

Principal Component Analysis

Dimensionality Reduction and the Maximum Variance Perspective

Based on Bishop PRML Chapter 12

November 10, 2025

The Dimensionality Challenge

Modern machine learning confronts us with high-dimensional data:

- ▶ Images: 28×28 grayscale = 784 dimensions
- ▶ Genomics: thousands of gene expressions per sample
- ▶ Text: vocabulary size in tens of thousands
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Problems we face:

- ▶ Cannot visualize beyond 3D
- ▶ Computational cost scales poorly with dimension
- ▶ Many algorithms struggle in high dimensions (curse of dimensionality)

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The central question: What does “meaningful” mean mathematically?

Real-World Applications

figures/eigenfaces.png

(a) Face recognition using eigenfaces

figures/genomics_pca.png

(b) Gene expression analysis

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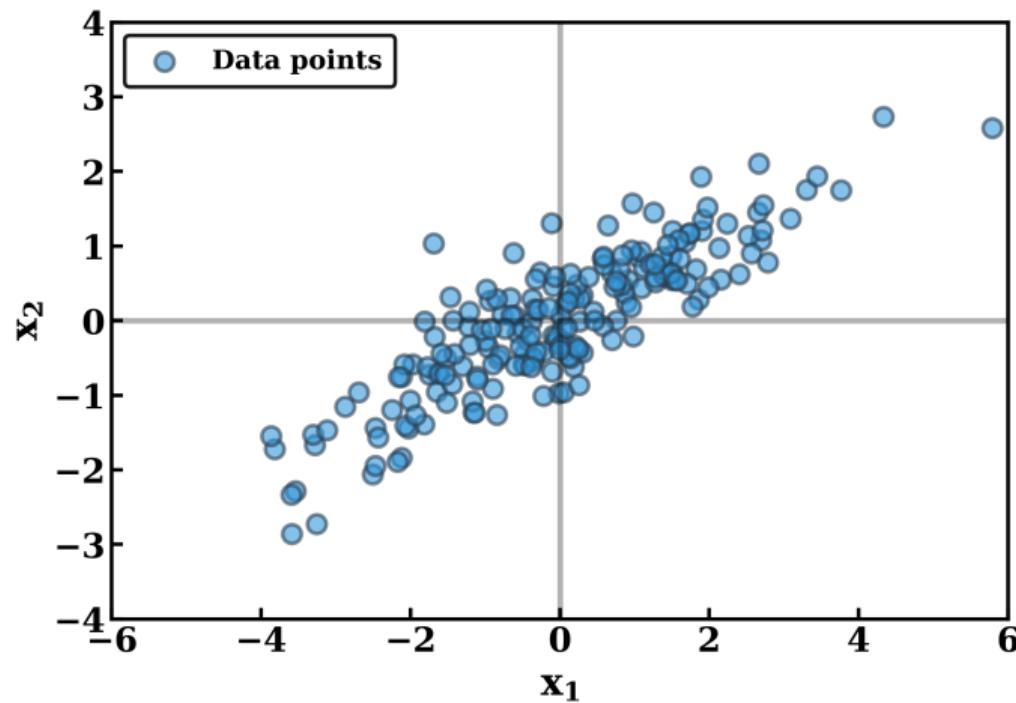
Which projection is “best”?

Principal Component Analysis provides an answer based on two equivalent perspectives:

1. **Maximum variance:** Keep directions with highest variance
2. **Minimum error:** Minimize information loss from projection

Both lead to the same solution.

A Simple 2D Example



Consider data naturally lying along an elongated cloud. There's clearly more “spread” in some directions than others.

Intuition: Direction of Spread

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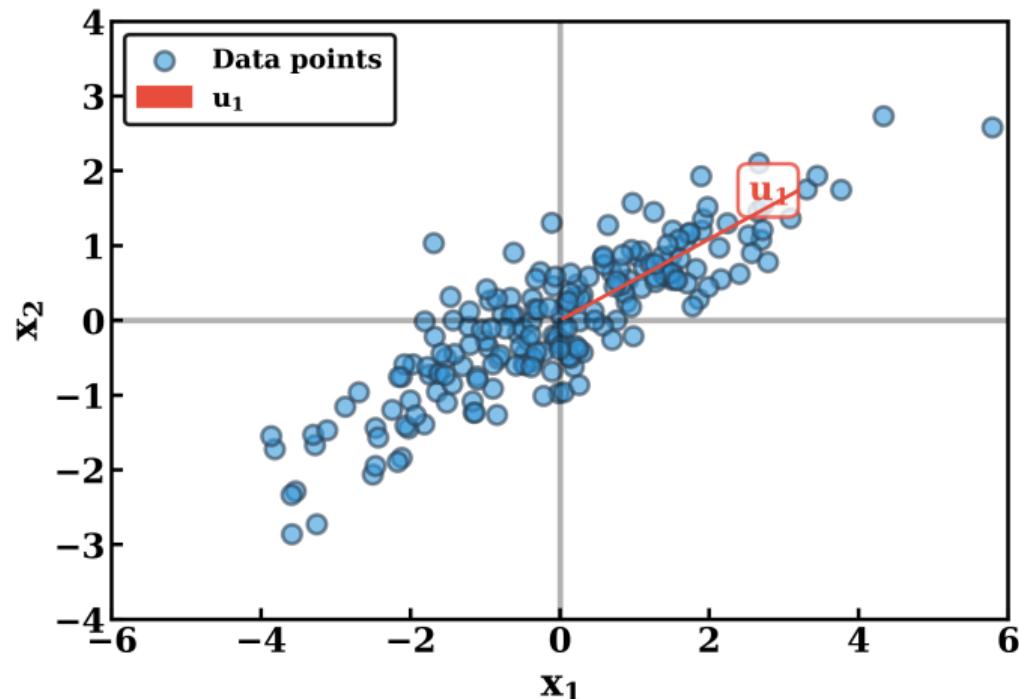
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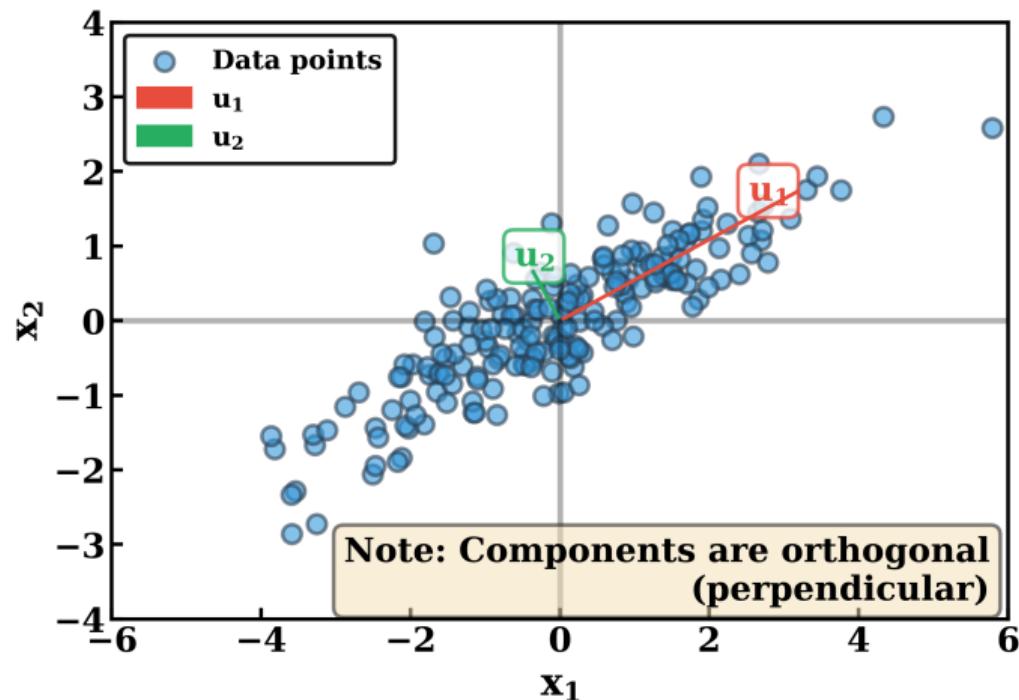
This direction of maximum variance is the **first principal component**.

