

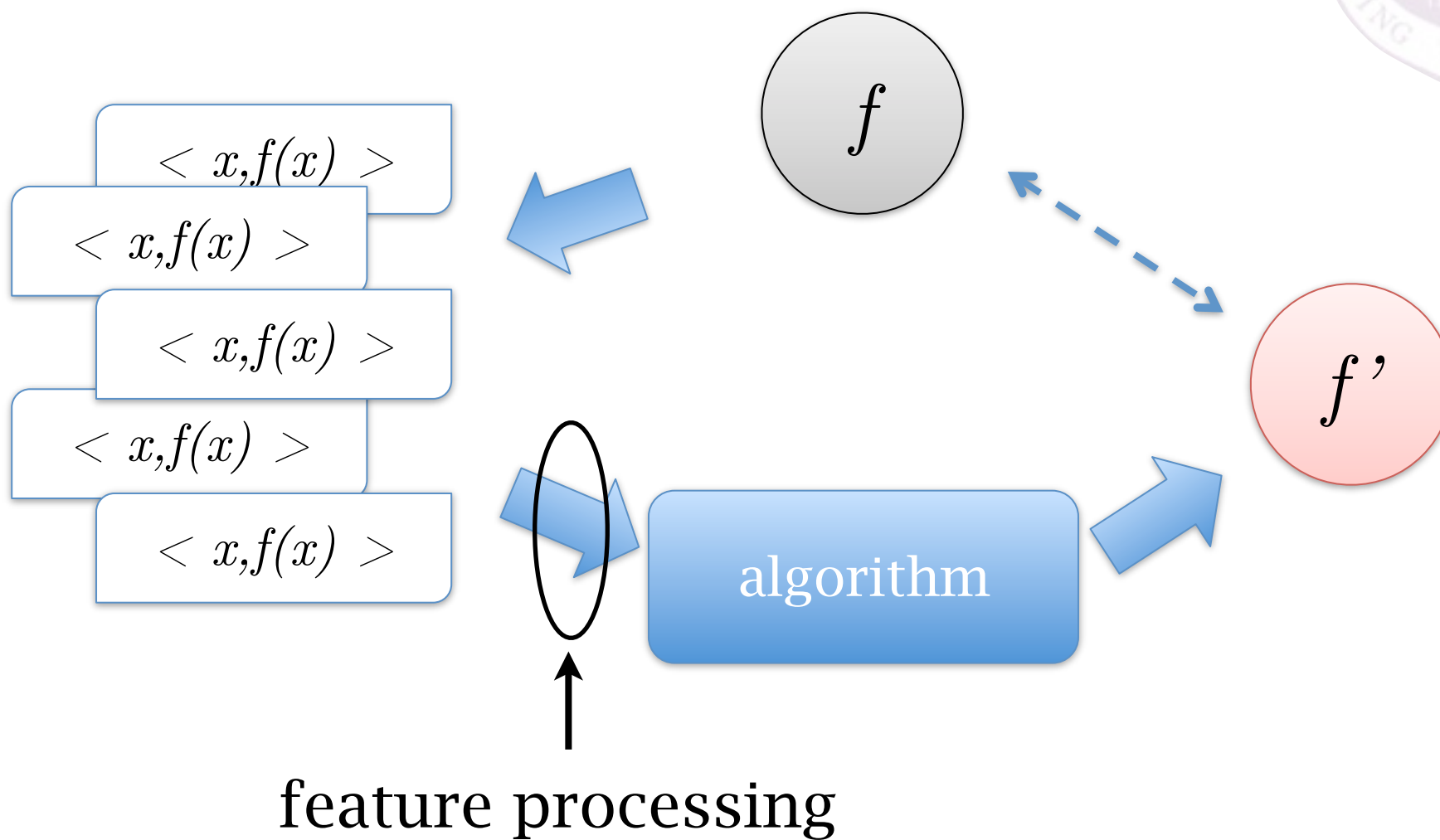
Lecture 10: Data Mining I

Feature Processing

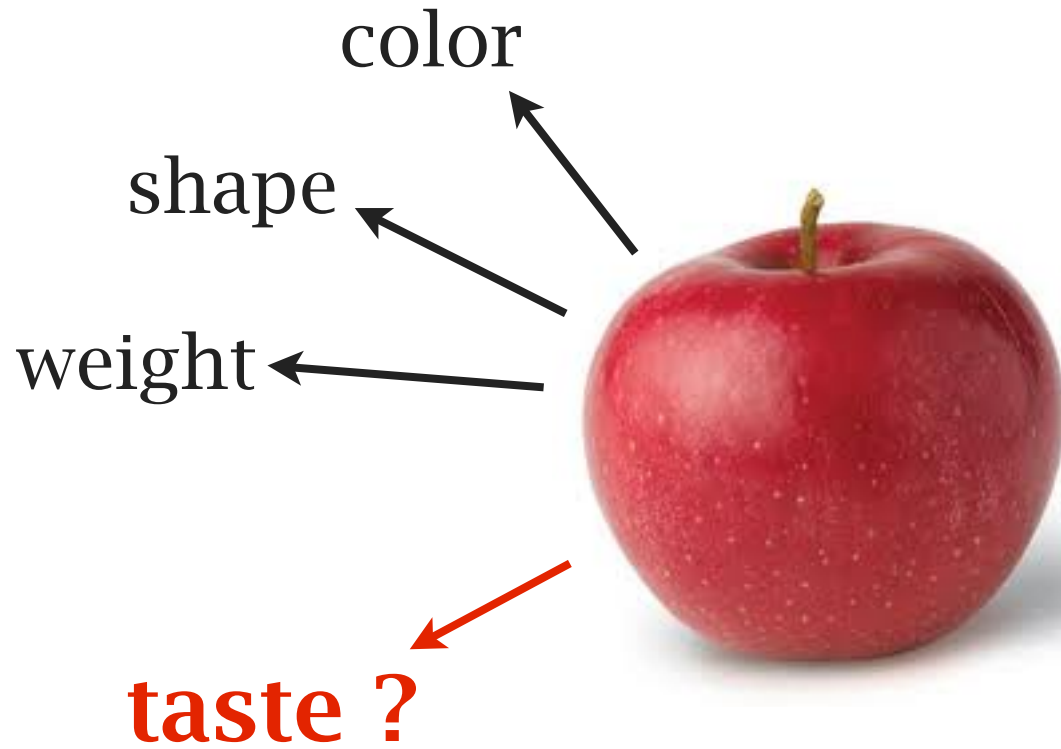
http://cs.nju.edu.cn/yuy/course_dm13ms.ashx



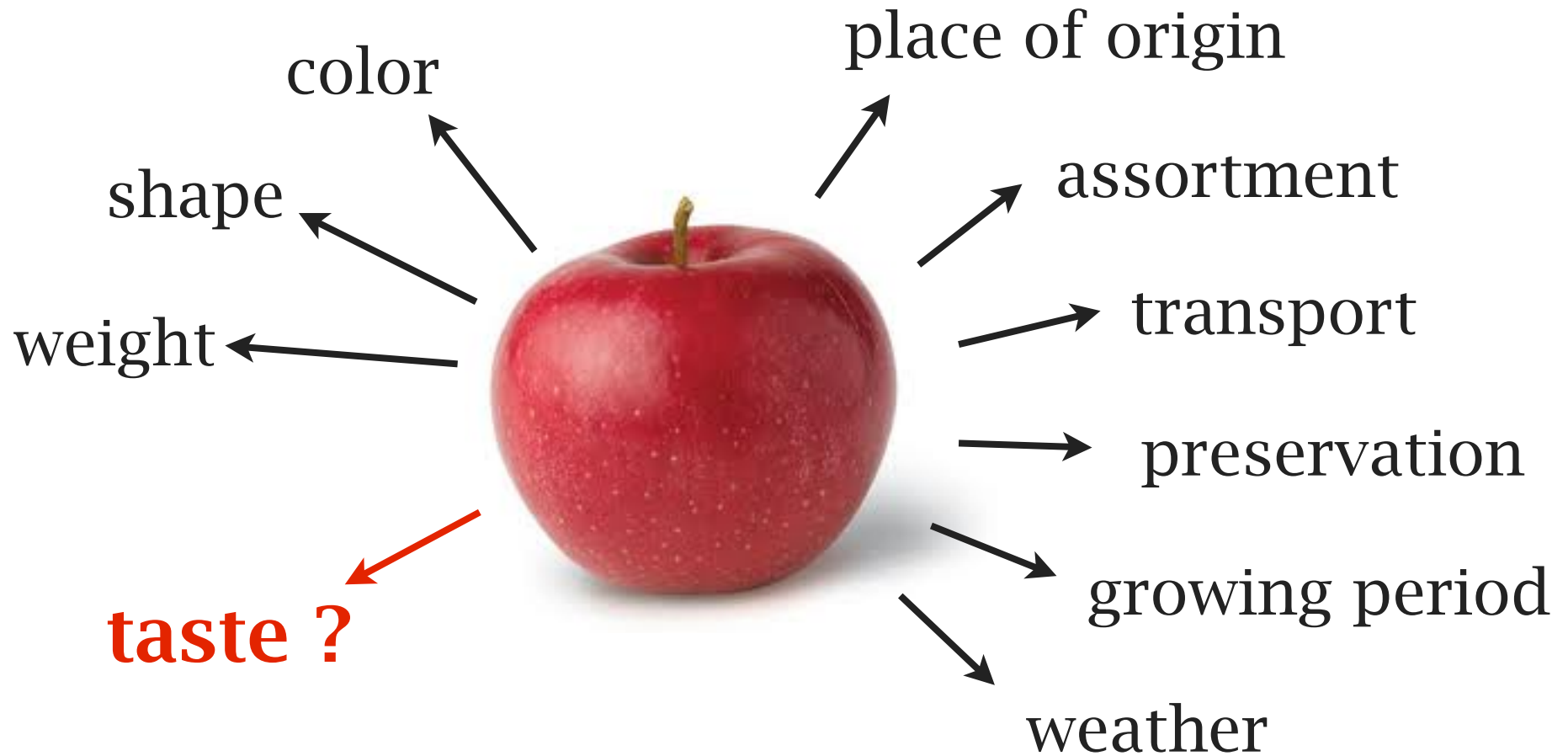
Position



The importance of features



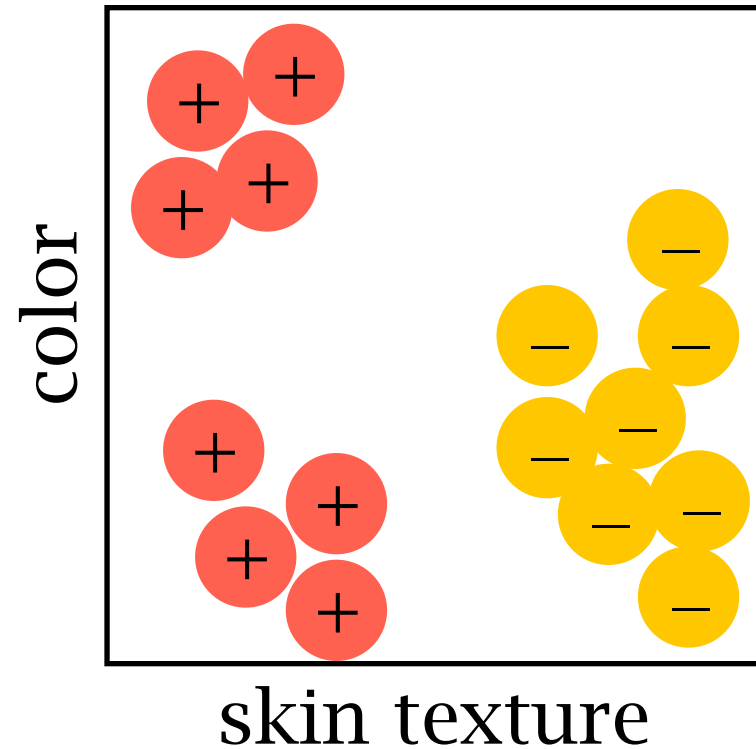
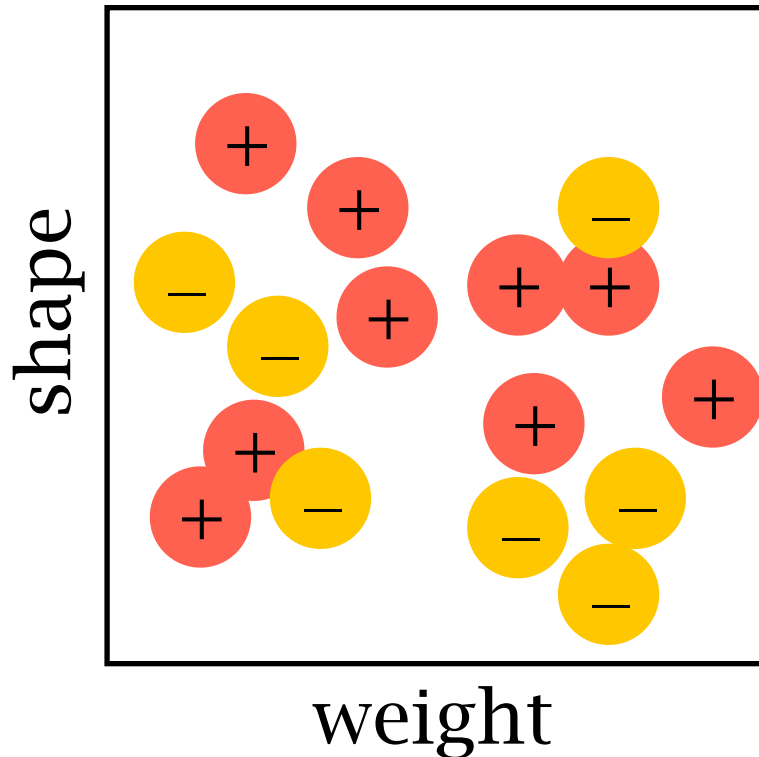
The importance of features



