Talk 11 Unsupervised Learning

Unsupervised Learning

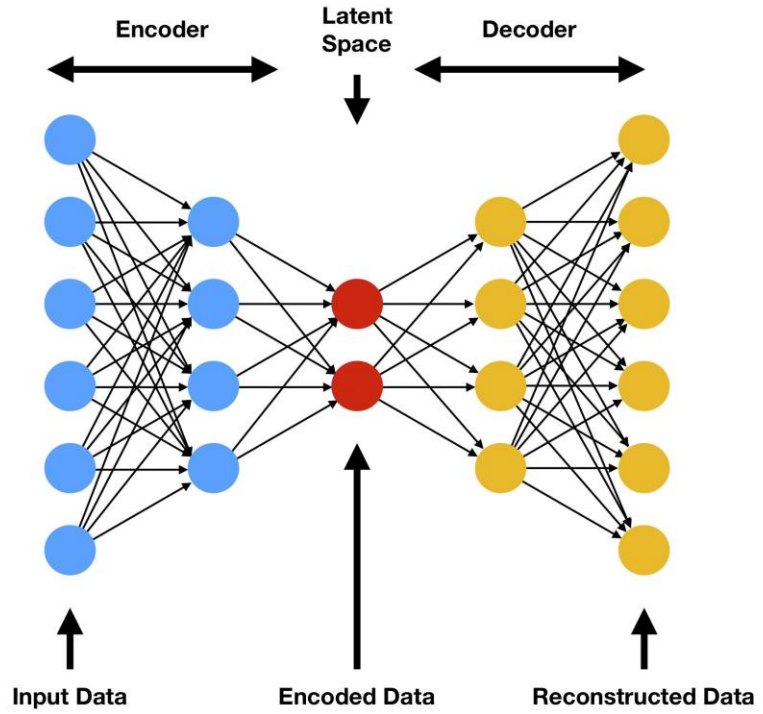
1. Introduction
2. Association Rules & Cluster Analysis
4. Self-Organizing Maps
5. Principal Components, Curves and Surfaces
6. Non-negative Matrix Factorization
7. Independent Component Analysis
8. Multidimensional Scaling
9. Nonlinear Dimension Reduction
10. The Google PageRank Algorithm

Motivation

- Supervised Learning: Large scale of labeled data
- Unsupervised Learning:
  - Latent structures in data: linear or nonlinear
  - Dimension reduction
  - Relations in data
- Semi-supervised learning
- Reinforcement learning

Statistical Learning for real world applications

- Linear dimension reduction
- Domain transform (time-spectral)
- Topic model: Semantic model
- Autoencoder: Mutual information
- Manifold embedding: non-linear dim. reduction
- **Information Bottleneck** for Classification



$$\mathrm{IB}(T) = -I(Y,T) + \beta\, I(T,X)$$

1. Introduction

- *Unsupervised learning* or "learning without a teacher."
- A set of N observations

$$\{x_1, x_2, \cdots, x_N\}, X \in R^p \sim \mathrm{P}(X)$$

- In low-dimensional problems (say p ≤ 3), there are a variety of effective nonparametric methods for directly estimating the density $P(X)$ itself at all X-values
- In high-dimensional problems, one must settle for estimating rather crude global models, such as Gaussian mixtures or various simple descriptive statistics that characterize $P(X)$.

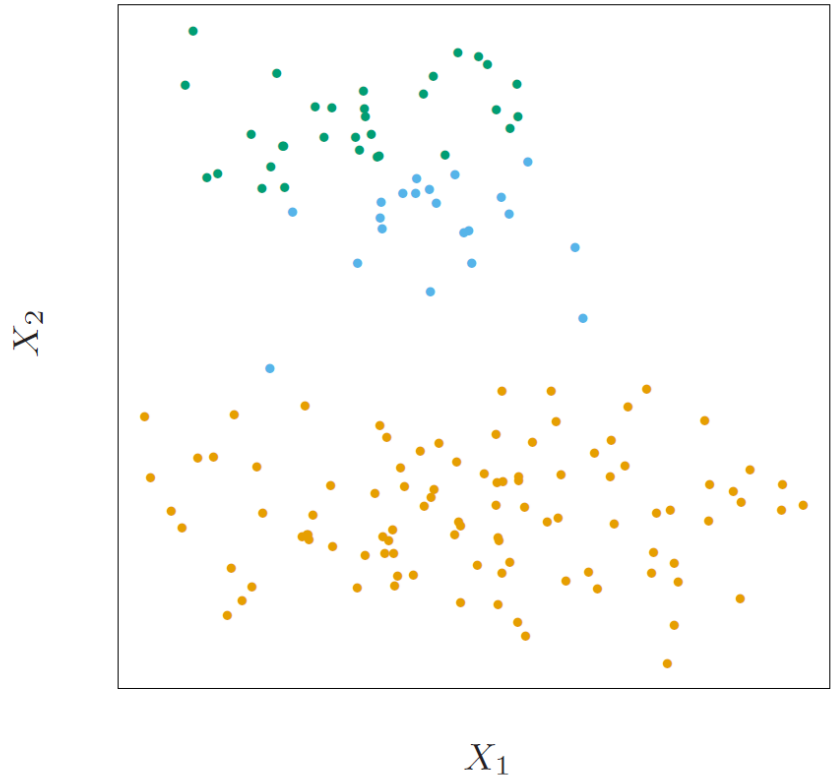
1. Introduction

- **Principal components, multidimensional scaling, self-organizing maps, and principal Curves**
  - To identify low-dimensional manifolds that represent high data density.
  - To find possible functions of a smaller set of “latent” variables.
- **Cluster analysis** attempts to find multiple convex regions of the X-space that contain modes of $Pr(X)$.
  - Whether or not $Pr(X)$ can be represented by a mixture of simpler densities representing distinct types or classes of observations.
- **Association rules** attempt to construct simple descriptions (conjunctive rules) that describe regions of high density in the special case of very high dimensional binary-valued data.

2. Cluster Analysis

- Cluster analysis, also called data segmentation, has a variety of goals.

All relate to grouping or segmenting a collection of objects into subsets or “clusters,” such that those within each cluster are more closely related to one another than objects assigned to different clusters.



2. Cluster Analysis

- Central to all of the goals of cluster analysis is the notion of the degree of similarity(相似值) (or dissimilarity（相异值）) between the individual objects being clustered.
- K-means clustering starts with guesses for three cluster centers.
  - for each data point, the closest cluster center (in Euclidean distance) is identified;
  - each cluster center is replaced by the coordinate-wise average of all data points that are closest to it.

Proximity Matrices

- Dissimilarities can then be computed by averaging over the collection of such judgments.
- Data represented by an $N \times N$ matrix $\boldsymbol{D}$,
  - N is the number of objects,
  - each element $d_{ii'}$ records the proximity between the i_{th} and i'_{th} objects.
- Most algorithms presume a matrix of dissimilarities with nonnegative entries and zero diagonal elements: $d_{ii} = 0, i = 1, 2, \ldots, N$.

Dissimilarities Based on Attributes

- Given measurements on variables

$$x_{ij}, \text{ for } i = 1, 2, \cdots, N, \text{ on vairables (attributes) } j = 1, 2, \cdots, p$$

- Dissimilarity between two objects

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} d(x_{ij}, x_{i'j})$$

- Most common distance

$$d(x_{ij}, x_{i'j}) = (x_{ij} - x_{i'j})^2$$

Dissimilarities Based on Attributes

- Alternatives for the attribute type: Quantitative variables

$$d(x_i, x_{i'}) = l(|x_i - x_{i'}|)$$

$$\rho(x_i, x_{i'}) = \frac{\sum_j (x_{ij} - \bar{x}_i)(x_{i'j} - \bar{x}_{i'})}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2 \sum_j (x_{i'j} - \bar{x}_{i'})^2}}, \quad with \quad \bar{x} = \sum_j x_{ij} / p$$

- If the observations is normalized

$$\sum_j (x_{ij} - x_{i'j})^2 \propto 2(1 - \rho(x_i, x_{i'}))$$

Dissimilarities Based on Attributes

- Alternatives for the attribute type: Ordinal Variables
  - The values of this type of variable are often represented as contiguous integers
  - Examples are academic grades (A, B, C, D, F)
- Error measures for ordinal variables are generally defined by replacing their M original values with

$$\frac{i-1/2}{M}, \quad i=1,\cdots,M$$

Dissimilarities Based on Attributes

- Alternatives for the attribute type: Categorical Variables
  - The degree-of-difference between pairs of values must be delineated explicitly.
- If the variable assumes M distinct values, these can be arranged in a symmetric M ×M matrix with elements

$$L_{rr'} = L_{r'r}, \quad L_{rr} = 0, \quad L_{rr'} \geq 0.$$

- The most common choice

$$L_{rr'} = 1, \text{ for all } r \neq r'$$

Object Dissimilarity

- Dissimilarity $D(x_i, x_{i'})$ between two objects or observations

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} w_j d(x_{ij}, x_{i'j}); \quad \sum_{j=1}^{p} w_j = 1$$

- The average object dissimilarity measure over all pairs of observations in the data set

$$\bar{D} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} D(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \bar{d}_j,$$

$$\bar{d}_j = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} d_j(x_{ij}, x_{i'j})$$

Combinatorial Algorithms

- Assign each observation to a group or cluster without regard to a probability model describing the data.

$$\{x_i\}_{i=1}^{N} \qquad x_i \Rightarrow C(i) = k, k = 1, \ldots, K$$

- The Loss function

$$W(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k} d(x_i, x_{i'})$$

- assigned to the same cluster tend to be close to one another.

