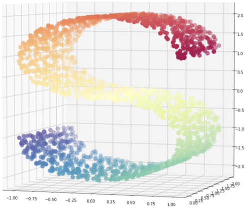
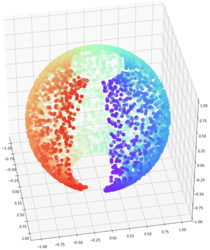
Mathematical techniques in data science

Lecture 15: Manifold learning

Reminders

- Final project presentations: 05/19
  (Check your scheduled time)
- Final project report due date: 05/23
- Course evaluation (05/09–05/16)

Manifold learning

- high-dimensional data often has a low-rank structure
- question: how can we discover low dimensional structures in data?

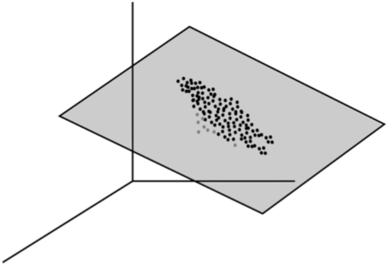
Some definitions

- Metric space: a space on which one can compute the distance between any two points
- Manifold: every point has a neighborhood that is homeomorphic to an open subset of an Euclidean space
- a manifold is locally Euclidean while globally its structure is more complex
- The dimension of a manifold is equal to the dimension of this Euclidean space

Topics

- Linear methods
  - *Principal component analysis*
  - **Multi-dimensional scaling (MDS)**
- Non-linear methods
  - **Isomap**
  - Spectral embedding
  - Locally linear embedding (LLE)
  - t-distributed Stochastic Neighbor Embedding (t-SNE)

Principal component analysis



Problem: How can we discover low dimensional structures in data?

- Principal components analysis: construct projections of the data that capture most of the *variability* in the data.
- Provides a low-rank approximation to the data.
- Can lead to a significant dimensionality reduction.

Multidimensional scaling

Multidimensional scaling (MDS)

- is a means of visualizing the level of similarity of individuals of a dataset
- seeks a low-dimensional representation of the data that respects the distances in the original high-dimensional space
- the goal of an MDS analysis is to find a spatial configuration of objects when all that is known is some measure of their general (dis)similarity

Problem settings

- The data to be analyzed is a collection of n objects on which a distance function is defined: d_{ij} is the distance between objects i and object j
- Given d_{ij}, MDS want to finds vector $z_1, z_2, \ldots, z_n \in \mathbb{R}^d$ such that

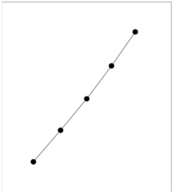
$$d_{ij} \approx \|z_i - z_j\|$$

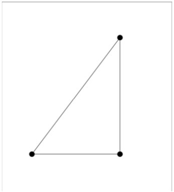
- MDS is formulated as an optimization problem

$$\min_{x_1,\ldots,x_n} \sum_{i<j} (d_{ij} - \|x_i - x_j\|)^2$$

Problem settings

$$D = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 2 & 3 \\ 2 & 1 & 0 & 1 & 2 \\ 3 & 2 & 1 & 0 & 1 \\ 4 & 3 & 2 & 1 & 0 \end{bmatrix} \qquad D = \begin{bmatrix} 0 & 3 & 4 \\ 3 & 0 & 5 \\ 4 & 5 & 0 \end{bmatrix}$$