The importance of features



features determine the instance distribution
good features lead to better mining results



Feature processing



a good feature set is more important
than a good classifier

feature selection

feature extraction

Feature selection



To select a set of good features from a given feature set

Improve mining performance
reduce classification error

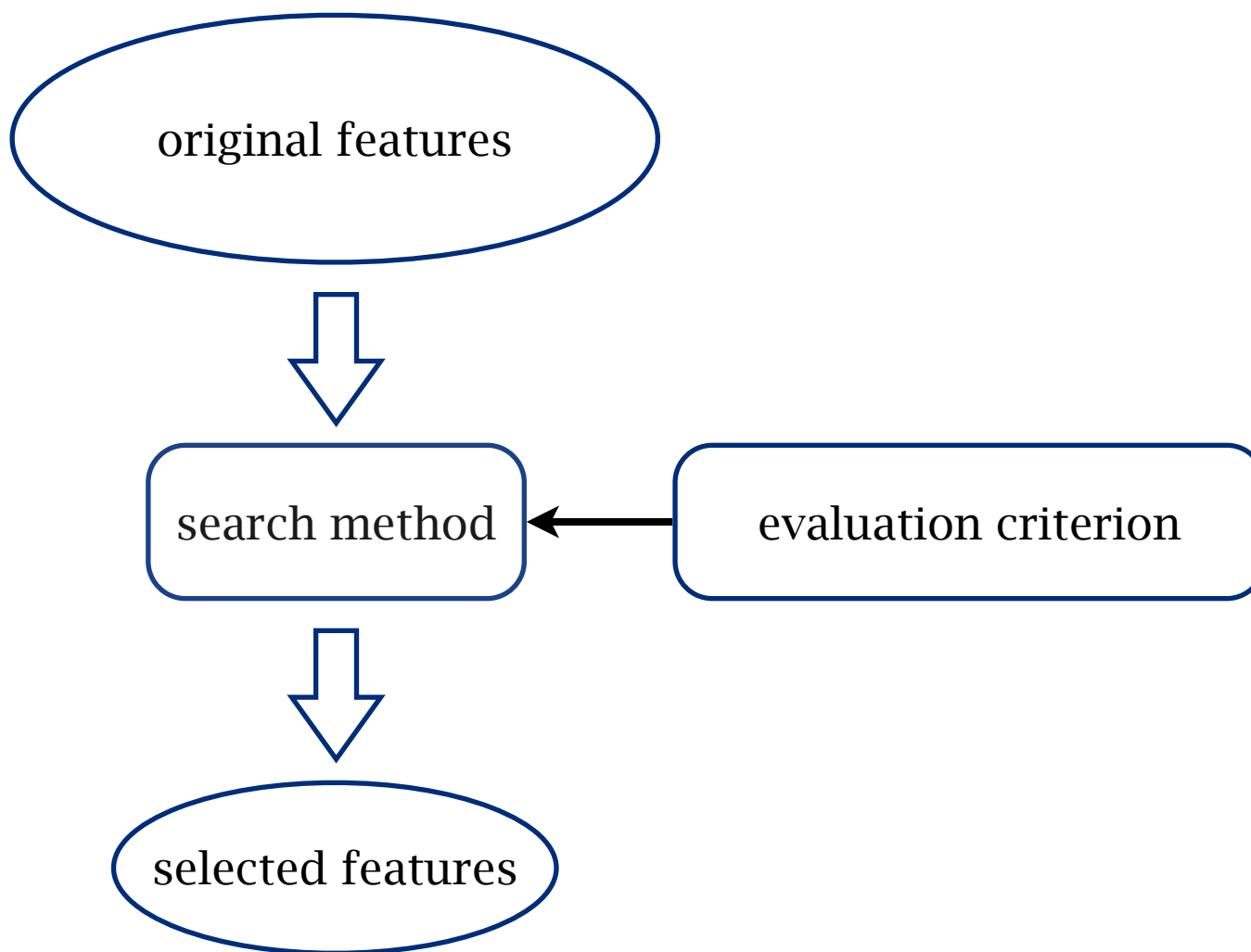
Reduce the time/space complexity of mining

Improve the interpretability

Better data visualization

Saving the cost of observing features

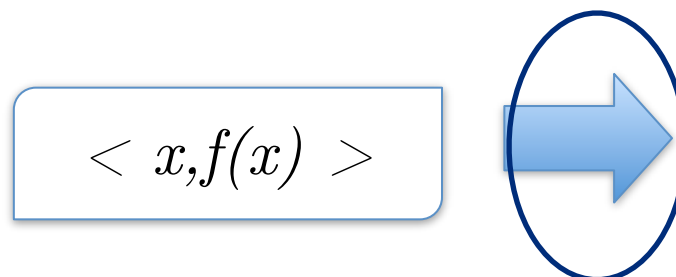
Feature selection



Evaluation criteria



classifier independent



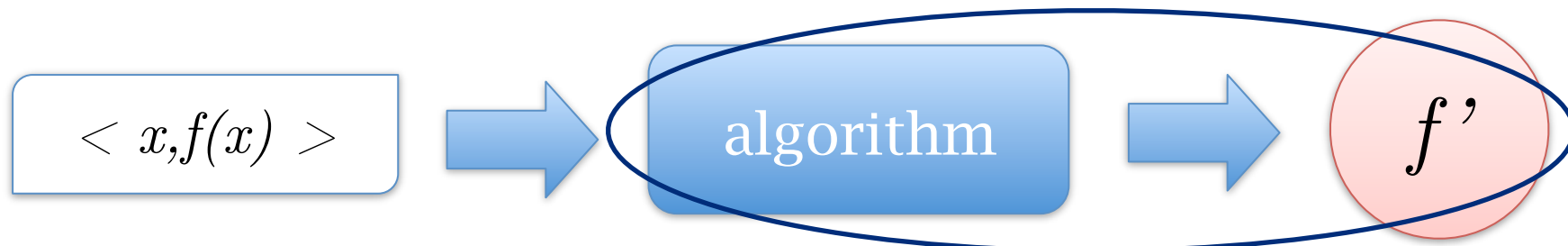
dependency based criteria

information based criteria

distance based criteria

classifier internal weighting

classifier dependent



Dependency based criteria

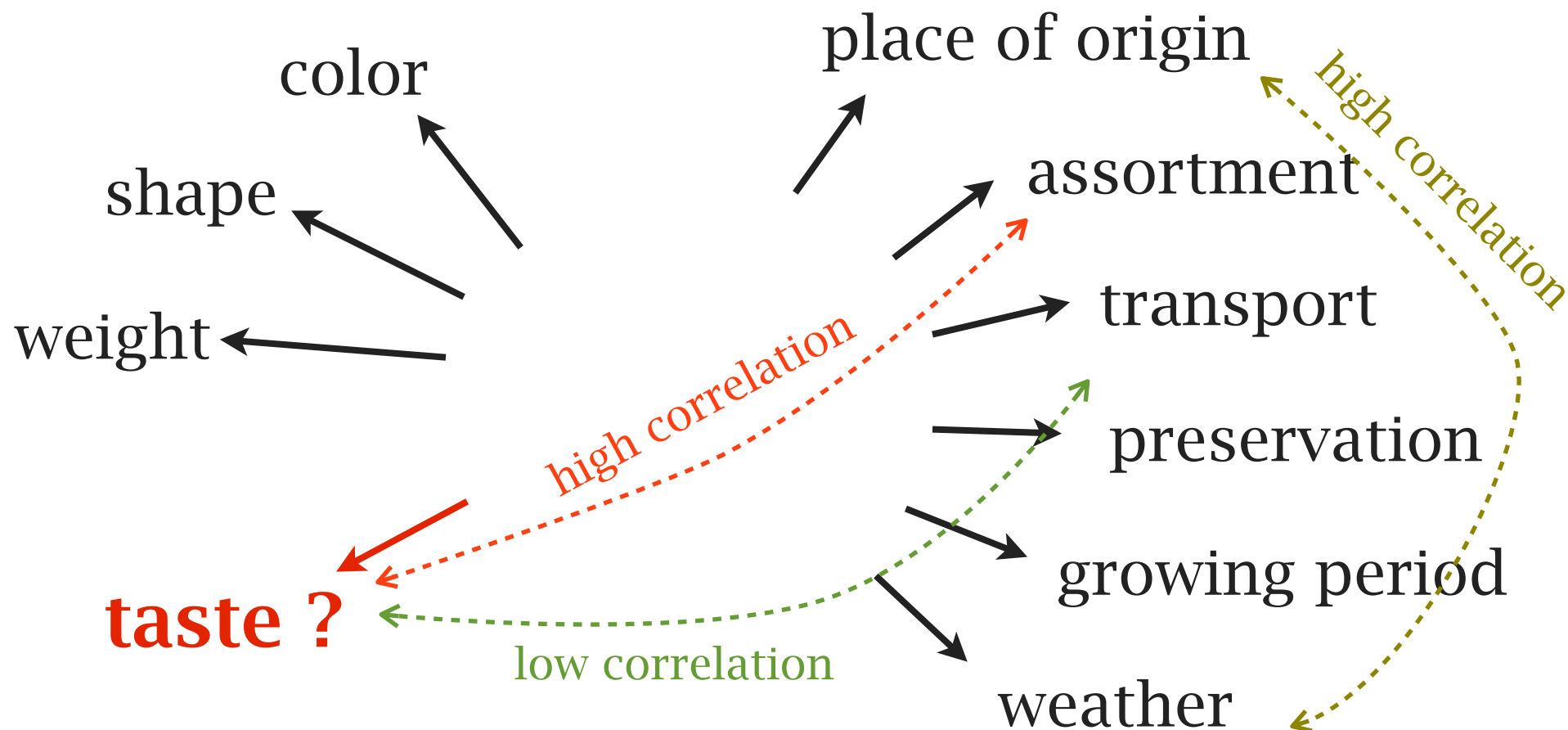


How a feature set is related with the class

correlation between a feature and the class

correlation between two features

search: select high correlated low redundant features



Information based criteria



How much a feature set provides information about the class

Information gain:

$$\text{Entropy: } H(X) = - \sum_i p_i \ln(p_i)$$

$$\text{Entropy after split: } I(X; \text{split}) = \sum_j \frac{\#\text{partition } j}{\#\text{all}} H(\text{partition } j)$$

$$\text{Information gain: } H(X) - I(X; \text{split})$$

A simple forward search



sequentially add the next best feature

- 1: F = original feature sets, C is the class label
- 2: $S = \emptyset$
- 3: **loop**
- 4: a = the best correlated/informative feature in F
- 5: v = the correlation/IG of a
- 6: **if** $v < \theta$ **then**
- 7: **break**
- 8: **end if**
- 9: $F = F / \{a\}$
- 10: $S = S \cup \{a\}$
- 11: **end loop**
- 12: **return** S

A simple forward search



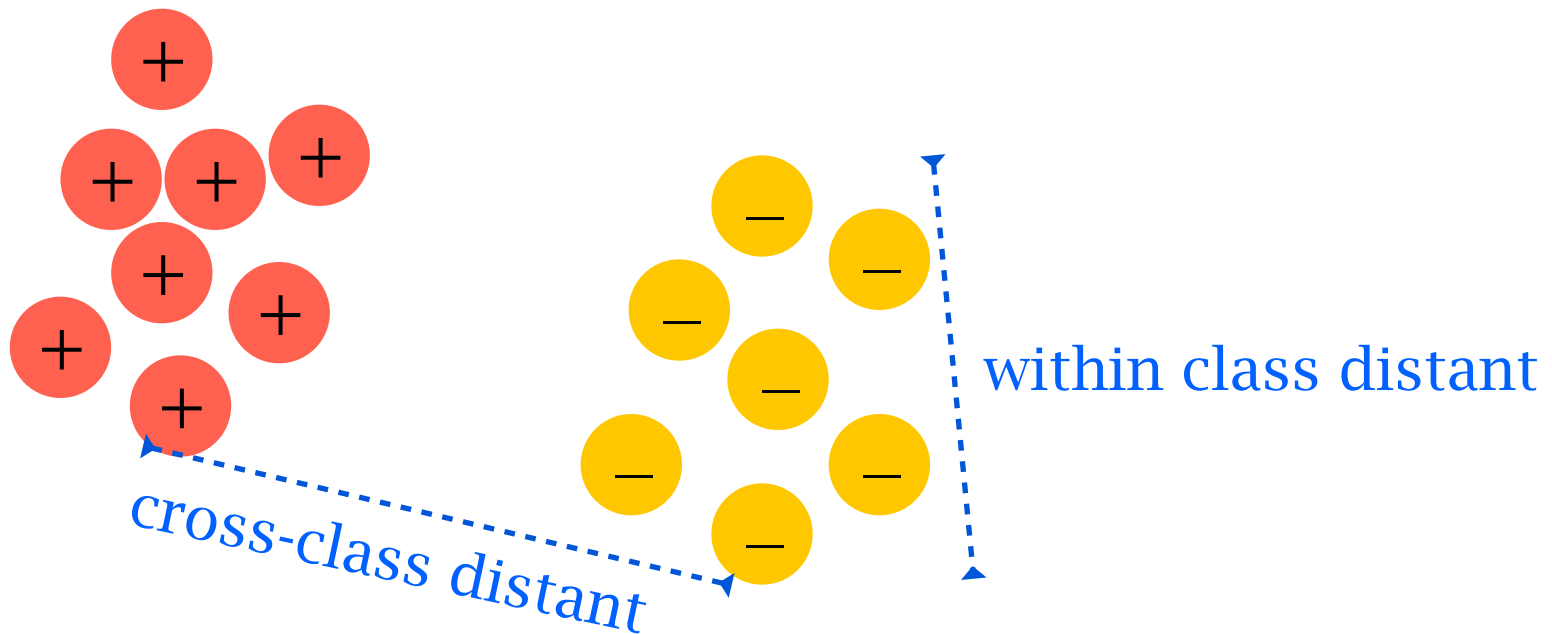
```
1:  $F$  = original feature sets,  $C$  is the class label
2:  $S = \emptyset$ 
3: loop
4:    $a$  = the best correlated/informative feature in  $F$ 
5:    $v$  = the correlation/IG of  $a$ 
6:   if  $v < \theta$  then
7:     break
8:   end if
9:    $F = F / \{a\}$ 
10:   $S = S \cup \{a\}$ 
11:  for  $a' \in F$  do
12:     $v'$  = the correlation/IG of  $a'$  to  $a$ 
13:    if  $v' > \alpha \cdot v$  then  $F = F / \{a'\}$ 
14:    end if
15:  end for
16: end loop
17: return  $S$ 
```

