

Introduction to Big Data Analysis

Dimensionality Reduction

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Outlines

Introduction

Principal Component Analysis

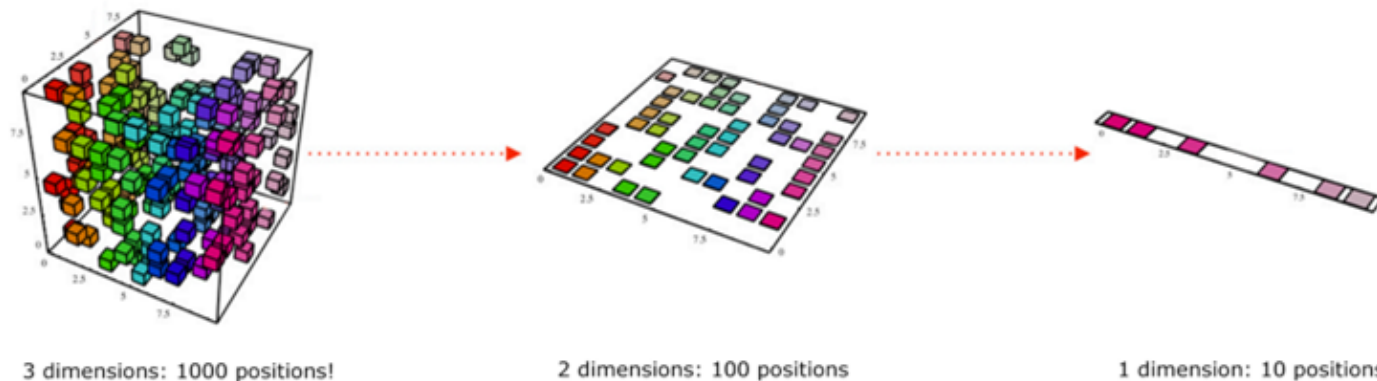
Linear Discriminant Analysis

Nonlinear Dimensionality Reduction

Feature Selection

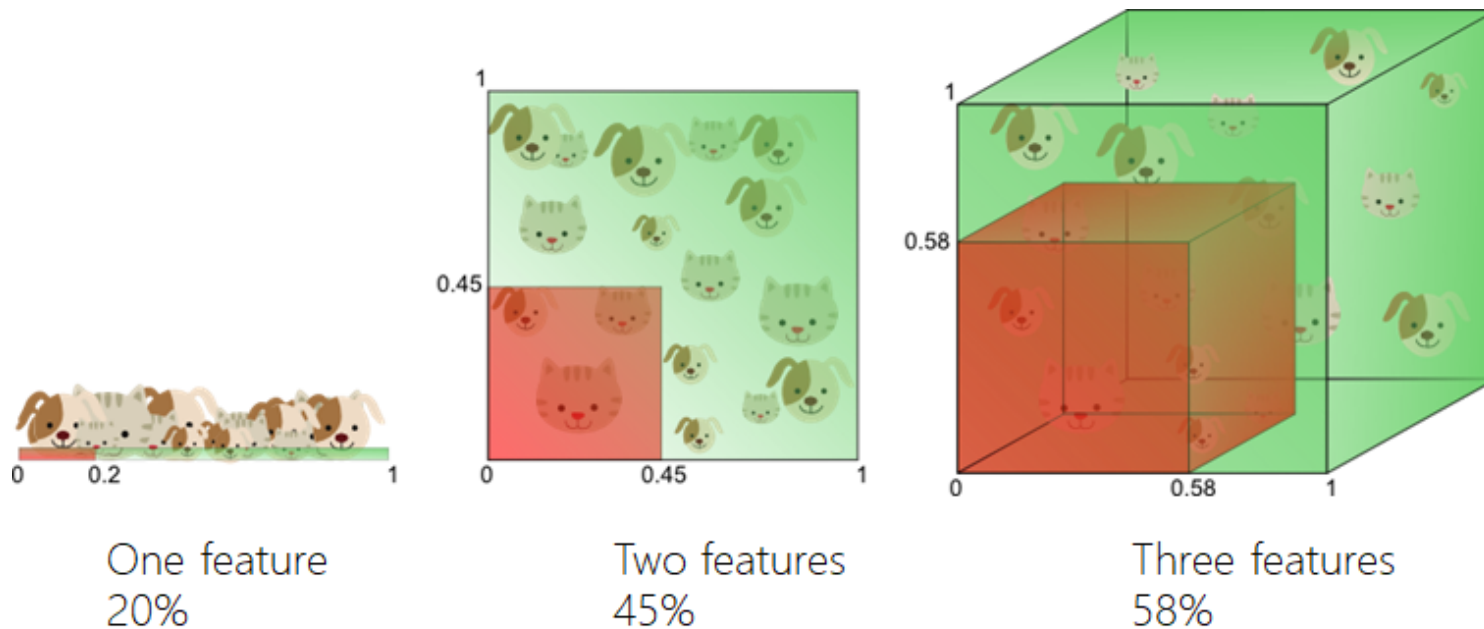
What is Dimensionality Reduction

- The process of reducing the number of random variables under consideration, via obtaining a set of “uncorrelated” principal variable
- By mapping from high-dimensional space to low-dimensional space
- Learning $f : \mathcal{X} \rightarrow \mathcal{Y}$, where $\dim \mathcal{X} = n$ and $\dim \mathcal{Y} = r$ with $n > r$.
- Including both unsupervised learning (mostly common) and supervised learning



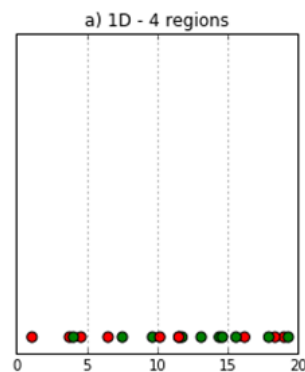
Why Need Dimensionality Reduction ?

- Curse of dimensionality
- Eg : classify cats and dogs using features, if we want to cover 20% of the feature space, how many data do we need ?
- However, the number of samples is limited in practice

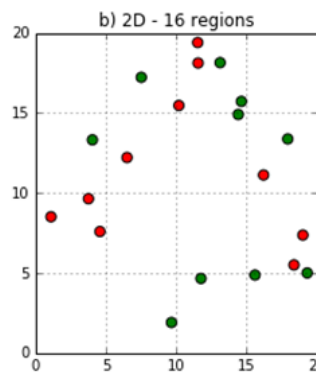


Why Need Dimensionality Reduction ? (Cont')

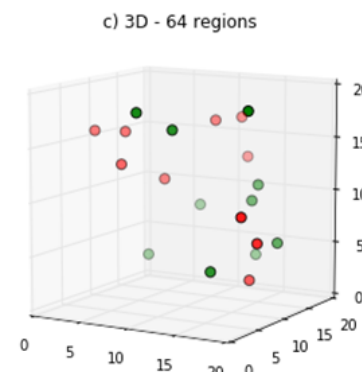
- Due to the sparsity of data in high dimensions, it is easy to overfit
- Hard to train a good model to classify the corner data (getting more in high dimensions)



Density: $20/4 = 5$



$20/16 = 1.25$

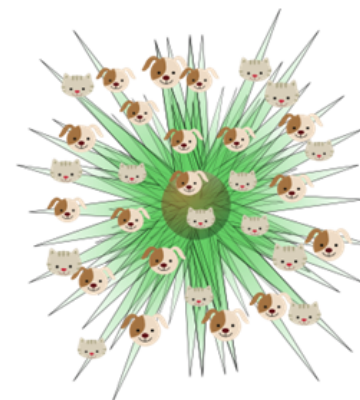
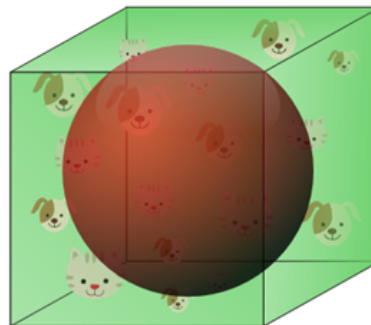
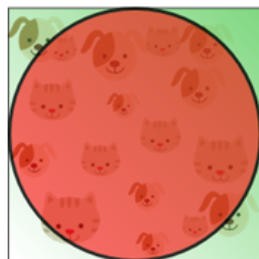