MDS is formulated as an optimization problem

$$\min_{x_1,\ldots,x_n} \sum_{i<j} \left(d_{ij} - \|x_i - x_j\|\right)^2$$

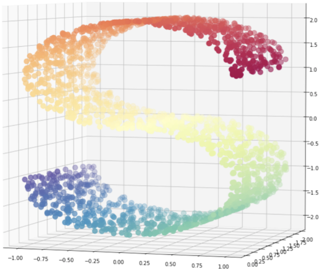
MDS

- MDS is formulated as an optimization problem

$$\min_{x_1,\ldots,x_n} \sum_{i<j} (d_{ij} - \|x_i - x_j\|)^2$$

- the idea is simple, but is easily generalizable

MDS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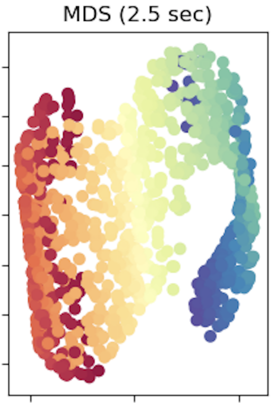
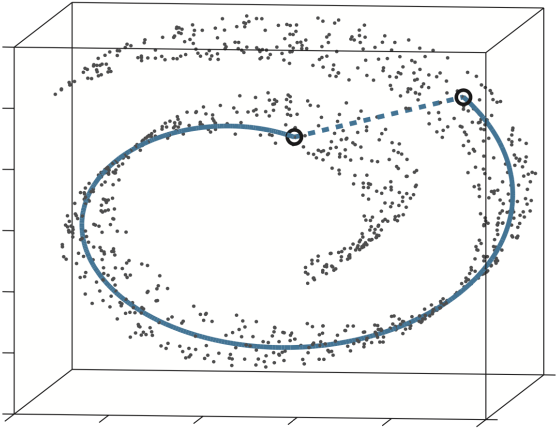

MDS (2.5 sec)

Isometric feature mapping (Isomap)

Distance on a manifold



Isomap

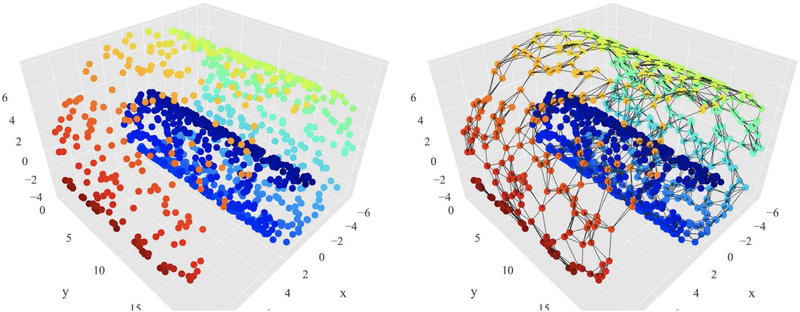
Isomap differs from MDS in one vital way - the construction of the distance matrix.

- In MDS, the distance between two points is just the euclidean distance
- In Isomap, the distances between points are the weight of the shortest path in a point-graph

Isomap: neighbor graph

- For each point, determine either
  - K nearest neighbors
  - all points in a fixed radius
- Construct a neighborhood graph.
  - each point is connected to other if it is a K nearest neighbor.
  - edge length equal to Euclidean distance between the points

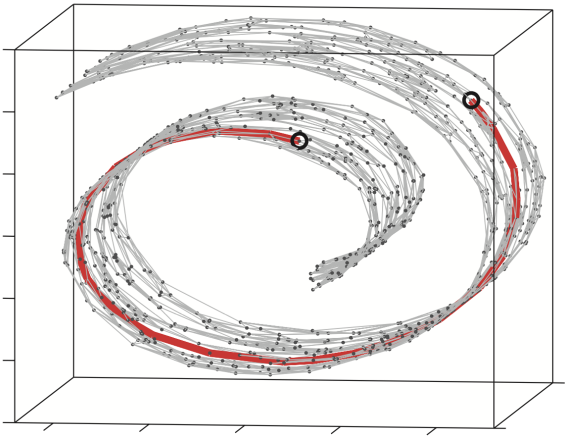
Neighbor graph



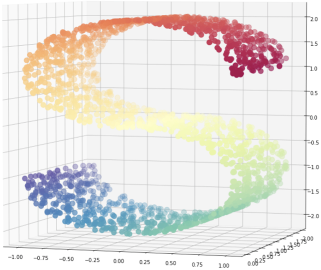
Isomap: compute intrinsic distance

- Compute shortest path between two nodes
  - Dijkstra's algorithm
  - Floyd–Warshall algorithm
- Compute lower-dimensional embedding using MDS
- The graph distance is non-Euclidean, so when embedded back into Euclidean space, some distortion occur