Combinatorial Algorithms

- The *total* point scatter

$$\mathrm{T} = \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} d(x_i, x_{i'}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\left(\sum_{C(i')=k} d(x_i, x_{i'}) + \sum_{C(i')\neq k} d(x_i, x_{i'})\right)$$

$$= W(C) + B(C)$$

- Between-Cluster Scatter:

$$\mathrm{B}(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')\neq k} d(x_i, x_{i'})$$

- Minimizing W(C) is equivalent to *maximizing* B(C).

K-means

- The within-point scatter can be written as

$$W(C)=\frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k}d(x_i,x_{i'})$$

$$=\frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k}\left\|x_i-x_{i'}\right\|^2$$

$$=\sum_{k=1}^{K}N_k\sum_{C(i)=k}\left\|x_i-\bar{x}_k\right\|^2$$

where N_k is the sample number of k-th class

K-means

Algorithm 14.1 *K-means Clustering.*

1. For a given cluster assignment C, the total cluster variance (14.33) is minimized with respect to $\{m_1, \ldots, m_K\}$ yielding the means of the currently assigned clusters (14.32).

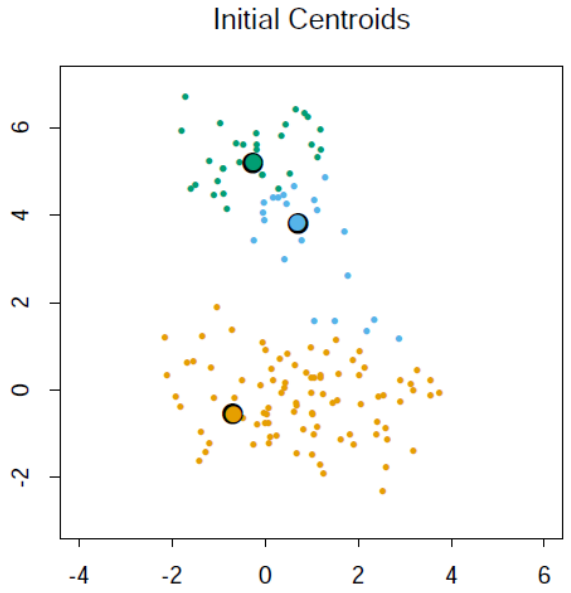
2. Given a current set of means $\{m_1, \ldots, m_K\}$, (14.33) is minimized by assigning each observation to the closest (current) cluster mean. That is,

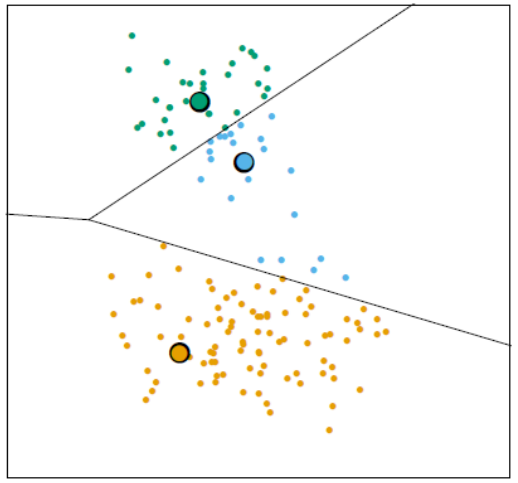
$$C(i) = \underset{1 \le k \le K}{\operatorname{argmin}} ||x_i - m_k||^2. \tag{14.34}$$

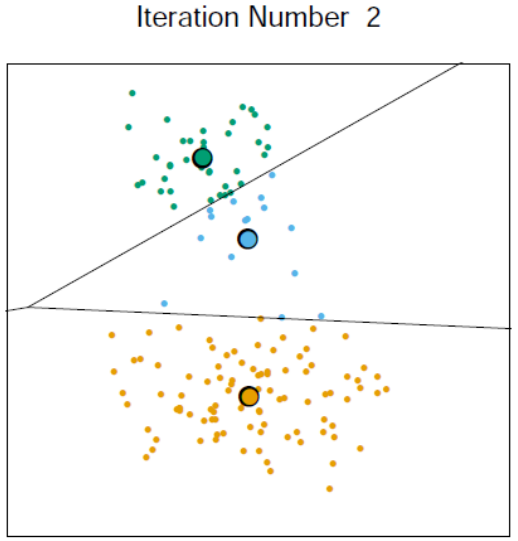
3. Steps 1 and 2 are iterated until the assignments do not change.

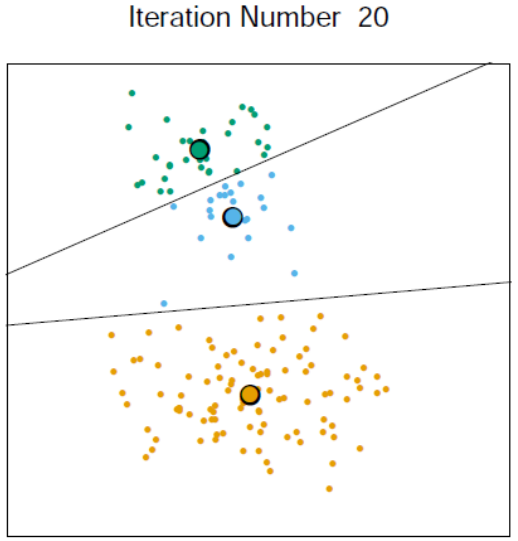
$$\bar{x}_S = \underset{m}{\operatorname{argmin}} \sum_{i \in S} ||x_i - m||^2. \tag{14.32}$$

$$\min_{C, \{m_k\}_1^K} \sum_{k=1} N_k \sum_{C(i)=k} ||x_i - m_k||^2. \tag{14.33}$$


Initial Centroids
6
4
2
0
-2
-4
-2
0
2
4
6


Initial Partition


Iteration Number 2


Iteration Number 20

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14.4 Self-Organizing Maps (SOMs)

Constrained version of K-means (VQ) with prototypes on a **topological map (grid)**

For K prototypes m_j in $\mathbb{R}^p$ placed on a given map

- Find closest m_j of considered x_i
- Move m_j and its neighbors m_k towards x_i

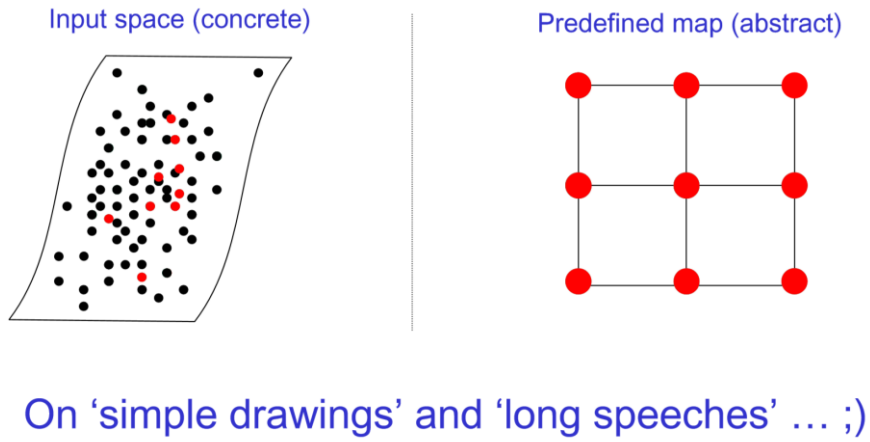
$$m_k = m_k + \alpha(x_i - m_k)$$

Running the algorithm moves the prototypes

inside the input distribution w.r.t. map constrains

l_j is integer pair of prototype m_j;

m_k *is* a set of neighbors of m_j



On ‘simple drawings’ and ‘long speeches’ … ;)

