

General Information:

Lecture (3 SWS): Mon 08.15 – 09:45 (H16) and Tue 08.15 – 09.45 (H16)
Exercises (1 SWS): Wed 12.15 – 13.15 (00.151-113) and Thu 12.30 – 13.30 (00.151-113)
Certificate: Oral exam at the end of the semester
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Manifold Learning

Exercise 1 The Sammon transform is historically seen one of the oldest techniques for dimensionality reduction. This exercise discusses how this approach works and examines some of its mathematical properties.

- (a) Explain the idea of the Sammon transform for dimensionality reduction. Write down the objective function of the Sammon transform.
- (b) Show that the Sammon transform is invariant with respect to
 - translation,
 - rotation,
 - and scaling

in the original feature space before applying the transform.

Hint: Use an orthogonal matrix \mathbf{R} to model a rotation of \mathbf{x} as $\mathbf{x}' = \mathbf{R}\mathbf{x}$, where \mathbf{x}' is the rotated sample.

Exercise 2 Locally linear embedding (LLE) is a manifold learning technique to perform a dimensionality reduction in two steps. First, weighting coefficients w_{ij} are determined to reconstruct each sample $\mathbf{x}_i \in \mathbb{R}^D$ from the neighborhood $\mathbf{x}_j \in \mathcal{N}(\mathbf{x}_i)$. In the second stage, the weights w_{ij} are used to find an embedding in a d -dimensional feature space ($d < D$) according to the minimization of:

$$E(\mathbf{x}'_1, \dots, \mathbf{x}'_n) = \sum_{i=1}^n \left\| \mathbf{x}'_i - \sum_{\mathbf{x}'_j \in \mathcal{N}(\mathbf{x}'_i)} w_{ij} \mathbf{x}'_j \right\|_2^2, \quad (1)$$

where $\mathbf{x}'_i \in \mathbb{R}^d$ are the embedded samples. Here, we examine the second step of the LLE algorithm.

- (a) Let us assume that $d = 1$ and thus x_i is a scalar. Derive an optimization problem associated with Eq.(1) that enforces unit covariance for the embedded samples.

Hint: Use a Lagrangian multiplier in your derivation.

- (b) Show that the derived optimization problem can be solved by an eigenvalue decomposition.

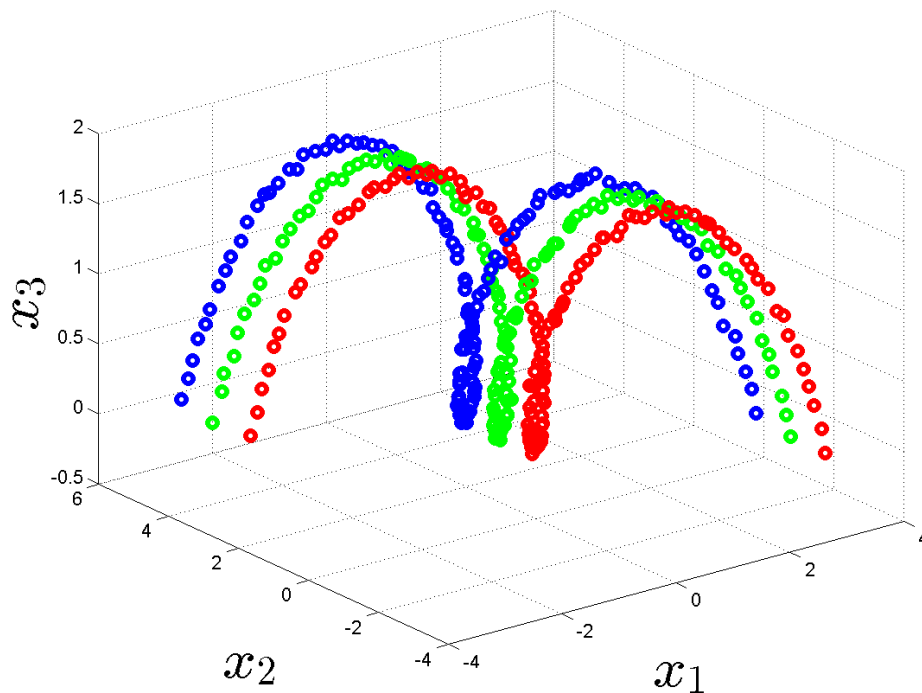


Figure 1: Original 3-dimensional samples used for dimensionality reduction.

- (c) Explain how \mathbf{x}_i can be determined for $d > 1$. Therefore, make use of the fact that the smallest eigenvalue in the derived eigenvalue decomposition is always zero.

Exercise 3 Matlab exercise In this exercise, we implement and apply the Isomap (**I**sometric feature **m**apping) algorithm, one of the most popular manifold learning techniques. Isomap employs classical multi-dimensional scaling (MDS) to exploit the geodesic distances of the samples in a high-dimensional feature space.

- (a) Explain the main steps of the Isomap algorithm.
- (b) We apply the Isomap algorithm for a dimensionality reduction of samples defined in a 3-dimensional feature space (see figure). Load the dataset `manifold3D.mat` provided on our web page into the Matlab workspace. The dataset consists of samples \mathbf{X} and a corresponding label matrix \mathbf{Z} .

Hint: \mathbf{Z} can be used for a color-coded visualization of the points in \mathbf{X} .

- (c) Visualize the original samples (Matlab: `scatter3` with colored points) and explain why a dimensionality reduction is beneficial.
- (d) Apply the Isomap algorithm to transform the 3-dimensional samples into a 2-dimensional feature space and visualize the samples after dimensionality reduction (Matlab: `scatter` with colored points).

You can employ Dijkstra's algorithm for shortest path calculation in Isomap. Use the `gaimac` toolbox (*Graph Algorithms in Matlab Code*) public available here (Matlab function `dijkstra`).

- (e) Apply a principal component analysis (PCA) for dimensionality reduction (reuse your code from the PR exercises if possible). Compare the outcome of Isomap and PCA and explain the main conceptual differences between both techniques.