Intrinsic distance



Isomap



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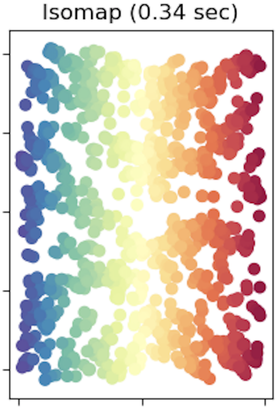


Isomap (0.34 sec)

Locally linear embedding

Locally linear embedding

- A manifold is locally Euclidean while globally its structure is more complex
- Locally, the relation between data points in a neighborhood is linear/affine
- Idea: try to preserve this linear structure

Locally linear embedding

1. For each data point x_i in p dimensions, we find its K-nearest neighbors $\mathcal{N}(i)$ in Euclidean distance.

2. We approximate each point by an affine mixture of the points in its neighborhood:

$$\min_{W_{ik}} ||x_i - \sum_{k \in \mathcal{N}(i)} w_{ik} x_k||^2 \tag{14.102}$$

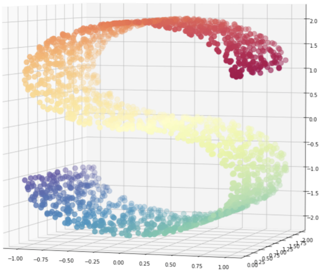
   over weights w_{ik} satisfying $w_{ik} = 0,\ k \notin \mathcal{N}(i),\ \sum_{k=1}^{N} w_{ik} = 1$. w_{ik} is the contribution of point k to the reconstruction of point i. Note that for a hope of a unique solution, we must have $K < p$.

3. Finally, we find points y_i in a space of dimension $d < p$ to minimize

$$\sum_{i=1}^{N} ||y_i - \sum_{k=1}^{N} w_{ik} y_k||^2 \tag{14.103}$$

   with w_{ik} fixed.

LLE



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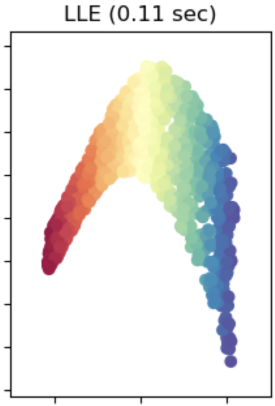


LLE (0.11 sec)

t-distributed stochastic neighbor embedding

t-SNE

- All methods proposed so far are great, and they work well if $\mathcal{M}$ is a manifold of low-dimension (2 dimension)
- Sometimes, even if the dimension of $\mathcal{M}$ is high, we still want to embed it to $\mathbb{R}^2$ for learning

t-SNE

- There are many problems with embedding high-dimensional manifold to low-dimensional space
- Structural differences
  - in ten dimensions, it is possible to have 11 data points that are mutually equidistant
  - there is no way to model this faithfully in a two-dimensional map
- Crowding problem:
  - the volume of a sphere centered on datapoint i scales as r^m, where r is the radius and m the dimensionality of the sphere
  - the area of the two-dimensional map that is available to accommodate moderately distant data points will not be nearly large enough compared with the area available to accommodate nearby data points

Stochastic neighbor embedding

- converting the high-dimensional Euclidean distances between data points into conditional probabilities that represent similarities
- The similarity of datapoint x_j to datapoint x_i is the conditional probability, $p_{j|i}$, that x_i would pick x_j as its neighbor if neighbors were picked in proportion to their probability density under a Gaussian centered at x_i

$$p_{ij} = \frac{\exp\left(-\|x_i - x_j\|^2/2\sigma^2\right)}{\sum_{k \neq l} \exp\left(-\|x_k - x_l\|^2/2\sigma^2\right)}$$

