AARHUS
UNIVERSITET

Computer Vision & Machine Learning

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This week

Introduction to ML

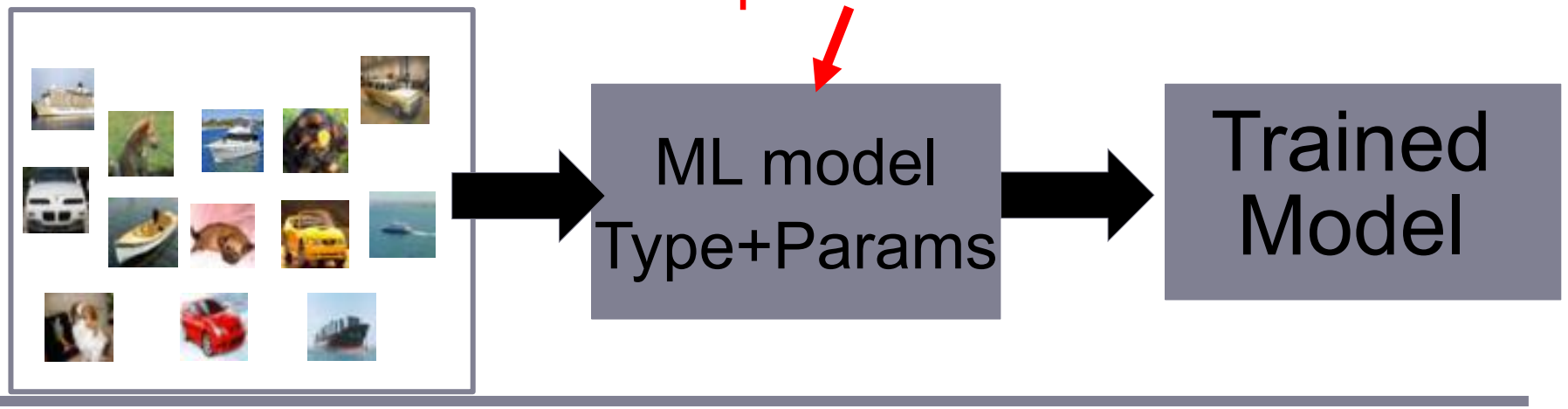
Data clustering

Subspace Learning

Multi-view Learning

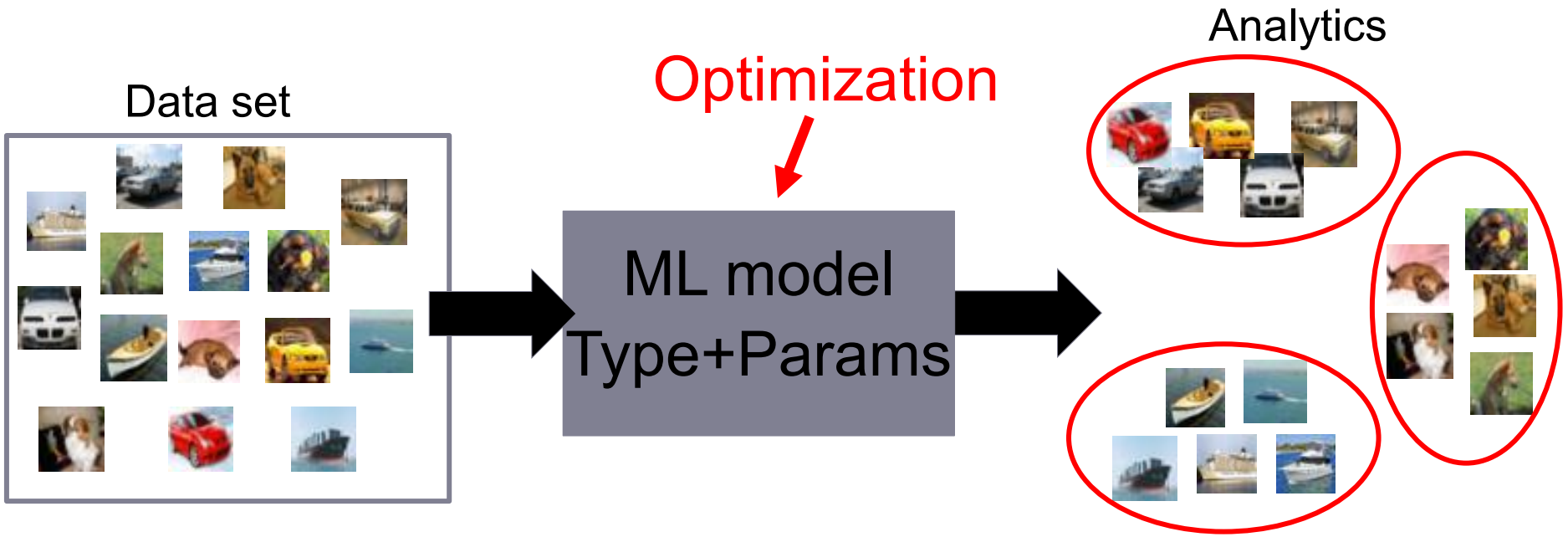
ML for out-of-sample analysis

Training phase



Test phase/Evaluation/Online process

ML for in-sample analysis



General processing steps

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    - Generic categories:
        - Unsupervised learning: We only have data!
        - Supervised learning: We have data and expert-given information (e.g. labels)

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1. Identify the type of the problem:
   - Generic categories:
     - Unsupervised learning: We only have data!
     - Supervised learning: We have data and expert-given information (e.g. labels)
   - More specific categories:
     - Clustering (determination of groups of items)
     - Dimensionality reduction (mapping from $\mathbb{R}^D$ to $\mathbb{R}^d$, d<D)
     - Regression (mapping from x ϵ $\mathbb{R}^D$ to y ϵ $\mathbb{R}^C$)
     - Classification (mapping from x ϵ $\mathbb{R}^D$ to y ϵ Z)

General processing steps

In order to apply a ML model we:

1. Identify the type of the problem
2. Define the “nature” of the problem:
   - Linear → the use of linear solutions, like lines and (hyper-)planes, can lead to good result
   - Non-linear → a good solution can be obtained by using nonlinear methods (defining e.g. parabolic solutions)

General processing steps

In order to apply a ML model we:

1. Identify the type of the problem
2. Define the “nature” of the problem
3. Other constraints:
   - Processing time limitations (e.g. for real-time operation)
   - Processing power limitations (e.g. for smart-phone apps)
   - Possible dependences on other software/hardware

General processing steps

In order to apply a ML model we:

1. Identify the type of the problem
2. Define the “nature” of the problem
3. Other constraints
4. Select the ML model to be used:
   - K-Means
   - Principal Component Analysis (PCA)
   - Linear Discriminant Analysis (LDA)
   - Support Vector Machine (SVM)
   - Multilayer Perceptron (MLP)
   - Convolutional Neural Network (CNN)
   - …

General processing steps

In order to apply a ML model we:

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5. Find the data for the learning (or otherwise the optimization of the parameters of the ML model)

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6. Apply the optimization

General processing steps

ML models are (most often) defined as problems trying to optimize an objective (otherwise called criterion)

This is done by:

- Finding exact (and unique) solutions → Convex optimization
  - For example: Linear Regression, Principal Component Analysis, etc.
  - The criteria of such models have a unique extreme (maximum/minimum) point w.r.t. their parameters

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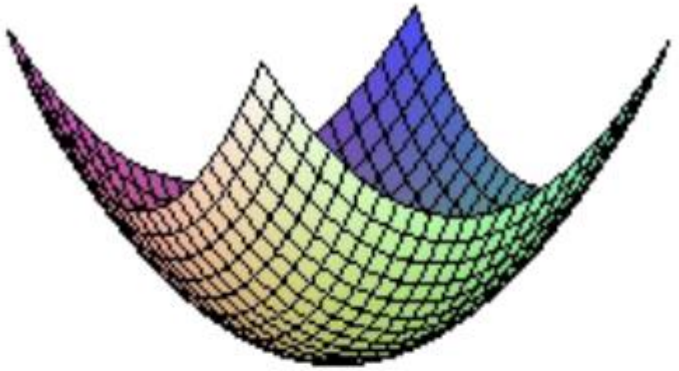
Optimization usually involves:

- Linear Algebra properties/equalities/expressions
- Calculus (differentiation, etc.)

