Lecture 11: Dimensionality Reduction and Subspace-based Methods

DD2421

Atsuto Maki

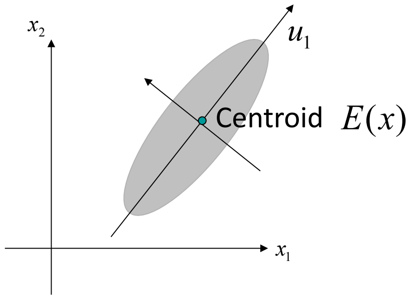
Autumn, 2017

Our keywords today:

- Dimensionality reduction
  - Principal Component Analysis (PCA)
- Discriminant function
  - Similarity measures: angle, projection length
- Subspace Methods

Principal Component Analysis (PCA)

1. Maximizing variance



Number of samples

Mean vector of x : $E(x) = (1/r)\sum x$

Covariance matrix: $\Sigma = E((x - E(x))(x - E(x))^T)$

1. Maximum variance criterion

Reduce the effective number of variables

(only dealing with components with larger variances)

$E((x^T u_i - E(x^T u_i))^2)$ → Maximize $(i = 1, \ldots, p)$

$= E((u_i^T (x - E(x)))^2)$

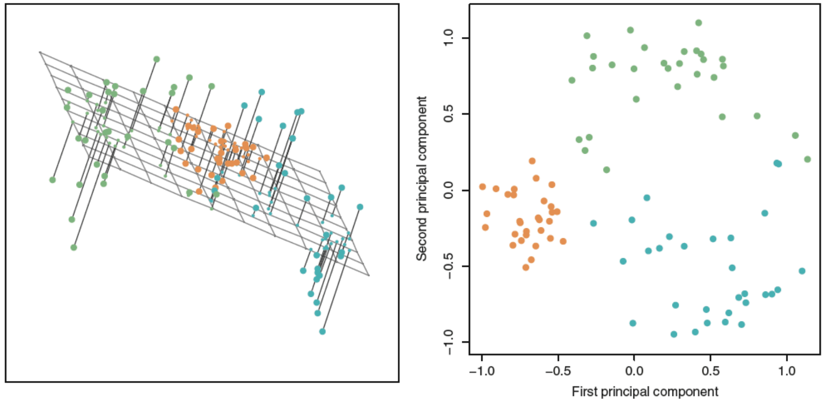
$= u_i^T \underbrace{E((x - E(x))(x - E(x))^T)}_{\text{Covariance matrix}} u_i = u_i^T \Sigma u_i$

Condition: $u_i^T u_j = \delta_{ij}$

$\max[\mathrm{tr}(U^T \Sigma U)]$

The transformation matrix U consists of p columns: the eigenvectors of the covariance matrix, Σ (corresponding to its p largest eigenvalues).

Example 3-d to 2-d: Ninety observations simulated in 3-d

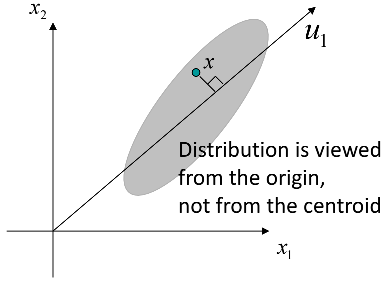


The first 2 principal component directions span the plane that best fits the data.
It minimizes the sum of squared distances from each point to the plane.

Figure from
An Introduction to Statistical Learning (James et al.)

Principal Component Analysis (PCA)

2. Min. approximation error



Autocorrelation matrix: $Q = E(xx^T)$

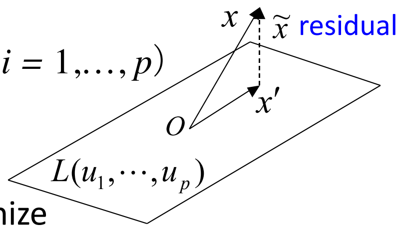
2. Minimum squared distance criterion

Averaged squared error between x and its approximation to be minimized by a set $\{u_1, \cdots, u_p\}$

$E(\| x - x' \|^2)$ →minimize $\quad (i = 1, \ldots, p)$

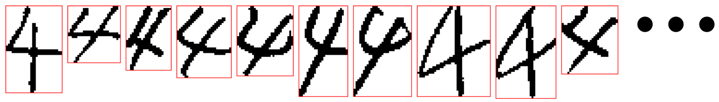
Approximated $x' = \sum_{i=1}^{p} (x^T u_i) u_i$

$\| x' \|^2 = \| x \|^2 - \| \tilde{x} \|^2$ →maximize



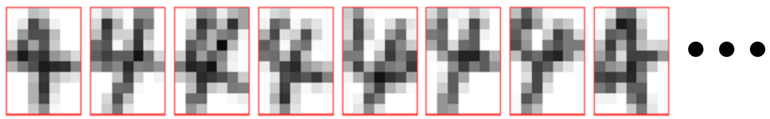
The basis consists of p eigenvectors of the autocorrelation matrix, Q (corresponding to its p largest eigenvalues).