$20/64 \approx 0.31$

In 2D, # of corners:
 $2^2 = 4$

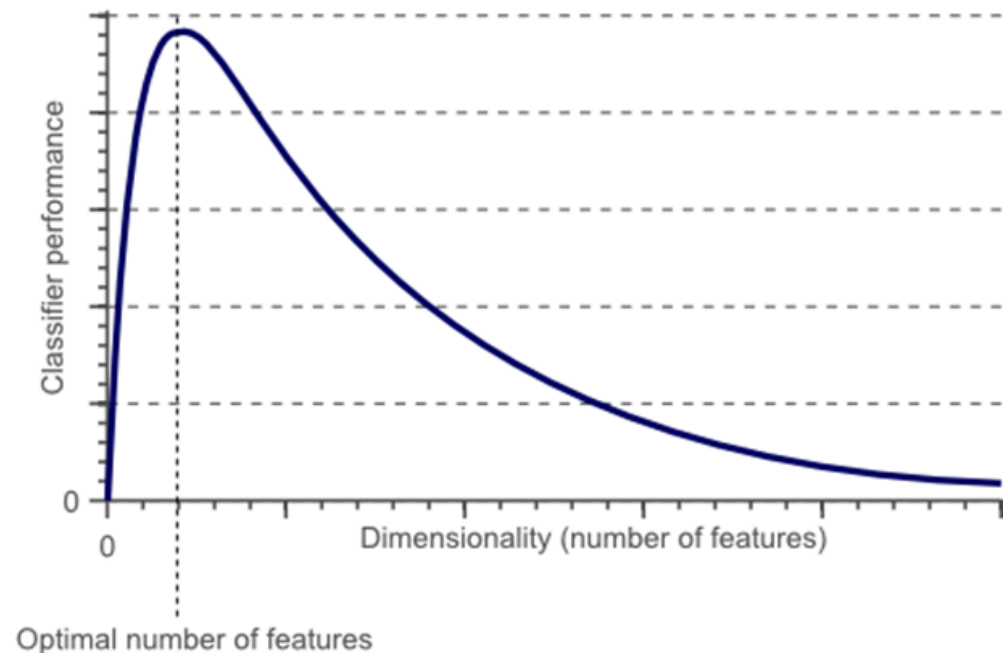
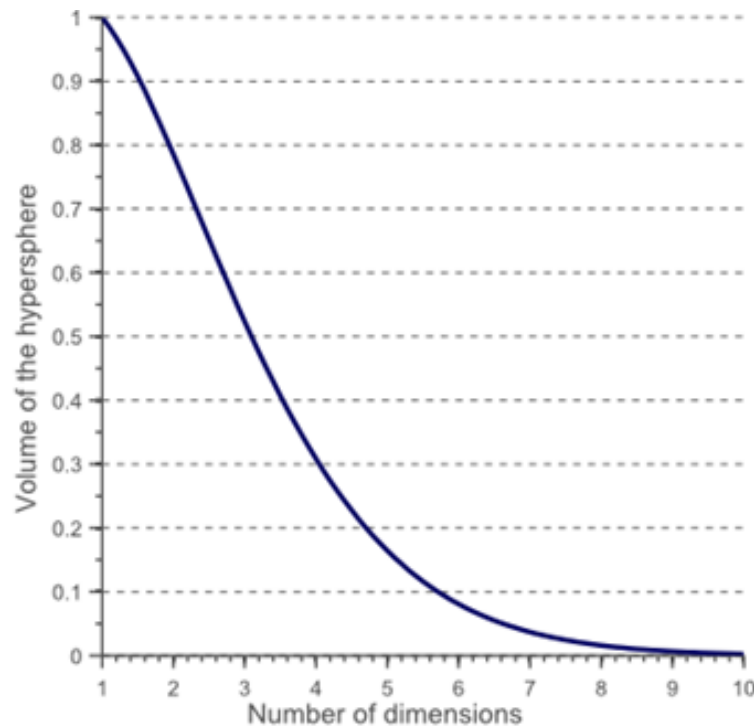
In 3D, # of corners:
 $2^3 = 8$

In 4D, # of corners:
 $2^8 = 256$



Curse of Dimensionality

- The volume of hypersphere decays to zero with the increase of dimension
- The performance gets worse with the increase of dimension



Roles of Dimensionality Reduction

- Data compression
- Denoising
- Feature extraction by mapping and feature selection (eg. Lasso)
- Reduce both spatial and time complexity, so that fewer parameters are needed and smaller computational power is required
- Data visualization

Methods in Dimensionality Reduction

- Linear dimensionality reduction :
 - Principal component analysis (PCA)
 - Linear discriminant analysis (LDA)
 - Independent component analysis (ICA)
- Nonlinear dimensionality reduction :
 - Kernel based methods (Kernel PCA)
 - Manifold learning (ISOMAP, Locally Linear Embedding (LLE), Multidimensional scaling (MDS), t-SNE)

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Variance and Covariance Matrix

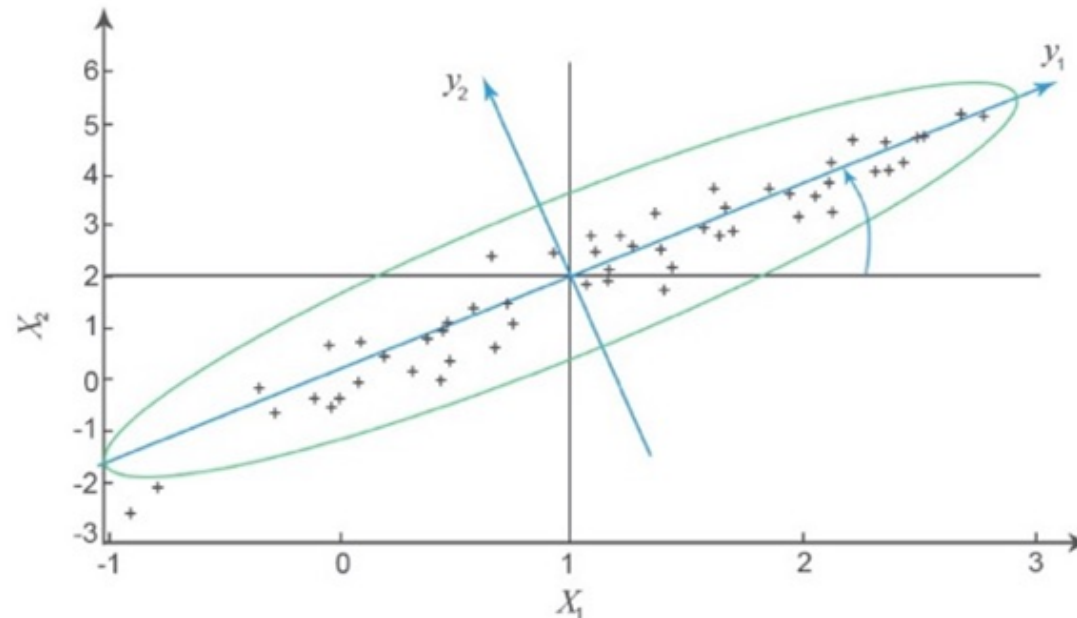
- Variance measures the variability or divergence of single variable : $\text{Var}(X) = E(X - EX)^2$, sample version $S^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$; standard deviation : $\text{Std}(X) = \sqrt{\text{Var}(X)}$
- For more variables, $\text{Cov}(X, Y) = E(X - EX)(Y - EY)$, sample version $C = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})$
- If $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)^T \in \mathbb{R}^{n \times p}$ is the sample matrix, then $C = \frac{1}{n-1} (X - \mathbf{1}_n \bar{\mathbf{x}}^T)^T (X - \mathbf{1}_n \bar{\mathbf{x}}^T) = \frac{1}{n-1} (X - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T X)^T (X - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T X) = \frac{1}{n-1} X^T J X$, where $J = \mathbf{I}_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T$ is a projection matrix with rank $n - 1$.

Principal Component Analysis (PCA)

- PCA transforms a set of strongly correlated variables to another set (**typically much smaller**) of **weakly correlated** variables by using orthogonal transformation
- The new variables are called principal components
- The new set of variables are linear combinations of the original variables whose variance information is inherited as much as possible
- Unsupervised learning
- Proposed by Karl Pearson, successfully used in economics by Stone (1947) : keep 97.4% information, 17 variables about income and expenditure are finally reduced to 3 variables (F1 : total income, F2 : rate of change in total income, F3 : economic development or recession)

Geometric Interpretation

- Assume a set of 2D data follows Gaussian distribution (but not limited to Gaussian distribution!), the reduction to 1D is successfully achieved by taking a direction with larger variance (larger variability of data)
- The direction in the major axis contains more information than the other direction, since smaller variance indicates the variables are almost the same



