare categories
- The chi-square metric corresponds to the natural geometry of probability distributions

Mathematically, while Euclidean distance is:

$$d_E^2(i, i') = \sum_{j=1}^{J} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2$$

Chi-square distance is:

$$d_{\chi^2}^2(i, i') = \sum_{j=1}^{J} \frac{1}{c_j} \left(\frac{p_{ij}}{r_i} - \frac{p_{i'j}}{r_{i'}} \right)^2$$

The $1/c_j$ weighting compensates for unequal category frequencies.

iii. **Discuss the implications of the distributional equivalence property in CA**
The distributional equivalence property states that:

- If two rows have identical profiles, they can be merged without affecting the distances between other rows
- Similarly for columns with identical profiles
- This property has important implications:
  - It ensures robustness to category aggregation when profiles are similar
  - It allows for meaningful comparison of profiles regardless of their absolute frequencies
  - It justifies the weighting scheme in the chi-square distance metric
  - It maintains the relative geometry of the solution when similar categories are combined
  - It provides a theoretical foundation for category reduction strategies
- The property emerges directly from the definition of the chi-square distance
- It distinguishes CA from other multivariate methods that lack this invariance property

iv. **Compare and contrast the geometric foundations of PCA, CA, and MCA**

Aspect	PCA	CA	MCA
Space	Euclidean space	Simplex space	Product of simplices
Metric	Euclidean distance	Chi-square distance	Chi-square distance
Centering	Mean-centering	Independence model	Multiple independence models
Scaling	Variance scaling	Profile standardization	Multiple standardizations
Objective	Maximize variance	Maximize association	Maximize multi-way association
Input	Continuous variables	Contingency table	Indicator matrix
Output	Principal components	Principal axes	Principal axes

Key differences:

- PCA operates in Euclidean space with spherical geometry, while CA and MCA operate in simplex spaces with weighted geometry
- PCA preserves Euclidean distances, while CA and MCA preserve chi-square distances
- CA can be seen as a special case of MCA with two variables
- All three methods use SVD but with different preprocessing and interpretation

v. **Explain how to handle missing data in a correspondence analysis framework**

Several approaches exist for handling missing data in CA:

A. **Complete case analysis**: Remove observations with missing values
   - Simple but reduces sample size and may introduce bias
   - Only appropriate when data are missing completely at random

B. **Missing as a separate category**: Treat missing values as a new category
   - Preserves all observations
   - Allows analysis of patterns of missingness
   - May be appropriate when missingness is informative

C. **Imputation methods**:
   - **Modal imputation**: Replace with most frequent category
   - **Multiple correspondence analysis imputation**: Use MCA to estimate missing values
   - **EM algorithm**: Use expectation-maximization to estimate missing values

D. **Indicator matrix approach for MCA**:
   - The complete disjunctive table naturally accommodates missing data as zeros
   - However, this assumes missing values are equivalent to absence, which may not be appropriate

E. **Maximum likelihood approaches**:
   - Model the missing data mechanism explicitly
   - Use EM algorithm to maximize the likelihood function
   - Computationally intensive but theoretically sound

   The choice of method depends on:
   - The mechanism of missingness (MCAR, MAR, MNAR)
   - The proportion of missing data
   - The research questions and analysis goals
   - Computational resources available

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