Lecture 7 Nonlinear dimensionality reduction: cMDS, ISOMAP, LLE, Laplacian Eigenmaps

Foundations of Data Science: Algorithms and Mathematical Foundations

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Multidimensional Scaling (MDS)

Isomap

Locally Linear Embedding (LLE)

Laplacian Eigenmaps

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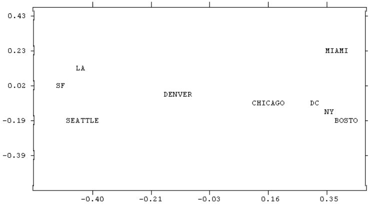
Laplacian Eigenmaps

Multidimensional Scaling (MDS)

- a means of visualizing the level of similarity of individual objects of a data set using the information contained in the **distance** matrix
- It aims to place each object in *p*-dimensional space such that the between-object distances are preserved as best as possible.

		1 BOST	2 NY	3 DC	4 MIAM	5 CHIC	6 SEAT	7 SF	8 LA	9 DENV
1	BOSTON	0	206	429	1504	963	2976	3095	2979	1949
2	NY	206	0	233	1308	802	2815	2934	2786	1771
3	DC	429	233	0	1075	671	2684	2799	2631	1616
4	MIAMI	1504	1308	1075	0	1329	3273	3053	2687	2037
5	CHICAGO	963	802	671	1329	0	2013	2142	2054	996
6	SEATTLE	2976	2815	2684	3273	2013	0	808	1131	1307
7	SF	3095	2934	2799	3053	2142	808	0	379	1235
8	LA	2979	2786	2631	2687	2054	1131	379	0	1059
9	DENVER	1949	1771	1616	2037	996	1307	1235	1059	0

(a) Input: Distance Matrix



(b) Output: 2-Dim. Embedding

Figure: Example of a 2-dimensional embedding produced by MDS given the matrix of distances among cities

Multidimensional Scaling (MDS)

- Suppose the data to be analyzed is a collection of n objects $x_i \in R^p, i = 1, \ldots, n$
- distance matrix D (size $n \times n$) containing **all** pairwise distances between the i^{th} and j^{th} object

$$D = \begin{bmatrix} D_{11} & D_{12} & D_{13} & \ldots & D_{1n} \\ D_{21} & D_{22} & D_{23} & \ldots & D_{2n} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ D_{n1} & D_{n2} & D_{n3} & \ldots & D_{nn} \end{bmatrix}, \tag{1}$$

$$D_{ij} = \| x_i - x_j \|^2, D_{ii} = 0. \tag{2}$$

- **Goal**: transform D into a cross-product matrix B, with $B_{ij} = x_j^\top x_i$ and find its eigen-decomposition
- yields an embedding of the n points into $\mathbb{R}^p$ that preserves pairwise (squared) distances
- often used for visualization if $p = \{2, 3\}$.

 Let us denote by s_i the sum of entries in row i of D

$$\begin{aligned} s_i = \sum_{j=1}^{n} D_{ij} &= \sum_{j=1}^{n} \| x_i - x_j \|^2 \\ &= \sum_{j=1}^{n} (\| x_i \|^2 + \| x_j \|^2 - 2x_i^\top x_j) \\ &= n \| x_i \|^2 + \sum_{j=1}^{n} \| x_j \|^2 - 2x_i^\top \sum_{j=1}^{n} x_j \qquad (3) \end{aligned}$$

- WLOG, assume points centered at the origin $\sum_{i=1}^{n} x_i = 0$

$$s_i = n \| x_i \|^2 + \sum_{j=1}^{n} \| x_j \|^2$$

$$s = \sum_{i=1}^{n} s_i = \sum_{i=1}^{n} \left(n \| x_i \|^2 + \sum_{j=1}^{n} \| x_j \|^2 \right) = n \sum_{i=1}^{n} \| x_i \|^2 + n \sum_{j=1}^{n} \| x_j \|^2$$

$$\implies s = 2n \sum_{i=1}^{n} \| x_i \|^2$$

Claim

$$D_{ij} - \frac{1}{n}s_i - \frac{1}{n}s_j + \frac{1}{n^2}s = -2x_i^{\mathsf{T}}x_j \tag{5}$$

Proof:

$$D_{ij} - \tfrac{1}{n}s_i - \tfrac{1}{n}s_j + \tfrac{1}{n^2}s$$

$$= \| x_i - x_j \|^2 - \frac{1}{n}\left(n \| x_i \|^2 + \sum_{j=1}^{n} \| x_j \|^2\right) - \frac{1}{n}\left(n \| x_j \|^2 + \sum_{i=1}^{n} \| x_i \|^2\right) + \frac{1}{n^2}2n\sum_{i=1}^{n} \| x_i \|^2 \tag{6}$$

$$= \| x_i - x_j \|^2 - \| x_i \|^2 - \| x_j \|^2 - \frac{2}{n}\sum_{i=1}^{n} \| x_i \|^2 + \frac{2}{n}\sum_{i=1}^{n} \| x_i \|^2 \tag{7}$$

$$= \| x_i \|^2 + \| x_j \|^2 - 2x_i^{\mathsf{T}}x_j - \| x_i \|^2 - \| x_j \|^2 \tag{8}$$

$$= -2x_i^{\mathsf{T}}x_j$$

The Gram matrix

- Consider the matrix
$$B = X^T X$$
- $X : p \times n$ of rank p (assuming $p < n$)
- $\text{rank}(B) = p, \quad p < n$

Spectral decomposition of B

$$B = U \Sigma U^T, \tag{9}$$

$$X = \Sigma^{\frac{1}{2}} U^T, \tag{10}$$

$$X^\intercal X = (U \Sigma^{\frac{1}{2}})(\Sigma^{\frac{1}{2}} U^\intercal) = U \Sigma U^T = B$$

Remark: When considering the spectrum of B, the largest eigenvalues correspond to the true intrinsic dimension of the data, while the remaining ones capture the noise.

