Dimensionality Reduction

- Typical PR problems involve dozens, hundreds, or even thousands of features
- For example, in bioinformatics:
  - Tumor classification involves 10,000+ features: 30,000+ genes or 60,000+ transcripts
  - Email or text classification: 1,000+ features; 2-grams, 3-grams, 4-grams, etc.
- Now, we need:
  - *high* classification accuracy, while
  - *reducing* computational complexity (in training and classification phases)
- While it is not easy to achieve **both**,
  - we may *substantially* improve one
  - while *slightly* diminishing the other
- How is this achieved?
  - Dimensionality reduction

- Feature generation:
  - Using combinations of original features generate new (fewer) ones
  - Linear combinations: Linear Dimensionality Reduction (LDR)
  - Nonlinear combinations (e.g., kernels): Nonlinear Dimensionality Reduction (NLDR)
- Feature selection:
  - A subset of features from original ones that delivers reasonable (or even better) classification performance

Linear Dimensionality Reduction

- **Aim:** Use linear combinations of original features to generate new (fewer) features in a lower dimensional space
- Main Schemes:
  - Unsupervised:
    - Principal Component Analysis (PCA)
    - Singular Value Decomposition (SVD)
    - Independent Component Analysis (ICA)
    - Nonnegative Matrix Factorization (NMF)
    - Linear Autoencoder
  - Supervised:
    - Linear Discriminant Analysis (LDA):
      - Fisher's Discriminant Analysis (FDA) or homoscedastic
      - Heteroscedastic Discriminant Analysis (HDA)
      - Chernoff Discriminant Analysis (CDA)

Principal Component Analysis

- Seeks a projection that best represents the data… in a sum of squared-errors sense.
- It better applies to *unsupervised* classification
- Unsuitable for *supervised* classification (though it can be applied, if no other method is suitable)

- Given $D = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$
- What is the vector $\mathbf{x}_0$ that best represents D in the sum of squared-errors sense?
- That is, we want to *minimize*

$$J_0(\mathbf{x}_0) = \sum_{k=1}^{n} \left\| \mathbf{x}_0 - \mathbf{x}_k \right\|^2$$

- The solution to this problem is given by $\mathbf{m} = \mathbf{x}_0$, where

$$\mathbf{m} = \frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k$$

  is the sample mean
- The mean is a *zero-dimensional* representation of *D*
- But… it does not reveal info about the dispersion of the samples in *D*
- Let's seek a *one-dimensional* representation
- say, the line $\mathbf{x} = \mathbf{m} + a\mathbf{e}$

  where:
  - the line passes through **m**
  - **e** is a unit vector in the direction of the line, and
  - scalar *a* is the distance from **x** to **m**

- If we represent $\mathbf{x}_k$ by $\mathbf{m} + a_k \mathbf{e}$, then minimizing the sum of squared errors implies minimizing:

$$J_1(a_1,\ldots,a_n,\mathbf{e}) = \sum_{k=1}^{n} \left\|(\mathbf{m} + a_k\mathbf{e}) - \mathbf{x}_k\right\|^2$$

$$= \sum_{k=1}^{n} a_k^2 \left\|\mathbf{e}\right\|^2 - 2\sum_{k=1}^{n} a_k \mathbf{e}^t(\mathbf{x}_k - \mathbf{m}) + \sum_{k=1}^{n} \left\|\mathbf{x}_k - \mathbf{m}\right\|^2$$

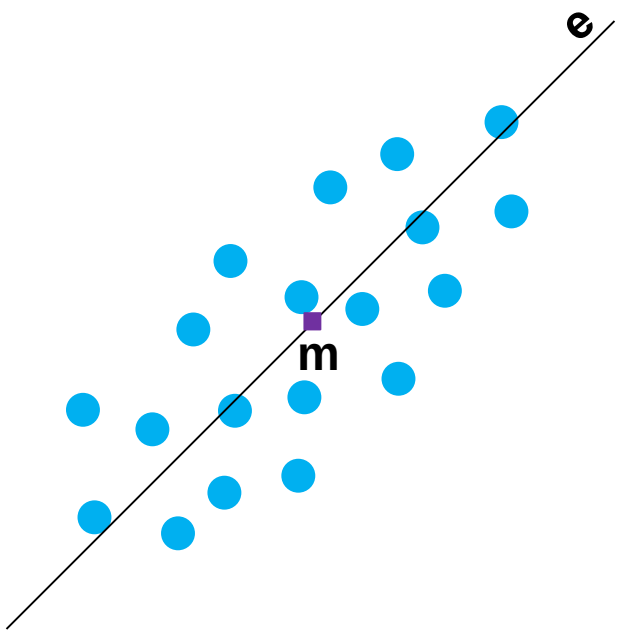
- whose solution is (where $\|\mathbf{e}\|^2 = 1$):

$$a_k = \mathbf{e}^t(\mathbf{x}_k - \mathbf{m})$$

Geometrically

- We project vector $\mathbf{x}_k$ onto the line, in the direction of **e** that passes through **m**
- What is the *best* direction of **e**?
- Lets introduce the *scatter matrix* **S**

$$\mathbf{S} = \sum_{k=1}^{n} (\mathbf{x}_k - \mathbf{m})(\mathbf{x}_k - \mathbf{m})^t$$



- Substituting a_k for the solution found, we have:

$$J_1(\mathbf{e}) = \sum_{k=1}^{n} a_k^2 - 2\sum_{k=1}^{n} a_k \mathbf{e}^t(\mathbf{x}_k - \mathbf{m}) + \sum_{k=1}^{n} \|\mathbf{x}_k - \mathbf{m}\|^2$$

$$= -\sum_{k=1}^{n} \left[\mathbf{e}^t(\mathbf{x}_k - \mathbf{m})\right]^2 + \sum_{k=1}^{n} \|\mathbf{x}_k - \mathbf{m}\|^2$$

$$= -\mathbf{e}^t\mathbf{S}\mathbf{e} + \sum_{k=1}^{n} \|\mathbf{x}_k - \mathbf{m}\|^2$$

- Then, the vector **e** that *minimizes* J_1 also *maximizes* $\mathbf{e}^t\mathbf{S}\mathbf{e}$
- Using the method of Lagrange multipliers, we differentiate:

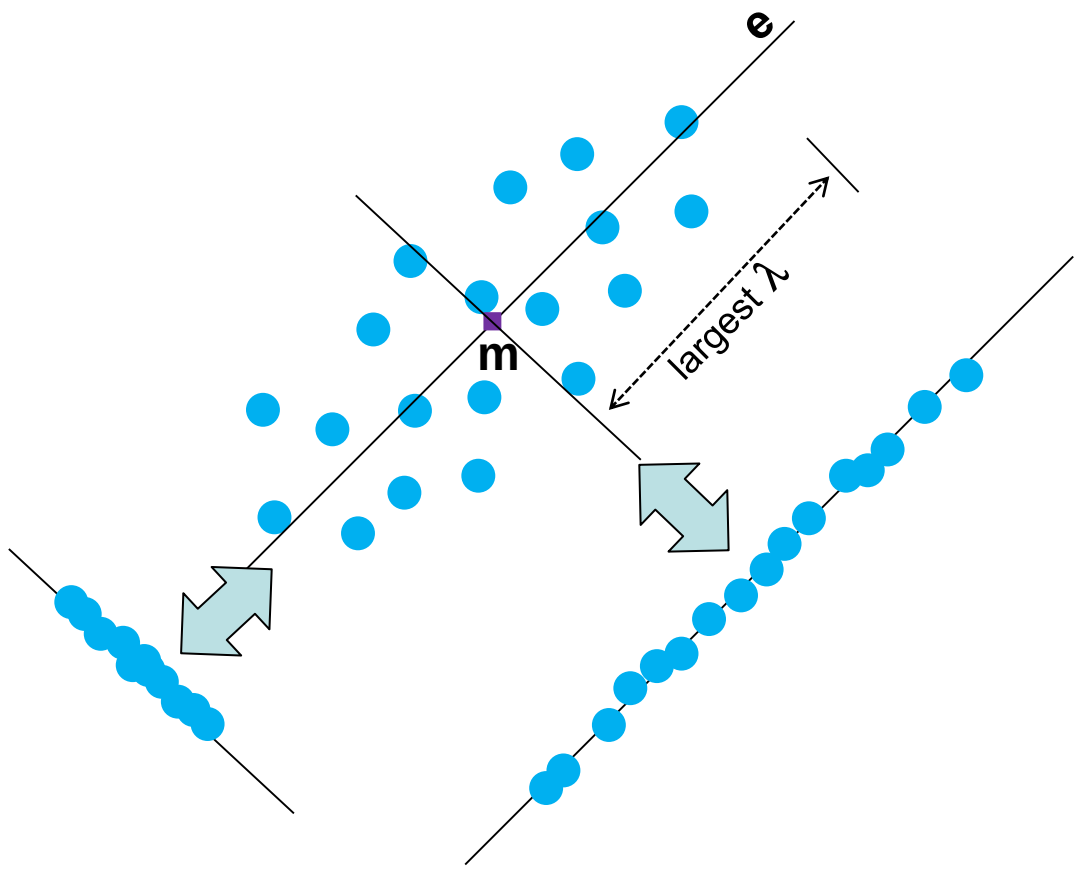
$$u = \mathbf{e}^t\mathbf{S}\mathbf{e} - \lambda(\mathbf{e}^t\mathbf{e} - 1) \qquad [\ \mathbf{e}^t\mathbf{e} - 1 = 0\ ]$$

- with respect to **e** obtaining

$$2\mathbf{S}\mathbf{e} - 2\lambda\mathbf{e} = \mathbf{0} \quad \text{or equivalently} \quad \mathbf{S}\mathbf{e} = \lambda\mathbf{e}$$

- Clearly, λ is an eigenvalue of **S**
- Since $\mathbf{e}^t\mathbf{S}\mathbf{e} = \lambda\mathbf{e}^t\mathbf{e} = \lambda$, then …
- maximizing $\mathbf{e}^t\mathbf{S}\mathbf{e}$ is equivalent to finding …

  the largest eigenvalue of **S**
- Thus, the **best** one-dimensional projection of the data in the sum-of-squared-error sense
  - is in the *direction* of the eigenvector **e**
  - having the *largest* eigenvalue λ
- Can be generalized to consider higher dimensions



- Then, the projection is onto a hyperplane:

$$\mathbf{x} = \mathbf{m} + \sum_{i=1}^{m} a_i \mathbf{e}_i$$

  and the aim is to find *m* vectors
- The solution is given by the *m* eigenvectors $\mathbf{e}_i$ of **S**
  having the *largest* eigenvalues λ_i
- Since **S** is *real* and *symmetric*,
  the eigenvectors are orthogonal
- They then form a basis in the *m*-dimensional space, and
  coefficients a_i are called the “principal components”

How to apply PCA?

Given $D = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$

- Find the scatter matrix $\mathbf{S}$
- Find the eigenvalue decomposition of $\mathbf{S}$:
  - $\mathbf{\Phi} = [\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_d]$ are the eigenvectors
  - $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ are the eigenvalues
- Arrange eigenvectors and eigenvalues such that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$
- Put the first *m* eigenvectors in a matrix

$$\mathbf{A} = \left[\boldsymbol{\phi}_1^t, \boldsymbol{\phi}_2^t, \ldots, \boldsymbol{\phi}_m^t\right]^t$$

- For each $\mathbf{x}_i$, perform $\mathbf{y}_i = \mathbf{A}\,\mathbf{x}_i$

Example

4 classes:

D_1={[1,10],[1,9],[1,7],[1,6],[1,5],[2,8],[2,9],[2,10],[3,9],[3,11],[4,9],[5,9],[6,9],[7,9],[5, 10],[5,11]}^{t}

D_2={[5,3],[6,1],[6,2],[7,1],[7,2],[7,3],[7,5],[8,2],[8,4]}^{t}

D_3={[8,6],[9,3],[9,4],[9,5],[10,2],[10,3],[10,4],[10,5],[10,6],[9,7],[11,3]}^{t}

D_4={[3,3],[3,4],[3,2],[2,2],[2,4],[3,5],[4,3]}^{t}

where $\mathbf{x} \in D \quad \text{and} \quad n = |D|$

- Calculate the sample mean: $\mathbf{m} = \frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k = \begin{bmatrix} 5.46 \\ 5.46 \end{bmatrix}$

- Calculate the *scatter matrix* **S**:

$$\mathbf{S} = \sum_{k=1}^{n} (\mathbf{x}_k - \mathbf{m})(\mathbf{x}_k - \mathbf{m})^t = \begin{bmatrix} 9.92 & -3.67 \\ -3.67 & 9.25 \end{bmatrix}$$

- The *eigenvectors* and *eigenvalues* of **S** are:

$$\mathbf{e}_1 = \begin{bmatrix} -0.67 & -0.74 \end{bmatrix}^t \qquad \lambda_1 = 5.90$$

$$\mathbf{e}_2 = \begin{bmatrix} -0.74 & 0.67 \end{bmatrix}^t \qquad \lambda_2 = 13.28$$

- Then, the largest eigenvalue is $\lambda_2 = 13.28$,

which corresponds to eigenvector $\mathbf{e}_2$

- Project the data D_1, D_2, D_3 and D_4 in the direction of $\mathbf{e}_2$

$$\mathbf{y}_i = \mathbf{e}_2 \mathbf{x}_i \quad \text{with } i = 1,\ldots,n$$

$$\mathbf{y}_1 = \begin{bmatrix} -0.74 & 0.67 \end{bmatrix} \begin{bmatrix} 1 \\ 10 \end{bmatrix} = 5.96$$

$$\mathbf{y}_2 = \begin{bmatrix} -0.74 & 0.67 \end{bmatrix} \begin{bmatrix} 1 \\ 9 \end{bmatrix} = 5.29$$

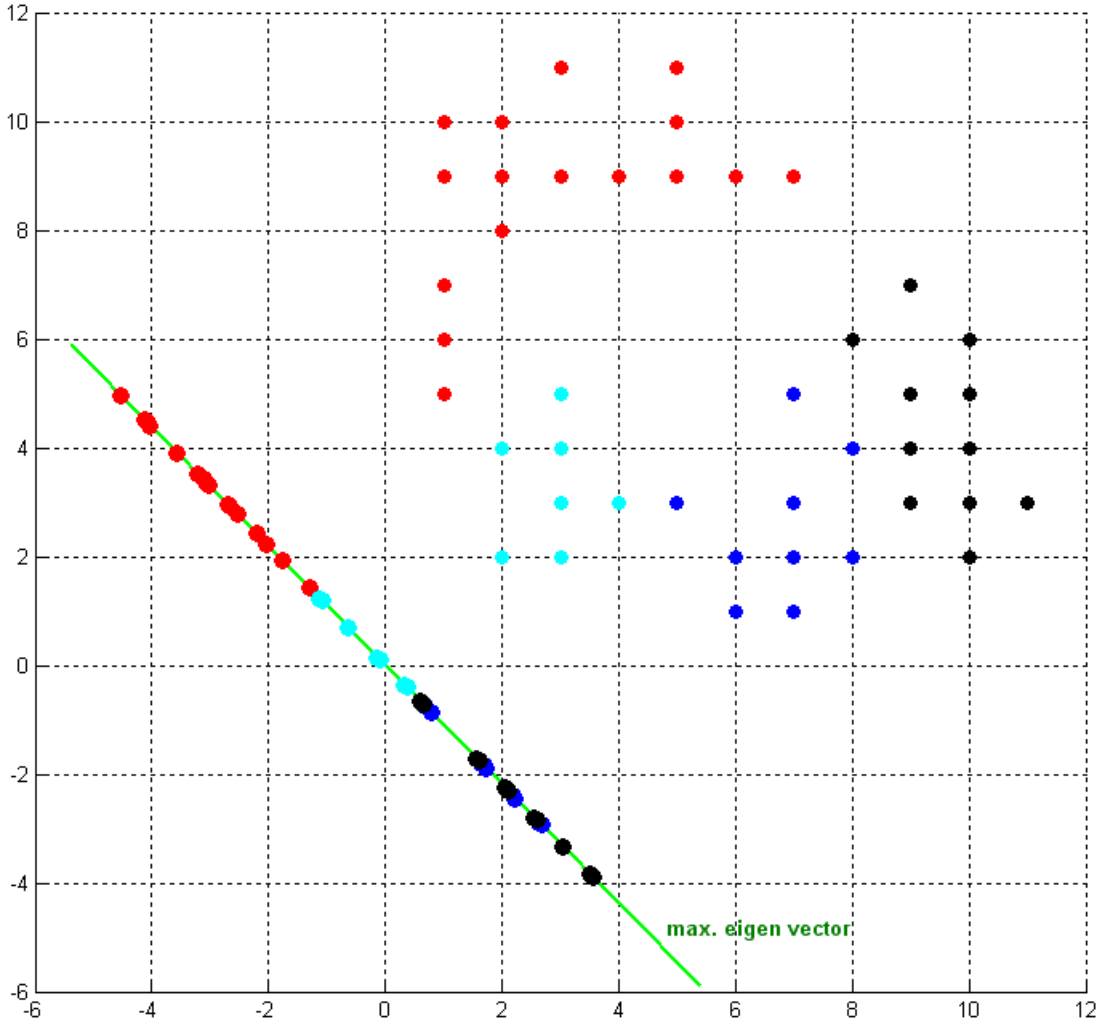
$$\mathbf{y}_3 = \begin{bmatrix} -0.74 & 0.67 \end{bmatrix} \begin{bmatrix} 1 \\ 7 \end{bmatrix} = 3.95$$

$$\vdots$$

$$\mathbf{y}_n = \begin{bmatrix} -0.74 & 0.67 \end{bmatrix} \mathbf{x}_n$$

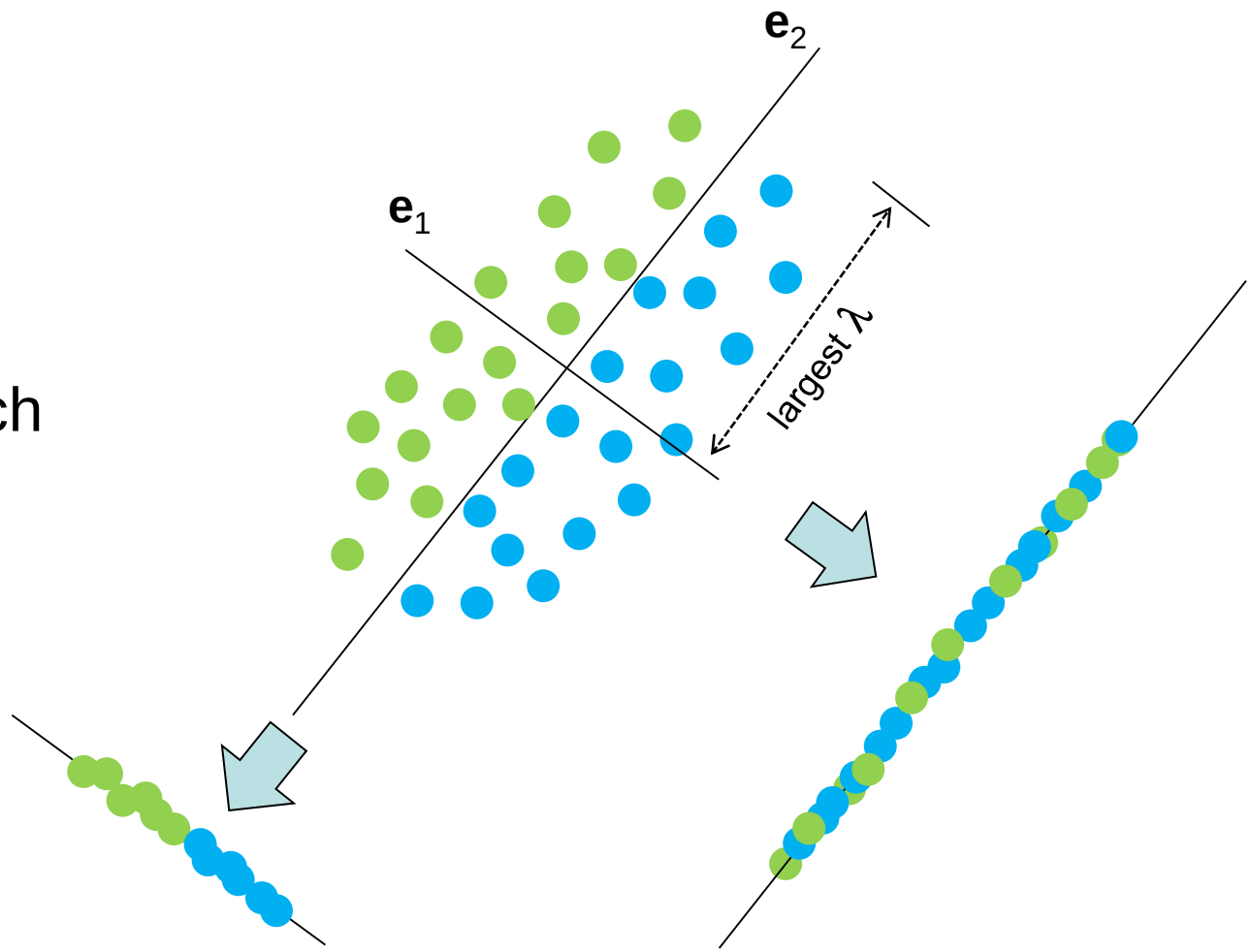
where $\mathbf{y}_i$ is the projection of $\mathbf{x}_i$ on the 1D space

Graphically



Example 2: Unsupervised vs Supervised LDR

- 2 dimensions
- 2 classes
- ≠ means
- Similar covariances
- PCA may not be the best approach for a supervised classification problem!

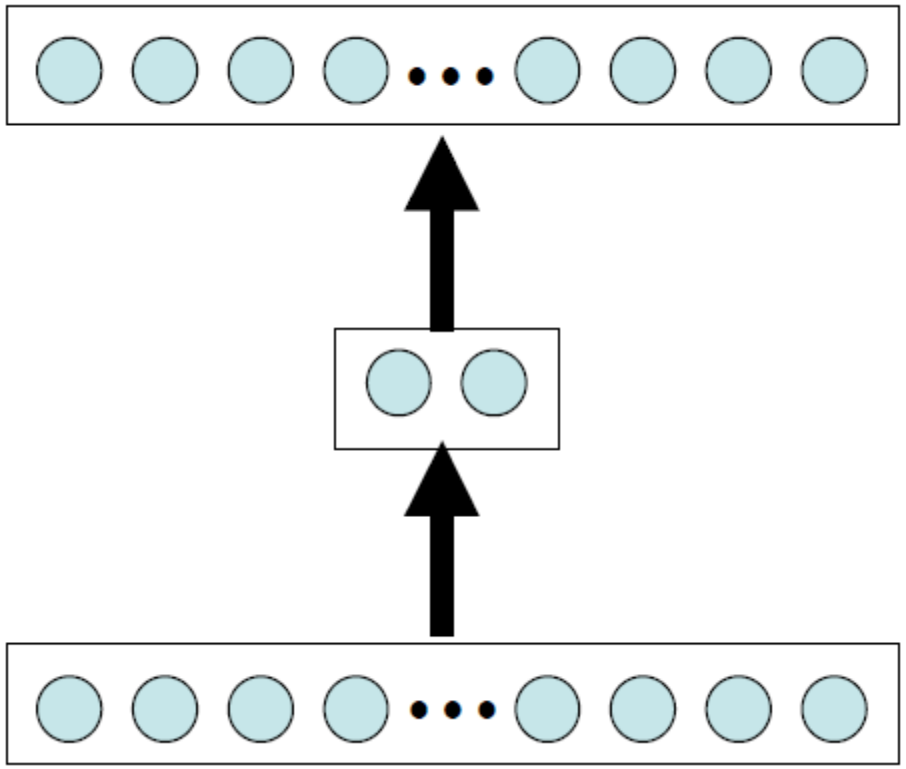


PCA vs Linear Autoencoder

- Autoencoder:
- Each layer implements a linear transformation
- Cost function:
- Minimize the reconstruction error

$$\mathcal{L} = \sum_{\mathbf{x}_i \in D} \|\mathbf{x}_i - \mathbf{A}^t \mathbf{A} \mathbf{x}_i\|_2^2$$

where $\mathbf{A}$ is the transformation matrix obtained by PCA



Singular Value Decomposition (SVD)

- Given $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$
- We can write:

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n]$$

- $\mathbf{X}$ is a matrix of rank $r \leq \min\{n, d\}$
- There exist unitary matrices $\mathbf{U}, \mathbf{V}$ such that

$$\mathbf{X} = \mathbf{U} \begin{bmatrix} \mathbf{\Lambda}^{1/2} & 0 \\ 0 & 0 \end{bmatrix} \mathbf{V}^t$$

where $\mathbf{0}$ is a matrix of zeros and

$\mathbf{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_r)$ contains the r nonzero eigenvalues of $\mathbf{X}^t\mathbf{X}$

SVD

- Removing zero sub-matrices, we can write the SVD of $\mathbf{X}$ as:

$$\mathbf{X} = [\mathbf{u}_1, \ldots, \mathbf{u}_r] \begin{bmatrix} \sqrt{\lambda_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sqrt{\lambda_r} \end{bmatrix} \begin{bmatrix} \mathbf{v}_1{}^t \\ \vdots \\ \mathbf{v}_r{}^t \end{bmatrix}$$

where $\mathbf{u}_i$ and $\mathbf{v}_i$ are the corresponding eigenvectors of the nonzero eigenvalues of $\mathbf{X}\mathbf{X}^t$ and $\mathbf{X}^t\mathbf{X}$ resp.