Visual: First Principal Component



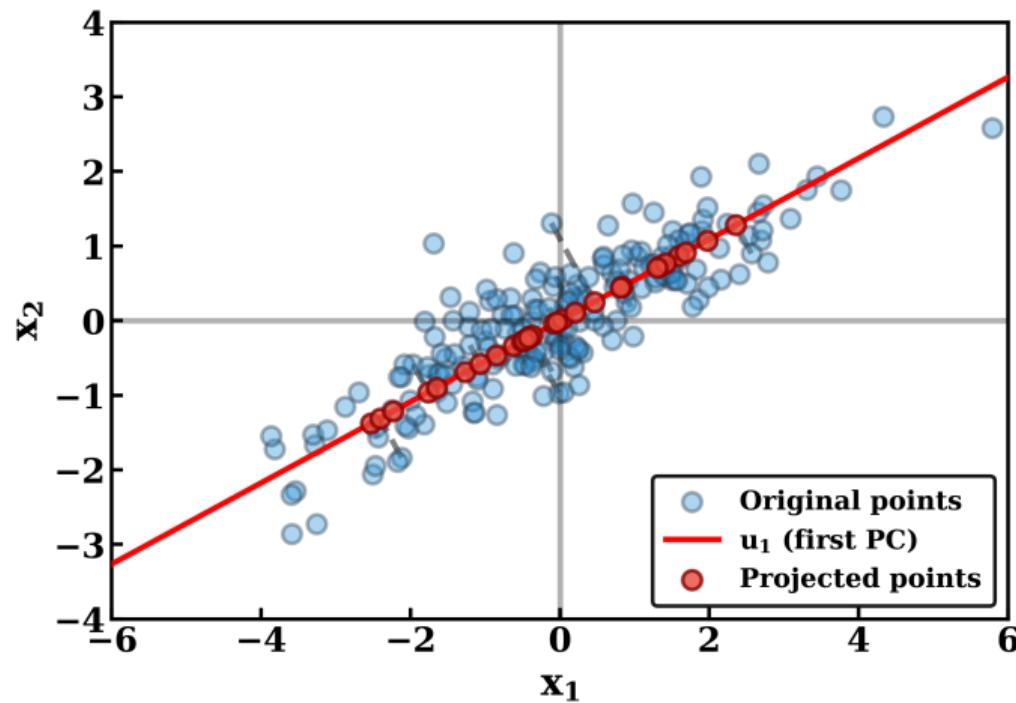
The first principal component u_1 points in the direction of maximum variance.

Visual: Second Principal Component



The second principal component u_2 is orthogonal to the first and captures the direction of next-highest variance.

Projection Intuition



Projecting onto u_1 reduces dimensionality from 2D to 1D while preserving maximum variance.

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- ▶ Variance in the perpendicular direction (\mathbf{u}_2 direction)
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What did we keep?

- ▶ Variance in the principal direction
- ▶ This is the “large” variance—more important
- ▶ The overall structure and spread of the data

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For dimensionality reduction: project data onto the top M principal components.

This captures as much variance as possible in M dimensions.

Setup: The Data Matrix

Consider a dataset of N observations, each in D dimensions:

$$\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N \quad \text{where } \mathbf{x}_n \in \mathbb{R}^D$$

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Why centering matters: PCA finds directions of maximum variance around the mean. Without centering, we'd be finding variance around the origin, which is not meaningful.

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(Without this constraint, we could make variance arbitrarily large by scaling \mathbf{u}_1 .)

The projection of each data point $\tilde{\mathbf{x}}_n$ onto \mathbf{u}_1 is:

$$\mathbf{u}_1^T \tilde{\mathbf{x}}_n$$

This is a scalar—the coordinate along \mathbf{u}_1 .

