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Lecture Pattern Analysis

Part 14: Isometric Feature Mapping (ISOMAP)

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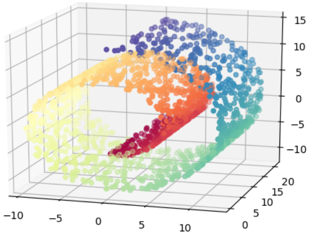
Introduction

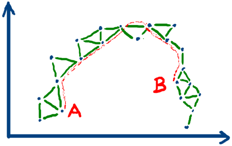
- PCA and MDS perform linear projections to transform the data
- Non-linear manifolds require a non-linear mapping
- One popular (academic) example for a non-linear manifold is the swiss roll:



- An orthogonal projection as done by PCA or MDS would “squash” the roll
- There are many non-linear manifold learning methods, e.g., “Sammon Mapping” and “Locally Linear Embedding” (LLE), and the modern t-SNE
- Key to these approaches is the MDS concept of distances between samples
- In Pattern Analysis, we look into ISOMAP and Laplacian Eigenmaps

ISOMAP

- ISOMAP is a straightforward “non-linearity hack” for MDS
- It preserves a non-linear manifold by exchanging the Euclidean distances of MDS by “geodesic” distances on the manifold
- More specifically, distances are calculated as shortest paths from a graph where each sample is connected to its nearest neighbors



- Algorithm:
  1. Define a graph where the edge weights are Euclidean distances to nearest samples (using k-NN or fixed distance threshold)
  2. The distance matrix are all-pairs shortest paths between the samples (e.g., via Floyd-Warshall algorithm or repeated use of Dijkstra’s algorithm)
  3. Perform MDS on the distance matrix