Lecture 14

Nonlinear PCA and Manifold Learning

Reading: Izenman 2008: Chapter 16.1-16.2; 16.5-16.6

DSA 8070 Multivariate Analysis

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Notes

Agenda

1. Nonlinear PCA

Notes

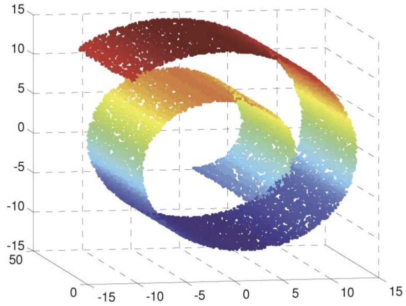
Motivation

- High-dimensional data often lie on low-dimensional manifolds
- Linear methods like PCA may fail to capture intrinsic geometry
- Goal: find lower-dimensional embedding that preserves structure

Notes

Swiss Roll Example: Motivation for Manifold Learning

- A classic synthetic example for nonlinear dimensionality reduction.
- Data lie on a 2-dimensional manifold smoothly embedded in $\mathbb{R}^3$.
- Structure: a flat rectangle "rolled up" into a spiral surface.



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Learning Objectives

By the end of this lecture, you will be able to:

- Understand the motivation behind manifold learning
- Describe key nonlinear dimensionality reduction techniques
- Implement and interpret, Nonlinear PCA methods, Isomap, LLE, and t-SNE in R
- Compare manifold methods to Linear PCA

Notes

Why Nonlinear PCA?

- Classical PCA assumes that the main structure of the data lies in a linear subspace of $\mathbb{R}^p$.
- For many data sets, structure is nonlinear:
  - Curved manifolds (e.g., Swiss roll)
  - Nonlinear functional relationships (e.g., quadratic curves)
- Idea: generalize PCA so that we still
  - Reduce dimension
  - Capture major modes of variation
  - Allow nonlinear transformations of the original variables
- There is no single unique "nonlinear PCA" – different methods generalize different properties of PCA

Notes

Polynomial PCA: Basic Idea

- Suppose $X \in \mathbb{R}^p$ is the original data vector
- Construct an expanded feature vector X' by adding polynomial terms, e.g. for quadratic PCA:

$$X' = (X_1, \dots, X_p,\ X_1^2, \dots, X_p^2,\ X_1X_2, \dots, X_{p-1}X_p)$$

- Apply ordinary PCA to the expanded data X':
    - Center X'
    - Compute covariance matrix of X'
    - Eigenvalues/eigenvectors give "principal components" in the polynomial feature space
- If the true relationship is approximately polynomial, small eigenvalues can correspond to approximate nonlinear constraints

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Polynomial PCA: Comments

- Advantages:
    - Simple conceptually: just augment features and run PCA
    - Can capture simple nonlinear structure (quadratic, cubic, etc.)
- Disadvantages:
    - Dimension of X' grows quickly with polynomial degree d and number of variables p
    - Risk of overfitting and numerical instability

Notes

Kernel PCA: PCA in Feature Space

- Instead of explicitly constructing polynomial (or other) features, map $x \in \mathbb{R}^p$ to a feature space H:

$$\Phi : \mathbb{R}^p \to H,$$

  and perform linear PCA on $\Phi(x_1), \dots, \Phi(x_n)$
- We never need $\Phi(x)$ explicitly, only inner products

$$K(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle_H$$

- A kernel $K(x_i, x_j)$ replaces the explicit feature map
- Kernel PCA = PCA in feature space defined by K

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Kernel PCA: Algorithm Sketch

1. Choose a kernel K, e.g.

$$K(x,y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right) \quad \text{(Gaussian / RBF kernel).}$$

