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

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

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

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

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

$\sum \boldsymbol{w}_1 = \alpha \boldsymbol{w}_1$ that is, $\boldsymbol{w}_1$ is an eigenvector of $\sum$
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 $\boldsymbol{w}_1$

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

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

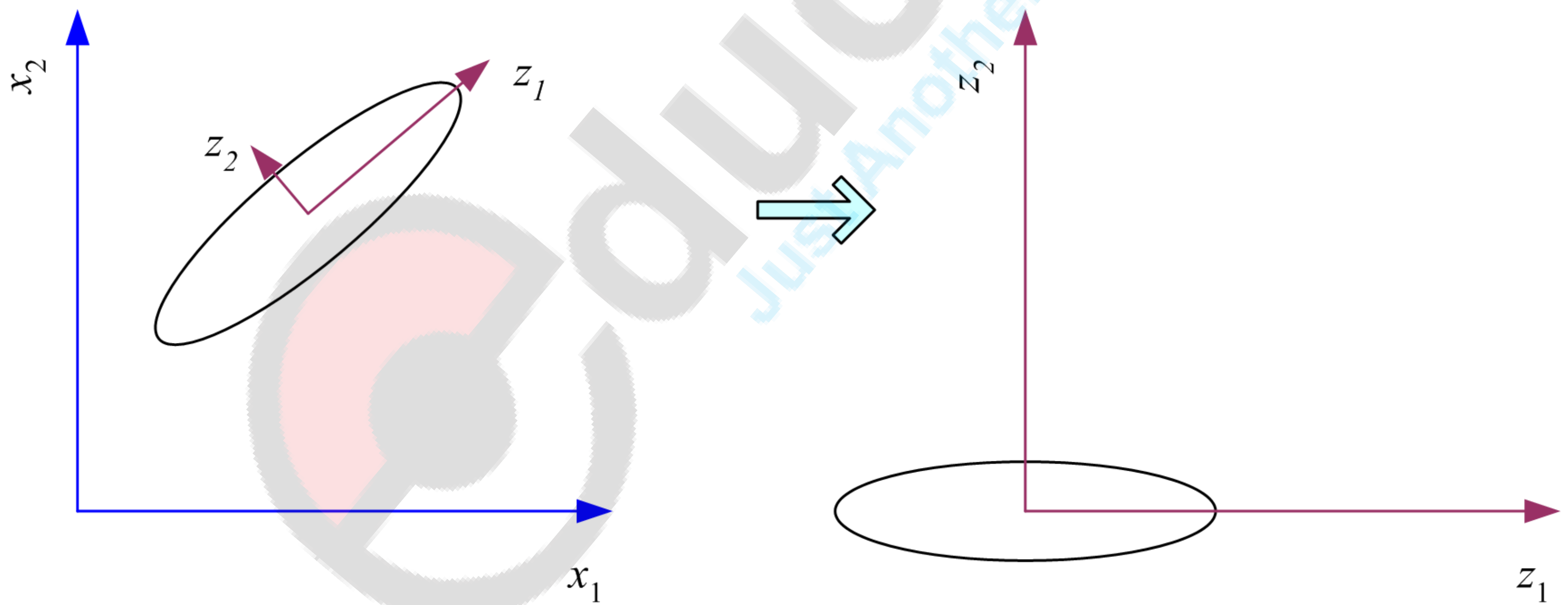
and so on.

