Computer Vision

CS308

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SUSTech CS Vision Intelligence and Perception

Week 7

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Content

- Brief Review
- Dimensionality Reduction
  - PCA
  - Manifold Learning
- Clustering
  - K-Means
  - Mean-Shift

Brief Review

Matching with Features

- Steps
  - Detect feature points in both images
  - Find corresponding pairs
  - Use these pairs to align images

Previous Lecture

Fitting: Issues

- If we know which points belong to the line, how do we find the "optimal" line parameters?
  - Least squares
- What if there are outliers?
  - Robust fitting, RANSAC
- What if there are many lines?
  - Voting methods: RANSAC, Hough transform
- What if we're not even sure it's a line?
  - Model selection

Machine Learning

Machine Learning Problems

- Taxonomy

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Dimensionality Reduction (Visualization)

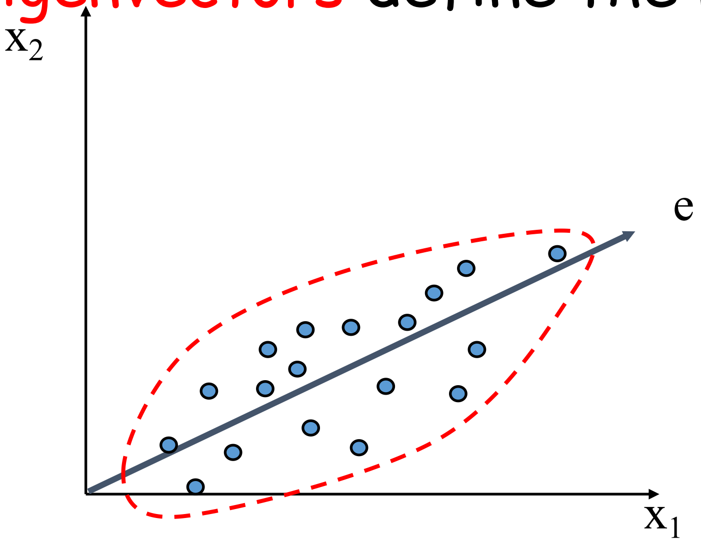
Dimensionality Reduction vs. Manifold Learning

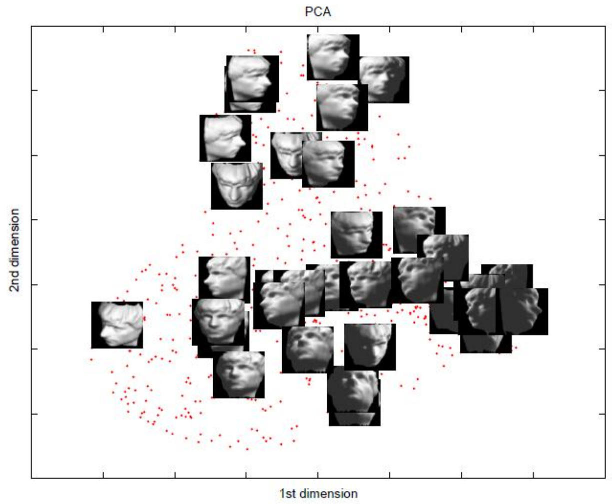
- Primary methods
  - ➢ Linear methods
    - ✓ Principal component analysis (PCA)

    保留数据点之间的距离来进行降维的方法。它通过最小化低维空间中距离的差异来实现数据的降维。
    - ✓ Multidimensional scaling (MDS)
  - ➢ Nonlinear methods
    - ✓ Kernel PCA
    - ✓ Locally linear embedding (LLE)
    - ✓ Isomap
    - ✓ Laplacian eigenmaps (LE)
    - ✓ T-distributed stochastic neighbor embedding

Principal Component Analysis (PCA)

- History: Karl Pearson, 1901
- Goal:
  - Find projections that capture the largest amounts of variation in data
  - Find the eigenvectors of the covariance matrix, and these eigenvectors define the new space

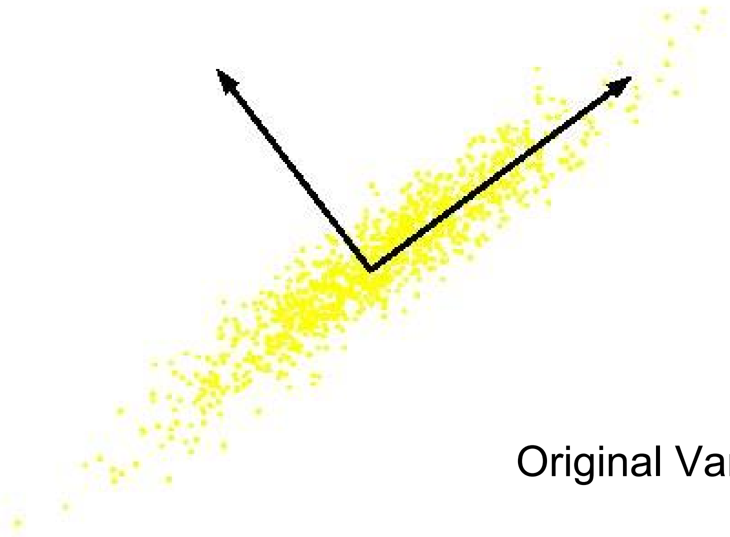




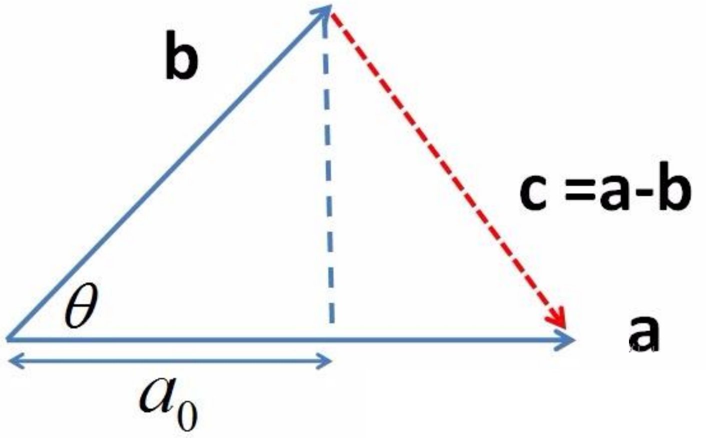
What is the original dimension of images?

Principal Component Analysis (PCA)

- Definition:
  - Given a set of data $X \in R^{d \times N}$, find the principal axes are those orthonormal axes onto which the variance retained under projection is maximal



Original Variable A



$$a \bullet b = |a||b| \cos \theta$$

PCA: One Attribute First

- Question: how much spread is in the data along the axis? (distance to the mean)
- Variance = Standard deviation^2

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

Temperature
42
40
24
30
15
18
15
30
15
30
35
30
40
30

PCA: Now Consider Two Dimensions

- Covariance: measures the correlation between X and Y
- $cov(X,Y)=0$: independent
- $cov(X,Y)>0$: move same direction
- $cov(X,Y)<0$: move opposition direction

90.81632653	57.14286
57.14285714	100

$$\operatorname{cov}(X,Y)=\frac{1}{n}\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})$$

X=Temperature	Y=Humidity
40	90
40	90
40	90
30	90
15	70
15	70
15	70
30	90
15	70
30	70
30	70
30	90
40	70
30	90

Covariance Matrix: Similarity Between Variables

- Contains covariance values between all possible dimensions (=attributes):

$$C^{nxn} = (c_{ij} \mid c_{ij} = \mathrm{cov}(Dim_i, Dim_j))$$

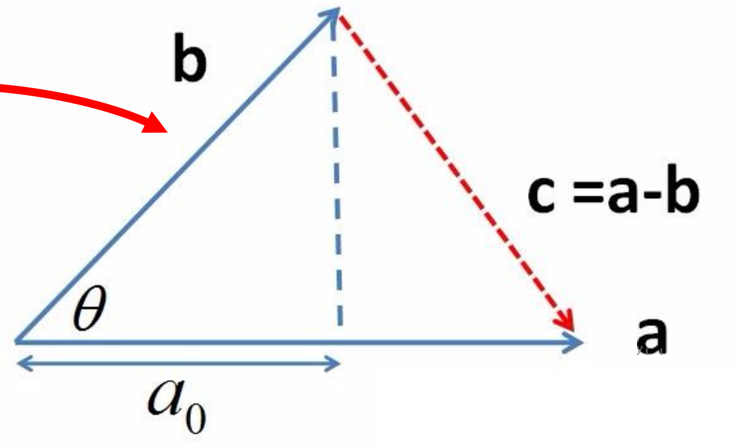
- Example for three attributes (x,y,z):

$$S = \begin{pmatrix} \mathrm{cov}(x,x) & \mathrm{cov}(x,y) & \mathrm{cov}(x,z) \\ \mathrm{cov}(y,x) & \mathrm{cov}(y,y) & \mathrm{cov}(y,z) \\ \mathrm{cov}(z,x) & \mathrm{cov}(z,y) & \mathrm{cov}(z,z) \end{pmatrix}$$