2. Form the $n \times n$ Gram matrix $K_{ij} = K(x_i, x_j)$
3. Center K in feature space:

$$\tilde{K} = K - \mathbf{1}K/n - K\mathbf{1}/n + \mathbf{1}K\mathbf{1}/n^2,$$

where $\mathbf{1}$ is the all-ones matrix

4. Compute eigenvalues/eigenvectors of $\tilde{K}$:

$$\tilde{K}\alpha^{(\ell)} = n\lambda_\ell \alpha^{(\ell)}$$

5. The coordinates of data point x_i on kernel PC ℓ are proportional to the ith component of $\alpha^{(\ell)}$

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Kernel PCA: Interpretation

- Kernel PCA finds directions of maximal variance in a nonlinear feature space.
- For suitable kernels, kernel PCA can:
  - capture curved manifolds,
  - partially “unfold” structures like the Swiss roll,
  - behave similarly to metric MDS based on a kernel-induced distance.
- The kernel choice (e.g., bandwidth σ in RBF kernel) controls the balance between:
  - local vs. global structure,
  - smooth vs. noisy embeddings.

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Kernel PCA vs Linear PCA (Swiss Roll)

Compare 2D linear PCA and RBF kernel PCA on the same Swiss roll dataset (coloured by height h)

Linear PCA

- Projects data onto a best linear 2D subspace
- Swiss roll remains curved and “folded”
- Colour gradient (in h) is not monotone along any axis

Kernel PCA (RBF)

- Applies PCA in a nonlinear feature space defined by the kernel
- Effectively unrolls the manifold into 2D
- Colour gradient in h varies smoothly across the embedding

Key message: Linear PCA is limited to global linear structure, whereas kernel PCA can recover nonlinear manifold structure when the kernel is chosen appropriately

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Takeaways: Nonlinear PCA

- Linear PCA can fail when the data lie on a nonlinear manifold
- Polynomial PCA:
  - PCA on explicitly expanded polynomial features
  - Simple but can be high-dimensional
- Kernel PCA:
  - PCA in an implicit feature space defined by a kernel
  - More flexible and scalable than explicit polynomial expansion

Notes

Manifold Learning: Core Idea

- Data points lie on a nonlinear subspace (manifold)
- Manifold learning tries to “unroll” this space
- Preserves local or global geometric relationships

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Isomap

- Combines classical MDS with geodesic distance
- Steps:
  1. Construct neighborhood graph (k-nearest or epsilon)
  2. Compute shortest path distances (Floyd-Warshall)
  3. Apply MDS on the geodesic distance matrix
- Captures global geometry

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Locally Linear Embedding (LLE)

- Preserves local linear relationships between neighbors
- Steps:
  1. Identify k-nearest neighbors
  2. Compute weights to reconstruct each point from neighbors
  3. Find embedding that preserves weights
- Sensitive to noise and parameter choice

Notes

t-SNE (t-distributed Stochastic Neighbor Embedding)

- Probabilistic approach to preserve pairwise similarities
- Converts distances to probabilities in high and low dimensions
- Optimizes Kullback-Leibler divergence between distributions
- Good for visualization (not true metric embedding)

Notes

UMAP (Uniform Manifold Approximation and Projection)

- Balances local and global structure preservation
- Faster than t-SNE and scales better
- Based on fuzzy simplicial sets and topological data analysis

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Comparison with PCA

- PCA is linear and global
- Manifold methods are nonlinear, and often local
- Use PCA when interpretability and simplicity matter
- Use t-SNE, Isomap, or UMAP for visualizing structure

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Nonlinear PCA vs. Manifold Methods

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- Polynomial PCA and kernel PCA:
  - Extend PCA using richer feature spaces
  - Remain variance-based methods
- Methods like Isomap, LLE:
  - Focus on preserving geodesic distances or local neighborhoods
  - Explicitly target manifold geometry

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Summary

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- Manifold learning methods uncover low-dimensional structures
- Isomap and LLE preserve distances or local geometry
- t-SNE and UMAP are widely used for high-dimensional data visualization

Notes