Lecture Slides for

INTRODUCTION TO

Machine Learning

2nd Edition

ETHEM ALPAYDIN

alpaydin@boun.edu.tr
http://www.cmpe.boun.edu.tr/~ethem/i2ml2e

CHAPTER 6:

Dimensionality Reduction

Why Reduce Dimensionality?

- Reduces time complexity: Less computation
- Reduces space complexity: Less parameters
- Saves the cost of observing the feature
- Simpler models are more robust on small datasets
- More interpretable; simpler explanation
- Data visualization (structure, groups, outliers, etc) if plotted in 2 or 3 dimensions

Feature Selection vs Extraction

- Feature selection: Choosing $k<d$ important features, ignoring the remaining $d - k$

    Subset selection algorithms

- Feature extraction: Project the

    original x_i , i =1,...,d dimensions to

    new $k<d$ dimensions, z_j , j =1,...,k

    Principal components analysis (PCA), linear discriminant analysis (LDA), factor analysis (FA)

Subset Selection

- There are 2^d subsets of d features
- Forward search: Add the best feature at each step
  - Set of features F initially Ø.
  - At each iteration, find the best new feature

    $j = \text{argmin}_i\, E\,(\,F \cup x_i\,)$
  - Add x_j to F if $E\,(\,F \cup x_j\,) < E\,(\,F\,)$

- Hill-climbing O(d^2) algorithm
- Backward search: Start with all features and remove one at a time, if possible.
- Floating search (Add k, remove l)

Principal Components Analysis (PCA)

- Find a low-dimensional space such that when ***x*** is projected there, information loss is minimized.
- The projection of ***x*** on the direction of ***w*** is: $z = \mathbf{w}^T\mathbf{x}$
- Find ***w*** such that Var(z) is maximized

$$\begin{aligned}
\mathrm{Var}(z) = \mathrm{Var}(\mathbf{w}^T\mathbf{x}) &= E[(\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\boldsymbol{\mu})^2] \\
&= E[(\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\boldsymbol{\mu})(\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\boldsymbol{\mu})] \\
&= E[\mathbf{w}^T(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\mathbf{w}] \\
&= \mathbf{w}^T E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T]\mathbf{w} = \mathbf{w}^T \boldsymbol{\Sigma} \mathbf{w}
\end{aligned}$$

where $\mathrm{Var}(\mathbf{x}) = E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T] = \boldsymbol{\Sigma}$

- Maximize Var(z) subject to $||\boldsymbol{w}||=1$

$$\max_{\mathbf{w}_1} \mathbf{w}_1^T \Sigma \mathbf{w}_1 - \alpha\left(\mathbf{w}_1^T \mathbf{w}_1 - 1\right)$$

  $\boldsymbol{\Sigma w}_1 = \alpha \boldsymbol{w}_1$ that is, $\boldsymbol{w}_1$ is an eigenvector of $\boldsymbol{\Sigma}$
  Choose the one with the largest eigenvalue for Var(z) to be max
- Second principal component: Max Var(z_2), s.t., $||\boldsymbol{w}_2||=1$ and orthogonal to $\boldsymbol{w}_1$

$$\max_{\mathbf{w}_2} \mathbf{w}_2^T \Sigma \mathbf{w}_2 - \alpha\left(\mathbf{w}_2^T \mathbf{w}_2 - 1\right) - \beta\left(\mathbf{w}_2^T \mathbf{w}_1 - 0\right)$$

  $\boldsymbol{\Sigma}\ \boldsymbol{w}_2 = \alpha\ \boldsymbol{w}_2$ that is, $\boldsymbol{w}_2$ is another eigenvector of $\boldsymbol{\Sigma}$

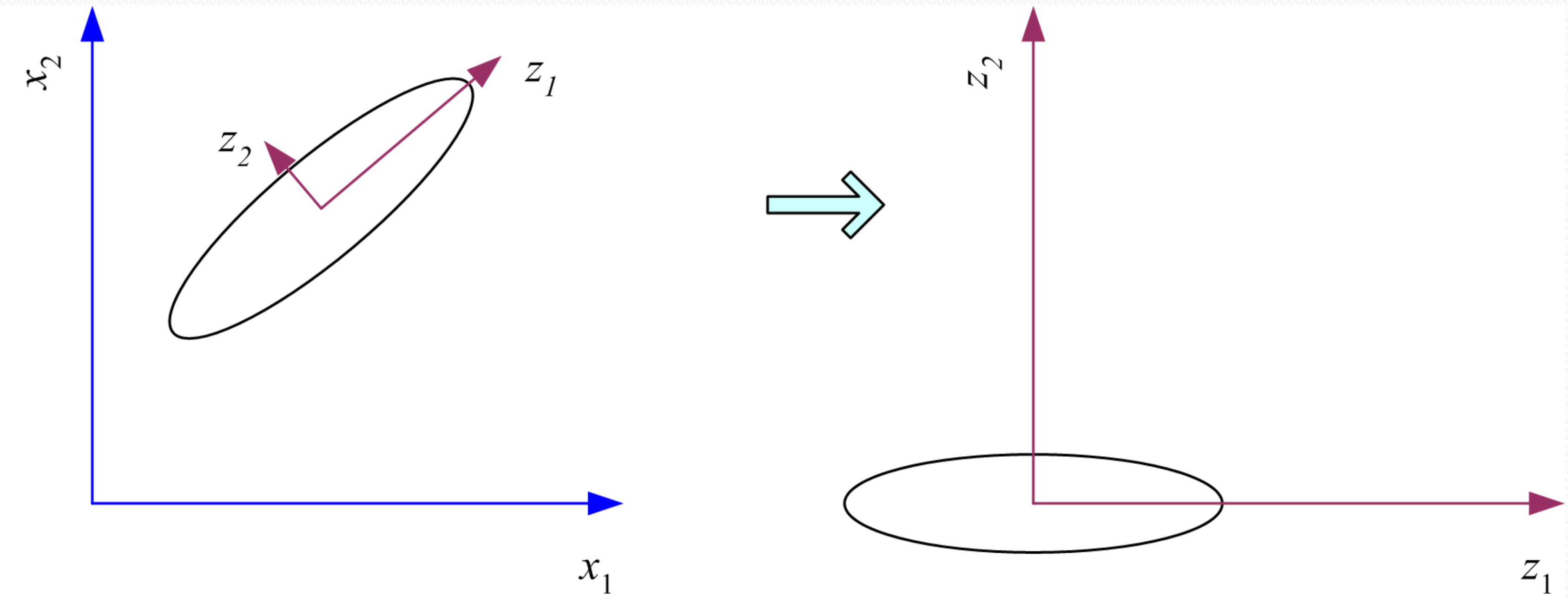
  and so on.