Formulation

- Variance on the first (one) dimension
  - ➢ $\mathrm{var}(U_1) = \mathrm{var}(\mathbf{w}^T X) = \mathbf{w}^T\mathbf{S}\mathbf{w}$
  - ➢ $\mathbf{S} = XX^T$: covariance matrix of X
- Objective: the variance retains the maximal
- Formulation

$$\max_{\mathbf{w}} \quad \mathbf{w}^T\mathbf{S}\mathbf{w}$$
$$\text{s.t.} \quad \mathbf{w}^T\mathbf{w} = 1$$



- Solving procedure
  - ➢ Construct Langrangian
  - ➢ Set the partial derivative on to zero
  - ➢ As $\mathbf{w} \neq \mathbf{0}$ then $\mathbf{w}$ must be an eigenvector of $\mathbf{S}$ with eigenvalue λ_1

$$L(\mathbf{w}, \lambda_1) = \mathbf{w}^T\mathbf{S}\mathbf{w} - \lambda_1(\mathbf{w}^T\mathbf{w} - 1)$$

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{S}\mathbf{w} = \lambda_1\mathbf{w}$$

$$\mathbf{w}^T\mathbf{S}\mathbf{w} = \lambda_1\mathbf{w}^T\mathbf{w} = \lambda_1$$

PCA: Another Interpretation

- A rank-k linear approximation model

$$x = f(\mathbf{y}) = \bar{\mathbf{x}} + U_k \mathbf{y}$$

- Fit the model with minimal reconstruction error

$$\min_{U_k, \mathbf{y}} \sum_{i=1}^{N} \left\| \mathbf{x}_i - U_k \mathbf{y}_i \right\|^2 \quad \text{suppose } \bar{\mathbf{x}} = \mathbf{0}$$

- Optimal condition

$$\frac{d}{d\mathbf{y}_i} = 0 \Rightarrow \mathbf{y}_i = U_k^T \mathbf{x}_i$$

- Objective
  - Can be expressed as SVD of X

$$\min_{U_k} \sum_{i=1}^{N} \left\| \mathbf{x}_i - U_k U_k^T \mathbf{x}_i \right\|^2 \qquad X = U \Sigma V^T$$

Σ

Diagonal matrix of eigenvalues

https://courses.cs.washington.edu/courses/cse446/17wi/slides/pca-annotated. $\text{error}_K = N \sum_{j=K+1}^{D} \mathbf{u}_j^T \Sigma \mathbf{u}_j$

PCA: Algorithm

- Step 1: Covariance matrix
- Step 2: Eigenvector decomposition

Algorithm 1 Direct PCA Algorithm

Input: Given data $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^N$, $\mathbf{x}_i \in \mathbb{R}^d$;

Recover basis: Calculate $XX^\top = \sum_{i=1}^N \mathbf{x}_i\mathbf{x}_i^\top$ and U as eigenvectors of $XX^\top$ for the top k eigenvalues.

Encode training data: $Y = U^\top X$, where Y is a $k \times N$ matrix of encodings of the original data.

Reconstruct training data: $\hat{X} = UY = UU^\top X$.

Encode test data: $y = U^\top x$, where y is a k-dimensional encoding of x.

Reconstruct test data: $\hat{x} = Uy = UU^\top x$.

Kernel Function: Similarity Between Samples

- Map the data into higher dimensional spaces: the data could become more easily separated or better structured
  - Support vector machine (SVM) -> Nonlinear SVM
  - Principal component analysis -> Kernel PCA

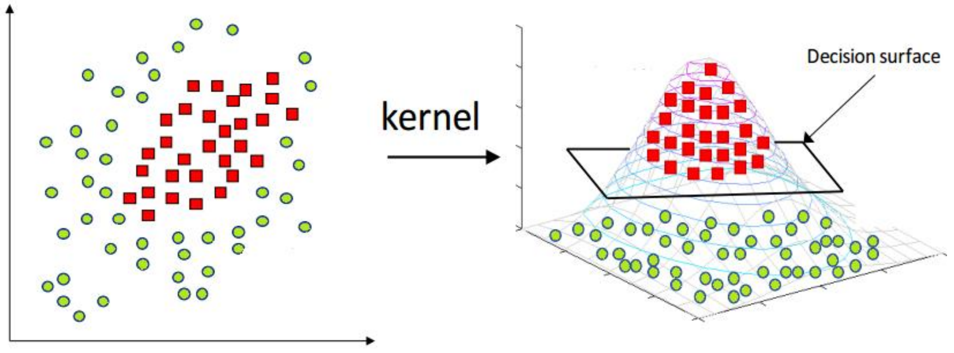
$k(x,y) = \langle \Phi(x), \Phi(y) \rangle$ $\quad \Phi : x \rightarrow \mathcal{H}$ $\quad x \mapsto \Phi(x)$

- Must be continuous, symmetric, and most preferably should have a positive (semi-) definite Gram matrix
- Kernel Functions
  - Linear Kernel
  - Polynomial Kernel
  - Gaussian Kernel

$$k(x,y) = x^T y + c$$

$$k(x,y) = (\alpha x^T y + c)^d$$

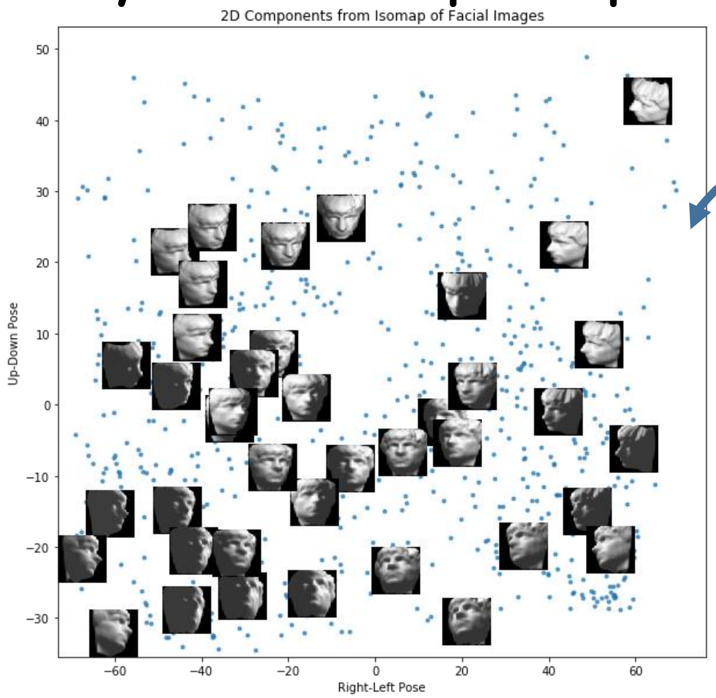
$$k(x,y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right)$$



http://crsouza.com/2010/03/17/kernel-functions-for-machine-learning-applications/

Kernel PCA

- History: S. Mika et al, NIPS, 1999
- Data may lie on or near a nonlinear manifold, not a linear subspace
- Find principal components that are nonlinearly to the input space via nonlinear mapping $\Phi : x \to \mathcal{H} \quad x \mapsto \Phi(x)$



- Objective $$\min_{U_k} \sum_{i=1}^{N} \left\| \Phi(\mathbf{x}_i) - U_k U_k^T \Phi(\mathbf{x}_i) \right\|^2$$