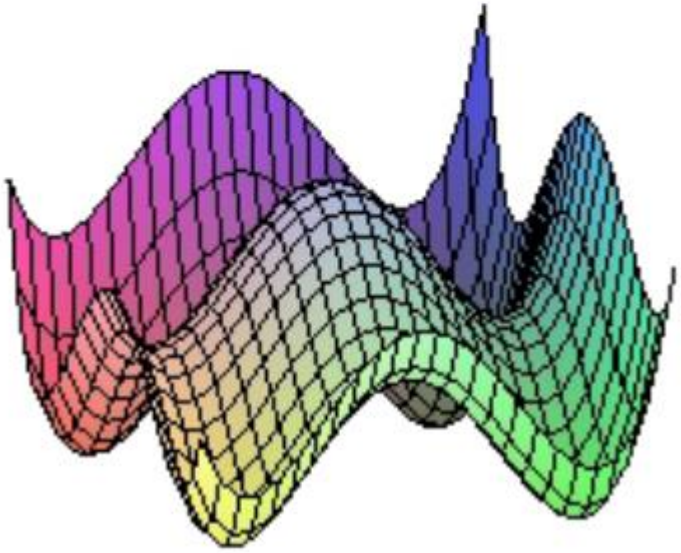
We will discuss how each model is optimized, along with its description

General processing steps

Convex criterion of two parameters



Non-convex criterion of two parameters



K-Means clustering

Unsupervised method:

- Available information is only the samples' representations x_i
- Goal: Define K groups of similar vectors

Mean vector of k-th

Criterion:

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

Euclidean distance between two vectors:

$$d(x_i, x_{i'}) = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = ||x_i - x_{i'}||^2$$

K-Means clustering

Iterative optimization (non-convex optimization problem)

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,

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

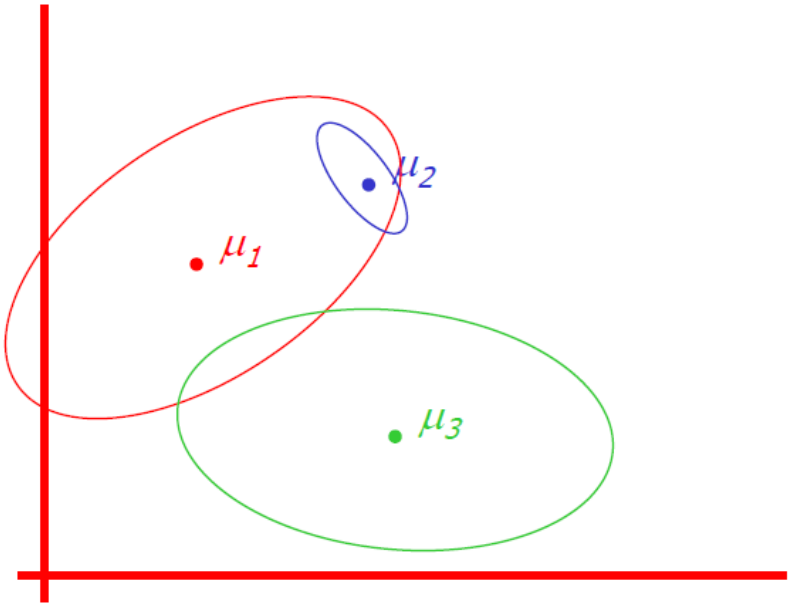
3. Steps 1 and 2 are iterated until the assignments do not change.

Demo

Mixture of Gaussians

K-Means assumes that all groups are represented by the corresponding mean vector m_k and have the same variance:

- This means that a sample x_i will be assigned to the group corresponding to the closest vector m_k, irrespectively to the *shape* of the groups
- An approach which uses such group shape information is the Gaussian Mixture Model (GMM)

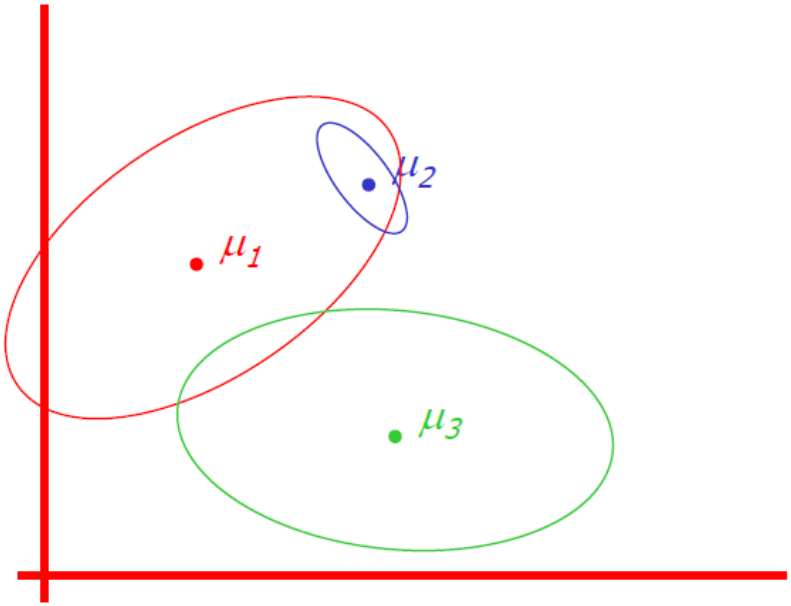


Mixture of Gaussians

GMM:

- There are K components/clusters
- The k-th cluster is associated with a vector m_k (mean vector)
- Each cluster generates data from a Gaussian with mean m_k and covariance Σ_k

Thus, in addition to defining the mean vector m_k as done in K-Means, we also need to determine the covariance Σ_k for each cluster.



Iterative process formed by two steps:

E-step: Compute the expected cluster label for all data

M-step: Update the mean vectors m_k and the covariance matrices Σ_k, k=1,…,K

K-Medoids clustering

K-Means uses the Euclidean distance function. By using different types of distances, it is extended to the K-medoids algorithm:

Algorithm 14.2 *K-medoids Clustering.*

1. For a given cluster assignment C find the observation in the cluster minimizing total distance to other points in that cluster:

$$i_k^* = \underset{\{i:C(i)=k\}}{\operatorname{argmin}} \sum_{C(i')=k} D(x_i, x_{i'}). \tag{14.35}$$

   Then $m_k = x_{i_k^*}$, $k = 1, 2, \ldots, K$ are the current estimates of the cluster centers.

2. Given a current set of cluster centers $\{m_1, \ldots, m_K\}$, minimize the total error by assigning each observation to the closest (current) cluster center:

$$C(i) = \underset{1 \le k \le K}{\operatorname{argmin}} D(x_i, m_k). \tag{14.36}$$

3. Iterate steps 1 and 2 until the assignments do not change.

Hierarchical clustering

The results of applying K-means or K-medoids clustering algorithms depend on the choice for the number of clusters to be searched and a starting configuration assignment.

In contrast, hierarchical clustering methods require the user to specify a measure of dissimilarity between (disjoint) groups of observations, based on the pairwise dissimilarities among the observations in the two groups.

Strategies:

- agglomerative (bottom-up): start at the bottom and at each level recursively merge a selected pair of clusters into a single cluster.
- divisive (top-down): start at the top and at each level recursively split one of the existing clusters at that level into two new clusters.

Both strategies lead to a (N-1)-level hierarchy

Agglomerative clustering

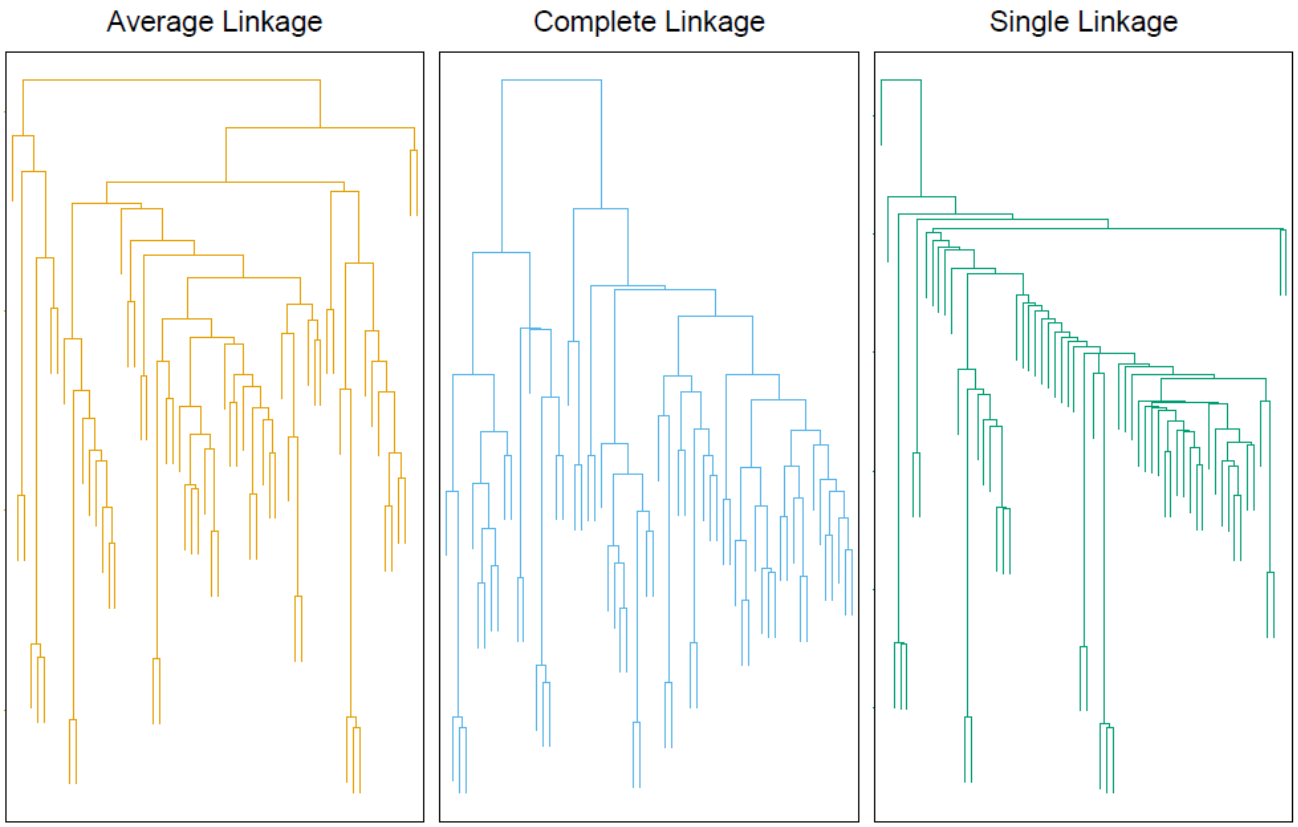
General process:

- Begin with every observation representing a singleton cluster
- At each of the N −1 steps, the closest two (least dissimilar) clusters are merged into a single cluster, producing one less cluster at the next higher level

Dissimilarity between groups G and H:

- Single linkage (or nearest-neighbor) approach: $d_{SL}(G,H) = \min_{\substack{i\in G \\ i'\in H}} d_{ii'}$
- Complete linkage (or furthest-neighbor) approach: $d_{CL}(G,H) = \max_{\substack{i\in G \\ i'\in H}} d_{ii'}$
- Group average approach: $d_{GA}(G,H) = \frac{1}{N_G N_H} \sum_{i\in G} \sum_{i'\in H} d_{ii'}$

Agglomerative clustering



Diameter D_G of a group of observations: the largest dissimilarity among its members:

$$D_G = \max_{\substack{i \in G \\ i' \in G}} d_{ii'}$$

SL → large D_G
CL → small D_G
AL → somewhere between SL-CL

FIGURE 14.13. *Dendrograms from agglomerative hierarchical clustering of human tumor microarray data.*

Divisive clustering

General process:

- Begin with the entire data set as single cluster
- Recursively divide one of the existing clusters into two clusters at each iteration (e.g. by applying K-Means with K=2)

Alternative method (not having randomness issues):

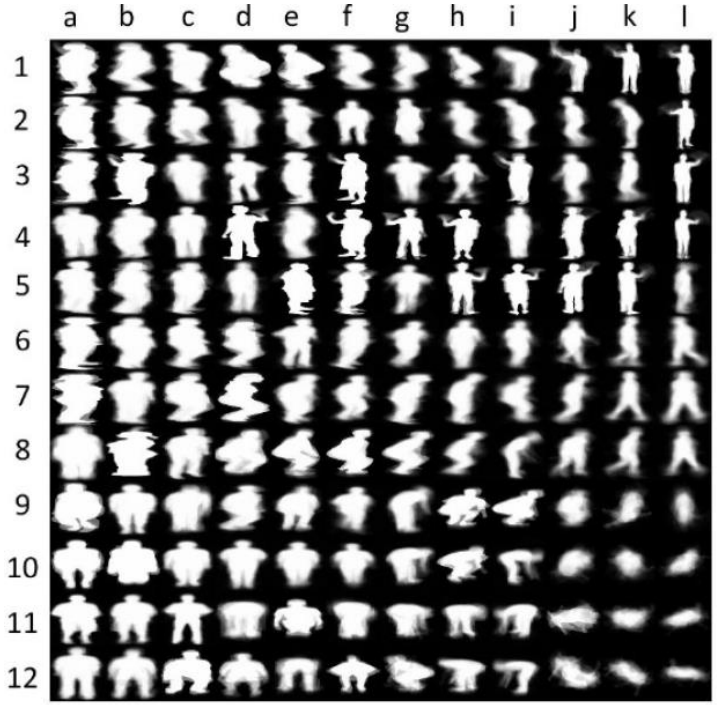
- Place all observations in a single cluster G
- Choose the sample whose average dissimilarity from all the other samples is largest. This is the first member of a second cluster H
- At each successive step the sample in G whose average distance from those in H, minus that for the remaining samples in G is largest, is transferred to H
- Stop when the corresponding difference in averages becomes negative.

Self-Organizing Map

Instead of clustering the input vectors, we want to learn vectors m_k, k=1,…,K that can represent the data well.

These vectors are constrained to belong to a topological map (e.g. a line or a HxW lattice).

A lattice of 12x12 prototypes
learnt using human body poses



Self-Organizing Map

Learning process:

- Initialization of the prototypes (e.g. as random vectors, or random samples)
- Use the input vectors x_i, i=1,…,N multiple times (epochs) for updating the prototypes
- At each iteration, a vector x_i is used to update the prototypes m_k:
  - find the closest (e.g. using Euclidean distance) prototype m_j to x_i
  - Update all prototypes m_k using

$$m_k \leftarrow m_k + \alpha h(\|\ell_j - \ell_k\|)(x_i - m_k)$$

h(·) is a decreasing function operating on the lattice coordinates of prototypes

Effect: For each sample x_i, the closest to it prototypes are updated to be more similar to it according to their similarities in the lattice.

Dimensionality Reduction

Goal: define a mapping from $\mathbb{R}^D$ to $\mathbb{R}^d$, where d < D

This mapping is defined using a set of data $x_i \in \mathbb{R}^D$, i=1,…,N and can be:

- Unsupervised
  - only the vectors x_i are known
  - the objective/criterion defining the mapping involves (geometric) relationships between the data (e.g. variance of the data)
- Supervised
  - vectors x_i are accompanied with class labels l_i
  - the objective/criterion defining the mapping involves class discrimination

Principal Component Analysis

Goal: define a mapping from $\mathbb{R}^D$ to $\mathbb{R}^d$, where d < D, such that the data in $\mathbb{R}^d$ will have the maximal variance.

This mapping is also called projection and for linear mappings is expressed using a matrix W ϵ $\mathbb{R}^{d \times D}$

Principal Component Analysis

Process:

- We define the data representations in $\mathbb{R}^d$ $\quad \mathbf{y}_i = \mathbf{W}^T \mathbf{x}_i$

- We define the variance using the representations y_i , i=1,…,N

$$\mathbf{S}_T = \sum_{i=1}^{N} (\mathbf{y}_i - \mathbf{m})(\mathbf{y}_i - \mathbf{m})^T = \sum_{i=1}^{N} \bar{\mathbf{y}}_i \bar{\mathbf{y}}_i^T = \bar{\mathbf{Y}} \bar{\mathbf{Y}}^T$$

- We express S_T as a function of the parameters **W**

$$\begin{aligned} \mathbf{S}_T &= \sum_{i=1}^{N} \left[\mathbf{W}^T (\mathbf{x}_i - \boldsymbol{\mu}) \right] \left[\mathbf{W}^T (\mathbf{x}_i - \boldsymbol{\mu}) \right]^T = \sum_{i=1}^{N} \mathbf{W}^T \bar{\mathbf{x}}_i \bar{\mathbf{x}}_i^T \mathbf{W} \\ &= \mathbf{W}^T \bar{\mathbf{X}} \bar{\mathbf{X}}^T \mathbf{W} = \mathbf{W}^T \tilde{\mathbf{S}}_T \mathbf{W}, \end{aligned}$$

- We optimize the following criterion $\quad \mathbf{W}^* = \arg\max \; Tr\left(\mathbf{W}^T \tilde{\mathbf{S}}_T \mathbf{W} \right)$

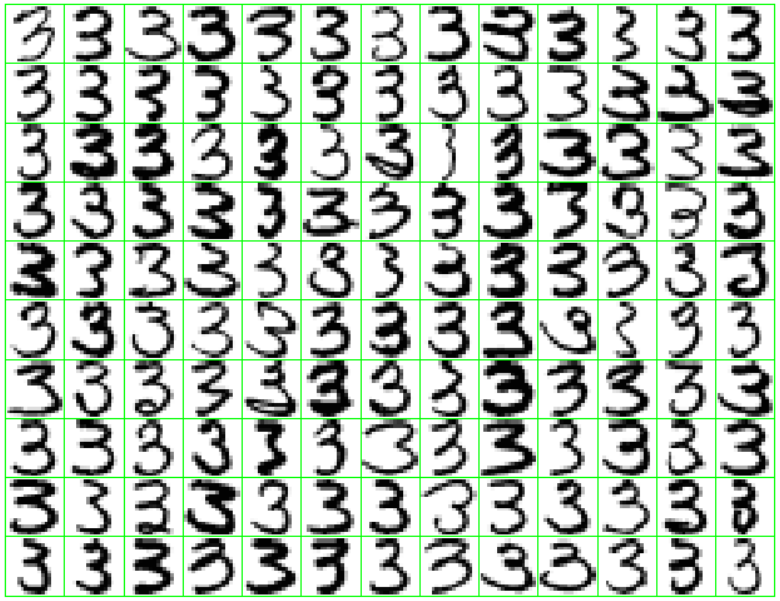
$$subject\ to \quad : \quad \mathbf{W}^T \mathbf{W} = \mathbf{I},$$

Principal Component Analysis

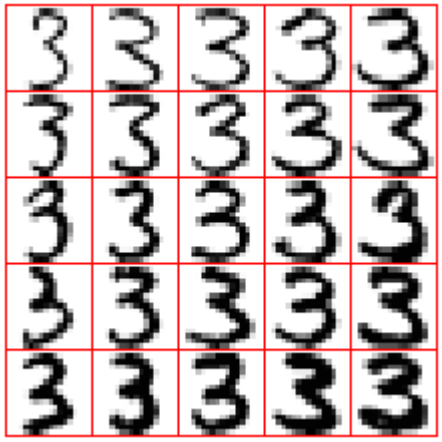
The matrix W is obtained by applying eigenanalysis to the matrix S_T

The same solution can be also obtained by applying Singular Value Decomposition to the matrix $\bar{X} = USV^T$ and keeping the right singular vectors V.