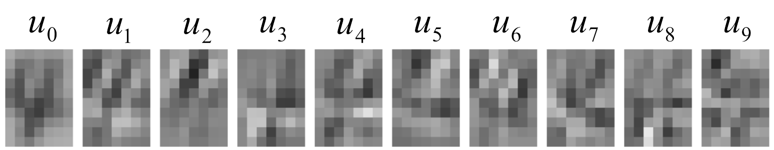
PCA example 1: Hand-written digits



Feature extraction

Pattern vectors: normalized & blurred patterns





(figure credit: Y.

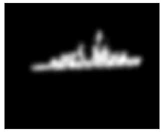
Example 2: Human face classificaiton

Basis vectors of a person: someone's *dictionary*

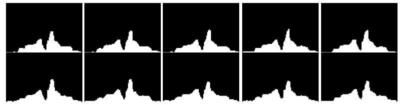
(Eigenvectors from a large collection of his/her face)

(figure credit: K. Fukui)

Example 3: Ship classification (profiles)



Profile vectors



Principal Component Analysis (PCA)

↓

Eigenvectors

↓

Dictionary

Eigenvectors for the greatest eigenvalues

Concept of subspace

Subspace L is a collection of n-d vectors:

spanned by a basis, a set of linearly independent vectors

$$L(b_1,\cdots,b_p) = \{z \mid z = \sum_{i=1}^{p} \xi_i b_i\} \qquad (\xi_i \in R, b_i \in R^n)$$

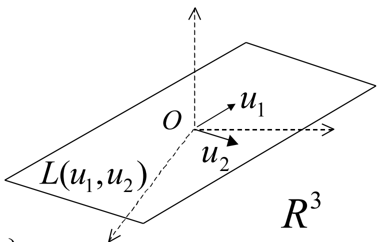
Dimension of a subspace:

the number of base vectors

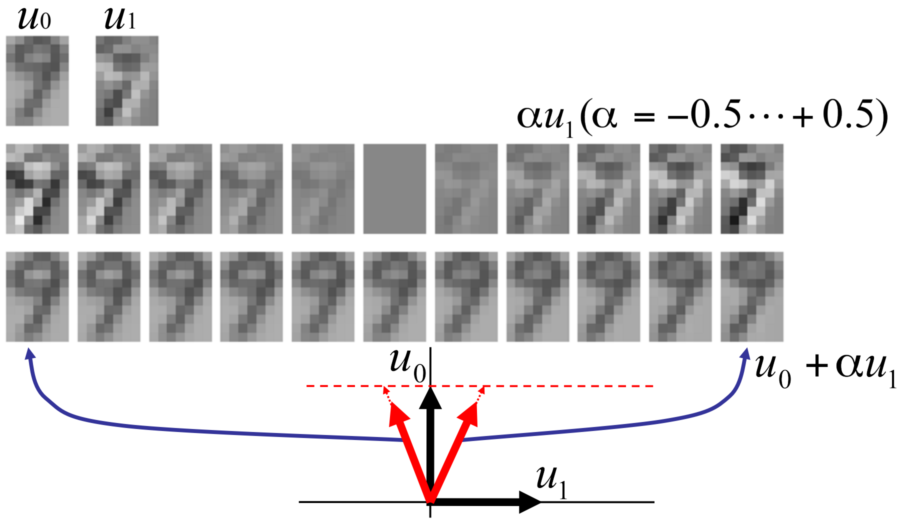
$$p = \dim(L) \quad << n$$

Conveniently represented

by orthonormal basis $\{u_1,\cdots,u_p\}$

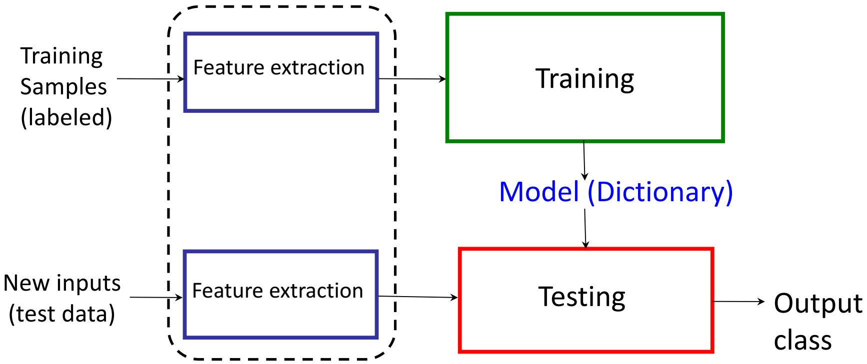


- Variations of "9" covered by a 2-d subspace



(figure credit: Y.