SVD

- We can also write:

$$\mathbf{X} = \sum_{i=1}^{r} \sqrt{\lambda_i}\mathbf{u}_i{\mathbf{v}_i}^t$$

- This is an exact representation of $\mathbf{X}$
- But we can do, instead, dimensionality reduction as follows:
  - Sort the eigenvalues: $\lambda_1 \geq \cdots \geq \lambda_r$
  - and pick the largest m eigenvalues $(m \leq r)$
- Then, an approximation of $\mathbf{X}$ is:

$$\mathbf{X} \cong \hat{\mathbf{X}} = \sum_{i=1}^{m} \sqrt{\lambda_i}\mathbf{u}_i{\mathbf{v}_i}^t$$

SVD

- In matrix form, $\widehat{\mathbf{X}}$ is expressed as:

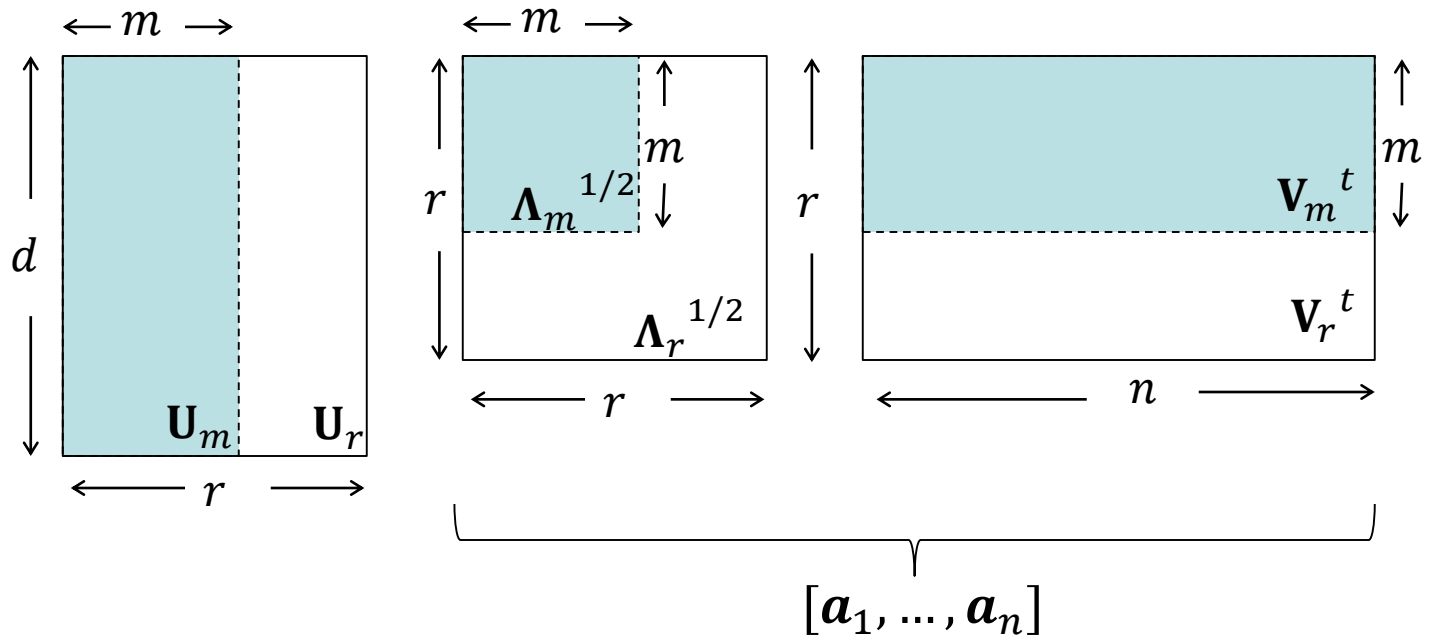
$$\widehat{\mathbf{X}} = \mathbf{U}_m \boldsymbol{\Lambda}_m{}^{1/2} \mathbf{V}_m{}^t = \mathbf{U}_m \, [\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n]$$

  where $\mathbf{U}_m = [\mathbf{u}_1, \ldots, \mathbf{u}_m]$ and $\mathbf{V}_m = [\mathbf{v}_1, \ldots, \mathbf{v}_m]$

- Each $\mathbf{x}_i$ is projected onto the m-dimensional subspace spanned by $\mathbf{U}_m$
- $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ are the corresponding vectors in the new space
- SVD vs PCA:
  - $\widehat{\mathbf{X}}$ is the best rank-m approximation of $\mathbf{X}$ in the Frobenius space
  - whereas the optimality of PCA is in terms of the mean square error

SVD

- SVD graphically:



- PCA vs SVD:
  - PCA is statistics-oriented
    - Uses the parameters of the distributions
  - SVD is data-oriented
    - Decomposes the data matrix itself

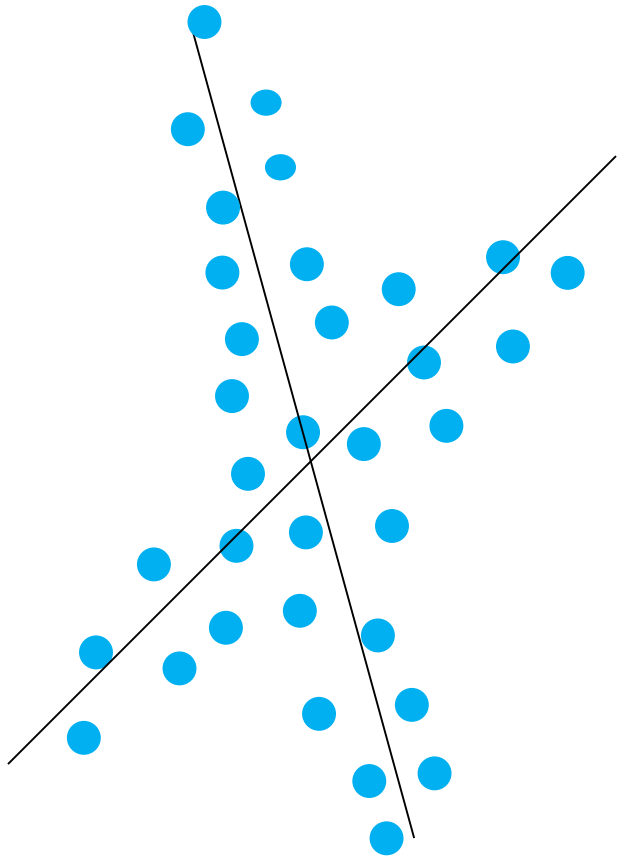
Independent Component Analysis (ICA)

- PCA focuses more on correlation of random variables (second order moments)
- Independent component analysis considers higher order moments

Given $\mathbf{Z} = \{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n\}$

For each $\mathbf{z}_t$, perform $\hat{\mathbf{x}}_t = \mathbf{W}^{-1}\mathbf{z}_t$

- Find $\mathbf{W}$ whose vectors are mutually independent
- Methods based on:
  - MLE + gradient
  - FastICA: based on Hessian matrix
    - Approximate Newton method
- PCA finds orthogonal vectors for projection, whereas
- ICA finds linearly independent vectors (not necessarily orthogonal)



The Cocktail Party Problem

- You’re in a cocktail party
- Many people talking at the same time
- We can we understand anything at all?
- Problem: Blind signal separation or blind source separation
- Applicable to EEG, financial or other types of data

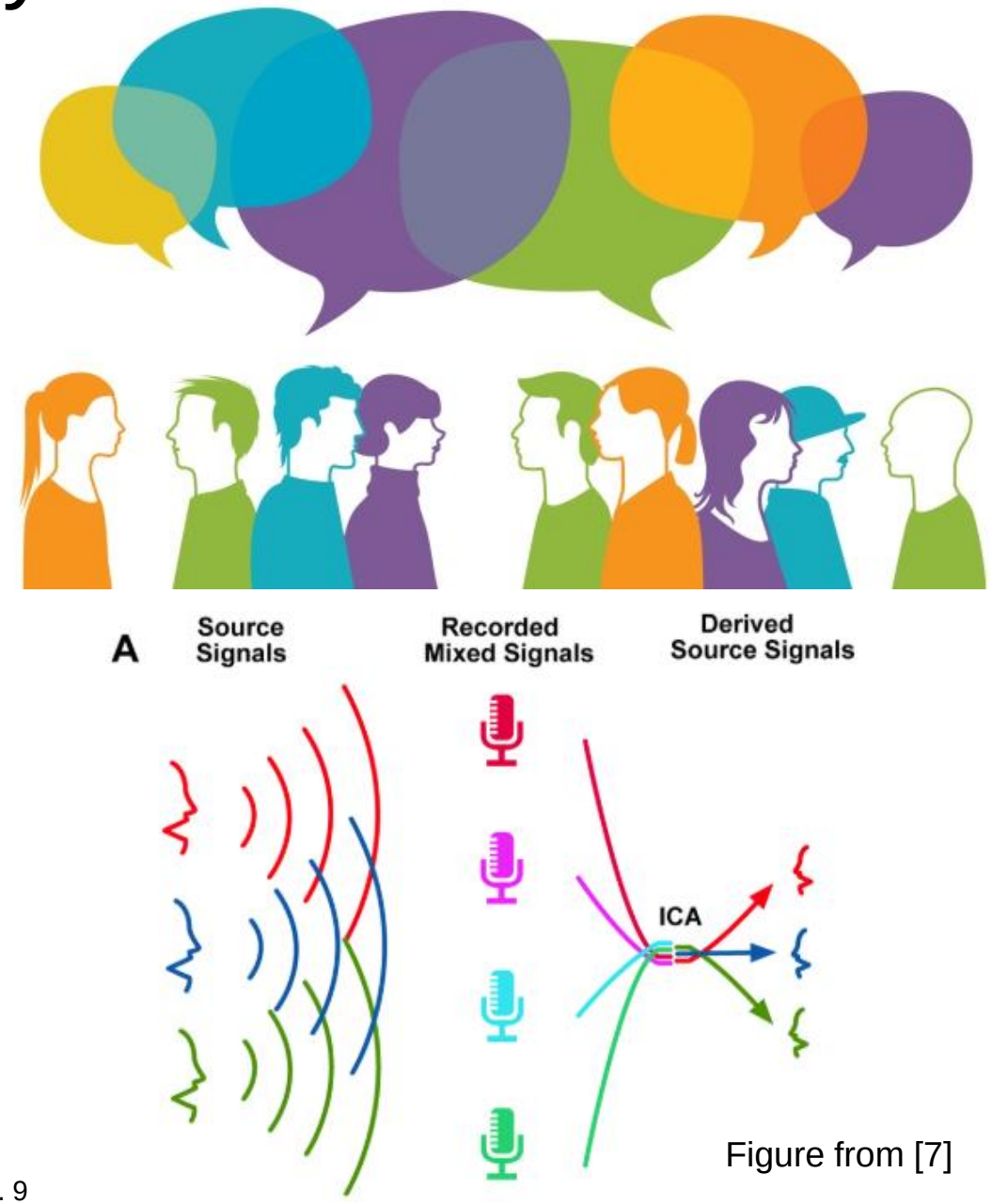
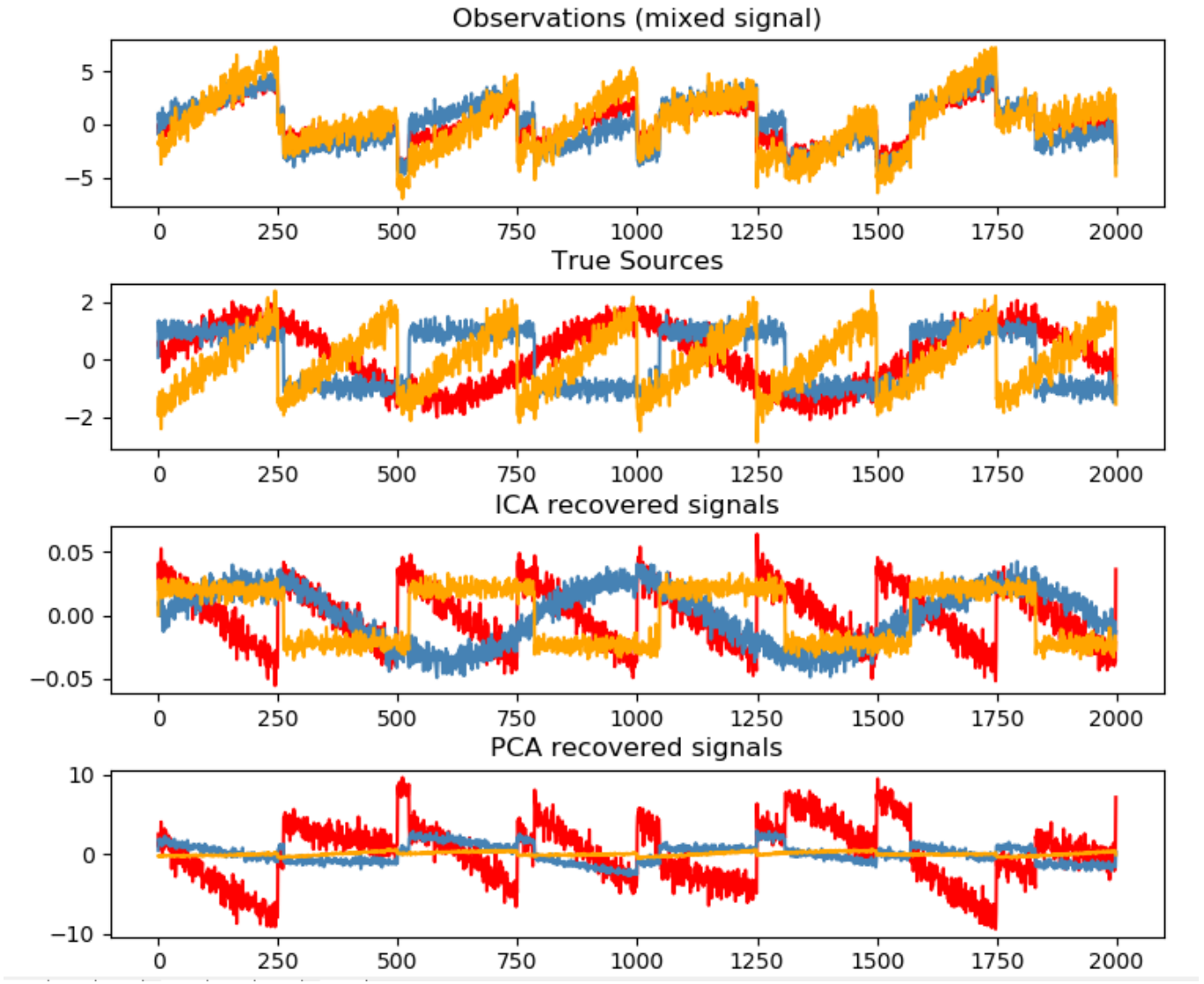


Figure from [7]

Musical Instruments

- Problem similar to the cocktail party
- 3 musical instruments played at the same time
- $d = l = 3$
- Data is sampled over time
- May not be the case in other applications



ICA – Problem Formulation

More formally:

- $\mathbf{x}_t \in \mathbb{R}^d$ are the observed signals
- t = time
- $\mathbf{z}_t \in \mathbb{R}^l$ is the source of signals
- Assume $d = l$
- i.e., we know how many people are talking at the same time
- Assume that

$$\mathbf{x}_t = \mathbf{W}\mathbf{z}_t + \boldsymbol{\epsilon}_t$$

where $\mathbf{W}$ is a $d \times l$ matrix

and $\boldsymbol{\epsilon}_t \sim N(\mathbf{0}, \boldsymbol{\Psi})$;

$\boldsymbol{\Psi}$ is aka "white noise"

In general, we assume $\boldsymbol{\Psi}$ is zero

- Given $\mathbf{Z}$, the aim is to find $\mathbf{W}$ whose rows are not necessarily orthogonal

where $\mathbf{z}_t$ follows a distribution:

$$p(\mathbf{z}_t) = \prod_{j=1}^{l} p_j(z_{tj})$$

- This distribution is like "mixture" of distributions.
- In case of PCA, we would be restricted to Gaussian distributions

Algorithms:

- MLE
- FastICA (uses 2nd order derivatives)
- Expectation maximization

Example – PCA vs ICA

- 2D data $\mathbf{Z}$ generated randomly
- 2 t-student data generated (true independent sources)
- Data mixed with matrix

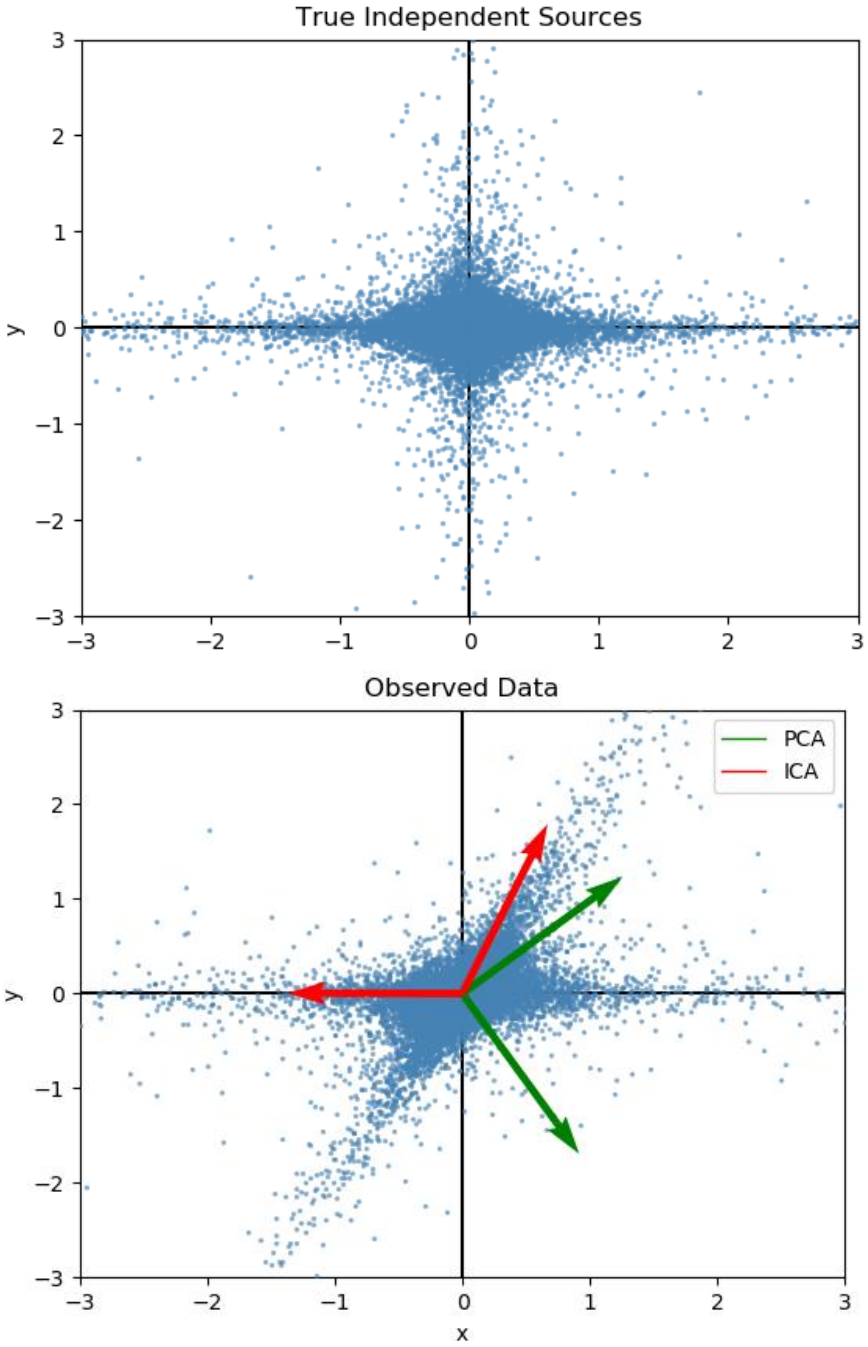
$$\mathbf{W} = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$$

- $\mathbf{W}$ is not orthogonal
- PCA and FastICA applied to Observed Data $\mathbf{X} = \mathbf{WZ}$
- Components of PCA are orthogonal but not capture the 2 signals
- Components of ICA are not orthogonal but represent the 2 signals better
- Apply inverse transformation

$$\hat{\mathbf{Z}} = \mathbf{W}^{-1}\mathbf{Z}$$

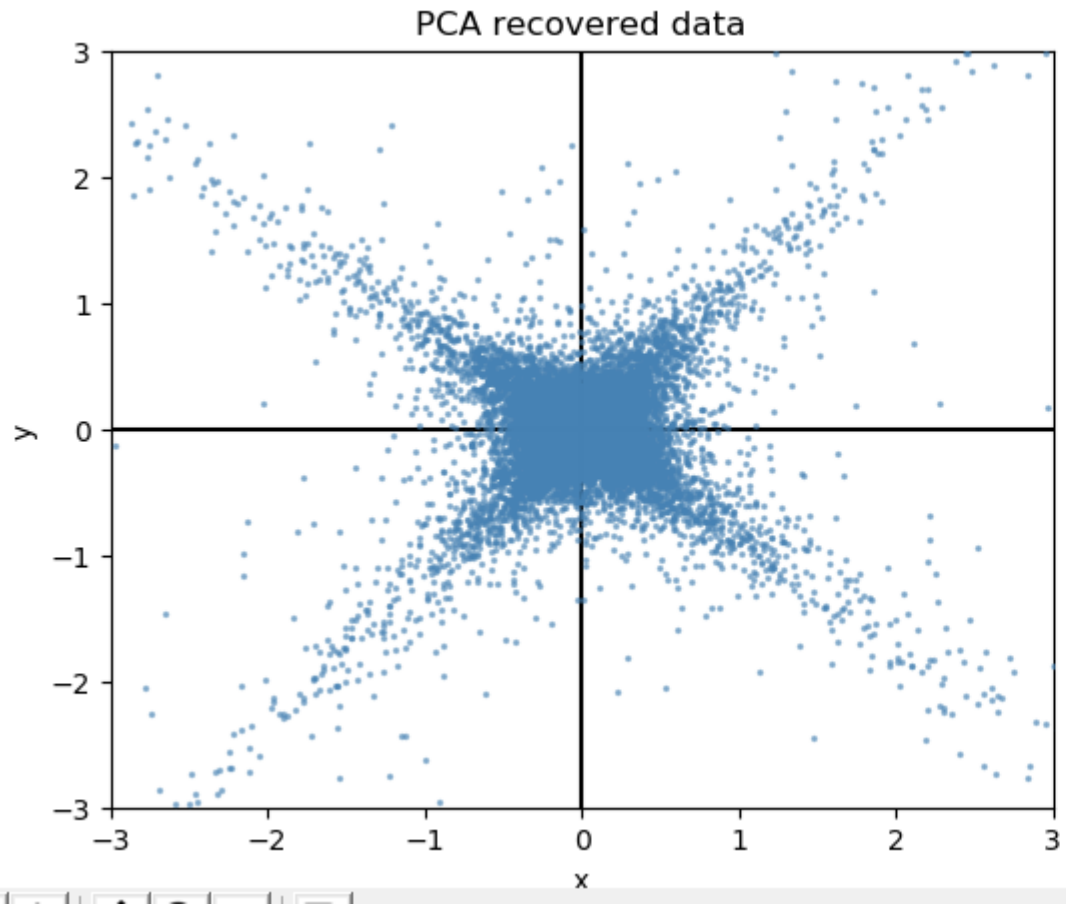
$$\text{where } \mathbf{W} = \begin{bmatrix} 1 & -0.5 \\ 0 & 0.5 \end{bmatrix}$$

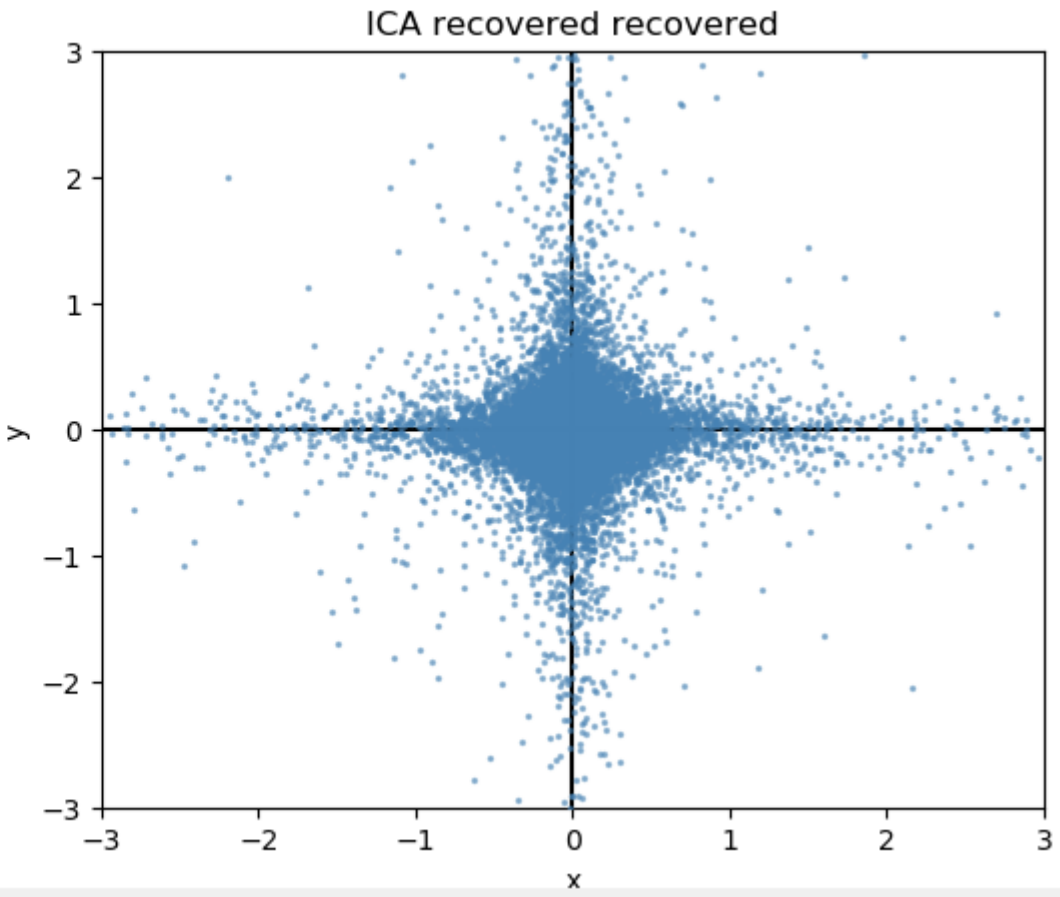
- The actual matrix obtained from FastICA $\widehat{\mathbf{W}}$ is slightly different from $\mathbf{W}$



Recovered data from PCA and ICA

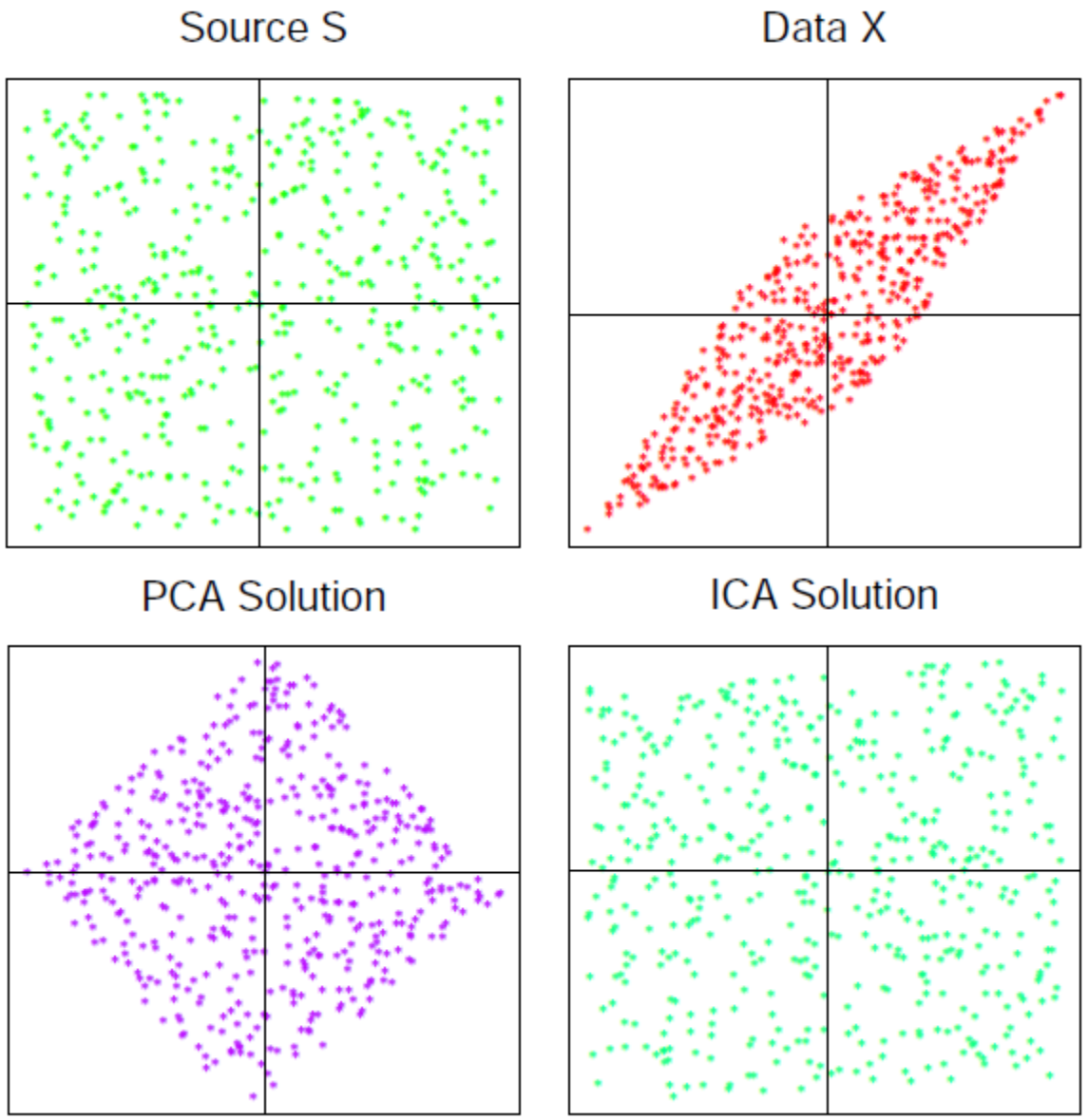
$$\hat{\mathbf{X}} = \mathbf{W}^{-1}\mathbf{Y}$$