Variance of Projections

The projected data are the scalars: $\mathbf{u}_1^T \tilde{\mathbf{x}}_1, \mathbf{u}_1^T \tilde{\mathbf{x}}_2, \dots, \mathbf{u}_1^T \tilde{\mathbf{x}}_N$

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Since the data are mean-centered, the mean of projections is zero:

$$\frac{1}{N} \sum_{n=1}^N \mathbf{u}_1^T \tilde{\mathbf{x}}_n = \mathbf{u}_1^T \left(\frac{1}{N} \sum_{n=1}^N \tilde{\mathbf{x}}_n \right) = \mathbf{u}_1^T \mathbf{0} = 0$$

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The sample variance of projections is:

$$\frac{1}{N} \sum_{n=1}^N (\mathbf{u}_1^T \tilde{\mathbf{x}}_n)^2$$

Goal: Maximize this quantity over choice of \mathbf{u}_1 .

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Note: \mathbf{S} is symmetric and positive semi-definite.

Variance in Matrix Form

The variance of projections can now be written as:

$$\begin{aligned}\frac{1}{N} \sum_{n=1}^N (\mathbf{u}_1^T \tilde{\mathbf{x}}_n)^2 &= \frac{1}{N} \sum_{n=1}^N \mathbf{u}_1^T \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^T \mathbf{u}_1 \\&= \mathbf{u}_1^T \left(\frac{1}{N} \sum_{n=1}^N \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^T \right) \mathbf{u}_1 \\&= \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1\end{aligned}$$

Our optimization problem:

$$\max_{\mathbf{u}_1} \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 \quad \text{subject to} \quad \mathbf{u}_1^T \mathbf{u}_1 = 1$$

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Form the Lagrangian:

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Taking the derivative with respect to \mathbf{u}_1 and setting to zero:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{u}_1} = 2\mathbf{S}\mathbf{u}_1 - 2\lambda_1\mathbf{u}_1 = \mathbf{0}$$

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This is an eigenvalue equation!

- ▶ \mathbf{u}_1 is an eigenvector of the covariance matrix \mathbf{S}
- ▶ λ_1 is the corresponding eigenvalue

See Bishop eq. 12.6

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Conclusion: The variance captured equals the eigenvalue λ_1 .

To maximize variance, choose the eigenvector with the **largest eigenvalue**.

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where \mathbf{u}_2 is the eigenvector with the second-largest eigenvalue λ_2 .

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General pattern: The i -th principal component is the eigenvector corresponding to the i -th largest eigenvalue.

Complete Solution

The covariance matrix has eigendecomposition:

$$\mathbf{S} = \sum_{i=1}^D \lambda_i \mathbf{u}_i \mathbf{u}_i^T$$

where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D \geq 0$.

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The variance captured by the i -th component is λ_i .

Summary of Maximum Variance Formulation

Problem: Find low-dimensional projection preserving maximum variance.

Solution:

1. Compute the sample covariance matrix \mathbf{S}
2. Find eigenvalues and eigenvectors of \mathbf{S}
3. Sort eigenvalues: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D$
4. The first M principal components are the eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_M$
5. Project data: $\mathbf{z}_n = \mathbf{U}_M^T \tilde{\mathbf{x}}_n$ where $\mathbf{U}_M = [\mathbf{u}_1 \cdots \mathbf{u}_M]$

Total variance captured: $\sum_{i=1}^M \lambda_i$

Total variance in data: $\sum_{i=1}^D \lambda_i = \text{tr}(\mathbf{S})$

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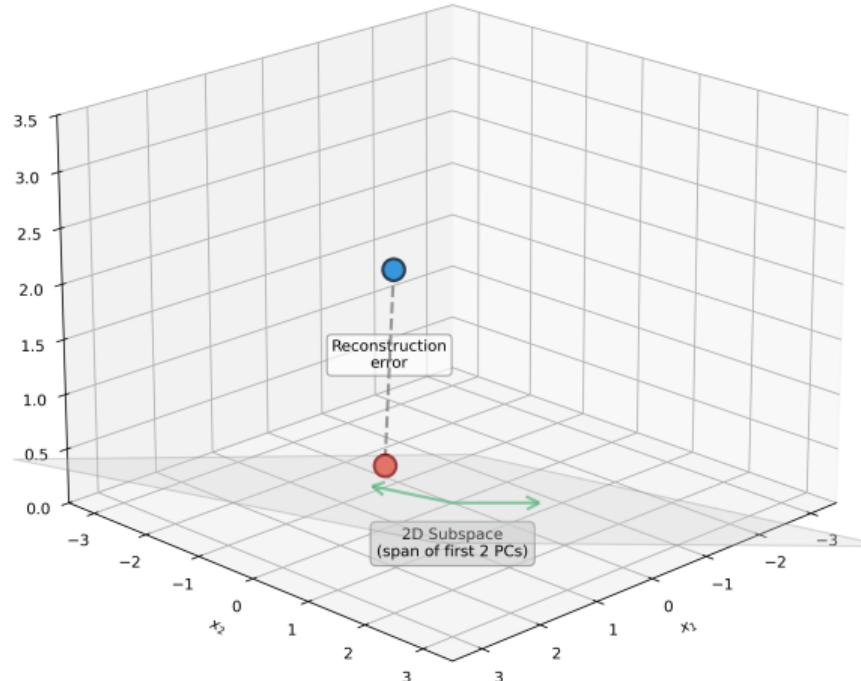
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Idea:

- ▶ Project data onto M -dimensional subspace
- ▶ Reconstruct back to original D dimensions
- ▶ Measure error between original and reconstruction
- ▶ Choose subspace that minimizes this error

The Projection Operation

- Original \vec{x}_n
- Reconstructed $\hat{\vec{x}}_n$



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Reconstruction back to D dimensions:

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(Note: $\mathbf{U}_M \mathbf{U}_M^T$ is the projection matrix onto the subspace.)