remove
redundant
features



Distance based criteria

Examples in the same class should be near
Examples in different classes should be far



select features to optimize the distance

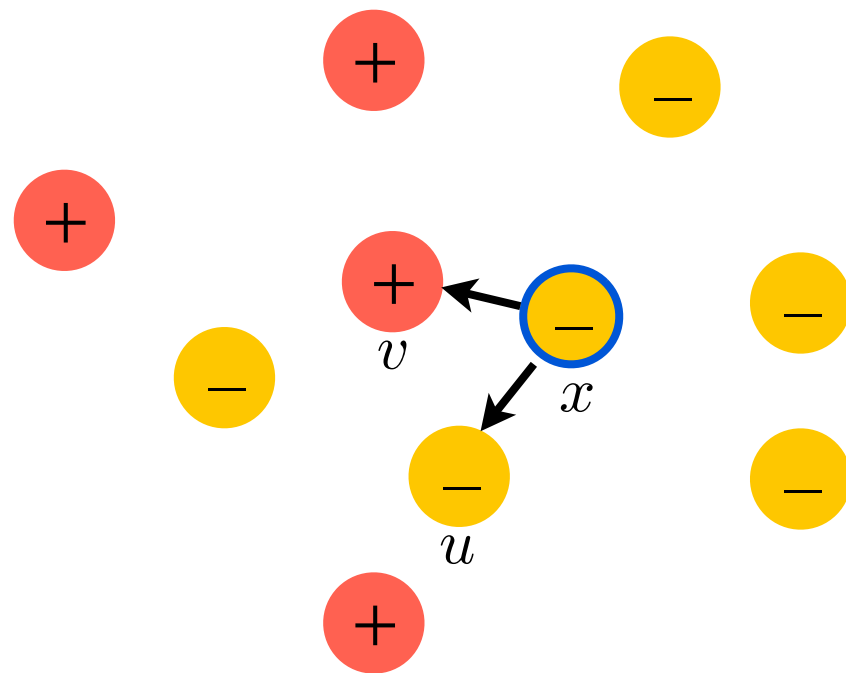
Distance based criteria



Relief: feature weighting based on distance

$$w = 0$$

1. random select an instance x
2. find the nearest same-class instance u (according to w)
3. find the nearest diff-class instance v (according w)
4. $w = w - |x - u| + |x - v|$
5. goto 1 for m times



select the features whose weights are above a threshold

Feature weighting from classifiers



Many classification algorithms perform feature selection and weighting internally

decision tree: select a set of features by recursive IG

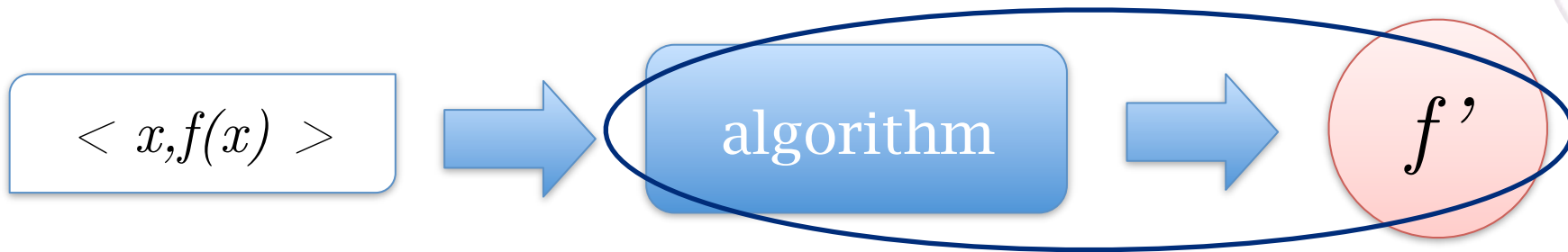
random forest: weight features by the frequency of using a feature

linear model: a natural feature weighting

select features from these models' internal feature weighting

note the difference to FS for classification

Classifier dependent feature selection



select features to maximize the performance of the following mining task

slow in speed

hard to search

hard to generalize the selection results

more accurate mining result

Classifier dependent feature selection



Sequential forward search:
add features one-by-one

F = original feature set

$S = \emptyset$

perf-so-far = the worst performance value

loop

for $a \in F$ **do**

$v(a)$ = the performance given features $S \cup \{a\}$

end for

ma = the best feature

$mv = v(ma)$

if mv is worse than perf-so-far **then**

break

end if

$S = S \cup ma$

perf-so-far = mv

end loop

return S

Classifier dependent feature selection



Sequential backward search:
remove features one-by-one

F = original feature set

perf-so-far = the performance given features F

loop

for $a \in F$ **do**

$v(a)$ = the performance given features $F/\{a\}$

end for

ma = the best feature to **remove**

$mv = v(ma)$

if mv is worse than perf-so-far **then**

break

end if

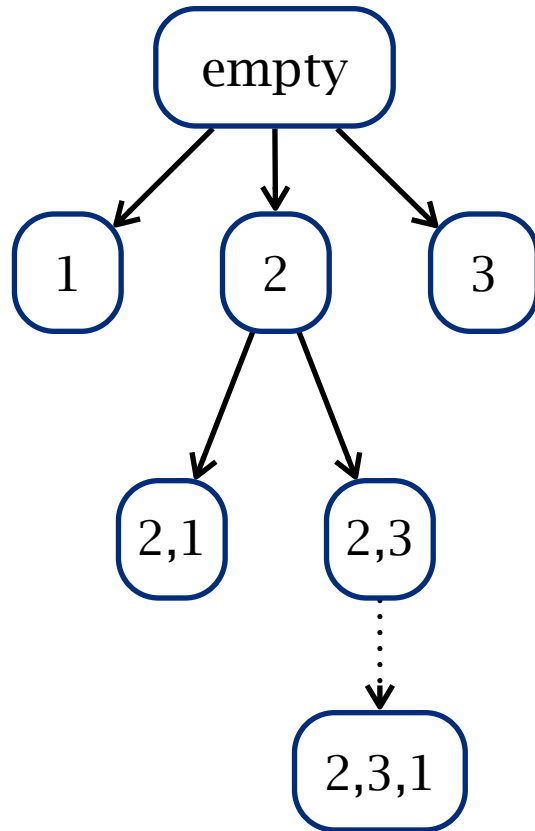
$F = F/\{ma\}$

perf-so-far = mv

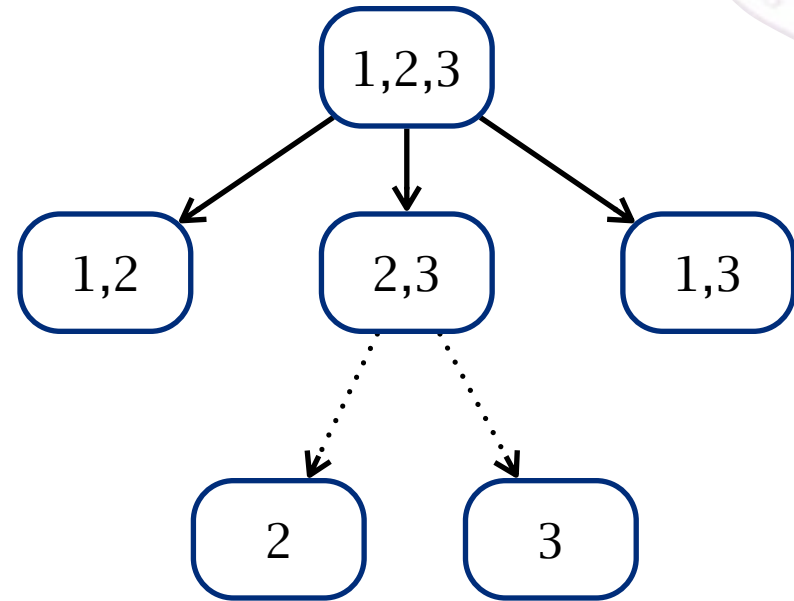
end loop

return S

Classifier dependent feature selection



forward
faster

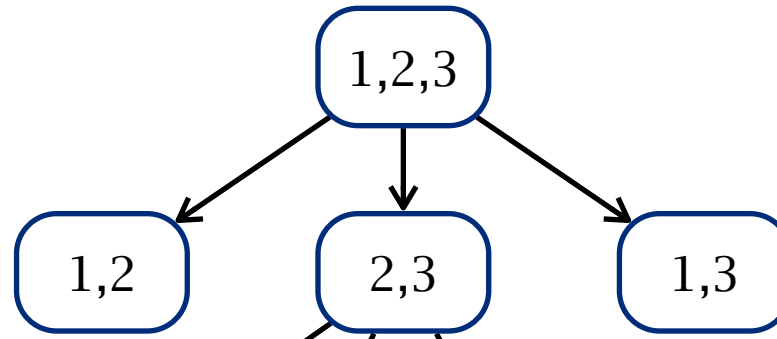


backward
more accurate

Classifier dependent feature selection



random init



backward

forward



backward



...

combined forward-backward search

Feature extraction



disclosure the inner structure of the data
to support a better mining performance

feature extraction construct new features
commonly followed by a feature selection
usually used for low-level features

digits bitmap:

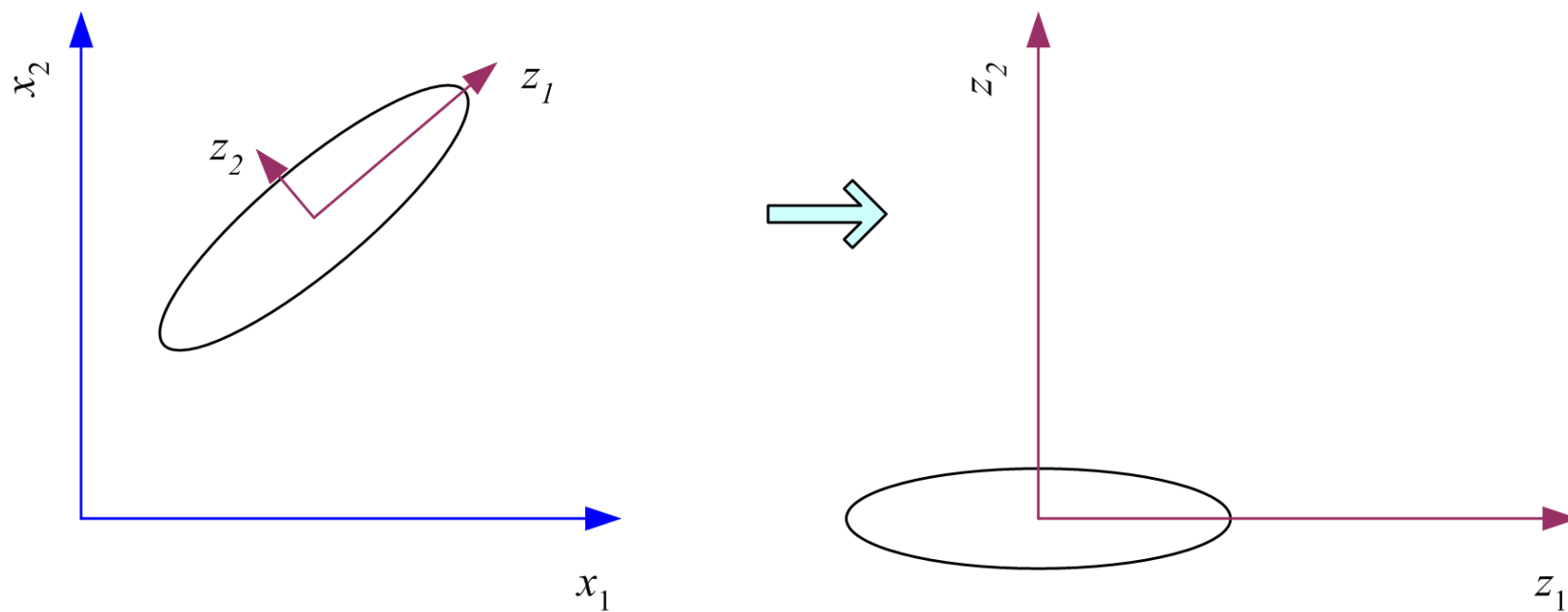
1	2	3	4	0	1
2	3	4	0	1	2
3	4	0	0	4	1
3	1	0	0	2	2
2	0	1	2	3	3
3	3	4	4	1	0