Example - ICA

- Source, S: 500 random points uniformly distributed on the plane
- Data, X: points after applying an arbitrary non-orthogonal linear transformation
- PCA captures the main diagonals but not the shape
- ICA recovers the original data with high accuracy



Nonnegative Matrix Factorization (NMF)

- Given $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$
- We can write:

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n]$$

- $\mathbf{X}$ is a matrix of rank $r \leq \min\{n, d\}$
- Recall SVD, which aims to find an approximation of $\mathbf{X}$:

$$\mathbf{X} \cong \widehat{\mathbf{X}} = \sum_{i=1}^{m} \sqrt{\lambda_i}\mathbf{u}_i{\mathbf{v}_i}^t$$

where $\widehat{\mathbf{X}}$ is the best rank-m approximation of $\mathbf{X}$

- Problems with PCA/SVD
  - Original matrix $\mathbf{X}$ is typically dense
  - Interpretation of basis vectors is difficult because it contains negative values
  - It is very difficult to obtain a good value of *m*
  - Can't deal with sparse matrices

$$\begin{bmatrix} 0 & 3.8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5.2 & 0 & 0 \\ 0 & 0 & -3.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10 & 0 \end{bmatrix}$$

NMF

- Given a sparse *n* x *d* matrix:

$$\mathbf{X} = [\mathbf{x}_1^t, \ldots, \mathbf{x}_n^t]^t$$

- Find two smaller matrices $\mathbf{P}$ and $\mathbf{Q}$ of dimensions *n* x *m* and *d* x *m* such that

$$\mathbf{X} \approx \widehat{\mathbf{X}} = \mathbf{P}\mathbf{Q}^t$$

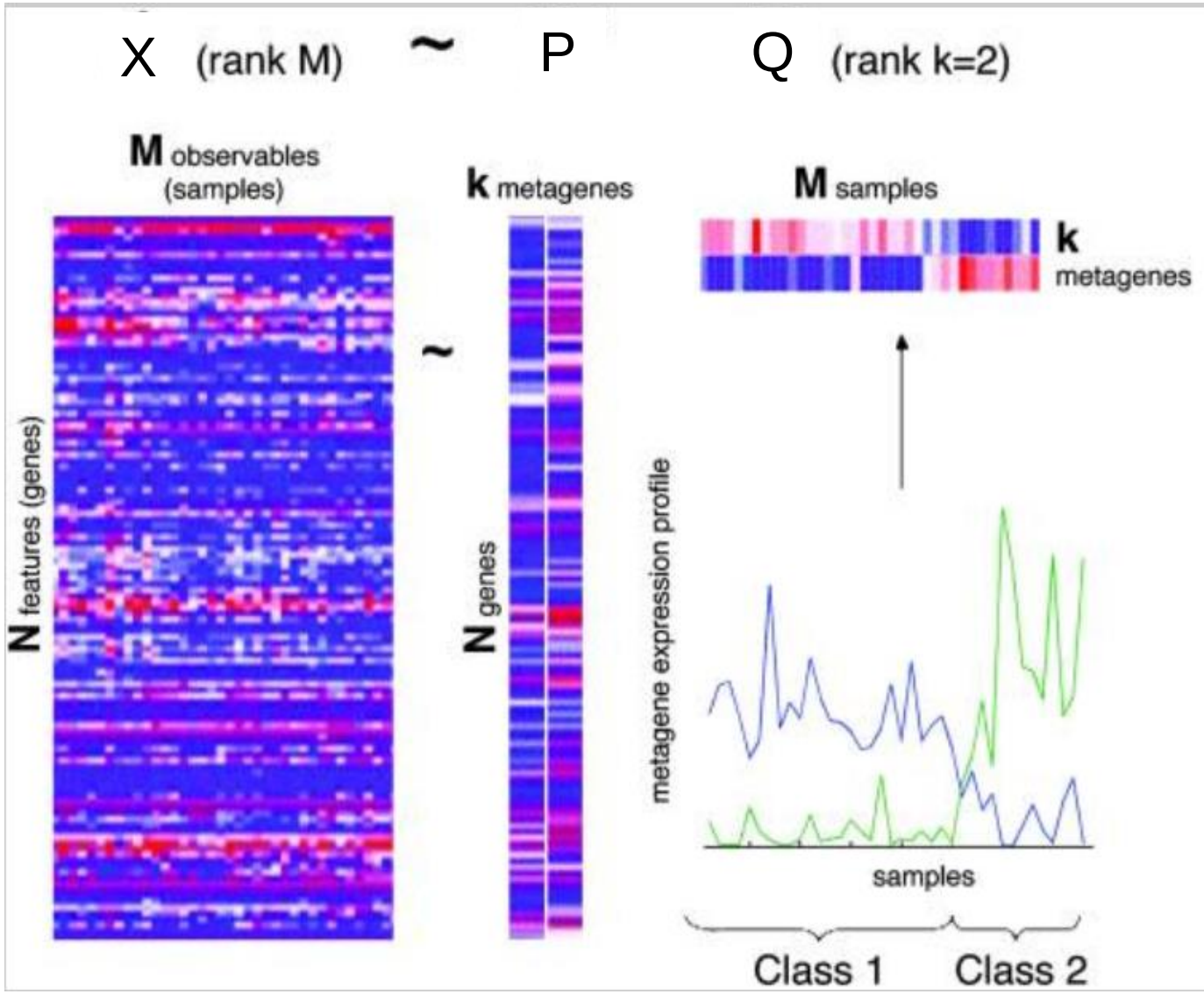
- i.e., $\widehat{\mathbf{X}}$ is an approximation of $\mathbf{X}$
- where $\widehat{\mathbf{X}}$, $\mathbf{P}$ and $\mathbf{Q}$ are nonnegative, i.e., they contain only positive values
- Ideally, $m \ll d$
- Example:

$$\underset{\mathbf{X}}{\begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}} \approx \underset{\mathbf{P}}{\begin{bmatrix} 1.58 & 0 \\ 1.57 & 0.01 \\ 0 & 1.42 \end{bmatrix}} \underset{\mathbf{Q}}{\begin{bmatrix} 0.32 & 0.32 & 0.63 & 0.63 & 0 \\ 0 & 0 & 0.7 & 0 & 0.7 \end{bmatrix}}$$

- The columns of $\mathbf{P}$ are the underlying basis vectors
- each of the d columns of $\widehat{\mathbf{X}}$ can be obtained from the columns of $\mathbf{P}$
- The columns of $\mathbf{Q}$ are the weights associated with each basis vector
- The columns of $\mathbf{P}$ are the new features, and the rows are the samples

NMF - Example

- Microarray data from [5]
- $\mathbf{X}$ contains *n* genes and *d* observables (M in the example)
- Aim is to find *m* metagenes (*k* in example)
- A smaller number of genes meaningful with biological data
  - Just 2 metagenes
  - Can divide data into 2 classes



NMF - Properties

- Basis vectors of $\mathbf{P}$ are not orthogonal
- can overlap samples/features
- Can restrict $\mathbf{P}$, $\mathbf{Q}$ to be sparse
- NMF is algorithm dependent
  - $\mathbf{P}$ and $\mathbf{Q}$ are not unique
- Solved as an optimization problem
- Objective function based on mean squared error

$$\min \left\| \widehat{\mathbf{X}} - \mathbf{PQ} \right\|_F^2$$

- such that $\mathbf{P}, \mathbf{Q} \geq 0$

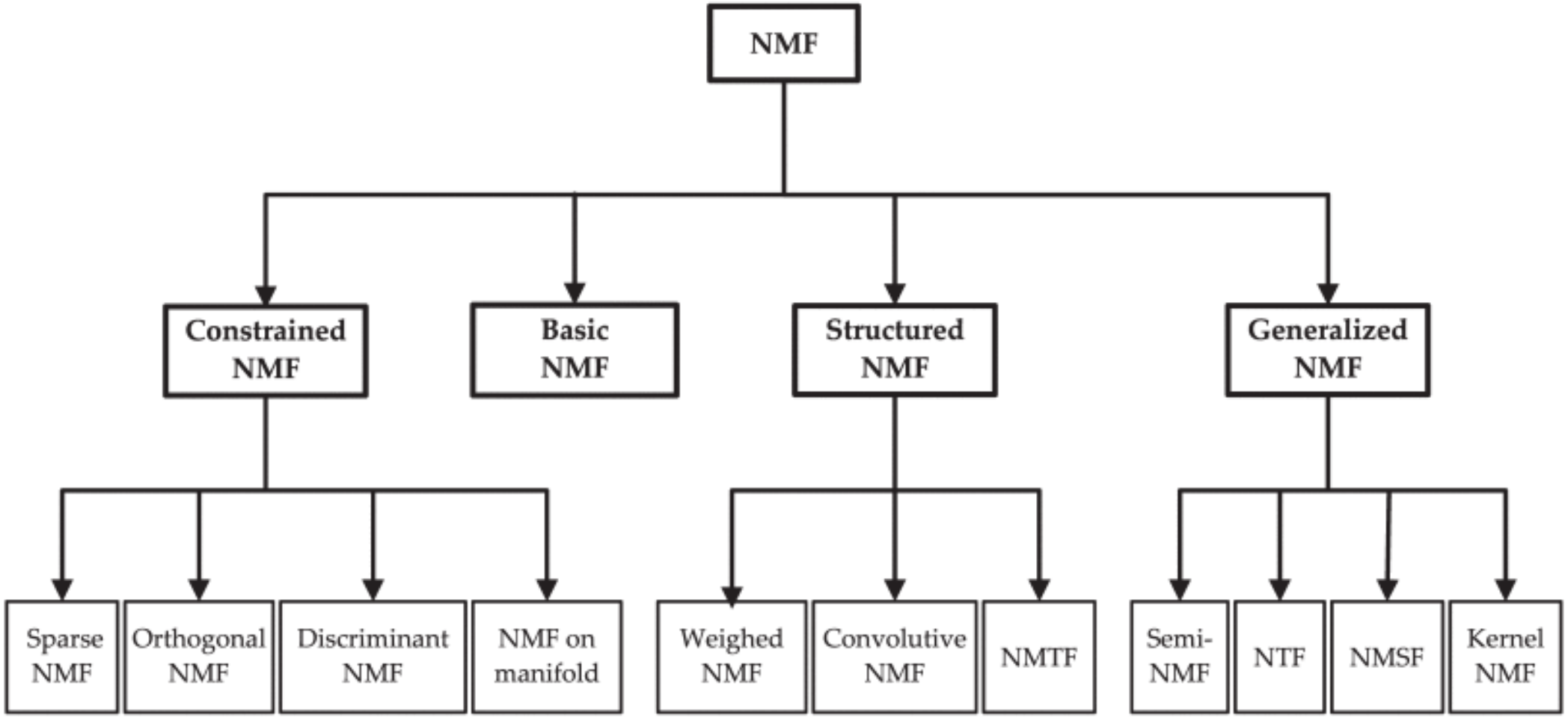
- Nonlinear optimization problem
- Convex in $\mathbf{P}$ or $\mathbf{Q}$ but not on both
- Difficult to obtain a global minimum
- Large number of unknowns, i.e., the values of $\mathbf{P}$ and $\mathbf{Q}$
- Optimization problem not easily solved
- Many algorithms exist

NMF - Algorithms

Four main categories:

- Basic NMF (BNMF), which only imposes the nonnegativity constraint.
- Constrained NMF (CNMF), which imposes some additional constraints as regularization.
- Structured NMF (SNMF), which modifies the standard factorization formulations.
- Generalized NMF (GNMF), which breaks through the conventional data types or factorization modes in a broad sense.

NMF – Algorithms – Schematic view



NMF - Algorithms

Constrained NMF – four subclasses:

- Sparse NMF (SPNMF), which imposes the sparseness constraint.
- Orthogonal NMF (ONMF), which imposes the orthogonality constraint.
- Discriminant NMF (DNMF), which involves the information for classification and discrimination.
- NMF on manifold (MNMF), which preserves the local topological properties.

NMF - Algorithms

Structured NMF – three subclasses:

- Weighed NMF (WNMF), which attaches different weights to different elements regarding their relative importance.
- Convolutive NMF (CVNMF), which considers the time-frequency domain factorization.
- Nonnegative Matrix Trifactorization (NMTF), which decomposes the data matrix into three factor matrices.

NMF - Algorithms

Generalized NMF – four subclasses:

- Semi-NMF, which relaxes the nonnegativity constraint only on the specific factor matrix
- Nonnegative Tensor Factorization (NTF), which generalizes the matrix-form data to higher dimensional tensors.
- Nonnegative Matrix-Set Factorization (NMSF), which extends the data sets from matrices to matrix-sets.
- Kernel NMF (KNMF), which is the nonlinear model of NMF.

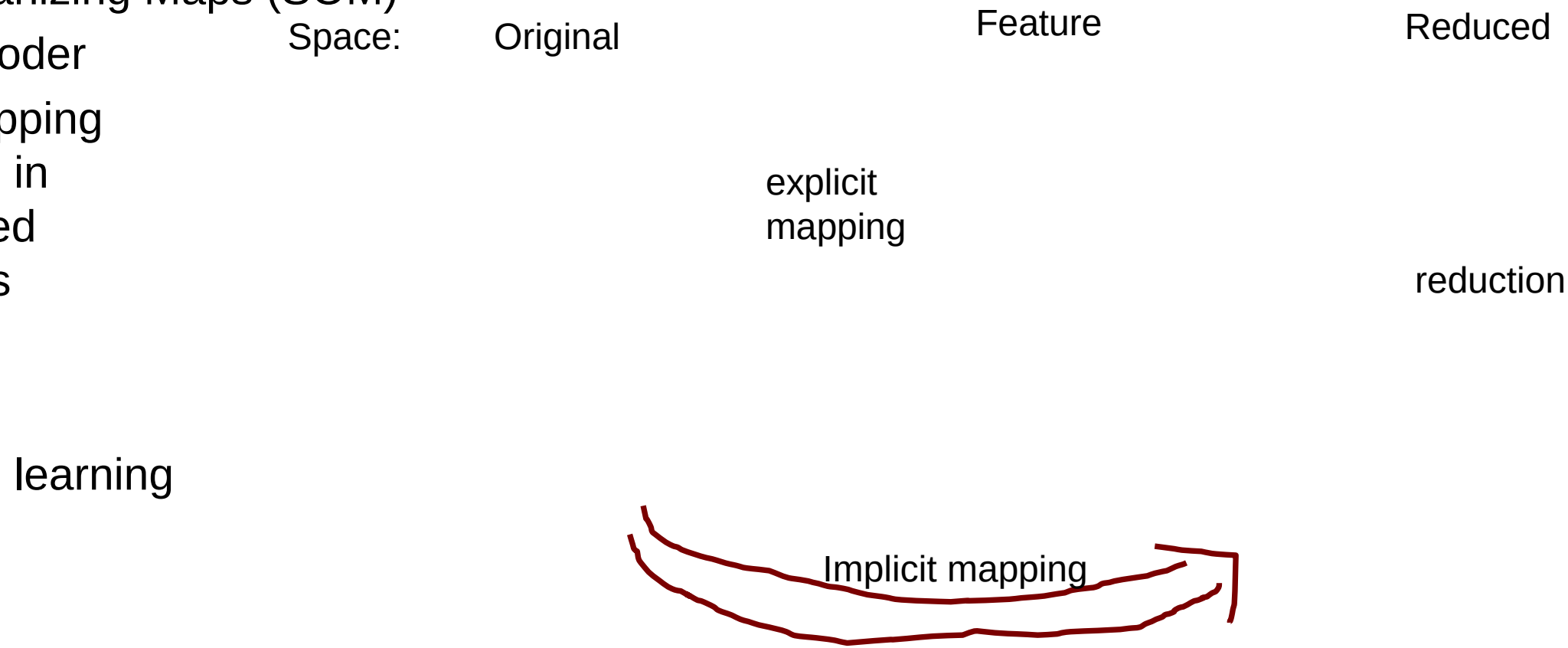
Nonlinear Dimensionality Reduction (NDR)

Methods:

- Kernel-based:
  - PCA, NMF, FDA, HDA, etc… (even SVM)
- Multi-dimensional Scaling (MDS)
- Self-organizing Maps (SOM)
- Autoencoder

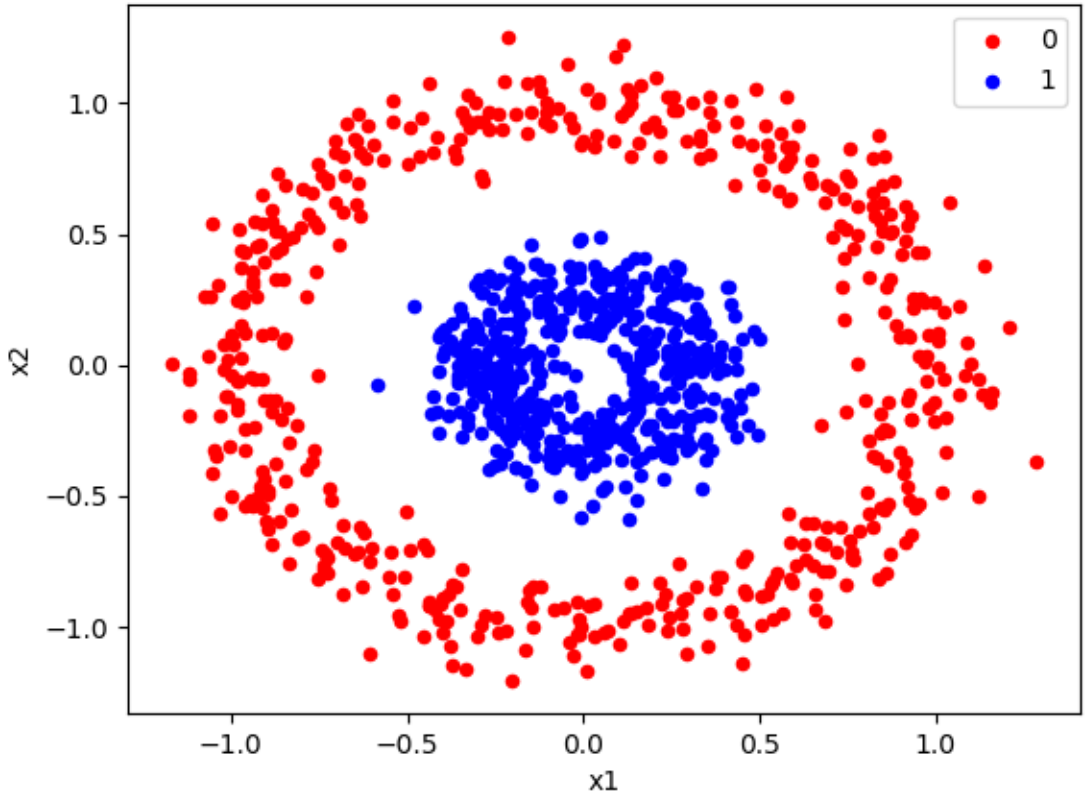
Explicit mapping not needed in kernel-based approaches

- KPCA
- KFDA
- Manifold learning

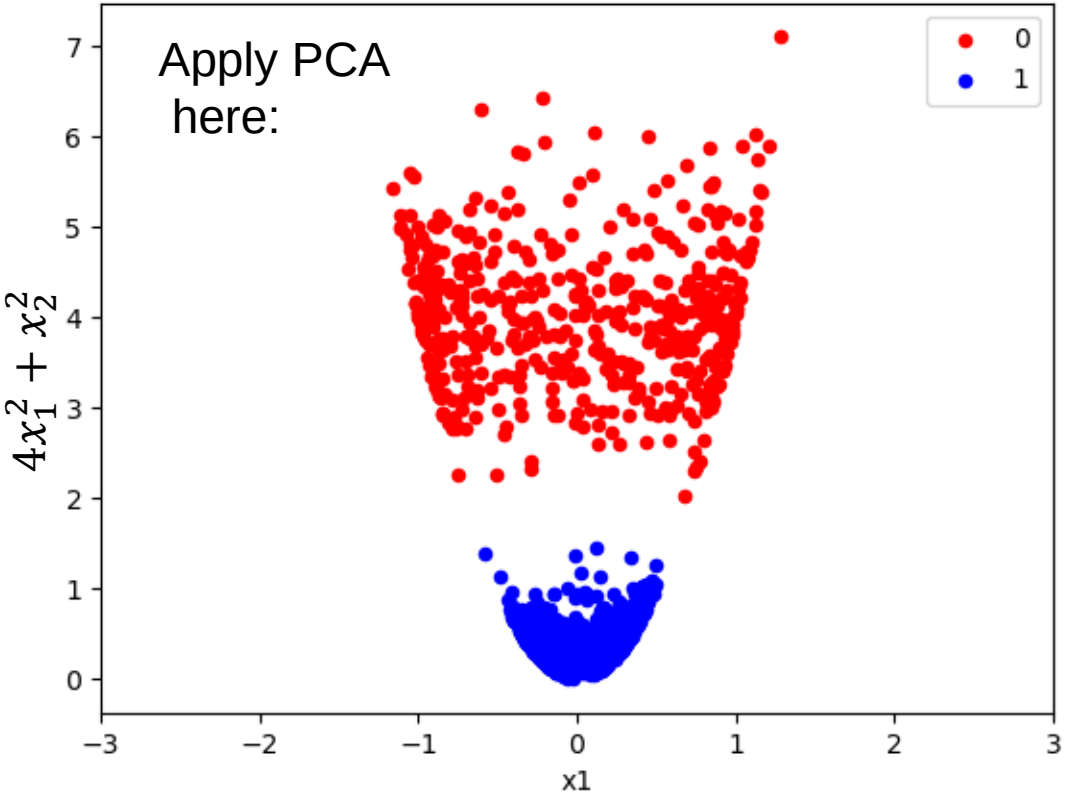


Kernel PCA – Motivation/Example

Original 2D space:



New 2D space:



Kernel PCA

- No known classes (unsupervised)
- Project vectors onto feature space:

$$\mathbf{x}_i \rightarrow \mathbf{\Phi}(\mathbf{x}_i)$$

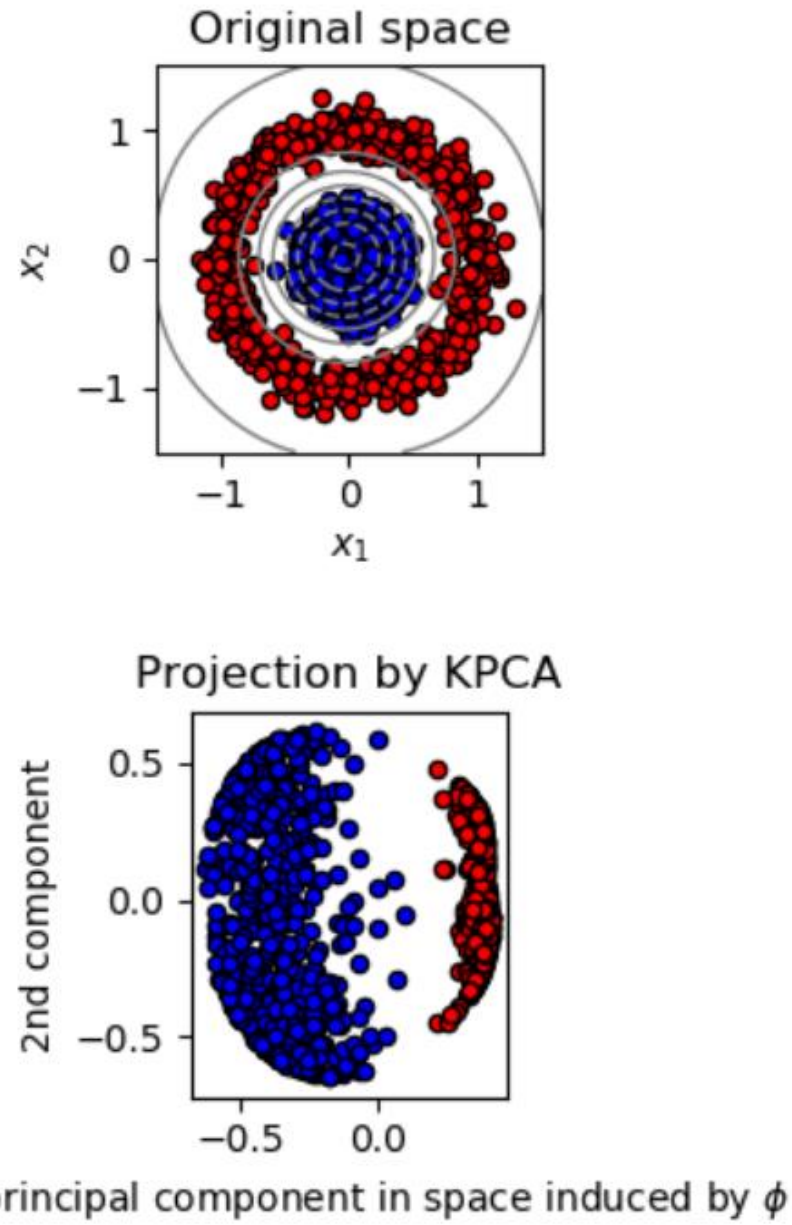
- Not needed, since the kernel trick allows us to use $k(\mathbf{x}, \mathbf{y})$ to replace $(\mathbf{\Phi}(\mathbf{x}) \cdot \mathbf{\Phi}(\mathbf{y}))$
- An eigenvector V of covariance in target space

$$\mathbf{V} = \sum_{i=1}^{n} \alpha_i \tilde{\mathbf{\Phi}}(\mathbf{x}_i)$$

- where

$$\tilde{\mathbf{\Phi}}(\mathbf{x}_i) = \mathbf{\Phi}(\mathbf{x}_i) - \frac{1}{n} \sum_{r=1}^{n} \mathbf{\Phi}(\mathbf{x}_r)$$

- α_i are the components of $\boldsymbol{\alpha}$



Kernel PCA

$\boldsymbol{\alpha}$ is an eigenvector of

$$\tilde{K}_{ij} = \left(\tilde{\boldsymbol{\Phi}}(\mathbf{x}_i) \cdot \tilde{\boldsymbol{\Phi}}(\mathbf{x}_j)\right)$$

choose length of $\boldsymbol{\alpha}$ such that:

$$||\mathbf{V}|| = 1 \Leftrightarrow ||\boldsymbol{\alpha}||^2 = 1/\lambda$$

for this, we need:

$$\tilde{K}_{ij} = K_{ij} - \frac{1}{n}\sum_{r=1}^{n} K_{ir} - \frac{1}{n}\sum_{r=1}^{n} K_{rj} + \frac{1}{n^2}\sum_{r,s=1}^{n} K_{rs}$$

where:

$$K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

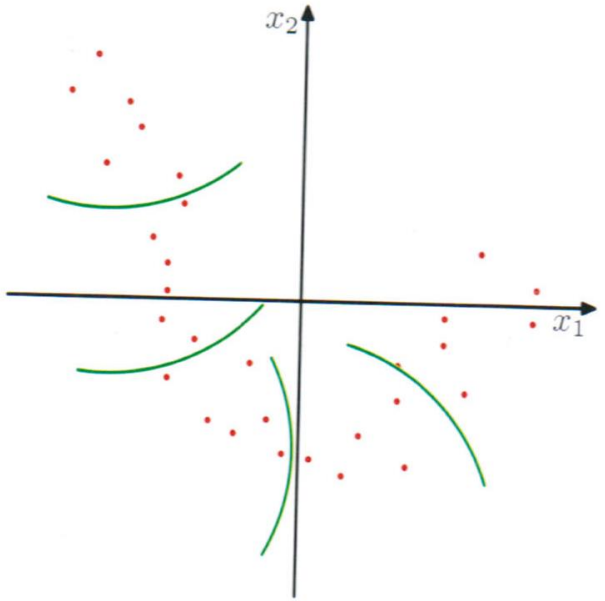
K is the Gram matrix and contains $k(\mathbf{x}_i, \mathbf{x}_j)$ for all pairs of vectors $\mathbf{x}_i$ and $\mathbf{x}_j$