- Solution found by SVD: $\Phi(X) = U \Sigma V^T$

  U contains the eigenvectors of $\boxed{\Phi(X)\Phi(X)^T}$

Kernel PCA

- Centering

$$\tilde{\Phi}(X) = \Phi(X) - E_x[\Phi(X)]$$

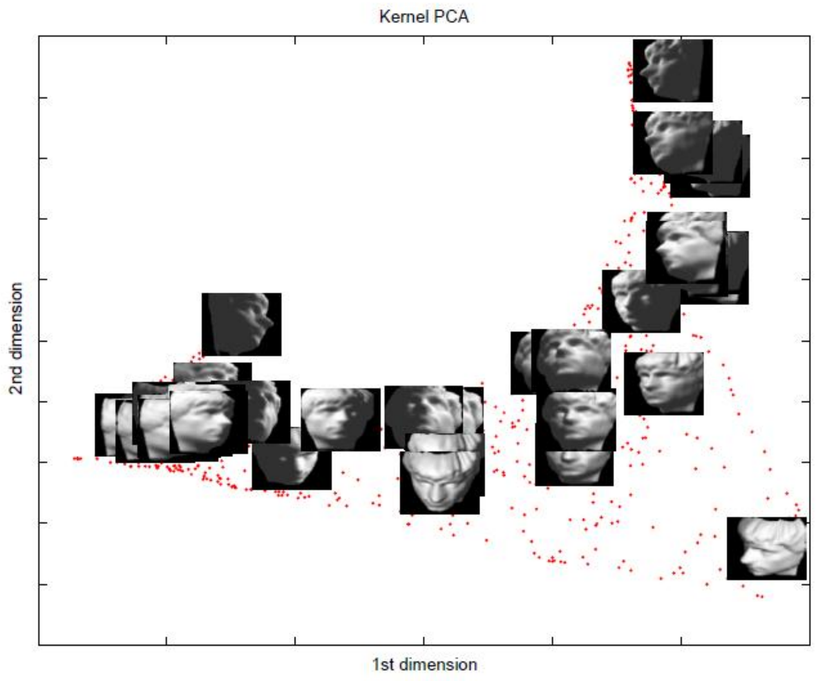
x, y both are the samples not the variables

$$\tilde{K}(x,y) = \tilde{\Phi}(x)\tilde{\Phi}(y)$$

$$\tilde{K}(x,y) = (\Phi(x) - E_x[\Phi(x)]).(\Phi(y) - E_y[\Phi(y)])$$

$$= K(x,y) - E_x[K(x,y)] - E_y[K(x,y)] + E_x[E_y[K(x,y)]]$$

- Issue: Difficult to calculate $\boxed{\Phi(X)\Phi(X)^T}$
  - ➢ Using $\boxed{\tilde{K}(x,y)}$ to calculate the eigenvectors



Two Matrices

$$X = \begin{pmatrix} ----- \\ ----- \\ \cdots\cdots \\ ----- \\ ----- \end{pmatrix}_{n\times D}$$

1. **Gram Matrix (Sample correlation matrix)**

$$K = (XX^T)_{n\times n} \qquad K\mu_i^T = \tau_i\mu_i^T \quad where\ i = \{1, 2, \cdots, n\}$$

$$K = (XX^T)_{n\times n} = \left(I - \frac{1}{n}1_n^T 1_n\right) E_X \left(I - \frac{1}{n}1_n^T 1_n\right)$$

$$where\ E_X(i,j) = d_{ij}$$

Similarity Between Samples

2. **Covariance Matrix**

$$C = \frac{1}{n}(X^T X)_{D\times D} = \frac{1}{n}\sum_i x_i^T x_i$$

$$Cv_i^T = \lambda_i v_i^T \quad where\ i = \{1, 2, \cdots, D\} \text{-------------} (0)$$

(a): $\lambda_i v_i^T = \frac{1}{n}\sum_j x_j^T < x_j, v_i >, \quad where \quad \lambda_i \neq 0$

Similarity Between Variables

Two Matrices

1. Relationship

- Existing coefficients: $v = \sum_{j=1}^{n} \alpha(j) x_j$
- For all samples x_k: $\lambda x_k v^T = x_k C v^T$-------------(1)

$$\lambda\, x_k \sum_{j=1}^{n} \alpha(j) {x_j}^T = x_k \left(\frac{1}{n}\sum_i {x_i}^T x_i\right) \sum_{j=1}^{n} \alpha(j) {x_j}^T \text{-----(2)}$$

- If set $K_{ij} = < x_i, x_j >$,

$$n\lambda K\alpha = K^2\alpha \text{ ---------------------------(3)}$$

$$n\lambda\alpha = K\alpha \text{--------------------------------(4)}$$

- Conclusion:

(b): $\alpha_i = X{v_i}^T = \sqrt{\lambda_i}\mu_i$; (c): $n\lambda_i = \tau_i$;

(d): $v_i x^T = \sum_{j=1}^{n} \alpha_i(j) x_j x^T$ (x is a new sample)

The required projection

Inner product

$$X = \begin{pmatrix} ----- \\ ----- \\ \cdots\cdots \\ ----- \\ ----- \end{pmatrix}_{n\times D}$$

(a): $\lambda_i {v_i}^T = \frac{1}{n}\sum_j {x_j}^T < x_j, v_i >$

$\boxed{a_i(j)}$

For Kernel PCA:

What do we know? Kernel

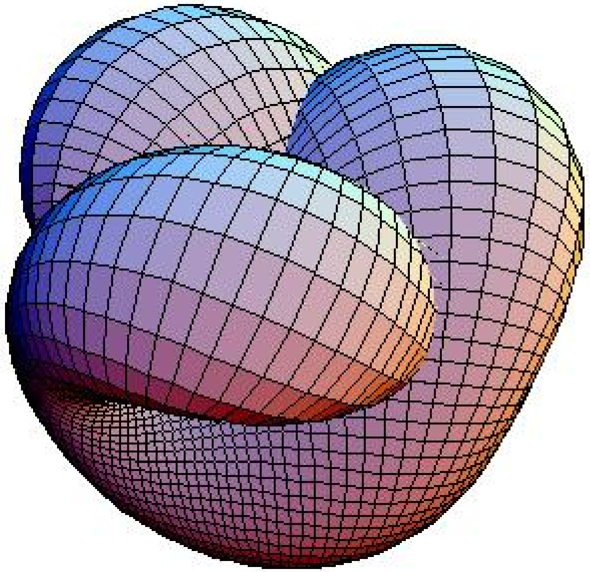
What do we not know? Covariance

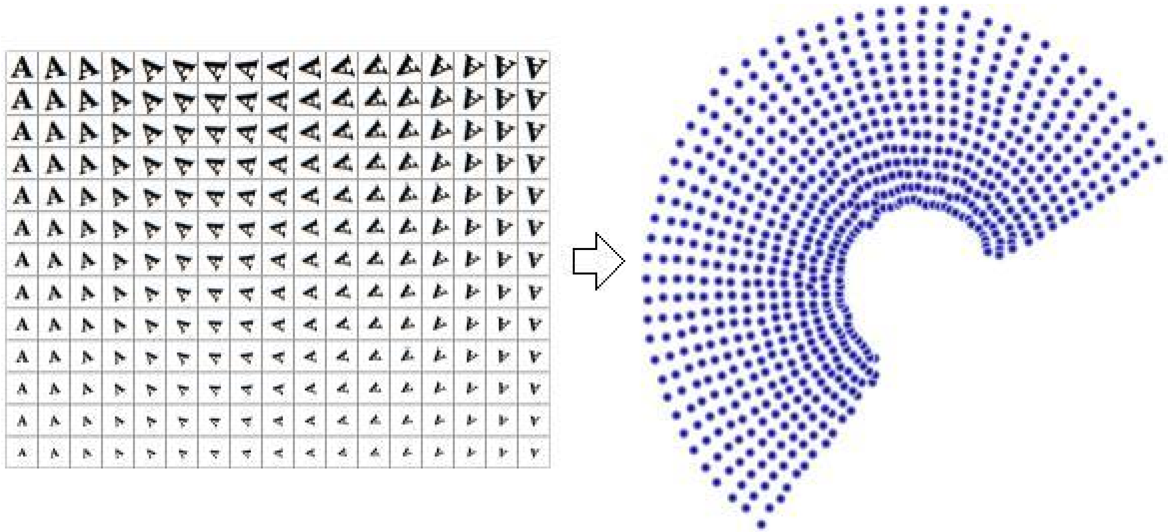
Manifold Learning

Manifold → Graph

在每个点的邻域内，它局部地类似于欧几里得空间。这意味着，尽管数据可能处于高维空间中，但我们可以假设数据的结构可以映射到较低维度的空间（流形上），并且在这个流形上，数据仍然保持其内在的结构。