Extended SOMs

l_j is integer pair of prototype m_j; m_k *is* a set of neighbors of m_j

$h(\|l_i - l_k\|)$ is a kernel function

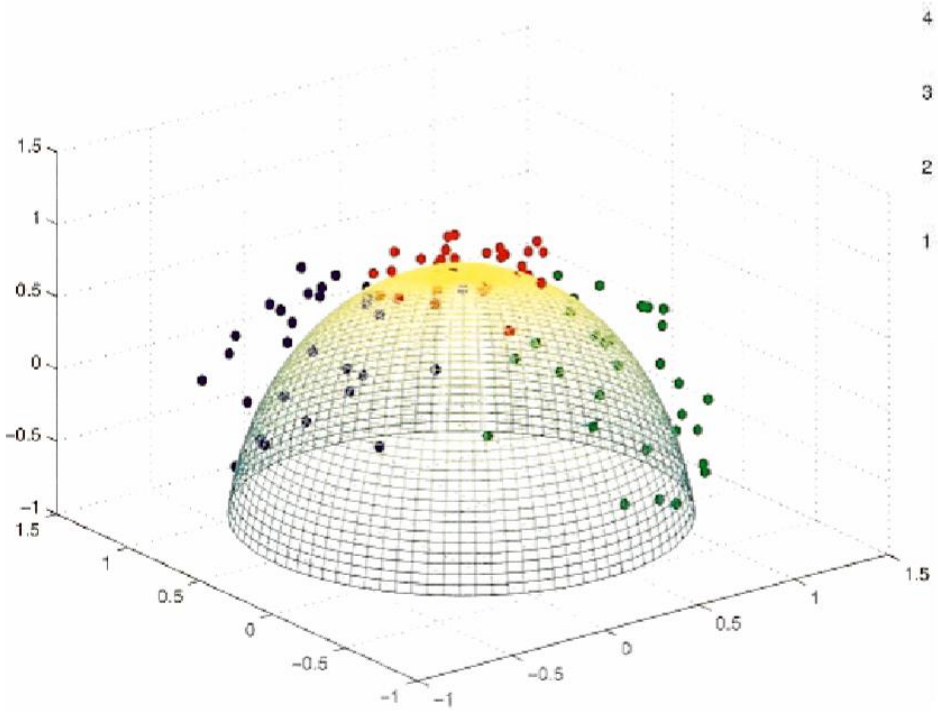
Enhanced version : $m_k = m_k + \alpha h(\|l_i - l_k\|)(x_i - m_k)$

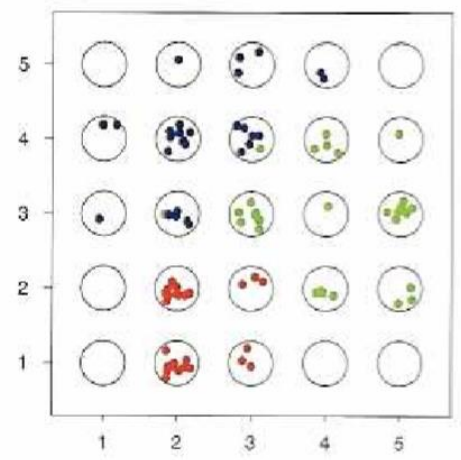
Batch one : $$m_j = \frac{\sum_k w_k x_k}{\sum_k w_k}$$

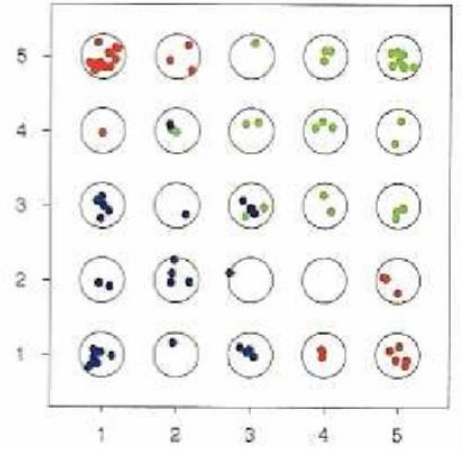
The sum is over points x_k that mapped (i.e., were closest to) neighbors m_k of prototype of m_j

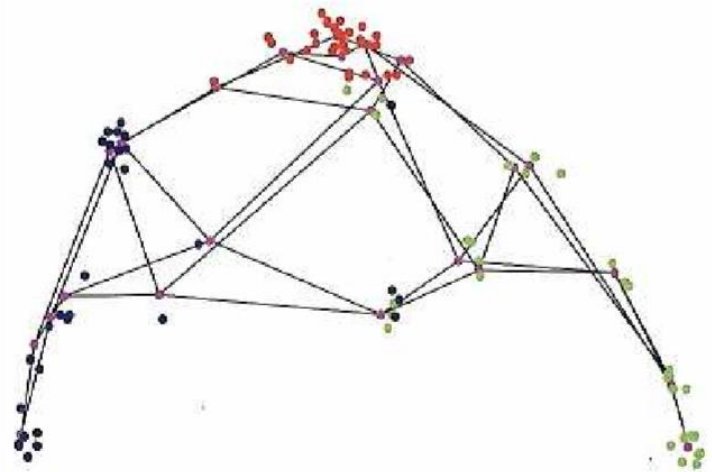
4. Self-Organizing Maps (SOMs)

- Can SOMs separate sphere data ?





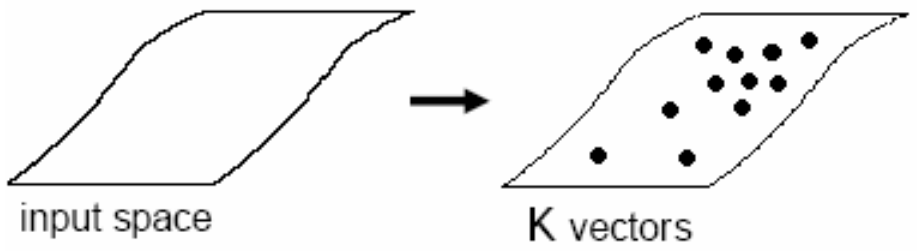




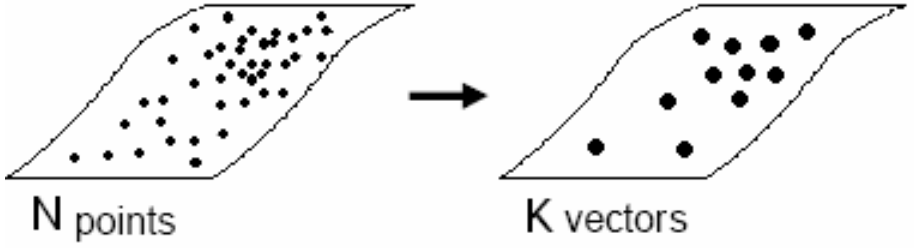
VQ aims to reduce the inputs (K≤N)

Vector Quantization (VQ) from 14.3.9 :

We aim to :

