Lecture 24: Non-linear dimensionality reduction techniques

Reading: ESL 14.5.4, 14.8, 14.9

STATS 202: Data mining and analysis

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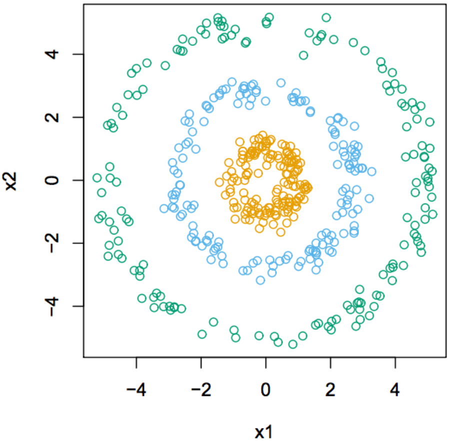
Overview

- Methods for unsupervised learning or exploratory data analysis.
- PCA is a linear dimensionality reduction method.
- If the data show non-linear patterns, these will be difficult to discover by PCA.
- Non-linear dimensionality reduction methods are useful to analyze data with a high signal to noise ratio, for example, images of physical objects.

Example. Shells



All directions have equal variance:
PCA wouldn't capture the obvious circular patterns.

Kernel PCA

- To make PCA non-linear, we transform the features through Φ.
- The feature map Φ gives rise to the kernel $\langle \Phi(x_i), \Phi(x_k) \rangle$.
- **Kernel PCA**:
  1. Find the vector g_1, in the expanded feature space, which maximizes the variance of the projections:

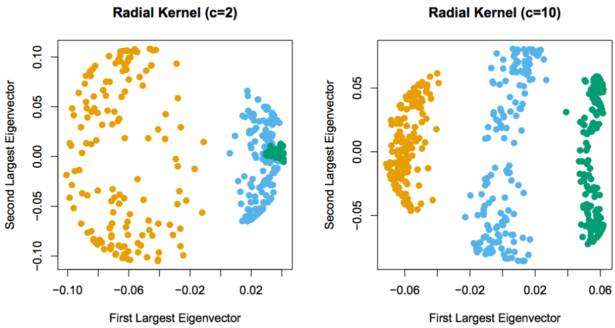
     $$\langle \Phi(x_1), g_1 \rangle, \langle \Phi(x_2), g_1 \rangle, \ldots, \langle \Phi(x_n), g_1 \rangle$$

  2. Find the vector g_2, orthogonal to g_1, which maximizes the variance of the projections:

     $$\langle \Phi(x_1), g_2 \rangle, \langle \Phi(x_2), g_2 \rangle, \ldots, \langle \Phi(x_n), g_2 \rangle$$

  3. ...

Example. Shells



The 1st principal component using the RBF kernel with $c = 1/\gamma = 10$ captures the distance from the center and clearly separates the three clusters.

How to choose the right kernel?

- In Kernel PCA, we have to choose the right kernel to obtain a meaningful visualization.
- This choice is not always easy.
- There are methods which use the data to learn the right kernel.
- These methods exploit the local structure of the data (similarity is only meaningful among nearest neighbors).
- We will talk about two examples:
  1. Locally linear embeddings
  2. Isomap

Locally linear embeddings (LLE)

Idea:

1. Represent each sample as a linear combination of neighbors:

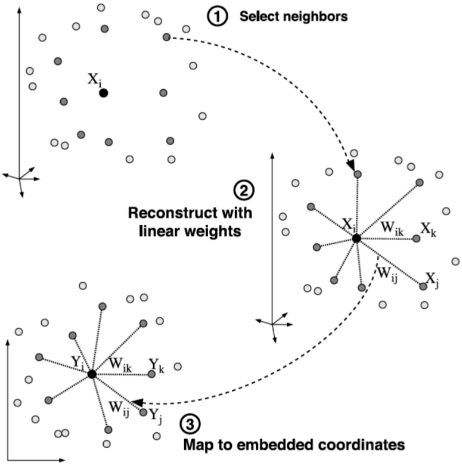
$$x_i \approx \sum_{k=1}^{n} x_j W_{ik}, \qquad W_{ik} > 0 \iff x_i, x_k \text{ are neighbors}$$