Linear Algebra

- Let $\{\mathbf{e}_i\}_{i=1}^p$ be the canonical basis in Euclidean space, want to find another orthonormal basis $\{\tilde{\mathbf{e}}_i\}_{i=1}^p$ such that the random vector $\mathbf{v} = \sum_{i=1}^p x_i \mathbf{e}_i$ can be expressed in the new basis by $\mathbf{v} = \sum_{i=1}^p \tilde{x}_i \tilde{\mathbf{e}}_i$, where $\text{Var}(\tilde{x}_1) \geq \dots \geq \text{Var}(\tilde{x}_p)$ and $\text{Cov}(\tilde{x}_i, \tilde{x}_j) \approx 0$ for $i \neq j$
- By linear algebra, the coordinate transformation is given by the linear transformation : $(\tilde{\mathbf{e}}_1, \dots, \tilde{\mathbf{e}}_p) = (\mathbf{e}_1, \dots, \mathbf{e}_p)W$, where $W \in \mathbb{R}^{p \times p}$ is an invertible matrix
- The component coefficients is transformed accordingly :
 $\mathbf{x} = W\tilde{\mathbf{x}}$

Eigendecomposition of Sample Covariance Matrix

- Assume we have n centralized samples $\{\mathbf{x}_i\}_{i=1}^n$ with $\frac{1}{n} \sum_{i=1}^n \mathbf{x}_i = \mathbf{0}_p$
- Then $X^T = (\mathbf{x}_1, \dots, \mathbf{x}_n) = W(\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n) = W\tilde{X}^T$
- The sample covariance matrix of X is $\text{Cov}(X) = \frac{1}{n-1} X^T X$
- The sample covariance matrix of \tilde{X} is $\text{Cov}(\tilde{X}) = \frac{1}{n-1} \tilde{X}^T \tilde{X} = \frac{1}{n-1} W^T X^T X W = W^T \text{Cov}(X) W$
- Its diagonals are the sample versions of $\text{Var}(\tilde{x}_1), \dots, \text{Var}(\tilde{x}_p)$, while its off-diagonals are the covariances between \tilde{x}_i and \tilde{x}_j
- Need that $\text{Cov}(\tilde{X})$ is nearly diagonal with decreasing diagonal entries for some W .
- Equivalent to do eigendecomposition : $\text{Cov}(X) = O \text{diag}(\lambda_1, \dots, \lambda_p) O^T$ with some orthogonal matrix $O \in \mathbb{R}^{p \times p}$ and $\lambda_1 \geq \dots \geq \lambda_p \geq 0$, then let $W = O$ completes the job

Interpretations

- Variances in the transformed variables : $\text{Var}(\tilde{x}_i) = \lambda_i$, eigenvalues of $\text{Cov}(X)$
- The new basis consists of the columns of $W = O$, i.e., the eigenvectors of $\text{Cov}(X)$
- The percentage $\frac{\lambda_i}{\sum_{j=1}^p \lambda_j}$ explains the importance of the new variable \tilde{x}_i
- Given a threshold t , we can choose the number of variables r such that the total contribution to the variance of the new r variables $\sum_{i=1}^r \frac{\lambda_i}{\sum_{j=1}^p \lambda_j}$ exceeds the threshold t . Thus these r directions $\mathbf{w}_1, \dots, \mathbf{w}_r$ are enough to represent the original n variables
- For any random vector $\mathbf{x} \in \mathbb{R}^p$, the corresponding r principal components are thus $\mathbf{w}_1^T \mathbf{x}, \dots, \mathbf{w}_r^T \mathbf{x}$

Another Viewpoint - Best Reconstruction

- Note that the new basis $\{\tilde{\mathbf{e}}_j\}_{j=1}^p$ is given by $\tilde{\mathbf{e}}_j = \mathbf{w}_j$;
- After the projection (if we keep the first r components), the projected point of each sample \mathbf{x}_i is $\tilde{x}_{i,1}\mathbf{w}_1 + \cdots + \tilde{x}_{i,r}\mathbf{w}_r$, where the coordinate is given by $\tilde{x}_{i,j} = \mathbf{w}_j^T \mathbf{x}_i$;
- The reconstruction error is the sum of all squared L^2 errors of all samples :

$$\begin{aligned}
 RE(W) &= \sum_{i=1}^n \left\| \sum_{j=1}^r \tilde{x}_{i,j} \mathbf{w}_j - \mathbf{x}_i \right\|_2^2 = \sum_{i=1}^n \left\| (W_r W_r^T - I) \mathbf{x}_i \right\|_2^2 \\
 &= \sum_{i=1}^n \mathbf{x}_i^T (I - W_r W_r^T) \mathbf{x}_i = \text{Tr} \left(\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T (I - W_r W_r^T) \right) \\
 &= \text{Tr}(X^T X (I - W_r W_r^T)) = \text{Tr}(X^T X) - \text{Tr}(W_r^T X^T X W_r)
 \end{aligned}$$

- Resulting in an optimization problem :

$$\min_{W_r} -\text{Tr}(W_r^T X^T X W_r), \quad \text{subject to } \underline{W_r^T W_r = I}$$

but $W_r^T W_r \neq I$.

PCA Algorithm

- Given the data matrix $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)^T \in \mathbb{R}^{n \times p}$ and a threshold t (in some other cases, the number of principal components r) :
 1. Centralize the data by their mean $\bar{\mathbf{x}} = \frac{1}{n} \mathbf{1}_n^T X$, and compute the sample covariance matrix $C = \frac{1}{n-1} (X - \mathbf{1}_n \bar{\mathbf{x}}^T)^T (X - \mathbf{1}_n \bar{\mathbf{x}}^T)$
 2. Compute the eigenvalues $\{\lambda_i\}_{i=1}^p$ and the corresponding eigenvectors $\{\mathbf{w}_i\}_{i=1}^p$
 3. Order the eigenvalues as $\lambda_{(1)} \geq \dots \geq \lambda_{(p)}$, and compose an orthogonal matrix W by the eigenvectors columnwise in the same order : $W = (\mathbf{w}_1, \dots, \mathbf{w}_p)$
 4. Compute the variance contribution of the first r eigenvalues : $\sum_{i=1}^r \frac{\lambda_i}{\sum_{j=1}^p \lambda_j}$, find a suitable r such that this variance contribution is greater than the threshold t
 5. Pick the first r columns in W and form a matrix $W_r = (\mathbf{w}_1, \dots, \mathbf{w}_r) \in \mathbb{R}^{p \times r}$
 6. Output $\tilde{X}_r = XW_r \in \mathbb{R}^{n \times r}$ as the projected data matrix, whose rows consist of data points in r dimensional subspace

An Example

- The data : the monthly prices of three brands of vehicles (Jeep : x_1 , Toyota : x_2 , Benz : x_3)
- The the covariance matrix is given by

$$C = \begin{pmatrix} 1 & \frac{2}{\sqrt{10}} & -\frac{2}{\sqrt{10}} \\ \frac{2}{\sqrt{10}} & 1 & -\frac{4}{5} \\ -\frac{2}{\sqrt{10}} & -\frac{4}{5} & 1 \end{pmatrix}$$

- Compute the characteristic polynomial :

$$\det(\lambda I - C) = \begin{vmatrix} \lambda - 1 & -\frac{2}{\sqrt{10}} & \frac{2}{\sqrt{10}} \\ -\frac{2}{\sqrt{10}} & \lambda - 1 & \frac{4}{5} \\ \frac{2}{\sqrt{10}} & \frac{4}{5} & \lambda - 1 \end{vmatrix}$$

- Solve for the eigenvalues : $\lambda_1 = 2.38$, $\lambda_2 = 0.42$, $\lambda_3 = 0.2$

An Example (Cont')

- Plug in each eigenvalues and solve for the corresponding eigenvectors, e.g., $(\lambda_1 I - C)\mathbf{w}_1 = \mathbf{0}$, or equivalently,

$$\begin{cases} 1.38w_{11} - \frac{2}{\sqrt{10}}w_{12} + \frac{2}{\sqrt{10}}w_{13} &= 0, \\ -\frac{2}{\sqrt{10}}w_{11} + 1.38w_{12} + 0.8w_{13} &= 0, \\ \frac{2}{\sqrt{10}}w_{11} + 0.8w_{12} + 1.38w_{13} &= 0. \end{cases}$$

- One can find three eigenvectors as $\mathbf{w}_1 = (0.54, 0.59, -0.59)^T$, $\mathbf{w}_2 = (0.84, -0.39, 0.39)^T$, $\mathbf{w}_3 = (0, 0.71, 0.71)^T$
- The three components are

$$\tilde{x}_1 = \mathbf{w}_1^T \mathbf{x} = 0.54x_1 + 0.59x_2 - 0.59x_3,$$

$$\tilde{x}_2 = \mathbf{w}_2^T \mathbf{x} = 0.84x_1 - 0.39x_2 + 0.39x_3,$$

$$\tilde{x}_3 = \mathbf{w}_3^T \mathbf{x} = 0.71x_2 + 0.71x_3.$$

- As $\lambda_1 \gg \lambda_2, \lambda_3$, the first principal component \tilde{x}_1 reflects the change of prices in all three brands of vehicles