- In mathematics, a manifold is a topological space that locally resembles Euclidean space near each point





Plot of the two-dimensional points that results from using a NLDR algorithm. In this case, Manifold Sculpting used to reduce the data into just two dimensions (rotation and scale).

https://scikit-learn.org/stable/modules/manifold.html

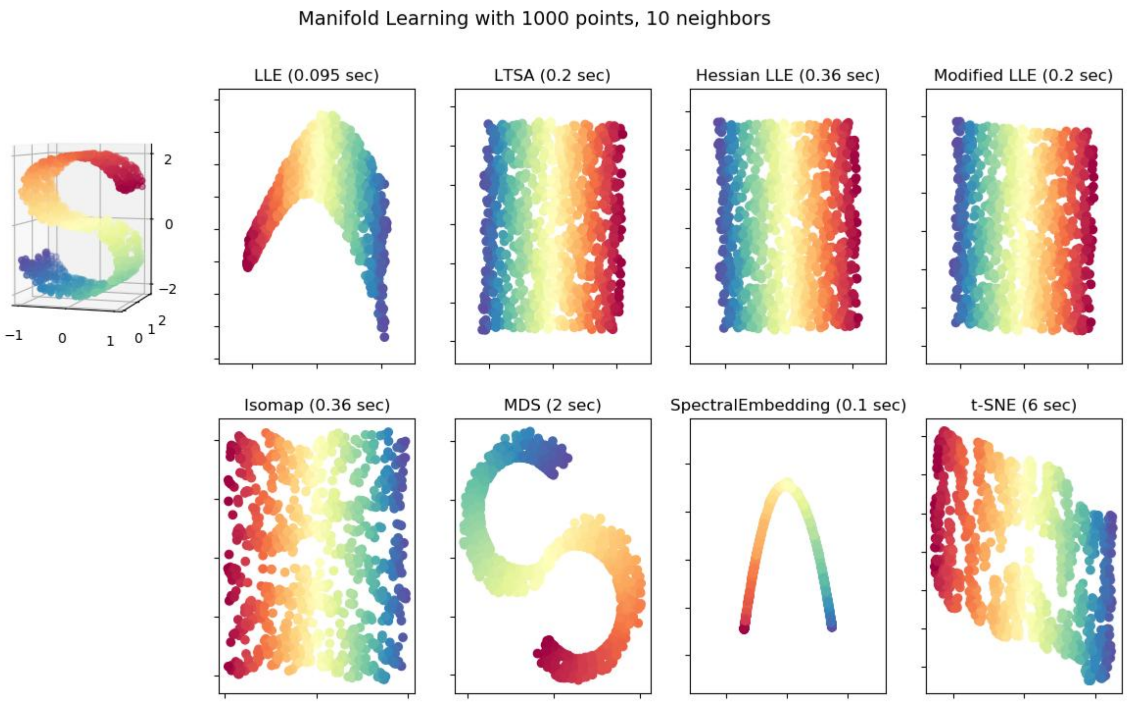
Nonlinear Dimensionality Reduction

LLE (Locally Linear Embedding)：保持局部邻域的线性结构。

Isomap：通过测量地理距离而非欧几里得距离来维护数据结构。

MDS (Multidimensional Scaling)：通过距离矩阵来缩减维度。

- High-dimensional data, meaning data that requires more than two or three dimensions to represent, can be **difficult** to interpret.
- One approach to **simplification** is to assume that the data of interest lie on an embedded non-linear manifold within the higher-dimensional space.
- If the manifold is of low enough dimension, the data can be **visualised** in the low-dimensional space.



Locally Linear Embedding (LLE)

- History: S. Roweis and L. Saul, Science, 2000
- Procedure
  - Identify the neighbors of each data point
  - Compute weights that best linearly reconstruct the point from its neighbors

$$\min_{\mathbf{w}} \sum_{i=1}^{N} \|\mathbf{x}_i - \sum_{j=1}^{k} w_{ij}\mathbf{x}_{N_i(j)}\|^2$$

Locally

  - Find the low-dimensional embedding vector which is best reconstructed by the weights determined in Step 2

$$\min_{Y} \sum_{i=1}^{N} \|\mathbf{y}_i - \sum_{j=1}^{k} w_{ij}\mathbf{y}_{N_i(j)}\|^2 \Longleftrightarrow \min_{Y} \quad \mathrm{tr}(Y^\top Y L)$$

Centering Y with unit variance

where $L = R - W$, R is diagonal and $R_{ii} = \sum_{j=1}^{N} W_{ij}$.

https://cs.nyu.edu/~roweis/lle/papers/lleintro.pdf

Laplacian Eigenmaps (LE)

- History: M. Belkin and P. Niyogi, 2003
- Similar to locally linear embedding
- Different in weights setting and objective function
  - ➢ Weights

$$W_{ij} = \begin{cases} 1 & i,j \text{ are connected} \\ \exp\left(\frac{-\|x_i - x_j\|^2}{s}\right) & \text{otherwise} \end{cases}$$

Locally

Has a different meaning to the weights in LLE

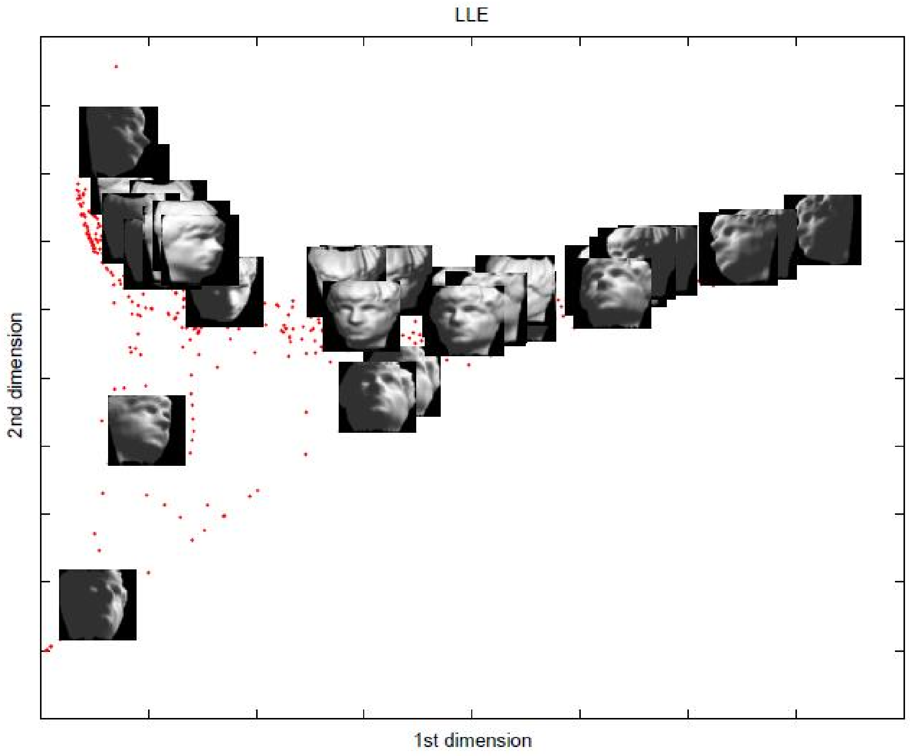
  - ➢ Objective

$$\min_{Y} \sum_{i=1}^{N}\sum_{j=1}^{N} (\mathbf{y}_i - \mathbf{y}_j)^2 W_{ij} \Leftrightarrow \min_{Y} \operatorname{tr}(YLY^\top)$$