2. Map each sample x_i to a point $\Psi(x_i)$ in 2 or 3 dimensional space, such that the local linear representation holds approximately:

$$\Psi(x_i) \approx \sum_{k=1}^{n} \Psi(x_j) W_{ik}.$$

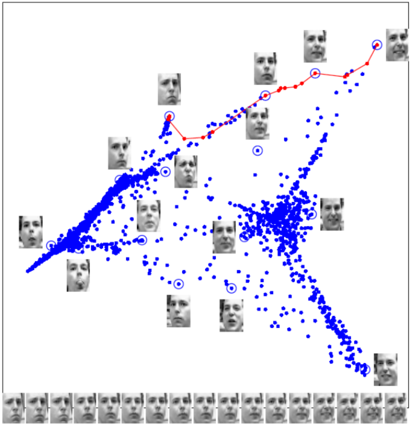
- In step 1, we find the weights W.
- In step 2, we fix W and find the optimal mapping Ψ.
- The second problem is solved by an eigendecomposition.

Locally linear embeddings (LLE)



From Roweis et al. (2000).

Example. Faces dataset



- 2000 images, 20×28 pixels.
- Number of features: $p = 560$.
- Applied LLE with 16 nearest neighbors to find a 2D projection.

Multidimensional scaling

Multidimensional scaling is a technique for projecting data onto a low-dimensional space, while preserving the distance between every pair of samples in the original dataset.

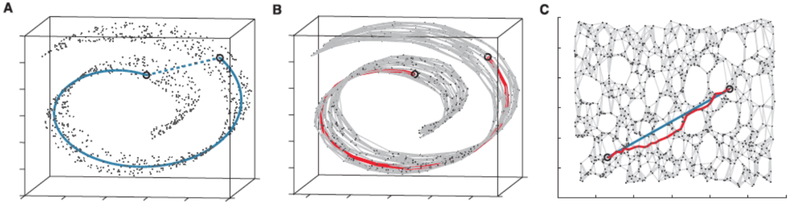
If $d(i,j)$ is the distance between x_i and x_j, we try to find a 2D representation $\Psi(x_i)$ of every sample, which minimizes:

$$\sum_{i,j} \left(d(i,j) - |\Psi(x_i), \Psi(x_j)|\right)^2$$

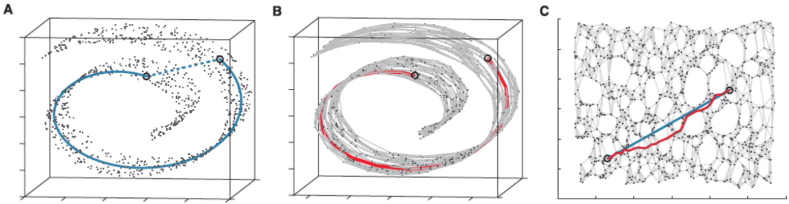
The function d can be any distance, not just the Euclidean distance between two samples.

Isomap

- Suppose that the data are clustered on a low dimensional **manifold** embedded in a high dimensional space.
- The relevant distance between two samples may not be the Euclidean distance on the space of predictors, but the shortest distance on the manifold.
- This distance is called the **geodesic**.

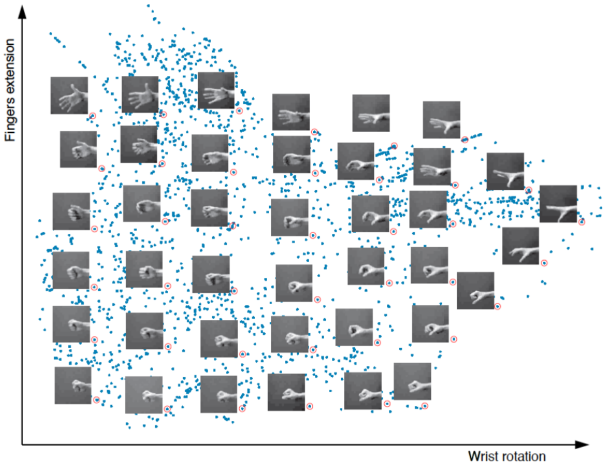


Isomap



- We don't know the manifold a priori.
- However, a nearest neighbor graph gives an approximation.
- **Idea:**
    1. Use the length of the shortest path on the graph as a proxy for the geodesic distance.
    2. Apply multidimensional scaling to visualize the manifold in a 2D space.

Example. Hands dataset



Summary

- Non-linear dimensionality reduction allows us to visualize complex data in low dimensions.
- This is useful when the samples concentrate on a non-linear manifold in high-dimensional space.
- Most methods exploit the nearest neighbor graph in some form or another.
- The data must have a good signal to noise ratio and high density. This is common in artificial intelligence tasks:
  1. Digit and letter recognition.
  2. Facial expression analysis.
  3. 3D physical models.