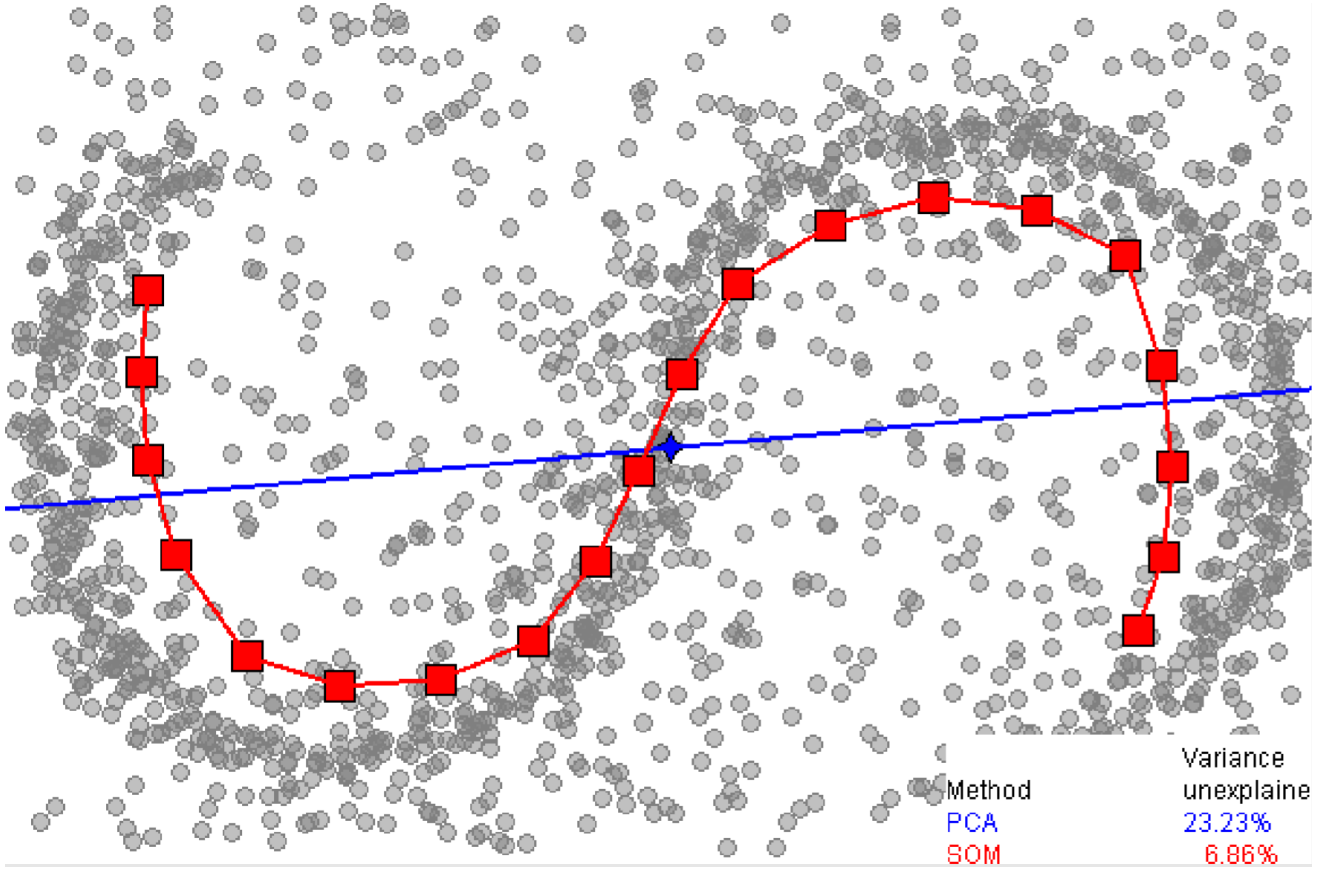


We use :



Neural VQ algorithms are an adaptative (iterated) version of K-means

4. Self-Organizing Maps (SOMs)



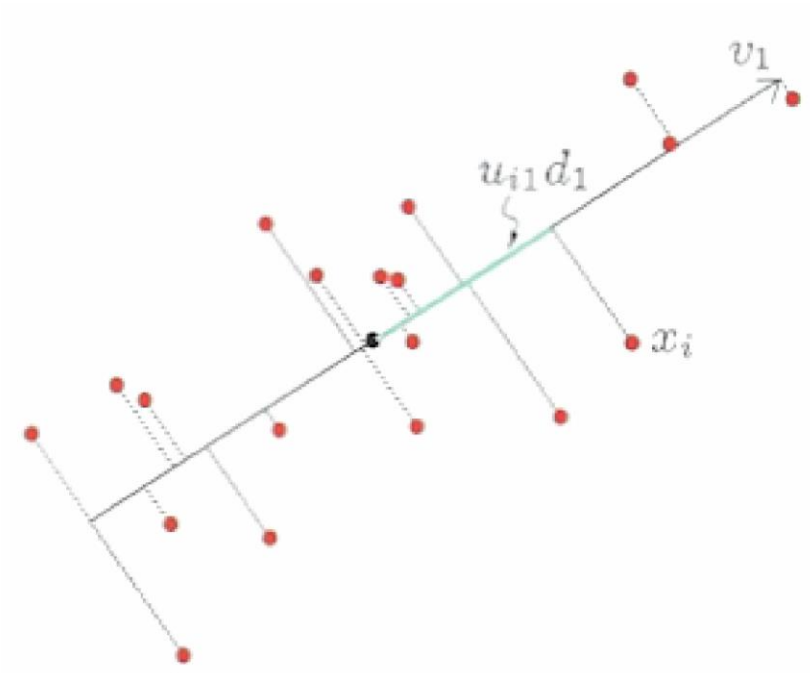
14.5 Principal Components (PCA)

Set of q directions towards which p-dimensional data are linearly projected

-> dimension reduction since $q \leq p$

Data : $x_1, x_2, \cdots, x_n$

Model : $f(\lambda) = (\mu + \lambda_i V_q)$



Model fitted by least squares

w.r.t. reconstruction error

$$\{\mu, \lambda_i, V_q\} = \text{var}\min_{\mu,\lambda,V_q} \sum_{i=1}^{n} \left\| x_i - (\mu + \lambda_i V_q) \right\|^2$$

14.5 Principal Components (PCA)

Principal Components are computed from matrix operations

1. Given V_q, solve the optimal problem

$$\hat{\mu} = \bar{x}, \quad \hat{\lambda}_i = V_q^T (x_i - \bar{x}).$$

2. Substitute them into original cost function

$$V_q = \text{var}\min_{V_q} \sum_{i=1}^{n} \left\| (x_i - \bar{x}) - V_q V_q^T (x_i - \bar{x}) \right\|^2$$

Data are usually centered, and $V_q V_q^T = H_q$ is the projection matrix. Solution V_q are the *q* first columns of V obtained from

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T = \mathbf{S}\mathbf{A}^T; \ \mathbf{U} \ \textit{is} \ \text{N} \times \text{p orthognal matrix } \text{U}^T\text{U=I}$$

14.5 Principal Components (PCA)

Given training data $\{x_i\}_{i=1}^N, x_i \in R^p$ Σ is its covariance matrix with eigenvectors $\{\mathbf{v}_j\}_{j=1}^p$ and eigenvalues $\lambda_1 > \lambda_2 > \cdots > \lambda_p$

Given an eigenvector $\mathbf{v}_j$, the projection of data to eigenvector $\mathbf{v}_j$ subspace is defined by :

$$\hat{\mu}_j, \{\hat{\beta}_{ji}\}_{i=1}^N = \arg\min \sum_{i=1}^N \left\| x_i - \mu - \mathbf{v}_j \beta_i \right\|^2 \quad \text{, where } \mathbf{v}_j^T \mathbf{v}_j = 1$$

1. Derive the solution to the optimal problem.
2. Prove that

$$\sum_{i=1}^N \left\| x_i - \hat{\mu}_k - \mathbf{v}_k \hat{\beta}_{ki} \right\|^2 < \sum_{i=1}^N \left\| x_i - \hat{\mu}_j - \mathbf{v}_j \hat{\beta}_{ji} \right\|^2, \text{ if } k < j.$$

14.5 Principal Components (PCA)

Solution:

$$\mu = mean(x) = \sum_{i=1}^{N} x_i / N$$

$$\beta_{ki} = V_k^T (x_i - \hat{\mu}), \quad i = 1, \cdots, N$$

Q2.

$$\sum_{i=1}^{N} \left\| x_i - \hat{\mu} - \mathbf{v}_k \hat{\beta}_{ki} \right\|^2 = \sum_{i=1}^{N} \left\| x_i - \hat{\mu} - \mathbf{v}_k \mathbf{v}_k^T (x_i - \hat{\mu}) \right\|^2$$

$$= \sum_{i=1}^{N} \left\| (\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^T)(x_i - \hat{\mu}) \right\|^2 = tr\left((\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^T) \mathbf{X}^T \mathbf{X} (\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^T)^{\mathrm{T}} \right)$$