Stochastic neighbor embedding

- Assume that the data points are mapped to $y_1, y_2, \ldots, y_n$ in low-dimension
- we construct a similar quantity for a y

$$q_{ij} = \frac{\exp\left(-\|y_i - y_j\|^2\right)}{\sum_{k \neq l} \exp\left(-\|y_k - y_l\|^2\right)}$$

- Goal: Minimize the difference between the two probabilities

$$\min_y \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

t-SNE

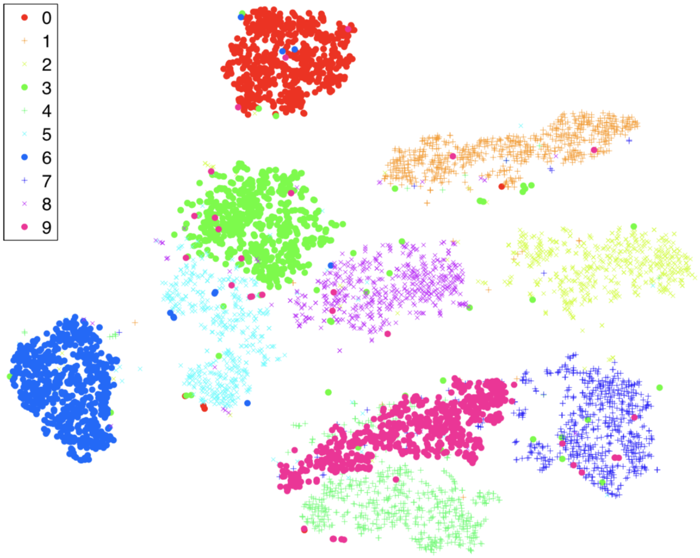
- employ a Student t-distribution with one degree of freedom (which is the same as a Cauchy distribution) as the heavy-tailed distribution in the low-dimensional map

$$q_{ij} = \frac{\left(1 + \|y_i - y_j\|^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \|y_k - y_l\|^2\right)^{-1}}$$

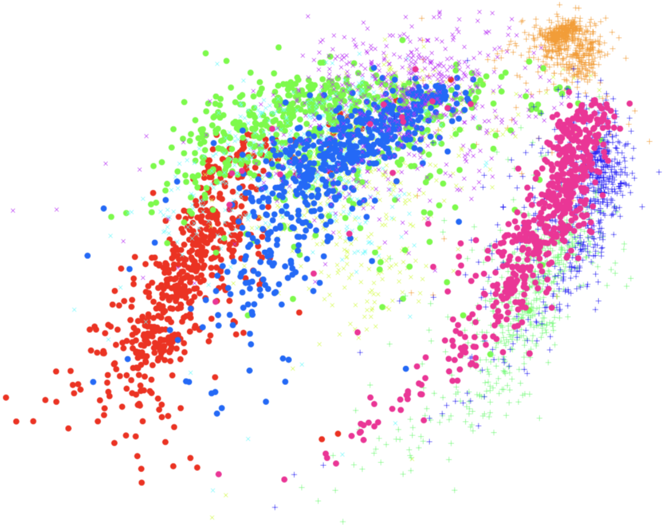
- Goal: Minimize the difference between the two probabilities

$$\min_y \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Visualization of MNIST by t-SNE



Visualization of MNIST by Isomap



Laplace eigenmap

The Laplace-Beltrami operator

- Let $\mathcal{M}$ be a manifold. We look for a map from the manifold such that points close together on the manifold are mapped close together
- Locally, we have

$$f(z) - f(x) \approx \langle \nabla f(x), z - x \rangle$$

  and $\|\nabla f(x)\|$ is a measure of local distortion by the map
- Idea:

$$\min_{\|f\|_{L_2(\mathcal{M})}=1} \int_{\mathcal{M}} \|\nabla f\|^2$$

The Laplace-Beltrami operator

- Idea:

$$\min_{\|f\|_{L_2(\mathcal{M})}=1} \int_{\mathcal{M}} \|\nabla f\|^2$$

- Define

$$\mathcal{L}(f) = -div \nabla f$$

then

$$\int_{\mathcal{M}} \|\nabla f\|^2 = \int_{\mathcal{M}} \mathcal{L}(f) f$$

The Laplace-Beltrami operator

- We have

$$\int_{\mathcal{M}} \|\nabla f\|^2 = \int_{\mathcal{M}} \mathcal{L}(f) f = \langle \mathcal{L}(f), f \rangle$$

- Problem: in manifold learning, we don't have information about the manifold, just a sample of it
- Question: how to approximate $\mathcal{L}(f)$ by the samples?