Claim

$$B = -\frac{1}{2}HDH \tag{11}$$

where H is the scaling matrix

$$H = I - \frac{1}{n}ee^{\mathsf{T}}$$

with $e = [1, \ldots, 1]^T$.

- Denote

$$S_{n\times 1} = [s_1, \ldots, s_n]^T$$

where (recall) $s_i = \sum_{j=1}^{n} D_{ij}$. Note the following hold true:

$$De = S \qquad \text{and} \qquad e^{\mathsf{T}}D = S^T \tag{12}$$

$$\begin{aligned} B &= -\frac{1}{2}HDH & (13)\\ &= -\frac{1}{2}(I - \frac{1}{n}ee^T)D(I - \frac{1}{n}ee^T) & (14)\\ &= -\frac{1}{2}(I - \frac{1}{n}ee^T)(D - \frac{1}{n}Dee^T) & (15)\\ &= -\frac{1}{2}(D - \frac{1}{n}Se^T - \frac{1}{n}ee^TD + \frac{1}{n^2}ee^TSe^T) & (16) \end{aligned}$$

We previously showed that $B_{ij} = -\frac{1}{2}(D_{ij} - \frac{1}{n}s_i - \frac{1}{n}s_j + \frac{1}{n^2}s) = x_i^T x_j$.

Final remarks on MDS

- classical MDS assumes Euclidean distances
- MDS can be generalized to incorporate additional nonnegative weights W_{ij} on each distance (useful when some distances are missing, or most distances are noisy, but some are known)
- The optimization involves minimizing an energy known in the literature as *stress*

$$\text{Stress}_D(x_1, \ldots, x_n) = \left(\sum_{1 \le i < j \le n} (d_{ij} - ||x_i - x_j||)^2 \right)^{1/2} \tag{17}$$

- one approach (De Leeuw) to minimize stress is to iteratively minimize a (simple convex) *majorizing* function of two variables
- for a generic function f, with input variable X, we say that $g(X, Y)$ majorizes $f(X)$ if $g(X, Y) \ge f(X)$ & $g(X, X) = f(X)$
- non-metric MDS (monotonic relationship btw. the item-item dissimilarities and the Euclidean distances btw. items)
- *ordinal embedding*: find an embedding of n points $\{\vec{x}_i\}_{i=1}^n$ in $\mathbb{R}^d$ s.t.

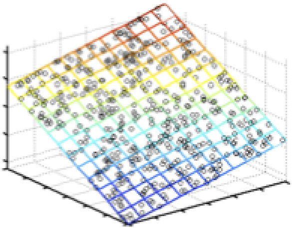
$$\forall (i, j, k, l) \in \mathcal{C}, \quad \|\vec{x}_i - \vec{x}_j\|_2 < \|\vec{x}_k - \vec{x}_l\|_2, \tag{18}$$

where $\mathcal{C}$ denotes the set of ordinal constraints.

Dimensionality Reduction

Data representation

- Inputs are real-valued vectors in a high-dimensional space
- Linear structure: data lives in a low-dimensional subspace
- Nonlinear structure: data lives on a low-dimensional submanifold



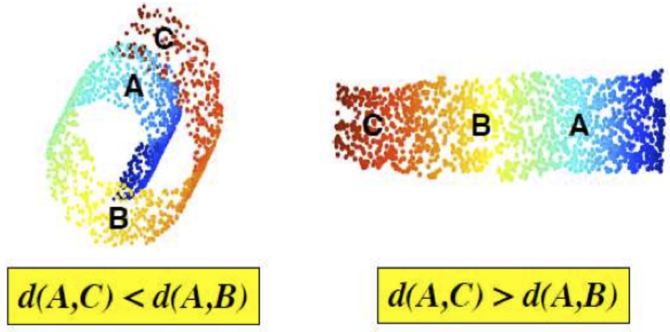
Dimensionality Reduction

- Inputs (high dimensional) $x_1, x_2, \ldots, x_n$ points in $\mathbb{R}^D$
- Outputs (low dimensional) $y_1, y_2, \ldots, y_n$ points in $\mathbb{R}^d (d << D)$

- Goals:
  - Nearby points remain nearby.
  - Distant points remain distant.

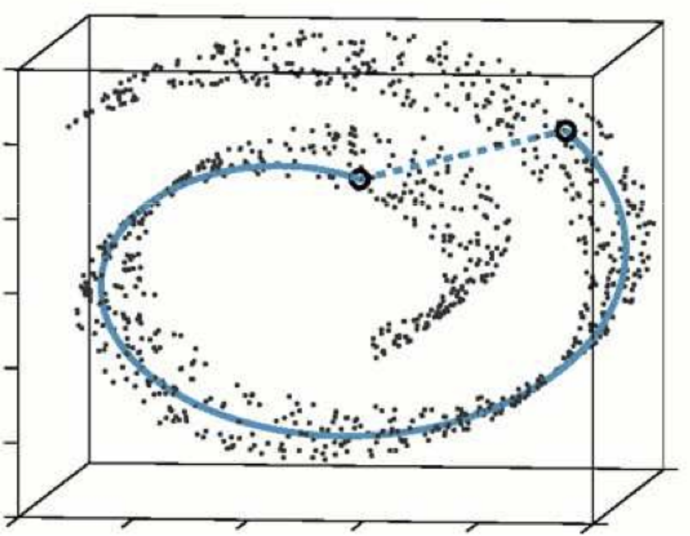
Non-metric MDS for manifolds?