Linear methods



Principal components analysis (PCA)

rotate the data to align the directions of the variance

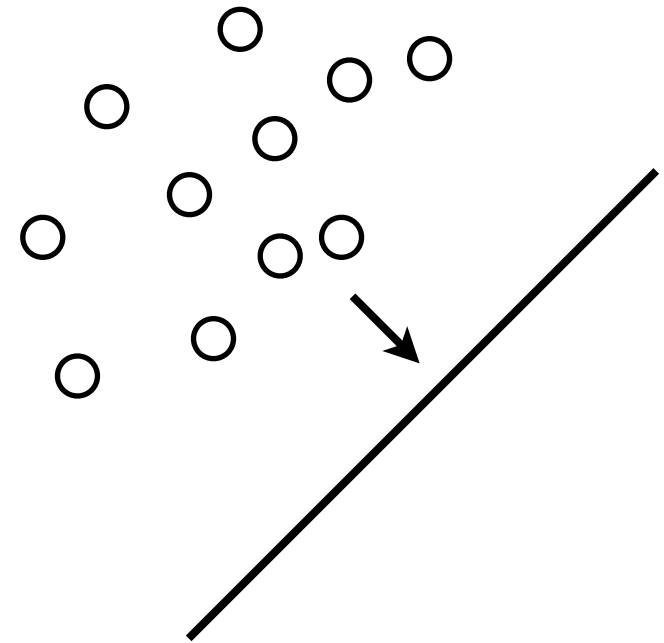


Linear methods



Principal components analysis (PCA)

the first dimension = the largest variance direction



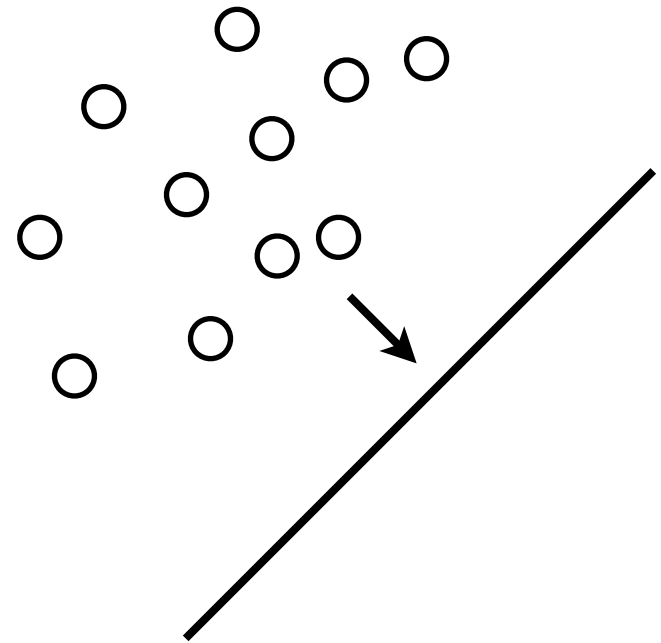
Linear methods



Principal components analysis (PCA)

the first dimension = the largest variance direction

$$z = \mathbf{w}^T \mathbf{x}$$



Linear methods

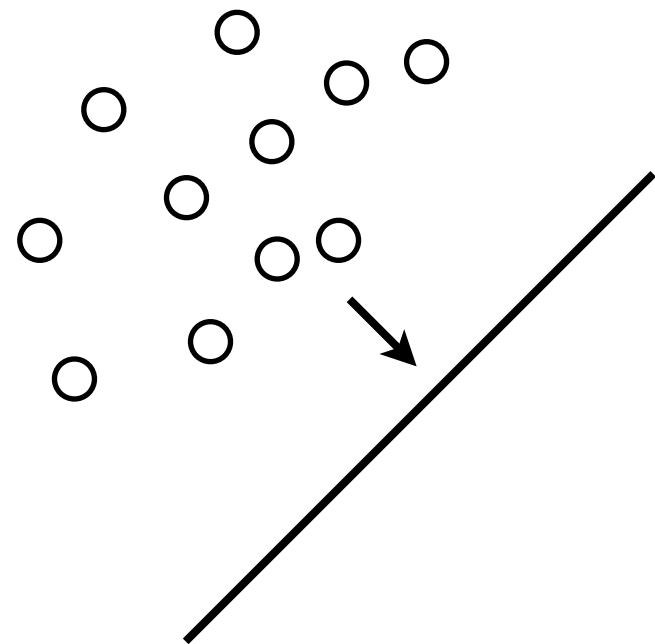


Principal components analysis (PCA)

the first dimension = the largest variance direction

$$z = \mathbf{w}^T \mathbf{x}$$

$$\text{Var}(z_1) = \mathbf{w}_1^T \Sigma \mathbf{w}_1$$



Linear methods



Principal components analysis (PCA)

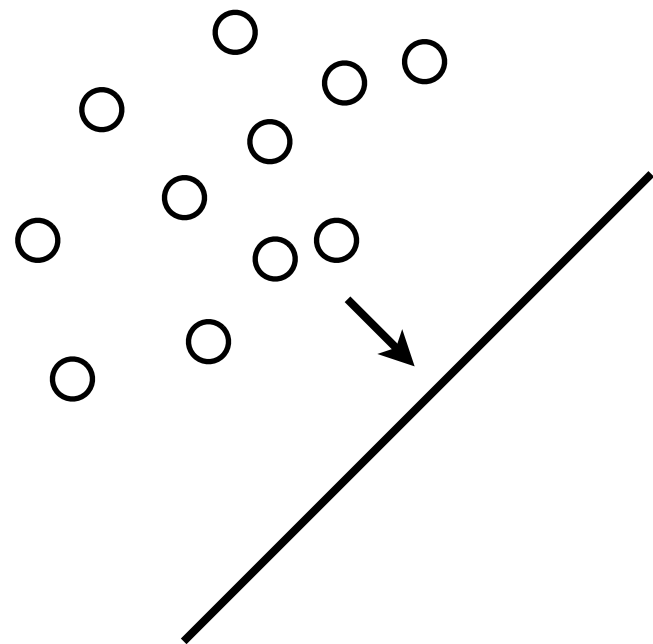
the first dimension = the largest variance direction

$$z = \mathbf{w}^T \mathbf{x}$$

$$\text{Var}(z_1) = \mathbf{w}_1^T \Sigma \mathbf{w}_1$$

find a unit \mathbf{w} to maximize the variance

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



Linear methods



Principal components analysis (PCA)

the first dimension = the largest variance direction

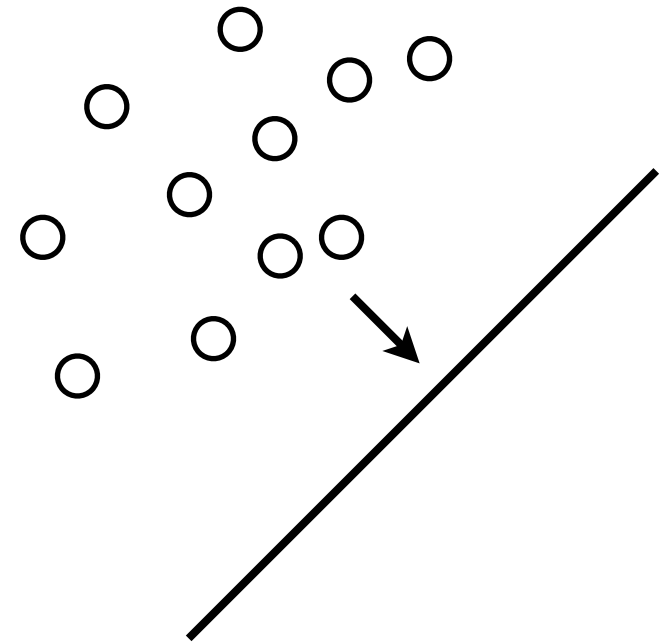
$$z = \mathbf{w}^T \mathbf{x}$$

$$\text{Var}(z_1) = \mathbf{w}_1^T \Sigma \mathbf{w}_1$$

find a unit \mathbf{w} to maximize the variance

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

$$2\Sigma \mathbf{w}_1 - 2\alpha \mathbf{w}_1 = 0, \text{ and therefore } \Sigma \mathbf{w}_1 = \alpha \mathbf{w}_1$$



Linear methods



Principal components analysis (PCA)

the first dimension = the largest variance direction

$$z = \mathbf{w}^T \mathbf{x}$$

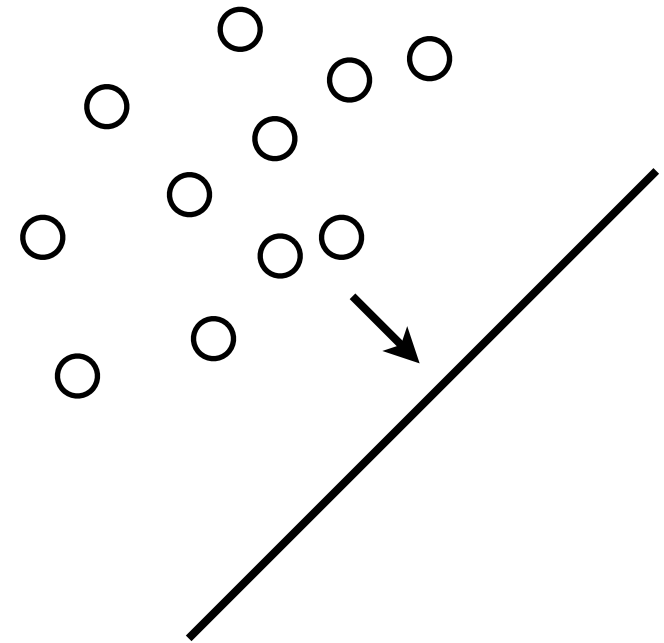
$$\text{Var}(z_1) = \mathbf{w}_1^T \Sigma \mathbf{w}_1$$

find a unit \mathbf{w} to maximize the variance

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

$2\Sigma\mathbf{w}_1 - 2\alpha\mathbf{w}_1 = 0$, and therefore $\Sigma\mathbf{w}_1 = \alpha\mathbf{w}_1$

$$\mathbf{w}_1^T \Sigma \mathbf{w}_1 = \alpha \mathbf{w}_1^T \mathbf{w}_1 = \alpha$$



Linear methods



Principal components analysis (PCA)

the first dimension = the largest variance direction

$$z = \mathbf{w}^T \mathbf{x}$$

$$\text{Var}(z_1) = \mathbf{w}_1^T \Sigma \mathbf{w}_1$$

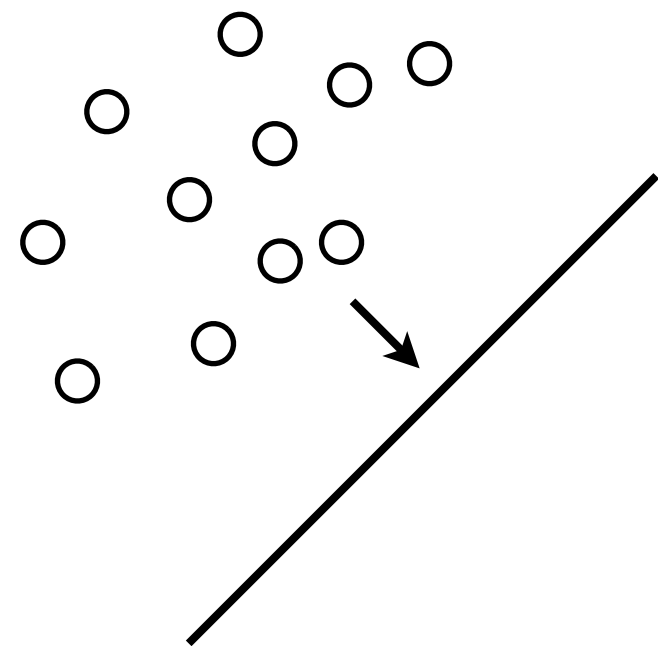
find a unit \mathbf{w} to maximize the variance

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

$2\Sigma\mathbf{w}_1 - 2\alpha\mathbf{w}_1 = 0$, and therefore $\Sigma\mathbf{w}_1 = \alpha\mathbf{w}_1$

$$\mathbf{w}_1^T \Sigma \mathbf{w}_1 = \alpha \mathbf{w}_1^T \mathbf{w}_1 = \alpha$$

\mathbf{w} is the eigenvector with the largest eigenvalue



Linear methods



Principal components analysis (PCA)

the second dimension = the largest variance
direction orthogonal to the first dimension

Linear methods



Principal components analysis (PCA)

the second dimension = the largest variance
direction orthogonal to the first dimension

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

Linear methods



Principal components analysis (PCA)

the second dimension = the largest variance direction orthogonal to the first dimension

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

$$2\Sigma \mathbf{w}_2 - 2\alpha \mathbf{w}_2 - \beta \mathbf{w}_1 = 0$$

Linear methods



Principal components analysis (PCA)

the second dimension = the largest variance direction orthogonal to the first dimension

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

$$2\Sigma \mathbf{w}_2 - 2\alpha \mathbf{w}_2 - \beta \mathbf{w}_1 = 0$$

$$\beta = 0 \quad \Sigma \mathbf{w}_2 = \alpha \mathbf{w}_2$$

Linear methods



Principal components analysis (PCA)

the second dimension = the largest variance direction orthogonal to the first dimension