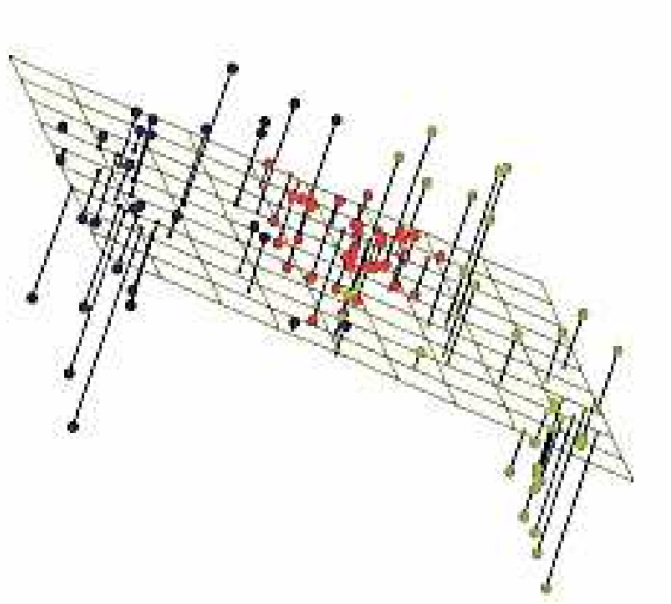
$$= tr\left(\mathbf{X}^T \mathbf{X} (\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^T) \right) = tr(\mathbf{X}^T \mathbf{X}) - tr(N \Sigma \mathbf{v}_k \mathbf{v}_k^T)$$

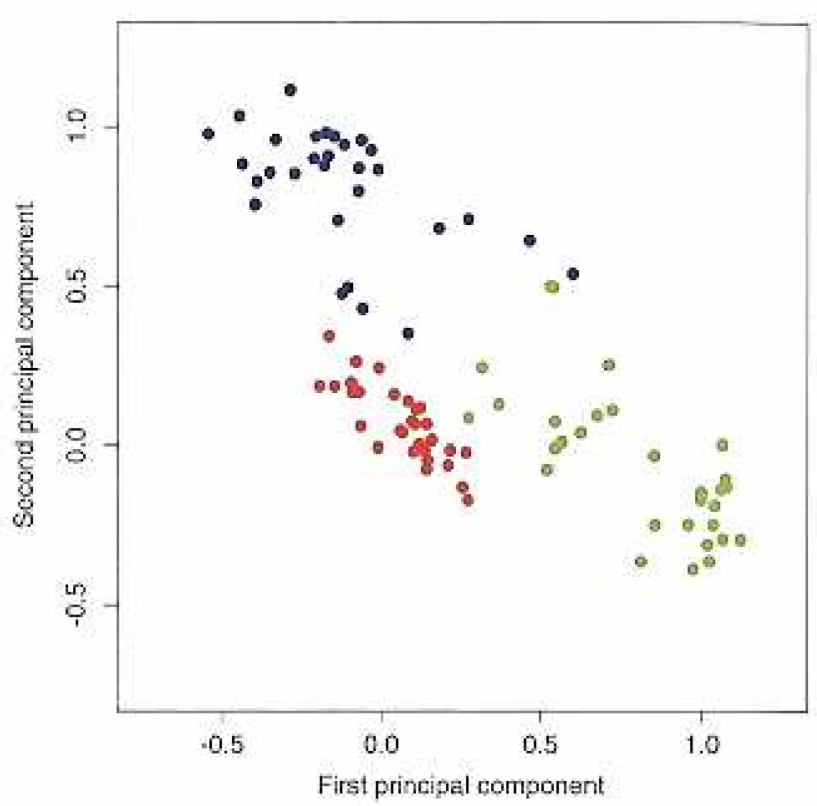
$$= tr(\mathbf{X}^T \mathbf{X}) - tr(N \Sigma \mathbf{v}_k \mathbf{v}_k^T) = tr(\mathbf{X}^T \mathbf{X}) - tr(N \lambda_k \mathbf{v}_k \mathbf{v}_k^T)$$

$$= tr(\mathbf{X}^T \mathbf{X}) - N \lambda_k$$

14.5. Principal Components (PCA)

- PCA can separate sphere data

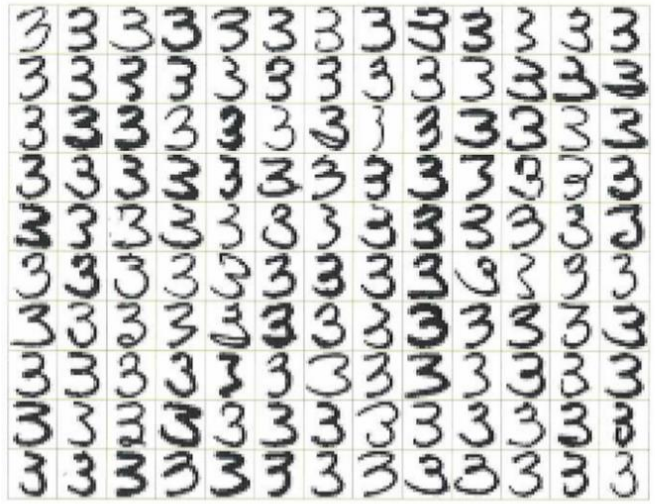




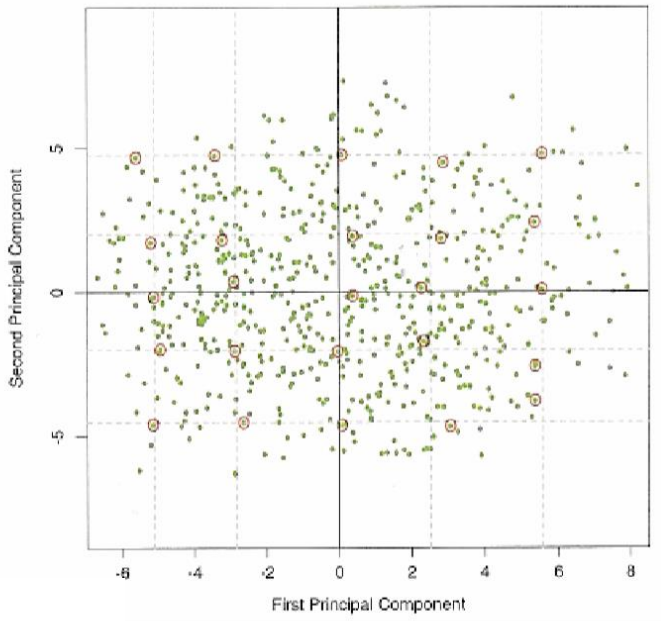
14.5. Principal Components (PCA)

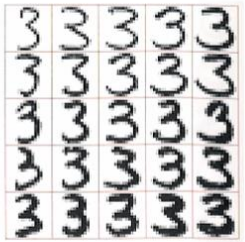
- PCA can be used for handwritten digits

Data in $\mathbb{R}^{256}$



2-D projections





$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

$$= \bar{x} + \lambda_1 \cdot + \lambda_2 \cdot .$$

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

14.5 Principal Curves (PCurves)

Let $f(\lambda)$ be a parametrized smooth curve in $\mathbb{R}^p$

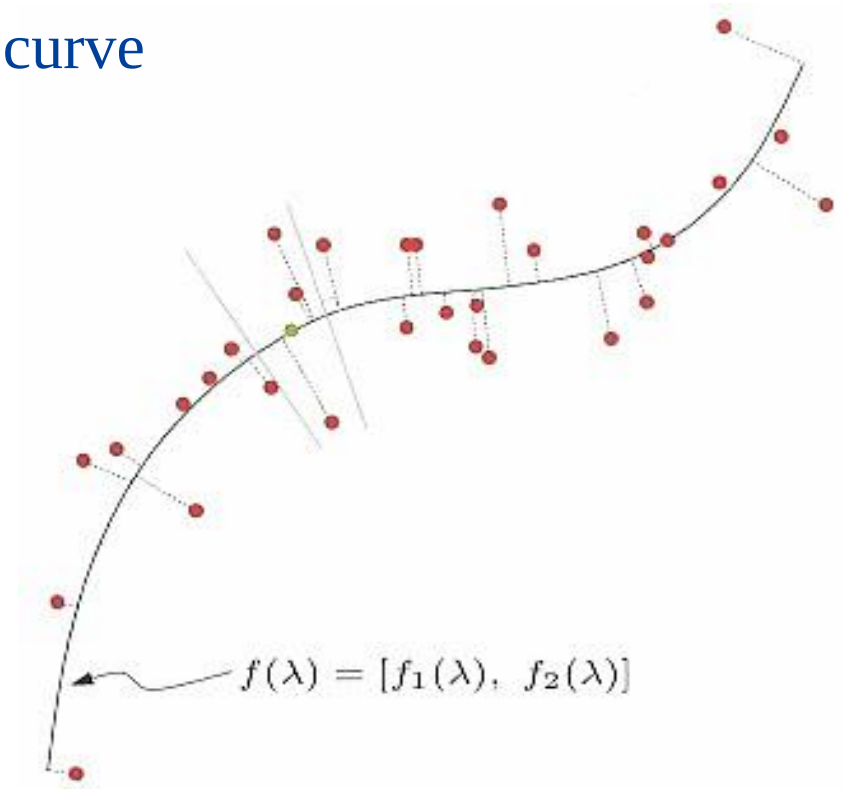
Each coordinate of *p*-dimensional $f(\lambda)$ is a smooth function of λ (e.g. arc-length)