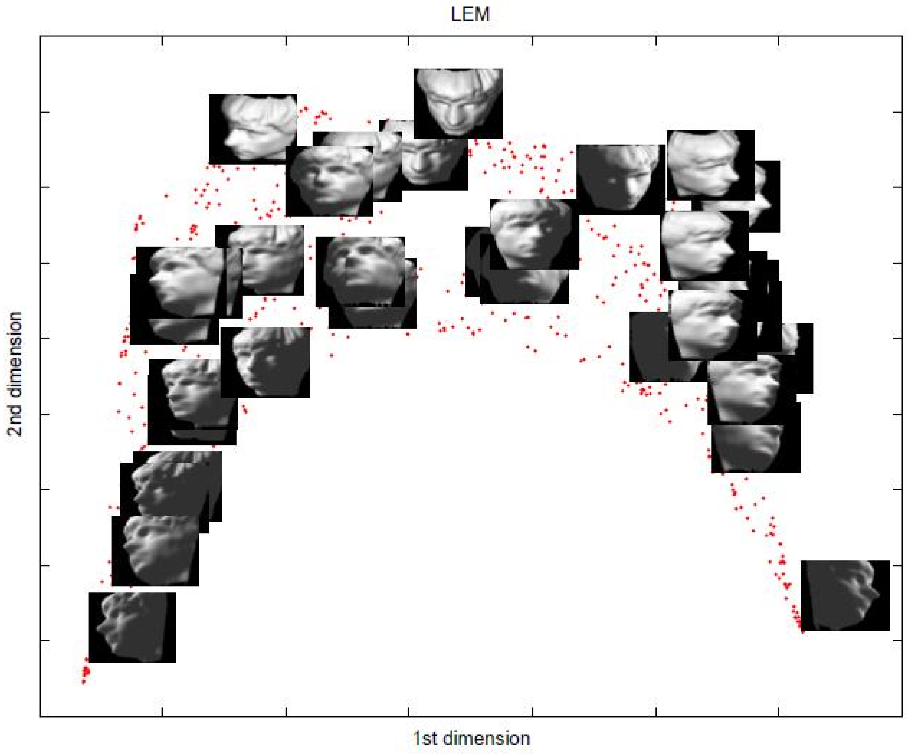
where $L = R - W$, R is diagonal and $R_{ii} = \sum_{j=1}^{N} W_{ij}$.

LLE and LE Examples

- Two-dimensional visualization



LLE



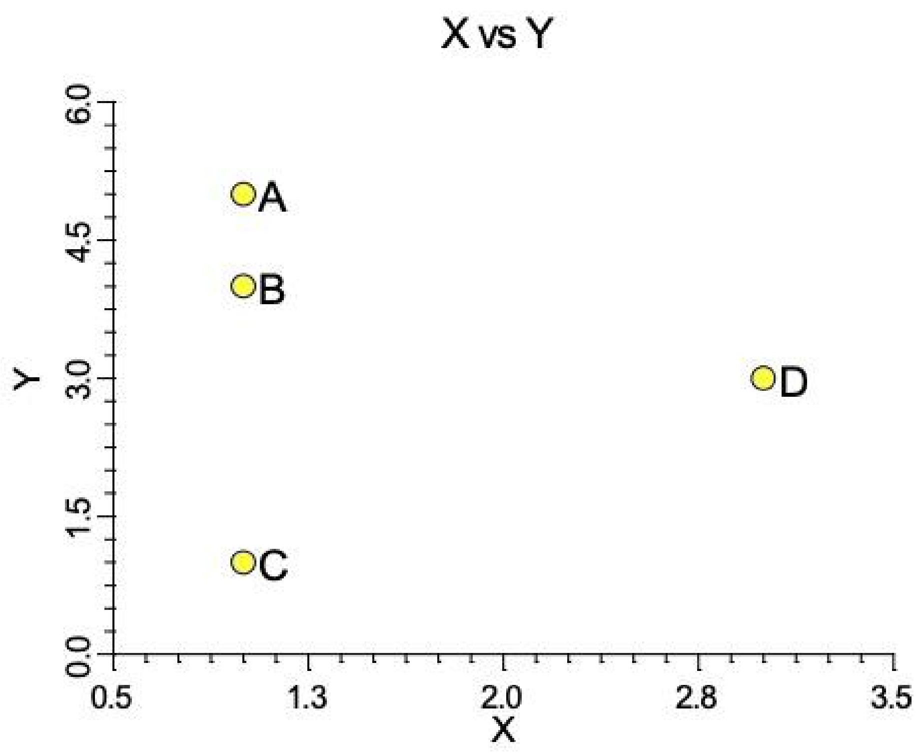
LE

Multidimensional Scaling (MDS)

- The following example will help explain what MDS does. Consider the following set of data

Original Data Matrix

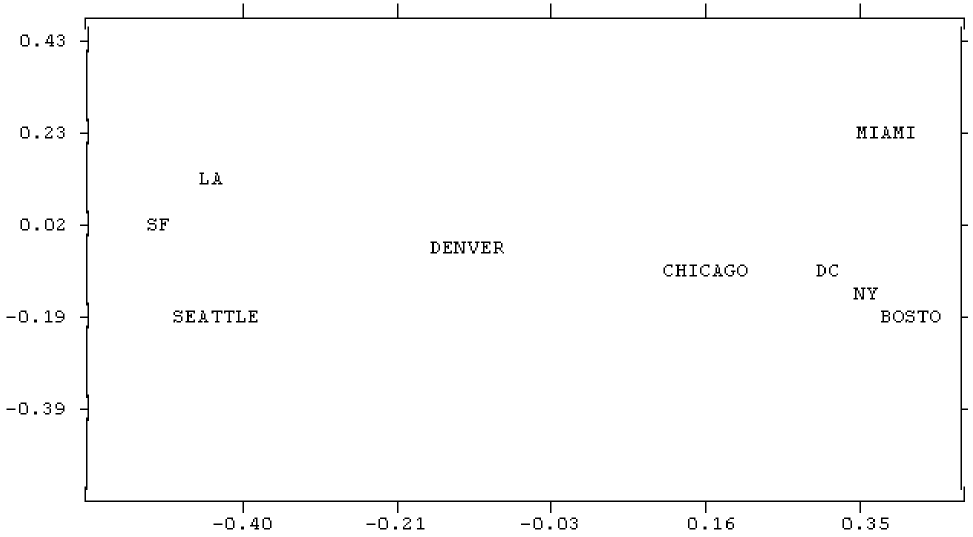
Label	X	Y
A	1	5
B	1	4
C	1	1
D	3	3



Multidimensional Scaling (MDS)

- Given the matrix of distances among cities, MDS produces this map

		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



- We may find the $N \times N$ Gram matrix $B = X^T X$, rather than X.

The solutions are not unique

Multidimensional Scaling (MDS)

- History: T. Cox and M. Cox, 2001
- Goal: attempts to preserve pairwise distances

Distance

$$\min_{Y} \sum_{i=1}^{N}\sum_{j=1}^{N}(d_{ij}^{(X)} - d_{ij}^{(Y)})^2$$

where $d_{ij}^{(X)} = \|x_i - x_j\|^2$ and $d_{ij}^{(Y)} = \|y_i - y_j\|^2$.

- Different formulation of PCA, but yields similar result form
- Transformation

Proximity matrix

Gram matrix B

$$\boxed{X^\top X = -\frac{1}{2} H D^{(X)} H} \quad \text{where } H = I - \frac{1}{N}\mathbf{1}\mathbf{1}^\top.$$

➢ Is equivalent to: $$\min_{Y} \sum_{i=1}^{N}\sum_{j=1}^{N}(x_i^\top x_j - y_i^\top y_j)^2$$

Inner product

http://fourier.eng.hmc.edu/e176/lectures/MultidimensionScaling.pdf

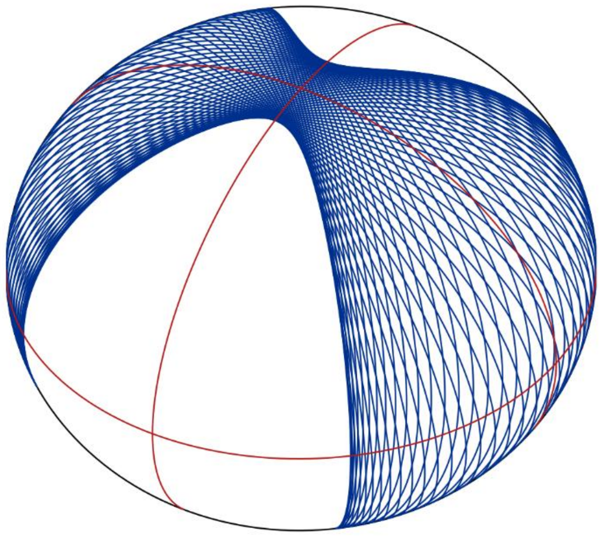
https://www.sjsu.edu/faculty/guangliang.chen/Math253S20/lec9mds.pdf