Heat kernel

In $\mathbb{R}^m$, we know that the heat equation

$$u_t(x,t) - \mathcal{L}u(x,t) = 0$$
$$u(x,0) = f(x)$$

has solution of the form

$$u(x,t) = \int H_t(x,y)f(y)dy$$

with

$$H_t(x,y) \approx (4\pi t)^{-m/2} e^{-\frac{|x-y|^2}{4t}}$$

when $t \approx 0$ and $x \approx y$, and

$$\lim_{t \to 0} \int H_t(x,y)f(y)dy = f(x)$$

Heat kernel

- We deduce that

$$\begin{aligned}\mathcal{L}f(x) = \mathcal{L}fu(x,0) &= -u_t(x,t)|_{t=0} \\ &\approx \frac{1}{t}\left[f(x) - (4\pi t)^{-m/2}\int e^{-\frac{|x-y|^2}{4t}} f(y)\right]\end{aligned}$$

- Sketchy maths
  - locally, $\mathcal{M}$ are just Euclidean space, and heat are transferred in a very similar way
  - If t is small, long term interaction on the manifold are killed
  - Laplace of a constant function is 0

Approximating the Laplace operator

$$\mathcal{L}f(x) \approx \frac{1}{t}\left[f(x) - (4\pi t)^{-m/2}\int e^{-\frac{|x-y|^2}{4t}} f(y)\right]$$

- Sketchy maths
  - locally, $\mathcal{M}$ are just Euclidean space, and heat are transferred in a very similar way
  - If t is small, long term interactions on the manifold are killed
  - Laplace of a constant function is 0
- Then $\mathcal{L}f(x_i)$ can be approximate by

$$C\left[f(x_i)\sum_{0<|x_i-x_j|<\epsilon} e^{-\frac{|x-y|^2}{4t}} - \sum_{0<|x_i-x_j|<\epsilon} e^{-\frac{|x_i-x_j|^2}{4t}} f(x_j)\right]$$

Approximating the Laplace operator

- $\mathcal{L}f(x_i)$ can be approximate by

$$C\left[f(x_i)\sum_{0<|x_i-x_j|<\epsilon} e^{-\frac{|x-y|^2}{4t}} - \sum_{0<|x_i-x_j|<\epsilon} e^{-\frac{|x_i-x_j|^2}{4t}} f(x_j)\right]$$

- Denote

$$W_{ij} = e^{-\frac{|x_i-x_j|^2}{4t}}, \quad |x_i - x_j| < \epsilon$$

and D is the diagonal matrix with entry $D_{ii} = \sum_j W_{ij}$

- We want to find f such that

$$\langle (D - W)f, f\rangle$$

is minimized

Laplace eigenmap

Step 1: Construct the neighbor graph

- For each point, determine either
    - K nearest neighbors
    - all points in a fixed radius
- each point is connected to its neghbours
- edge length equal to ~~Euclidean distance between the points~~

$$W_{ij} = e^{-\frac{|x_i - x_j|^2}{4t}}$$

Laplace eigenmap

Step 2: Embedding by Laplace operator's eigenvectors

- Define $L = D - W$
- We want to minimize

$$\min_{\langle Df, f \rangle = 1} \langle Lf, f \rangle$$

- Solve for eigenvectors $\{f_1, f_2, \ldots, f_m\}$
- Map

$$x \to (\langle f_1, x \rangle, \langle f_2, x \rangle, \ldots, \langle f_m, x \rangle)$$