Then $f(\lambda) = E(x \mid \lambda_f(x) = \lambda)$ is a principal curve

Related concepts

-responsability

-principal points



14.5 Principal Curves (PCurves)

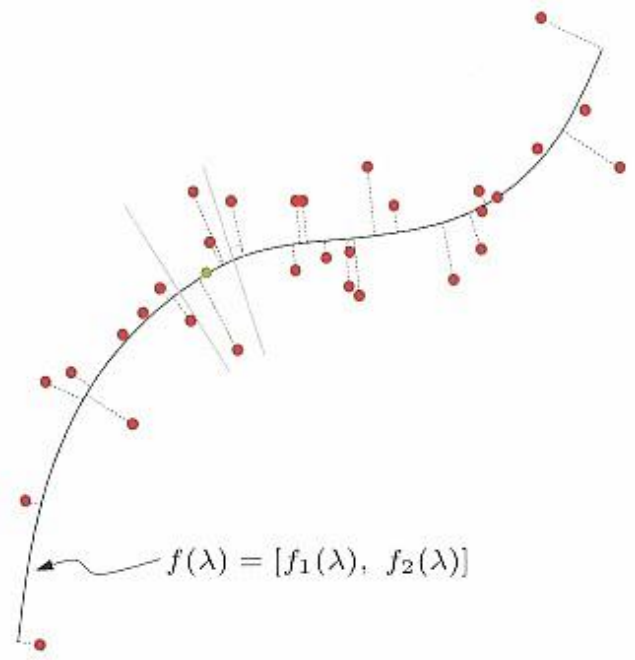
- PCurves can be obtained automatically
- Procedure:

1. Consider the PCurve coordinates one by one

$$\hat{f}(\lambda) = E(x_j \mid \lambda_f(x_j) = \lambda)$$

$$\hat{\lambda}_f(x) = \arg\min_{\lambda} \left\| x - \hat{f}(\lambda) \right\|^2$$

2. Those two steps are repeated until convergence



14.5 Principal Surfaces (PSurfaces)

Generalization to more than one parameter (but rarely more than two)

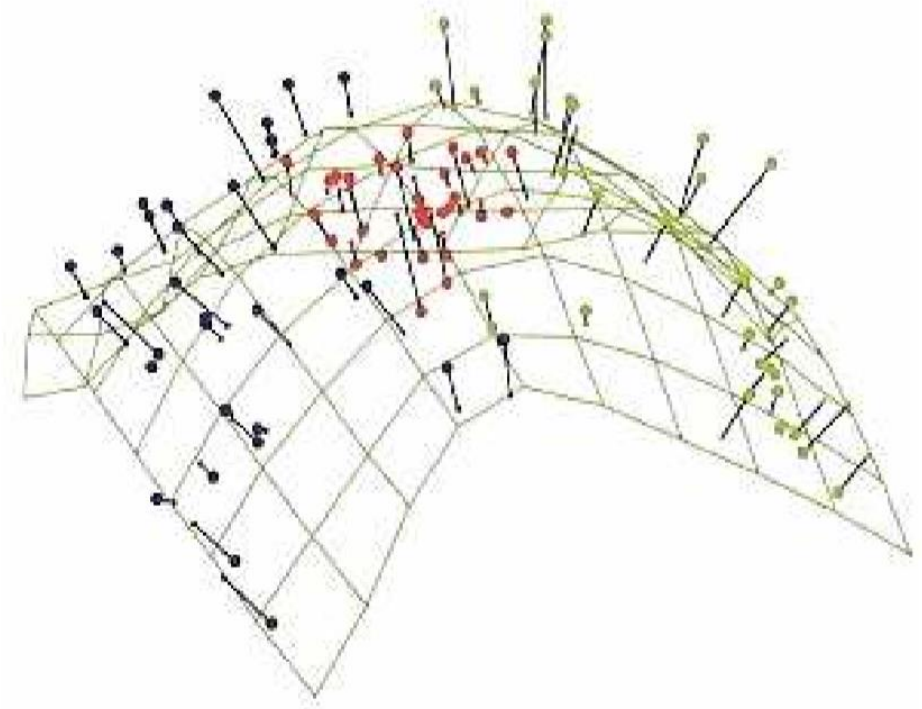
$$f(\lambda_1, \lambda_2) = [f_1(\lambda_1, \lambda_2), f_2(\lambda_1, \lambda_2), \cdots, f_p(\lambda_1, \lambda_2)]$$

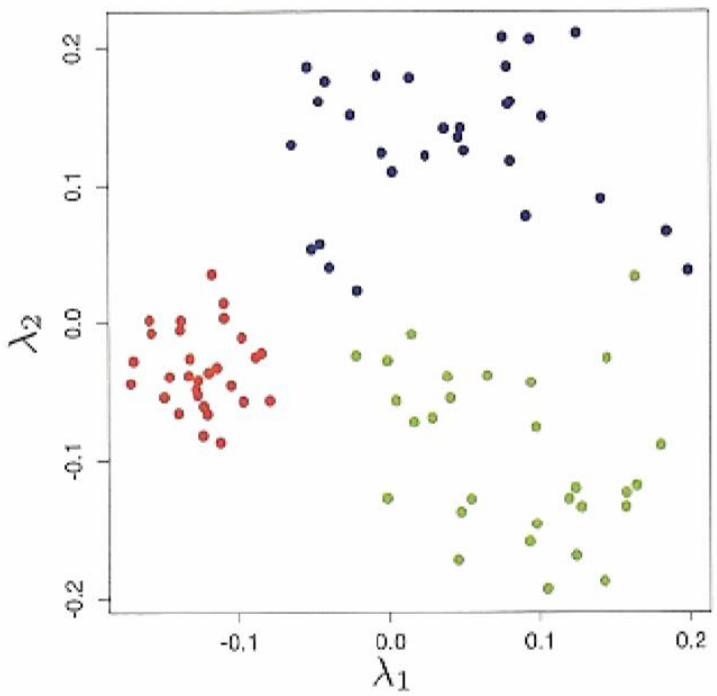
Algorithm for PCurves can be applied for PSurfaces

Links with the SOMs

5. Principal Curves (PCurves)

- PSurfaces can separate sphere data





14.6 Factor Analysis (FA)

Goal : find the latent variables within the observed ones

Latent representation of data (using SVD)

$$\mathbf{X} = \mathbf{UDV}^T = \mathbf{SA}^T;\ \mathbf{U}\ is\ \mathrm{N}\times\mathrm{p}\ \text{orthognal matrix}\ \mathrm{U}^T\mathrm{U}=\mathrm{I}$$

where $\mathbf{S} = \sqrt{N}\mathbf{U}$ and $\mathbf{A}^T = \dfrac{\mathbf{DV}^T}{\sqrt{N}}$

We have the following relations

$$\begin{cases} X_1 = a_{11}S_1 + a_{12}S_2 + \cdots + a_{1p}S_p \\ X_2 = a_{21}S_1 + a_{22}S_2 + \cdots + a_{2p}S_p \\ \vdots \\ X_p = a_{p1}S_1 + a_{p2}S_2 + \cdots + a_{pp}S_p \end{cases}$$

PCA estimates a latent variable model

$$\begin{cases} X_1 = a_{11}S_1 + a_{12}S_2 + \cdots + a_{1p}S_p \\ X_2 = a_{21}S_1 + a_{22}S_2 + \cdots + a_{2p}S_p \\ \vdots \\ X_p = a_{p1}S_1 + a_{p2}S_2 + \cdots + a_{pp}S_p \end{cases}$$

Due to hypothesis on X there are many solutions

$$\mathbf{X} = \mathbf{AS} = \mathbf{AR}^T\mathbf{RS} = \mathbf{A}^*\mathbf{S}^*$$

as

$$Cov(\mathbf{S}^*) = \mathbf{R}Cov(\mathbf{S})\mathbf{R}^T = \mathbf{I}$$

$\mathbf{S}^*$ is also the factor basis

Factor Analysis

Idea : use $q < p$

factor *loadings*

$$\begin{cases} X_1 = a_{11}S_1 + a_{12}S_2 + \cdots + a_{1q}S_q + \varepsilon_1 \\ X_2 = a_{21}S_1 + a_{22}S_2 + \cdots + a_{2q}S_q + \varepsilon_2 \\ \vdots \\ X_p = a_{p1}S_1 + a_{p2}S_2 + \cdots + a_{pq}S_q + \varepsilon_p \end{cases}$$

or $\mathbf{X} = \mathbf{AS} + \boldsymbol{\varepsilon}$, with ε_j is mutually independent