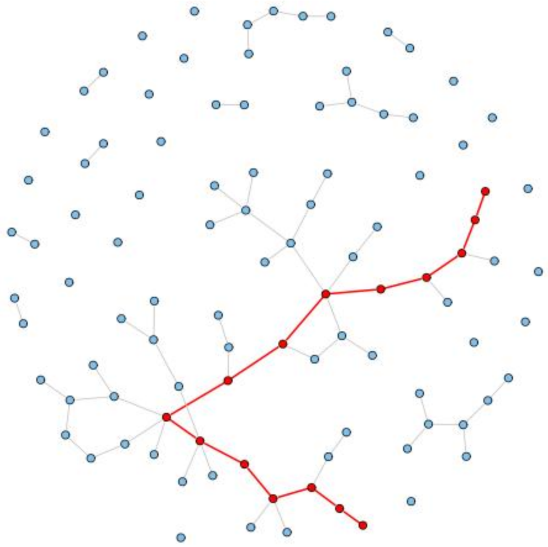
Multidimensional Scaling (MDS)

- Steps of a Classical MDS algorithm:
  - Set up the squared proximity matrix
  - Apply double centering $\boxed{-\frac{1}{2} H D^{(X)} H}$
  - Determine the largest k eigenvalues and corresponding eigenvectors
  - The original coordinate is $X = \Lambda^{1/2} V'$, if we have had
  - The NEW coordinate is $X_k = \Lambda_k^{1/2} V_k'$

Isomap

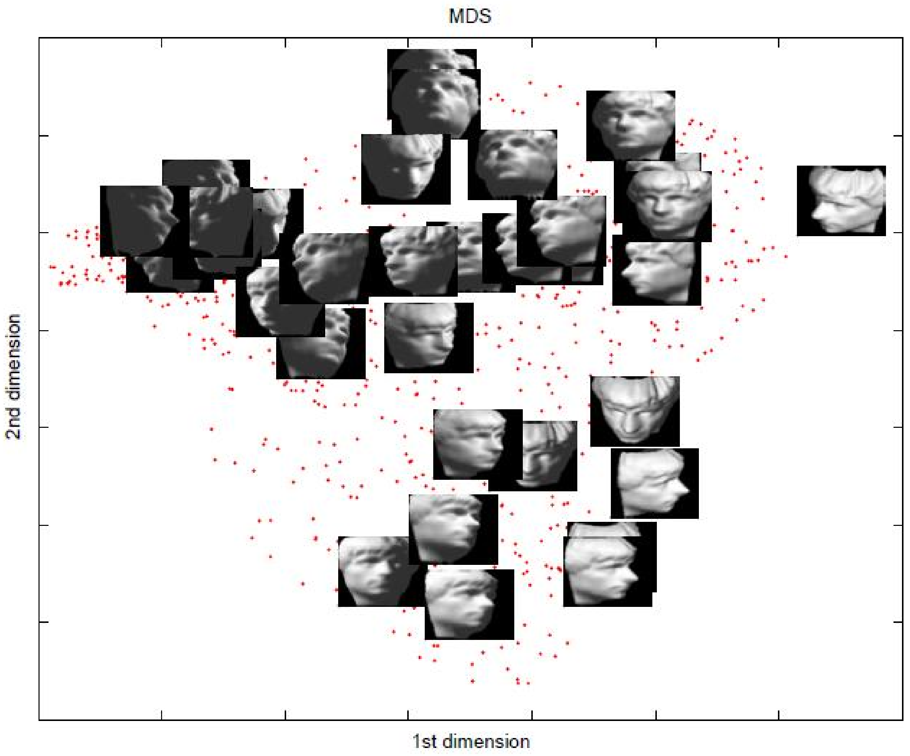
- History: J. Tenenbaum et al, Science 2000
  - ➢ A nonlinear generalization of classical MDS
  - ➢ Perform MDS, not in the original space, but in the geodesic space
- Procedure-similar to LLE
  - ➢ Find neighbors of each data point - graph
  - ➢ Compute geodesic pairwise distances (e.g., shortest path distance) between all points
  - ➢ Embed the data via MDS



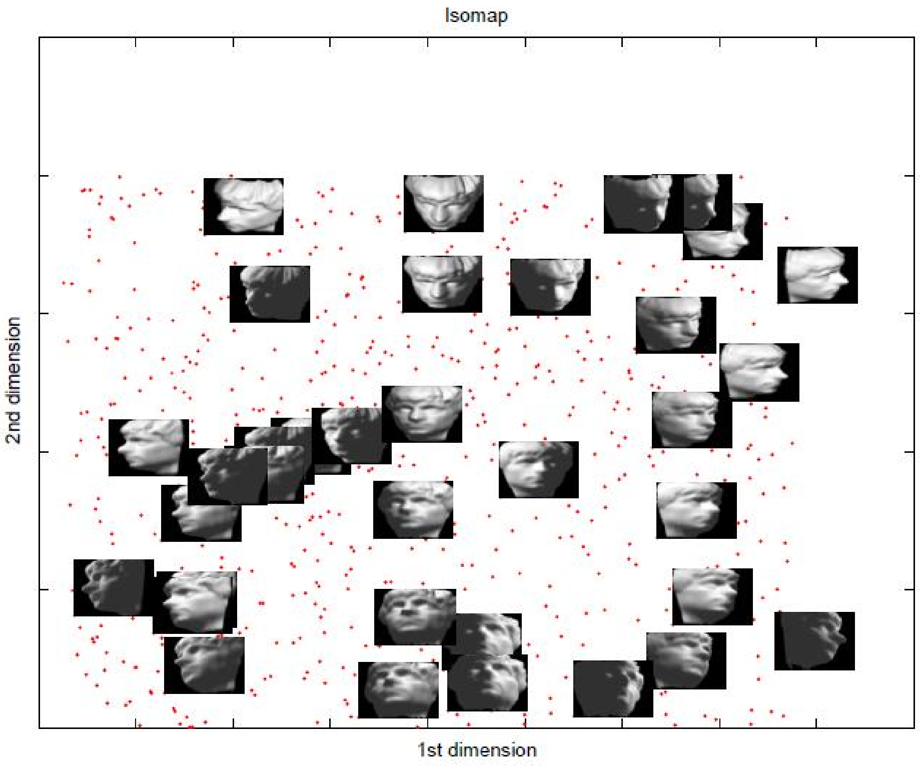


MDS and Isomap Example

- Two-dimensional visualization



MDS



Isomap

Intrinsic of Manifold Learning

- Preserve the local similarities (smoothness)

Manifold → graph

Revisiting PCA

- Maximizing the variance

  =

- Minimizing the reconstruction error

  =

- Preserving the similarities or distances (classical MDS)

- OTHERS
  - Local reconstruction error (LLE)
  - Local similarities (LE)

Stochastic Neighbor Embedding

- The similarity of data point x_j to data point x_i is the conditional probability: $p_{j|i}$

$$p_{j|i} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$

The relationships are only related to point ***i***

- For the low-dimensional counterparts, a similar conditional probability is defined as: $q_{j|i}$

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

What is preserved? Similarity distribution

Stochastic Neighbor Embedding

- SNE minimizes the sum of Kullback-Leibler divergences over all data points using a gradient descent method. The cost function C is given by

$$C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

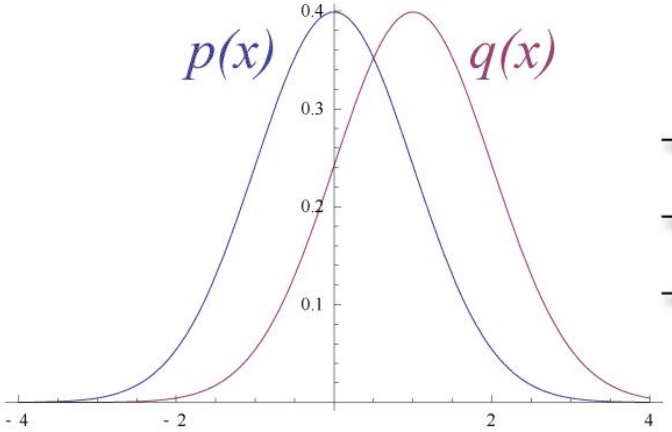
  - P_i: conditional probability distribution over all others given x_i
  - Q_i: conditional probability distribution over all other map points given map point y_i