What PCA does

$$\boldsymbol{z} = \mathbf{W}^T(\boldsymbol{x} - \boldsymbol{m})$$

where the columns of **W** are the eigenvectors of ∑, and ***m*** is sample mean

Centers the data at the origin and rotates the axes

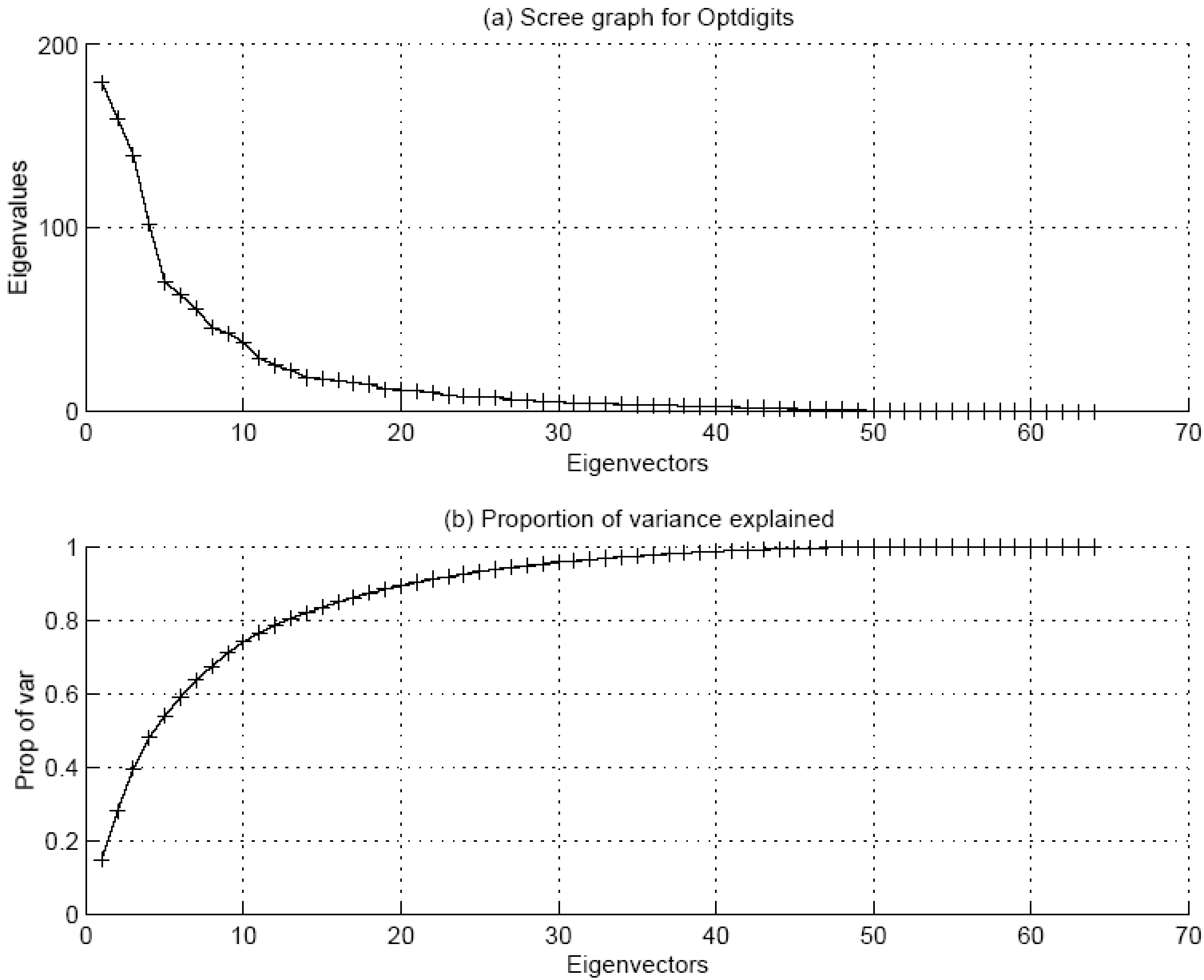


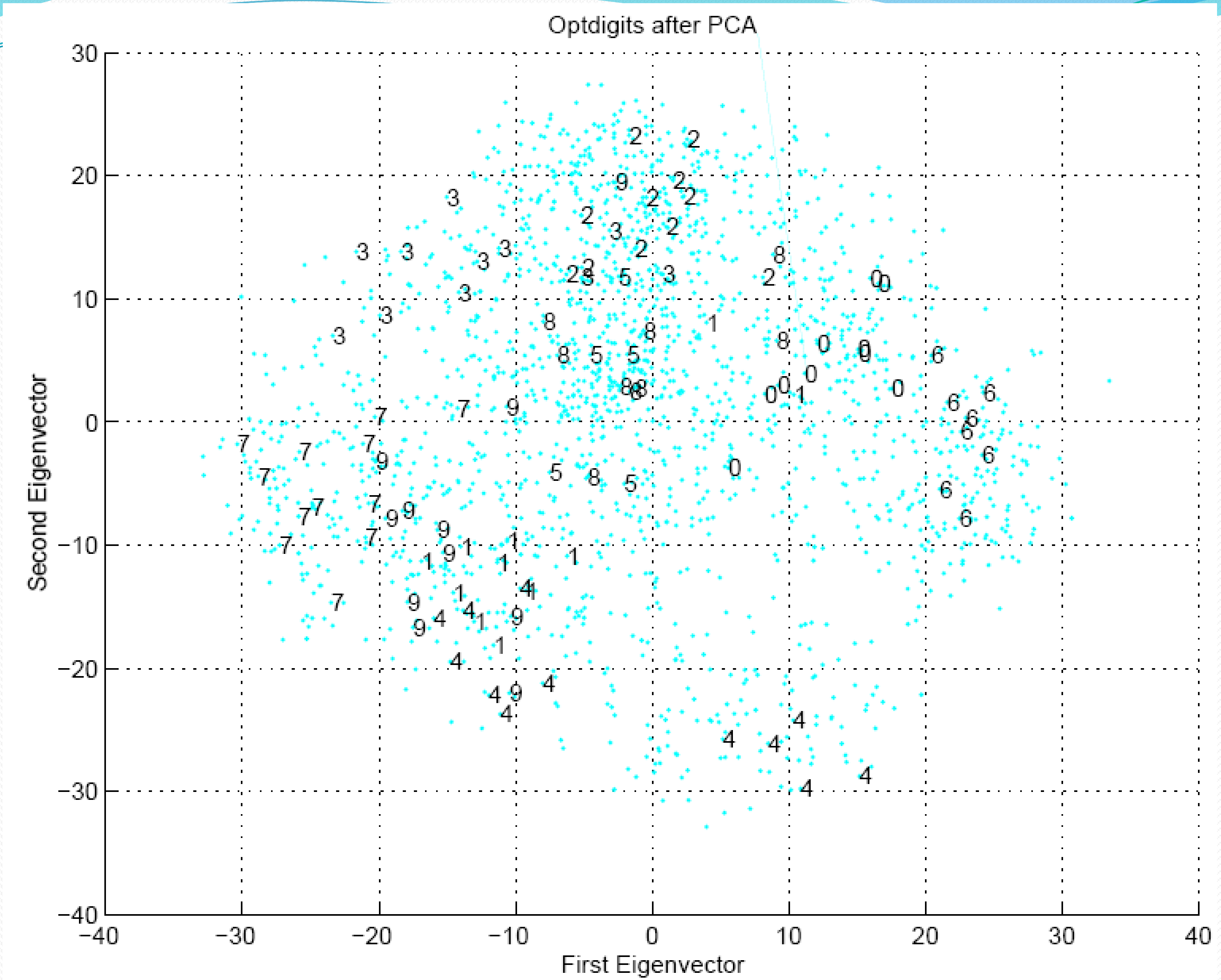
How to choose k ?

- Proportion of Variance (PoV) explained

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$

  when λ_i are sorted in descending order
- Typically, stop at PoV>0.9
- Scree graph plots of PoV vs *k*, stop at "elbow"


(a) Scree graph for Optdigits
Eigenvalues
200
100
0
0
10
20
30
40
50
60
70
Eigenvectors
(b) Proportion of variance explained
Prop of var
1
0.8
0.6
0.4
0.2
0
0
10
20
30
40
50
60
70
Eigenvectors


Optdigits after PCA
Second Eigenvector
First Eigenvector
30
20
10
0
−10
−20
−30
−40
−40
−30
−20
−10
0
10
20
30
40

Factor Analysis

- Find a small number of factors $\boldsymbol{z}$, which when combined generate $\boldsymbol{x}$:

$$x_i - \mu_i = v_{i1}z_1 + v_{i2}z_2 + \dots + v_{ik}z_k + \varepsilon_i$$

where z_j, $j = 1,\dots,k$ are the latent factors with

$E[\, z_j \,]=0$, $\mathrm{Var}(z_j)=1$, $\mathrm{Cov}(z_i, z_j)=0$, $i \neq j$,

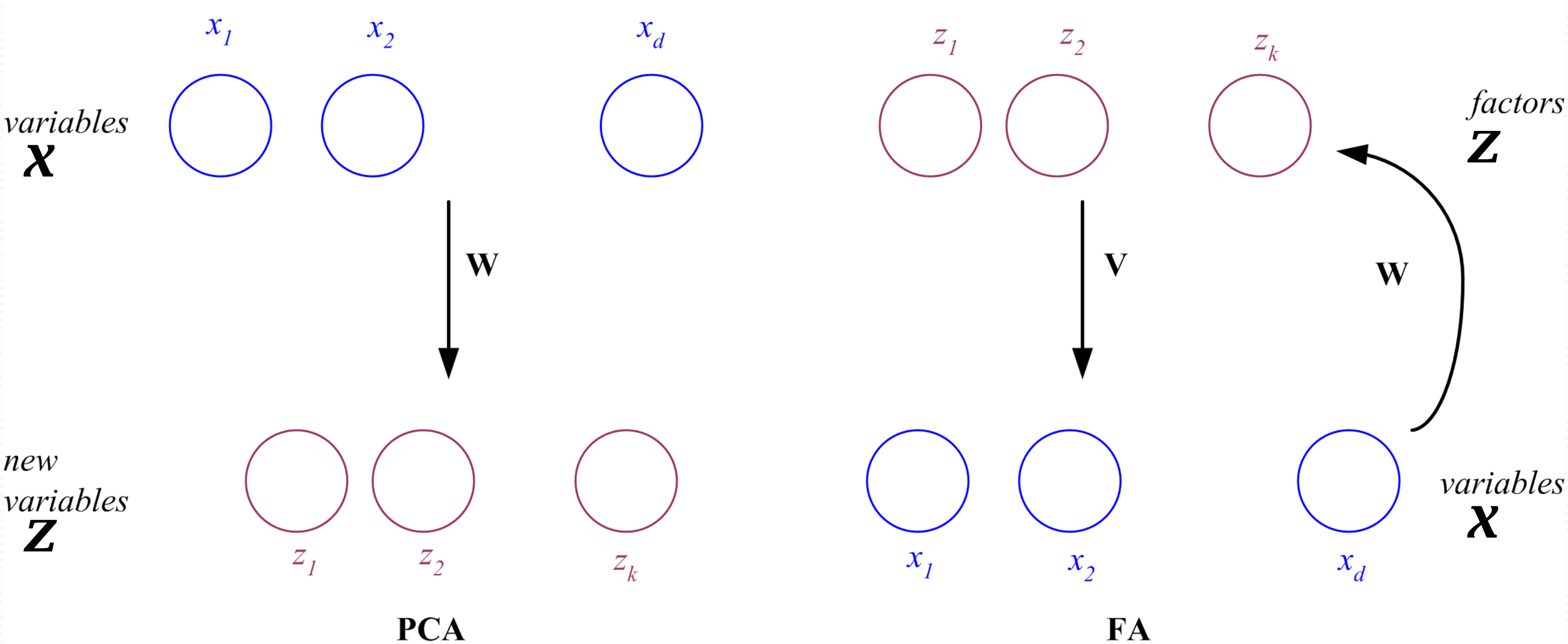
ε_i are the noise sources

$E[\, \varepsilon_i \,]= \psi_i$, $\mathrm{Cov}(\varepsilon_i , \varepsilon_j) =0$, $i \neq j$, $\mathrm{Cov}(\varepsilon_i , z_j) =0$,

and v_{ij} are the factor loadings

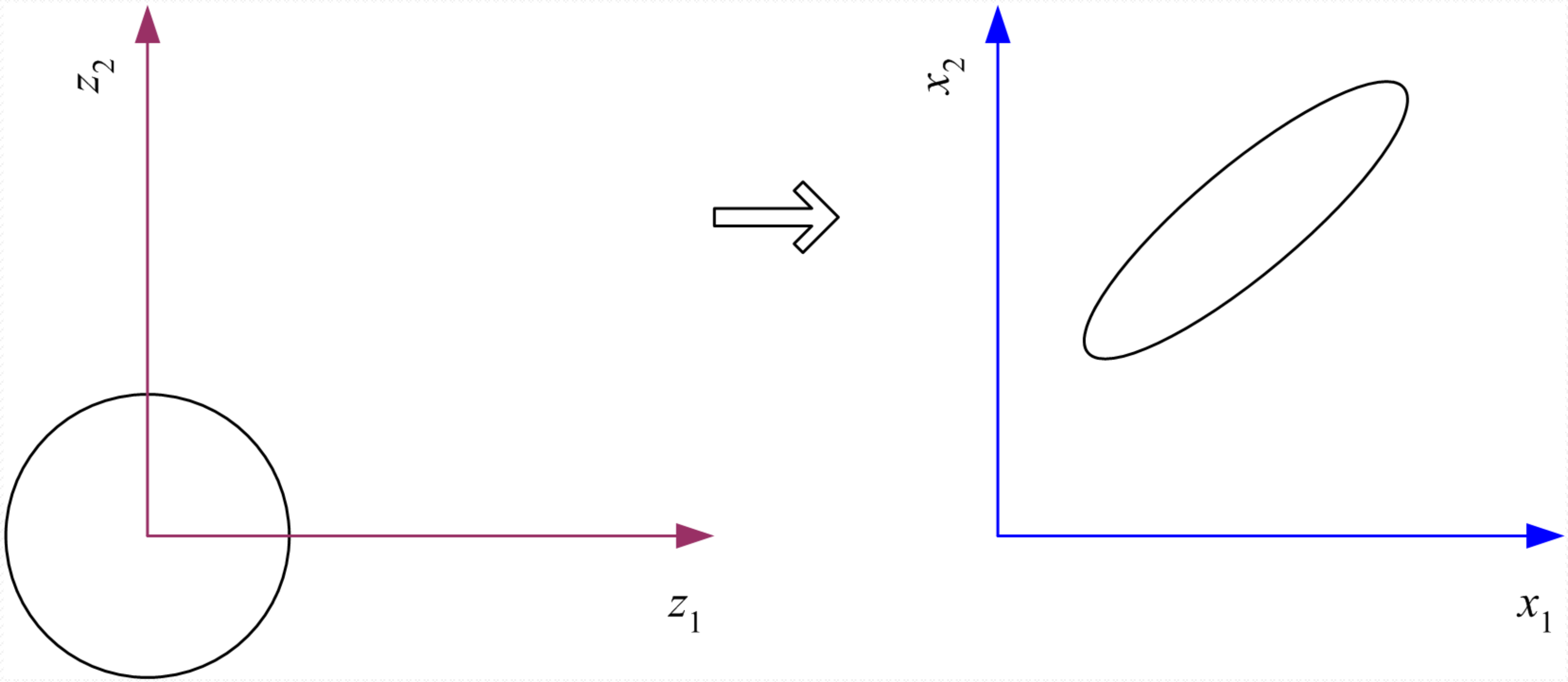
PCA vs FA

- PCA From $\boldsymbol{x}$ to $\boldsymbol{z}$ $\boldsymbol{z} = \mathbf{W}^T(\boldsymbol{x} - \boldsymbol{\mu})$
- FA From $\boldsymbol{z}$ to $\boldsymbol{x}$ $\boldsymbol{x} - \boldsymbol{\mu} = \mathbf{V}\boldsymbol{z} + \boldsymbol{\varepsilon}$



Factor Analysis

- In FA, factors z_j are stretched, rotated and translated to generate $\boldsymbol{x}$