Implementation of Kernel PCA

- Compute the Gram matrix K
- Compute the *m* dominant eigenvalues and eigenvectors of K
  - $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_m$
- Compute the *m* projections of each dimension of $\mathbf{x}$, y_k, onto each of the dominant eigenvectors
  - $y_k = \langle \mathbf{V}_k, \boldsymbol{\phi}(\mathbf{x}) \rangle = \sum_{i=1}^{d} \alpha_i^k \mathbf{K}(\mathbf{x}_i, \mathbf{x}), \ k = 1, \ldots, m$
- $\mathbf{y} = [y_1, \ldots, y_m]^t$ is the new vector

Kernel PCA: Example 1

original space



feature space

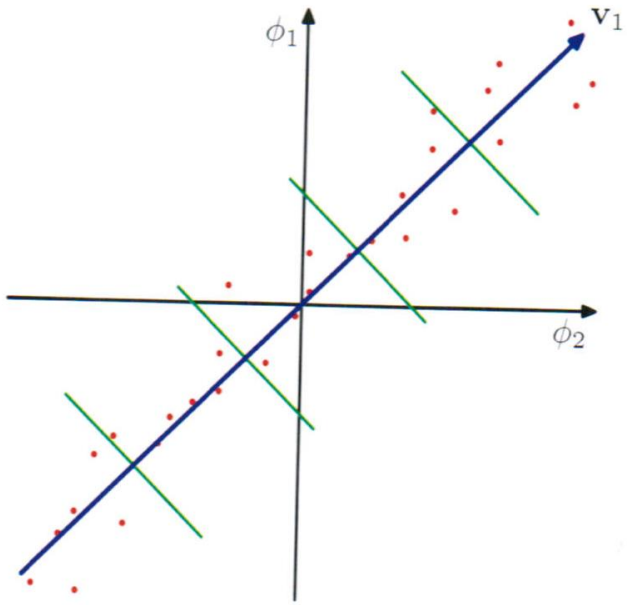
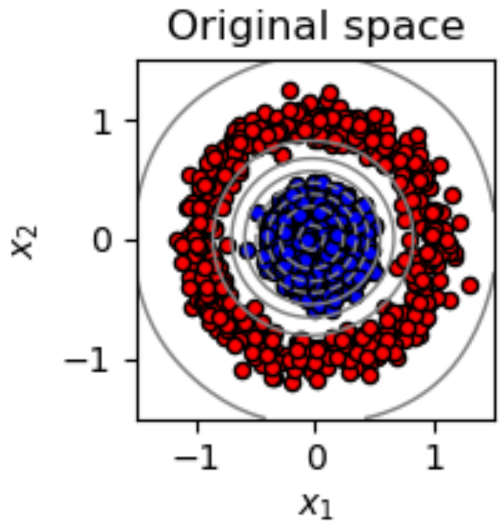
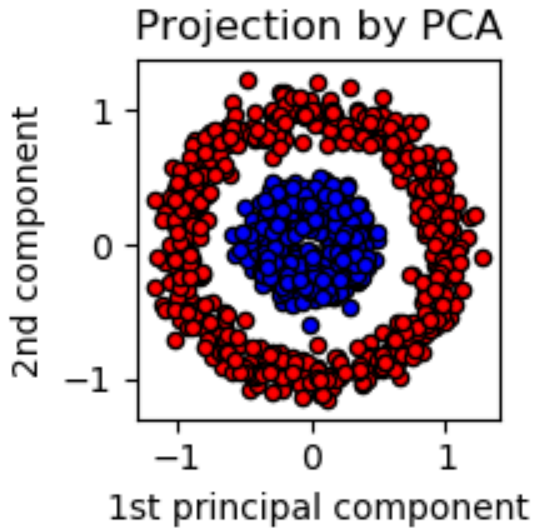


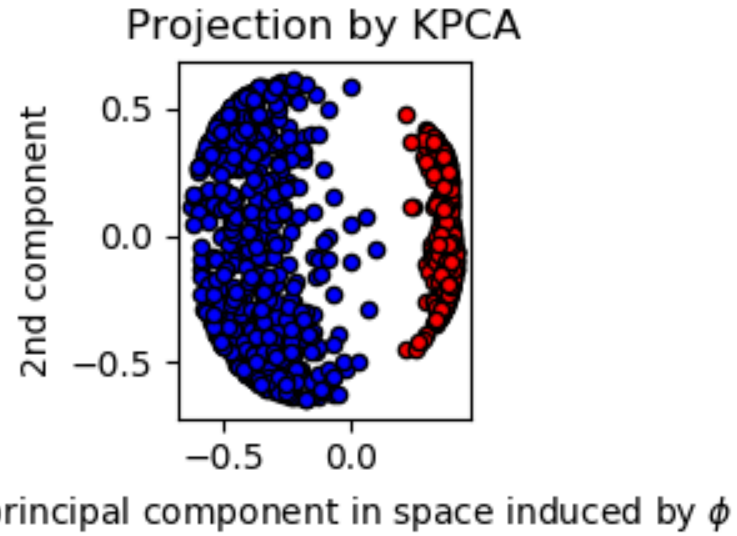
Figure from (Bishop, 2006)

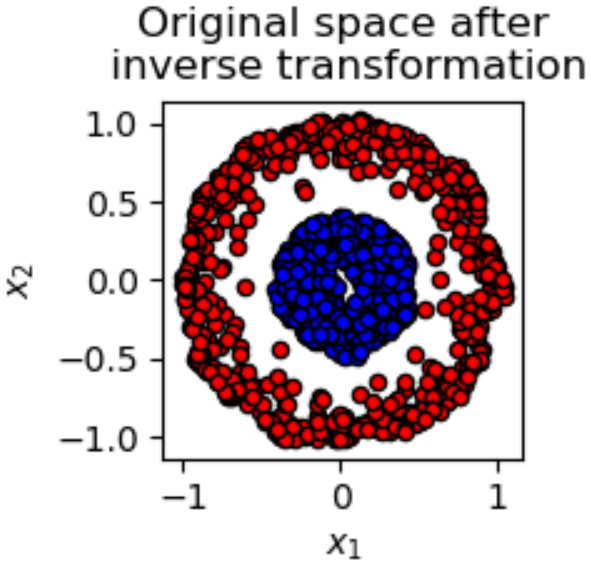
KPCA – Example 2

- 2D data points
- Cluster in cluster
- or “double doughnut”
- RBF kernel:
- $k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}\right)$
- Gamma $= \sigma = 4$



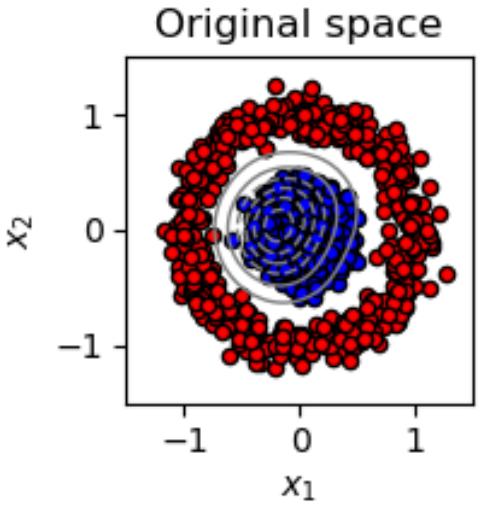


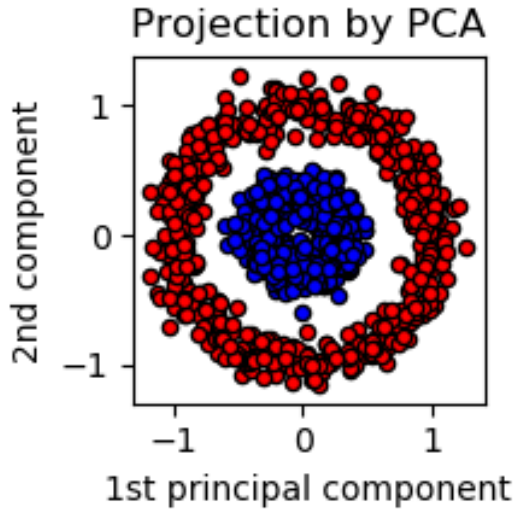


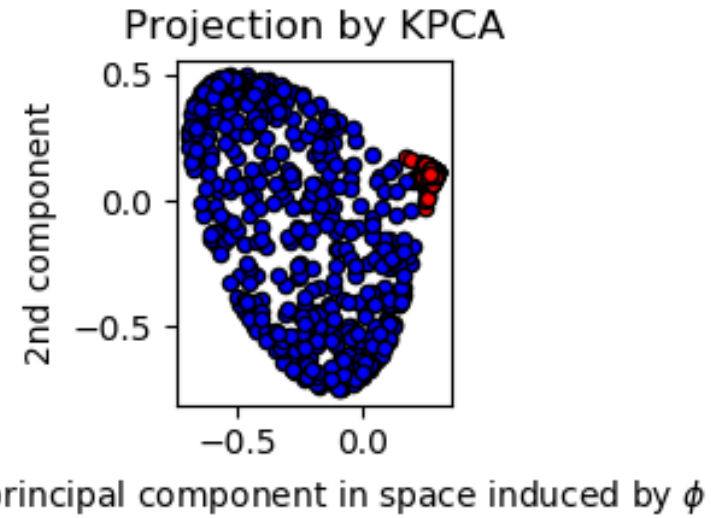


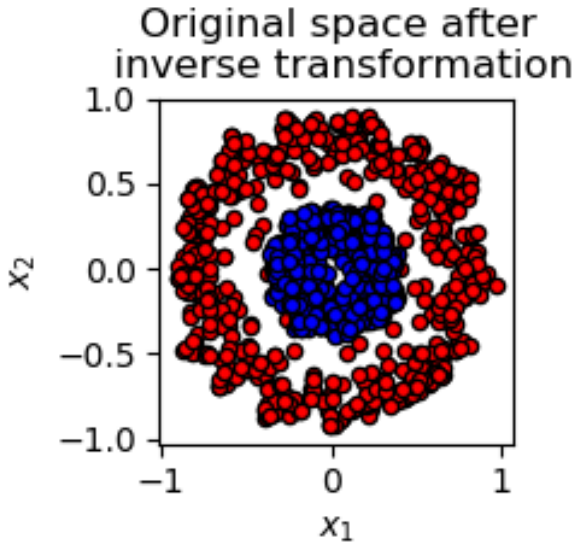
KPCA – Example 2

- 2D data points
- Cluster in cluster
- or “double doughnut”
- RBF kernel
- $k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}\right)$
- Gamma $= \sigma = 10$



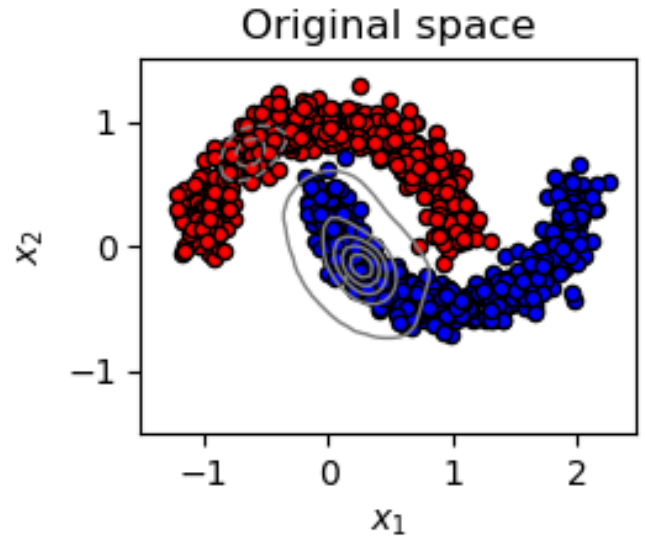


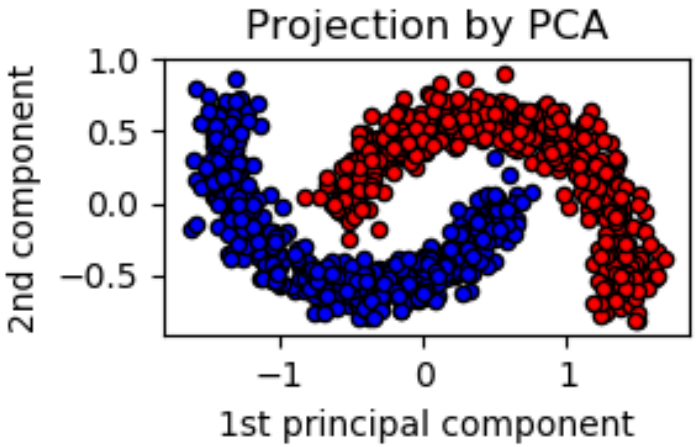


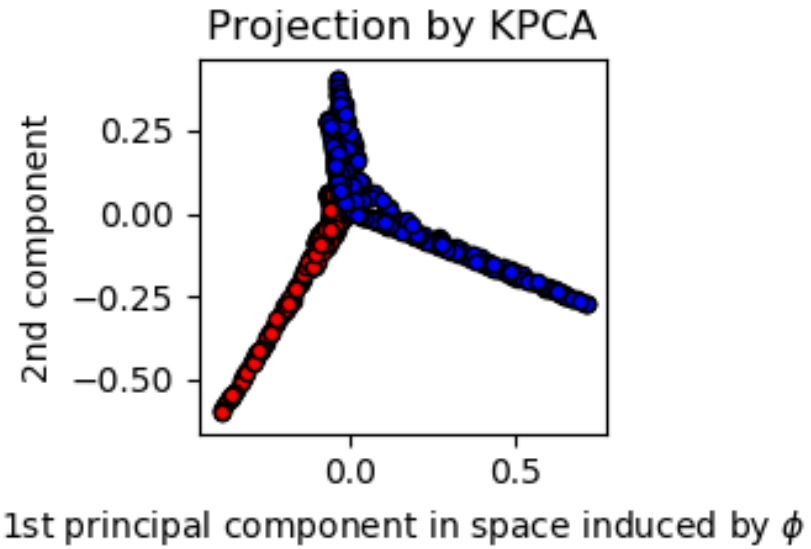


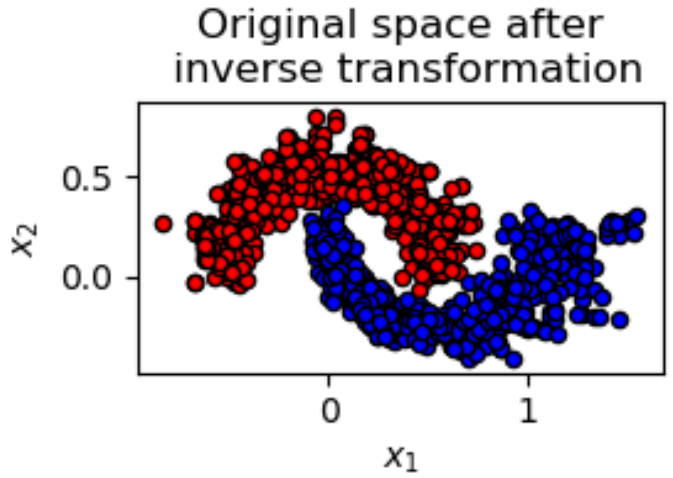
KPCA – Example 2

- 2D data points
- Moons dataset
- RBF kernel
- $k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}\right)$
- Gamma $= \sigma = 40$





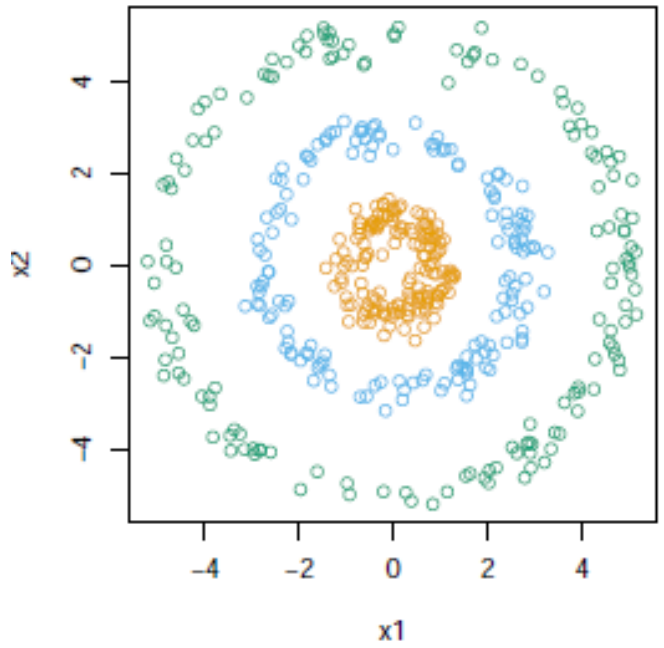




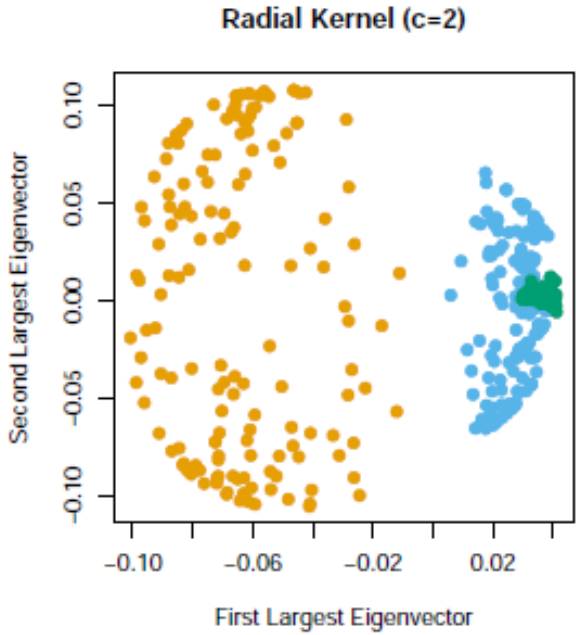
KPCA – Example 3

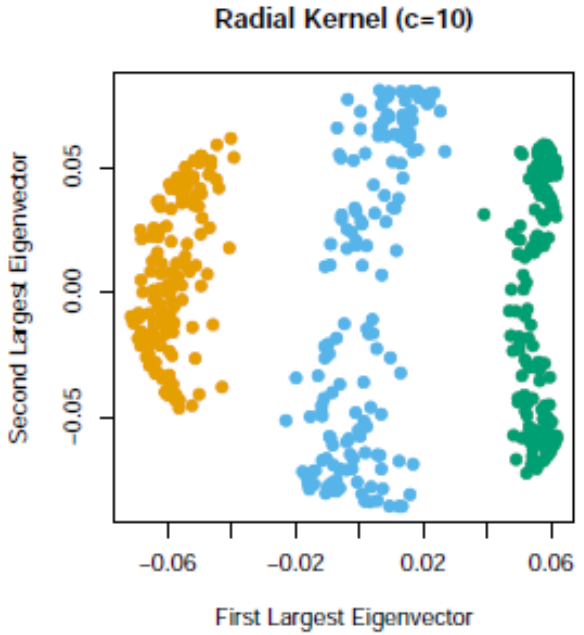
- 2D data points
- 3 circles
- RBF kernel:

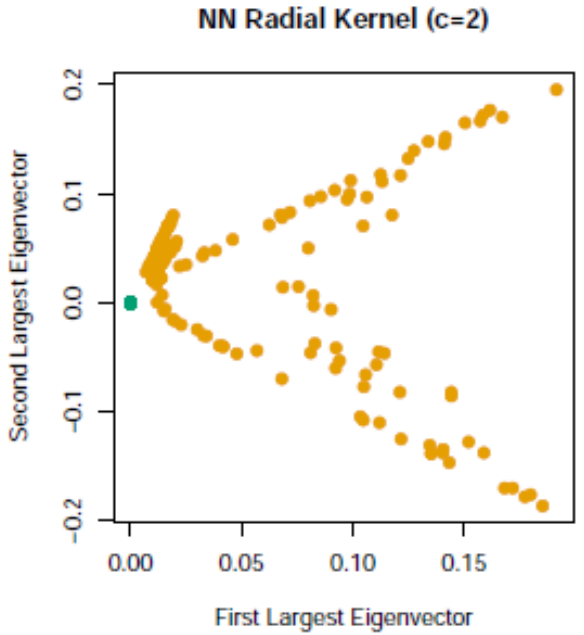
$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{c}\right)$$

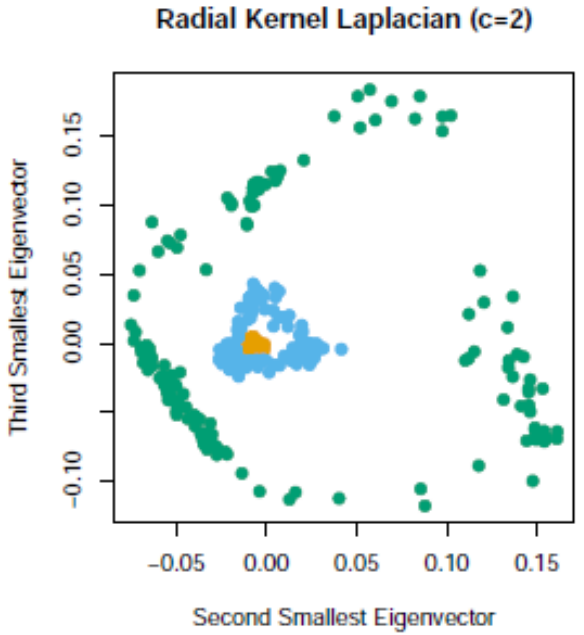


Example from [12]



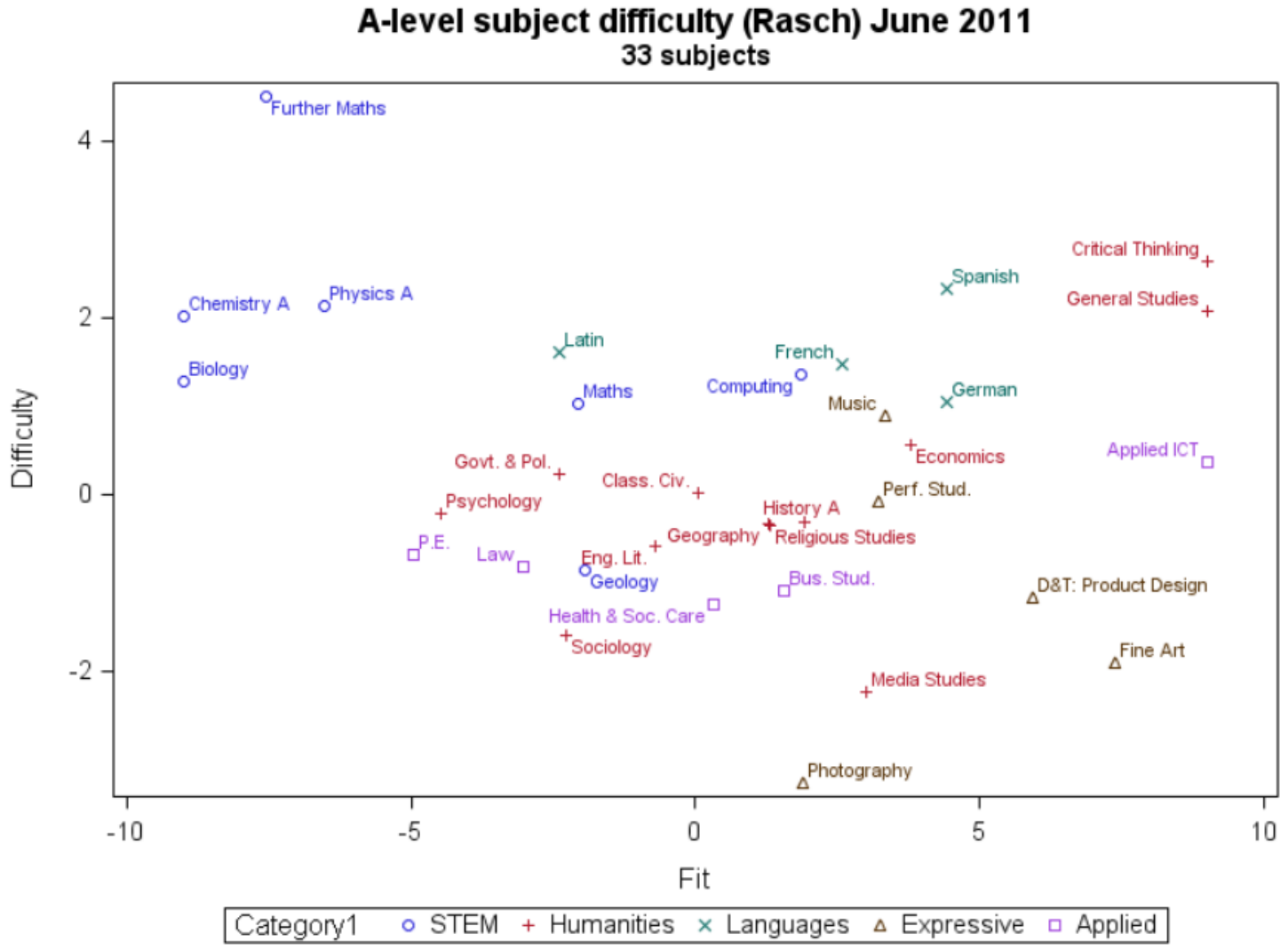






Multidimensional Scaling (MDS)

- MDS is a dimensionality reduction technique
- Aims at mapping high-dimensional data onto a lower-dimensional space
- Similarities between points in high dimensional (original) space are preserved in lower dimensional (new) space
- 2 cases of MDS
  - Metric MDS: Uses a metric to measure distance between points in original space
    - E.g., Euclidean, Manhattan, Mahalanobis, etc.
  - Non-metric MDS: Any kind of function is used to measure distance between points
    - E.g., Correlation, No. of occurrences, Edit distance, BLAST Alignment Score, etc.



Metric MDS

Input: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, where $\mathbf{x}_i \in \mathbb{R}^d$

- Let d_{ij} be the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$
- d_{ij} is a metric
- Typically, Euclidean distance is used
- $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$
- Other metrics can be used too

Aim:

- Find k-dimensional representation of $\mathbf{X}$:

$$\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n\}$$

where $\mathbf{y}_i \in \mathbb{R}^k$

- by minimizing the stress function:

$$S_M(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n) = \sum_{i \neq i'} (d_{ii'} - \|\mathbf{y}_i - \mathbf{y}_{i'}\|)^2$$

Known as Kruskal-Shephard scaling

- S_M can be minimized via gradient descent algorithm

Variation of least squares:

- Sammon mapping, which minimizes:

$$S_{Sm}(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n) = \sum_{i \neq i'} \frac{(d_{ii'} - \|\mathbf{y}_i - \mathbf{y}_{i'}\|)^2}{d_{ii'}}$$

Better for preserving smaller pairwise distances

Why?