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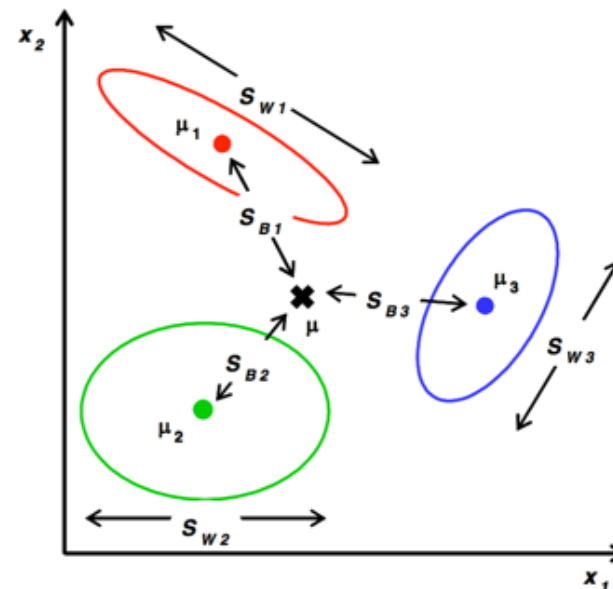
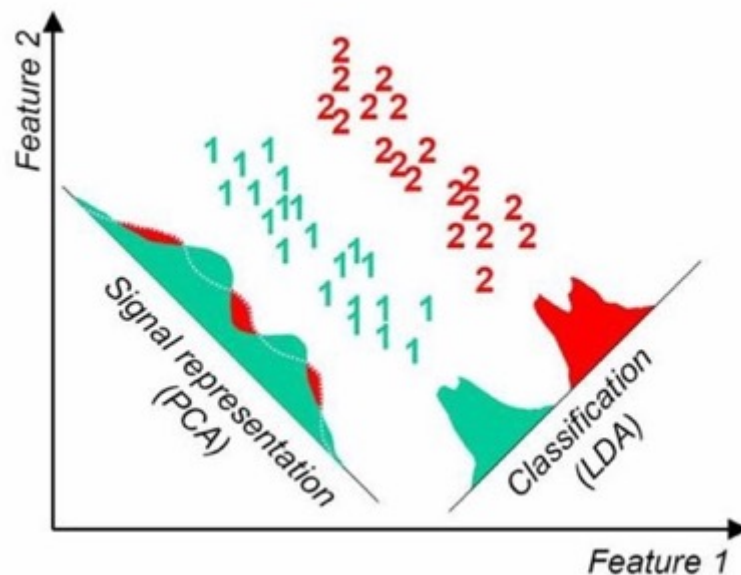
Linear Discriminant Analysis

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Linear Discriminant Analysis (LDA)

- Supervised learning : based on the labels, do linear projection in order to maximize the between-class point scatter (variability) in low dimensions
- Initially proposed by R. Fisher for two-class classification (1936)
- Generalized by C. R. Rao (1948) to K classes $\{C_1, \dots, C_K\}$



Basic Concepts

- The number of samples in each class is $n_k = \sum_{i:\mathbf{x}_i \in C_k} 1$, whereas the total number of samples is $n = \sum_{k=1}^K n_k$
- The mean of samples in class k is $\mu_k = \frac{1}{n_k} \sum_{i:\mathbf{x}_i \in C_k} \mathbf{x}_i$, whereas the mean of all samples is $\mu = \sum_{k=1}^K \frac{n_k}{n} \mu_k$
- Before projection, the between-class point scatter is $S_b = \sum_{k=1}^K \frac{n_k}{n} (\mu_k - \mu)(\mu_k - \mu)^T$; after projection $W_r \in \mathbb{R}^{p \times r}$, the between-class point scatter is $\tilde{S}_b = W_r^T S_b W_r$
- Before projection, the within-class point scatter (variance) for each class C_k is $S_k = \frac{1}{n_k} \sum_{i:\mathbf{x}_i \in C_k} (\mathbf{x}_i - \mu_k)(\mathbf{x}_i - \mu_k)^T$, thus the total within-class point scatter is $S_w = \sum_{k=1}^K \frac{n_k}{n} S_k$; after projection, the within-class point scatter for each class C_k is $\tilde{S}_k = W_r^T S_k W_r$, and the total within-class point scatter is $\tilde{S}_w = W_r^T S_w W_r$

Optimization Problem

- Need to find the optimal directions (columns of W_r) such that the between-class point scatter \tilde{S}_b is maximized and within-class point scatter \tilde{S}_w is minimized, i.e.,

$$\max_{\mathbf{w}} J(\mathbf{w}) = \frac{\mathbf{w}^T S_b \mathbf{w}}{\mathbf{w}^T S_w \mathbf{w}}$$

- This is equivalent to solve

$$\max_{\mathbf{w}} J_b(\mathbf{w}) = \mathbf{w}^T S_b \mathbf{w}, \quad \text{subject to} \quad \mathbf{w}^T S_w \mathbf{w} = 1$$

- By introducing a Lagrange multiplier λ , we define Lagrangian as $L(\mathbf{w}, \lambda) = \mathbf{w}^T S_b \mathbf{w} - \lambda(\mathbf{w}^T S_w \mathbf{w} - 1)$
- The optima is obtained as the solution to the equation

$$\nabla_{\mathbf{w}} L = 2S_b \mathbf{w} - 2\lambda S_w \mathbf{w} = \mathbf{0} \quad \Rightarrow \quad S_w^{-1} S_b \mathbf{w} = \lambda \mathbf{w}$$

- The optimal directions are the eigenvectors of $S_w^{-1} S_b$

An Example

- Given two sets of data : class 1 is $\{(4, 1)^T, (2, 4)^T, (2, 3)^T, (3, 6)^T, (4, 4)^T\}$, and class 2 is $\{(9, 10)^T, (6, 8)^T, (9, 3)^T, (8, 7)^T, (10, 8)^T\}$
- Class means : $\mu_1 = (3, 3.6)^T$, $\mu_2 = (8.4, 7.6)^T$, the point scatter metrics are

$$S_1 = \begin{pmatrix} 0.8 & -0.4 \\ -0.4 & 2.6 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 1.84 & -0.28 \\ -0.28 & 5.36 \end{pmatrix},$$

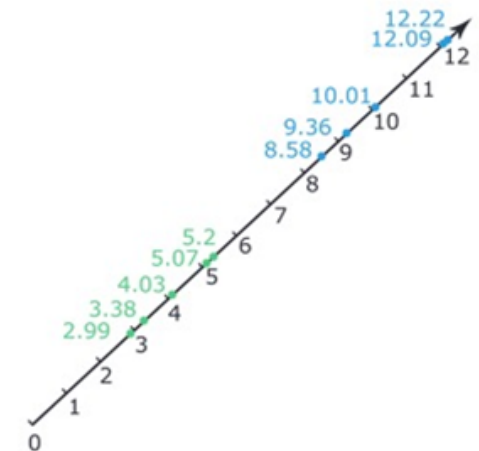
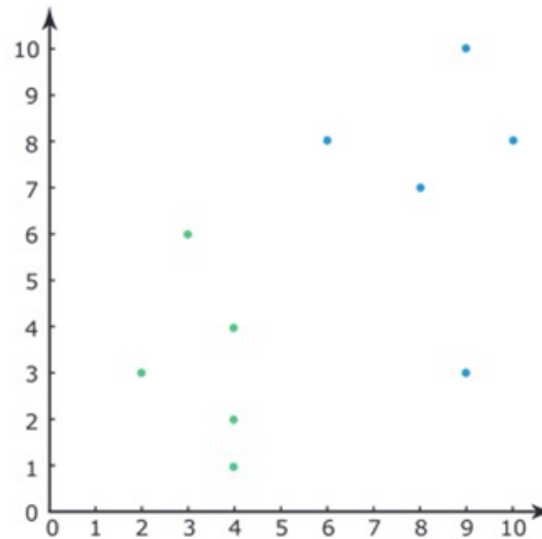
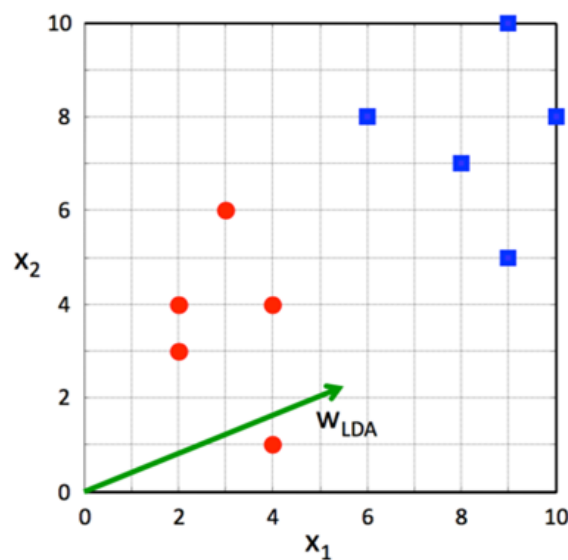
$$S_b = \begin{pmatrix} 7.29 & 4.86 \\ 4.86 & 3.24 \end{pmatrix}, \quad S_w = \begin{pmatrix} 1.32 & -0.34 \\ -0.34 & 4 \end{pmatrix}.$$