Multidimensional Scaling

- Given pairwise distances between N points,

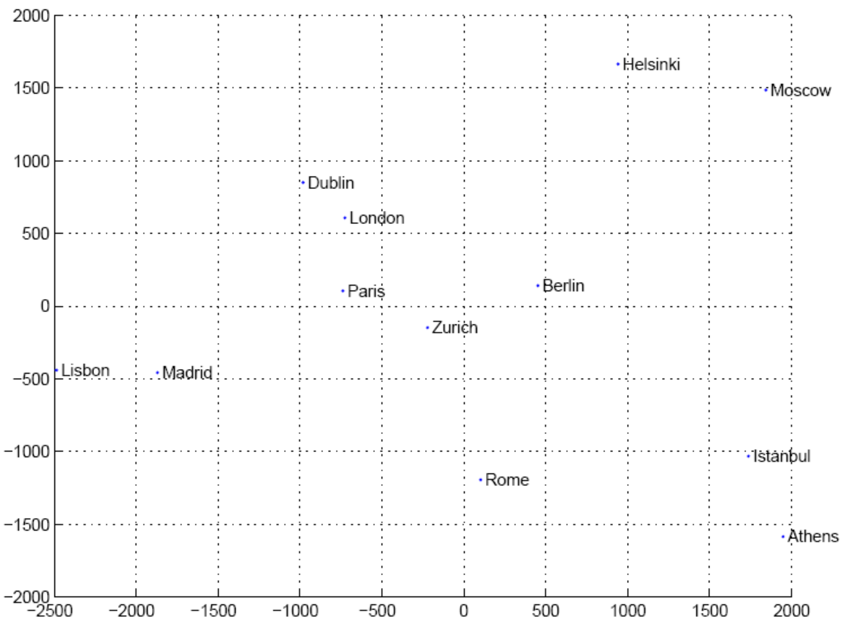
  d_{ij}, $i,j = 1,\ldots,N$

  place on a low-dim map s.t. distances are preserved.
- $\boldsymbol{z} = \boldsymbol{g}(\boldsymbol{x} \mid \vartheta)$ Find ϑ that min Sammon stress

$$E(\theta \mid \mathcal{X}) = \sum_{r,s} \frac{\left(\|\mathbf{z}^r - \mathbf{z}^s\| - \|\mathbf{x}^r - \mathbf{x}^s\|\right)^2}{\|\mathbf{x}^r - \mathbf{x}^s\|^2}$$

$$= \sum_{r,s} \frac{\left(\|\mathbf{g}(\mathbf{x}^r \mid \theta) - \mathbf{g}(\mathbf{x}^s \mid \theta)\| - \|\mathbf{x}^r - \mathbf{x}^s\|\right)^2}{\|\mathbf{x}^r - \mathbf{x}^s\|^2}$$

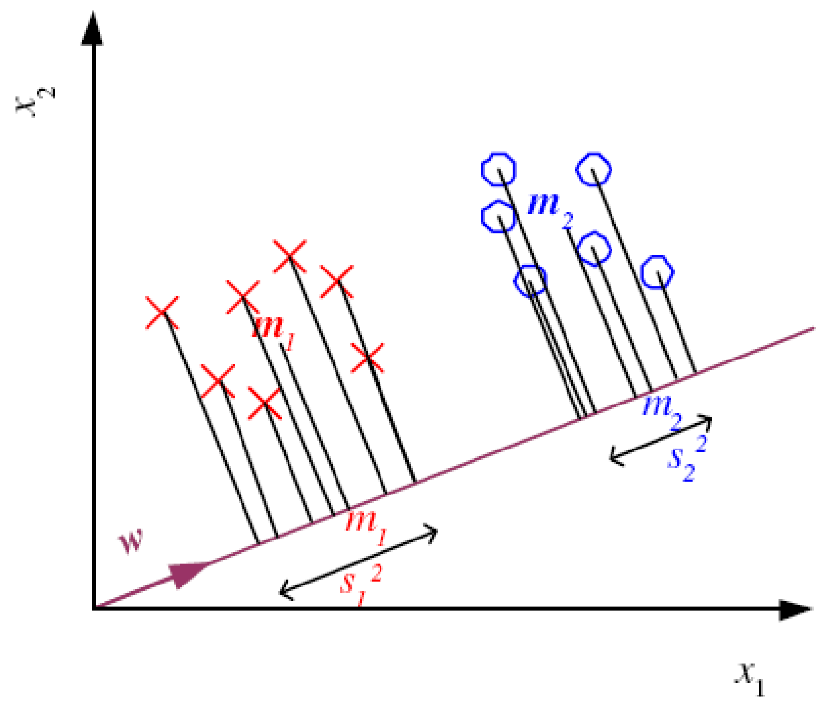
Map of Europe by MDS



Map from CIA – The World Factbook: http://www.cia.gov/

Linear Discriminant Analysis

- Find a low-dimensional space such that when ***x*** is projected, classes are well-separated.
- Find ***w*** that maximizes



$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

$$m_1 = \frac{\sum_t \mathbf{w}^T \mathbf{x}^t r^t}{\sum_t r^t} \qquad s_1^2 = \sum_t \left(\mathbf{w}^T \mathbf{x}^t - m_1\right)^2 r^t$$

- Between-class scatter:

$$(m_1 - m_2)^2 = \left(\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2\right)^2$$
$$= \mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\mathbf{w}$$
$$= \mathbf{w}^T\mathbf{S}_B\mathbf{w} \text{ where } \mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T$$

- Within-class scatter:

$$s_1^2 = \sum_t \left(\mathbf{w}^T\mathbf{x}^t - m_1\right)^2 r^t$$
$$= \sum_t \mathbf{w}^T\left(\mathbf{x}^t - \mathbf{m}_1\right)\left(\mathbf{x}^t - \mathbf{m}_1\right)^T\mathbf{w}r^t = \mathbf{w}^T\mathbf{S}_1\mathbf{w}$$
$$\text{where } \mathbf{S}_1 = \sum_t \left(\mathbf{x}^t - \mathbf{m}_1\right)\left(\mathbf{x}^t - \mathbf{m}_1\right)^T r^t$$
$$s_1^2 + s_1^2 = \mathbf{w}^T\mathbf{S}_W\mathbf{w} \text{ where } \mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$$

Fisher's Linear Discriminant

- Find ***w*** that max

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{\left|\mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)\right|^2}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- LDA soln:

$$\mathbf{w} = c \cdot \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- Parametric soln:

$$\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$$

$$\text{when } p(\mathbf{x}|C_i) \sim \mathcal{N}(\mu_i, \Sigma)$$

K>2 Classes

- Within-class scatter:

$$\mathbf{S}_W = \sum_{i=1}^{K} \mathbf{S}_i \qquad \mathbf{S}_i = \sum_t r_i^t \left(\mathbf{x}^t - \mathbf{m}_i\right)\left(\mathbf{x}^t - \mathbf{m}_i\right)^T$$