What PCA does

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

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

Centers the data at the origin and rotates the axes

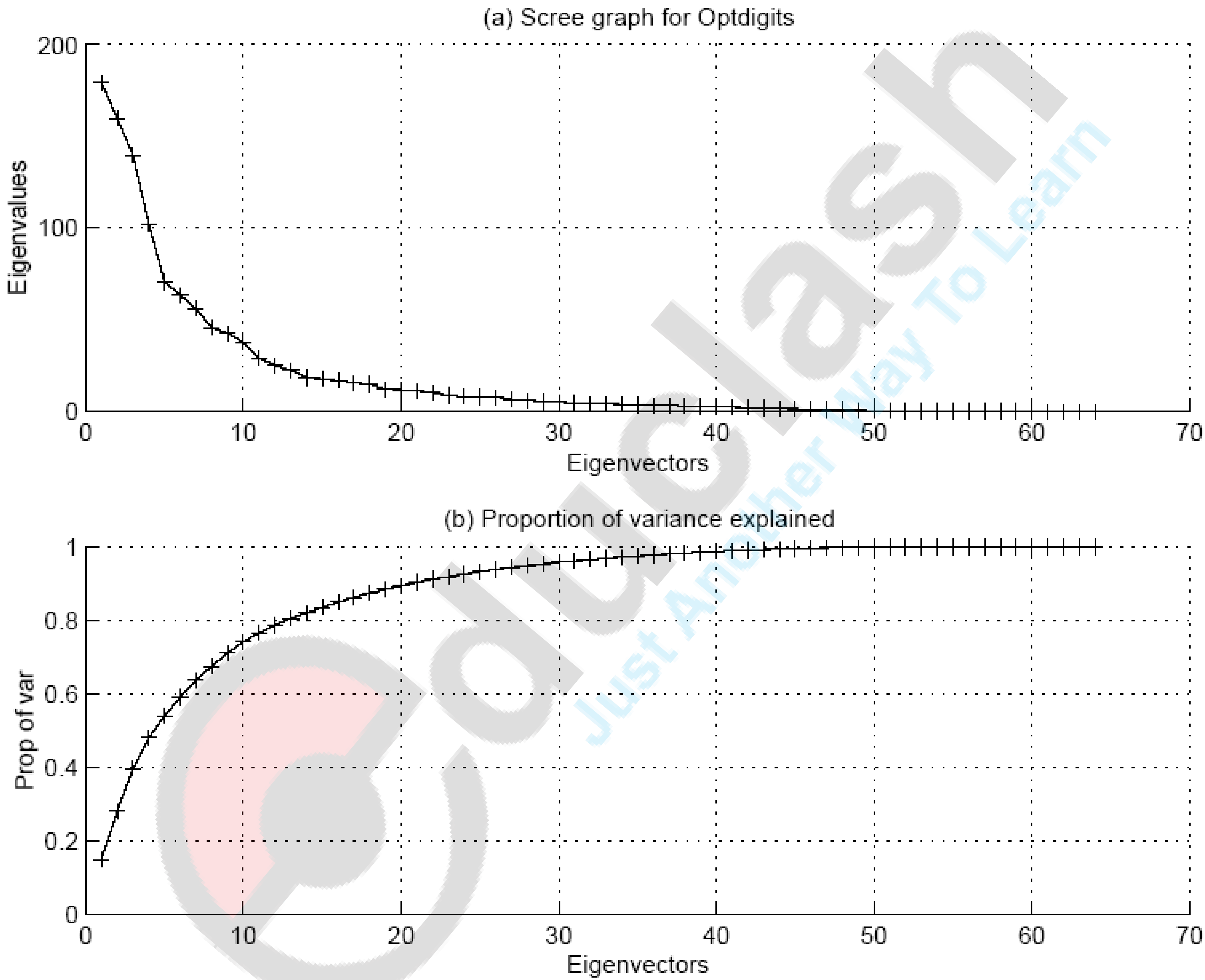


How to choose k ?

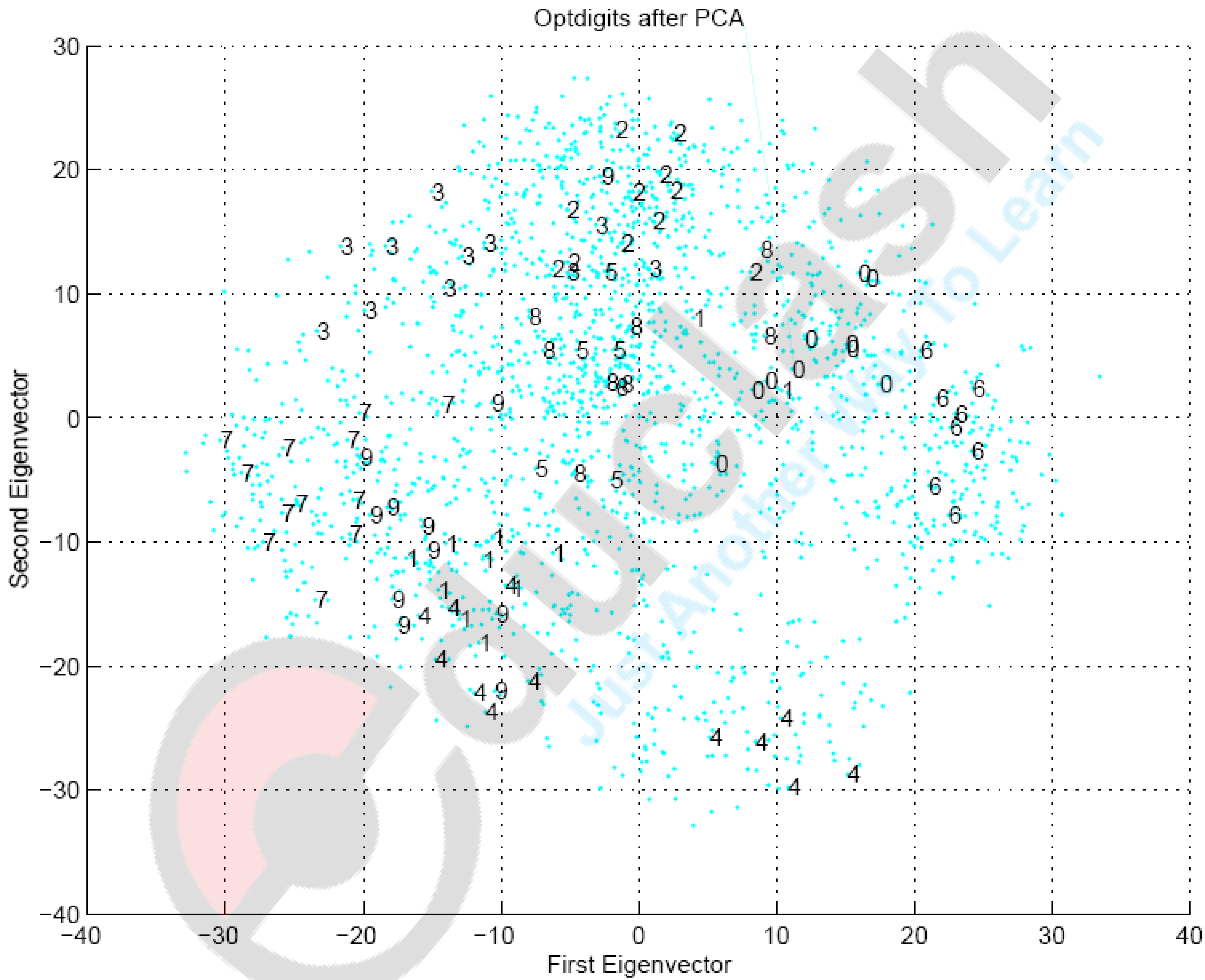
- Proportion of Variance (PoV) explained