- The eigenvalue of $S_w^{-1}S_b$ is solved from

$$0 = \det(\lambda I - S_w^{-1}S_b) = \begin{vmatrix} \lambda - 5.97 & -3.98 \\ -1.72 & \lambda - 1.15 \end{vmatrix} \Rightarrow \lambda = 7.11$$

An Example (Cont')

- The optimal directions is $\mathbf{w}^* = (0.96, 0.28)^T$
- After projection, the data become 1D :
 - Class 1 : {4.12, 3.03, 2.75, 4.55, 4.95}
 - Class 2 : {11.42, 7.98, 9.48, 9.63, 11.83}



PCA vs. LDA

Rk: 都是线性降维

- PCA
 - Start from sample covariance matrix and find directions with maximal variances
 - Unsupervised learning, used as pre-training step, must be coupled with other learning methods
- LDA
 - Make use of labels and find projections after which the classification becomes more obvious
 - Supervised learning, can be used as classification or coupled with other learning methods

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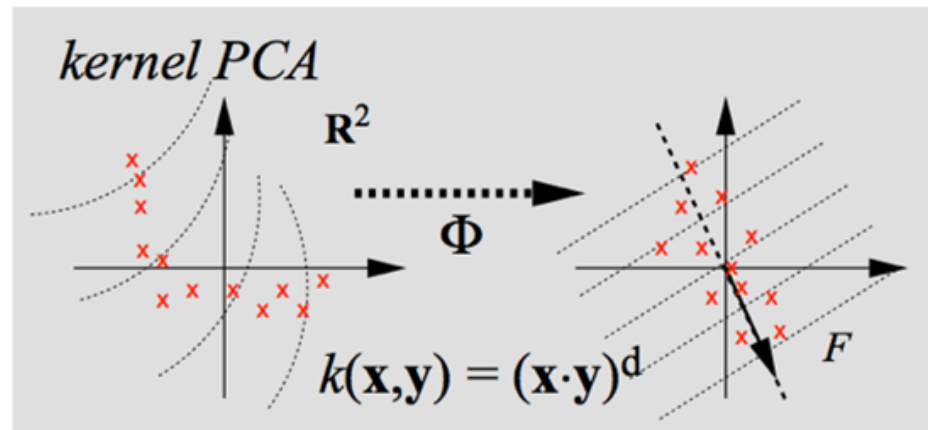
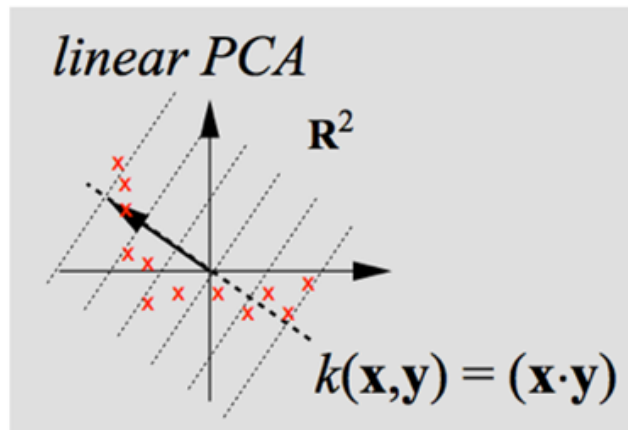
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Kernel PCA

- PCA works well for Gaussian distribution
- If the data do not follow Gaussian, we can find a map $\phi : \mathbb{R}^p \rightarrow \mathbb{R}^q$ so that $\phi(\mathbf{x})$ (almost) follows Gaussian
- We can do PCA for the transformed data $\{\phi(\mathbf{x}_i)\}_{i=1}^n$
- Similar to nonlinear SVM, kernel trick can be used to avoid explicit computation of ϕ



Covariance Matrix in Transformed Space

- Assume the transformed data are centralized :

$$\mu = \frac{1}{n} \sum_{i=1}^n \phi(\mathbf{x}_i) = 0$$

- Covariance Matrix $\tilde{C} = \frac{1}{n-1} \sum_{i=1}^n \phi(\mathbf{x}_i) \phi(\mathbf{x}_i)^T$

- Do PCA for transformed data is equivalent to find the eigenvalues and eigenvectors of \tilde{C}

- Let λ be an eigenvalue of \tilde{C} and $\mathbf{v} \in \mathbb{R}^q$ be the corresponding eigenvector, i.e., $\tilde{C}\mathbf{v} = \lambda\mathbf{v}$.

- It can be shown that $\mathbf{v} = \sum_{i=1}^n \alpha_i \phi(\mathbf{x}_i)$ where $\alpha_i = \frac{1}{\lambda(n-1)} \phi(\mathbf{x}_i)^T \mathbf{v}$

- Furthermore, $\alpha_i = \frac{1}{\lambda(n-1)} \sum_{j=1}^n K(\mathbf{x}_i, \mathbf{x}_j) \alpha_j$, where

$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ is kernel function

- It is sufficient to solve the eigenvalue problem :

$K\alpha = \lambda(n-1)\alpha$ where $K = (K(\mathbf{x}_i, \mathbf{x}_j))_{i,j}$ is kernel matrix and

$\alpha = (\alpha_i)$ is the coefficient vector of \mathbf{v}

$$\tilde{C}\vec{v} = \frac{1}{n-1} \sum_{i=1}^n \phi(\vec{x}_i) \frac{\phi(\vec{x}_i)^T \vec{v}}{(1 \times n) \times (n \times 1)} = \frac{1}{n-1} \sum_{i=1}^n \phi(\vec{x}_i)^T \vec{v} \phi(\vec{x}_i)$$

承似成立. $\exists \phi$ st 可以有张量能力.

$$\lambda \vec{v} = \sum_{i=1}^n \lambda \alpha_i \phi(\vec{x}_i)$$

$$\tilde{C}\vec{v} = \lambda \vec{v} : \text{张量分解}$$

$$\alpha_i = \frac{1}{\lambda(n-1)} \phi(\vec{x}_i)^T \vec{v}$$

$$\Rightarrow \alpha_i = \frac{1}{\lambda(n-1)} \sum_{j=1}^n \alpha_j \phi(\vec{x}_i)^T \phi(\vec{x}_j)$$

$$\Leftrightarrow \vec{\alpha} = \frac{1}{\lambda(n-1)} K(\vec{x}_i, \vec{x}_j) \cdot \vec{\alpha}$$

Kernel PCA Algorithm

1. Choose a kernel function $K(x, y)$ satisfying the necessary properties
2. Compute the kernel matrix $K = (K(\mathbf{x}_i, \mathbf{x}_j))_{i,j}$
3. Compute the eigenvalues $\lambda_1 \geq \dots \geq \lambda_q$ and eigenvectors $\alpha^{(1)}, \dots, \alpha^{(q)}$ of K
4. For any new sample \mathbf{x} , the j component after projection is

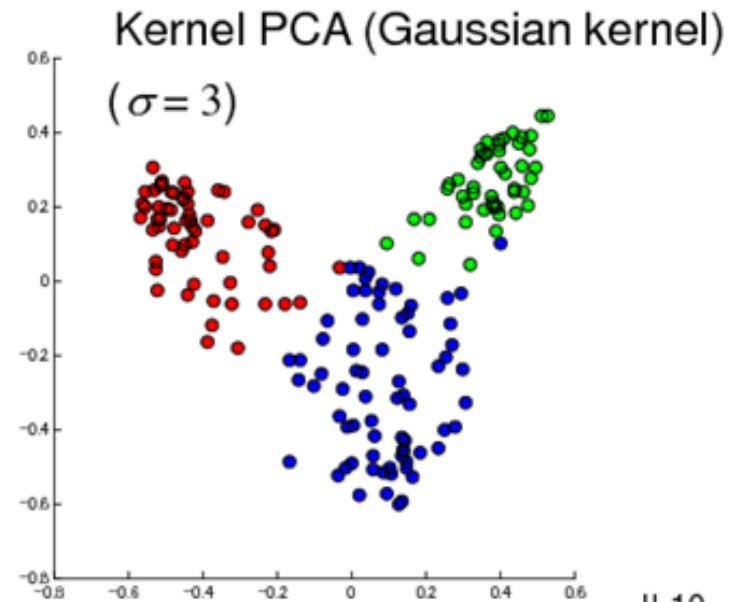
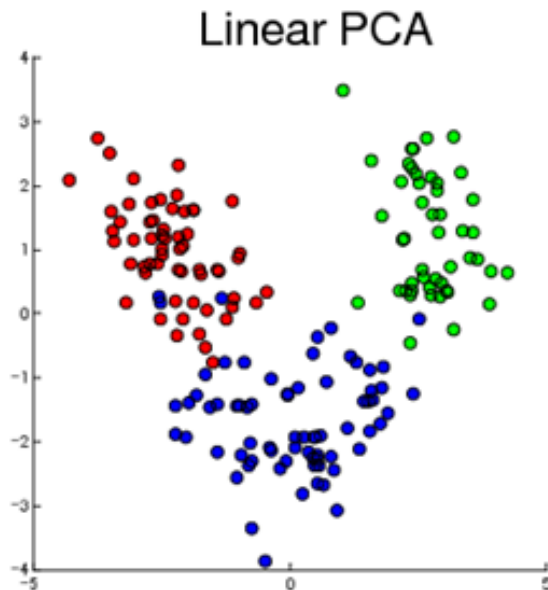
$$z_j = \mathbf{v}_j^T \phi(\mathbf{x}) = \sum_{i=1}^n \alpha_i^{(j)} K(\mathbf{x}_i, \mathbf{x})$$

Kernel PCA : An Example

■ Wine data (from UCI repository)

13 dim. chemical measurements of for three types of wine. 178 data.
Class labels are **NOT** used in PCA, but shown in the figures.