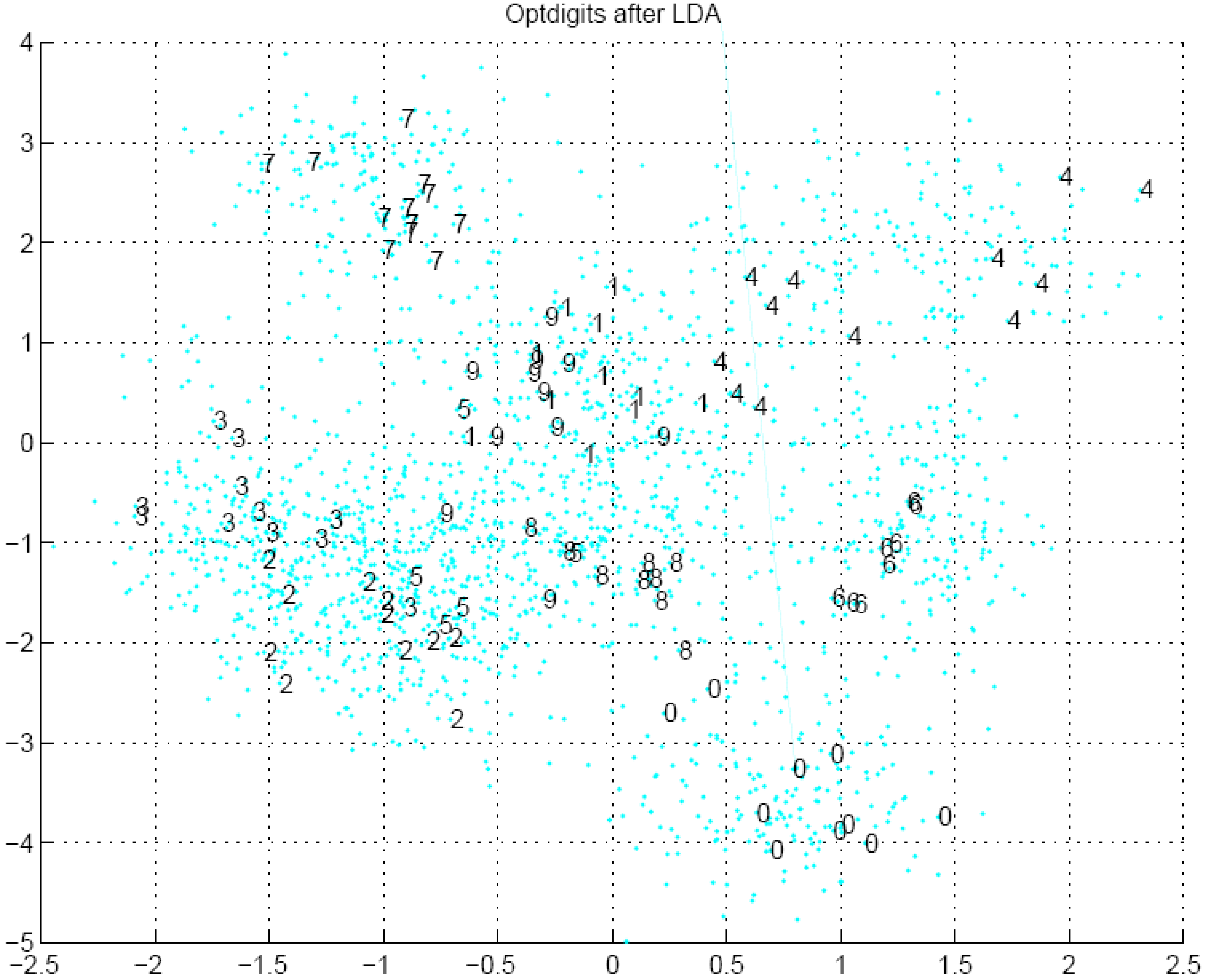
- Between-class scatter:

$$\mathbf{S}_B = \sum_{i=1}^{K} N_i \left(\mathbf{m}_i - \mathbf{m}\right)\left(\mathbf{m}_i - \mathbf{m}\right)^T \qquad \mathbf{m} = \frac{1}{K}\sum_{i=1}^{K} \mathbf{m}_i$$

- Find **W** that max

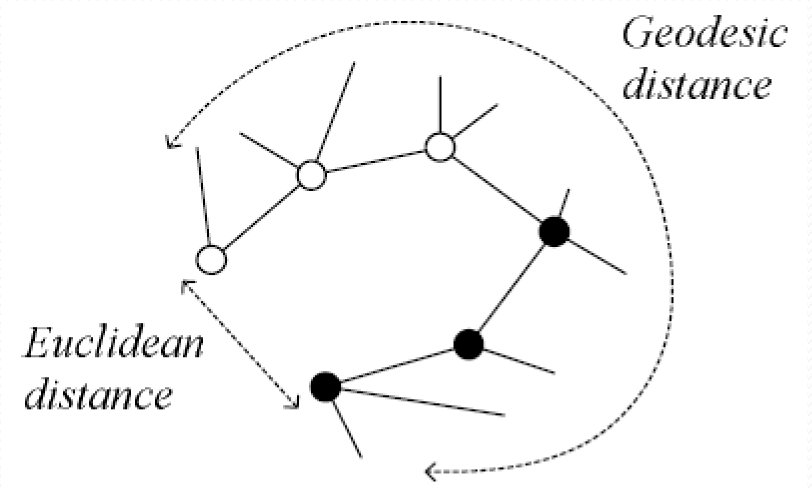
$$J(\mathbf{W}) = \frac{\left|\mathbf{W}^T \mathbf{S}_B \mathbf{W}\right|}{\left|\mathbf{W}^T \mathbf{S}_W \mathbf{W}\right|}$$

The largest eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$
Maximum rank of K-1


Optdigits after LDA

Isomap

- Geodesic distance is the distance along the manifold that the data lies in, as opposed to the Euclidean distance in the input space