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

  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
Eigenvectors
(b) Proportion of variance explained
Prop of var
Eigenvectors



Optdigits after PCA
Second Eigenvector
First Eigenvector

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

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

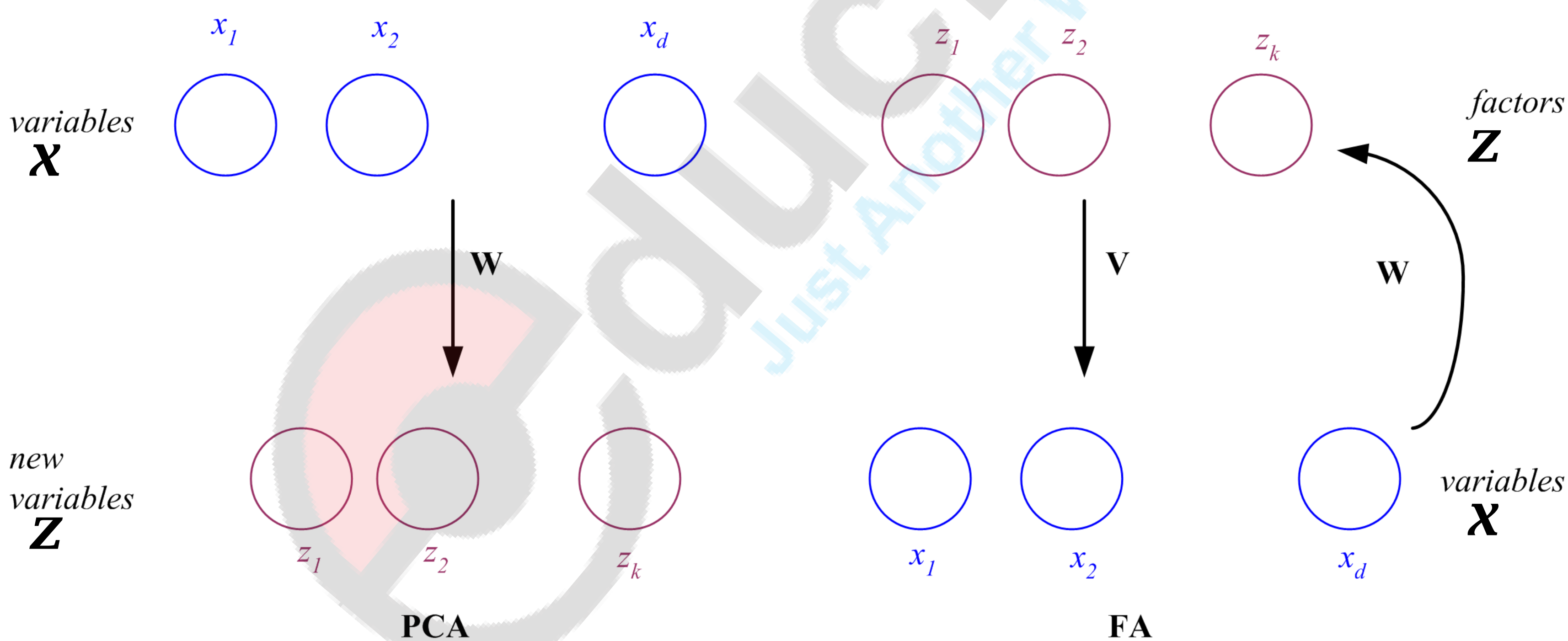
  ε_i are the noise sources

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

  and v_{ij} are the factor loadings

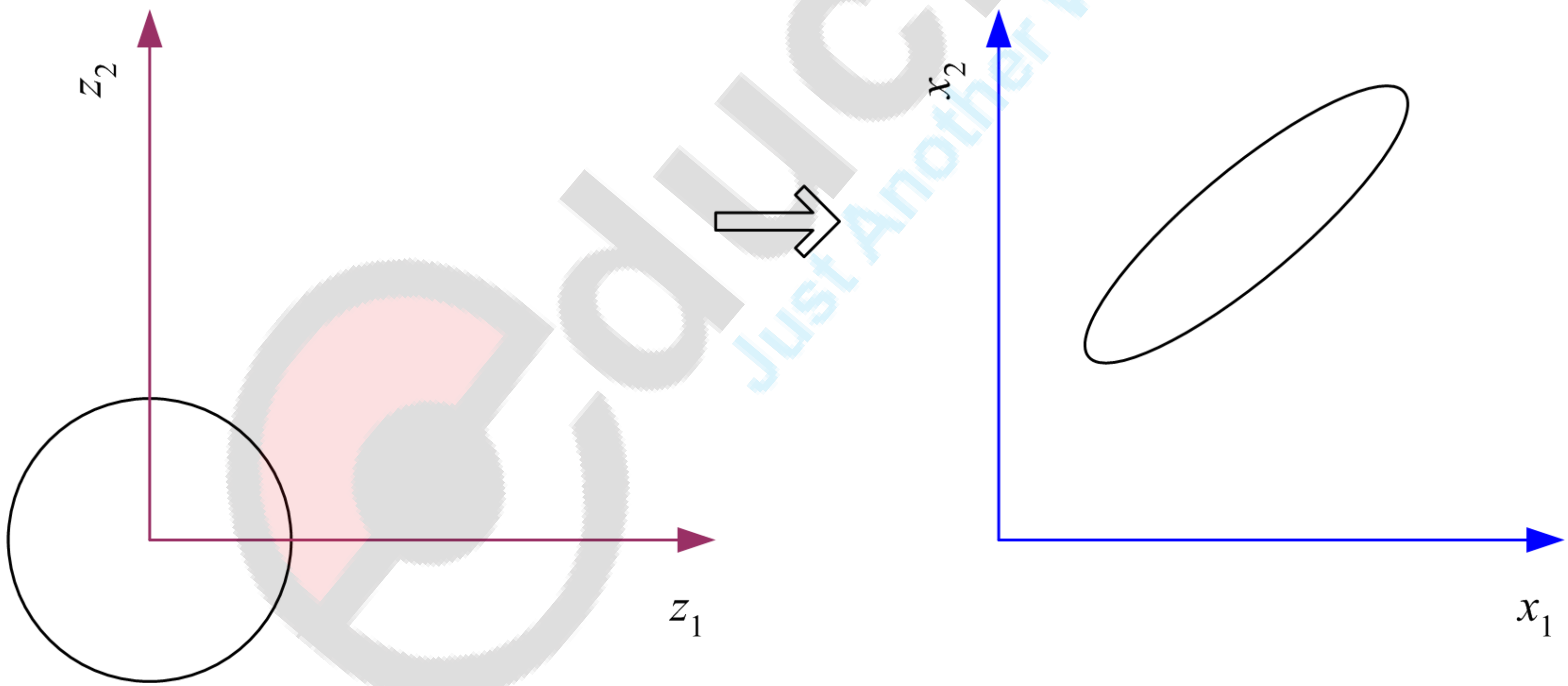
PCA vs FA

- PCA   From x to z $z = W^T(x - \mu)$
- FA   From z to x $x - \mu = Vz + \varepsilon$