- Local similarities are important

Classical MDS

- Mean vector in original space:

$$\mathbf{m}_x = \sum_{i=1}^{n} \mathbf{x}_i$$

Mean vector in new space:

$$\mathbf{m}_y = \sum_{i=1}^{n} \mathbf{y}_i$$

- Instead of samples, start with similarities using inner product:

$$s_{ii'} = (\mathbf{x}_i - \mathbf{m}_x)^t(\mathbf{x}_{i'} - \mathbf{m}_x)$$

- Aim is to minimize:

$$S_C(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n) = \sum_{i,i'} \left(s_{ii'} - (\mathbf{y}_i - \mathbf{m}_x)^t(\mathbf{y}_{i'} - \mathbf{m}_y)\right)^2$$

over $\mathbf{y}_i \in \mathbb{R}^k$

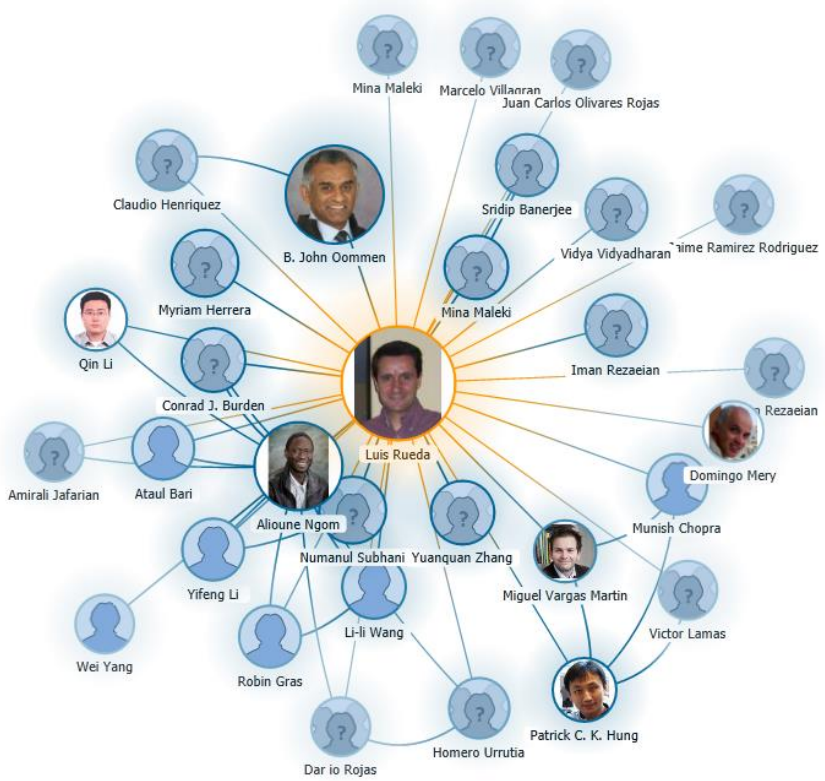
- Intereresting… because
- it can be shown that it's equivalent to find the largest eigenvalues of

$$\mathbf{S} = \{(\mathbf{x}_i - \mathbf{m}_x)^t(\mathbf{x}_{i'} - \mathbf{m}_x)\}_{ii'}$$

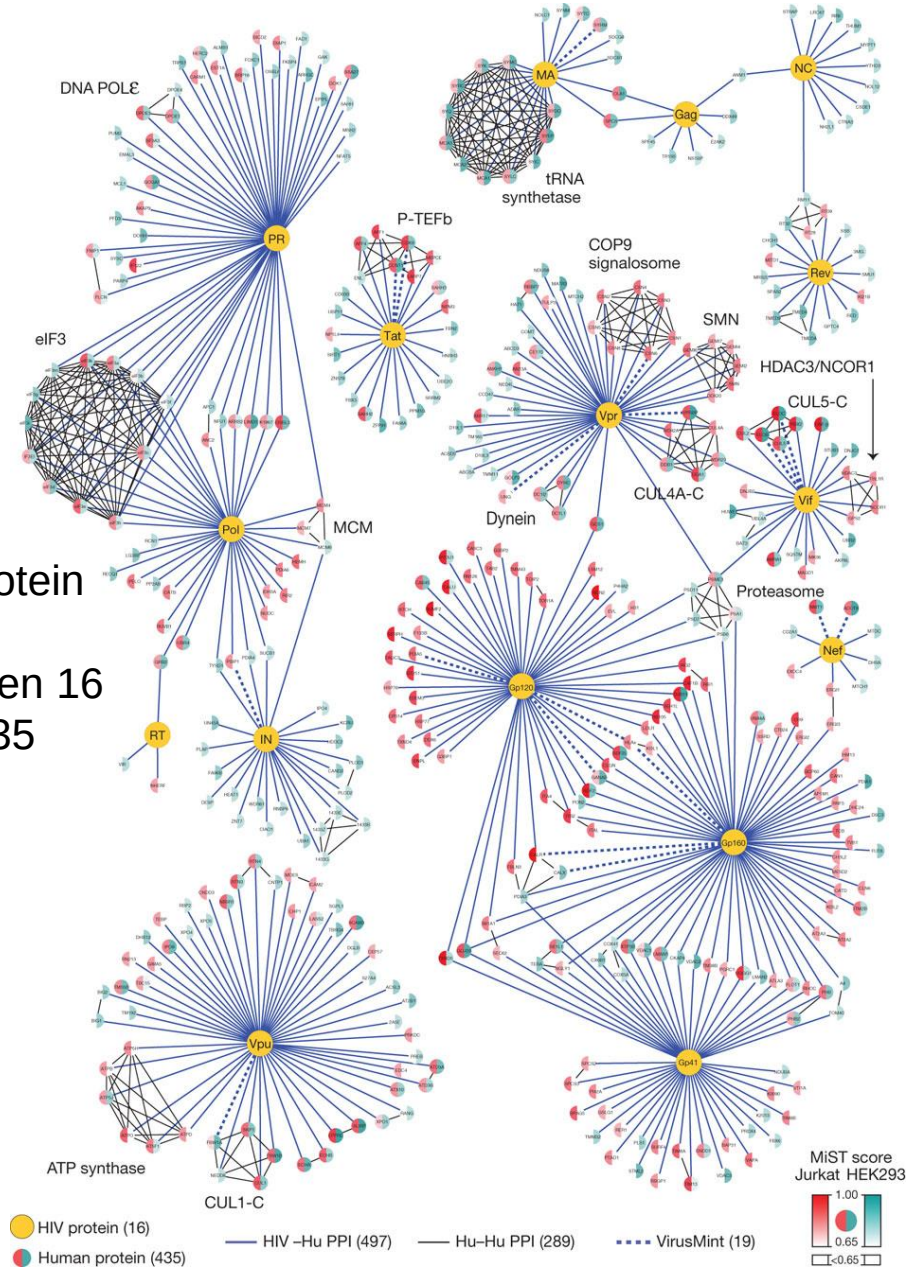
- and choose the corresponding eigenvectors
- Then, metric MDS is similar to PCA, and also to SVD
- However, life's not that easy in many real problems:
  - Network data: PPI, social networks, semantics of words, protein complexes
  - Graphs in general, in which data lies in very high-dimensional spaces
  - Relationships among text or strings: e.g., similarity between two DNA sequences via alignment or between strings via Edit distance

Real problems – Non-metric Data

- Research gate



497 HIV–human protein interactions (blue) representing between 16 HIV proteins and 435 human factors [6]



Real problems – Non-metric Data

- **Edit distance between two strings:**

  X = *excused* is transformed into

  Y = *exhausted*

- Steps:
  - First, substitute *h* for *c*, yielding
    X = *exhused*
  - Second, insert *a*, obtaining
    X = *exhaused*
  - Third, insert *t*, obtaining
    X = *exhausted*
  - Since the cost of each operation is 1, the distance between X and Y is 3

DNA sequence alignment

- Uses a scoring system that assigns:
  - score values for **each** pair of symbols
  - e.g. nucleic acid or amino acid pairs
  - penalty values to single gaps
- Score = sum of pair scores – sum of gap penalties

Example: *X* = **TGATAGCCAG** *Y* = **AGAGCA**

```
T - G A T A G C C A G
- A G A G - - C - A -
```

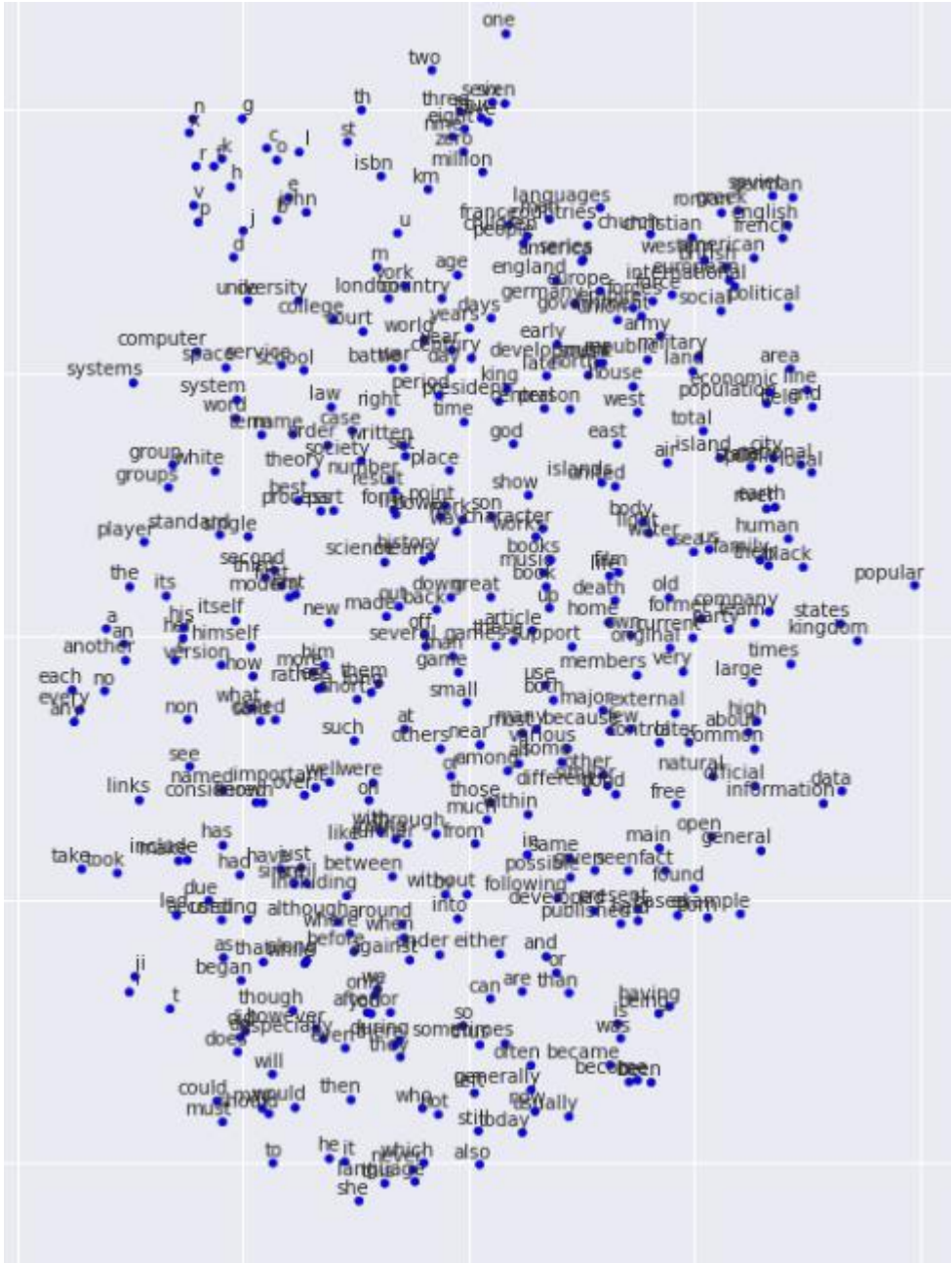
Score = -4-4+6+6+2-4-4+6-4+6-4 = 2

Non-metric Data

List of words:

…
can
college
common
computer
could
….

Embedding in 2D space

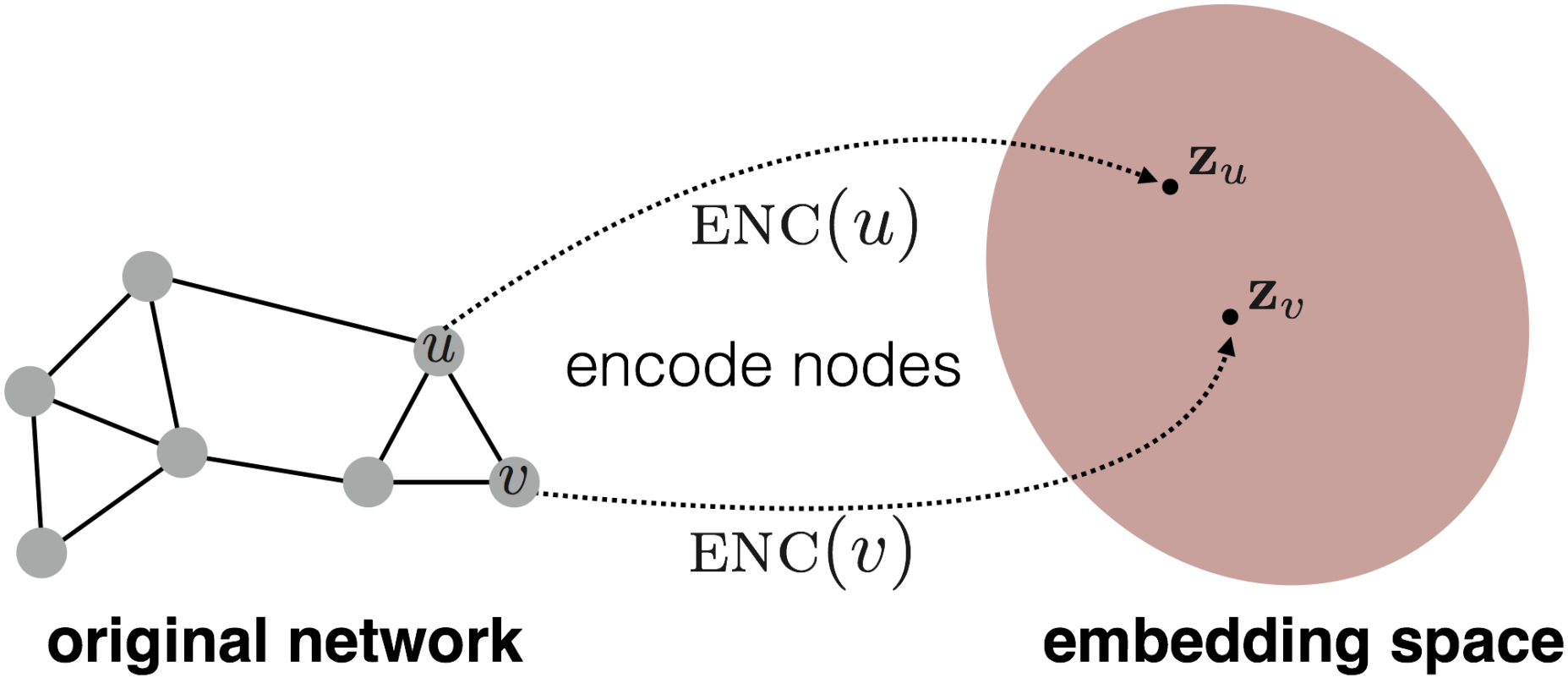


- Words in alphabetical (or some other) order
- Similarity based on meaning, rather than on spelling
  - Non-metric (e.g., non-Euclidean) in higher dimensional space

https://www.tensorflow.org/tutorials/representation/word2vec ref [9]

Real problems – Node Embedding in Graphs

- Aim is to encode nodes [10]
- Similarity in original network (graph) preserved in embedding space



Non-metric MDS

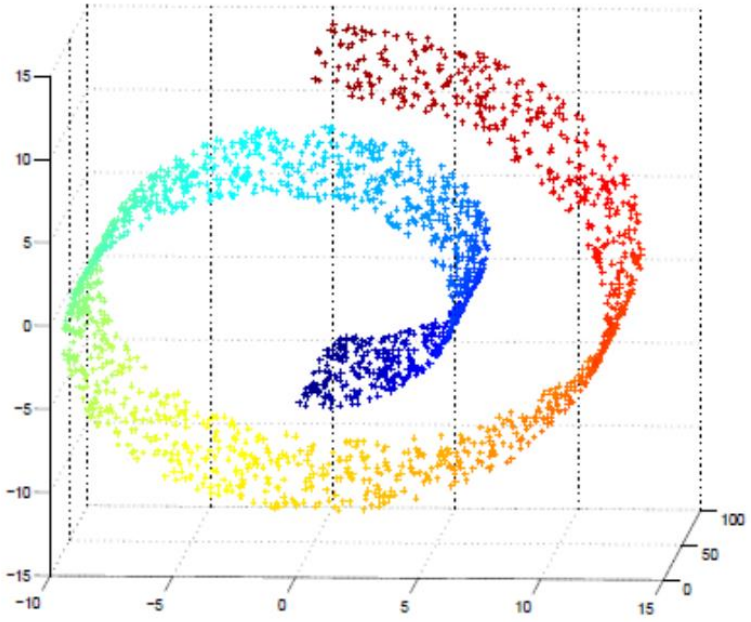
- Shephar-Kruskal non-metric MDS works with any distance measure
- Only requires a matrix distance $\{\Delta_{ij}\}$
- Aim: minimize the stress function:

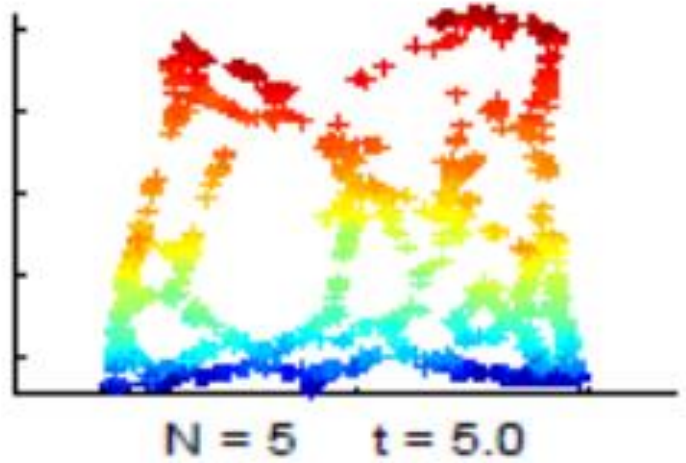
$$S_M(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n) = \frac{\sum_{i \neq i'} \left[\|\mathbf{y}_i - \mathbf{y}_{i'}\| - g(\Delta_{ij})\right]^2}{\sum_{i \neq i'} \|\mathbf{y}_i - \mathbf{y}_{i'}\|^2}$$

over $\mathbf{y}_i$, where g is an arbitrarily increasing function

- If g is fixed, S_M can be minimized using the gradient descent
- with $\mathbf{y}_i$ fixed, isotonic regression can be used to find best monotonic approximation of $g(\Delta_{ij})$ to $\|\mathbf{y}_i - \mathbf{y}_{i'}\|$

These two steps repeated until desired solution is found





Local MDS

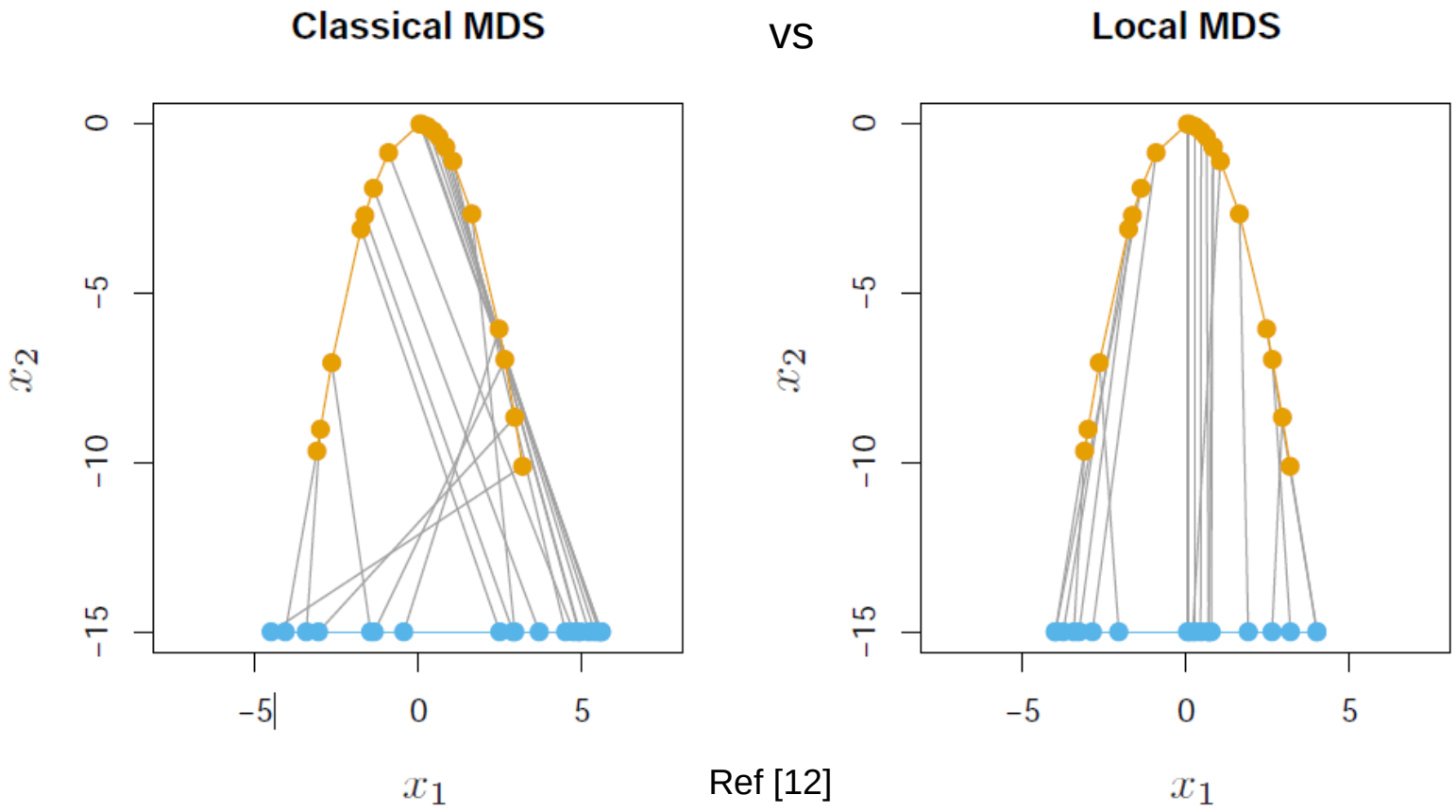
- Local MDS is good for manifold representation and graph embedding
- Aim for nonlinear dimensionality reduction and for capturing neighborhood relationships in high-dimensional and/or complex data

Main approaches:

- Isomap
- Laplacian eigenmaps
- Local linear embedding (LLE)

Example:

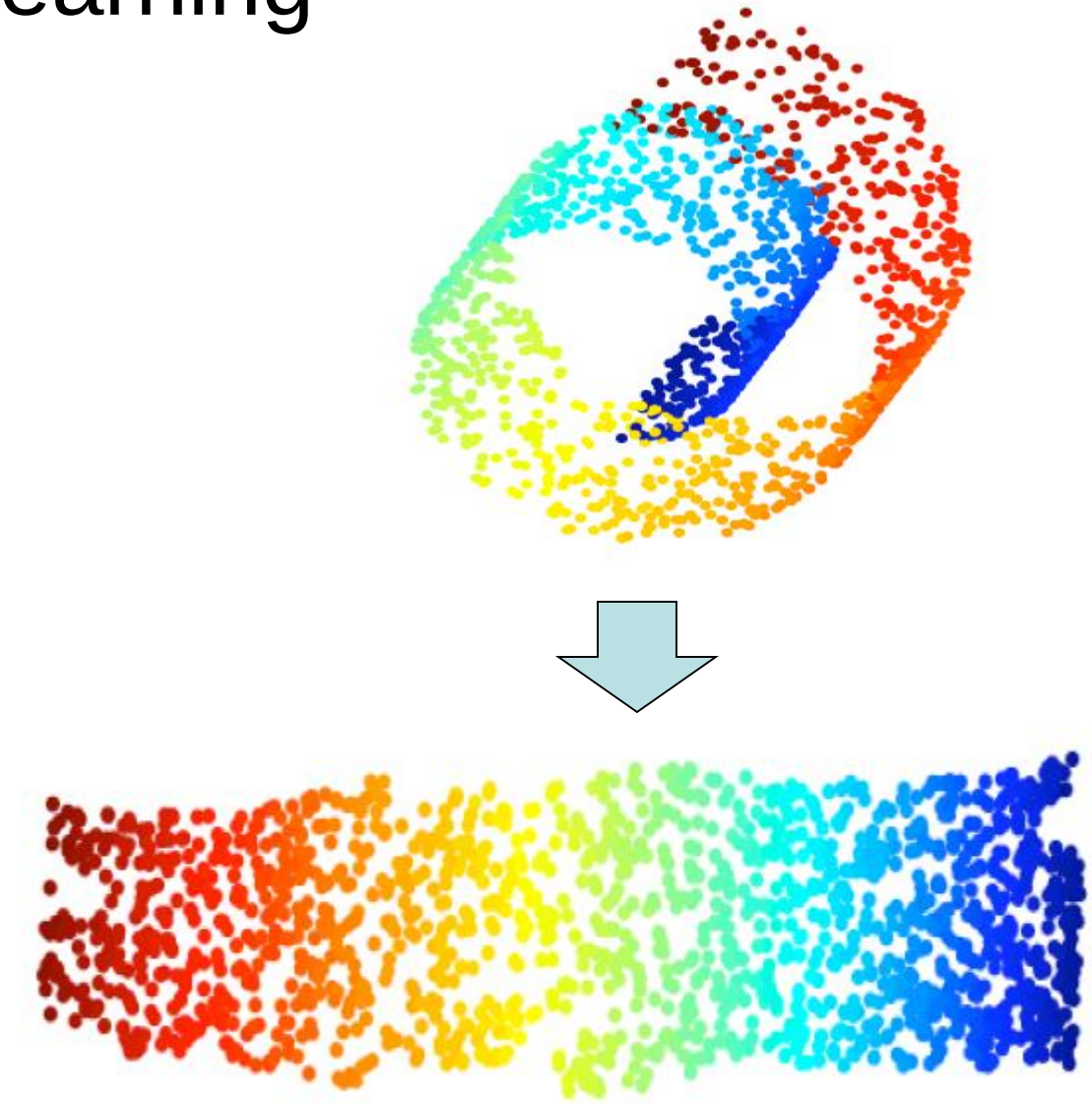
- Data lies in parabola in 2D
- Projected onto 1D space



Ref [12]

Manifold Learning

- Manifolds are techniques for NDR
- Assume higher dimensional data lie on a lower dimensional space via nonlinear mapping
- Transformation called “manifold embedding”
- Can be seen as special case of KPCA
- Most well-known techniques
  - Isomap
  - Laplacian eigenmaps
  - Locally linear embedding (LLE)