Input data



Principal Components



Demo

$3 = \bar{3} + \lambda_1 \cdot$  $+ \lambda_2 \cdot$  $+ \ldots$

Non-negative Matrix Factorization

NMF is useful for modeling non-negative data, such as images.

It is obtained by calculating a factorization of the matrix X ϵ $\mathbb{R}^{N \times D}$ as follows:

$$\mathbf{X} \approx \mathbf{WH}$$

The matrices W and H are found by minimizing:

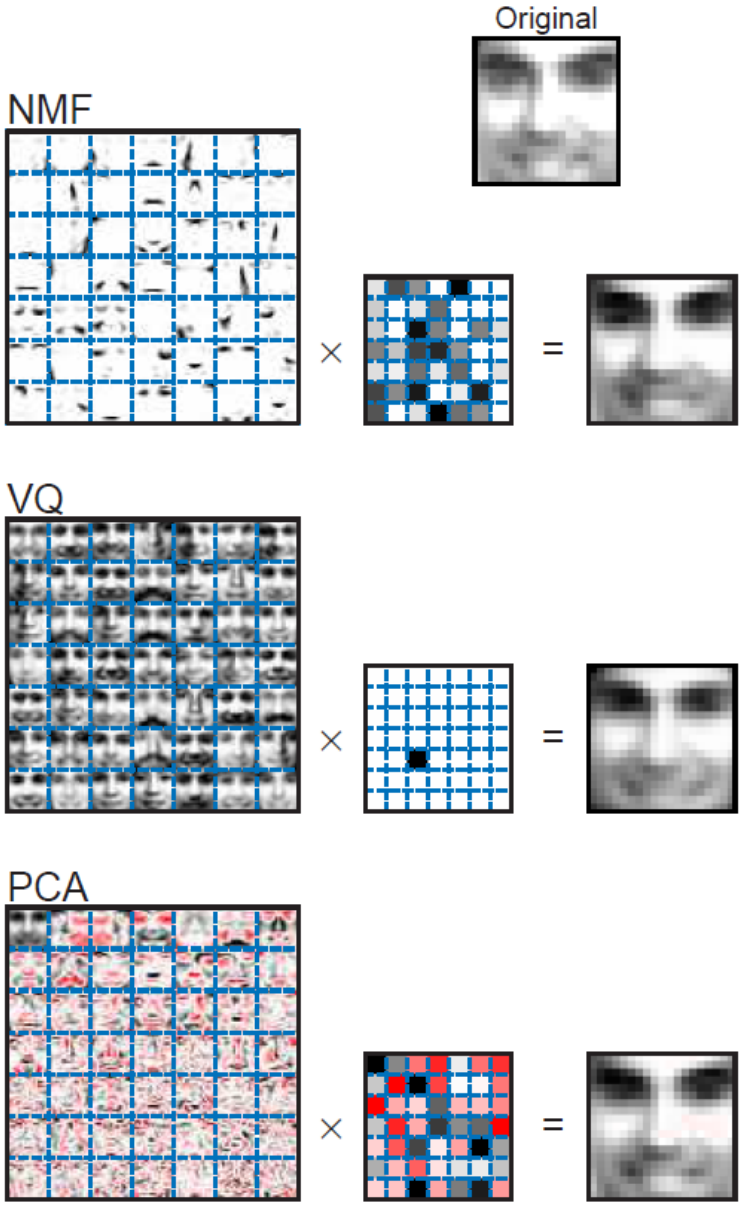
$$L(\mathbf{W}, \mathbf{H}) = \sum_{i=1}^{N} \sum_{j=1}^{p} [x_{ij} \log(\mathbf{WH})_{ij} - (\mathbf{WH})_{ij}]$$

Iterative process formed by two steps:

- Keeping H fixed, update W as $w_{ik} \leftarrow w_{ik} \frac{\sum_{j=1}^{p} h_{kj} x_{ij} / (\mathbf{WH})_{ij}}{\sum_{j=1}^{p} h_{kj}}$

- Keeping W fixed, update H as $h_{kj} \leftarrow h_{kj} \frac{\sum_{i=1}^{N} w_{ik} x_{ij} / (\mathbf{WH})_{ij}}{\sum_{i=1}^{N} w_{ik}}$

Examples

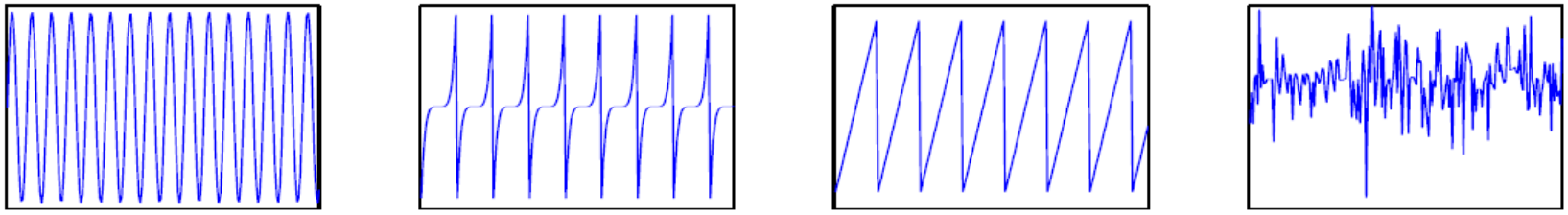


Independent Component Analysis

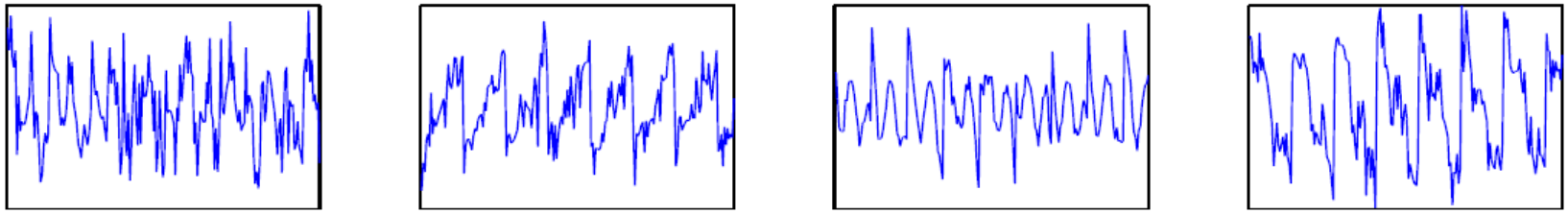
Some motivation first!

Blind source separation problem:

- There is a number of “source signals”:



- Due to some reason, we observe only linear mixtures of the above signals:



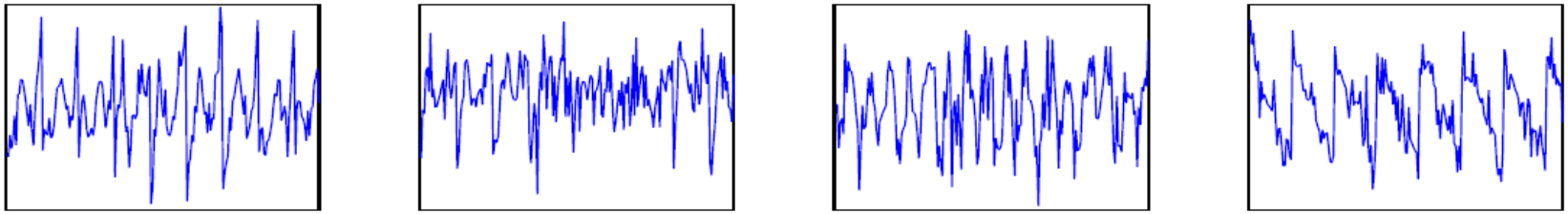
- We want to estimate (separate) the original signals, based on the observations

Independent Component Analysis

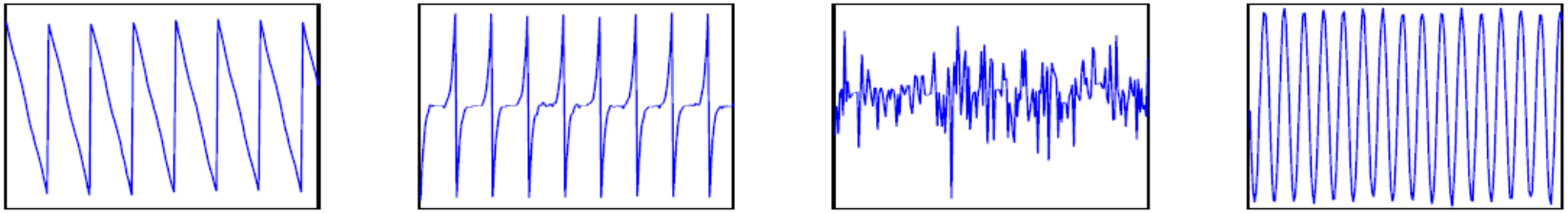
Some motivation first!