- The (rank) ordering of Euclidean distances is NOT preserved in ”manifold learning”
- Euclidean distance can be misleading (*dumbbell* cloud of points)



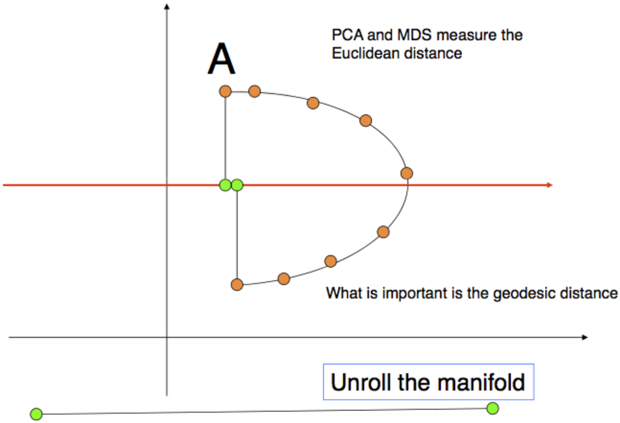
Preserving structure

- To preserve structure preserve the geodesic distance and not the Euclidean distance!

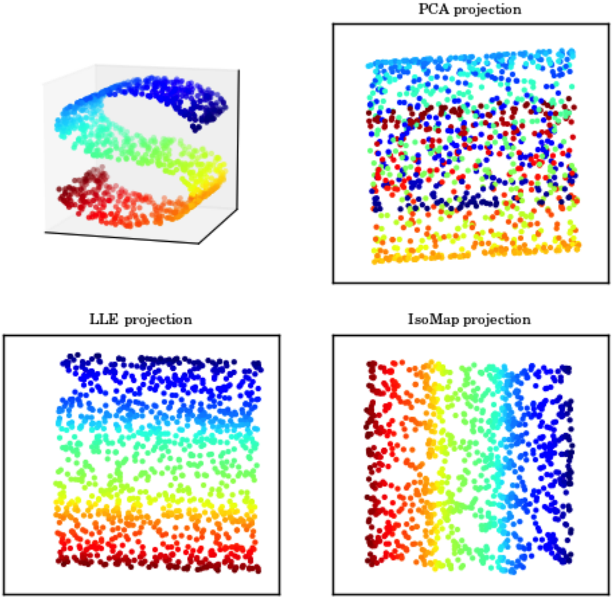


Nonlinear manifolds

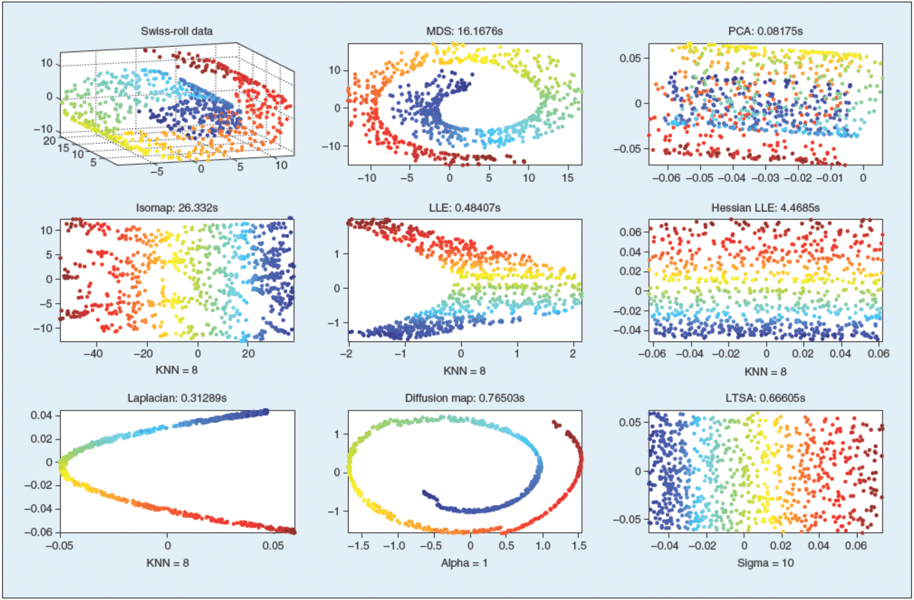
- PCA and MDS measure the Euclidean distance
- what matters most is the geodesic distance (shortest path distance)



Preserving structure



Lots of methods



Graph-Based Methods

- Isomap Algorithm
  - Global approach: Preserves global pairwise distances
  - Joshua B Tenenbaum, Vin de Silva, John C Langford, *A global geometric framework for nonlinear dimensionality reduction*
  - Science (2000)
  - 16,377 (2023) citations
- Locally Linear Embedding (LLE) Algorithm
  - Local approach: Nearby points should map nearby
  - Roweis, Sam T., and Lawrence K. Saul. *"Nonlinear dimensionality reduction by locally linear embedding"*, Science (2000)
  - 18,000 (2023) citations
- Laplacian Eigenmaps Algorithm
  - Local approach: minimizes approx. the same value as LLE
  - Belkin, Mikhail, and Partha Niyogi. *Laplacian eigenmaps for dimensionality reduction and data representation*, Neural computation (2003)
  - 9,300 (2023) citations