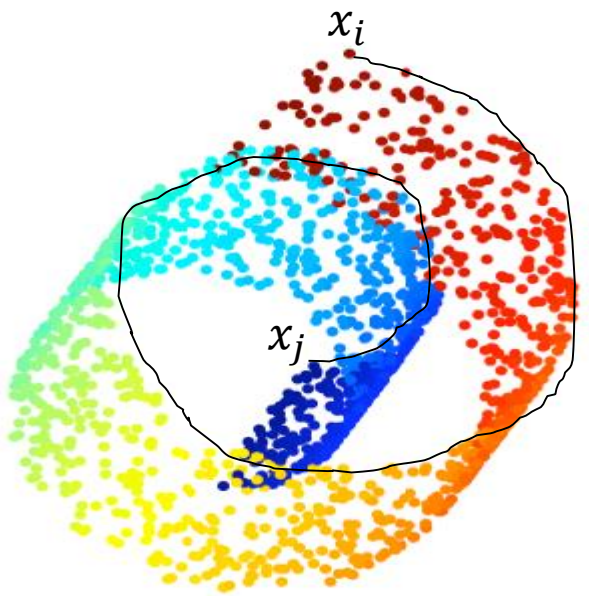


Isomap

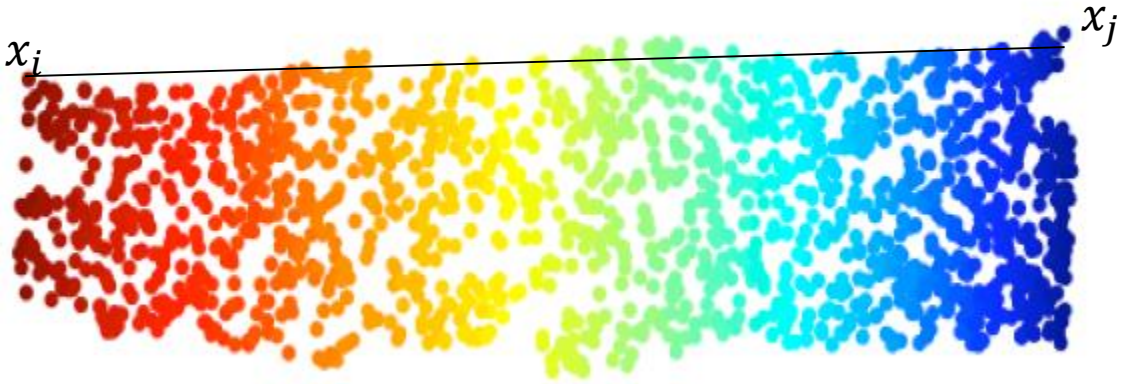
- Extract low dimensional representation of data
- Preserve pairwise distance between points measured by geodesic distances
- Use L_2-norm to measure distances
- Use nearest neighbors only (not all points)

Main steps:

- Find t nearest neighbors
- Construct adjacency graph
- Compute approximate geodesic distances
- Find singular values via eigen decomposition



Unroll the Swiss roll



Isomap - Algorithm

Input: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$

Step 1:

- Find t nearest neighbors for each point $\mathbf{x}_i$
- Use L_2-norm to construct undirected neighborhood graph $G = (V, E)$
- V are the points as vertices
- E are the links between neighbors as edges

Step 2:

- Compute approximate geodesic distances Δ_{ij} for all pairs of vertices $(\mathbf{x}_i, \mathbf{x}_j)$
- Find all-pairs shortest distances in G using dynamic programming (e.g., Floyd-Warshall algorithm)

Step 3:

- Convert squared distance matrix into $m \times m$ similarity matrix:

$$\mathbf{K}_{Iso} = -\frac{1}{2}\mathbf{H}\Delta\mathbf{H}$$

where

- Δ is the squared distance matrix
- $\mathbf{H} = \mathbf{I}_m - \frac{1}{m}\mathbf{1}\mathbf{1}^t$ is the centering matrix
- $\mathbf{I}_m$ is the $m \times m$ identity matrix
- $\mathbf{1}$ is a column vector of all ones

Isomap

Step 4:

- Find optimal k-dimensional representation

$$\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n\}$$

such that:

$$\mathbf{Y} = \underset{\mathbf{Y}'}{\operatorname{argmin}} \sum_{i,j} \left(\left\| \mathbf{y}'_i - \mathbf{y}'_j \right\|_2^2 - \Delta_{ij}^2 \right)$$

Solution given by:

- $\mathbf{Y} = \left(\mathbf{\Sigma}_{Iso,k}\right)^{1/2} \mathbf{U}_{Iso,k}^t$

where

- $\mathbf{\Sigma}_{Iso,k}$ is the diagonal matrix of the top k singular values of $\mathbf{K}_{Iso}$ and
- $\mathbf{U}_{Iso,k}^t$ are the associated singular vectors
- $\mathbf{K}_{Iso}$ can be viewed as a kernel matrix
- If positive semidefinte, Isomap resembles KPCA (typical of a smooth manifold)

Complexity

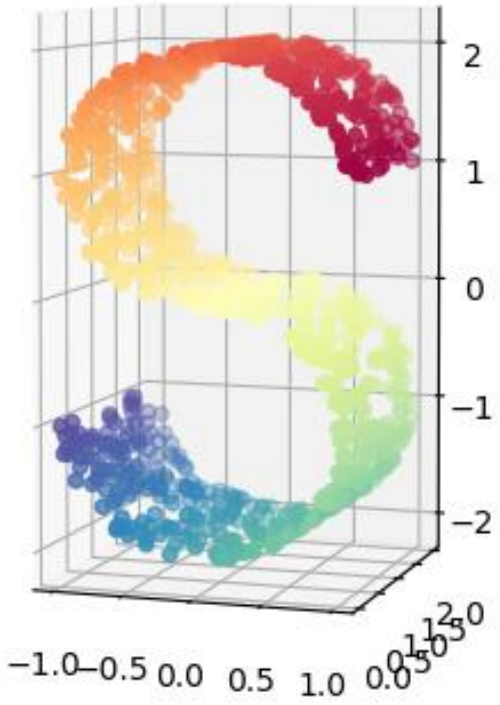
- t-NN is $O(n^2 d)$
- Djikstra's for shortest path: $O(n^2 \log n + n^2 k)$
- Embedding: top k eigenvectors found in $O(n^2 k)$
- Optimizations can be done via approximation

Big Data

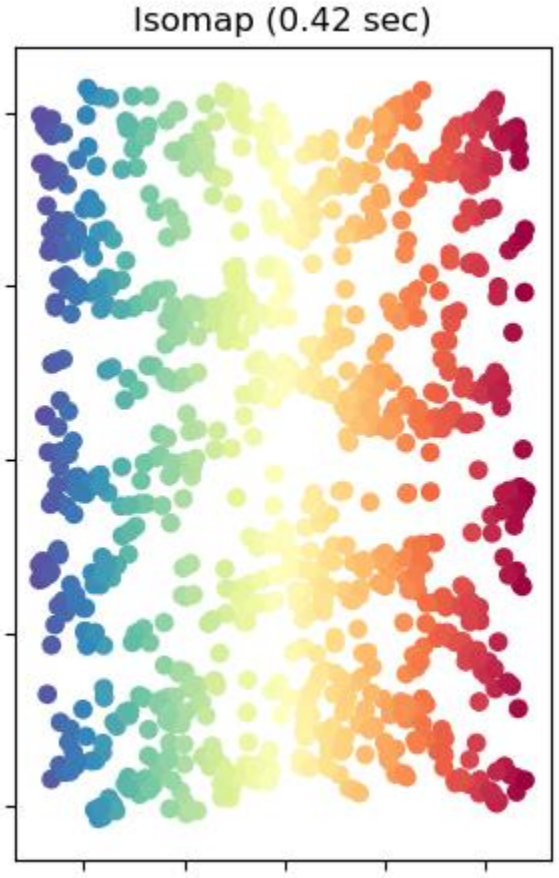
- Too expensive to find all shortest paths
- Can compute shortest paths in part of Gram matrix
- Use diagonalization of sub-matrix

Isomap – Example: S data

- Original data, S-shaped in 3D



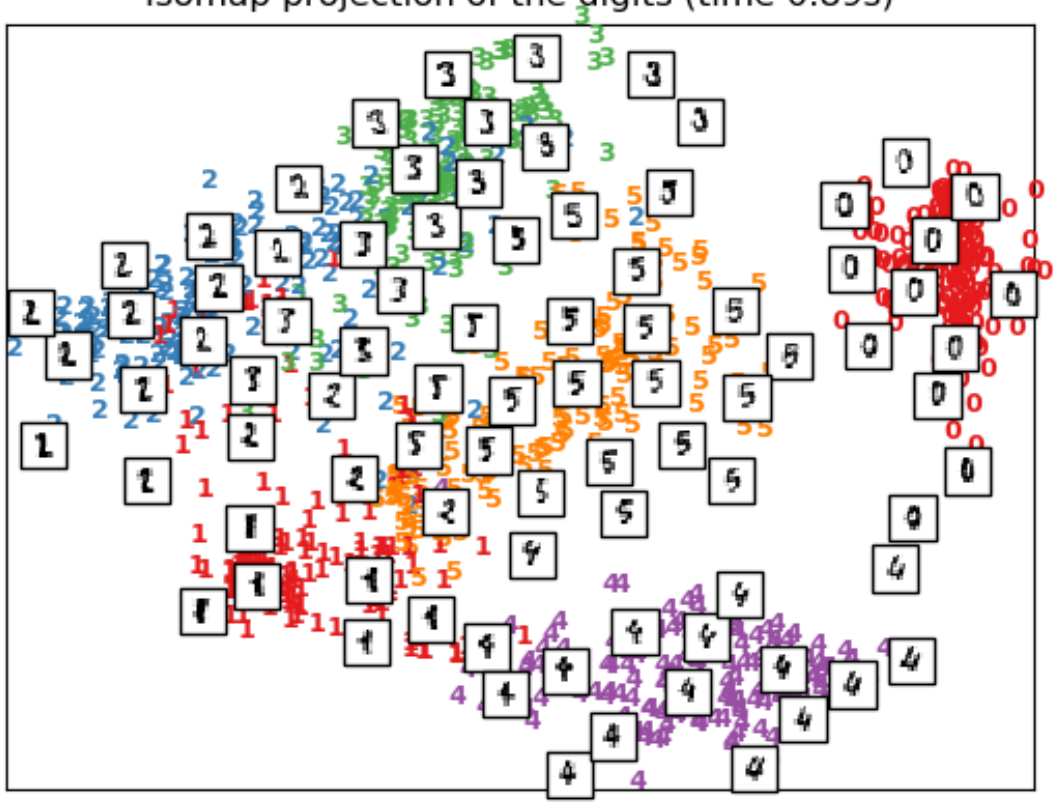
- Isomap
- $t = 10$



Isomap – Digits example

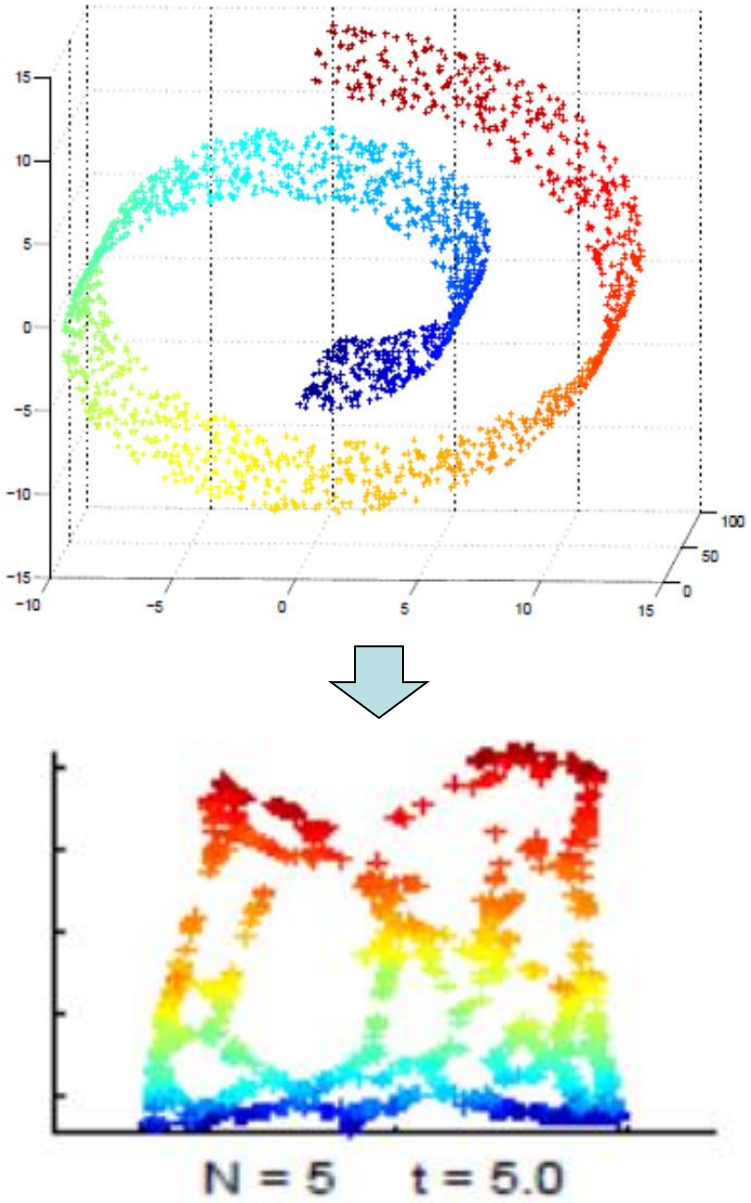
A selection from the 64-dimensional digits dataset

Isomap projection of the digits (time 0.89s)



Laplacian Eigenmaps

- Key idea: preserve local information only
- Find lower-dimensional representation
- Try to preserve neighborhood relations in lower dimension
- Use information of the spectral (frequency) domain
- Derive a weight matrix $\mathbf{W}$
- Matrix constructed via a kernel
  - Most commonly used kernel is RBF
- Perform eigen decomposition of the graph Laplacian matrix
- Can be applied to high-dimensional non-Euclidean weighted graphs



Laplacian Eigenmaps

Input: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$

Step 1:

- Find t nearest neighbors for each point $\mathbf{x}_i$

Step 2:

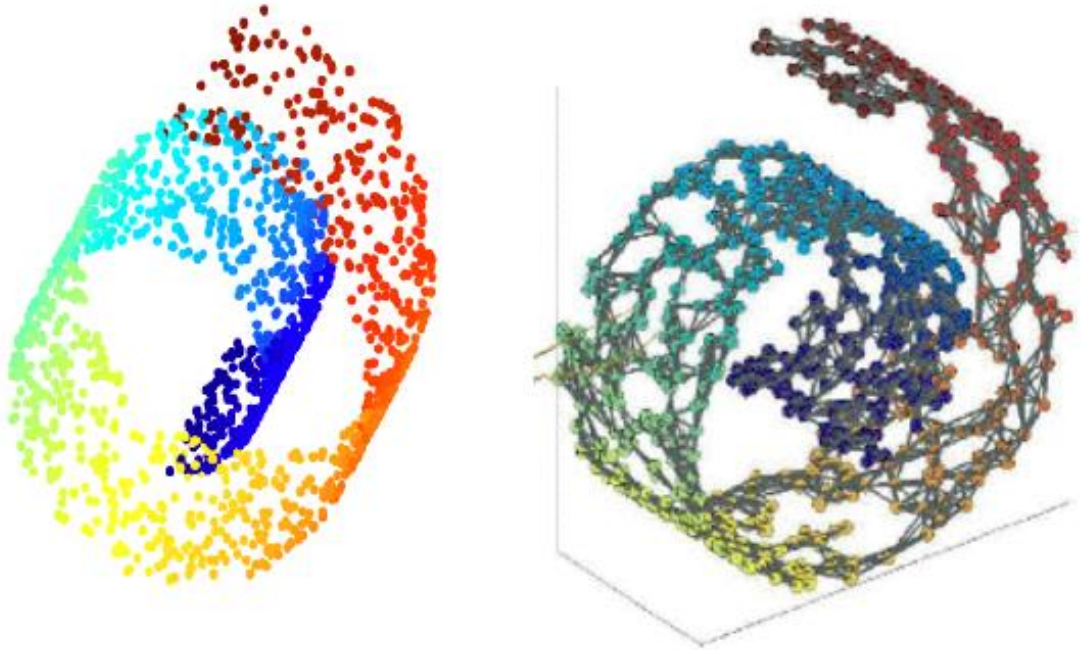
- Construct undirected neighborhood graph $G = (V, E, \mathbf{W})$
- V are the points as vertices
- E are the links between neighbors as edges
- $\mathbf{W}$ is a sparse, symmetric $\mathrm{n} \times n$ matrix where $w_{ij} = k(x_i, x_j)$ if $\mathbf{x}_i$ and $\mathbf{x}_j$ are neighbors
  = 0 otherwise

Commonly used kernel: RBF

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

- Sparsity of G depends on t
  - Small $t \Rightarrow G$ is very sparse
  - Large $t \Rightarrow G$ is very dense

- Example: From Swiss roll to Sparse Graph



Laplacian Eigenmaps

Step 3:

- Construct the diagonal matrix $\mathbf{D}$

  where $d_{ij} = \sum_j w_{ij}$

- It's basically the degree of each node placed on the diagonal of $\mathbf{D}$

Step 4:

- Find the k-dimensional representation of the data
- Minimize the weighted distance between neighbors in the new space:

$$\mathbf{Y} = \underset{\mathbf{Y}'}{\operatorname{argmin}} \sum_{i,j} w_{ij} \left\| \mathbf{y}'_i - \mathbf{y}'_j \right\|_2^2$$

- Neighbor inputs in original space are mapped to points that are close to each other in new space, using info in $\mathbf{W}$

Solution:

$$\mathbf{Y} = \mathbf{U}_{L,k}^t$$

where

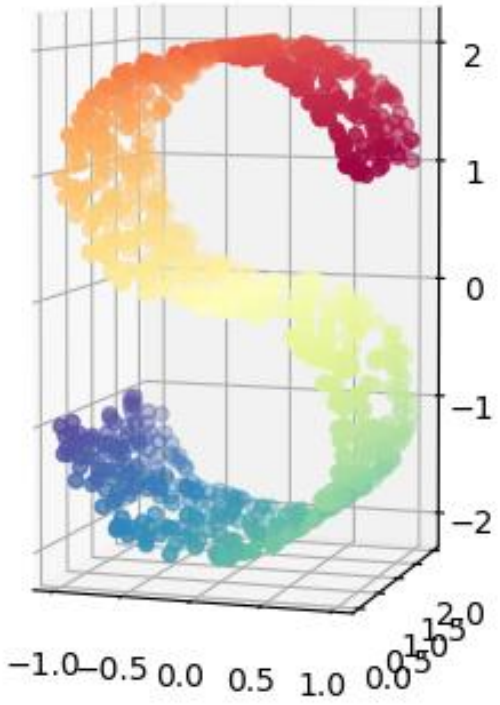
- $\mathbf{L} = \mathbf{D} - \mathbf{W}$ is the graph Laplacian
- $\mathbf{U}_{L,k}^t$ are the bottom k singular vectors (associated smallest eigenvalues)
  excluding the singular value 0

Interpretation:

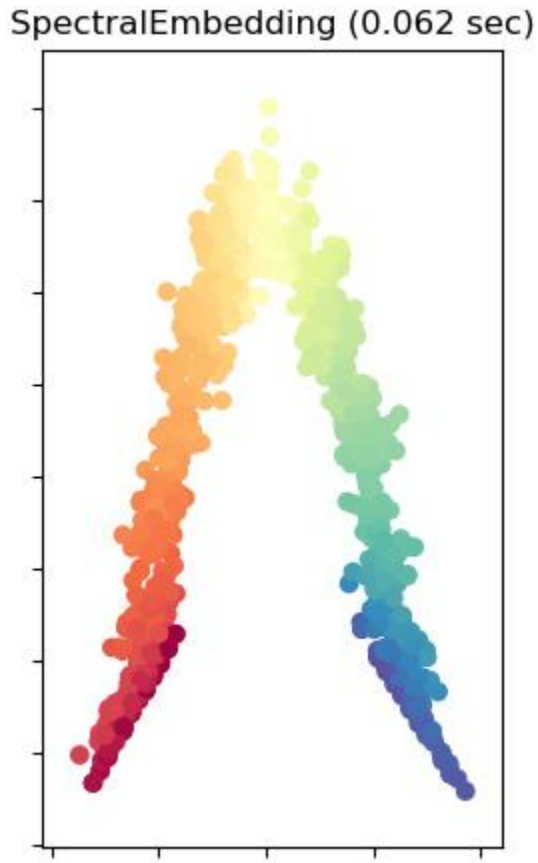
- Find the largest singular vectors of $\mathbf{L}^+$, the pseudoinverse of $\mathbf{L}$
- If we consider $\mathbf{K}_L = \mathbf{L}^+$, we can view Laplacian Eigenmaps as a particular case of KPCA

Laplacian Eigenmaps – Example: S data

- Original data, S-shaped in 3D

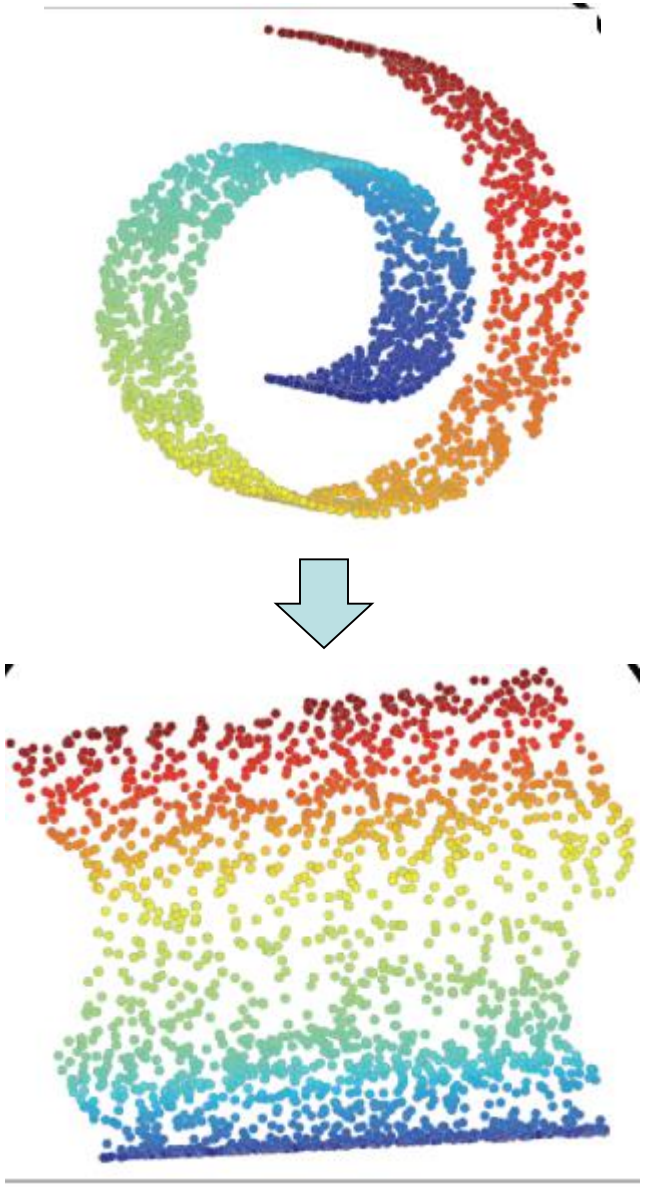


- Laplacian eigenmaps
- $t = 10$



Local Linear Embedding (LLE)

- Also aims at mapping high dimensional data to lower dimensional data
- Preserves the local linear structure of nearby input data points
- Unlike the Isomap, the outputs are derived from the bottom eigenvectors of a sparse matrix
- Also based on nearest neighbors
- Constructs the sparse matrix based on distances to those neighbors



Local Linear Embedding (LLE)

Input: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$

Step 1:

- Find t nearest neighbors for each point $\mathbf{x}_i$

Step 2:

- Construct sparse, symmetric $n \times n$ matrix $\mathbf{W}$
- i^{th} row of $\mathbf{W}$ sums to one
- The reconstruction error is:

$$\left(\mathbf{x}_i - \sum_{j \in \mathcal{N}_i} w_{ij}\mathbf{x}_j\right)^2 = \left(\sum_{j \in \mathcal{N}_i} w_{ij}(\mathbf{x}_i - \mathbf{x}_j)\right)^2$$

$$= \sum_{j,k \in \mathcal{N}_i} w_{ij} w_{ik} \mathbf{C}'_{jk} \qquad (1)$$

- $\mathcal{N}_i$ is the set of indices of the of the neighbors of x_i
- $\mathbf{C}'_{jk} = (\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_k)^t$ is the local covariance matrix

- Minimizing (1) with constraint $\sum_j w_{ij} = 1$ gives solution:

$$w_{ij} = \frac{\sum_k (\mathbf{C}')^{-1}_{jk}}{st \sum (\mathbf{C}')^{-1}_{st}}$$

Step 4:

- Find the k-dimensional representation of the data
- Minimize the weighted distance between neighbors in the new space:

$$\mathbf{Y} = \underset{\mathbf{Y}'}{\operatorname{argmin}} \sum_i \left(\mathbf{y}'_i - \sum_j w_{ij} \boldsymbol{y}'_j\right)^2 \qquad (2)$$

Local Linear Embedding (LLE)

Solution:

$$\mathbf{Y} = \mathbf{U}_{M,k}^{t}$$

where

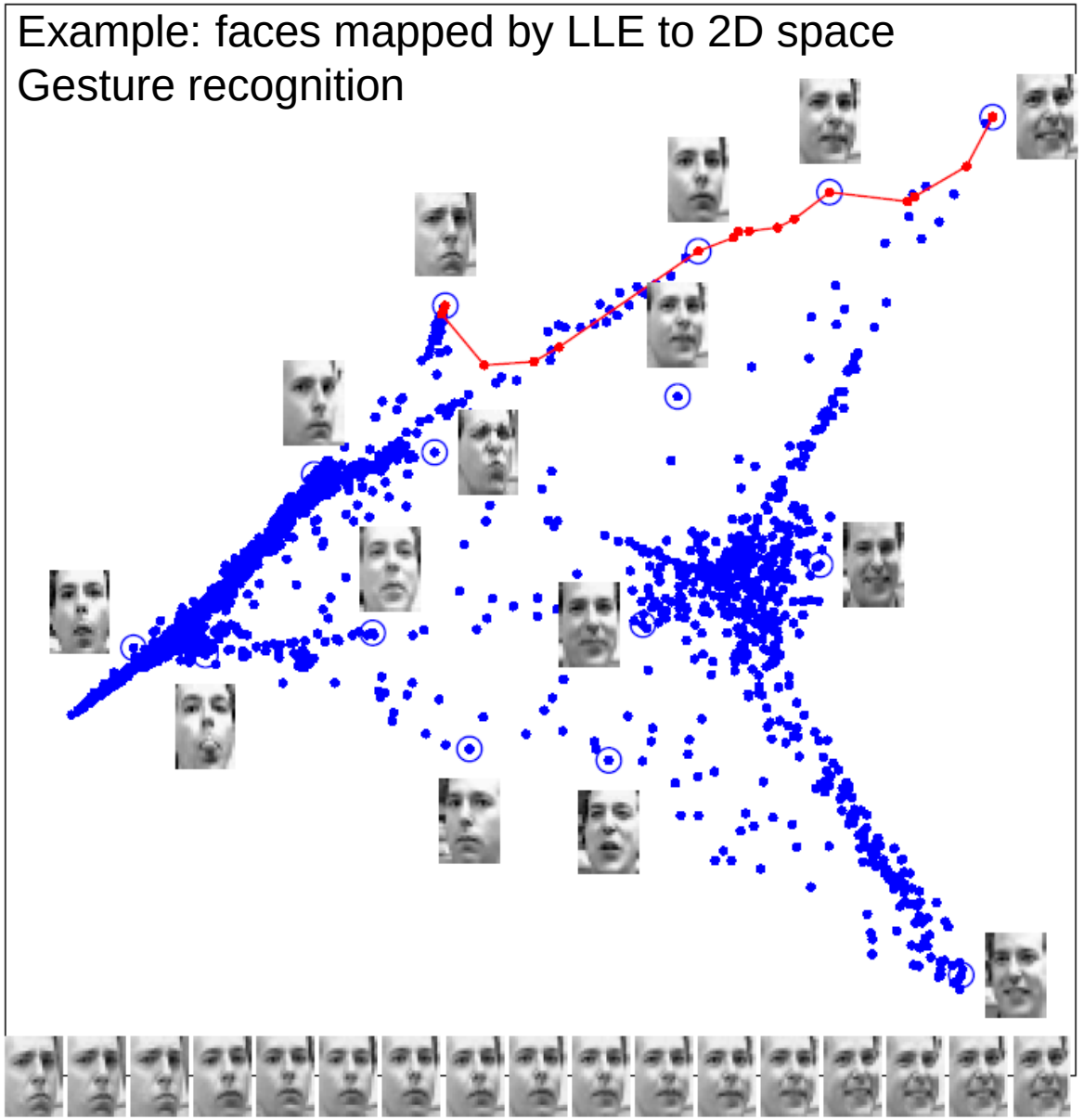
- $\mathbf{M} = (\mathbf{I} - \mathbf{W}^t)(\mathbf{I} - \mathbf{W}^t)$
- $\mathbf{U}_{M,k}^{t}$ are the bottom k singular vectors (associated smallest eigenvalues)
  excluding the singular value 0