Blind source separation problem:

- PCA (optimized to find components with maximal variance) fails:



- If we use information on statistical independence we can recover:



Independent Component Analysis

The observation matrix X is modelled hidden variables s:

$$\mathbf{X} = \mathbf{AS}$$

where:

- the matrix A is called “mixing matrix”
- the vectors forming the matrix S are called “independent components”

Assumptions and restrictions:

- The number of Independent Components is equal to the number of observations
  → A is a square matrix. Then, we can use $S = A^{-1} X = W^T X$
- s_i are statistically independent → $p(s_1,s_2) = p(s_1)p(s_2)$
- Since both A and S are not known, any arbitrary scaling of the first can be cancelled by inverting it to the second → we restrict $||s_i||_2 = 1$.

Independent Component Analysis

Pre-processing steps:

1. Data centering: $x_i \leftarrow x_i - \mu$
2. Data whitening: $S_T = U\Sigma U^T$ and $x_i = (U\Sigma^{-1/2}U^T)\, x_i$

$$Obj(\mathbf{W}) = \sum_{t=1}^{T} G(\mathbf{W}^T \mathbf{x}_t) - \Lambda(\mathbf{W}^T\mathbf{W} - \mathbf{I})$$

$$\frac{\partial Obj}{\partial \mathbf{W}} = \mathbf{X}g(\mathbf{W}^T\mathbf{X})^T - \Lambda\mathbf{W} = \mathbf{0}$$

Fixed Point Algorithm

Input: $\mathbf{X}$

Random init of $\mathbf{W}$

Iterate until convergence:

$$\mathbf{S} = \mathbf{W}^T\mathbf{X}$$

$$\mathbf{W} = \mathbf{X}g(\mathbf{S})^T$$

$$\mathbf{W} = \mathbf{W}\sqrt{(\mathbf{W}^T\mathbf{W})^{-1}}$$

Output: $\mathbf{W}$, $\mathbf{S}$

Independent Component Analysis

Criterion: Find the A that leads to the most independence between the components of $Y = W^T X$.

We use the mutual information I(Y) : $$I(Y) = \sum_{j=1}^{p} H(Y_j) - H(Y)$$

Where H(Y) is the differential entropy of Y with density g(y)

$$H(Y) = -\int g(y) \log g(y) dy$$

Random Projections

The transformation y = W x, when W ϵ $\mathbb{R}^{d \times D}$ is a random matrix is referred to as RP

It has been shown that for a random matrix W such that each element of it is distributed normally with zero mean and variance 1/d, the ratio

$$\frac{\|W\mathbf{x}_1 - W\mathbf{x}_2\|}{\|\mathbf{x}_1 - \mathbf{x}_2\|}$$

is close to 1.

The above means that the pair-wise distances between vectors in $\mathbb{R}^D$ and $\mathbb{R}^d$ are very similar

Linear Discriminant Analysis

Supervised method:

- Each vector x_i is followed by a class label $l_i \in \{1,\ldots,C\}$

Goal: Define a mapping $y_i = W^T x_i$, when $W \in \mathbb{R}^{d \times D}$, enhancing class discrimination:

- increasing class compactness == minimizing within-class variance
- increasing distance between classes == increasing between-class variance

Demo

Linear Discriminant Analysis

Process:

- Define within-class variance (μ_k is the mean vector of k-th class)

$$\mathbf{S}_w = \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

- Define between-class variance

$$\mathbf{S}_b = \sum_{k=1}^{K} N_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$

- Maximize the Fisher ratio

$$\mathcal{J}(\mathbf{W}) = \frac{Tr(\mathbf{W}^T \mathbf{S}_b \mathbf{W})}{Tr(\mathbf{W}^T \mathbf{S}_w \mathbf{W})}$$

Several solutions for J(W) have been proposed. The most common one is the solution of the generalized eigen-value problem

$$\mathbf{S}_b \mathbf{w} = \lambda \mathbf{S}_w \mathbf{w}$$

Graph-based Subspace Learning

Let us consider a graph G = {V,E}:

- V = $\{v_1,\ldots,v_N\}$ is called the vertex set of the graph
- E = $\{e_{ij}\}$ is called the edge set of the graph
  - e_{ij} is an edge connecting v_i and v_j
  - e_{ij} can indicate a link between the i-th and j-th vertices (unweighted graph)
  - e_{ij} can be associated with a weight value w_{ij} showing how strong is the link between the i-th and j-th vertices (weighted graph)

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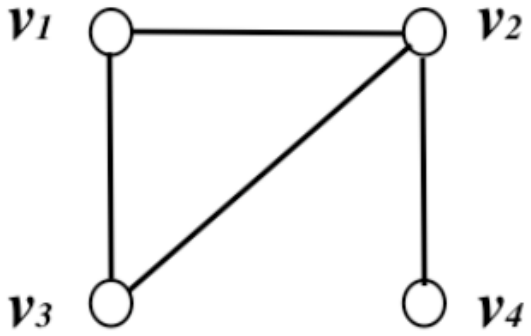
The graph can be:

- fully connected → there is an edge between every pair of nodes (and the associated weight)
- partially connected → each vertex is connected only with some other vertices (those which are more similar to it – according to a similarity/distance metric)

Graph-based Subspace Learning

The adjacency matrix A ϵ $\mathbb{R}^{N \times N}$ of the graph is defined as:

$$\mathbf{A} := \begin{cases} A_{ij} = 1 & \text{if there is an edge } e_{ij} \\ A_{ij} = 0 & \text{if there is no edge} \\ A_{ii} = 0 \end{cases}$$



$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

The weight matrix W ϵ $\mathbb{R}^{N \times N}$ of the graph has the same form, but each element denotes the strength of connection (similarity) between the corresponding vertices.

Graph-based Subspace Learning

Let us associate a feature vector $f(v_i)$ to each vertex i of an undirected weighted graph:

- We want the relation between the vectors representing the graph vertices to be the same as those expressed by the corresponding weights w_{ij}
- Example of graph weights (Gaussian kernel):

$$w_{ij} = \exp\left(-\|\boldsymbol{v}_i - \boldsymbol{v}_j\|^2/\sigma^2\right)$$

$$0 \leq w_{\min} \leq w_{ij} \leq w_{\max} \leq 1$$

this means that if w_{ij} is high, the representations of vertices i and j should be close using the Euclidean distance, i.e. the vertex representations to minimize:

$$\frac{1}{2}\sum_{e_{ij}} w_{ij}(f(v_i) - f(v_j))^2 = \boldsymbol{f}^\top \mathbf{L} \boldsymbol{f}$$

Graph-based Subspace Learning

$$\frac{1}{2}\sum_{e_{ij}} w_{ij}(f(v_i) - f(v_j))^2 = \boldsymbol{f}^\top \mathbf{L}\boldsymbol{f}$$

L is the Laplacian matrix: L = D – W

D is a diagonal matrix (called Degree matrix) having elements $D_{ii} = \sum_j w_{ij}$

Laplacian Embedding

Define low-dimensional representations f by optimizing:

$$\arg\min_{\boldsymbol{f}} \boldsymbol{f}^\top \mathbf{L}\boldsymbol{f} \text{ with: } \boldsymbol{f}^\top \boldsymbol{f} = 1 \text{ and } \boldsymbol{f}^\top \mathbf{1} = 0$$

Solution is obtained by solving the eigenanalysis problem $\mathbf{L}\boldsymbol{f} = \lambda \boldsymbol{f}$

Graph Embedding

GE defines two graphs:

- an (intrinsic) graph G expressing properties of the data that we want the embedding to enhance/minimize
- a penalty graph G^p, expressing properties of the data that we want the embedding to penalize/maximize

Graph Embedding

GE defines two graphs:

- an (intrinsic) graph G expressing properties of the data that we want the embedding to enhance/minimize
- a penalty graph G^p, expressing properties of the data that we want the embedding to penalize/maximize