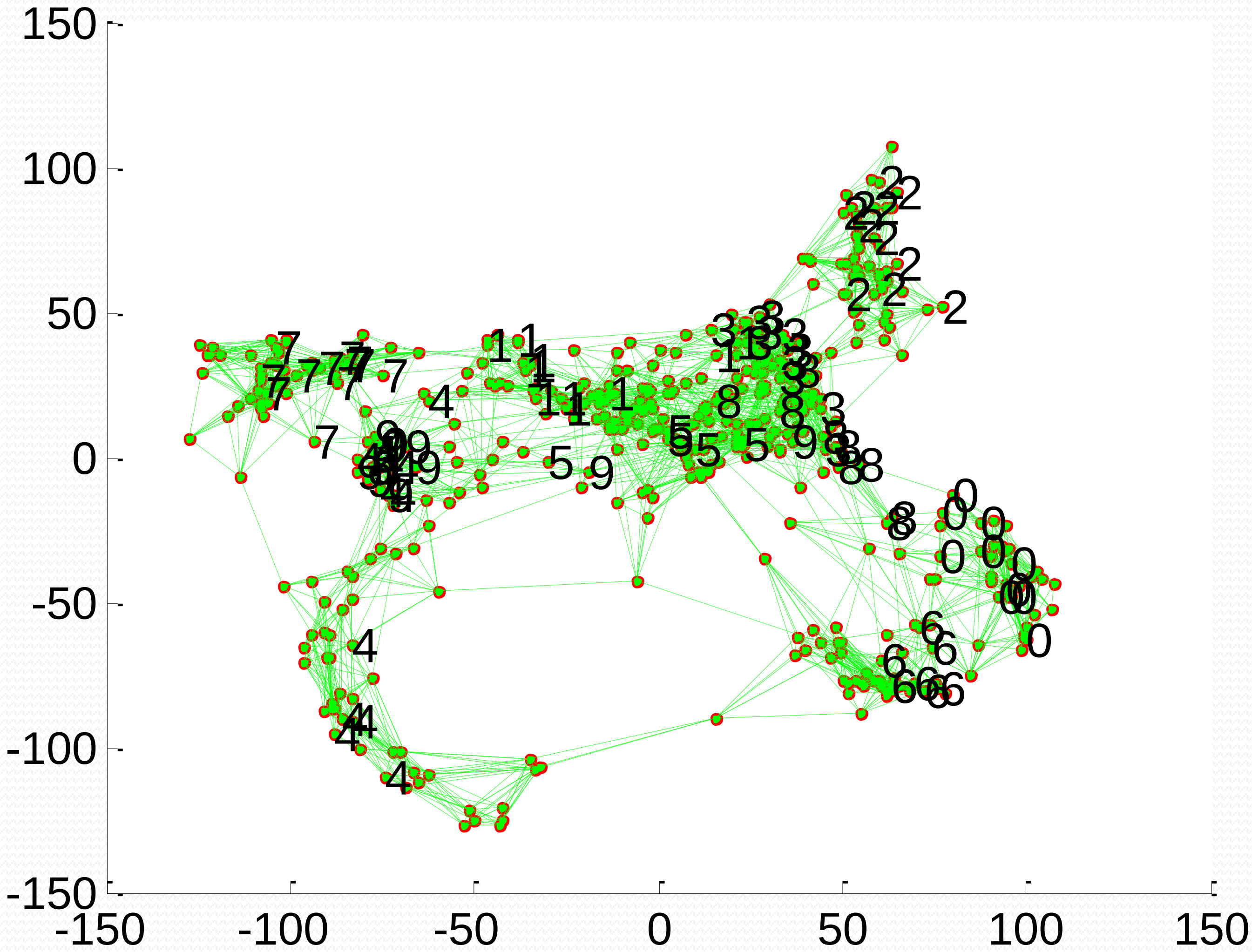
Isomap

- Instances r and s are connected in the graph if

  $||\boldsymbol{x}^r - \boldsymbol{x}^s|| < \varepsilon$ or if $\boldsymbol{x}^s$ is one of the *k* neighbors of $\boldsymbol{x}^r$

  The edge length is $||\boldsymbol{x}^r - \boldsymbol{x}^s||$
- For two nodes r and s not connected, the distance is equal to the shortest path between them
- Once the *N*x*N* distance matrix is thus formed, use MDS to find a lower-dimensional mapping

Optdigits after Isomap (with neighborhood graph).