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}, $i,j = 1,\dots,N$

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

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

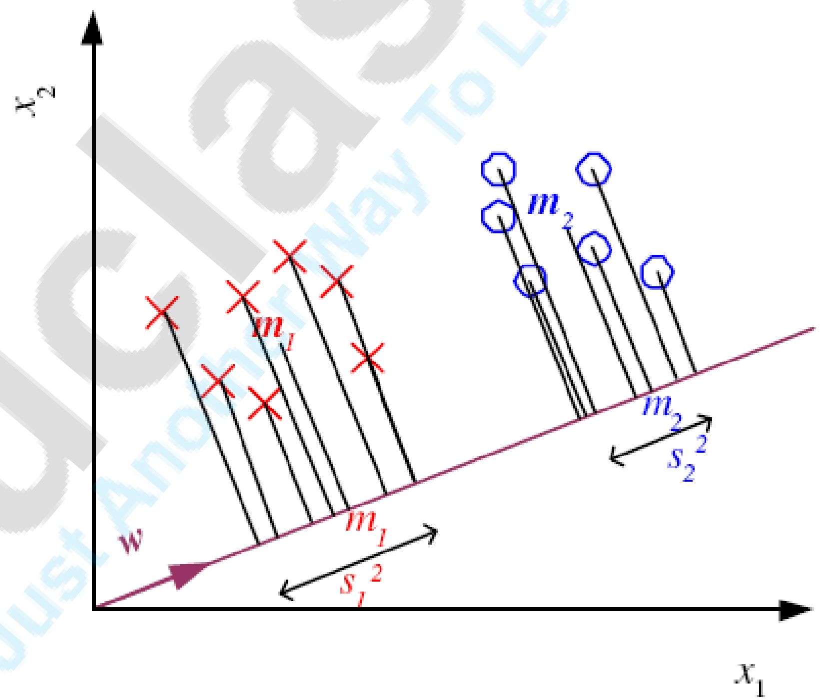
$$= \sum_{r,s} \frac{\left(\|\mathbf{g}(\mathbf{x}^r \mid \theta) - \mathbf{g}(\mathbf{x}^s \mid \theta)\| - \|\mathbf{x}^r - \mathbf{x}^s\|\right)^2}{\|\mathbf{x}^r - \mathbf{x}^s\|^2}$$

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:

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

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:

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

- Between-class scatter:

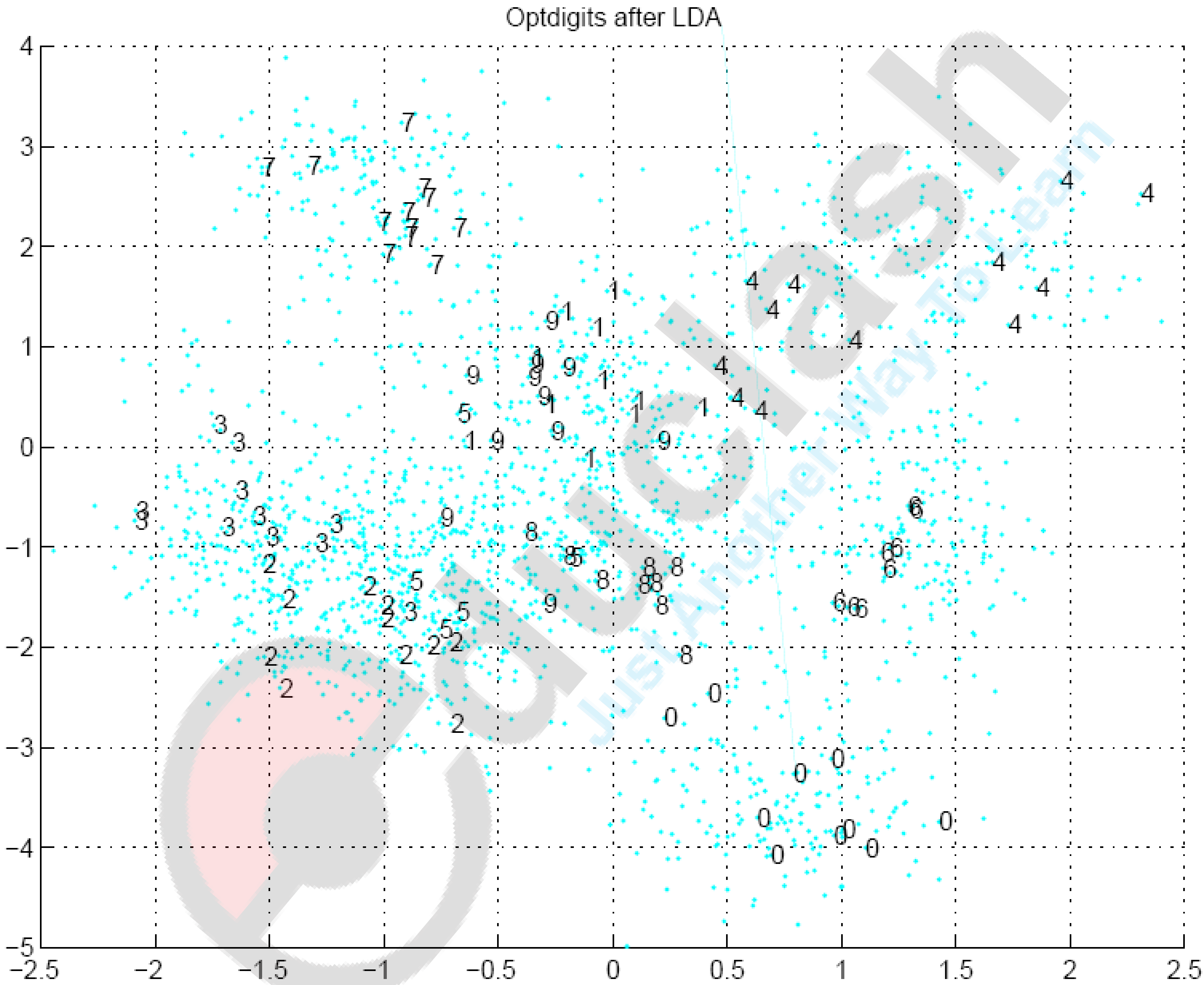
$$\mathbf{S}_B = \sum_{i=1}^{K} N_i (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T \qquad \mathbf{m} = \frac{1}{K} \sum_{i=1}^{K} \mathbf{m}_i$$