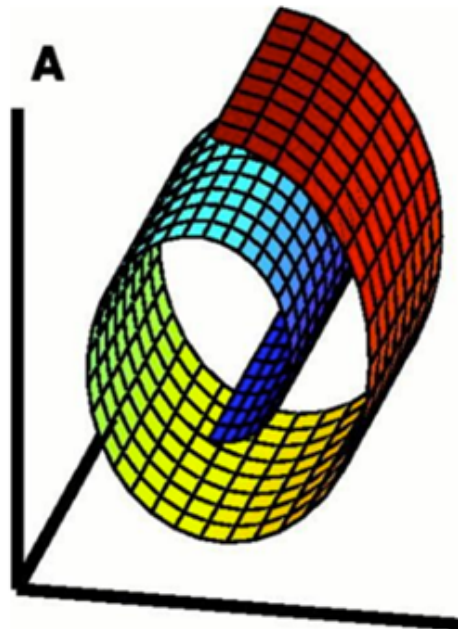
First two principal components:



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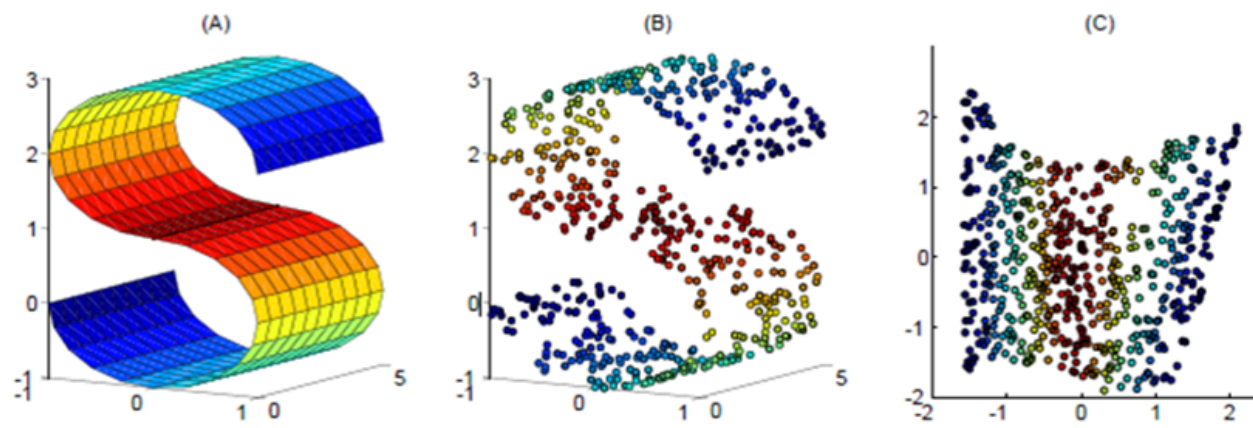
Manifolding Learning

- A manifold is a topological space that locally resembles Euclidean space near each point. It generalizes the concepts of curves and surfaces in Euclidean space.
- The dimension of a manifold is the minimal number of coordinates to represent a point on the manifold
- Some dimensionality reduction methods are based on the concept of manifold : ISOMAP, LLE, MDS, t-SNE



Locally Linear Embedding (LLE)

- Reduce the number of free coordinates while keeping the local geometric structure of the data, e.g., if \mathbf{x}_A and \mathbf{x}_B are neighbor in high dimension, after the dimension reduction (transformation), they must be close to each other in low dimension
- The clustering effect should also be inherited



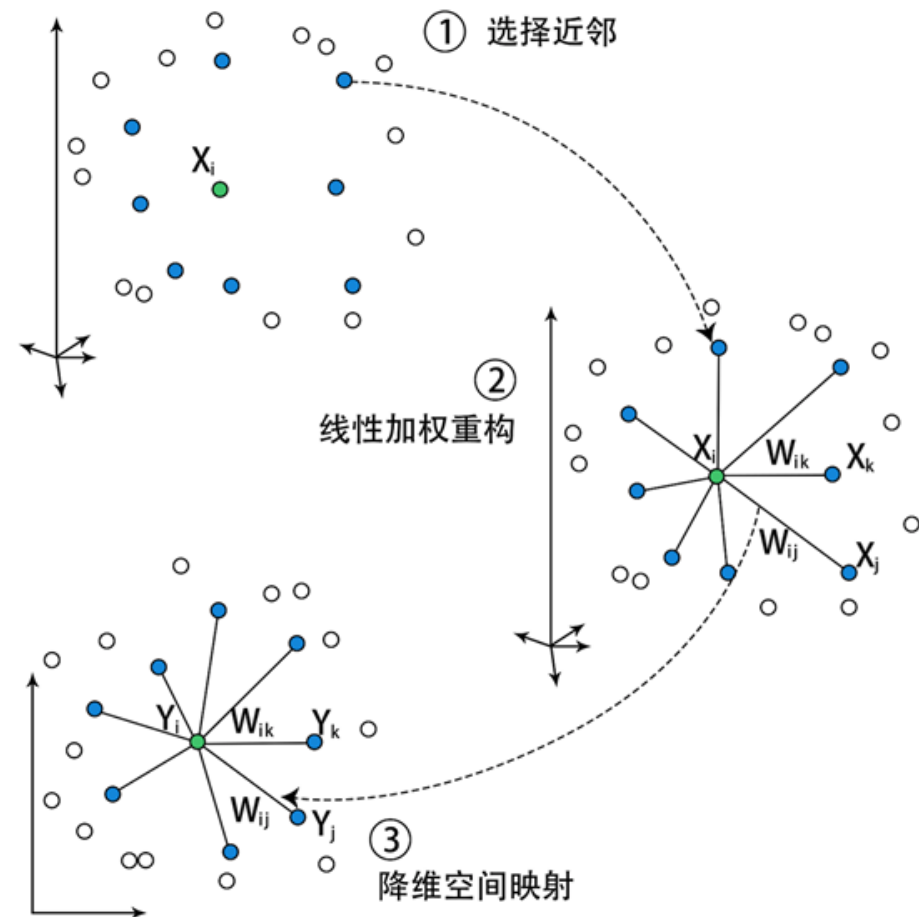
LLE Reconstruction

- Assume each data point is locally linearly dependent of its neighbors : it can be written as the linear combination of its K nearest neighbors $\{\mathbf{x}_{k_{ij}}\}_{j=1}^K$, with the KNN indices $\{k_{ij}\}_{j=1}^K$
- The weight is determined by the optimization for each \mathbf{x}_i :

$$\min_{\mathbf{w}} \left\| \mathbf{x}_i - \sum_{j=1}^K w_{ik_{ij}} \mathbf{x}_{k_{ij}} \right\|_2^2$$

$$\text{subject to } \sum_{j=1}^K w_{ik_{ij}} = 1, \quad w_{ij} \geq 0$$

where $w_{ij} = 0$ if $j \notin \{k_{ij}\}_{j=1}^K$



Low Dimensional Representation

- In r ($r < p$) dimensional space, find n points such that the local structure (e.g., clustering effect) is preserved

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \sum_{i=1}^n \left\| \mathbf{y}_i - \sum_{j=1}^n w_{ij} \mathbf{y}_j \right\|_2^2$$

- This is equivalent to the matrix minimization problem

$$\min_{\mathbf{Y}} \text{Tr}(\mathbf{Y}^T \mathbf{M} \mathbf{Y}), \quad \text{s.t.} \quad \mathbf{Y} \mathbf{Y}^T = \mathbf{I},$$

where $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_n)^T \in \mathbb{R}^{n \times r}$ and $\mathbf{M} = (\mathbf{I} - \mathbf{W})^T (\mathbf{I} - \mathbf{W})$ with $\mathbf{W} = (w_{ij})_{i,j=1}^n$ being the weight matrix (not necessarily symmetric)