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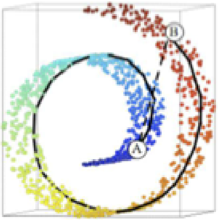
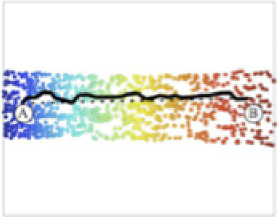
Laplacian Eigenmaps

Isomap - Key Idea

Use geodesic instead of Euclidean distances in MDS:

- For neighboring points: the Euclidean distance is a good approximation to the geodesic distance
- For distant points estimate: the distance by a series of short hops between neighboring points
  - Find shortest paths in a graph with edges connecting neighboring data points





Assumptions

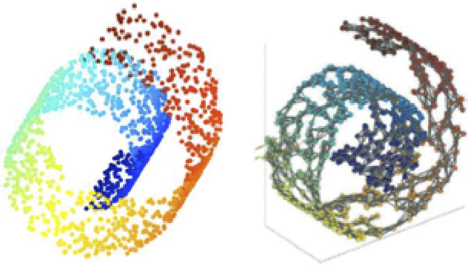
- Graph is connected.
- Neighborhoods on the graph reflect neighborhoods on the manifold (no *shortcuts* connect different portions of swiss roll.)

Isomap: Step 1 - Building adjacency graph

Neighbourhood selection - many options:

- k-nearest neighbours
- inputs within radius r
- prior knowledge.

Graph is discretized approximation of submanifold:



Computation (in $\mathbb{R}^d$)

- kNN scales naively as $O(n^2 d)$
- fast methods exploit data structures: $O(nd + kn)$, $O(ndk)$
- approximate nearest neighbor $O\left(\frac{1}{\epsilon^d} \log n\right)$

Isomap: 2 - Estimate geodesics

- Dynamic programming
  - Weight edges by local distances.
  - Compute shortest paths through graph.
- Geodesic distances
  - Estimate by lengths of shortest paths: denser sampling = better estimates.
- Computation
  - Djikstra's algorithm for shortest paths $O(n^2 \log n + n^2 m)$

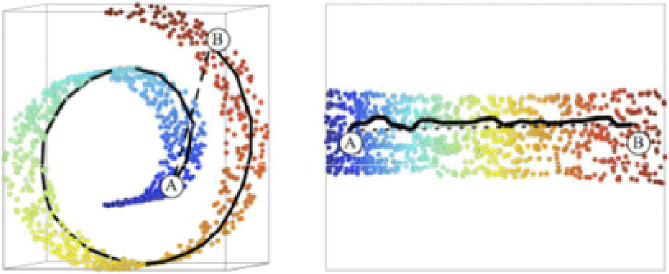
Isomap: 3 - Classical/Metric MDS

- Embedding
  - Top d eigenvectors of Gram matrix yield the desired embedding (recall the previous material on cMDS)
- Dimensionality
  - Number of significant eigenvalues yield estimate of dimensionality (look for a large spectral gap)
- Computation
  - Top d eigenvectors can be computed in $O(n^2 d)$

Summary of the ISOMAP Algorithm:

1. k-nearest neighbors
2. shortest paths through graph
3. MDS on geodesic distances

Swiss Roll

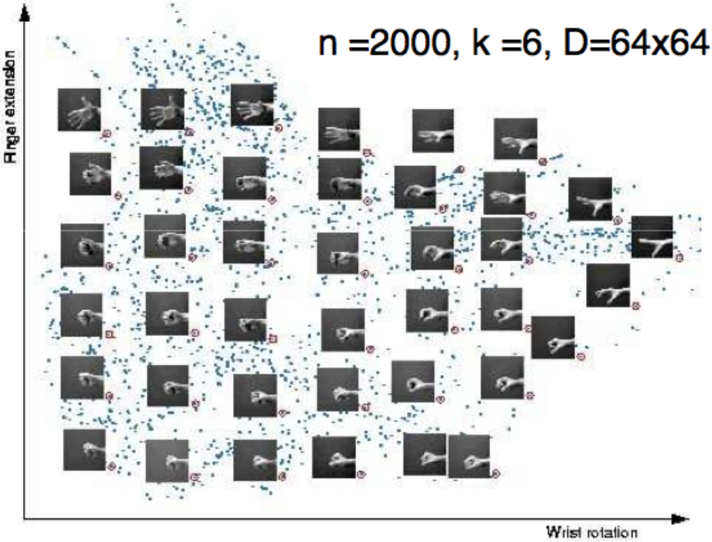


n (points) =1024

k (neighbors) =12

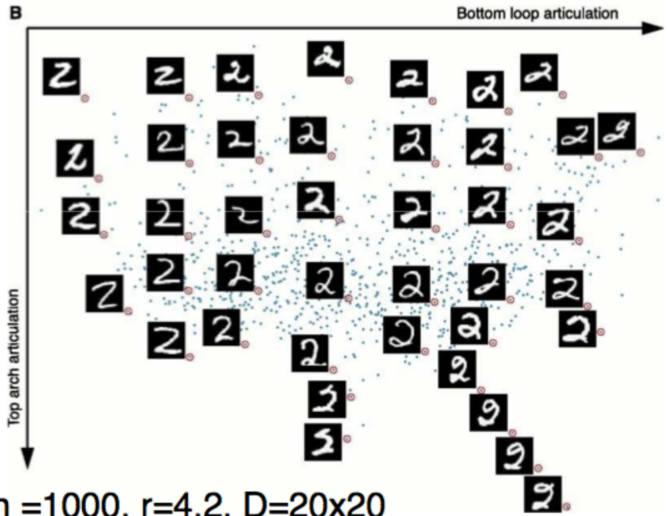
Hands

Isomap: Two-dimensional embedding of hand images (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)