Reconstruction Error

The reconstruction error for point n is:

$$\|\tilde{\mathbf{x}}_n - \hat{\mathbf{x}}_n\|^2 = \|\tilde{\mathbf{x}}_n - \mathbf{U}_M \mathbf{U}_M^T \tilde{\mathbf{x}}_n\|^2$$

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The total reconstruction error across all data points:

$$J = \frac{1}{N} \sum_{n=1}^N \|\tilde{\mathbf{x}}_n - \mathbf{U}_M \mathbf{U}_M^T \tilde{\mathbf{x}}_n\|^2$$

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Goal: Choose the M -dimensional subspace (i.e., choose \mathbf{U}_M) to minimize J .

Equivalence to Maximum Variance

It can be shown that:

$$\sum_{n=1}^N \|\tilde{\mathbf{x}}_n - \hat{\mathbf{x}}_n\|^2 + \sum_{n=1}^N \|\hat{\mathbf{x}}_n\|^2 = \sum_{n=1}^N \|\tilde{\mathbf{x}}_n\|^2 = \text{constant}$$

Equivalence to Maximum Variance

It can be shown that:

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Therefore:

Minimizing reconstruction error \iff Maximizing captured variance

Both formulations yield the same solution! See Bishop §12.1.1

Intuitive Connection

Variance decomposition

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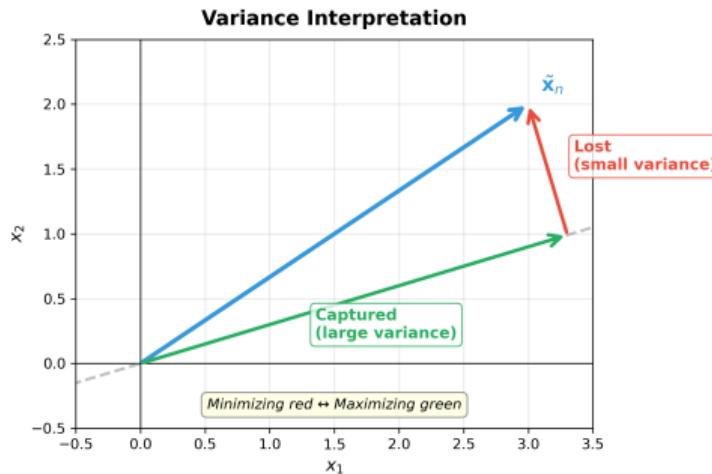
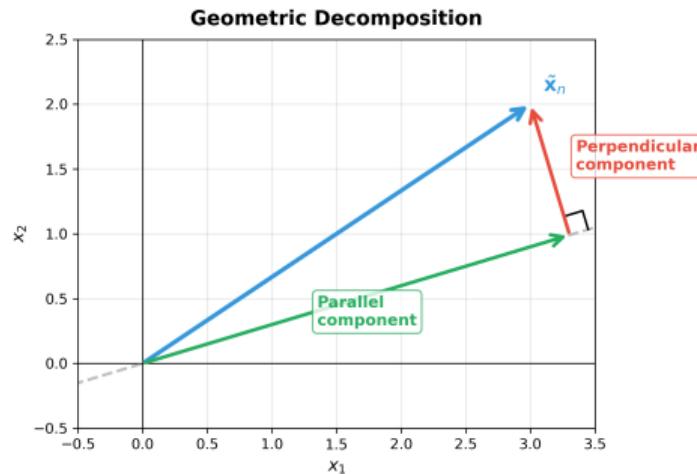
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Both perspectives lead to the same principal components.

Geometric Interpretation



The PCA Algorithm

Input: Data matrix \mathbf{X} of size $N \times D$, desired dimension M

Algorithm:

1. Compute mean: $\bar{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n$

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7. Project: $\mathbf{z}_n = \mathbf{U}_M^T \tilde{\mathbf{x}}_n$ for all n

Output: Low-dimensional representations $\mathbf{z}_1, \dots, \mathbf{z}_N$

Computational Considerations

Covariance matrix: $D \times D$ (can be very large!)

- ▶ For $D = 10,000$ features, \mathbf{S} requires ~ 800 MB (double precision)
- ▶ Eigendecomposition: $O(D^3)$ complexity

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Standard implementations (scikit-learn, R, MATLAB) use SVD internally.

How Many Components?

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No single correct answer—depends on application:

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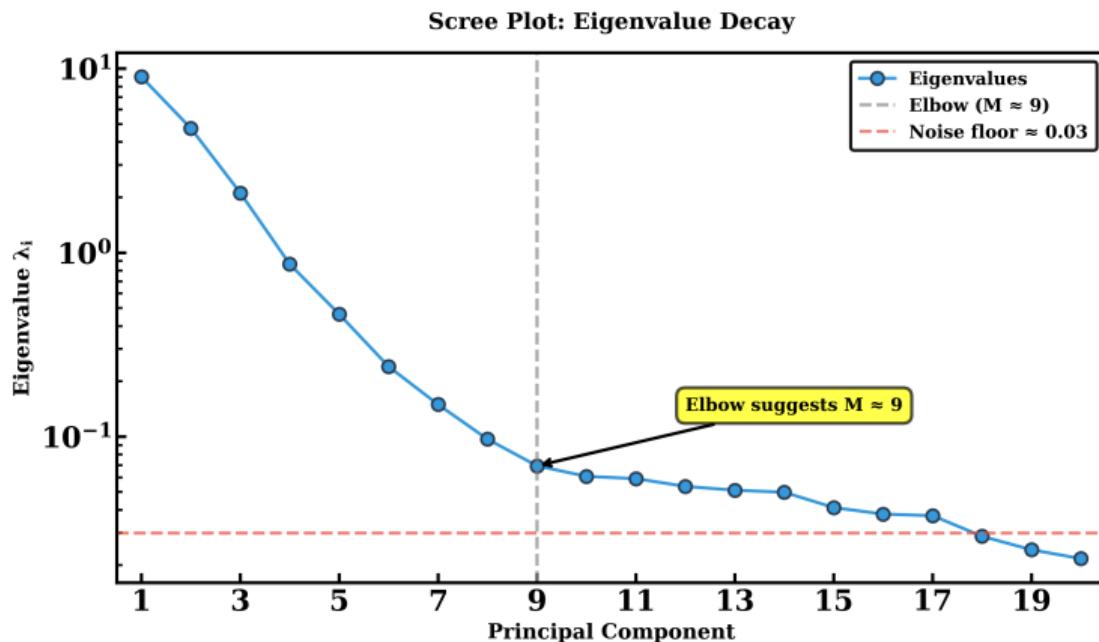
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Several diagnostic tools help us decide:

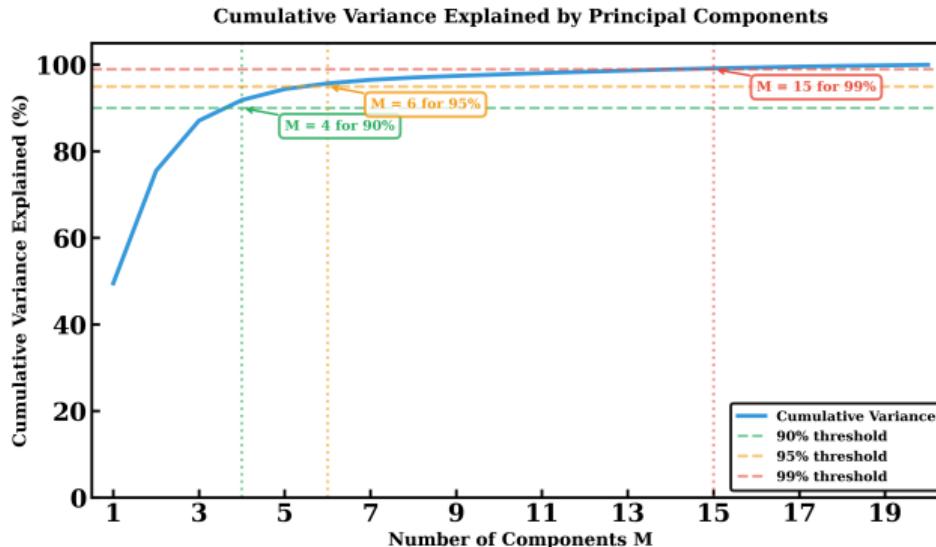
1. Scree plot (eigenvalue spectrum)
2. Cumulative variance explained
3. Cross-validation on downstream task
4. Domain knowledge

Scree Plot



Look for the “elbow” where eigenvalues drop off sharply, then plateau.

Cumulative Variance Explained



Proportion of variance explained by first M components:

$$\frac{\sum_{i=1}^M \lambda_i}{\sum_{i=1}^D \lambda_i}$$

Common thresholds: 90%, 95%, or 99% variance explained.

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Standard practice: Standardize features to unit variance

$$x_{nd} \leftarrow \frac{x_{nd} - \bar{x}_d}{\sigma_d}$$

where σ_d is the standard deviation of feature d .

This ensures all features contribute on equal footing.

Practical Example Setup

We'll work through PCA on a classic dataset.

Iris Dataset:

- ▶ 150 samples of iris flowers
- ▶ 4 features: sepal length, sepal width, petal length, petal width
- ▶ 3 species: setosa, versicolor, virginica

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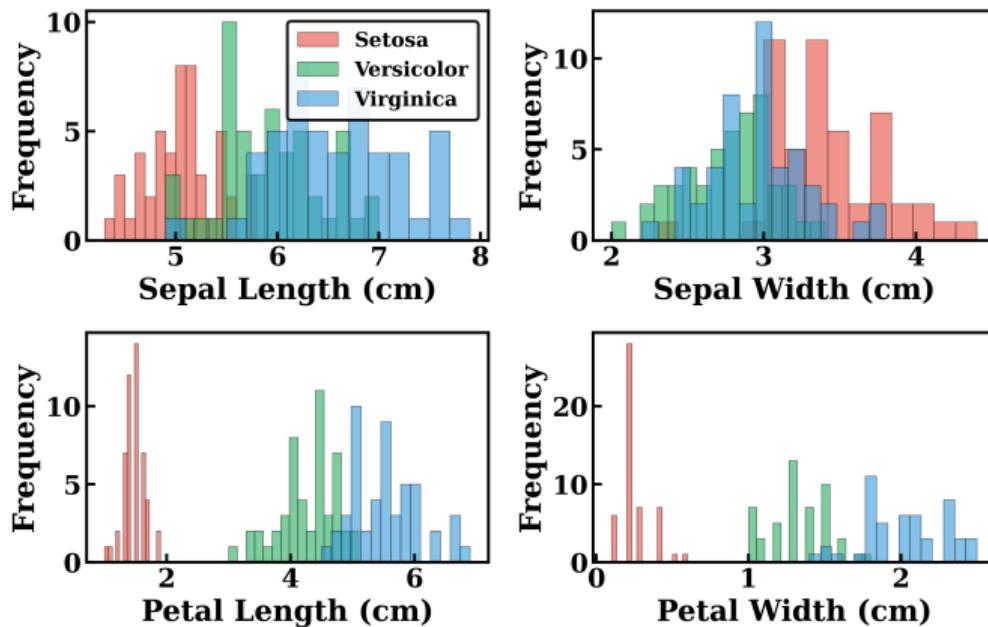
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This is a perfect example because:

- ▶ Low enough dimension to understand fully
- ▶ Real biological data with known structure
- ▶ Widely recognized in ML community