- LLE is equivalent to KPCA if the kernel matrix $\mathbf{K}_{LLE}$ is given by the pseudoinverse of $\mathbf{M}$

Variant of LLE:

- Choose $\ell < n$ random points constrained to equal the corresponding inputs
- For ℓ sufficiently large, (2) can be minimized by solving a MSE problem

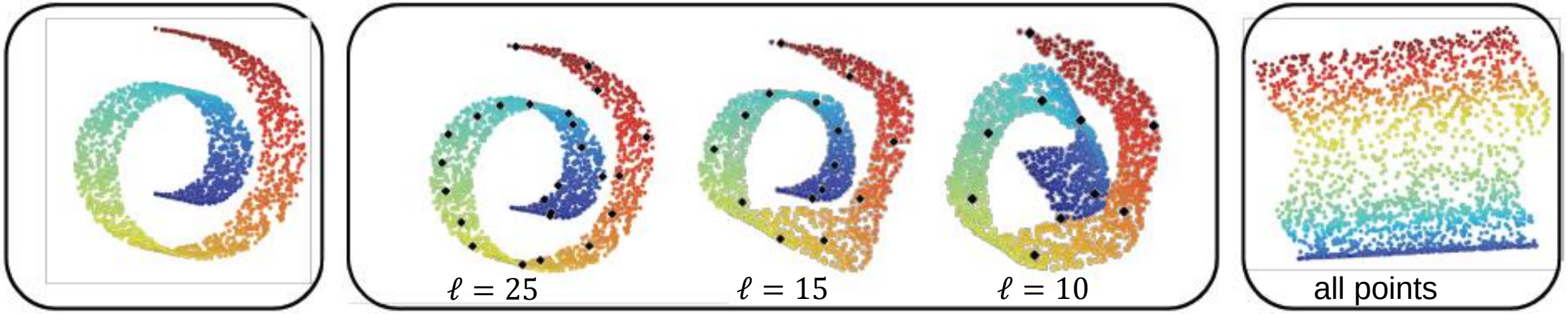
Example: faces mapped by LLE to 2D space
Gesture recognition



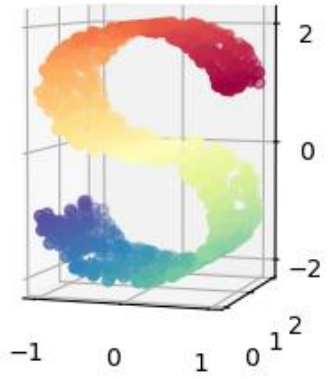
LLE Example – Effect of ℓ

Swiss roll data

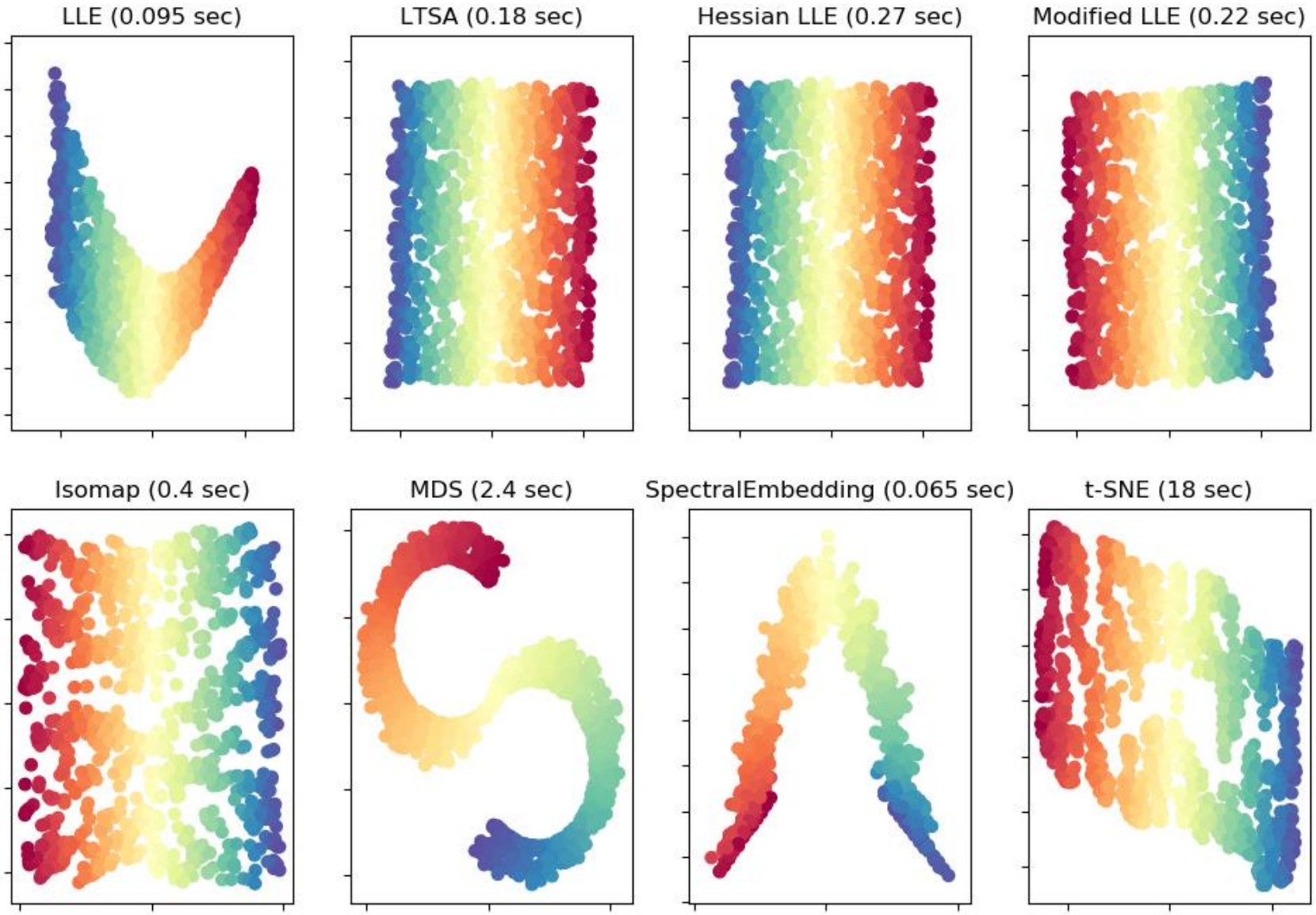
$t = 20$ nearest neighbors



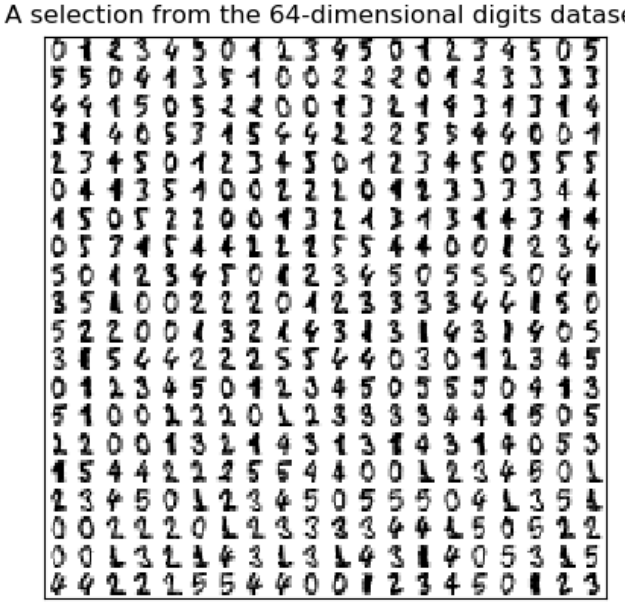
Manifold – S data - Comparison

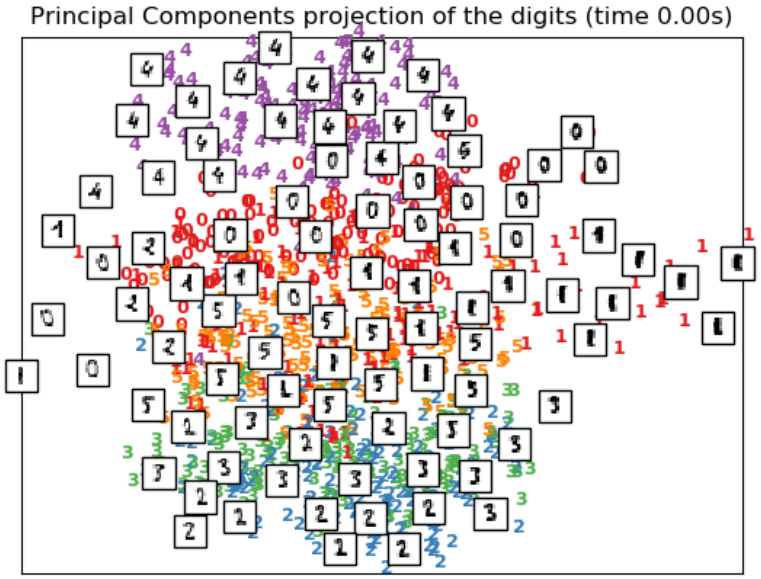


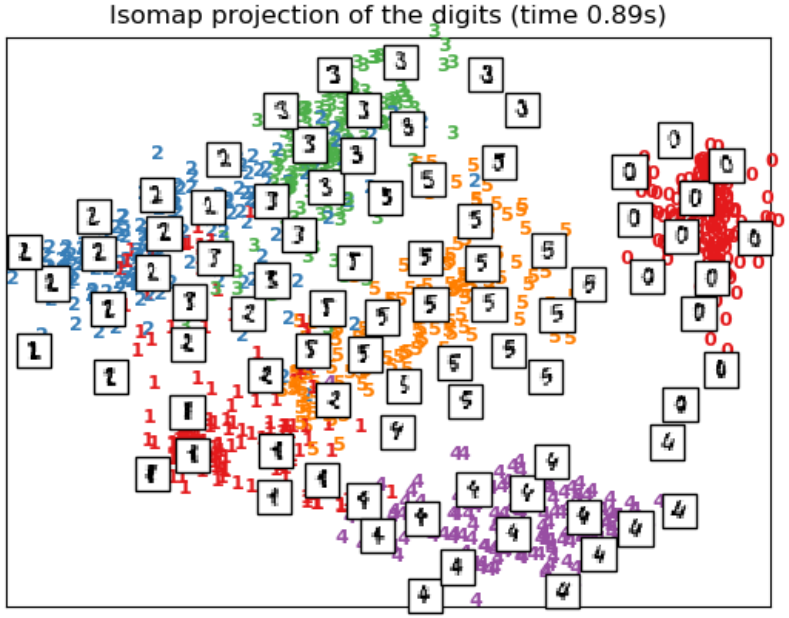
$t = 10$
nearest neighbors

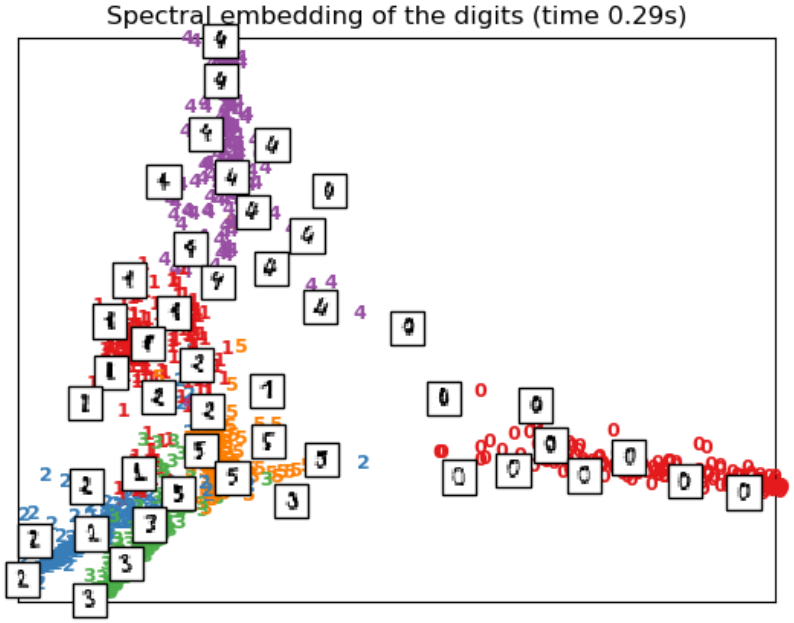


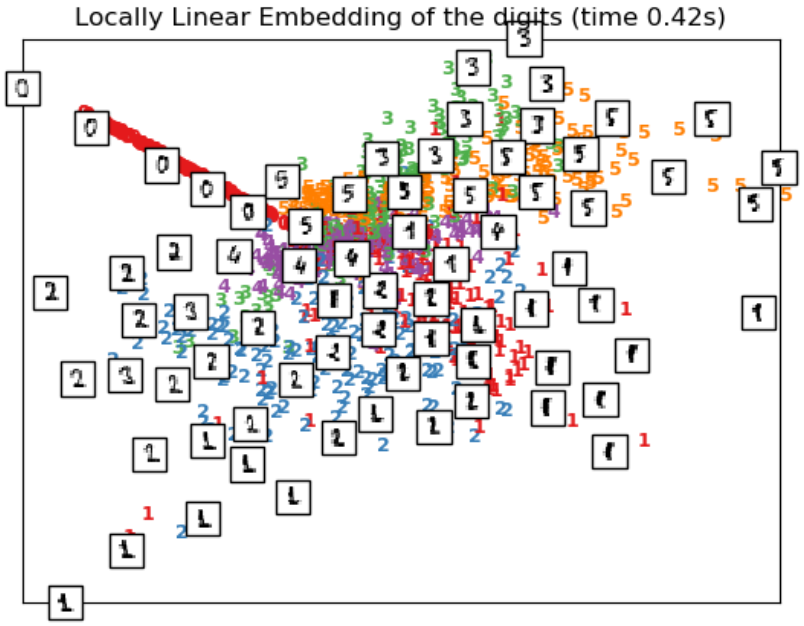
Digits: PCA vs Isomap, LLE, Laplacian, MDS

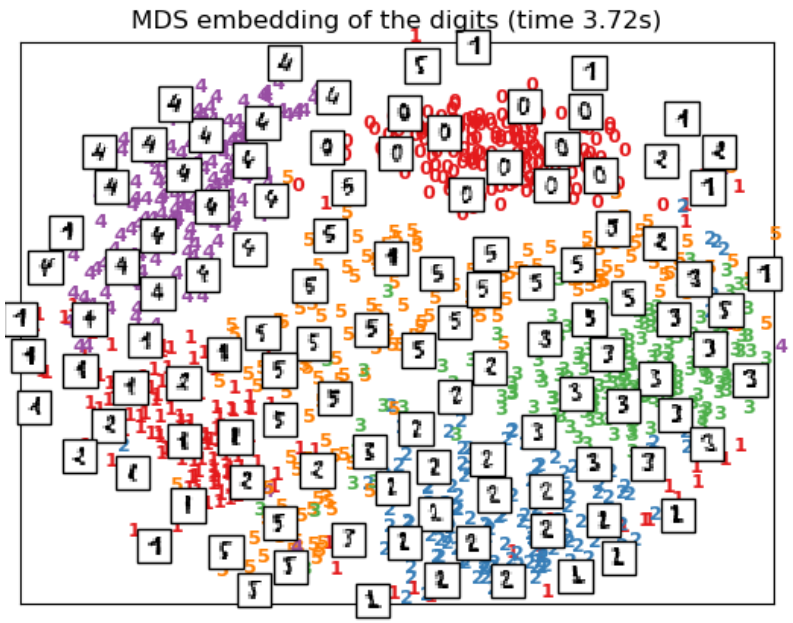












Nonlinear Autoencoder

Autoencoder:

- Each layer parameterizes a nonlinear transformation

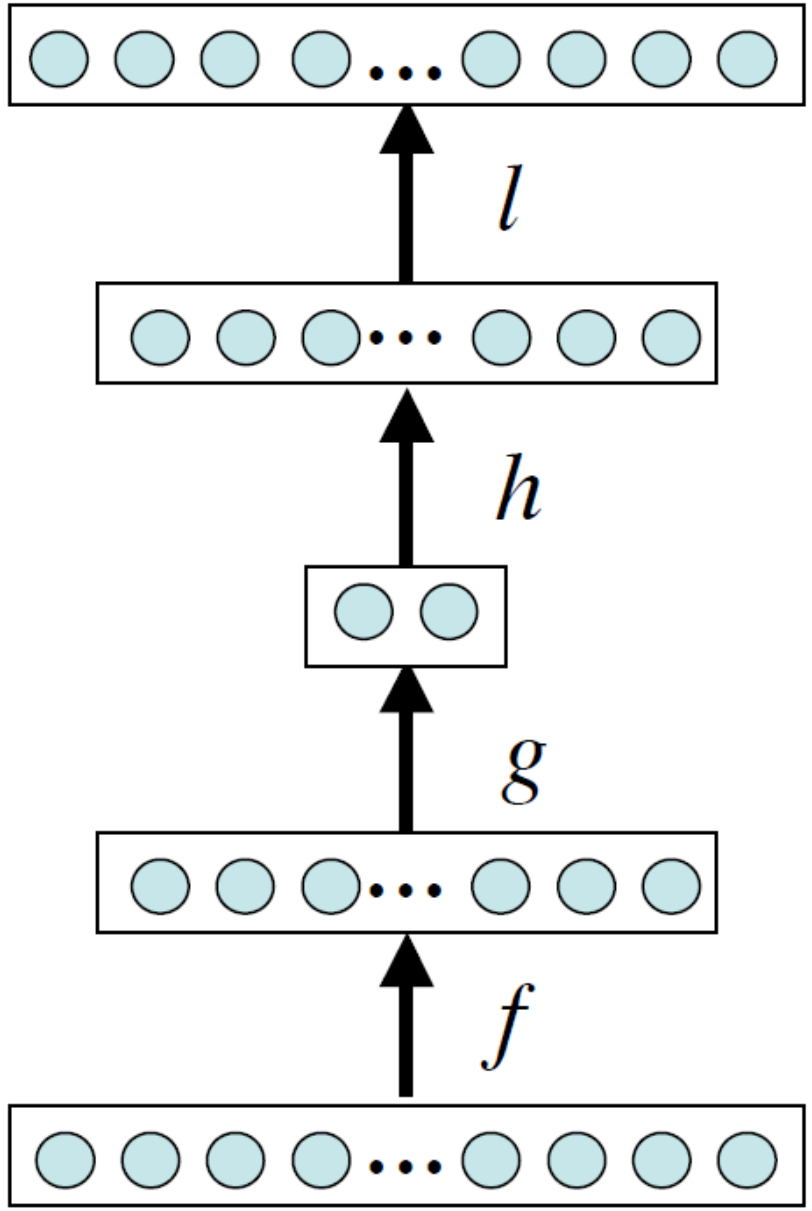
Cost function:

- Minimize the reconstruction error

$$\mathcal{L} = \sum_{\mathbf{x}_i \in D} \left\| \mathbf{x}_i - l_w(h_w(g_w f(\mathbf{x}_i))) \right\|_2^2$$

here, f and g are encoding functions

while h and l are decoding functions



Linear Discriminant Analysis

- Given a dataset $D = D_1 \cup D_2 \cup \ldots \cup D_k$ of n labeled samples, which belong to k classes:

$$D_1 = \{\mathbf{x}_{11}, \mathbf{x}_{12}, \ldots, \mathbf{x}_{1n_1}\}$$

$$D_2 = \{\mathbf{x}_{21}, \mathbf{x}_{22}, \ldots, \mathbf{x}_{2n_2}\}$$

$$\ldots$$

$$D_k = \{\mathbf{x}_{k1}, \mathbf{x}_{k2}, \ldots, \mathbf{x}_{kn_k}\}$$

where:

- each $\mathbf{x}_{ij}$ that $\in$ to class ω_i

$$n = \sum_{i=1}^{k} n_i$$

Consider the linear transformation $\mathbf{y} = \mathbf{A}\,\mathbf{x}$,

where $\mathbf{A}$ is an $m \times d$ matrix

- The projection is onto the m-dimensional space
- Then, the samples $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ in the d-dim. space
  - correspond to $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$ in the m-dim. space
  - where $m < d$ (ideally, $m <<< d$)
- Once projection/transformation is performed:
  - Classify the data using *any* classifier

Assumptions

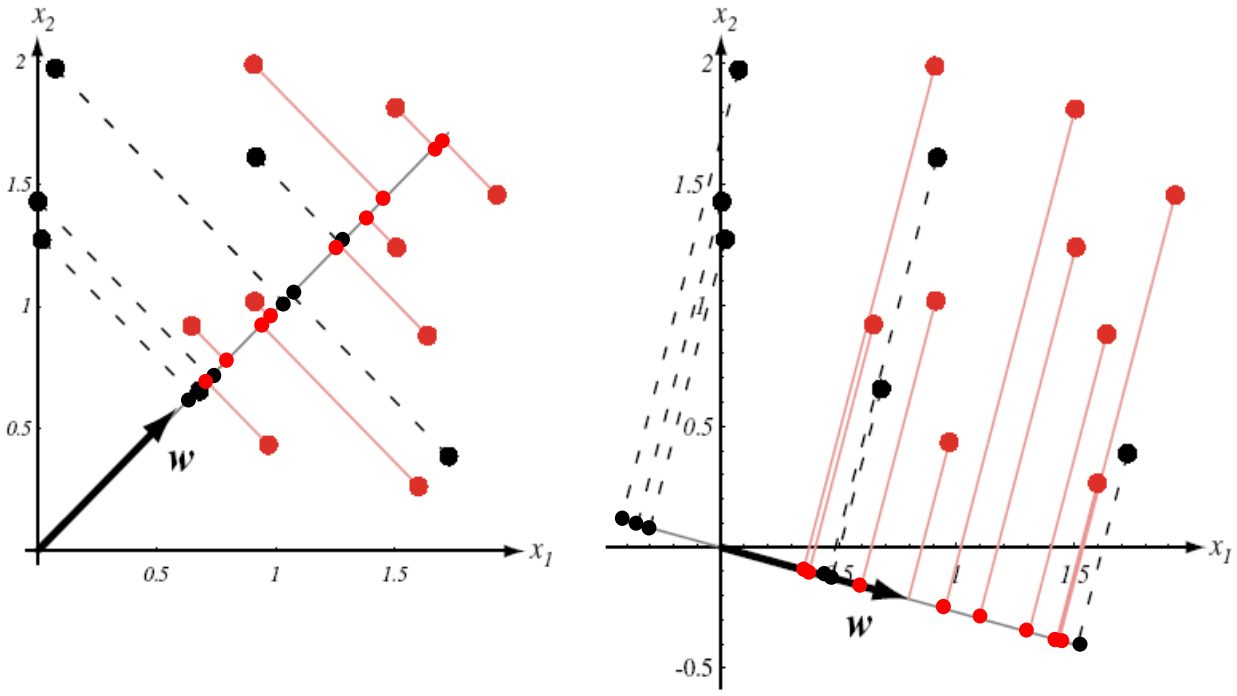
- Prior probabilities known:
  - $p_1, p_2, \ldots, p_k$
- Means known:
  - $\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_k$
- Covariances known:
  - $\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_k$
- If not known, estimate them!
- So, we have:

$$p_i = \frac{|D_i|}{|D|}, \quad \mathbf{m}_i = \frac{1}{|D_i|}\sum_{\mathbf{x}\in D_i}\mathbf{x}, \qquad \mathbf{S}_i = \frac{1}{|D_i|}\sum_{\mathbf{x}\in D_i}(\mathbf{x}-\mathbf{m}_i)(\mathbf{x}-\mathbf{m}_i)^t$$

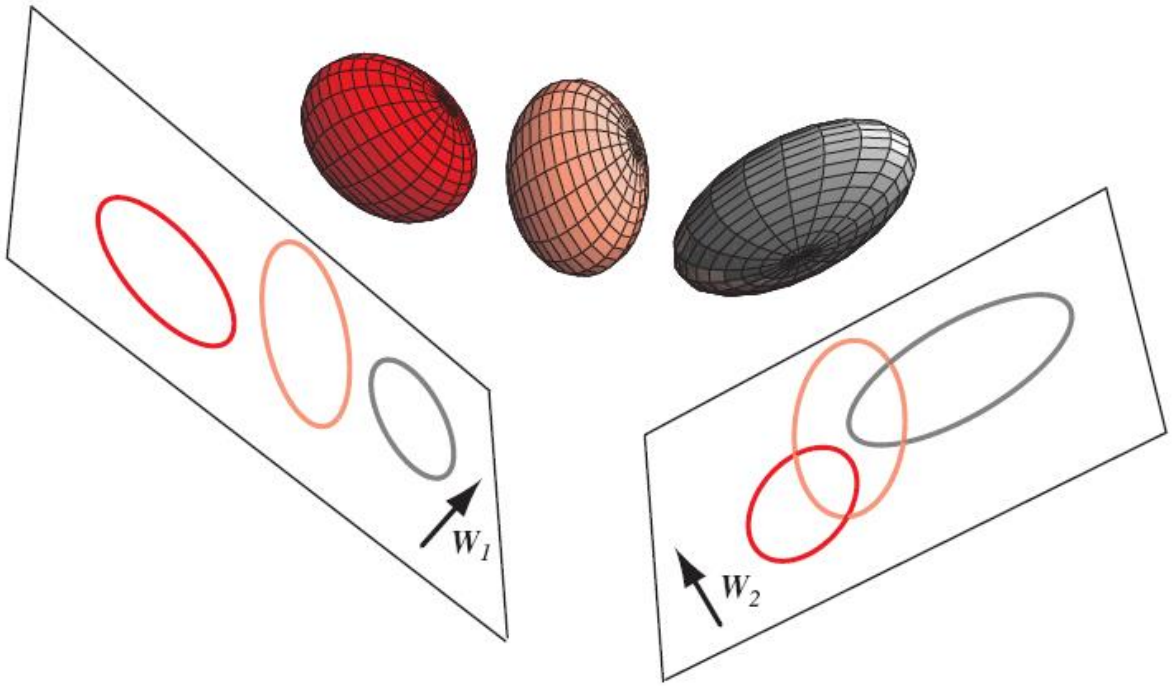
- **Important:**
  - Can apply LDR even when data are *not* normal

Examples

From 2D to 1D:



From 3D to 2D:



Fisher's Discriminant Analysis (FDA)

- FDA can be seen as an LDR method as well
- **Fisher's criterion** aims to maximize:

$$J(\mathbf{w}) = \frac{\mathbf{w}^t \mathbf{S}_E \mathbf{w}}{\mathbf{w}^t \mathbf{S}_W \mathbf{w}}$$

$$J_F(\mathbf{A}) = tr\left\{(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}(\mathbf{A}\mathbf{S}_E\mathbf{A}^t)\right\}$$

where $\mathbf{S}_E$ is the *between-class* scatter given by:

$$\mathbf{S}_E = \sum_{i=1}^{k} p_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t$$

- with **m** being the *total mean vector* computed as:

$$\mathbf{m} = \sum_{i=1}^{c} p_i \mathbf{m}_i$$

- $\mathbf{S}_W$ is the *within-class* scatter matrix (as in the two-class case):

$$\mathbf{S}_W = \sum_{i=1}^{k} p_i \mathbf{S}_i$$

- The solution is given by the eigenvectors that correspond to the *largest* eigenvalues of:

$$\mathbf{S}_W^{-1}\mathbf{S}_E$$

Note:

- Found only if $\mathbf{S}_W^{-1}$ exists
- For *c* classes *at most c* – 1 eigenvalues are > 0, while the others are 0 and yield **no classification** at all

Heteroscedastic Discriminant Analysis (HDA)

- FDA is a homoscedastic criterion:
  - Maximizes the Mahalanobis distance between the means
  - and when the covariance matrices are equal
- HDA is heteroscedastic:
  - Takes correlations between random variables to project data onto lower dimensional spaces
  - Uses directed distance matrices
  - Starts from the Chernoff distance in original space
  - Also called the “Chernoff criterion” or “Loog-Duin (LD)”
  - More details in ref. [1]

Mathematical Formulation

- For two classes, maximize:

$$J_{LD_2}(\mathbf{A}) = tr\left\{(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}\left[\mathbf{A}\mathbf{S}_E\mathbf{A}^t - \mathbf{A}\mathbf{S}_W^{\frac{1}{2}}\frac{p_1\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_1\mathbf{S}_W^{-\frac{1}{2}}) + p_2\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_2\mathbf{S}_W^{-\frac{1}{2}})}{p_1p_2}\mathbf{S}_W^{\frac{1}{2}}\mathbf{A}^t\right]\right\}$$

  where log(**B**) = **F** log(**L**) **F**$^{-1}$, with **F** being the eigenvectors of **B** and **L** the eigenvalues.