- Find **W** that max

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

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

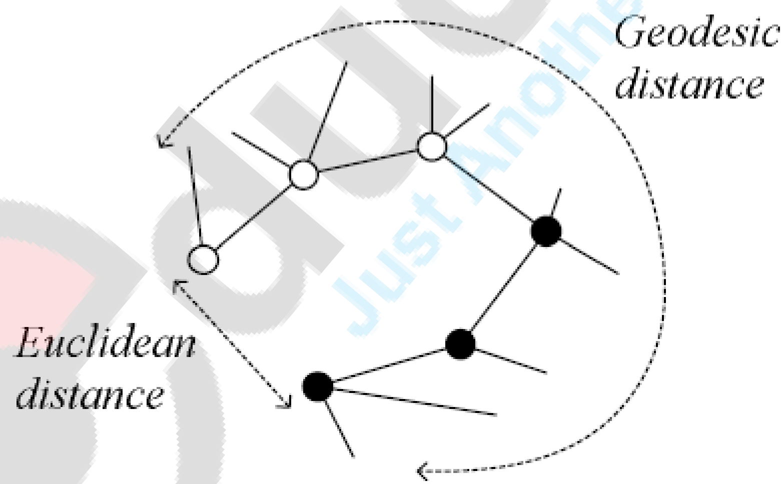
Maximum rank of K-1



Optdigits after LDA
4
3
2
1
0
−1
−2
−3
−4
−5
−2.5
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2
2.5

Isomap

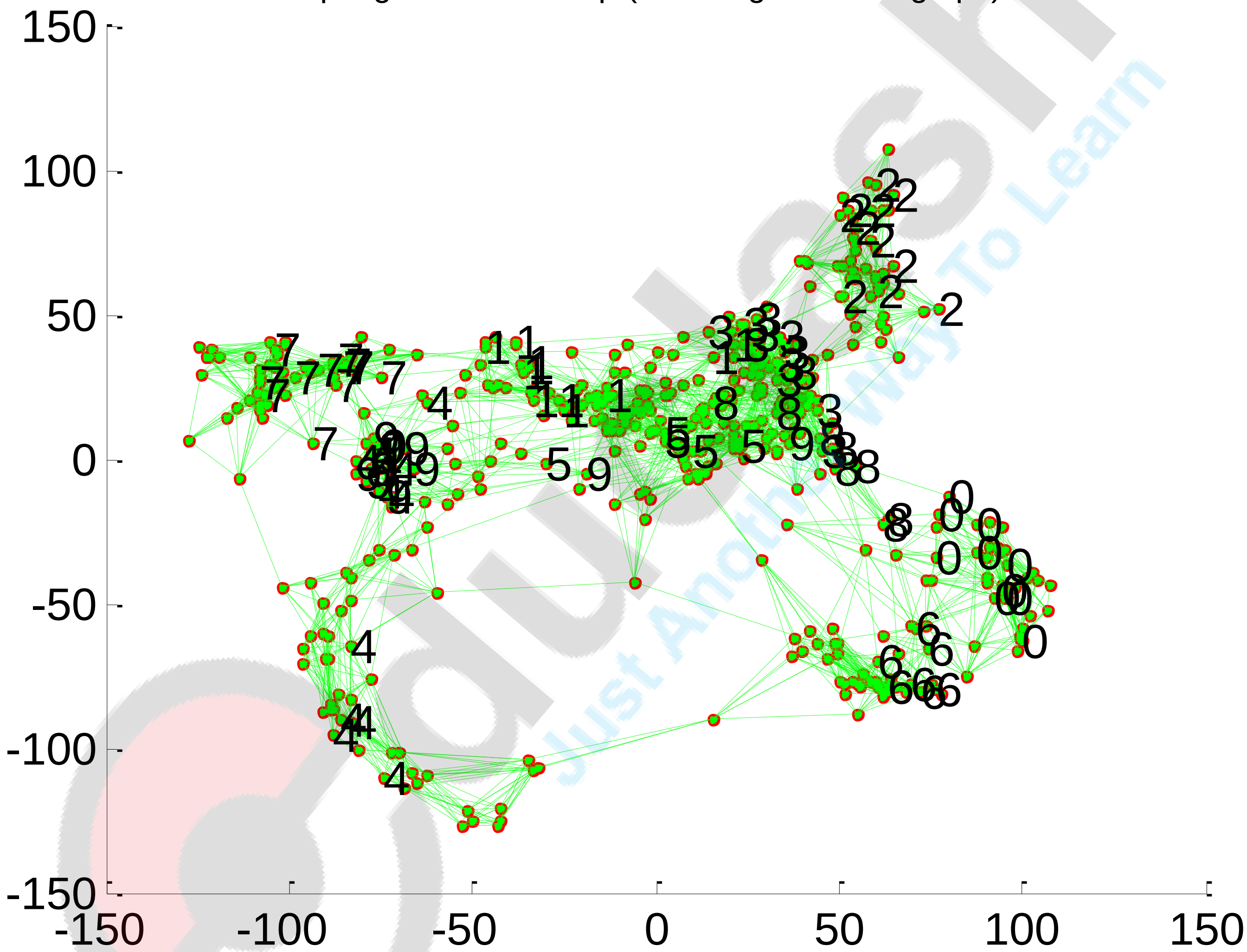
- Geodesic distance is the distance along the manifold that the data lies in, as opposed to the Euclidean distance in the input space