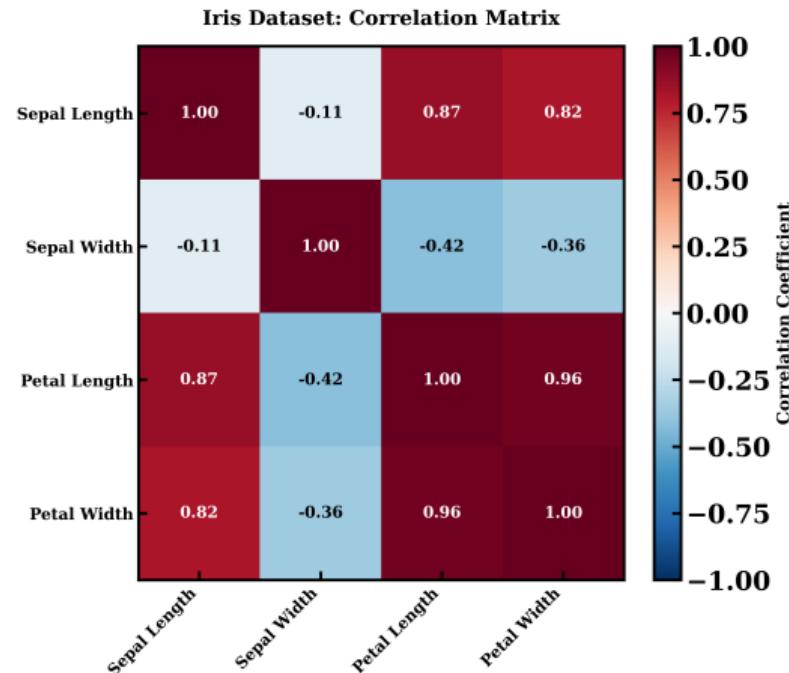
Example: Original High-Dimensional Data

Iris Dataset: Feature Distributions by Species



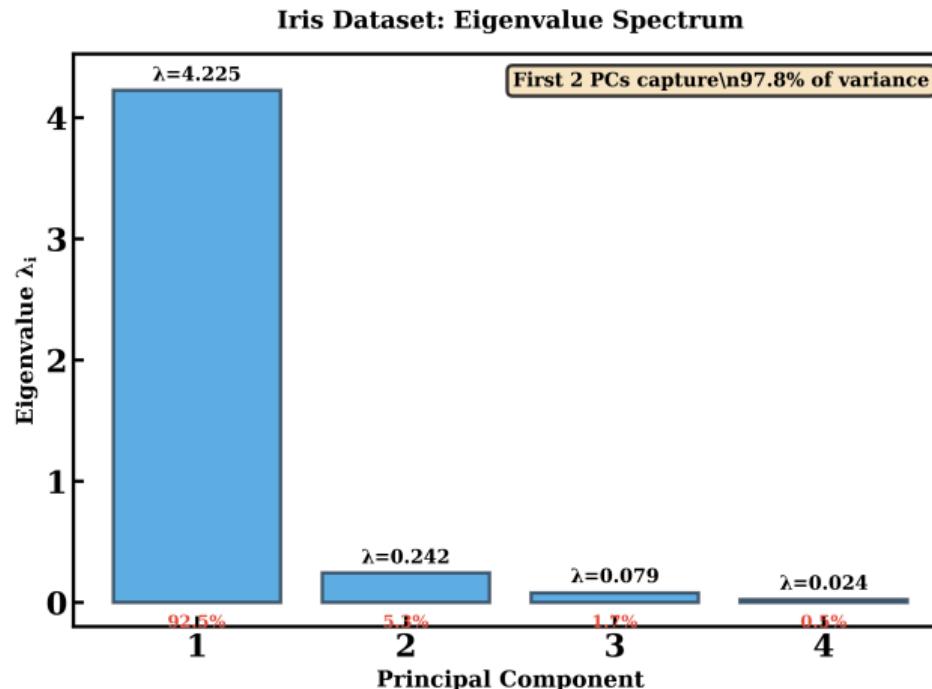
Feature histograms colored by species reveal distinct distributions, especially for petal dimensions.

Covariance Structure



The covariance matrix reveals strong correlations between certain features (e.g., petal dimensions).

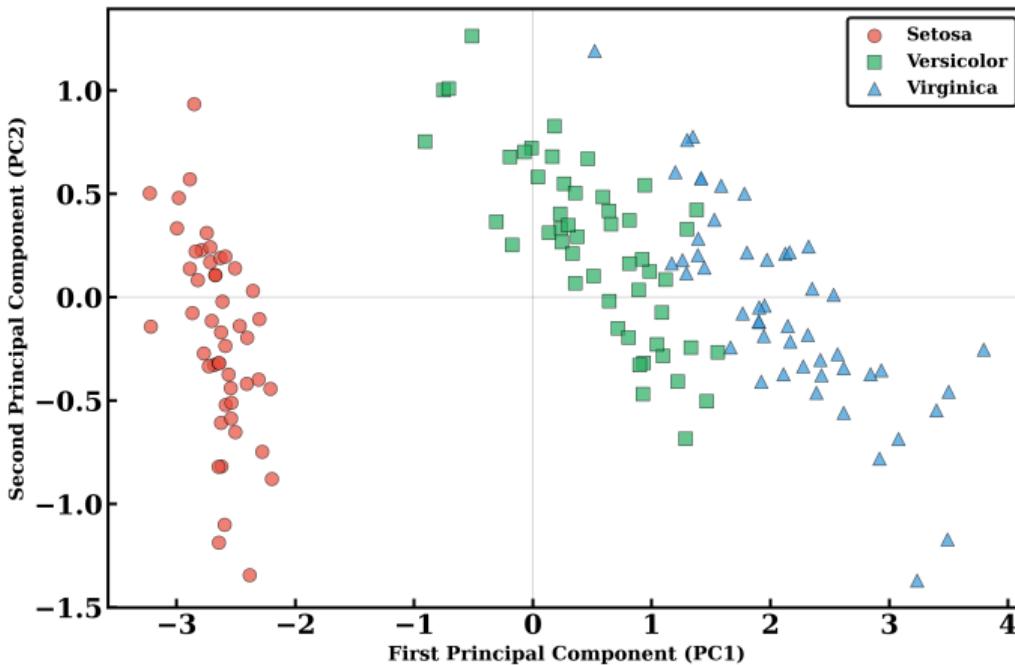
Eigenvalue Spectrum



First two components capture ~98% of variance—excellent for 2D visualization!