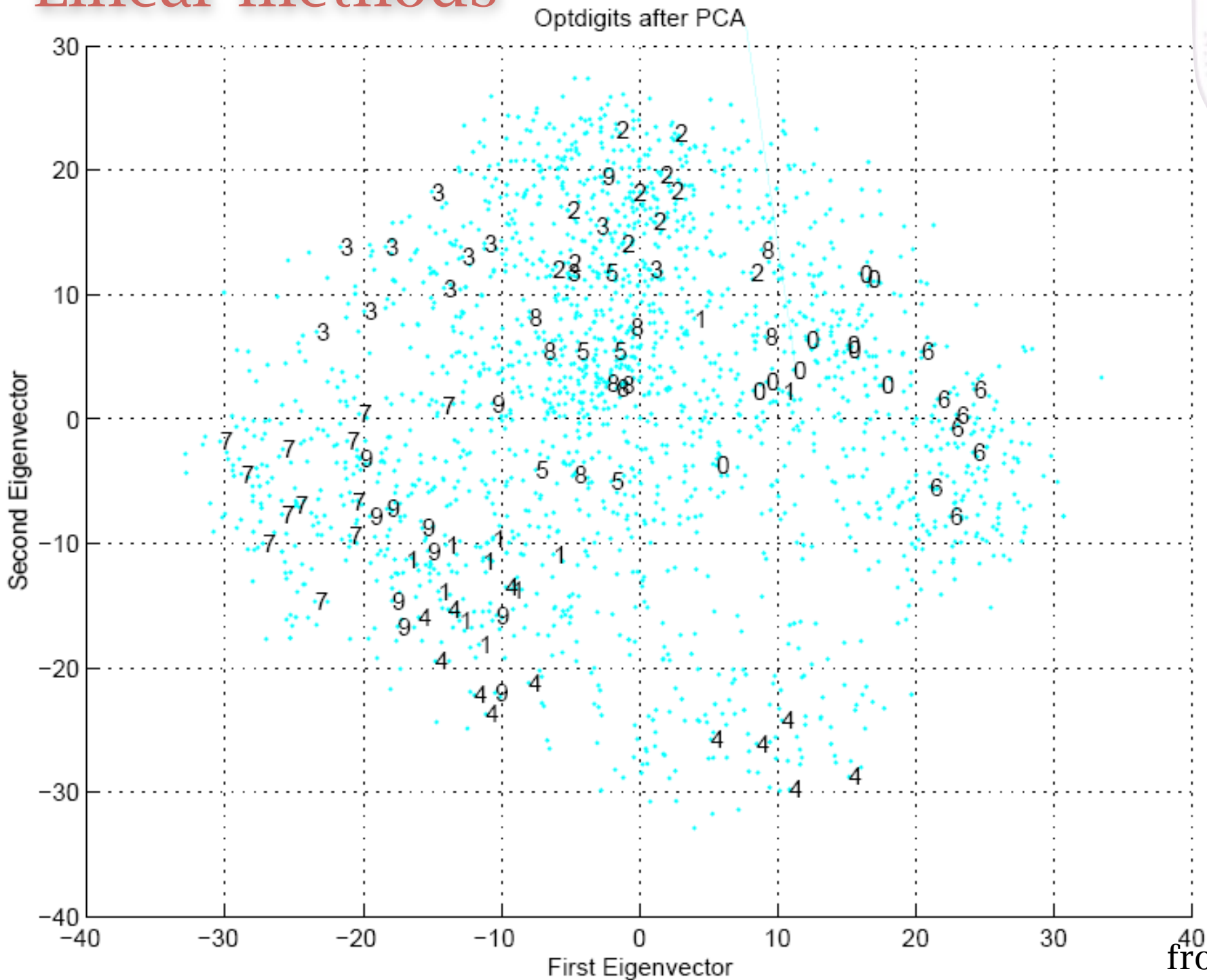
$$\max_{\mathbf{w}_2} \mathbf{w}_2^T \Sigma \mathbf{w}_2 - \alpha (\mathbf{w}_2^T \mathbf{w}_2 - 1) - \beta (\mathbf{w}_2^T \mathbf{w}_1 - 0)$$

$$2\Sigma \mathbf{w}_2 - 2\alpha \mathbf{w}_2 - \beta \mathbf{w}_1 = 0$$

$$\beta = 0 \quad \Sigma \mathbf{w}_2 = \alpha \mathbf{w}_2$$

\mathbf{w} 's are the eigenvectors sorted by the eigenvalues

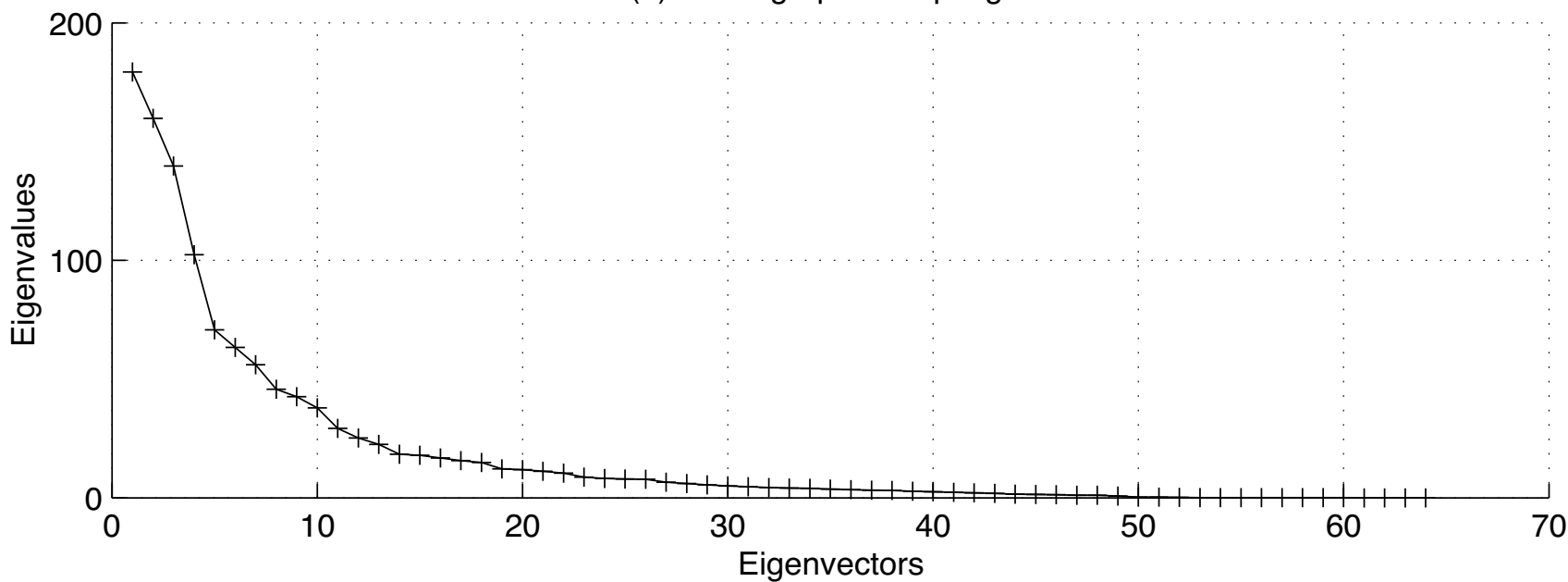
Linear methods



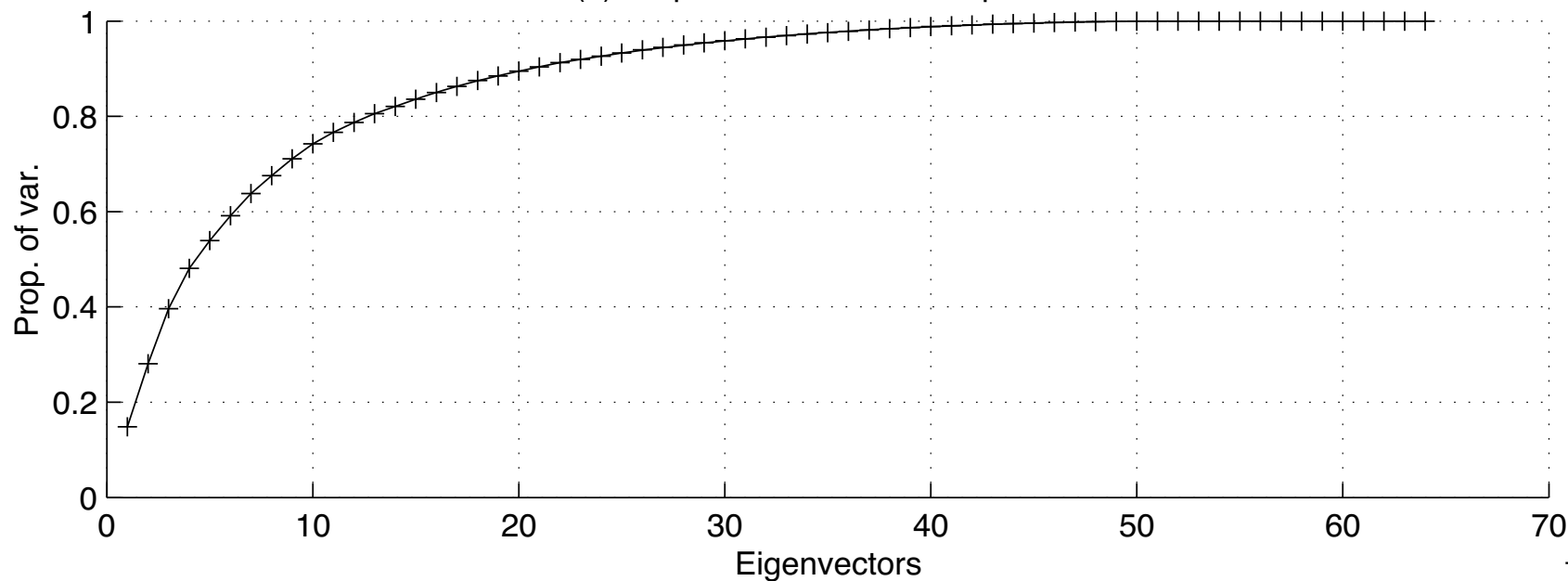
Linear methods



(a) Scree graph for Optdigits



(b) Proportion of variance explained



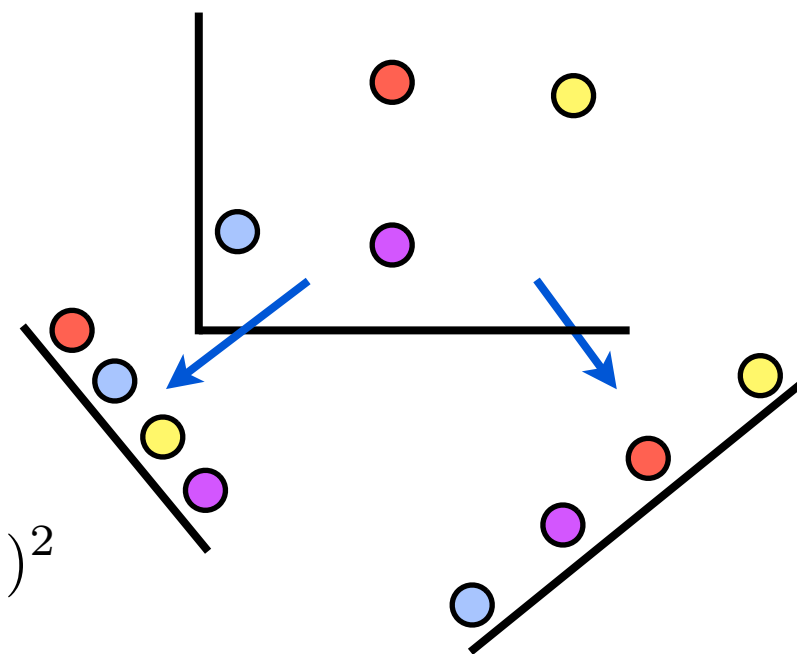
Linear methods



Multidimensional Scaling (MDS)

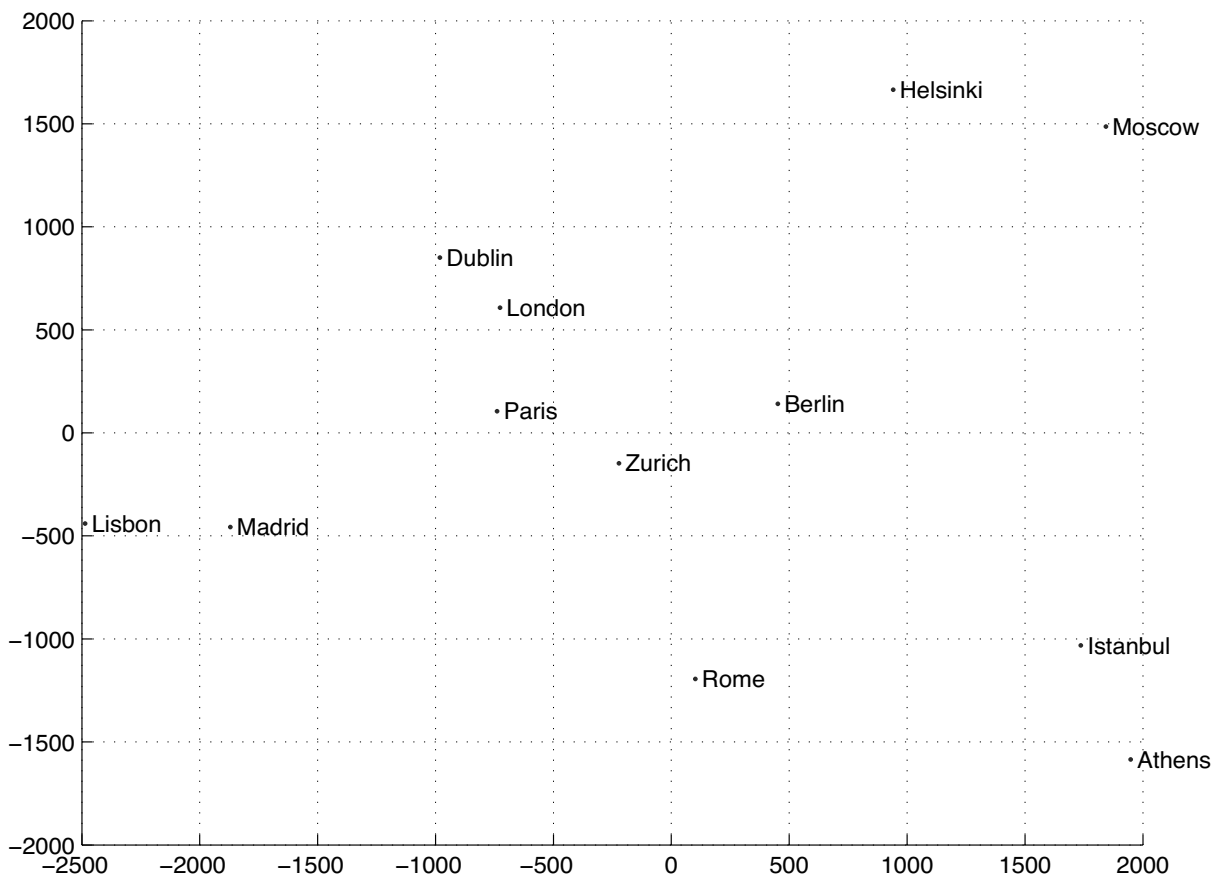
keep the distance into a lower dimensional space

for linear transformation,
 W is an $n \times k$ matrix



$$\arg \min_W \sum_{i,j} (\| \mathbf{x}_i^\top W - \mathbf{x}_j^\top W \| - \| \mathbf{x}_i - \mathbf{x}_j \|)^2$$