The digit 2

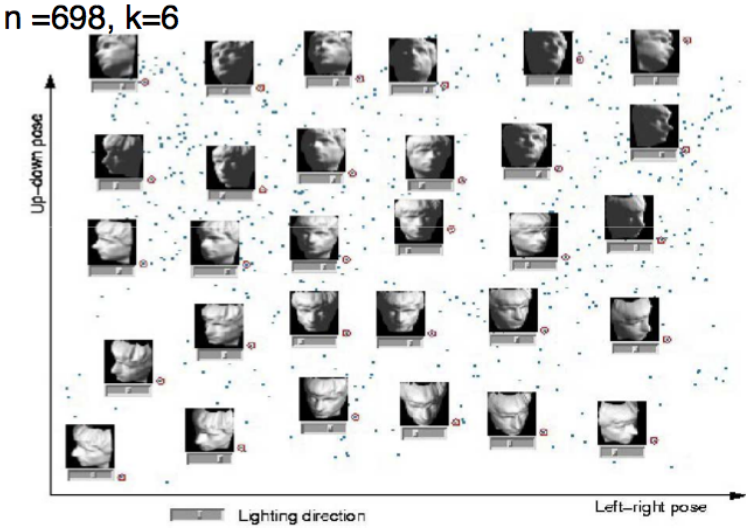
Isomap: two-dimensional embedding of hand-written ‘2’ (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)



n =1000, r=4.2, D=20x20

Faces

Isomap: three-dimensional embedding of faces (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)



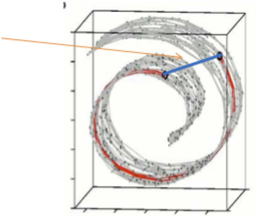
Properties of Isomap

Strengths

- preserves the global data structure
- performs global optimization
- non-parametric (the only parameter is the neighbourhood size)
- provable convergence guarantees
  - given that x_i is sampled sufficiently dense, ISOMAP will approximate closely the original distance as measured in manifold M
  - approx. geodesic distance in M by short Euclidean distance hops

Weaknesses

- very slow: need to compute pairwise shortest path between all sample pairs (i, j): Global + Non-sparse + Cubic complexity $O(n^3)$
- sensitive to "shortcuts"



ISOMAP- Theoretical considerations

-Convergence proof rests upon the idea that one can approximate the geodesic distance in M by short Euclidean distance hops.

-Consider the following quantities for a pair of points $x, y \in M$

- $d_M(x, y) = \inf_\gamma\{\text{length}(\gamma)\}$
  where γ varies over the set of smooth arcs connecting x to y in M
- $d_G(x, y) = \min_P(||x_0 - x_1|| + \ldots + ||x_{p-1} - x_p||)$
  where P varies over all paths along the edges of G starting from the source node $x = x_0$ and ending at $y = x_p$
- $d_S(x, y) = \min_P(d_M(x_0, x_1) + \ldots + d_M(x_{p-1}, x_p))$
- one can show that $d_M \approx d_S$ and $d_S \approx d_G$, leading to the desired result that $d_G \approx d_M$

Main result in [Bernstein, de Silva, Langford, and Tenenbaum 2000]: (under a long list of assumptions), the following is valid for all $x, y \in M$

$$(1 - \lambda_1)d_M(x, y) \leq d_G(x, y) \leq (1 + \lambda_2)d_M(x, y), \tag{19}$$

where λ_1, λ_2 relate to the minimum radius of curvature of M, and to a certain δ-sampling condition for every point on M.

Multidimensional Scaling (MDS)

Isomap

Locally Linear Embedding (LLE)

Laplacian Eigenmaps

Locally Linear Embedding (LLE)

Assumption:

- data lies on a manifold: each sample and its neighbors lie on an approximately linear subspace

Approach:

1. Approximate the data cloud by a set of linear patches
2. Glue these patches together on a low-dimensional subspace in such a way that the neighborhood relationships between patches are preserved.

Properties:

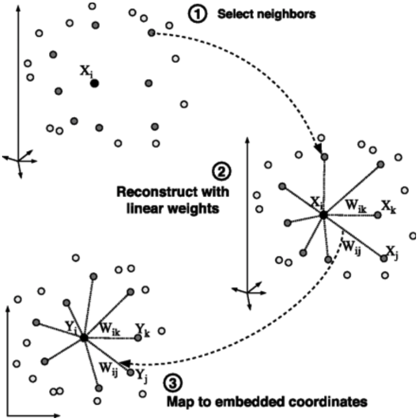
1. can obtain highly nonlinear embeddings
2. not prone to get stuck at local minima
3. sparse graphs lead to sparse problems, hence scalable

`https://cs.nyu.edu/~roweis/lle/algorithm.html`

• Roweis, Sam T., and Lawrence K. Saul. *Nonlinear dimensionality reduction by locally linear embedding*, Science (2000): 2323-2326.