Let us assume that L, B are the Laplacian matrices of G and G^p, respectively. Then, GE optimizes the following criterion:

$$y^* = \arg \min_{y^T B y = d} \sum_{i \neq j} \|y_i - y_j\|^2 W_{ij} = \arg \min_{y^T B y = d} y^T L y$$

y_i is the vector associated with vertex i and d is a constant value

Graph Embedding

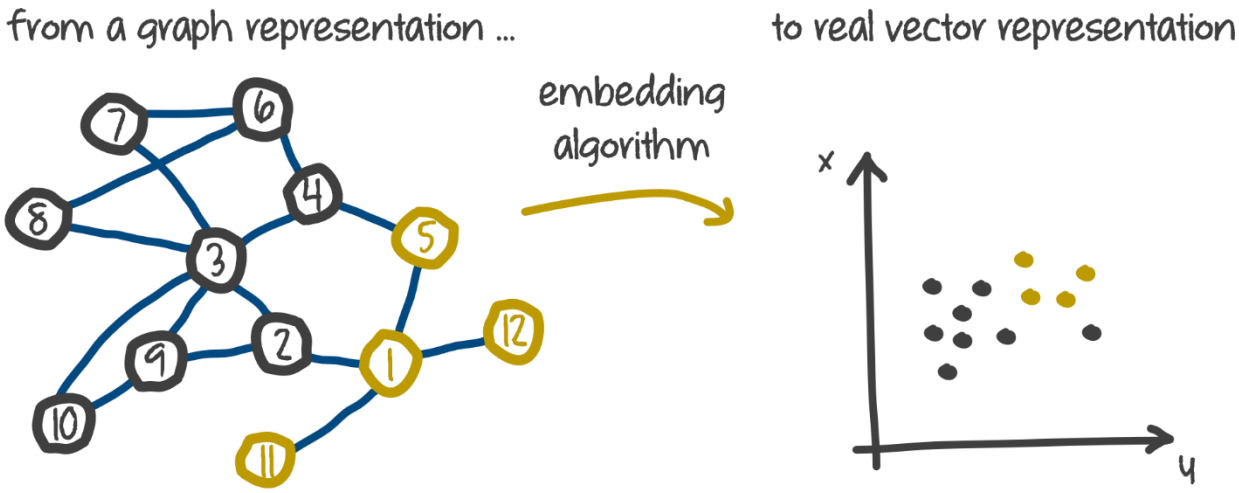
If we define a linear mapping: $y_i = w^T x_i$, then the projection w is obtained by:

$$w^* = \underset{\substack{w^T XBX^T w=d \\ \text{or } w^T w=d}}{\arg\min} \sum_{i \neq j} \|w^T x_i - w^T x_j\|^2 W_{ij} = \underset{\substack{w^T XBX^T w=d \\ \text{or } w^T w=d}}{\arg\min} w^T XLX^T w$$

And is calculated by solving the generalized eigenanalysis problem: $\tilde{L}v = \lambda \tilde{B}v$

where $\tilde{L} = XLX^T$

$\tilde{B} = XBX^T$



Graph Embedding

Let us take again a look at the scatter matrices of LDA:

$$\mathbf{S}_w = \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

Using $\mathbf{1}_k \in \mathbb{R}^N$ a vector having its elements for which $l_i = k$ equal to one and the remaining elements equal to zero and $\mathbf{J}_k \in \mathbb{R}^{N \times N}$ the diagonal matrix of 1_k

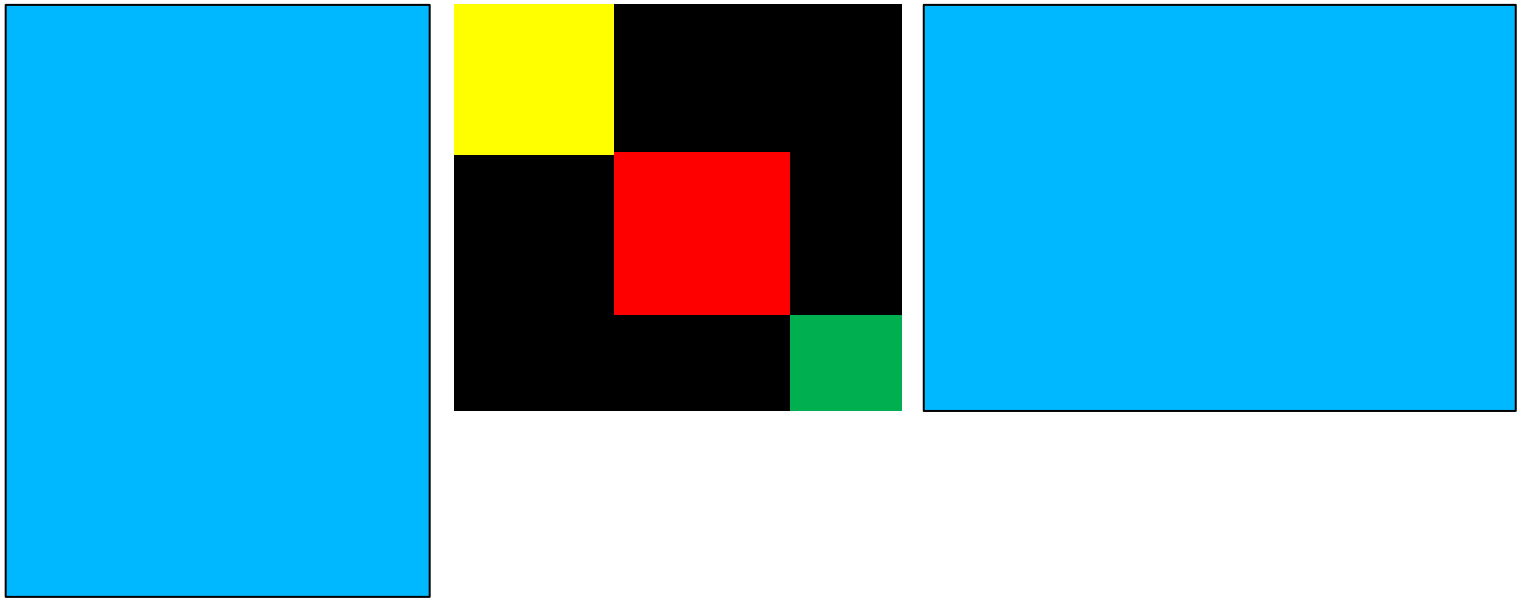
$$\begin{aligned}
\mathbf{S}_w &= \sum_{k=1}^{K} \left(\mathbf{X}\mathbf{J}_k - \frac{1}{N_k}\mathbf{X}\mathbf{1}_k\mathbf{1}_k^T \right) \left(\mathbf{X}\mathbf{J}_k - \frac{1}{N_k}\mathbf{X}\mathbf{1}_k\mathbf{1}_k^T \right)^T \\
&= \sum_{k=1}^{K} \mathbf{X} \left(\mathbf{J}_k - \frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T \right) \left(\mathbf{J}_k - \frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T \right)^T \mathbf{X}^T \\
&= \mathbf{X} \left(\sum_{k=1}^{K} \left(\mathbf{J}_k - \frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T \right) \left(\mathbf{J}_k - \frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T \right)^T \right) \mathbf{X}^T \\
&= \mathbf{X}\mathbf{L}_w\mathbf{X}^T.
\end{aligned}$$

Graph Embedding

Let us take again a look at the scatter matrices of LDA:

$$\mathbf{S}_w = \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

$\mathbf{S}_w =$ $\mathbf{X}$ $\mathbf{L}_w$ $\mathbf{X}^T$



Graph Embedding

Similarly:

$$\mathbf{S}_b = \sum_{k=1}^{K} N_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$

$$\begin{aligned}
\mathbf{S}_b &= \sum_{k=1}^{K} N_k \left(\frac{1}{N_k}\mathbf{X}\mathbf{1}_k\mathbf{1}_k^T - \frac{1}{N}\mathbf{X}\mathbf{1}\mathbf{1}_k^T\right)\left(\frac{1}{N_k}\mathbf{X}\mathbf{1}_k\mathbf{1}_k^T - \frac{1}{N}\mathbf{X}\mathbf{1}\mathbf{1}_k^T\right)^T \\
&= \mathbf{X}\left(\sum_{k=1}^{K} N_k \left(\frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T - \frac{1}{N}\mathbf{1}\mathbf{1}_k^T\right)\left(\frac{1}{N_k}\mathbf{1}_k\mathbf{1}_k^T - \frac{1}{N}\mathbf{1}\mathbf{1}_k^T\right)^T\right)\mathbf{X}^T \\
&= \mathbf{X}\mathbf{L}_b\mathbf{X}^T.
\end{aligned}$$

and

$$\mathcal{J}(\mathbf{W}) = \frac{Tr(\mathbf{W}^T\left(\mathbf{X}\mathbf{L}_b\mathbf{X}^T\right)\mathbf{W})}{Tr(\mathbf{W}^T\left(\mathbf{X}\mathbf{L}_w\mathbf{X}^T\right)\mathbf{W})}$$

Graph Embedding

Similarly:

$$\mathbf{S}_b = \sum_{k=1}^{K} N_k(\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$