Linear methods



from [Intro. ML]

Linear methods



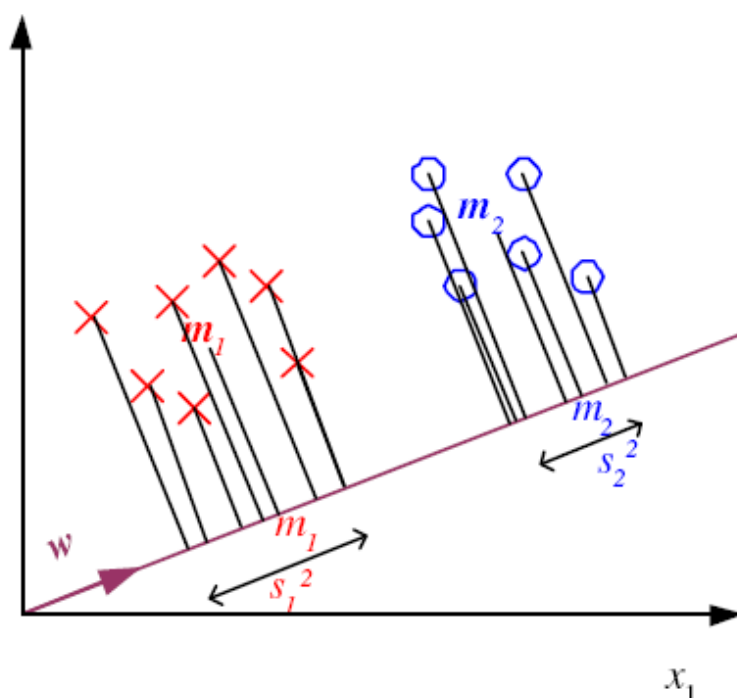
Linear Discriminant Analysis (LDA)

find a direction such that the two classes are well separated

$$Z = \mathbf{w}^T \mathbf{x}$$

m be the mean of a class

s^2 be the variance of a class



maximize the criterion

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

Linear methods

Linear Discriminant Analysis (LDA)



Linear methods



Linear Discriminant Analysis (LDA)

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T \mathbf{m}_1 - \mathbf{w}^T \mathbf{m}_2)^2 \\ &= \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2) (\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_B \mathbf{w}\end{aligned}$$

Linear methods



Linear Discriminant Analysis (LDA)

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T \mathbf{m}_1 - \mathbf{w}^T \mathbf{m}_2)^2 \\ &= \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2) (\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_B \mathbf{w}\end{aligned}$$

$$\begin{aligned}s_1^2 &= \sum_t (\mathbf{w}^T \mathbf{x}^t - m_1)^2 r^t \\ &= \sum_t \mathbf{w}^T (\mathbf{x}^t - \mathbf{m}_1) (\mathbf{x}^t - \mathbf{m}_1)^T \mathbf{w} r^t \\ &= \mathbf{w}^T \mathbf{S}_1 \mathbf{w}\end{aligned}$$

Linear methods



Linear Discriminant Analysis (LDA)

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T \mathbf{m}_1 - \mathbf{w}^T \mathbf{m}_2)^2 \\ &= \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2) (\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_B \mathbf{w}\end{aligned}$$

$$\begin{aligned}s_1^2 &= \sum_t (\mathbf{w}^T \mathbf{x}^t - m_1)^2 r^t \\ &= \sum_t \mathbf{w}^T (\mathbf{x}^t - \mathbf{m}_1) (\mathbf{x}^t - \mathbf{m}_1)^T \mathbf{w} r^t \\ &= \mathbf{w}^T \mathbf{S}_1 \mathbf{w}\end{aligned}$$

$$s_1^2 + s_2^2 = \mathbf{w}^T \mathbf{S}_W \mathbf{w} \quad \mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$$

Linear methods



Linear Discriminant Analysis (LDA)

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T \mathbf{m}_1 - \mathbf{w}^T \mathbf{m}_2)^2 \\ &= \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2) (\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_B \mathbf{w}\end{aligned}$$

$$\begin{aligned}s_1^2 &= \sum_t (\mathbf{w}^T \mathbf{x}^t - m_1)^2 r^t \\ &= \sum_t \mathbf{w}^T (\mathbf{x}^t - \mathbf{m}_1) (\mathbf{x}^t - \mathbf{m}_1)^T \mathbf{w} r^t \\ &= \mathbf{w}^T \mathbf{S}_1 \mathbf{w}\end{aligned}$$

$$s_1^2 + s_2^2 = \mathbf{w}^T \mathbf{S}_W \mathbf{w} \quad \mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$$

The objective becomes:

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)|^2}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

Linear methods



Linear Discriminant Analysis (LDA)

The objective becomes:

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)|^2}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

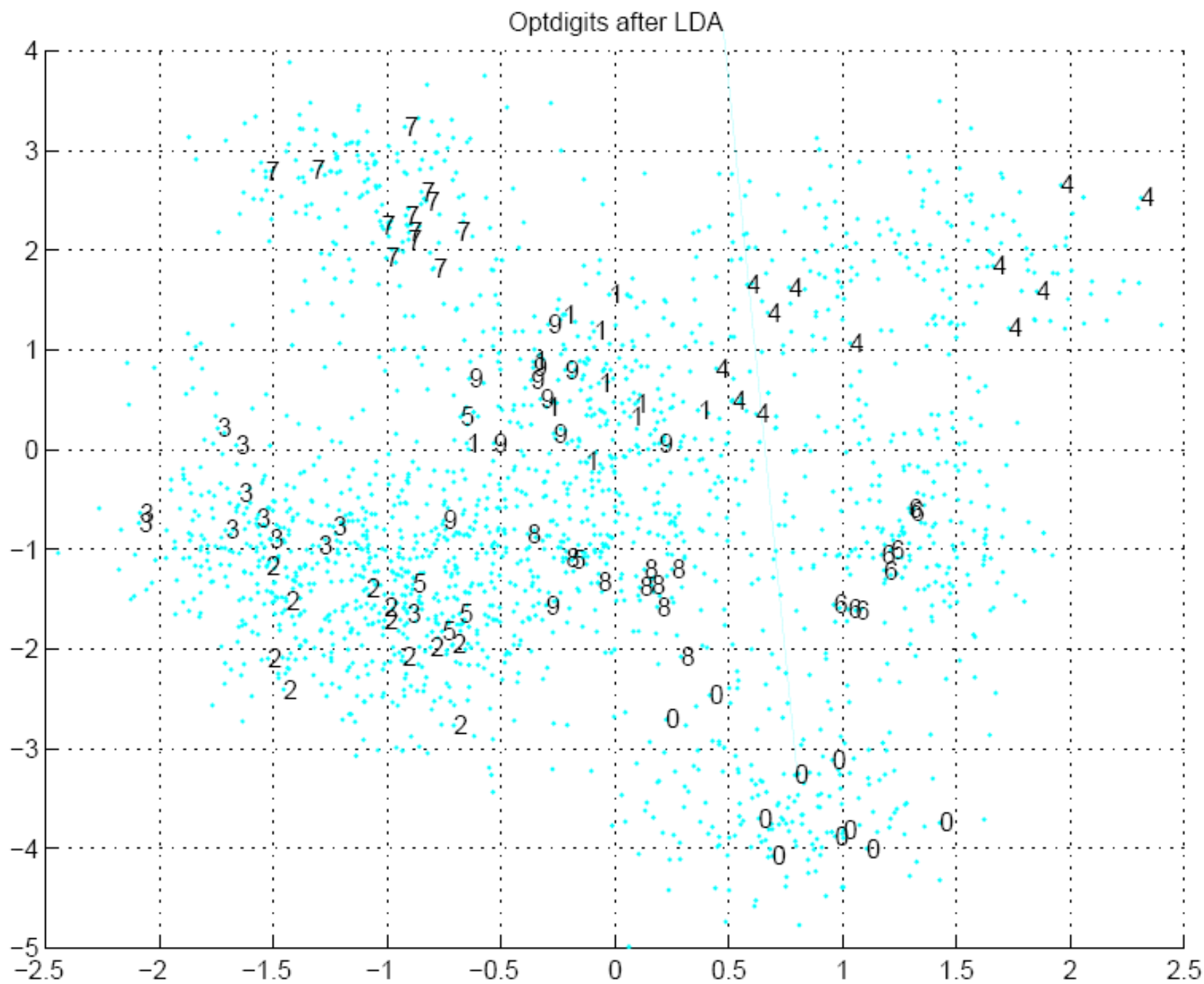
$$\frac{\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \left(2(\mathbf{m}_1 - \mathbf{m}_2) - \frac{\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \mathbf{S}_W \mathbf{w} \right) = 0$$

Given that $\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2) / \mathbf{w}^T \mathbf{S}_W \mathbf{w}$ is a constant, we have

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

just take $c = 1$ and find \mathbf{w}

Linear methods



from [Intro. ML]

Example: Face recognition

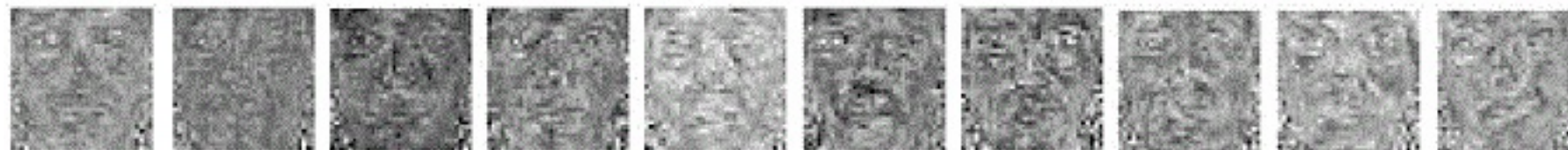


PCA and LDA are commonly used to extract features for face recognition.

Basis of eigenface (PCA):



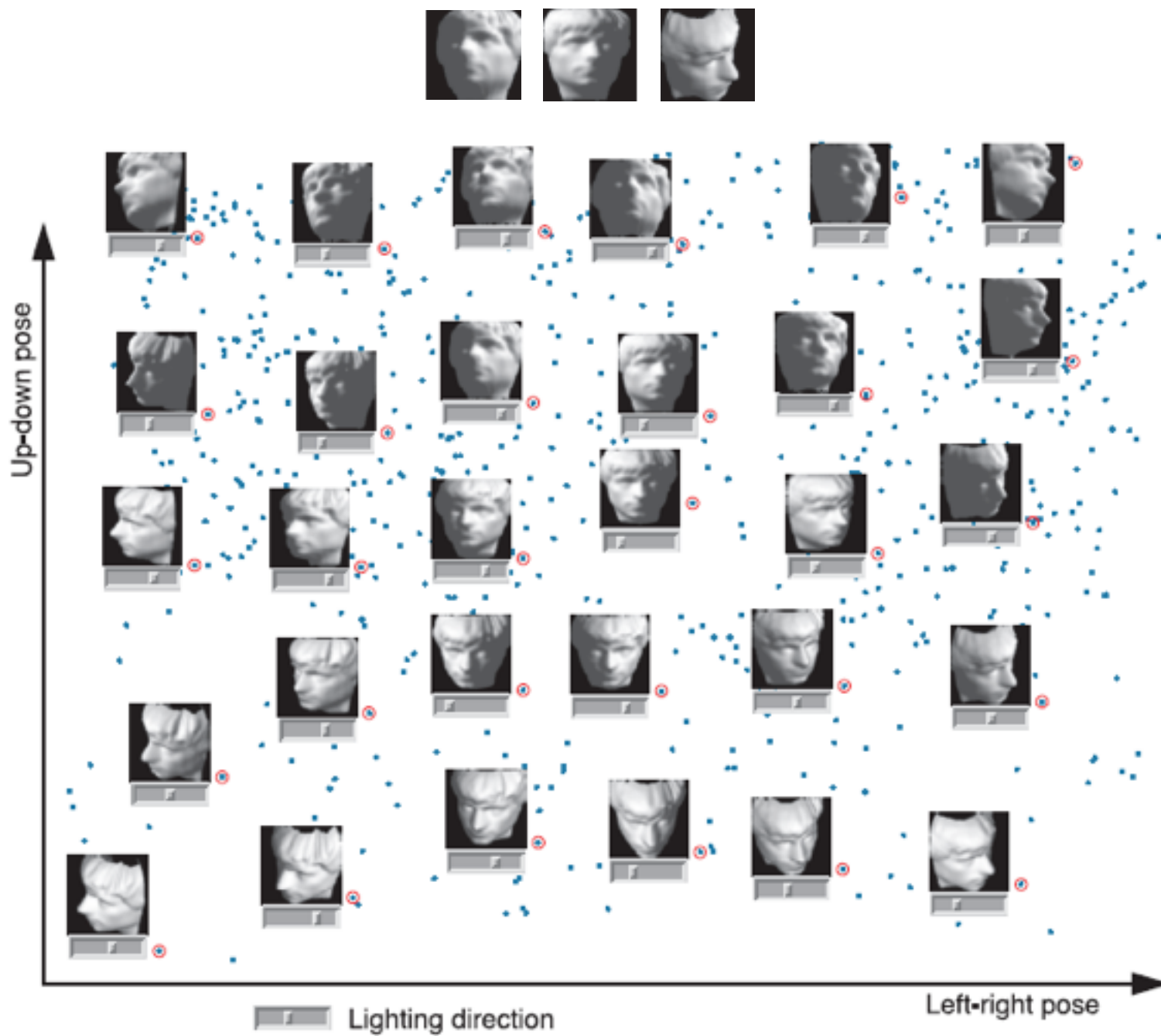
Basis of Fisherface (LDA):