- Solution given by the eigenvectors (whose eigenvalues are the *largest*) of:

$$\mathbf{S}_{LD_2} = \mathbf{S}_W^{-1}\left[\mathbf{S}_E - \mathbf{S}_W^{\frac{1}{2}}\frac{p_1\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_1\mathbf{S}_W^{-\frac{1}{2}}) + p_2\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_2\mathbf{S}_W^{-\frac{1}{2}})}{p_1p_2}\mathbf{S}_W^{\frac{1}{2}}\right]$$

Multi-class case

The heteroscedastic criterion (HDA):

$$J_{LD}(\mathbf{A}) = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} p_i p_j tr\left\{(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}\mathbf{A}\mathbf{S}_W^{\frac{1}{2}} \left[(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_{ij}\mathbf{S}_W^{-\frac{1}{2}})^{-\frac{1}{2}}\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_{E_{ij}}\mathbf{S}_W^{-\frac{1}{2}}(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_{ij}\mathbf{S}_W^{-\frac{1}{2}})^{-\frac{1}{2}} + \frac{1}{\pi_i\pi_j}\left(\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_{ij}\mathbf{S}_W^{-\frac{1}{2}}) - \pi_i\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_i\mathbf{S}_W^{-\frac{1}{2}}) - \pi_j\log(\mathbf{S}_W^{-\frac{1}{2}}\mathbf{S}_j\mathbf{S}_W^{-\frac{1}{2}})\right)\right]\mathbf{S}_W^{\frac{1}{2}}\mathbf{A}^t\right\},$$

where:

$$\mathbf{S}_{E_{ij}} = (\mathbf{m}_i - \mathbf{m}_j)(\mathbf{m}_i - \mathbf{m}_j)^t,\ \pi_i = \frac{p_i}{p_i+p_j},\ \pi_j = \frac{p_j}{p_i+p_j},\ \text{and}\ \mathbf{S}_{ij} = \pi_i\mathbf{S}_i + \pi_j\mathbf{S}_j$$

$$\mathbf{S}_W = \sum_{i=1}^{k} p_i\mathbf{S}_i$$

- Solution given by the eigenvectors (whose eigenvalues are the *largest*) of:

$$\mathbf{S}_{LD} = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} p_i p_j \mathbf{S}_W^{-1} \mathbf{S}_W^{\frac{1}{2}} \Big[(\mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_{ij} \mathbf{S}_W^{-\frac{1}{2}})^{-\frac{1}{2}} \mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_{E_{ij}} \mathbf{S}_W^{-\frac{1}{2}} (\mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_{ij} \mathbf{S}_W^{-\frac{1}{2}})^{-\frac{1}{2}} + \frac{1}{\pi_i \pi_j} \Big(\log(\mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_{ij} \mathbf{S}_W^{-\frac{1}{2}}) - \pi_i \log(\mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_i \mathbf{S}_W^{-\frac{1}{2}}) - \pi_j \log(\mathbf{S}_W^{-\frac{1}{2}} \mathbf{S}_j \mathbf{S}_W^{-\frac{1}{2}}) \Big) \Big] \mathbf{S}_W^{\frac{1}{2}}$$

Chernoff Discriminant Analysis (CDA)

- HDA uses Chernoff distance in original space:
  - To create directed distance matrices
  - This does not, however, guarantee to maximize the Chernoff distance in transformed space
- CDA (unlike HDA) aims to maximize Chernoff distance in transformed space:
  - Chernoff distance is a good approximation of Bayes' classification error (for normal distributions)
  - Can be used even if distributions are not normal
  - Maximizing Chernoff distance in transformed space may not guarantee minimizing error
  - But works very well in many cases, including practical cases. See ref. [2]

Mathematical Formulation

Two-class criterion:

- Maximize:

$$J^*_{c_{12}}(\mathbf{A}) = p_1 p_2 (\mathbf{A}\mathbf{m}_1 - \mathbf{A}\mathbf{m}_2)^t [\mathbf{A}\mathbf{S}_W\mathbf{A}^t]^{-1} (\mathbf{A}\mathbf{m}_1 - \mathbf{A}\mathbf{m}_2) + \log\left(\frac{|\mathbf{A}\mathbf{S}_W\mathbf{A}^t|}{|\mathbf{A}\mathbf{S}_1\mathbf{A}|^{p_1}|\mathbf{A}\mathbf{S}_2\mathbf{A}|^{p_2}}\right)$$

- or equivalently:

$$J^*_{c_{12}}(\mathbf{A}) = tr\left\{p_1 p_2 (\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}\mathbf{A}\mathbf{S}_E\mathbf{A}^t + \log(\mathbf{A}\mathbf{S}_W\mathbf{A}^t) - p_1\log(\mathbf{A}\mathbf{S}_1\mathbf{A}^t) - p_2\log(\mathbf{A}\mathbf{S}_2\mathbf{A}^t)\right\}$$

- The gradient:

$$\begin{aligned}\frac{\partial J^*_{c_{12}}}{\partial \mathbf{A}} = {} & 2p_1p_2\left[\mathbf{S}_E\mathbf{A}^t(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1} - \mathbf{S}_W\mathbf{A}^t(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}(\mathbf{A}\mathbf{S}_E\mathbf{A}^t)(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1}\right]^t \\ & +2\left[\mathbf{S}_W\mathbf{A}^t(\mathbf{A}\mathbf{S}_W\mathbf{A}^t)^{-1} - p_1\mathbf{S}_1\mathbf{A}^t(\mathbf{A}\mathbf{S}_1\mathbf{A}^t)^{-1} - p_2\mathbf{S}_2\mathbf{A}^t(\mathbf{A}\mathbf{S}_2\mathbf{A}^t)^{-1}\right]^t\end{aligned}$$

- The criterion is maximized via the gradient algorithm.

Algorithm **Chernoff_LDA_Two**

Input: Threshold τ

begin

$\mathbf{A}^{(0)} \leftarrow \max_{\mathbf{A}}\{J^*_{c_{12}}(\mathbf{A}_F), J^*_{c_{12}}(\mathbf{A}_{LD})\}$ // Max. of Fisher's and

$k \leftarrow 0$

repeat

$\eta_k \leftarrow max_{\eta>0}\phi_{k_{12}}(\eta)$

$\mathbf{B} \leftarrow \mathbf{A}^{(k)} + \eta_k \nabla J^*_{c_{12}}(\mathbf{A}^{(k)})$

Decompose $\mathbf{B}$ into $\mathbf{R}$ and $\mathbf{Q}$

$\mathbf{A}^{(k+1)} \leftarrow \mathbf{Q}$

$k \leftarrow k + 1$

until $|J^*_{c_{12}}(\mathbf{A}^{(k-1)}) - J^*_{c_{12}}(\mathbf{A}^{(k)})| < \tau$

return $\mathbf{A}^{(k)}$, $J^*_{c_{12}}(\mathbf{A}^{(k)})$

end

Multi-class case

- Maximize:

$$J_c^*(\mathbf{A}) = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} J_{c_{ij}}^*(\mathbf{A})$$

where:

$$J_{c_{ij}}^*(\mathbf{A}) = tr\left\{p_i p_j (\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t)^{-1}\mathbf{A}\mathbf{S}_{E_{ij}}\mathbf{A}^t + \log(\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t) - p_i \log(\mathbf{A}\mathbf{S}_i\mathbf{A}^t) - p_j \log(\mathbf{A}\mathbf{S}_j\mathbf{A}^t)\right\}$$

- Gradient:

$$\nabla J_c^*(\mathbf{A}) = \frac{\partial J_c^*(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial}{\partial \mathbf{A}} \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} J_{c_{ij}}^*(\mathbf{A}) = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \nabla J_{c_{ij}}^*(\mathbf{A})$$

$$\nabla J_{c_{ij}}^*(\mathbf{A}) = \frac{\partial J_{c_{ij}}^*}{\partial \mathbf{A}} = 2p_i p_j \left[\mathbf{S}_{E_{ij}}\mathbf{A}^t(\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t)^{-1} - \mathbf{S}_{W_{ij}}\mathbf{A}^t(\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t)^{-1}(\mathbf{A}\mathbf{S}_{E_{ij}}\mathbf{A}^t)(\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t)^{-1}\right]^t$$
$$+2\left[\mathbf{S}_{W_{ij}}\mathbf{A}^t(\mathbf{A}\mathbf{S}_{W_{ij}}\mathbf{A}^t)^{-1} - p_i\mathbf{S}_i\mathbf{A}^t(\mathbf{A}\mathbf{S}_i\mathbf{A}^t)^{-1} - p_j\mathbf{S}_j\mathbf{A}^t(\mathbf{A}\mathbf{S}_j\mathbf{A}^t)^{-1}\right]^t$$

Algorithm (multi-class)

Algorithm **Chernoff_LDA_Multi**

Input: Threshold τ

begin

$\mathbf{A}^{(0)} \leftarrow \max_{\mathbf{A}}\{J^*_{c12}(\mathbf{A}_F), J^*_{c12}(\mathbf{A}_{LD})\}$ // Max. of Fisher's and Loog-Duin

$k \leftarrow 0$

repeat

$\eta_k \leftarrow max_{\eta>0}\phi_k(\eta)$

$\mathbf{B} \leftarrow \mathbf{A}^{(k)} + \eta_k \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} \nabla J^*_{c_{ij}}(\mathbf{A}^{(k)})$

Decompose $\mathbf{B}$ into $\mathbf{R}$ and $\mathbf{Q}$

$\mathbf{A}^{(k+1)} \leftarrow \mathbf{Q}$

$k \leftarrow k+1$

until $|J^*_{c_{ij}}(\mathbf{A}^{(k-1)}) - J^*_{c_{ij}}(\mathbf{A}^{(k)})| < \tau$

return $\mathbf{A}^{(k)}, \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} J^*_{c_{ij}}(\mathbf{A}^{(k)})$

end

Dealing with Singular Matrices

- Find a function of A as follows $f(\mathbf{A}) = \mathbf{\Phi}\, f(\mathbf{\Lambda})\, \mathbf{\Phi}^{-1}$, where

$$f(\mathbf{\Lambda}) = \begin{bmatrix} f(\lambda_1) & 0 & 0 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \vdots & \cdots & \vdots \\ 0 & 0 & f(\lambda_k) & 0 & \cdots & 0 \\ 0 & 0 & 0 & \mathbf{0} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & \cdots & \mathbf{0} \end{bmatrix}$$

Make zero all these values in the diagonal

- 0's in bold replace singular values of $f(\lambda_{k+1}), \ldots, f(\lambda_d)$
- For example, log(0), 0^{-1}, $0^{-1/2}$, etc.
- This will let us compute $\mathbf{S}_W^{-1}$, log($\mathbf{S}_W$), etc.
- It's similar to SVD

Example 1:

- Given: $\mathbf{x}_1 \sim N(\mathbf{m}_1, \mathbf{S}_1)$ and $\mathbf{x}_2 \sim N(\mathbf{m}_2, \mathbf{S}_2)$

$$\mathbf{m}_1 = [0.5001, 0.4947]^t, \quad \mathbf{m}_2 = [2.1069, 1.4324]^t$$

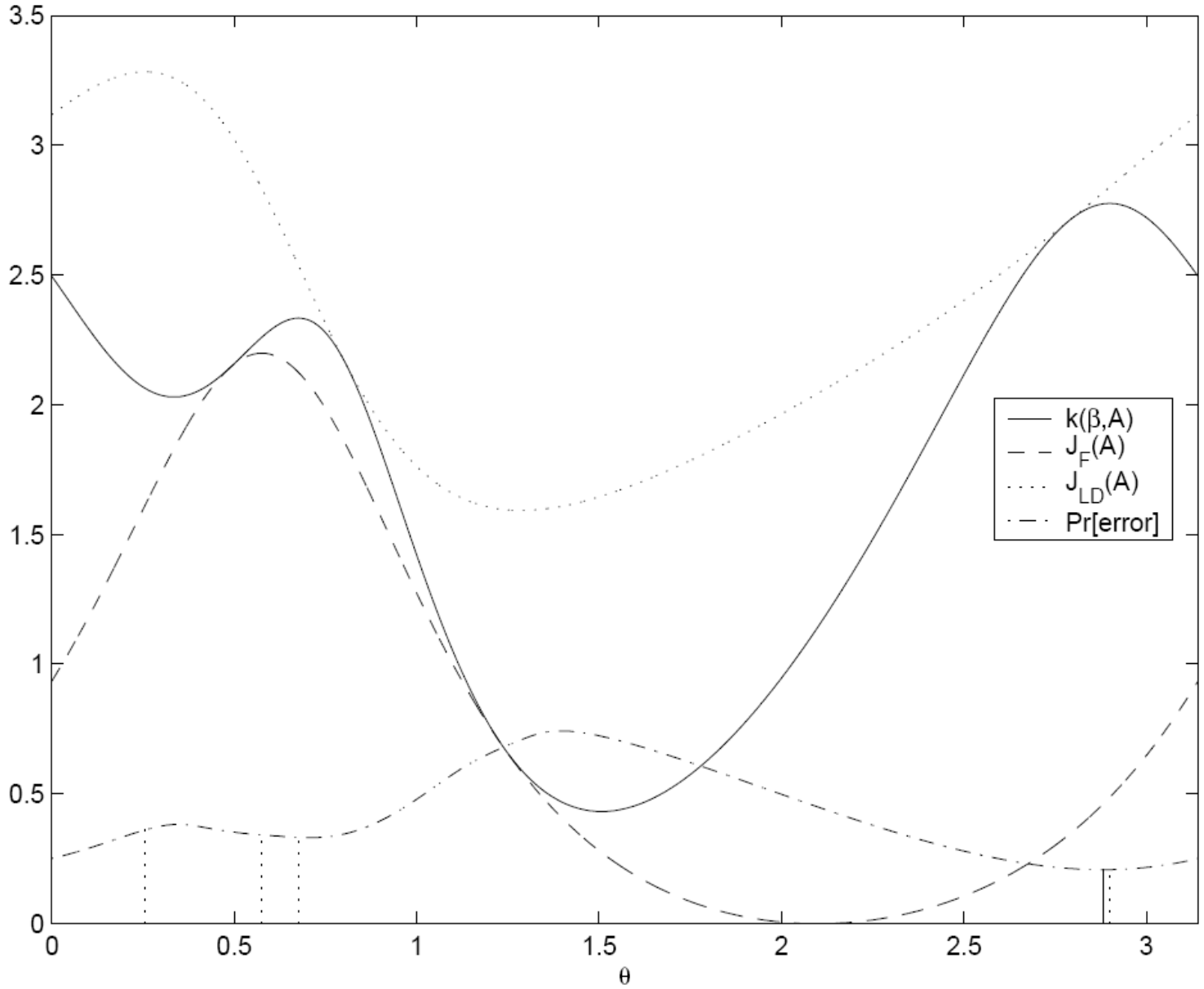
$$\mathbf{S}_1 = [0.8205, 0.4177; 0.4177, 2.8910]$$

$$\mathbf{S}_2 = [5.1150, -4.3990; -4.3990, 5.7119]$$

$$p_1 = p_2 = 0.5$$

- Linear transformation: **y** = **A x**
  where **x** is 2D, **y** is 1D, and **A** is 1×2.
- Let $\beta = 1/2$
- Plot J_F, J_{LD}, and J_c^* or $k(\beta,\mathbf{A})$ for all values of θ
  where θ is the angle between **A** and $[1,0]^t$

Plots of Criterion Functions



Example 2:

Given: $\mathbf{x}_1 \sim N(\mathbf{m}_1, \mathbf{S}_1)$ and $\mathbf{x}_2 \sim N(\mathbf{m}_2, \mathbf{S}_2)$

$$\mathbf{m}_1 = [0.6083 \quad 2.2414]^t, \quad \mathbf{m}_2 = [3.5014 \quad 6.3859]^t$$

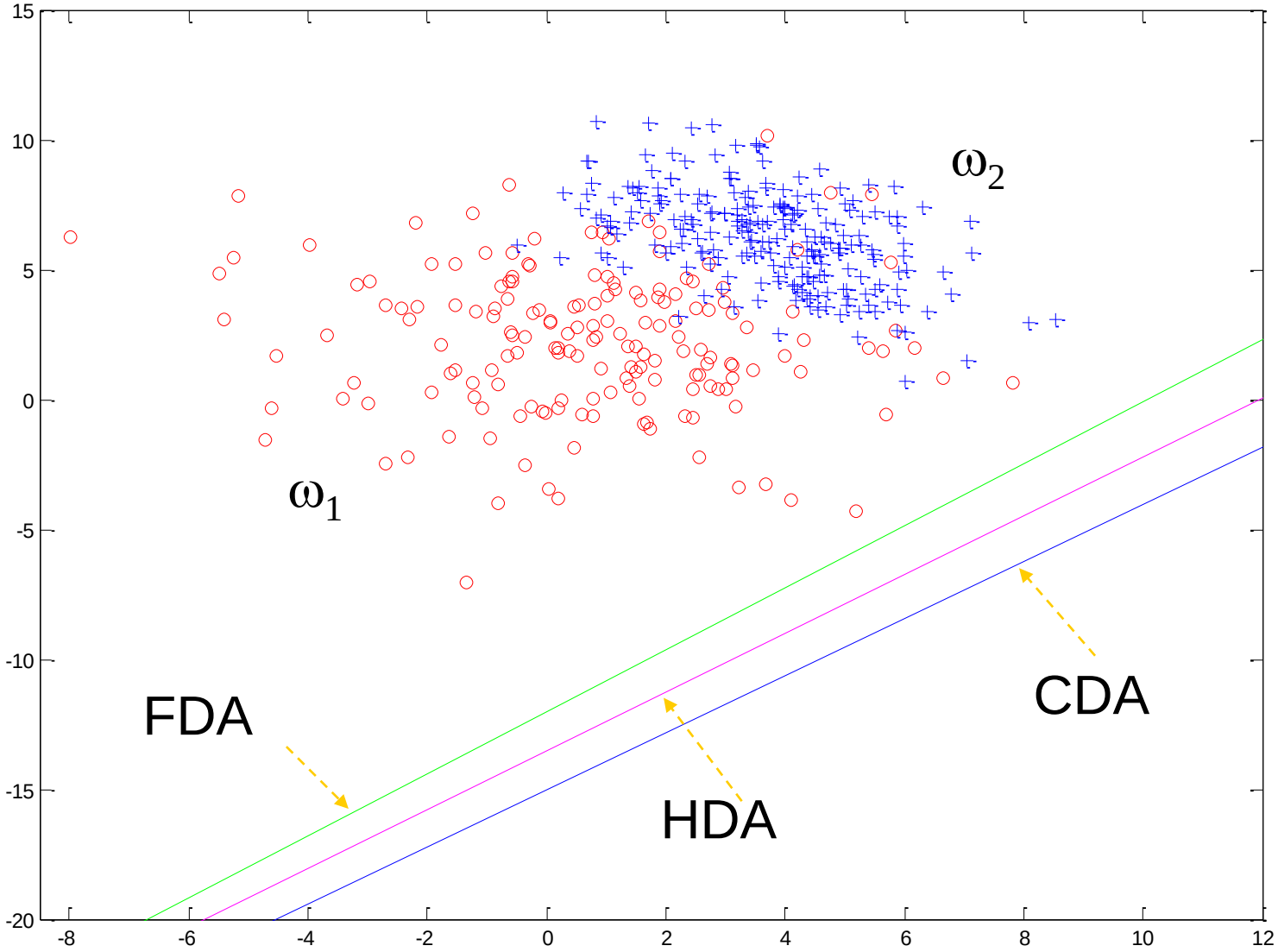
$$\mathbf{S}_1 = \begin{bmatrix} 6.9311 & -0.4091 \\ -0.4091 & 6.7122 \end{bmatrix}, \quad \mathbf{S}_2 = \begin{bmatrix} 2.7743 & -1.5834 \\ -1.5834 & 3.4662 \end{bmatrix}$$

$p_1 = 0.4358, \quad p_2 = 0.5642$

	Chernoff Dist.	**A**
Fisher	7.7708	[0.6431 0.7658]
Loog-Duin	7.7880	[0.6620 0.7495]
Gradient*	7.7907	[0.6731 0.7397]

***** Optimal for this example.

Graphically



- Difference almost not noticeable in 2D → 1D
- But significant in larger dimensions:
  e.g., 50D → 10D

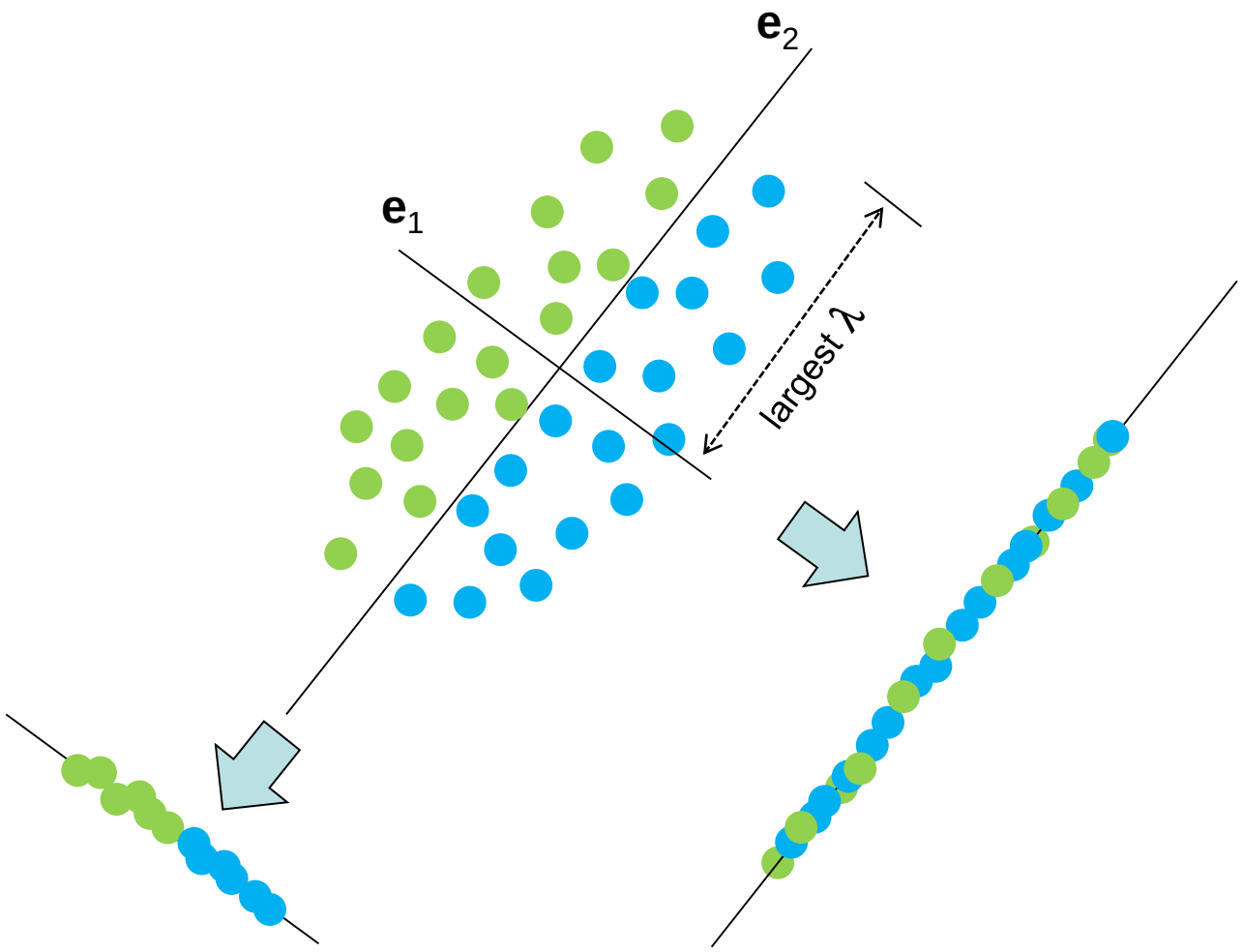
PCA vs LDA

PCA considers *all* classes *together* as a source of information about how *disperse* the data points are

- Better applicable to:
  - *Unsupervised* learning problems (classes not known)
  - When no LDA method can be applied (due to ill-conditioned matrices, for example)

LDA takes information about individual classes into account to maximize separability in new space

- Better applicable to:
  - *Supervised* classification (classes are *known*)
  - Lower dimension still gives good (desired) separability and sometimes even better!



Dimensionality Reduction in Scikit

- The sklearn.decomposition module includes matrix decomposition algorithms, including among others PCA, NMF or ICA.
- It also includes:
  - kernel PCA
  - SVD
  - Manifold learning
    - https://scikit-learn.org/stable/modules/manifold.html#manifold
- Main link:
  - http://scikit-learn.org/stable/modules/classes.html#module-sklearn.decomposition
- LDA is included in sklearn.discriminant_analysis:
  - http://scikit-learn.org/stable/modules/classes.html#module-sklearn.discriminant_analysis

Sample Dataset Generation in Scikit

- The sklearn.datasets module includes utilities for generating and loading datasets.
- Typical datasets:
  - Synthetic: S-shape, Swiss roll, Circles, Blobs, Moons, etc.
  - Real datasets: Iris, Breast cancer, Faces, News groups, etc.

- Main link:
  - https://scikit-learn.org/stable/modules/classes.html#module-sklearn.datasets

References - Acknowledgments

The material presented in this chapter has been taken from the following sources (among others):

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