First Two Principal Components

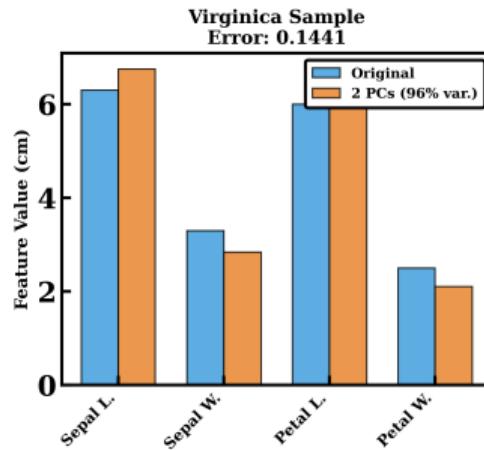
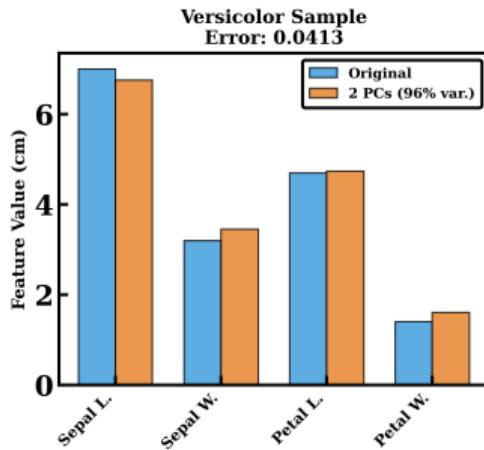
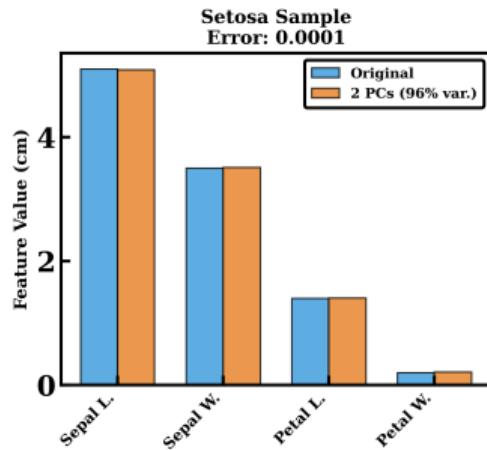
Iris Dataset Projected onto First Two Principal Components



The 2D projection preserves species separation well. Setosa is distinctly separated; some overlap between versicolor and virginica.

Reconstruction Quality

Reconstruction Quality: Original vs. 2 Principal Components



With 2 components (98% variance), reconstruction is excellent. Original and reconstructed feature values are very close.

Interpretation of Components

What do the principal components actually represent?

The first principal component \mathbf{u}_1 has loadings:

$$\mathbf{u}_1 = [0.362, -0.082, 0.857, 0.359]$$

for sepal length, sepal width, petal length, and petal width respectively.

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The second principal component focuses on contrasts between sepal and petal dimensions.

Note: Component interpretation is data-dependent and requires domain knowledge!

Assumptions of PCA

PCA makes several implicit assumptions:

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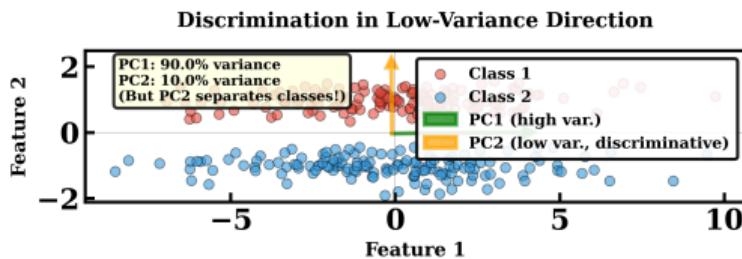
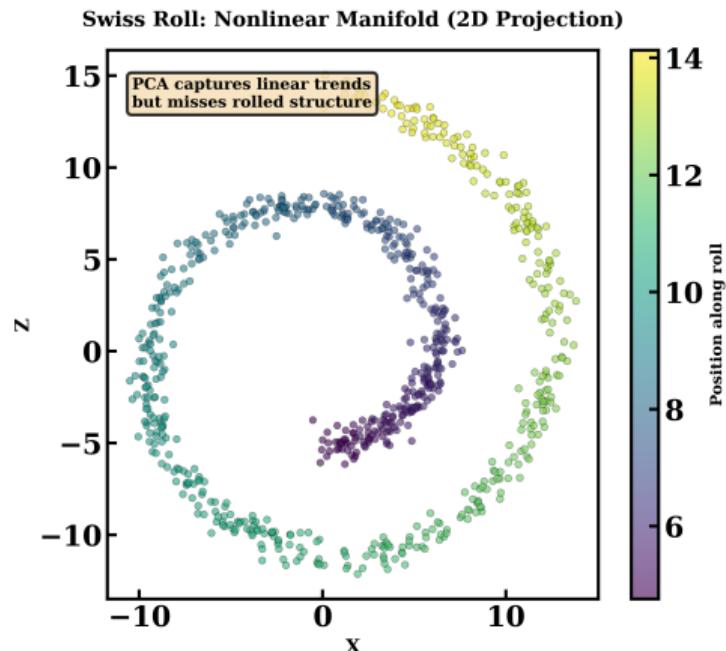
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3. Orthogonality

- ▶ Components must be uncorrelated (orthogonal)
- ▶ Sometimes natural structure isn’t orthogonal

When PCA Struggles



PCA fails when data has nonlinear structure or when discriminative information lies in low-variance directions.