$\mathbf{S}_b$ = $\mathbf{X}$ $\mathbf{L}_b$ $\mathbf{X}^T$

Graph Embedding

And the criterion of LDA is given by:

$$\mathcal{J}(\mathbf{W}) = \frac{Tr(\mathbf{W}^T \left(\mathbf{X}\mathbf{L}_b\mathbf{X}^T\right)\mathbf{W})}{Tr(\mathbf{W}^T \left(\mathbf{X}\mathbf{L}_w\mathbf{X}^T\right)\mathbf{W})}$$

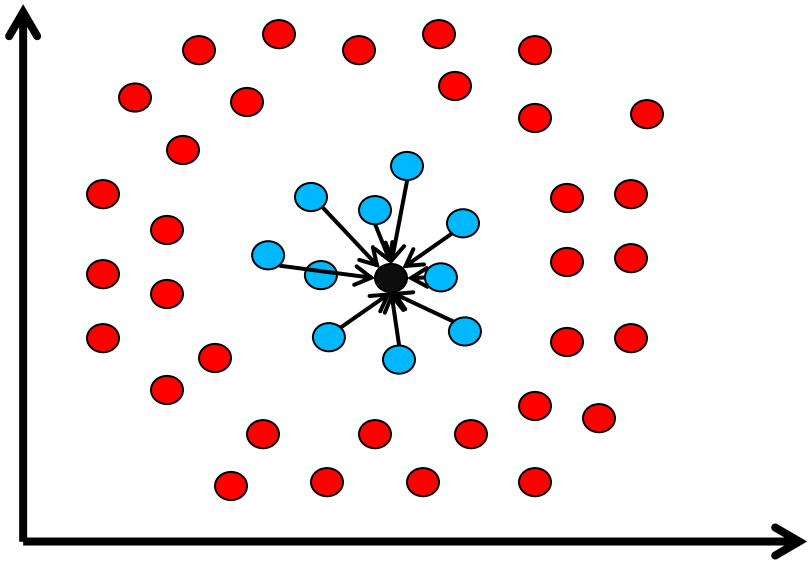
The above expression is simple, yet powerful:

- Use of different $L_{(?)}$ matrices leads to the description of different relationships for the data (and/or classes)
- Examples:
  - Linear Discriminant Analysis
  - Principal Component Analysis
  - Local Fisher Discriminant Analysis
  - Marginal Discriminant Analysis
  - Class-Specific Discriminant Analysis

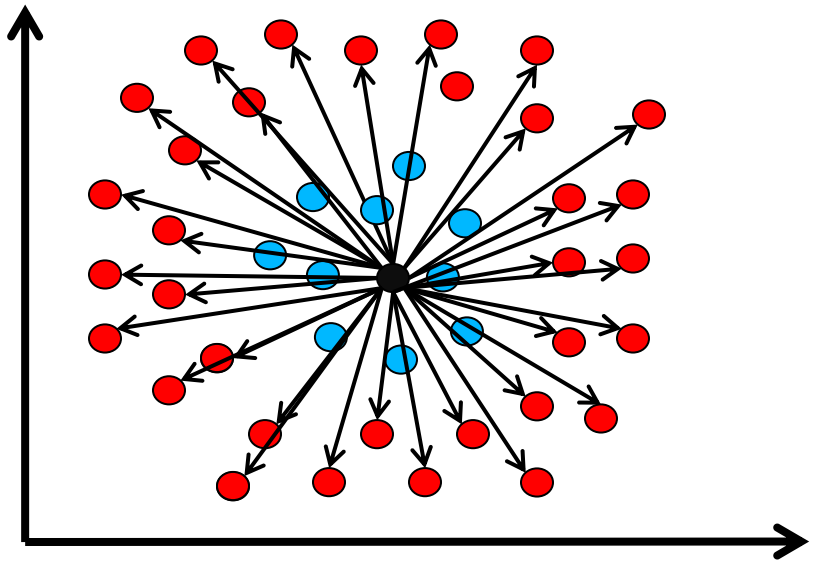
Graph Embedding

Example: Class-specific Discriminant Analysis

Intra-class scatter $\mathbf{S}_i$



Out-of-class scatter $\mathbf{S}_p$



Spectral Clustering

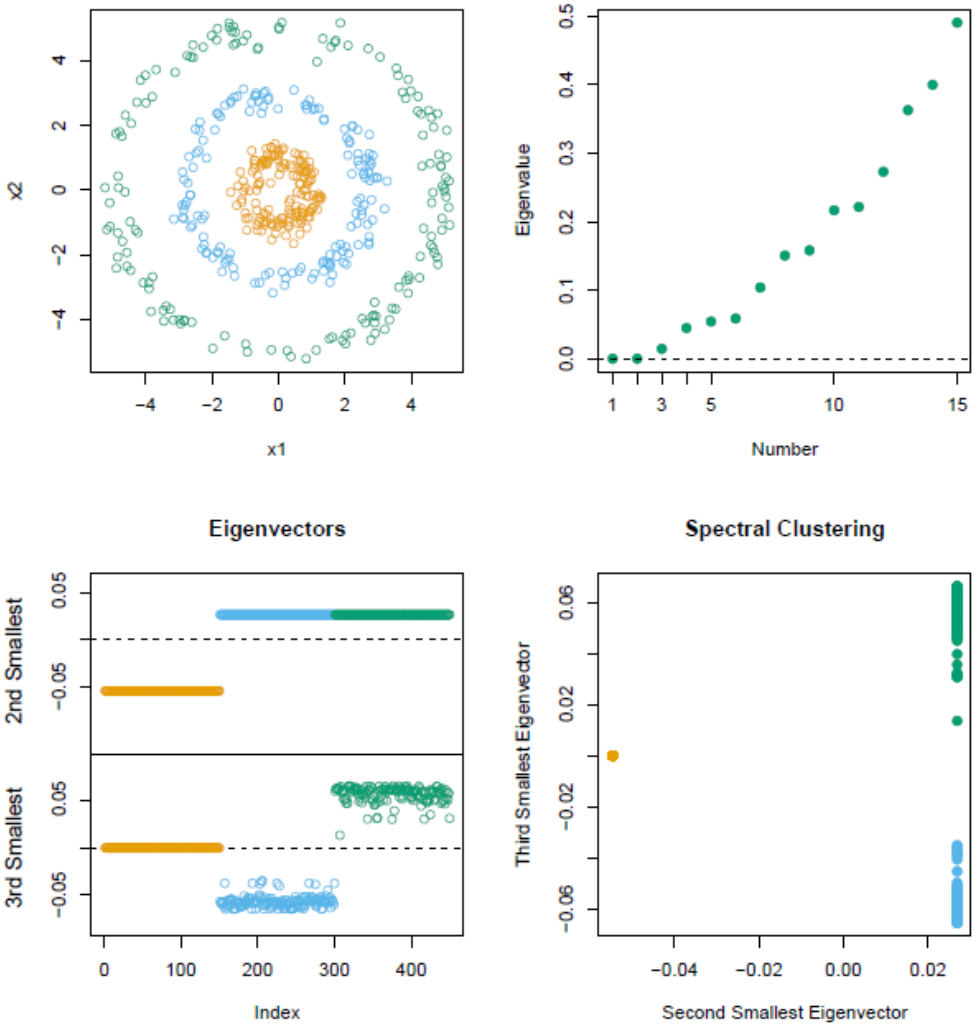
Spectral Clustering exploits a data transformation based on the spectrum (eigenanalysis) of a graph Laplacian matrix for applying non-linear clustering.

Process:

- Construct a fully connected graph G = {V,E,W} using $x_i \in \mathbb{R}^D$, i=1,..,N
- Calculate the graph Laplacian matrix L = D – W
- Apply eigenanalysis to L and keep the eigen-vectors corresponding to the d smallest eigenvalues, in order to form new d-dimensional data representations y_i.
- Apply a clustering algorithm (K-Means) using y_i.
- Assign the cluster labels to x_i.

Spectral Clustering

Example:



Multi-view Embedding

Until now we used one representation for each sample. However, there are cases where a sample can be represented based on different modalities/views (e.g. a video can be represented by a vector encoding visual information and another vector encoding sound information).