Manifold learning



Manifold learning

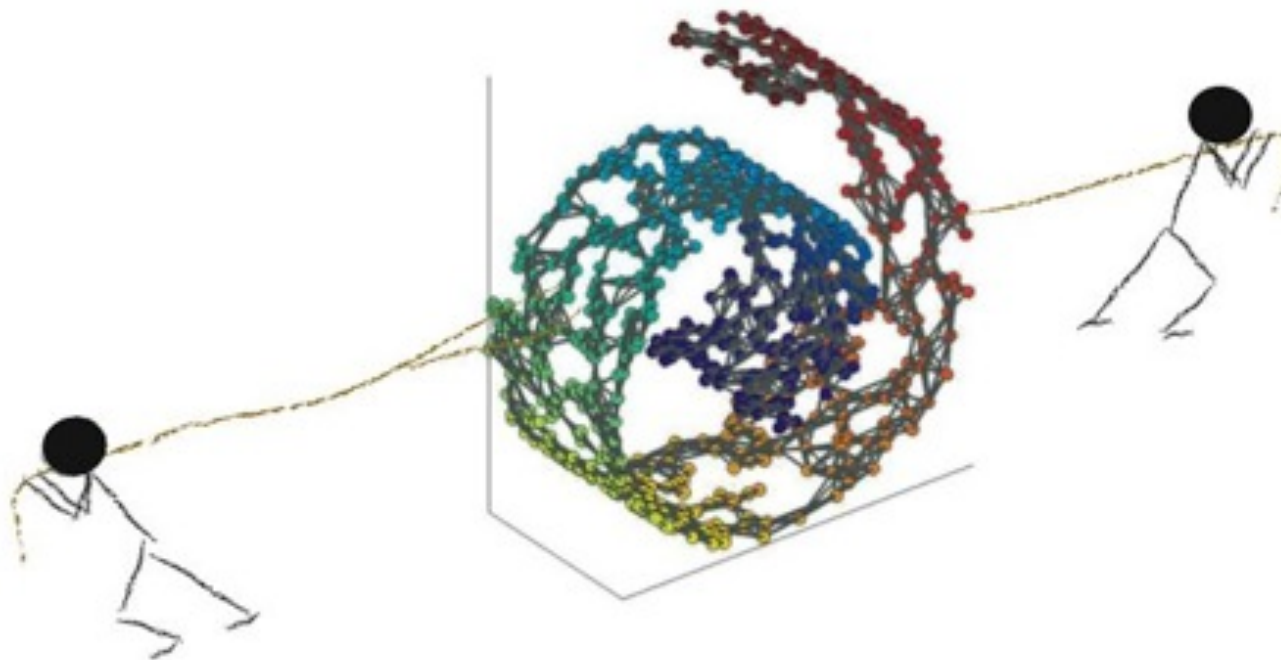


Manifold learning



A low intrinsic dimensional data embedded in a high dimensional space

cause a bad distance measure

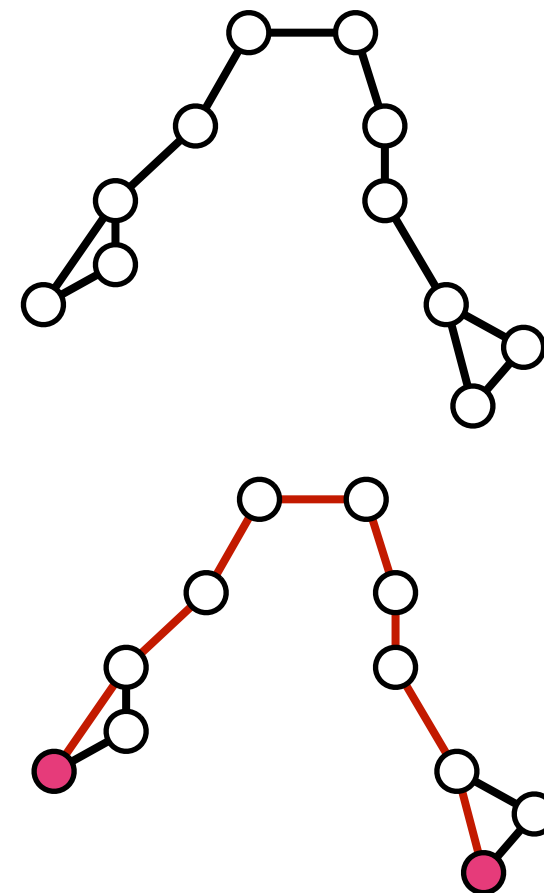


Manifold learning



ISOMAP

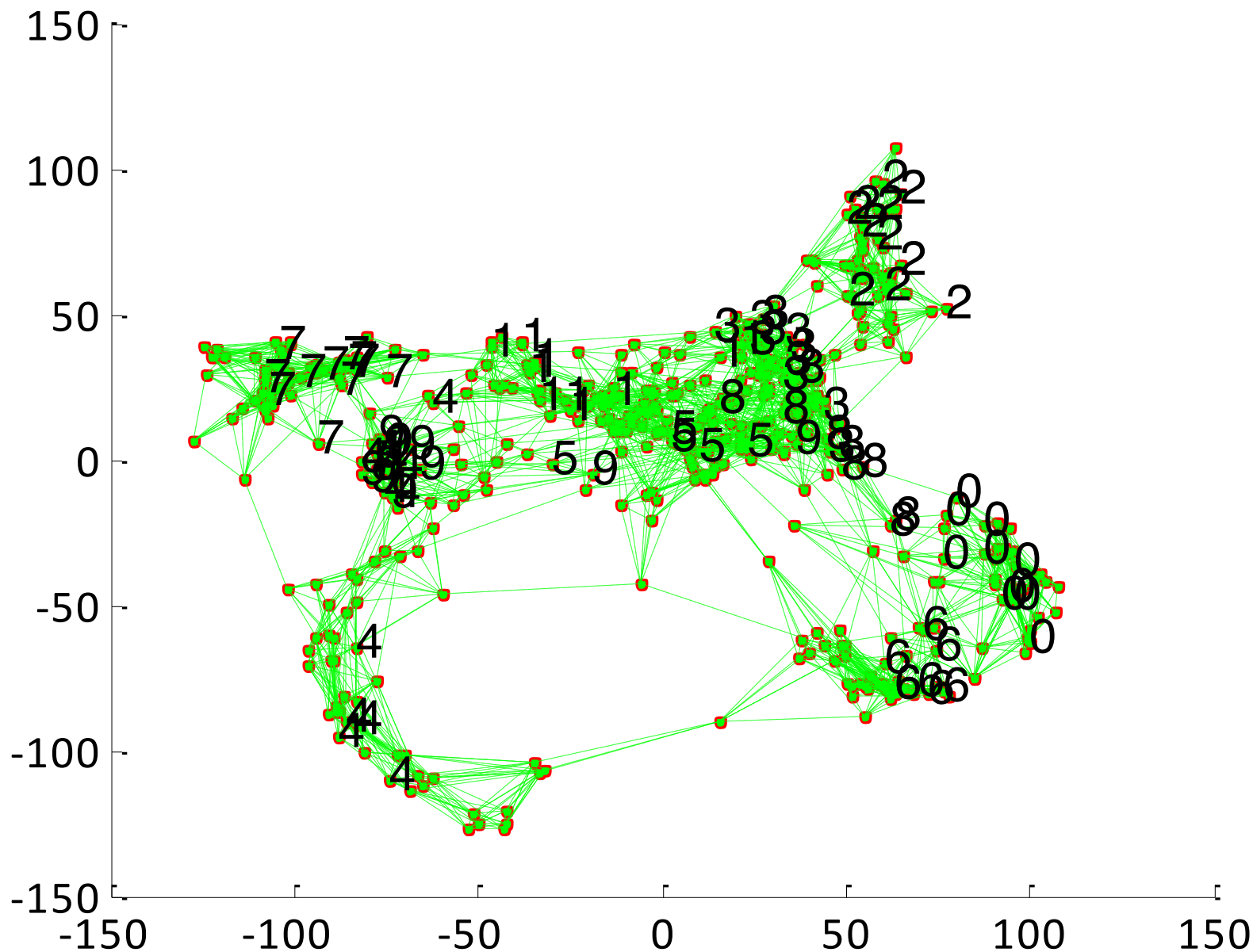
1. construct a neighborhood graph (kNN and ϵ -NN)
2. calculate distance matrix as the shortest path on the graph
3. apply MDS on the distance matrix



Manifold learning



Optdigits after Isomap (with neighborhood graph).



Manifold learning



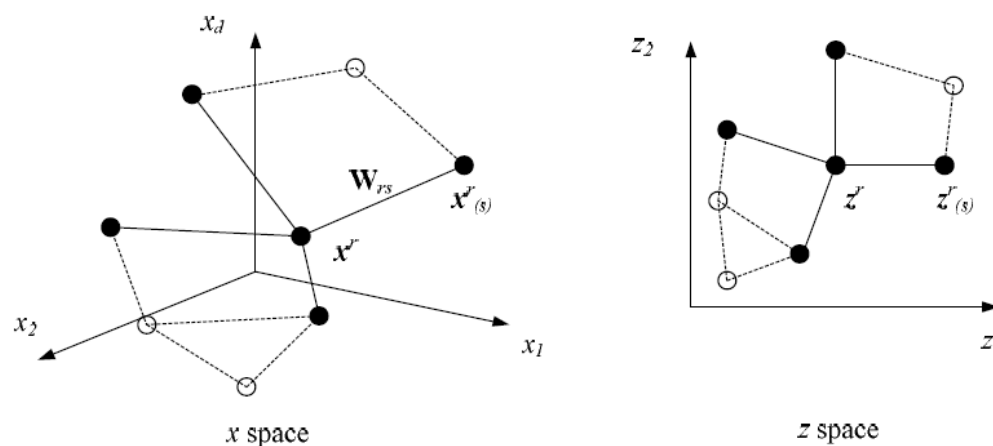
Local Linear Embedding (LLE):

1. find neighbors for each instance
2. calculate a linear reconstruction for an instance

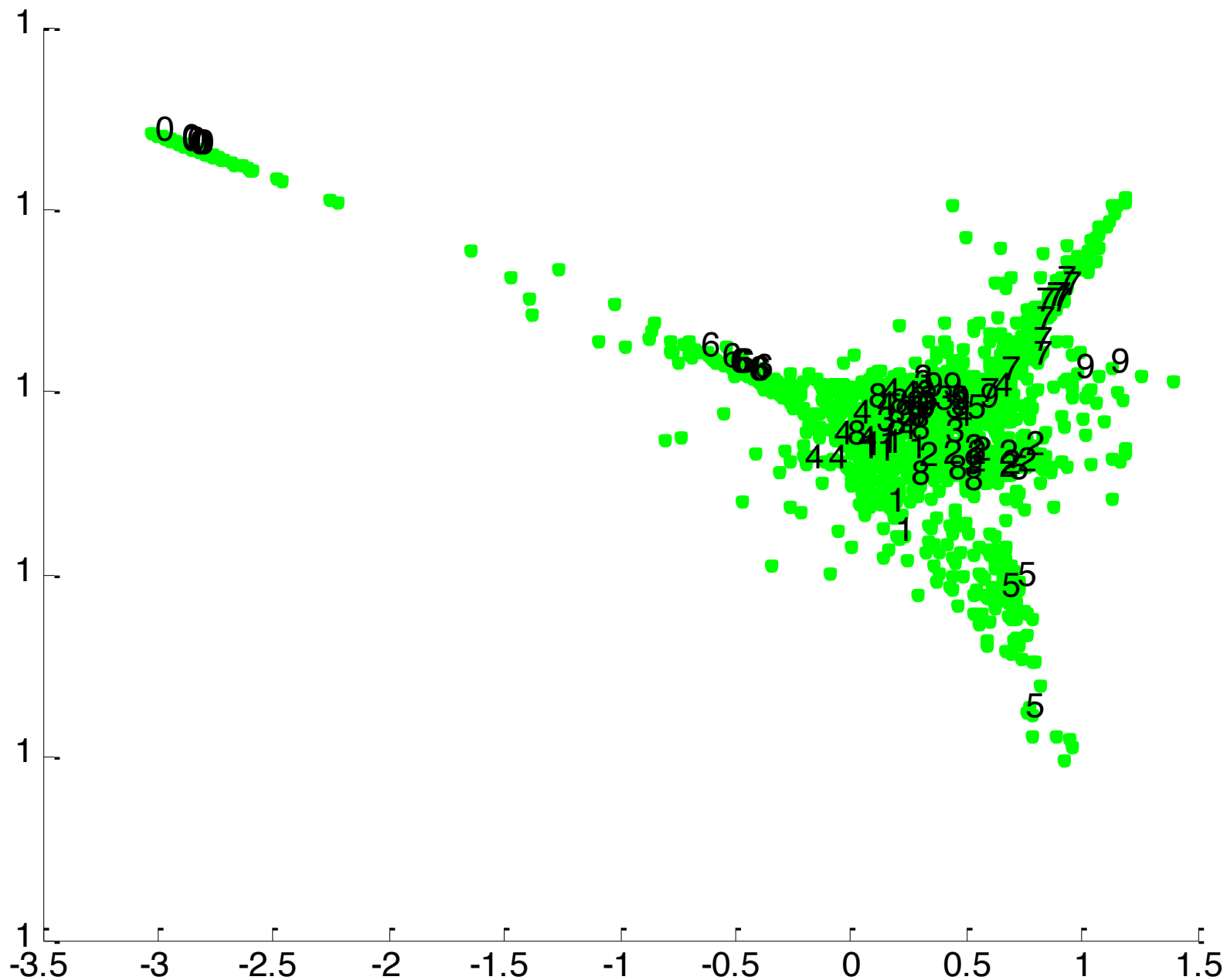
$$\sum_r \left\| \mathbf{x}^r - \sum_s \mathbf{W}_{rs} \mathbf{x}_{(r)}^s \right\|^2$$