- The gradient has a surprisingly simple form

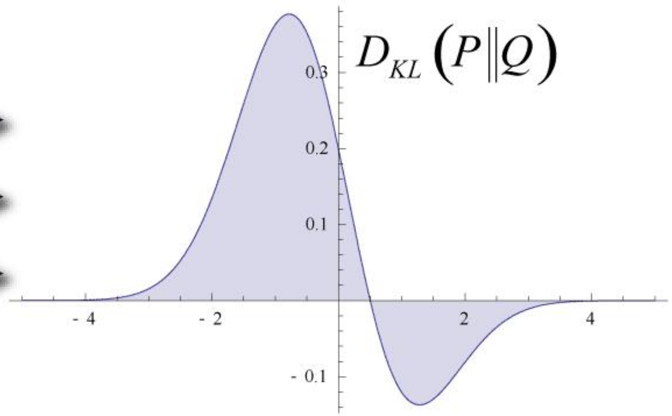
$$\frac{\delta C}{\delta y_i} = 2 \sum_j (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})(y_i - y_j)$$

Kullback-Leibler Divergences

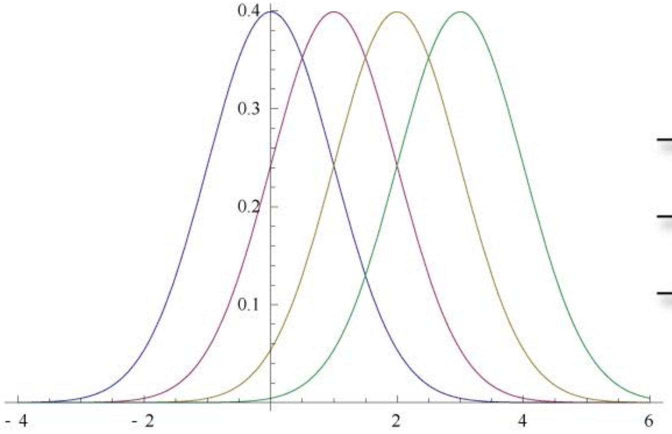
$$D_{\mathrm{KL}}(P \parallel Q) = \int_{-\infty}^{\infty} p(x) \log\left(\frac{p(x)}{q(x)}\right) dx$$

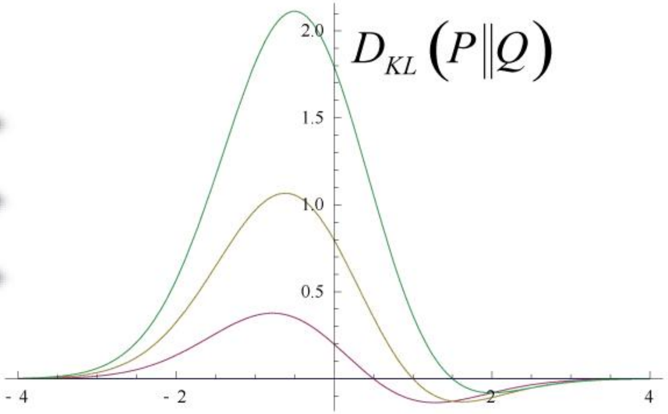


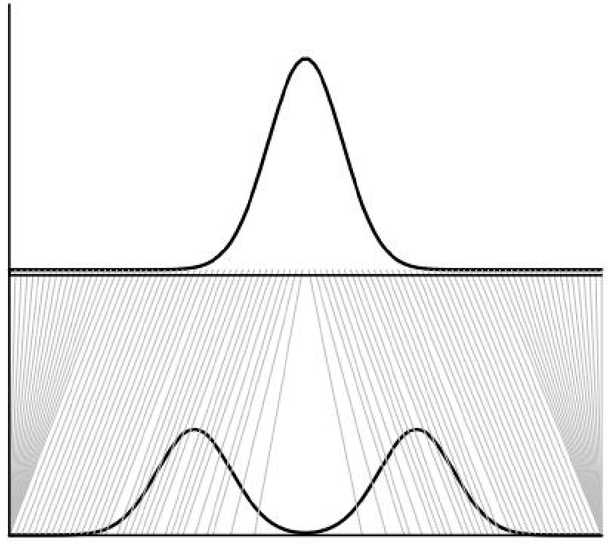
Original Gaussian PDF's



KL Area to be Integrated







Wasserstein distance

Kantorovich–Rubinstein metric

Earth Mover's Distance

Symmetric SNE

- In symmetric SNE, the pairwise similarities in the low-dimensional map is:

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

All points

- The pairwise similarities in the high-dimensional space is:

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

- The gradient of symmetric SNE is fairly similar to that of asymmetric SNE

$$\frac{\delta C}{\delta y_i} = 4 \sum_j (p_{ij} - q_{ij})(y_i - y_j)$$

T-distributed Stochastic Neighbor Embedding (T-SNE)

- The crowding problem
  - 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
  - For example, it is possible to have 11 data points that are mutually equidistant in a ten-dimensional manifold but it is not possible to model this faithfully in a two-dimensional map. Therefore, if the small distances can be modeled accurately in a map, most of the moderately distant data points will be too far away in the two-dimensional map

T-distributed Stochastic Neighbor Embedding (T-SNE)

- Employ a Student t-distribution with one degree of freedom

v=1

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

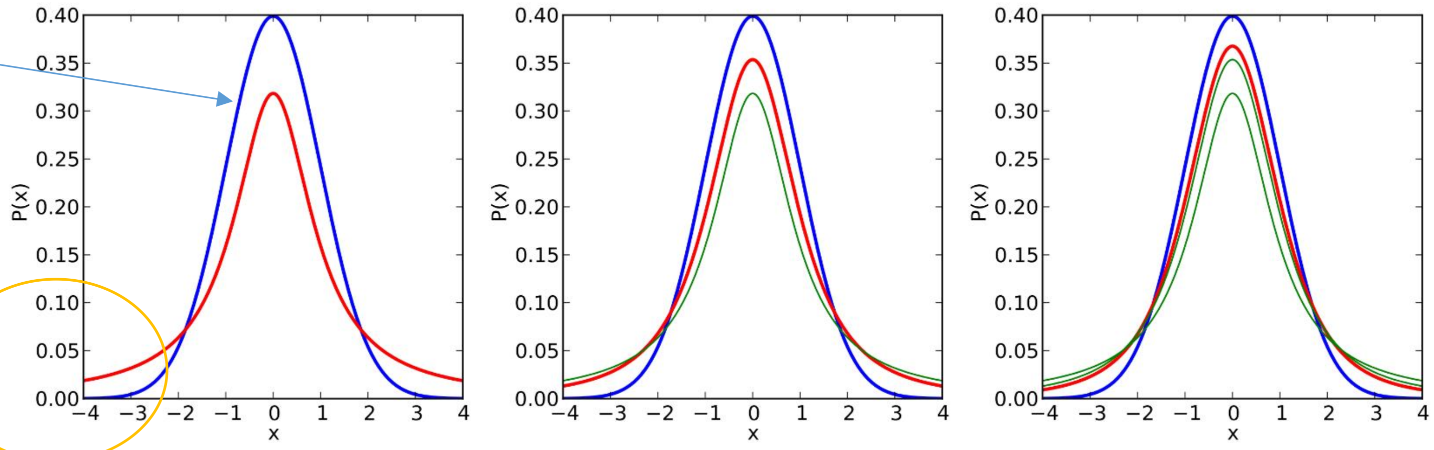
$$f(t) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi}\,\Gamma(\frac{\nu}{2})}\left(1+\frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

- The gradient of the Kullback-Leibler divergence

$$\frac{\delta C}{\delta y_i} = 4\sum_j (p_{ij} - q_{ij})(y_i - y_j)\left(1+\|y_i - y_j\|^2\right)^{-1}$$