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

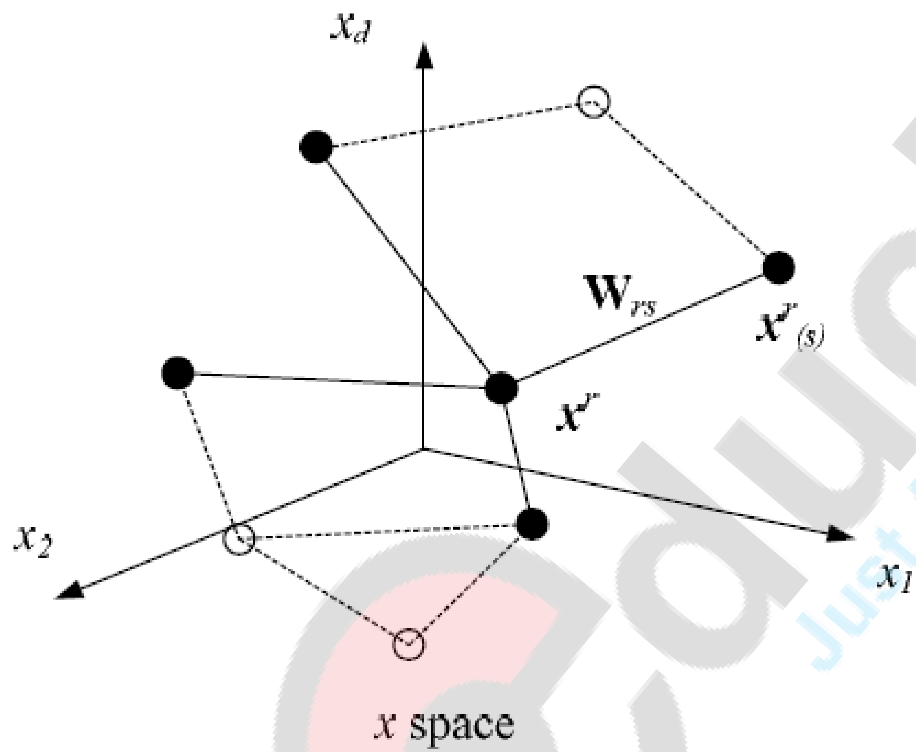
Locally Linear Embedding

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

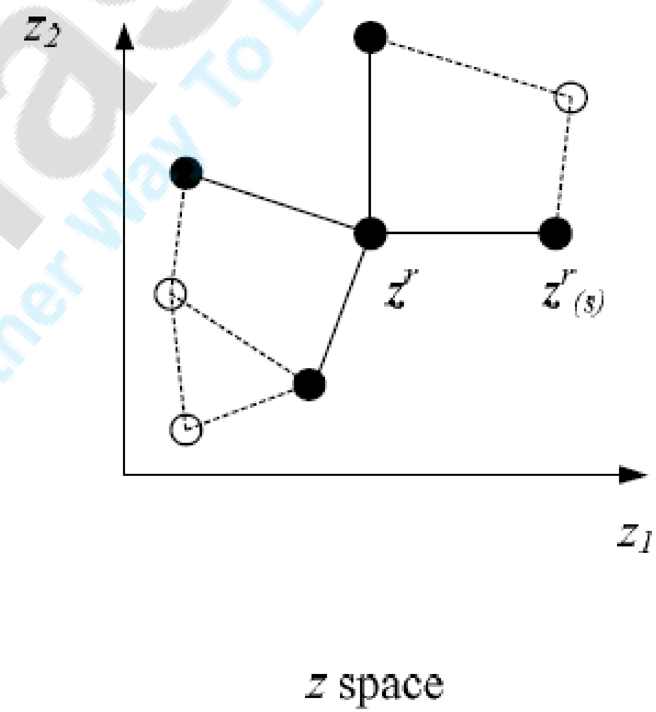
$$E(\mathbf{W} \mid X) = \sum_r \left\| \mathbf{x}^r - \sum_s \mathbf{W}_{rs} \mathbf{x}^s_{(r)} \right\|^2$$