Background: Schematic of classification



Training phase

- Given: Limited number of labeled data
  (samples whose classes are known)
- The dimensionality often too high for limited number of samples

One approach to this is to find redundant variables and discard them, i.e. *dimensionality reduction*
(without losing essential information)

Information compression: to extract the class characteristics and throw away the rest!

Testing phase

- Various ways to measure the distance
  - Euclidean / Mahalanobis distance
  - Angle between vectors
  - Projection length on subspaces

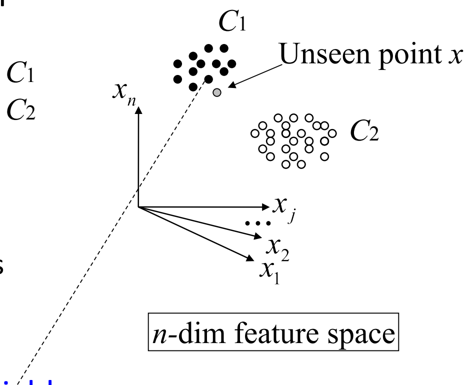
    …
- Classification methods
  - Discriminant function
  - Subspace method

    …

Nearest Neighbor methods (revisiting)

- Binary classification
  - N_1 samples of class C_1
  - N_2 samples of class C_2
  - Unseen data x

  → Compute distances to $N_1 + N_2$ samples



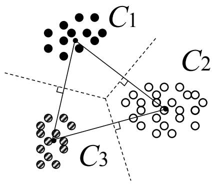
- Find the nearest neighbour

→ classify x to the same class

Discriminant function

- Need to remember all the samples?
  - In k-NN we simply used all the training data
  - Still cover only a small portion of possible patterns
- Define a class by a few representative patterns
  - e.g. the centroid of class distribution

Extreme case: one vector per class



Formulation: one prototype per class

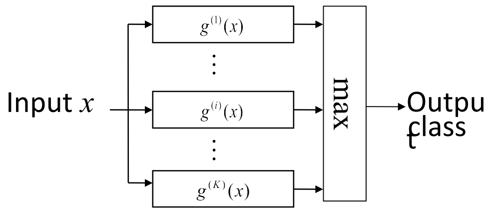
- K classes: $C^{(1)},\cdots,C^{(K)}$
- K prototypes: $a^{(1)},\cdots,a^{(K)}$

Consider Euclidean distances between the new input x and the prototypes: $\|x-a^{(i)}\|^2 = \|x\|^2 - 2a^{(i)^T}x + \|a^{(i)}\|^2$

→ Choose the class that minimises the distance.

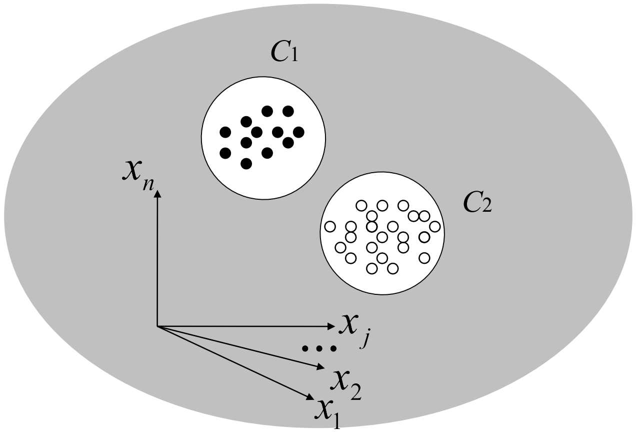
Discriminant function

$$g^{(i)}(x) \equiv a^{(i)^T}x - \frac{1}{2}\|a^{(i)}\|^2$$



Setting the “don’t know” category

- Reject if the distance is above the threshold



Direction cosine as similarity

Think of the new input and the prototype as vectors.
Compute cosine between the input vector x and vector $a^{(i)}$

$$g^{(i)}(x) = \frac{(x^T a^{(i)})}{\|x\|\,\|a^{(i)}\|} = \cos A$$

“Simple similarity”

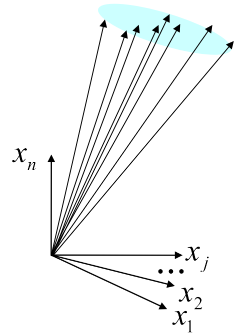
$0 \le \cos^2 A \le 1$ (The closer it is to 1, the more likely to be in $C^{(i)}$)

Now let’s extend the class representative to
a set of basis vectors → spans a subspace

Subspace Methods

- Exploit localization of pattern distributions

Samples in the same class such as a digit (or face images of a person) are similar to each other.
They are localized in a *subspace* spanned by a set of basis u_i .