Google Scholar: 14957(2020); 16416 (2021); 17136 (2022); 18,000 (2023)

LLE: Main Steps



Steps

1. Nearest neighbour search.
2. Solve for reconstruction weights W & Least-squares fits.
3. Compute embedding coordinates Y using weights W

Step 1: nearest neighbour search

For each node X_i, $i = 1, \ldots, n$

- compute the distance from X_i to every other point X_j
- find the K smallest distances
- assign the corresponding points to be neighbours of X_j

More efficient computationally:

- use standard algorithms for k-nearest neighbor (k-nn) search
- or even settle for approximation algorithms, that compute k-nearest neighbors
- *Randomized approximate nearest neighbors algorithm*, Peter Wilcox Jones, Andrei Osipov, and Vladimir Rokhlin, PNAS 2011 `https://www.pnas.org/content/108/38/15679.full`
- *nearest neighbor search* is an established area in theoretical computer science.

Step 2: computing the reconstruction weights W

- characterize local geometry of each neighbourhood by weights W_{ij}
- compute weights by reconstructing each input (linearly) from neighbours (assume neighbours lie on locally linear patches of a low-dimensional manifold)

Minimize reconstruction error

- write each point as a linear combination of its neighbors
- weights chosen to minimize the reconstruction error

$$\min_{W} \sum_{i=1} \left(X_i - \sum_j W_{ij} X_j \right)^2 \tag{20}$$

- set $W_{ij} = 0$, if X_j is not a neighbor of X_i
- weights must sum to one: $\sum_{ij} W_{ij} = 1$ (invariance to translation)
- optimal weights W_{ij} obey an important **symmetry**: for any particular data point, they are invariant to rotations, rescalings, and translations of that data point and its neighbors
- weights characterize intrinsic geometric properties of each neighborhood, as opposed to properties that depend on a particular frame of reference.

Step 3: computing the LLE Embedding

- aim to find points $y_i \in \mathbb{R}^d, i = 1, \ldots, n$ to minimize

$$\sum_{i=1}^{n} \left\| y_i - \sum_{j=1}^{n} w_{ij} y_j \right\|^2 \tag{21}$$

- subject to

$$\sum_{i=1}^{n} y_i y_i^T = I_{d \times d} \tag{22}$$

$$\sum_{i=1}^{n} y_i = 0_{d \times 1} \tag{23}$$

- condition (22) means that the points are uncorrelated
- condition (23) centers outputs on origin
- (22) + (23) impose unit covariance matrix
- this eliminates the trivial solution $y_i = 0, i = 1, \ldots, n$
- explicitly, if we denote by $y_i(k)$ the k^{th} entry of y_i, we get

$$\left(\sum_{i=1}^{n} y_i y_i^T \right)_{kj} = \sum_{i=1}^{n} (y_i y_i^T)_{kj} = \sum_{i=1}^{n} y_i(k) y_i(j) = (Y^T Y)_{kj} \tag{24}$$

Step 3: computing the LLE Embedding

- (from prev slide), if we denote by $y_i(k)$ the k^{th} entry of y_i, we get

$$\left(\sum_{i=1}^{n} y_i y_i^T\right)_{kj} = \sum_{i=1}^{n} (y_i y_i^T)_{kj} = \sum_{i=1}^{n} y_i(k) y_i(j) = (Y^T Y)_{kj}$$

- where $k, j = 1, \ldots, d$
- Y is an $n \times d$ matrix given by

$$Y = \begin{pmatrix} - & y_1^T & - \\ - & y_2^T & - \\ & \vdots & \\ - & y_n^T & - \end{pmatrix} \tag{25}$$

- think of $Y^T Y$ as a scaled version of the covariance matrix for the vectors y_i.

Step 3: computing the LLE Embedding

- to find the embedding $y_i \in \mathbb{R}^d$ we seek, recall we aim to minimize

$$\sum_{i=1}^{n} \left\| y_i - \sum_{j=1}^{n} w_{ij} y_j \right\|^2 \tag{26}$$

$$= \sum_{i=1}^{n} \left(y_i - \sum_{k=1}^{n} w_{ik} y_k \right)^T \left(y_i - \sum_{l=1}^{n} w_{il} y_l \right)$$

$$= \sum_{i=1}^{n} y_i^T y_i - \sum_{i=1}^{n} y_i^T \sum_{l=1}^{n} w_{il} y_l - \sum_{i=1}^{n} \sum_{k=1}^{n} w_{ik} y_k^T y_i + $$

$$+ \sum_{i=1}^{n} \sum_{k=1}^{n} w_{ik} y_k^T \sum_{l=1}^{n} w_{il} y_l \tag{27}$$

$$= \sum_{i,j=1}^{n} \delta_{ij} y_i^T y_j - \sum_{i,j=1}^{n} w_{ij} y_i^T y_j - \sum_{i,j=1}^{n} w_{ji} y_i^T y_j + $$

$$+ \sum_{k,l=1}^{n} \left(\sum_{i=1}^{n} w_{ik} w_{il} \right) y_k^T y_l \tag{28}$$

Step 3: computing the LLE Embedding

$$= \sum_{i,j=1}^{n} \delta_{ij} y_i^T y_j - \sum_{i,j=1}^{n} w_{ij} y_i^T y_j - \sum_{i,j=1}^{n} w_{ji} y_i^T y_j + \sum_{i,j=1}^{n} \left(\sum_{k=1}^{n} w_{ki} w_{kj} \right) y_i^T y_j$$

$$= \sum_{i,j=1}^{n} \left(\delta_{ij} - w_{ij} - w_{ji} + \sum_{k=1}^{n} w_{ki} w_{kj} \right) y_i^T y_j \quad (29)$$

$$= \sum_{i,j=1}^{n} M_{ij} y_i^T y_j \quad (30)$$

where

$$M_{ij} = \delta_{ij} - w_{ij} - w_{ji} + \sum_{k=1}^{n} w_{ki} w_{kj} \quad (31)$$