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Solutions:

- ▶ Robust PCA variants (using robust covariance estimators)
- ▶ Outlier detection and removal before PCA
- ▶ Regularization methods

Connections to Other Methods

PCA is related to many other techniques:

Probabilistic PCA (Bishop §12.2)

- ▶ Probabilistic latent variable model
- ▶ Provides principled handling of missing data
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Kernel PCA

- ▶ Nonlinear generalization using kernel trick
- ▶ Can capture curved manifold structure

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Autoencoders

- ▶ Neural network approach to dimensionality reduction
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Supervised alternatives

- ▶ Linear Discriminant Analysis (LDA): uses class labels
- ▶ Partial Least Squares: considers both features and targets
- ▶ Better when goal is prediction, not just description

Practical Pitfalls

Common mistakes when applying PCA:

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3. Wrong number of components

- ▶ Too few: lose important information
- ▶ Too many: keep noise, computational waste
- ▶ Always validate on downstream task when possible

Implementation Options

Three main approaches in Python:

1. NumPy (manual implementation)

- ▶ Full control, educational value
- ▶ Use `np.cov()` and `np.linalg.eig()`
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3. SciPy

- ▶ Lower-level linear algebra routines
- ▶ `scipy.linalg` for SVD-based approach
- ▶ More flexible but requires more code

Scikit-learn Example: Basic Usage

```
1 import numpy as np
2 from sklearn.decomposition import PCA
3 from sklearn.preprocessing import StandardScaler
4
5 # Load your data (N samples, D features)
6 X = np.loadtxt('data.csv', delimiter=',')
7
8 # IMPORTANT: Standardize features to unit variance
9 scaler = StandardScaler()
10 X_scaled = scaler.fit_transform(X)
11
12 # Fit PCA - reduce to 2 dimensions
13 pca = PCA(n_components=2)
14 X_reduced = pca.fit_transform(X_scaled)
15
16 # X_reduced now has shape (N, 2)
17 print(f"Reduced data shape: {X_reduced.shape}")
```

Key points: **always** standardize first, then fit PCA.

Analyzing Results

```
1 # Variance explained by each component
2 print("Variance explained ratio:")
3 print(pca.explained_variance_ratio_)
4 # Output: [0.729, 0.229] (example values)
5
6 # Cumulative variance
7 print("Cumulative variance:")
8 print(pca.explained_variance_ratio_.cumsum())
9 # Output: [0.729, 0.958]
10
11 # Access principal components (shape: n_components x n_features)
12 components = pca.components_
13 print(f"PC1 loadings: {components[0]}")
14
15 # Reconstruct original data (with information loss)
16 X_reconstructed = pca.inverse_transform(X_reduced)
17
18 # Compute reconstruction error
19 reconstruction_error = np.mean((X_scaled - X_reconstructed)**2)
20 print(f"Mean squared error: {reconstruction_error:.4f}")
```

Choosing Number of Components

```
1 # Strategy 1: Fit with all components first, then decide
2 pca_full = PCA()
3 pca_full.fit(X_scaled)
4
5 # Plot scree plot
6 import matplotlib.pyplot as plt
7 plt.figure(figsize=(8, 5))
8 plt.plot(range(1, len(pca_full.explained_variance_) + 1),
9         pca_full.explained_variance_, 'bo-')
10 plt.xlabel('Principal Component')
11 plt.ylabel('Eigenvalue')
12 plt.title('Scree Plot')
13 plt.show()
14
15 # Strategy 2: Specify variance threshold automatically
16 pca_auto = PCA(n_components=0.95) # Keep 95% variance
17 pca_auto.fit(X_scaled)
18 print(f"Number of components selected: {pca_auto.n_components_}")
19
20 # Strategy 3: Cross-validation on downstream task
21 # (use GridSearchCV with your classifier/regressor)
```

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What is PCA?

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Key assumptions:

- ▶ Linearity of projections
- ▶ Variance indicates importance
- ▶ Orthogonality of components

When to Use PCA

Excellent for:

- ▶ Exploratory data analysis
- ▶ Visualization of high-dimensional data (reduce to 2D/3D)
- ▶ Preprocessing for supervised learning (reduce features, speed up training)
- ▶ Noise reduction (keep top components, discard noisy ones)
- ▶ Compression (store low-dimensional representation)
- ▶ When data is approximately Gaussian with linear structure

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Consider alternatives when:

- ▶ Data lies on nonlinear manifold → Kernel PCA, t-SNE, UMAP
- ▶ Discriminative task with labels → LDA, supervised methods
- ▶ Need interpretable/sparse components → Sparse PCA, Factor Analysis
- ▶ Outliers present → Robust PCA

Looking Ahead

Topics we haven't covered:

Probabilistic PCA (Bishop §12.2)

- ▶ Latent variable model: $\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$
- ▶ Principled treatment of noise and missing data
- ▶ Enables Bayesian inference, model selection

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Probabilistic PCA (Bishop §12.2)

- ▶ Latent variable model: $\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$
- ▶ Principled treatment of noise and missing data
- ▶ Enables Bayesian inference, model selection

Advanced topics:

- ▶ Kernel PCA for nonlinear dimensionality reduction
- ▶ Factor Analysis and its relationship to PCA
- ▶ Modern deep learning approaches (variational autoencoders)
- ▶ Manifold learning methods (Isomap, LLE, t-SNE, UMAP)

Looking Ahead

Topics we haven't covered:

Probabilistic PCA (Bishop §12.2)

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For supervised learning:

- ▶ Linear Discriminant Analysis (uses class labels)
- ▶ Canonical Correlation Analysis (two sets of variables)

References and Further Reading

Primary source:

- ▶ Bishop, C.M. (2006). *Pattern Recognition and Machine Learning*. Chapter 12 (§12.1)

Additional resources:

- ▶ Jolliffe, I.T. (2002). *Principal Component Analysis*. Springer. [Comprehensive treatment]
- ▶ Shlens, J. (2014). "A Tutorial on Principal Component Analysis." arXiv:1404.1100 [Accessible tutorial]
- ▶ James et al. (2013). *An Introduction to Statistical Learning*. Chapter 10.2 [Practical perspective]

Software documentation:

- ▶ Scikit-learn PCA guide:
scikit-learn.org/stable/modules/decomposition.html

Questions?