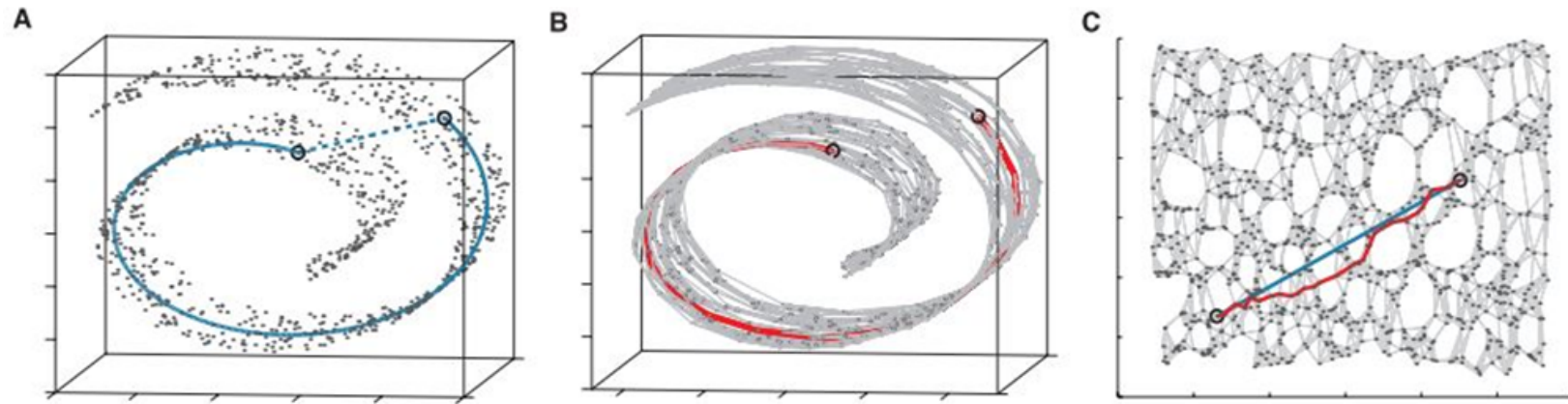
- This is solved by eigen-decomposition : The columns of \mathbf{Y} consist of the r eigenvectors corresponding to the r smallest eigenvalues of \mathbf{M}

Summary of LLE

- Only one tuning parameter K
- Linear algebra computation
- Only local information, no global information
- No explicit mapping as in PCA ($\tilde{X}_r = XW_r$)

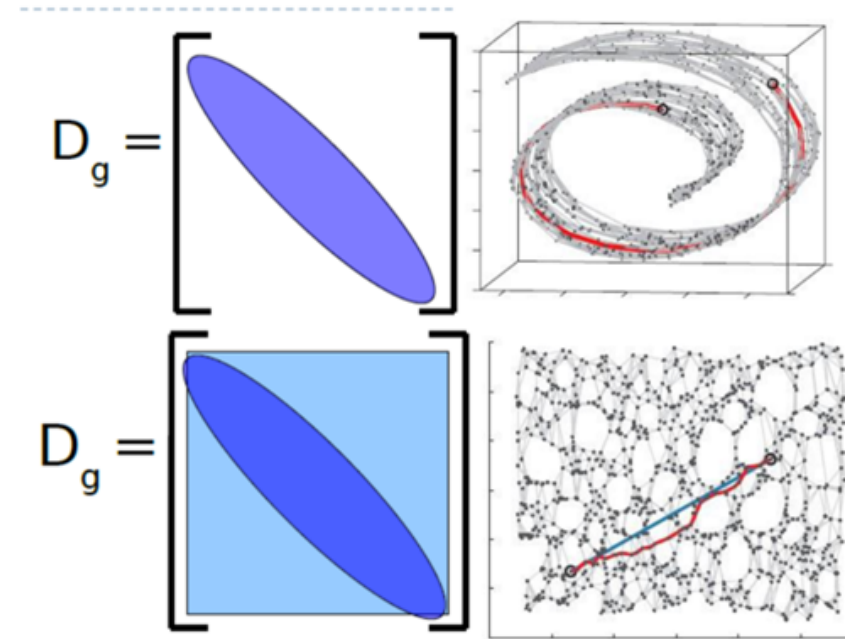
The Motivation of ISOMAP

- The distance between two points may be different in different metrics (manifold metric vs. Euclidean metric)
- Geodesic distance could be a good metric instead of Euclidean distance
- Computation of geodesic distance, minimal path in graph



ISOMAP Algorithm

- Construct KNN graph $G = (V, E)$:
 - For each \mathbf{x}_i , find its K nearest neighbors $\{\mathbf{x}_j\}_{j \in N(i)}$
 - The weight of the edge $\langle i, j \rangle$ between \mathbf{x}_i and \mathbf{x}_j is the Euclidean distance for each $j \in N(i)$
- Use Floyd algorithm to compute the minimal path between each pair of vertices (i, j) as the geodesic distance $d_G(i, j)$
- Find the low dimensional representation (e.g. by MDS) :



$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \sum_{i \neq j} (d_G(i, j) - \|\mathbf{y}_i - \mathbf{y}_j\|)^2$$

将d(i,j)换成d_G(i,j) : 高维空间中的距离可能出现问题

Floyd Algorithm (Complexity $O(n^3)$)

1. Initialization :

$$d_G(i, j) = \begin{cases} d_x(i, j), & \text{if } \langle i, j \rangle \in E \\ \infty, & \text{otherwise} \end{cases}$$

2. For each pair (i, j) , update the distance as follows : for each $k = 1, \dots, n$, $d_G(i, j) = \min\{d_G(i, j), d_G(i, k) + d_G(k, j)\}$
3. The final output $d_G(i, j)$ is the geodesic distance between i and j

Summary of ISOMAP

- Only one tuning parameter K
- High computational power
- Preserve the global information
- Sensitive to noise

Multidimensional Scaling (MDS)

- For data points in high dimensional space, $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^p$, find the distance or dissimilarity matrix $\{d_{ij}\}_{i,j}^n$, e.g.,

$$d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$$
- Find $\{\mathbf{y}_i\}_{i=1}^n \subset \mathbb{R}^r$ ($r < p$), such that the distance information is preserved :

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} S_M(\mathbf{y}_1, \dots, \mathbf{y}_n)$$

where $S_M(\mathbf{y}_1, \dots, \mathbf{y}_n) = \sum_{i \neq j} (d_{ij} - \|\mathbf{y}_i - \mathbf{y}_j\|)^2$ is the stress function. This is called least square or Kruskal-Shephard scaling

- Alternative objective function (Sammon mapping) :

$$S_{S_M}(\mathbf{y}_1, \dots, \mathbf{y}_n) = \sum_{i \neq j} \frac{(d_{ij} - \|\mathbf{y}_i - \mathbf{y}_j\|)^2}{d_{ij}}$$
 takes care of small d_{ij}
- This is nonconvex minimization

t-distributed Stochastic Neighbor Embedding (t-SNE)

- Developed by Laurens van der Maaten and Geoffrey Hinton
- Effective for data visualization in 2D and 3D, applications in computer security research, music analysis, cancer research, especially for bioinformatic data
- Often display clusters in low dimensional space (may be false findings)
- With special parameter choices, approximates a simple form of spectral clustering

Similarity in High Dimensional Space

- For data points in high dimensional space, $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^p$, find the similarity of \mathbf{x}_i and \mathbf{x}_j in the form of probability p_{ij}
- The similarity of data point x_j to data point x_i is the conditional probability, $p_{j|i}$, that x_j would pick x_i as its neighbor if neighbors were picked in proportion to their probability density under a Gaussian centered at x_i :

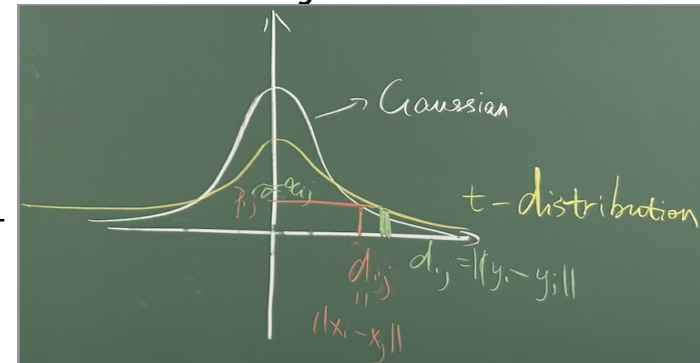
$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$$