Parameters are given by the covariance matrix

$$\boldsymbol{\Sigma} = \mathrm{AA}^T + \mathrm{D}_\varepsilon$$

with

$$\mathrm{D}_\varepsilon = \mathrm{diag}[\mathrm{var}(\varepsilon_1), \cdots, \mathrm{var}(\varepsilon_p)]$$

PCA and FA are related

FA can be further generalized

$$\begin{cases} X_1 = a_{11}S_1 + a_{12}S_2 + \cdots + a_{1q}S_q + \varepsilon_1 \\ X_2 = a_{21}S_1 + a_{22}S_2 + \cdots + a_{2q}S_q + \varepsilon_2 \\ \vdots \\ X_p = a_{p1}S_1 + a_{p2}S_2 + \cdots + a_{pq}S_q + \varepsilon_p \end{cases}$$

PCA : *all* variability in an item should be used

FA : only the variability in common is used

In most cases, the methods yield similar results PCA is preferred for data reduction

FA is preferred for structure detection

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6. **Non-negative Matrix Factorization**
7. Independent Component Analysis
8. Multidimensional Scaling
9. Nonlinear Dimension Reduction
10. The Google PageRank Algorithm

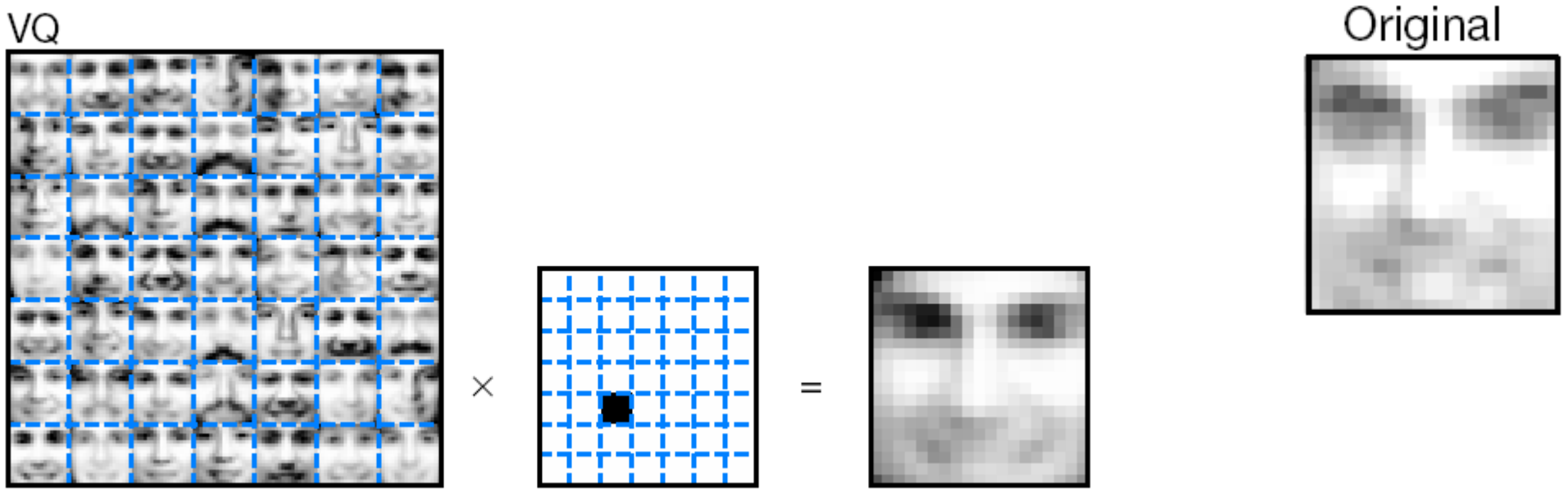
Problem

Given a set of images:

1. Create a set of basis images that can be linearly combined to create new images
2. Find the set of weights to reproduce every input image from the basis images
    - One set of weights for each input image

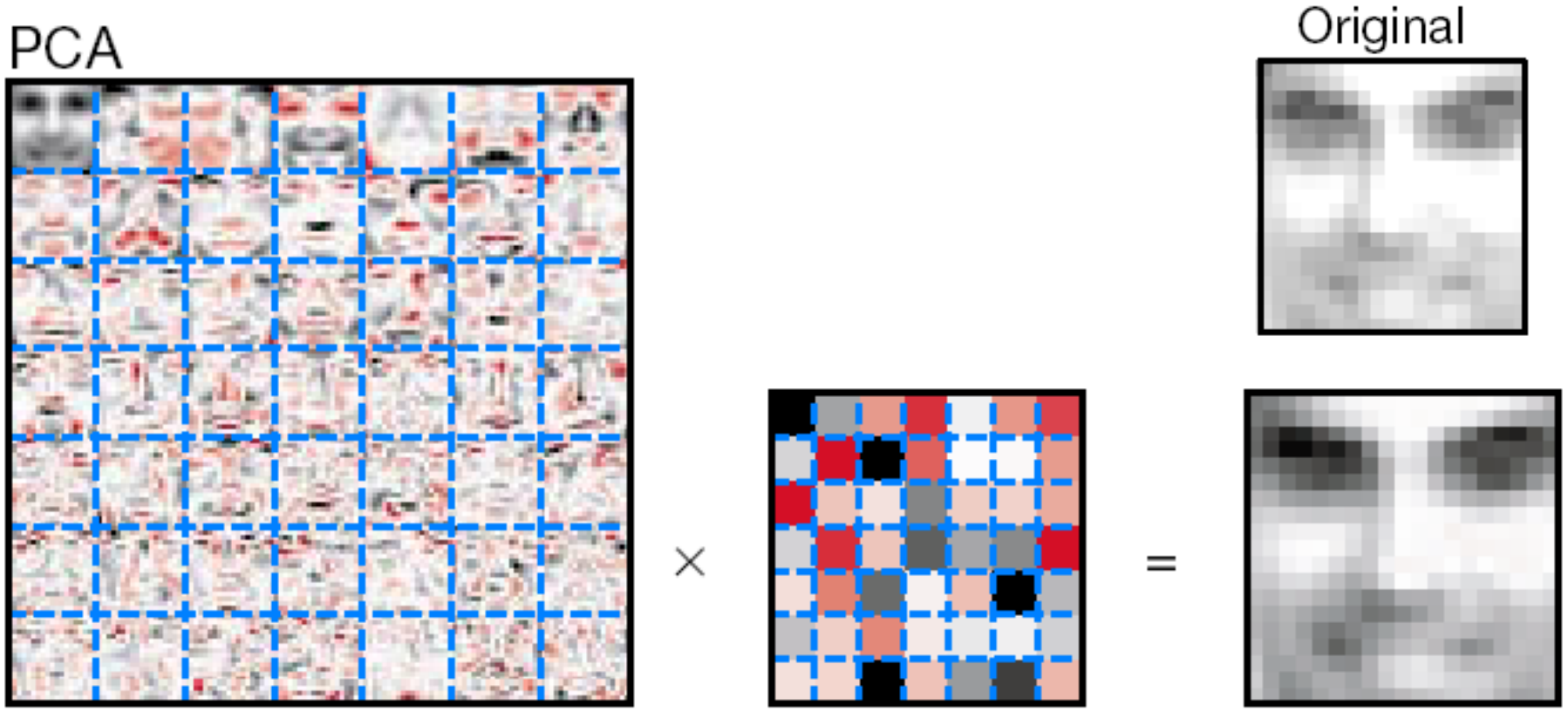
Vector Quantization

- The reconstructed image is the basis image that is closest to the input image.