Matlab source from http://web.mit.edu/cocosci/isomap/isomap.html

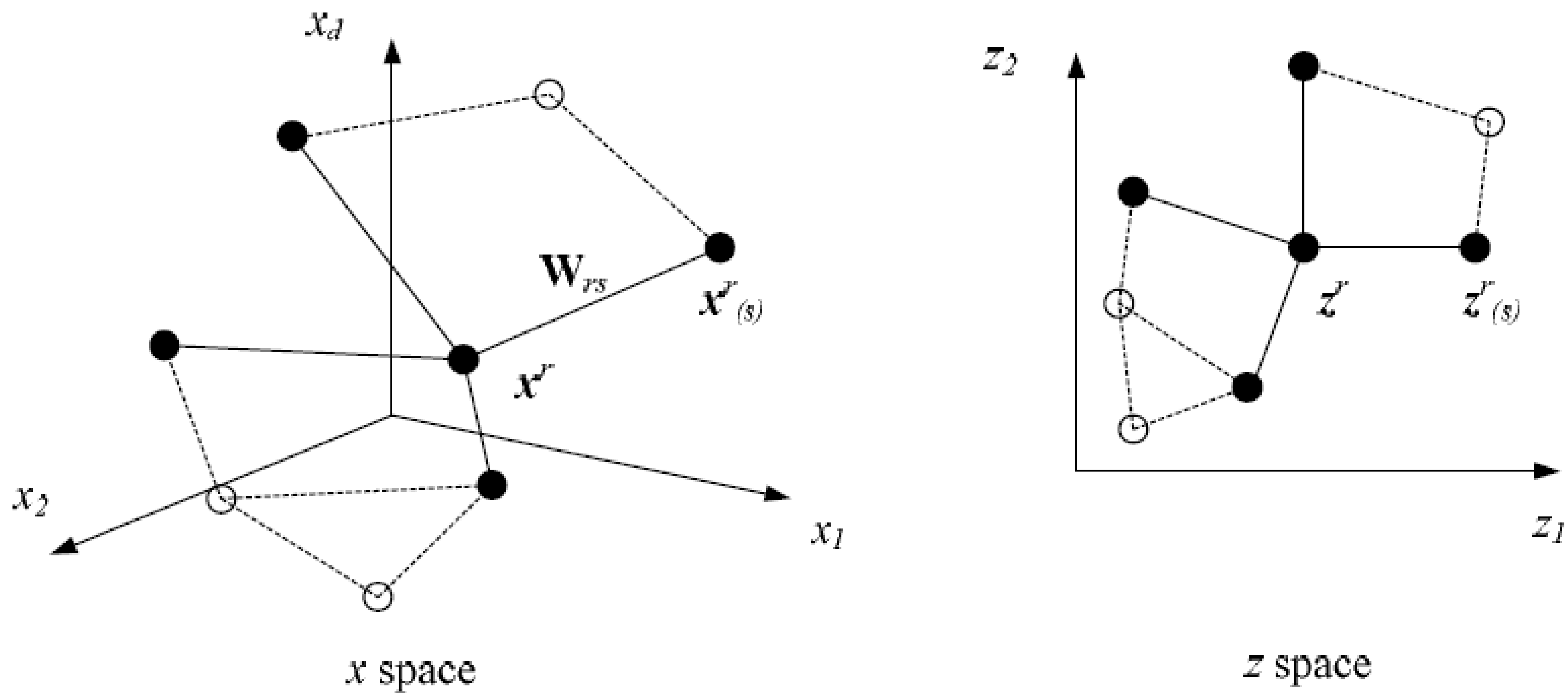
Locally Linear Embedding

1. Given $\boldsymbol{x}^r$ find its neighbors $\boldsymbol{x}^s_{(r)}$
2. Find $\mathbf{W}_{rs}$ that minimize

$$E(\mathbf{W} \mid X) = \sum_r \left\| \mathbf{x}^r - \sum_s \mathbf{W}_{rs} \mathbf{x}^s_{(r)} \right\|^2$$

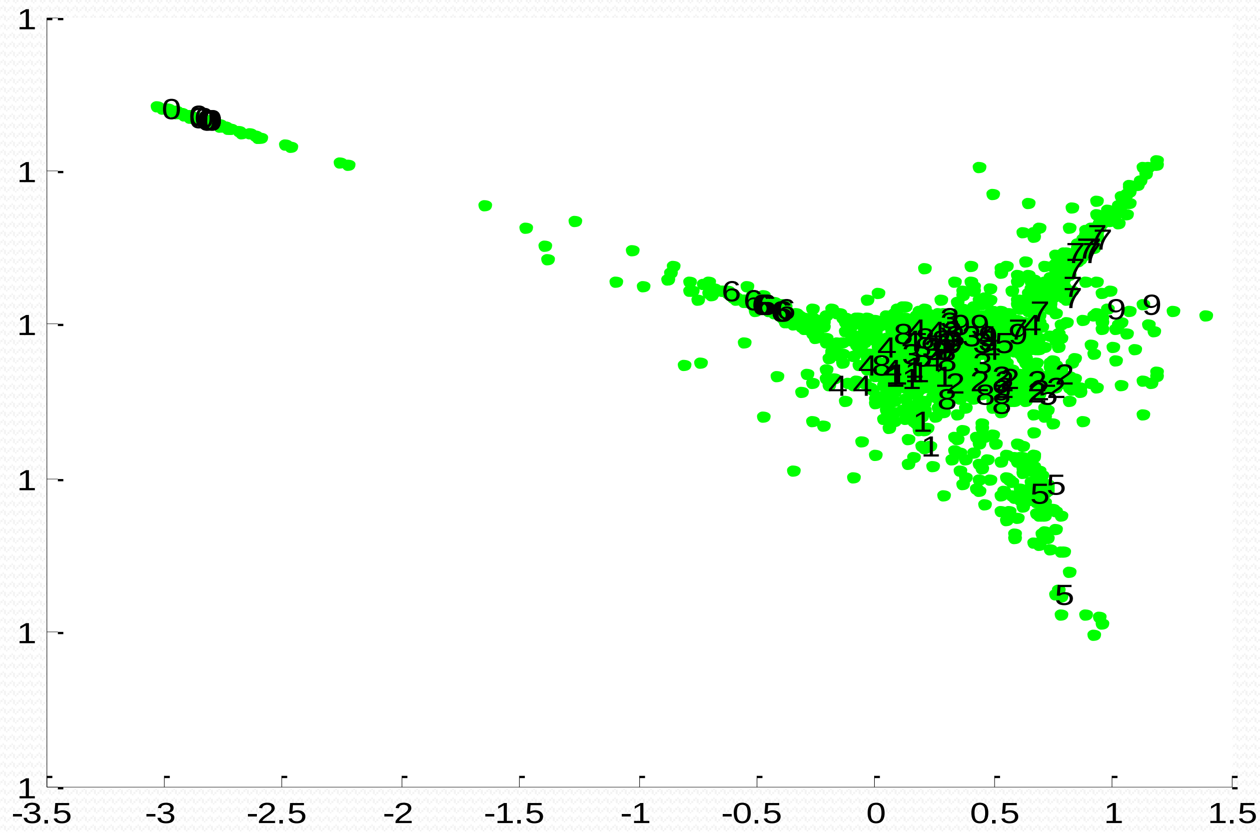
3. Find the new coordinates $\boldsymbol{z}^r$ that minimize

$$E(\mathbf{z} \mid \mathbf{W}) = \sum_r \left\| z^r - \sum_s \mathbf{W}_{rs} z^s_{(r)} \right\|^2$$



x_d
$\mathbf{W}_{rs}$
$x^r_{(s)}$
x^r
x_2
x_1
x space
z_2
z^r
$z^r_{(s)}$
z_1
z space

LLE on Optdigits



Matlab source from http://www.cs.toronto.edu/~roweis/lle/code.html