- $p_{ij} = (p_{j|i} + p_{i|j}) / 2n$, $p_{ii} = 0$
- The bandwidth is adapted to the density of the data : smaller values of σ_i are used in denser parts of the data space

Similarity in Low Dimensional Space

- t-SNE aims to learn a set of low dimensional data $\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^r$ that reflects the similarity p_{ij} as well as possible
- The similarity between the data point \mathbf{y}_i and \mathbf{y}_j follows t-distribution : (assume $q_{ii} = 0$)

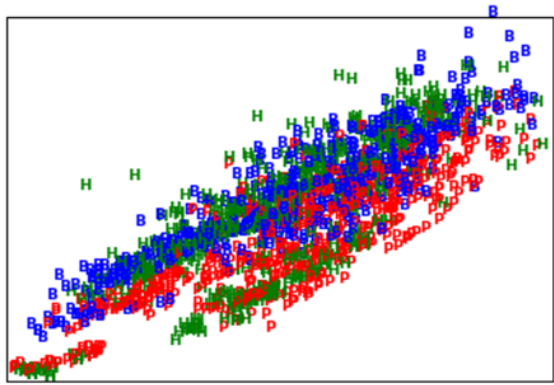
$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$



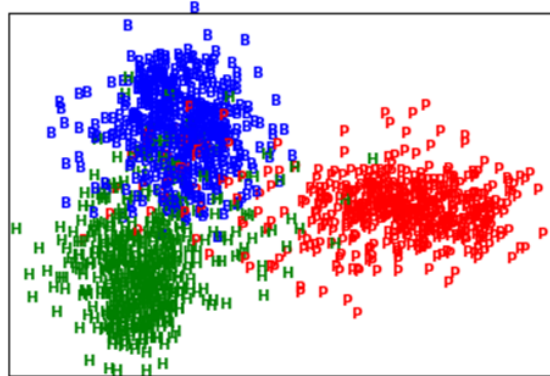
- t-distribution is heavy tailed so that large p_{ij} (dissimilar data pair) leads to even larger q_{ij} (falls apart)
- The closedness between the two similarity measures p_{ij} and q_{ij} is given by the Kullback-Leibler divergence :

$$D_{KL}(P \| Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

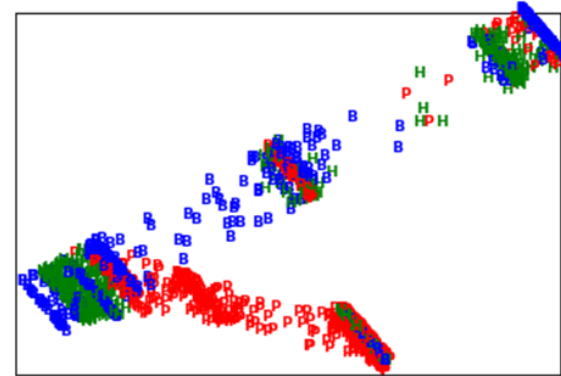
Comparison (Optical Character Recognition)



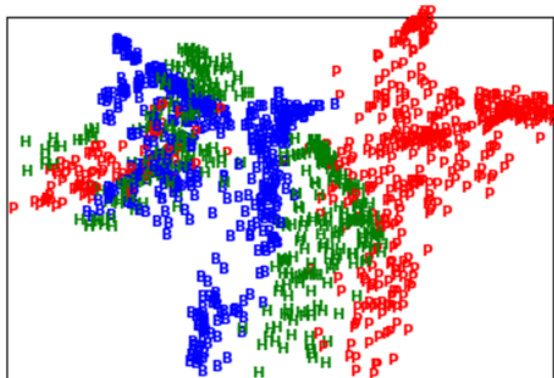
PCA



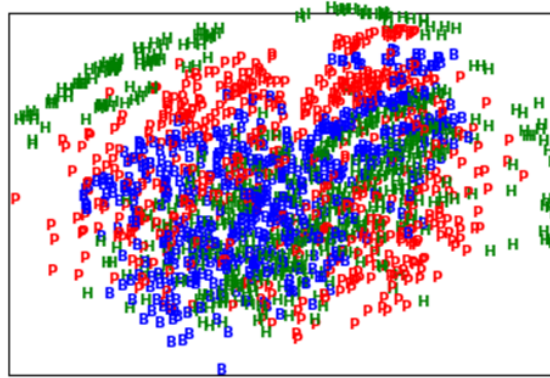
LDA



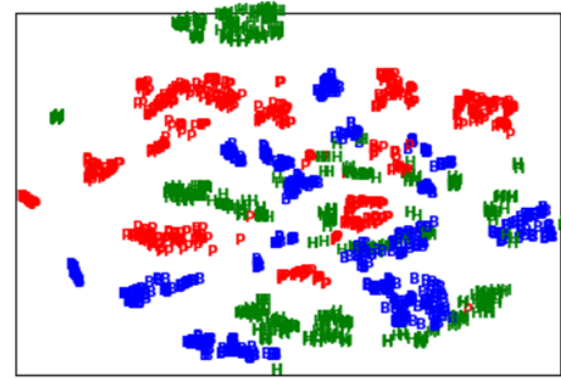
LLE



ISOMAP



MDS



t-SNE

Outlines

Introduction

Principal Component Analysis

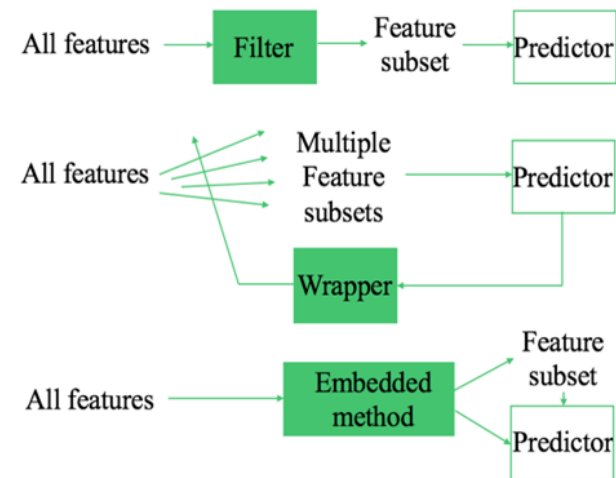
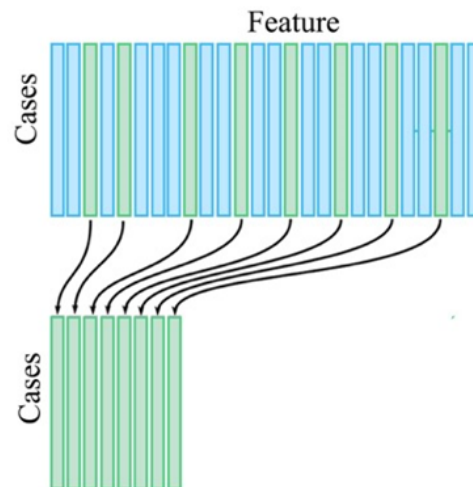
Linear Discriminant Analysis

Nonlinear Dimensionality Reduction

Feature Selection

What is Feature Selection

- Low computational cost, better accuracy (avoid overfitting), and better interpretation,
- Feature engineering : feature extraction and selection. Feature extraction is according to the knowledge of the professions, usually done by expertise in the professional areas
- Three types : Filter, Wrapper, and Embedded



Subset Selection

- Subset search :
 - Forward search (forward stepwise, forward stagewise) :
 $\emptyset \Rightarrow \{x_1\} \Rightarrow \{x_1, x_4\} \Rightarrow \dots$
 - Backward search (backward stepwise) :
 $\{x_1, x_2, \dots, x_p\} \Rightarrow \{x_1, x_2, \dots, x_p\} \setminus \{x_4\} \Rightarrow \dots$
 - Bidirectional search
- Evaluation metrics :
 - Distances : Euclidean, Manhattan, point scatter matrices, Kullback-Leibler divergence, etc.
 - Information : mutual information, information gain (IG), etc.
 - Correlations : Pearson correlation, Maximal information coefficients (MIC)
- Stopping rules : number of features, number of iterations, non-incremental metrics, attaining optimality, etc.
- Validation and comparison

Three Types of Feature Selection

- Filter : filter the features by their correlations (or MIC, IG) with response variables
- Wrapper : use accuracy, precision, recall, AUC, etc.
 - Akaike Information Criteria (AIC) : $AIC = -2 \ln(L) + 2k$
 - Bayes Information Criteria (BIC) : $BIC = -2 \ln(L) + k \ln(n)$
 - Minimize AIC or BIC, where L is likelihood function, k is the number of features (parameters), n is the number of samples
- Embedded :
 - Random forest : feature importance
 - Regularization : Ridge and LASSO
 - Recursive feature elimination (RFE) : select the best (worst) feature according to the coefficients (e.g. linear regression), then do this recursively to find the feature importance

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