- M is an $n \times n$ symmetric matrix $M = (I - W)^T (I - W)$
- M is non-negative (all its eigenvalues are non-negative)
- denoting by $\mathbf{1}_n$ the all-ones vector of length n, and observing that the rows of W sum to 1, yields

$$M\mathbf{1} = (I - W)^T (I - W)\mathbf{1} = (I - W)^T (\mathbf{1} - \mathbf{1}) = 0 \quad (32)$$

- $\mathbf{1}$ is an eigenvector with corresponding eigenvalue $\lambda = 0$.

Denote by Y_k the k^{th} column of Y defined in (25)

$$Y_k = \begin{pmatrix} y_1(k) \\ \vdots \\ y_n(k) \end{pmatrix} \tag{33}$$

Note that

$$\sum_{k=1}^{d} Y_k^T M Y_k = \sum_{k=1}^{d} \left(\sum_{j=1}^{n} Y_k(j) \ \ (MY_k)(j) \right) \tag{34}$$

$$= \sum_{k=1}^{d} \left(\sum_{j=1}^{n} Y_k(j) \sum_{i=1}^{n} M_{ji} Y_k(i) \right) \tag{35}$$

$$= \sum_{i,j=1}^{n} M_{ij} \left(\sum_{k=1}^{d} Y_k(j) Y_k(i) \right) \tag{36}$$

$$= \sum_{i,j=1}^{n} M_{ij} \left(\sum_{k=1}^{d} y_j(k) y_i(k) \right) = \sum_{i,j=1}^{n} M_{ij} y_i^T y_j \tag{37}$$

which is where we left off in (30) for the original objective function.

Computing the Locally Linear Embedding (LLE) (cont.)

Altogether, the initial objective function

$$\sum_{i=1}^{n} \left\| y_i - \sum_{j=1}^{n} w_{ij} y_j \right\|^2 \tag{38}$$

becomes

$$\begin{array}{cl} \min\limits_{Y_1, \ldots, Y_d} & \sum_{k=1}^{d} Y_k^T M Y_k \\ \text{s.t.} & Y^T Y = I_d, \\ & Y_k \mathbf{1}_n = 0, \forall k = 1, \ldots, d \end{array} \tag{39}$$

Also note that

$$\sum_{i,j=1}^{n} M_{ij} y_i^T y_j = \text{trace}(Y^T M Y) \tag{40}$$

To minimize the obj in (39) subject to the constraints, we next consider the Lagrangian.

Computing the Locally Linear Embedding (LLE) (cont.)

- To minimize the obj in (39) subject to the constraints, we next consider the Lagrangian

$$L(Y_1, \ldots, Y_d,\ \phi_1, \ldots, \phi_d) = \sum_{k=1}^{d} Y_k^T M Y_k - \sum_{k=1}^{d} \phi_k (Y_k^T Y_k - 1) \quad (41)$$

- This is actually a *relaxation* since we discarded
  - all the off-diagonal constraints from $Y^T Y = I_d$
  - and also the centering constraints $Y_k \mathbf{1}_n = 0$
- It will turn out that the solution of the relaxed problem will satisfy all the required constraints in (39)
- consider the partials

$$\frac{\partial L}{\partial Y_k} = (M + M^T) Y_k - 2\phi_k Y_k \quad (42)$$

Computing the Locally Linear Embedding (LLE) (cont.)

- taking partials

$$\frac{\partial L}{\partial Y_k} = (M + M^T)Y_k - 2\phi_k Y_k \tag{43}$$

- leads to

$$MY_k = \phi_k Y_k \tag{44}$$

  making Y_k an eigenvector of M

- since M is symmetric, the condition $Y^T Y = I_d$ holds
- also, the all-ones vector $\mathbf{1}_n$ is an eigenvector, and thus all other eigenvectors satisfy $Y_k \mathbf{1}_n = 0$
- L is thus a sum of d eigenvalues, which is minimized by choosing Y_k to be the d eigenvectors corresponding to the d smallest eigenvalues, ignoring the first trivial eigenvector $\mathbf{1}_n$.

Multidimensional Scaling (MDS)

Isomap

Locally Linear Embedding (LLE)

Laplacian Eigenmaps

Laplacian Eigenmaps

Belkin, Mikhail, and Partha Niyogi. *Laplacian eigenmaps and spectral techniques for embedding and clustering*" Advances in neural information processing systems. 2002

Google Scholar citations: 5858 (2023); 5458 (2022); 5062 (2021); 4435 (2020);

Laplacian Eigenmaps

- Input: a set $\{x_1, \ldots, x_n\}$ of n points, $x_i \in \mathbb{R}^D$
- Output: find a set $\{y_1 \ldots, y_n\}, y_i \in \mathbb{R}^D$ such that y_i represents x_i as best as possible.
- Assumption: $x_i \in \mathcal{M}$, where $\mathcal{M}$ is a manifold embedded in $\mathbb{R}^D$.