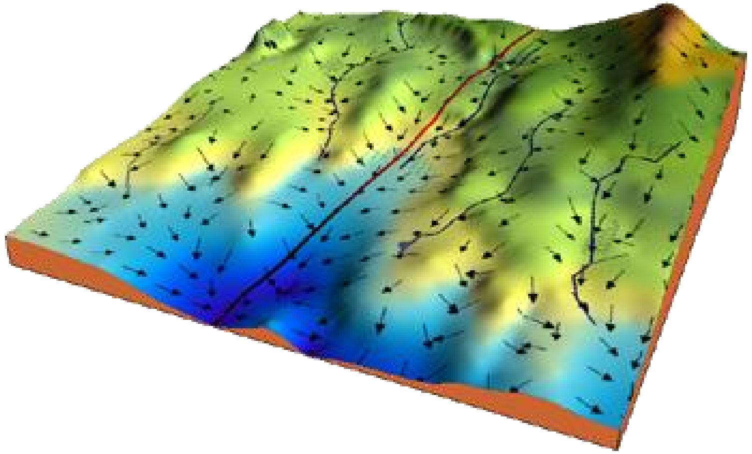
Gaussian

When distances lose the ability to discriminate



Density of the t-distribution (red) for 1, 2, 3 degrees of freedom compared to the standard normal distribution (blue)

Gradient Descent Method



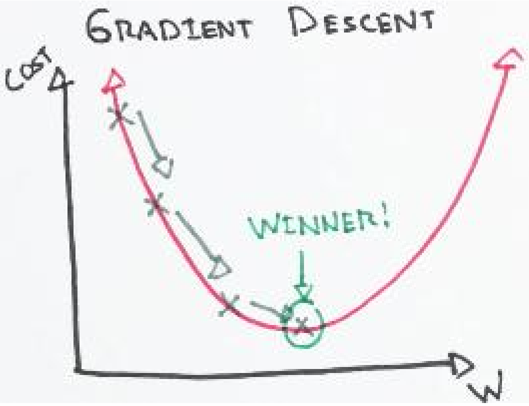
- Hypothesis space: linear function (m,b)
- Given the cost function

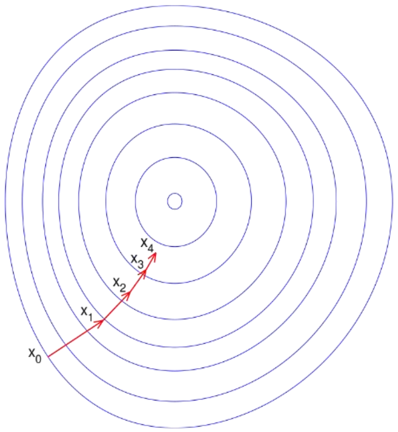
$$f(m,b) = \frac{1}{N}\sum_{i=1}^{n}(y_i - (mx_i + b))^2$$

- Gradient descent

$$f'(m,b) = \begin{bmatrix} \frac{df}{dm} \\ \frac{df}{db} \end{bmatrix} = \begin{bmatrix} \frac{1}{N}\sum -2x_i(y_i - (mx_i + b)) \\ \frac{1}{N}\sum -2(y_i - (mx_i + b)) \end{bmatrix}$$

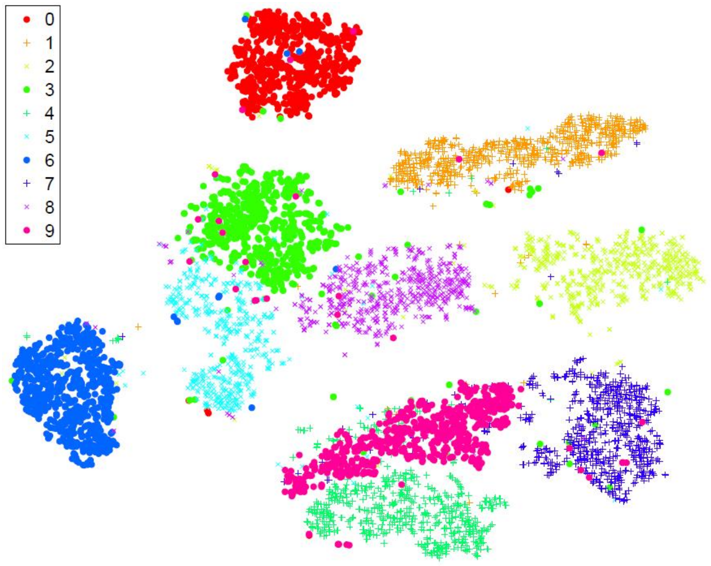
- Types of Gradient Descent:
  - ➢ Batch Gradient Descent
  - ➢ Stochastic Gradient Descent



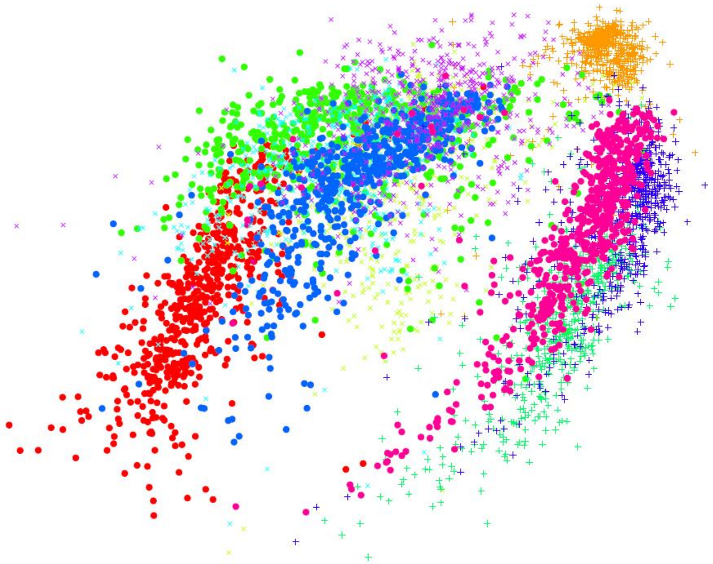


2D Visualization

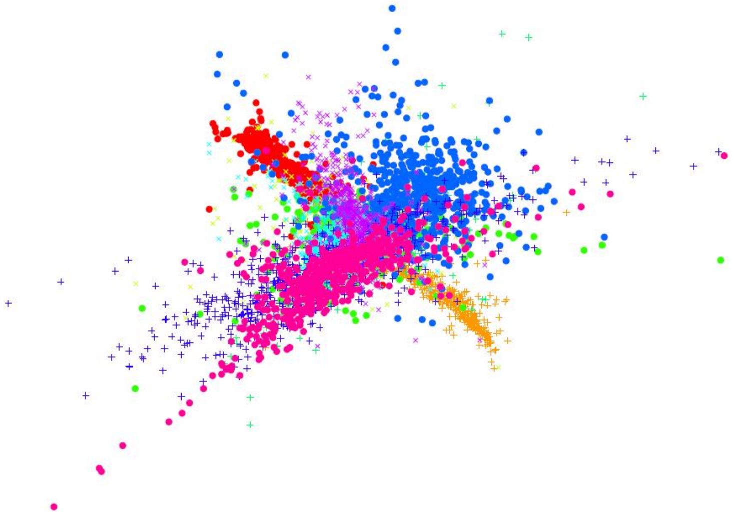
- Comparison



T-SNE



Isomap

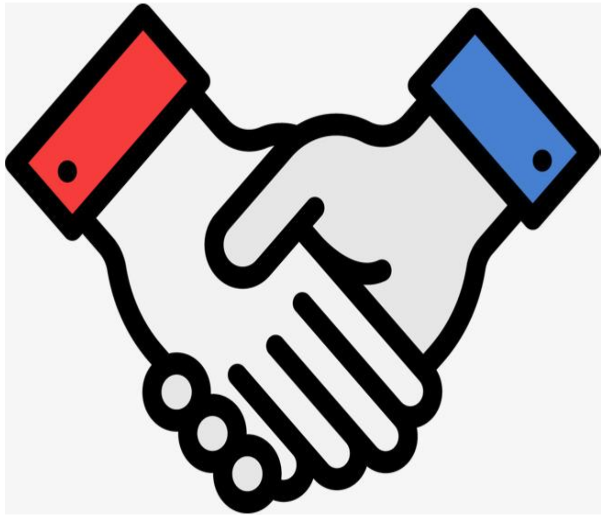


LLE

Conclusions

Conclusion

- Dimensionality Reduction
  - Linear
    - ✓ PCA
    - ✓ MDS
  - Manifold Learning (Nonlinear)
    - ✓ LLE
    - ✓ LE
    - ✓ Isomap
    - ✓ T-SNE



Thanks

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