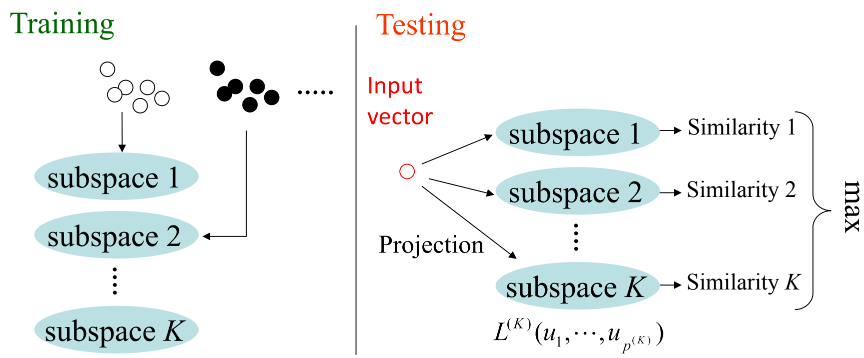


u_i : reference vectors (orthonormal basis)

a.k.a CLAFIC
CLAss-Featuring Information Compression

Framework of Subspace Method

1. Training: for each class, compute a low-dimensional subspace that represents the distribution in the class.
   $\omega^{(1)}, \cdots, \omega^{(K)}$
2. Testing: determine the class of new unknown input by comparing which subspace best approximates the input.



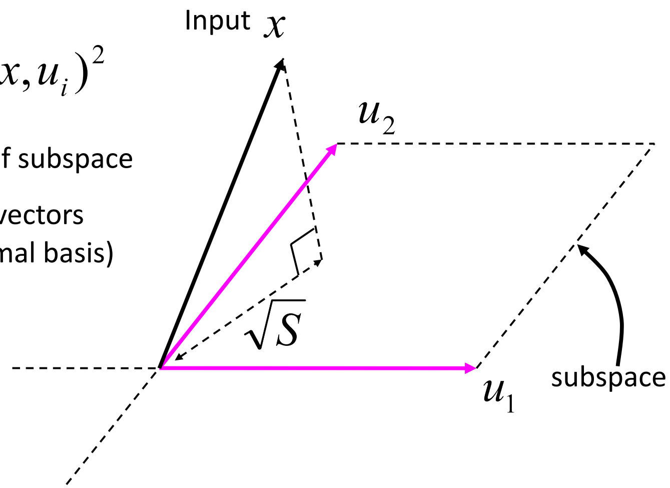
Similarity in Subspace Method

Projection length to the subspace

$$S = \sum_{i=0}^{p-1} (x, u_i)^2$$

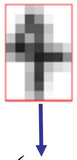
p: dimension of subspace

u_i : reference vectors (orthonormal basis)



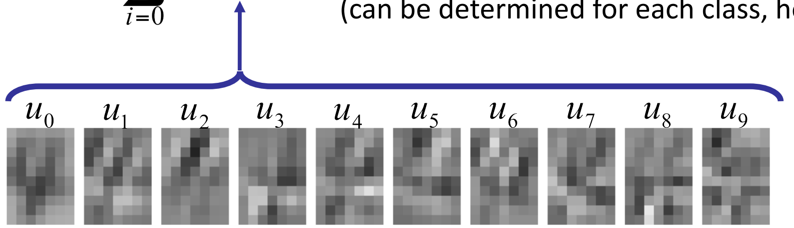
Similarity in Subspace Method (example)

Projection length to the subspace



$$S = \sum_{i=0}^{p-1} (x, u_i)^2$$

p: the dimensionality of class subspace (can be determined for each class, how?)