Algorithm:

- Construct a graph $G = (V, E)$, undirected and symmetric, where $V = x_1, \ldots, x_n$, and $(x_i, x_j) \in E$ if x_i is "close" to x_j, where "close" means, for example, that
  - x_i and x_j are at most ϵ distance apart
  - or that x_i is within the K nearest neighbors of x_j (or vice versa for symmetry).
- Choose weights for each edge; use a Gaussian Kernel

$$W_{ij} = \begin{cases} e^{-||x_i - x_j||^2/t} & \text{if } (x_i, x_j) \in E \\ 0 & \text{otherwise.} \end{cases} \quad (45)$$

- alternatively, we can use a "parameter-free" approach: $W_{ij} = 1$ if $(x_i, x_j) \in E$, and $W_{ij} = 0$ otherwise.

Laplacian Eigenmaps

- Define the diagonal matrix D of row sums of W

$$D_{ii} = \sum_j W_{ij} \tag{46}$$

- Build graph Laplacian $L = D - W$ (symmetric, positive definite)
- Find eigenvectors of the generalized eigenvector problem

$$Lf = \lambda Df \tag{47}$$

- let $f_0, \ldots, f_d$ be the solutions to the eigenvalue problem ordered such that $0 = \lambda_0 \leq \ldots \leq \lambda_d$, that is

$$\begin{aligned} L\, f_0 &= \lambda D\, f_0 \\ L\, f_1 &= \lambda D\, f_1 \\ &\vdots \\ L\, f_d &= \lambda D\, f_d \end{aligned} \tag{48}$$

- drop $f_0 = [1, \ldots, 1]^T$ and define the embedding of x_i into $\mathbb{R}^d$

$$x_i \mapsto (f_0(i), \ldots, f_d(i)) \tag{49}$$

Laplacian Eigenmaps - Analysis

- considering the mapping of the original points x_i to the line.
- nearby points in $\mathbb{R}^D$ (corresponding to connected points in the graph G) should be mapped to nearby points on the line.
- denote this map by $(y_1, \ldots, y_n)$, with $y_i \in \mathbb{R}$.
- a reasonable criterion for such a map is

$$\min_{y_1,\ldots,y_n} \sum_{i,j} (y_i - y_j)^2 W_{ij}. \tag{50}$$

- if x_i and x_j are close, then W_{ij} is large, thus there is heavy penalty if those are mapped apart.

Laplacian Eigenmaps - derivation ($\mathbb{R}$)

$$\begin{aligned}\sum_{i,j}(y_i - y_j)^2 W_{ij} &= \sum_{i,j}(y_i^2 - 2y_iy_j + y_j^2)W_{ij}\\ &= \sum_i y_i^2 \sum_j W_{ij} - 2\sum_{i,j} y_iy_jW_{ij} + \sum_j y_j^2 \sum_i W_{ij}\\ &= \sum_i y_i^2 D_{ii} - 2\sum_{i,j} y_iy_jW_{ij} + \sum_j y_j^2 D_{jj}\\ &= \sum_{i,j} y_iy_jD_{ij} + \sum_{i,j} y_iy_jD_{ij} - 2\sum_{i,j} y_iy_jW_{ij}\\ &= 2\sum_{i,j} y_iy_j(D - W)_{ij} = 2y^TLy\end{aligned}$$

- which also shows that L is positive semidefinite
- the minimization problem is $\operatorname{argmin}\ y^TLy$
- to remove an arbitrary scaling from the embedding & eliminate the trivial solution, add the constraint $y^TDy = 1$

$$\operatorname*{argmin}_{y^TDy=1}\ y^TLy \tag{51}$$

Laplacian Eigenmaps

- D_{ii} construed as a measure of the importance of vertex i
- the normalization $D^{-1}L$ (equivalent to the normalization above), has a probabilistic interpretation
- consider the Lagrangian
$$H = y^T L y + \lambda(y^T D y - 1) \tag{52}$$
- differentiate and equate to zero
$$(L + L^T)y = \lambda(D + D^T)y, \tag{53}$$
- which amounts to
$$Ly = \lambda D y \tag{54}$$
- thus, y is an eigenvector; enforce $y^T D y = 1$ by dividing y by the scaling factor $(\sum_i y_i^2 D_{ii})^{1/2}$
- for y an eigenvector, the objective function evaluates to $y^T L y = \lambda y^T D y = \lambda$ due to the constraint
- optimal solution: eigenvector of the smallest eigenvalue
- $\mathbf{1}_n$ is an eigenvector with eigenvalue 0 (due to the row stochastic normalization); discard this solution
- use eigenvector corresponding to the next smallest eigenvalue

Laplacian Eigenmaps - the d-dimensional case

- so far we looked at the case of embedding into 1-D
- in the more general case, we are looking for a d-dimensional embedding, that is, a matrix

$$Y = (y_1, \ldots, y_d), \quad y_i \in \mathbb{R}^n \tag{55}$$

- the i^{th} row is the embedding of the i point in $\mathbb{R}^d$. Each column is of length n and gives one of the coordinates.
- in this setting, we aim to minimize

$$\sum_{i,j} ||y^{(i)} - y^{(j)}||^2 W_{ij} = \ldots = 2\,\mathrm{trace}(Y^T L Y) \tag{56}$$

where $y^{(i)}$ is the i-th row of Y, that is the d-dimensional representation of x_i
- the minimization problem becomes

$$\min_{Y^T D Y = I} trace(Y^T L Y) \tag{57}$$

- as before, the solution is given by the eigenvectors of L corresponding to the lowest eigenvalues, after discarding the constant eigenvector $\mathbf{1}_n$ corresponding to eigenvalue $\lambda = 0$