3. find low dimensional instances preserving the reconstruction

$$\sum_r \left\| \mathbf{z}^r - \sum_s \mathbf{W}_{rs} \mathbf{z}^s \right\|^2$$



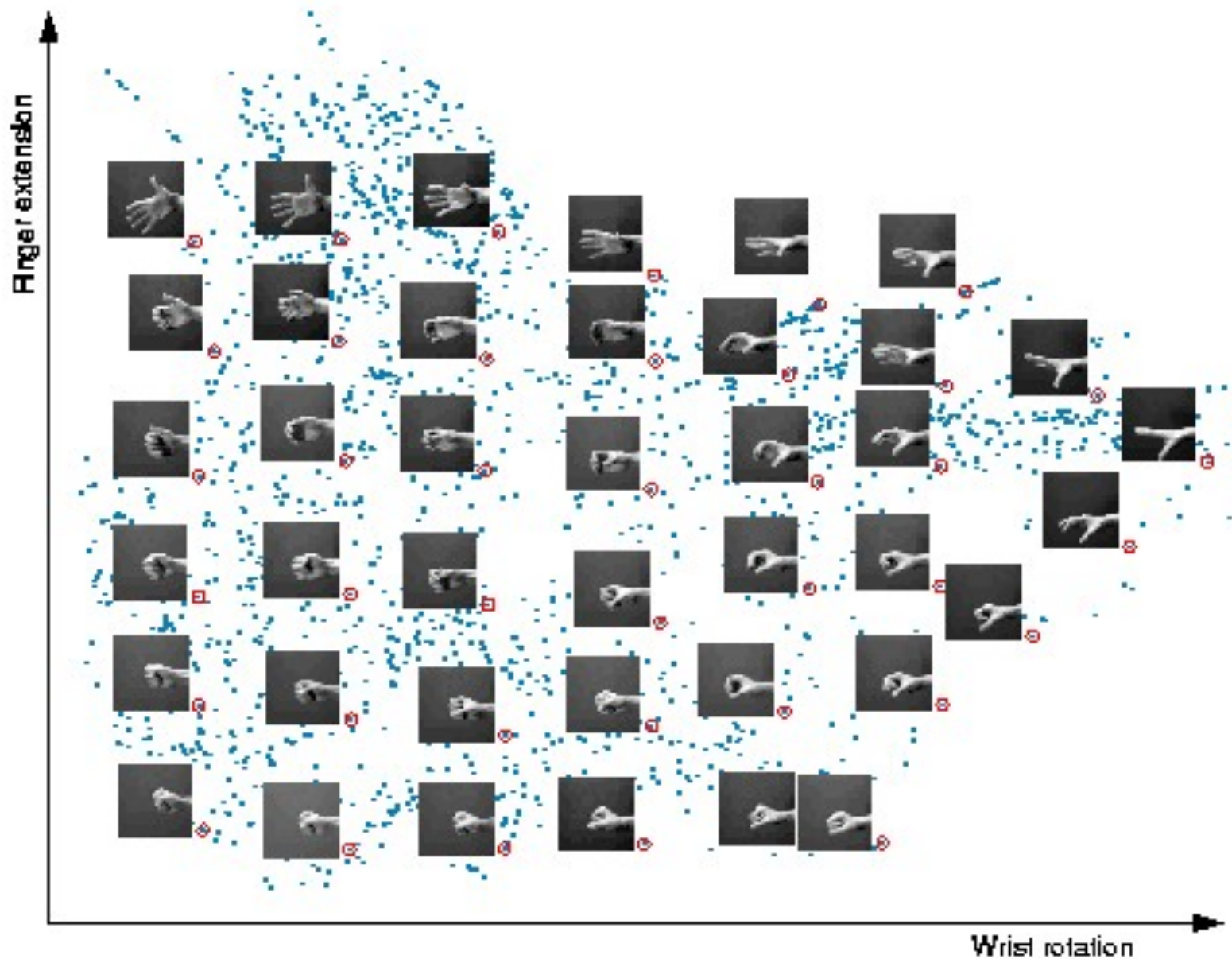
Manifold learning



from [Intro. ML]

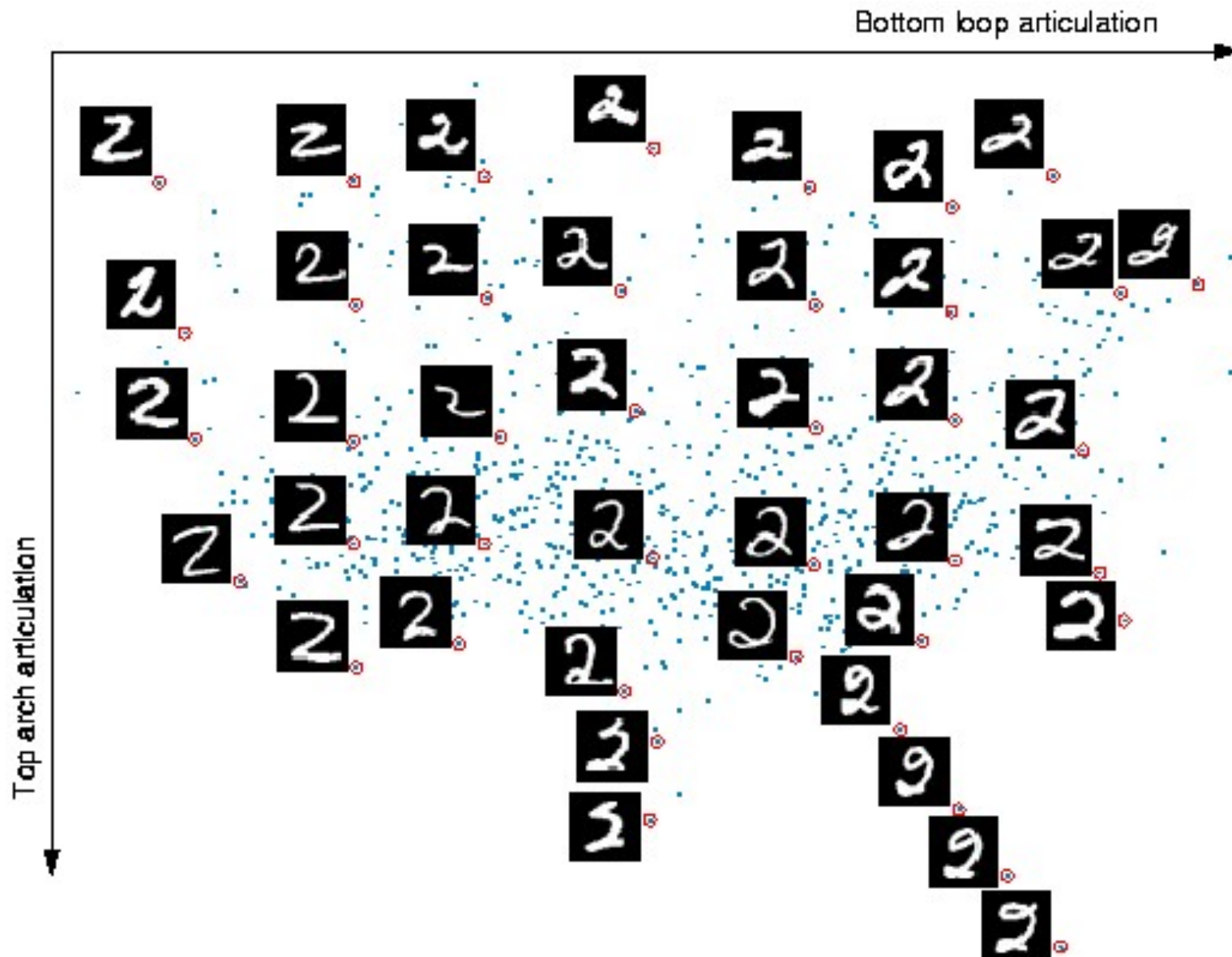
Manifold learning

more manifold learning examples



Manifold learning

more manifold learning examples

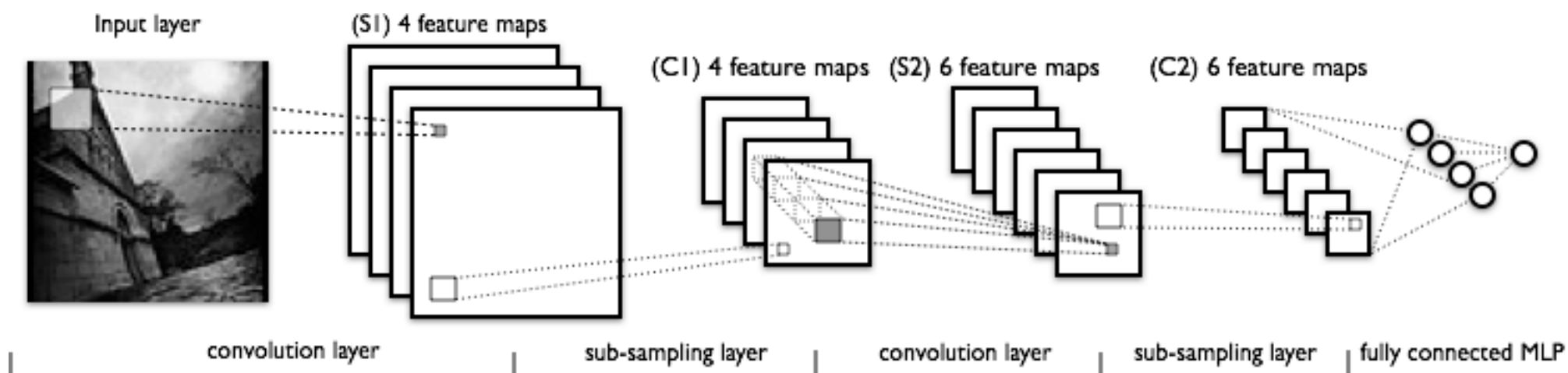




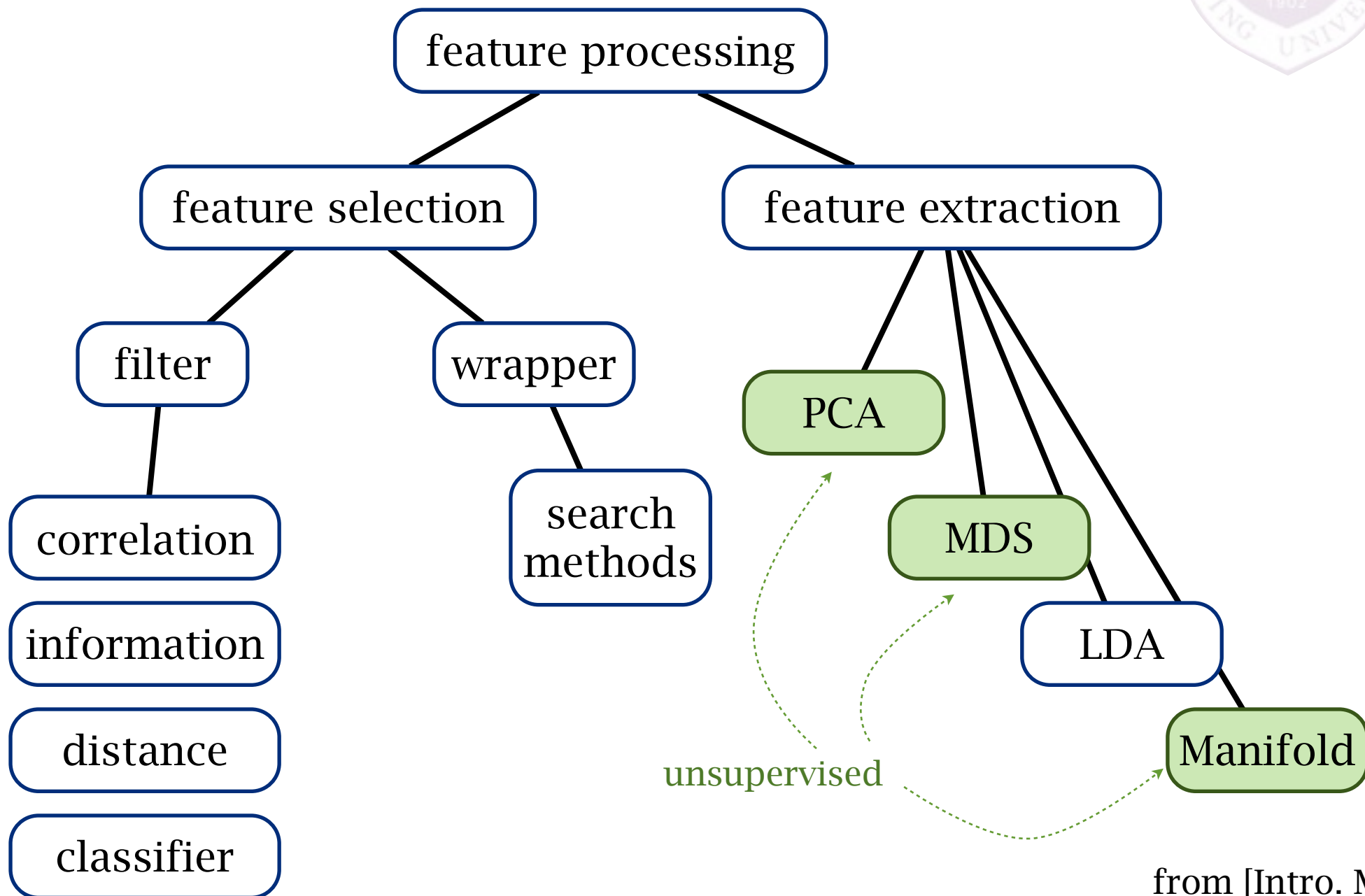
Other feature extraction methods

Most feature extractions are case specific

Convolutional Neural Networks (CNN/LeNet)
for general image feature extraction



A summary of approaches



习题



特征是否越多越好？为什么？

特征选择(feature selection)和特征抽取(feature extraction)各适合应用在什么场景？

主成分分析(PCA)和线性判别分析(LDA)哪一种是需要类别标记的？