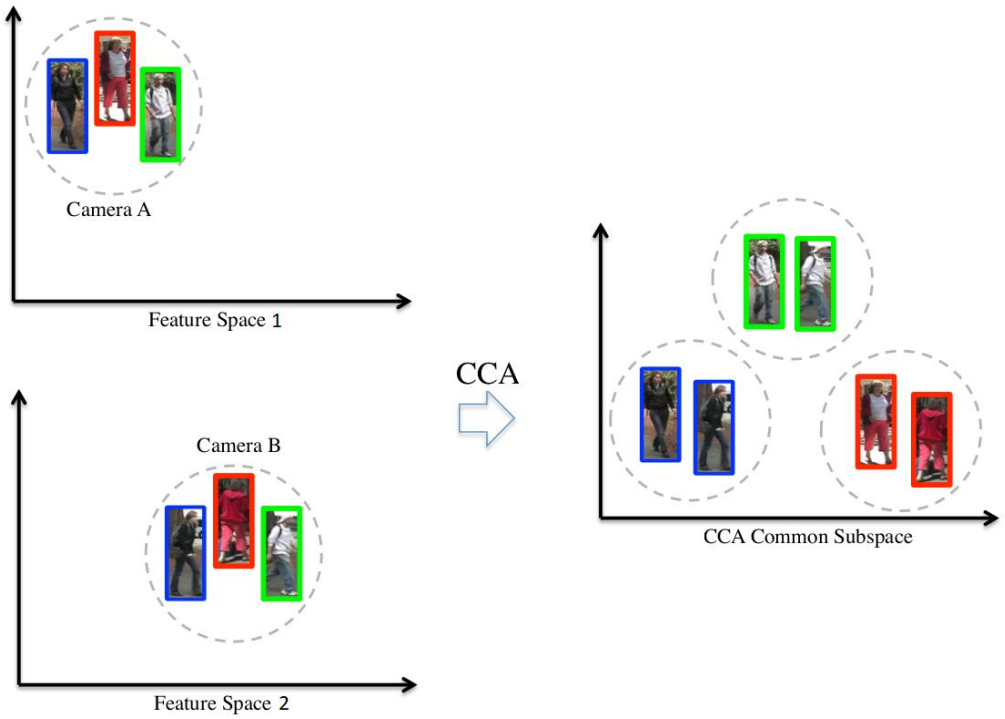
In Multi-view Embedding with V views:

- Each sample is represented by V vectors → V data matrices X_1, X_2, …, X_V
- We want to jointly use the information encoded in all V matrices to enhance performance

Multi-view Embedding

Canonical Correlation Analysis:

- Given two data views ($X_1 \in \mathbb{R}^{D_1 \times N}$ and $X_2 \in \mathbb{R}^{D_2 \times N}$) we want to determine data representations in a common (sub-)space $\mathbb{R}^d$ such that data correlation is maximized



Multi-view Embedding

Canonical Correlation Analysis:

- Given two data views ($X_1 \in \mathbb{R}^{D_1 \times N}$ and $X_2 \in \mathbb{R}^{D_2 \times N}$) we want to determine data representations in a common (sub-)space $\mathbb{R}^d$ such that data correlation is maximized
- For linear projections we have: $Y_1 = W_1^T X_1$ and $Y_2 = W_2^T X_2$
- $W_1 \in \mathbb{R}^{D_1 \times d}$ and $W_2 \in \mathbb{R}^{D_2 \times d}$ are obtained by optimizing:

$$\mathcal{J} = \arg\max_{\mathbf{W}_1, \mathbf{W}_2} \operatorname{corr}(\mathbf{W}_1^\top \mathbf{X}_1, \mathbf{W}_2^\top \mathbf{X}_2)$$

$$= \arg\max_{\mathbf{W}_1, \mathbf{W}_2} \frac{\mathbf{W}_1^\top \boldsymbol{\Sigma}_{12} \mathbf{W}_2}{\sqrt{\mathbf{W}_1^\top \boldsymbol{\Sigma}_{11} \mathbf{W}_1} \cdot \sqrt{\mathbf{W}_2^\top \boldsymbol{\Sigma}_{22} \mathbf{W}_2}}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix} = \frac{1}{N} \begin{bmatrix} \bar{\mathbf{X}}_1 \bar{\mathbf{X}}_1^\top & \bar{\mathbf{X}}_1 \bar{\mathbf{X}}_2^\top \\ \bar{\mathbf{X}}_2 \bar{\mathbf{X}}_1^\top & \bar{\mathbf{X}}_2 \bar{\mathbf{X}}_2^\top \end{bmatrix}$$

centered data

Multi-view Embedding

Multi-view Discriminant Analysis:

- Define data projections $Y_1 = W_1^T X_1$ and $Y_2 = W_2^T X_2$ using a generalization of the within-class and between-class variance

$$\mathbf{S}_W^M = \sum_{i=1}^{V}\sum_{j=1}^{V}\mathbf{W}_i^\top\mathbf{X}_i\left(\mathbf{I} - \sum_{c=1}^{C}\frac{1}{N_c}\mathbf{e}_c\mathbf{e}_c{}^\top\right)\mathbf{X}_j^\top\mathbf{W}_j$$

$$\mathbf{S}_B^M = \sum_{i=1}^{V}\sum_{j=1}^{V}\mathbf{W}_i^\top\mathbf{X}_i\left(\sum_{c=1}^{C}\frac{1}{N_c}\mathbf{e}_c\mathbf{e}_c{}^\top - \frac{1}{N}\mathbf{e}\,\mathbf{e}^\top\right)\mathbf{X}_j^\top\mathbf{W}_j$$

- $W_1 \in \mathbb{R}^{D_1 \times d}$ and $W_2 \in \mathbb{R}^{D_2 \times d}$ are obtained by optimizing:

$$\mathcal{J} = \arg\max_{\mathbf{W}} \frac{\mathrm{Tr}(\mathbf{S}_B^M)}{\mathrm{Tr}(\mathbf{S}_W^M)}$$

Multi-view Embedding

Generalized Multi-view Embedding:

- Define two graphs G and G' with graph Laplacians L and L', respectively.
- Define the projections $Y_1 = W_1^T X_1$ and $Y_2 = W_2^T X_2$, where $W_1 \in \mathbb{R}^{D_1 \times d}$ and $W_2 \in \mathbb{R}^{D_2 \times d}$ are obtained by optimizing:

$$\mathcal{J} = \underset{\mathbf{W}^\top \mathbf{W} = \mathbf{I}}{\arg\max} \frac{\sum_{v=0}^{V} \sum_{i=0}^{N} \sum_{j=0}^{N} \mathbf{S}'_{vij} \|\mathbf{W}_v^\top \mathbf{X}_{vi} - \mathbf{W}_v^\top \mathbf{X}_{vj}\|^2}{\sum_{v=0}^{V} \sum_{i=0}^{N} \sum_{j=0}^{N} \mathbf{S}_{vij} \|\mathbf{W}_v^\top \mathbf{X}_{vi} - \mathbf{W}_v^\top \mathbf{X}_{vj}\|^2}$$

$$= \underset{\mathbf{W}^\top \mathbf{W} = \mathbf{I}}{\arg\max} \frac{\mathrm{Tr}(\mathbf{W}^\top \mathbf{X} \mathbf{L}' \mathbf{X}^\top \mathbf{W})}{\mathrm{Tr}(\mathbf{W}^\top \mathbf{X} \mathbf{L} \mathbf{X}^\top \mathbf{W})}.$$

Multi-view Embedding

Generalized Multi-view Embedding:

- Define two graphs G and G' with graph Laplacians L and L', respectively.
- Define the projections $Y_1 = W_1^T X_1$ and $Y_2 = W_2^T X_2$, where $W_1 \in \mathbb{R}^{D_1 \times d}$ and $W_2 \in \mathbb{R}^{D_2 \times d}$
- Generalization of many multi-view methods of the form:

$$\mathcal{J} = \arg\max_{\mathbf{W}} \frac{\mathrm{Tr}(\mathbf{W}^\top \mathbf{P} \mathbf{W})}{\mathrm{Tr}(\mathbf{W}^\top \mathbf{Q} \mathbf{W})}$$

where the projection matrices $W = [W_1^T W_2^T \ldots W_V^T]^T$ are obtained by solving:

$$\mathbf{P}\mathbf{W} = \rho\, \mathbf{Q}\mathbf{W}$$

Multi-view Embedding

$$\mathbf{PW} = \rho\,\mathbf{QW}$$

	$\mathbf{P}$	$\mathbf{Q}$
MvCCA	$\begin{bmatrix} \mathbf{0} & \boldsymbol{\Sigma}_{12} & \cdots & \boldsymbol{\Sigma}_{1V} \\ \boldsymbol{\Sigma}_{21} & \mathbf{0} & \cdots & \boldsymbol{\Sigma}_{2V} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma}_{V1} & \boldsymbol{\Sigma}_{V2} & \cdots & \mathbf{0} \end{bmatrix}$	$\begin{bmatrix} \boldsymbol{\Sigma}_{11} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_{22} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{\Sigma}_{VV} \end{bmatrix}$
MvPLS	$\begin{bmatrix} \mathbf{0} & \boldsymbol{\Sigma}_{12} & \cdots & \boldsymbol{\Sigma}_{1V} \\ \boldsymbol{\Sigma}_{21} & \mathbf{0} & \cdots & \boldsymbol{\Sigma}_{2V} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma}_{V1} & \boldsymbol{\Sigma}_{V2} & \cdots & \mathbf{0} \end{bmatrix}$	$\begin{bmatrix} \mathbf{I} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{I} \end{bmatrix}$
MvMDA	$\begin{bmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} & \cdots & \mathbf{P}_{1V} \\ \mathbf{P}_{21} & \mathbf{P}_{22} & \cdots & \mathbf{P}_{21} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{P}_{V1} & \mathbf{P}_{V2} & \cdots & \mathbf{P}_{VV} \end{bmatrix}$	$\begin{bmatrix} \mathbf{Q}_{11} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_{22} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{Q}_{VV} \end{bmatrix}$