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

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

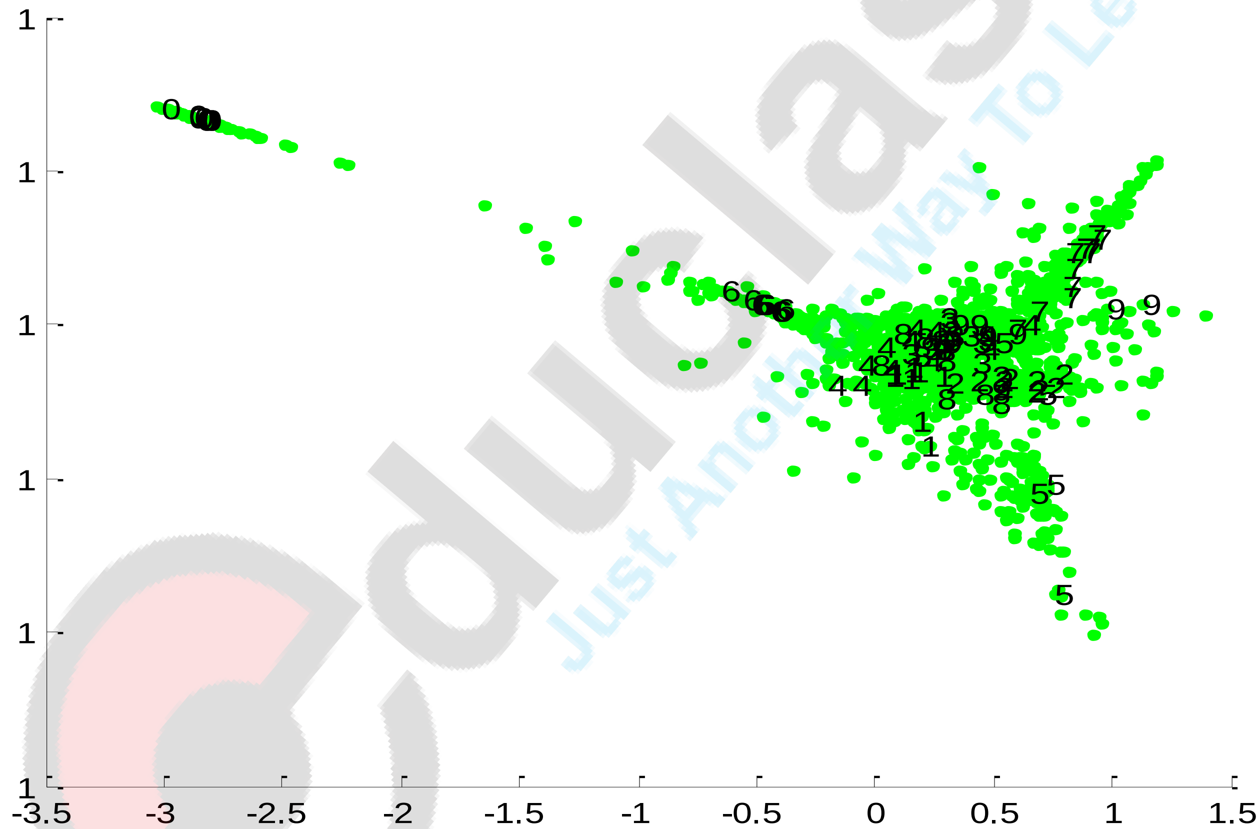


x_d
$\mathbf{W}_{rs}$
$x^{r}_{(s)}$
x^{r}
x_2
x_1
x space



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