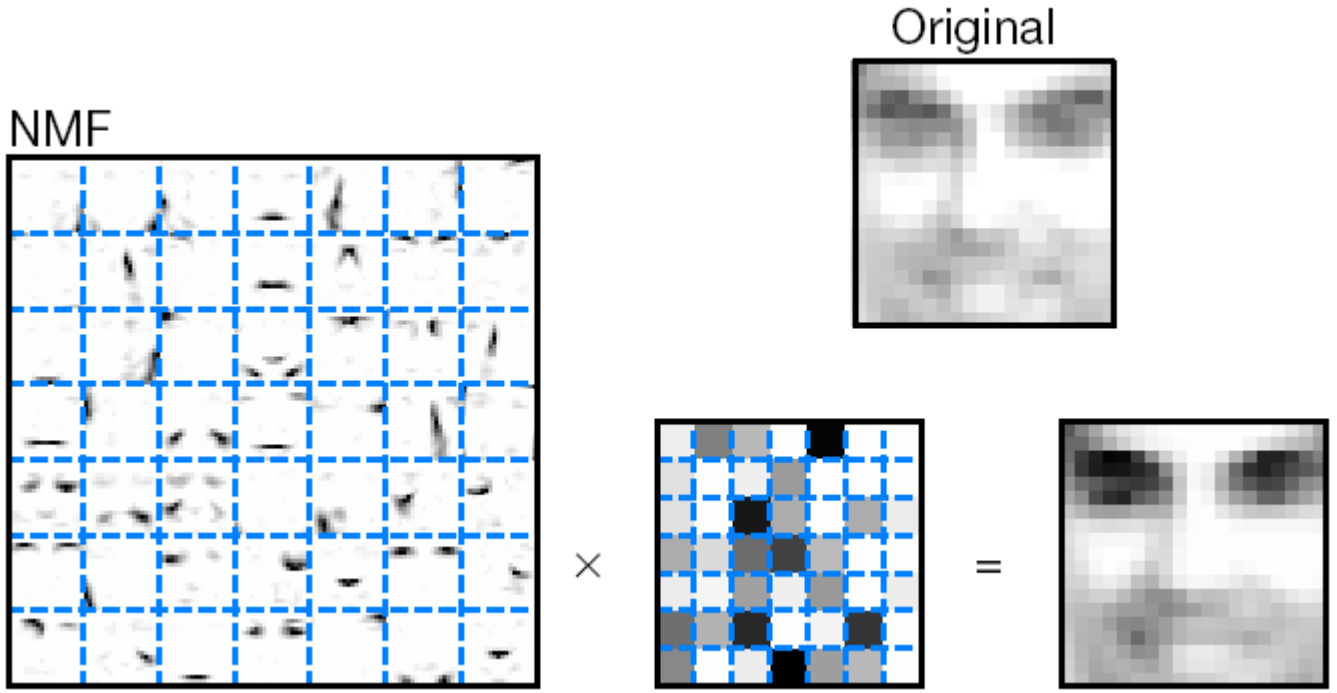
PCA

- Find a set of orthogonal basis images
- The reconstructed image is a linear combination of the basis images



Non-negative Matrix Factorization

- Like PCA, except the coefficients in the linear combination cannot be negative



The cool idea

- By constraining the weights, we can control how images are represented into the weighted sum of basis functions

- In this case, constraining the weights leads to “parts-based” basis images

Objective function

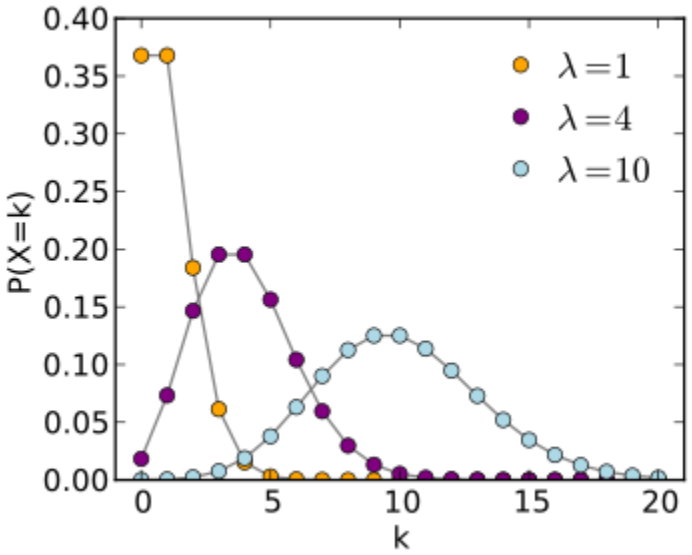
- Let the value of a pixel in an original input image be X.

$$X = WH + \varepsilon, \qquad W \in R^{N \times r}, H \in R^{r \times p}$$

- Let $(WH)_{ij}$ be the reconstructed pixel.
- If we consider X to be a noisy version of $(WH)_{ij}$, then the Poisson PDF of V is

$$P(x \mid (WH)_{ij}) = \frac{(WH)_{ij}^{x} e^{-(WH)_{ij}}}{x!}$$

$$P(x \mid \lambda) = \frac{\lambda^{x} e^{-\lambda}}{x!}$$



Objective function

$$P(x \mid (WH)_{ij}) = \frac{(WH)_{ij}^{x} e^{-(WH)_{ij}}}{x!}$$

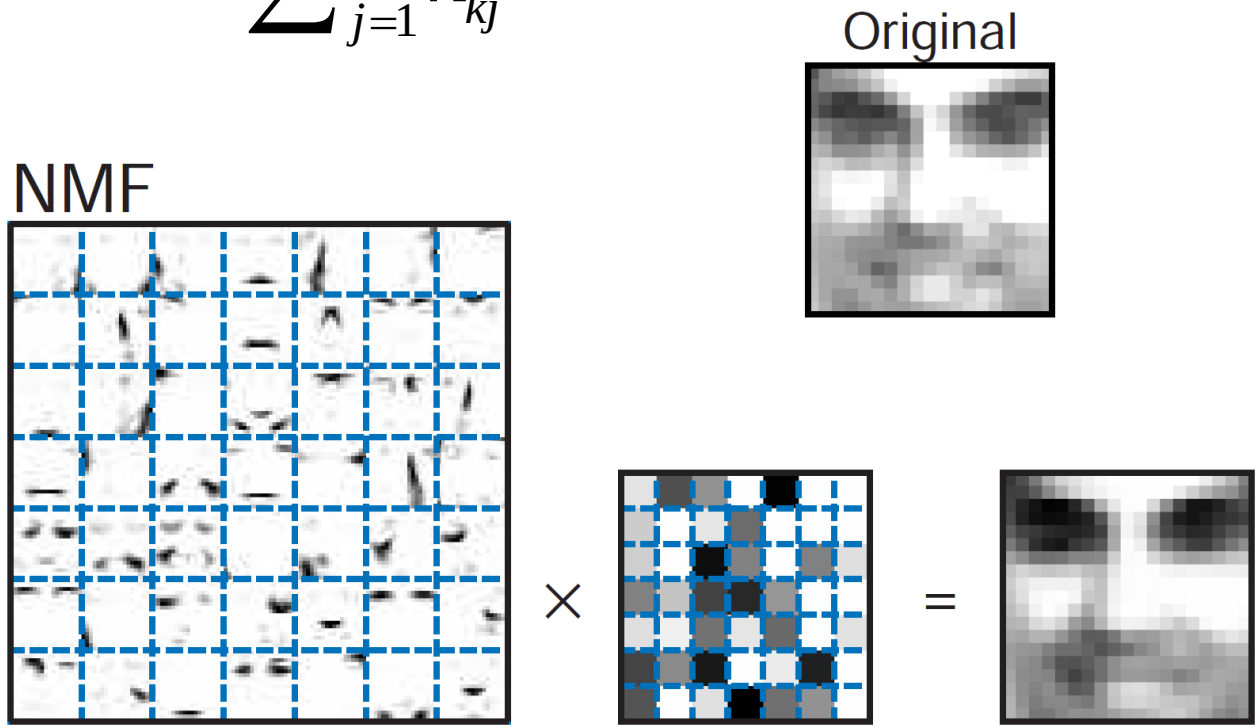
- Now we will maximize the log probability of this PDF over W and H, leaving the relevant objective function to be:

$$L(W, H) = \sum_{i=1}^{N} \sum_{j}^{p} \left[x_{ij} \log(WH)_{ij} - (WH)_{ij} \right]$$

Deriving Update Rules

- Gradient Descent Rule： (Alternating algorithm)

$$w_{ik} \leftarrow w_{ik} \frac{\sum_{j=1}^{p} h_{kj} x_{ij} / (WH)_{ij}}{\sum_{j=1}^{p} h_{kj}}; \qquad h_{kj} \leftarrow h_{kj} \frac{\sum_{i=1}^{N} w_{ik} x_{ij} / (WH)_{ij}}{\sum_{i=1}^{N} w_{ik}}$$



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