Dimensionality of a class subspace

Eigenvalues of autocorrelation matrix Q: $\lambda_1 \geq \ldots \lambda_j \ldots \geq \lambda_p \geq 0$

The number of dimensions to be used:

- Too low → low capability to represent the class
- Too high→ issue of overlapping across classes

• Cumulative contributions

$$a(p^{(i)}) = \frac{\sum_{j=1}^{P^{(i)}} \lambda_j}{\sum_{j=1}^{p} \lambda_j}$$

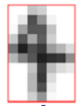
Choose a dimension $p^{(i)}$ for each class $\omega^{(i)}$

$a(p^{(i)}) \leq \kappa \leq a(p^{(i)}+1)$ (κ: common value)

The projection length to the subspace is made uniform.

Experiments still needed to find a good dimensionality

Similarity in weighted Subspace Method



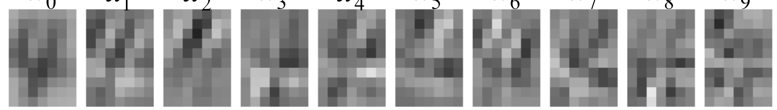
$$S = \sum_{i=0}^{p-1} \mu_i (x, u_i)^2$$

p: the dimension of subspace

weight: μ_i

$\mu_0 \quad \mu_1 \quad \mu_2 \quad \mu_3 \quad \mu_4 \quad \mu_5 \quad \mu_6 \quad \mu_7 \quad \mu_8 \quad \mu_9$

$u_0 \quad u_1 \quad u_2 \quad u_3 \quad u_4 \quad u_5 \quad u_6 \quad u_7 \quad u_8 \quad u_9$

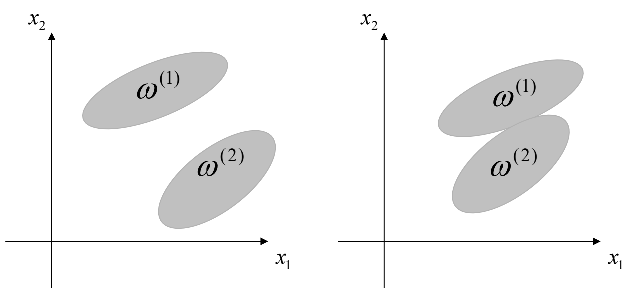


(figure credit: Y.

Useful dimension for classification?

Ideal distributions of input pattern vectors:

- Patterns from an identical class be close
- Patterns from different classes be apart



→ Overlapping distributions harmful for classification

Ratio of between-classes variance to within-class variance

Within-class variance

$$\sigma_W^2 = \frac{1}{r} \sum_{i=1}^{K} \sum_{x \in \omega^{(i)}} (x - E^{(i)}(x))^T (x - E^{(i)}(x))$$

Average in class $\omega^{(i)}$

Total # of samples

Between-class variance

$$\sigma_B^2 = \frac{1}{r} \sum_{i=1}^{K} r^{(i)} (E^{(i)}(x) - E(x))^T (E^{(i)}(x) - E(x))$$

Average overall

Number of samples in class $\omega^{(i)}$

Within-class var. between-class var. ratio

$$J_\sigma = \frac{\sigma_B^2}{\sigma_W^2}$$

Between-class variance / Within-class var in ave

In short: distance between classes normalized by distance within class

→ the larger the better!

Fisher's method

Find a subspace most suitable to classification
(discriminant analysis)

Given pattern distributions in 2 classes

$\Rightarrow$ Optimal axis direction where J is maximized

Scatter matrix represents variation within class

$$S_i \equiv \sum_{x\in\omega^{(i)}} (x - E^{(i)}(x))(x - E^{(i)}(x))^T$$

Within-class: $S_W \equiv S_1 + S_2$

Between-classes: $S_B \equiv \sum_{i=1,2} r^{(i)}(E^{(i)}(x) - E(x))(E^{(i)}(x) - E(x))^T$

$$\dots = \frac{r^{(1)}r^{(2)}}{r}(E^{(1)}(x) - E^{(2)}(x))(E^{(1)}(x) - E^{(2)}(x))^T$$

From n-d feature space to 1-d space by Matrix A

A is an n x 1 matrix → n-dim vector a in practice

→ The pattern will become a scalar by $y = A^T x$

Scatter matrix in the space after the transformation:

$$\hat{S}_i \equiv \sum_{x\in\omega^{(i)}} (y - E^{(i)}(y))(y - E^{(i)}(y))^T$$
$$= \sum_{y\in\omega^{(i)}} A^T (x - E^{(i)}(x))(x - E^{(i)}(x))^T A = A^T S_i A$$

Within-class: $\hat{S}_W \equiv \hat{S}_1 + \hat{S}_2 = A^T S_1 A + A^T S_2 A = A^T S_W A$

Between-class: $\hat{S}_B \equiv \sum_{i=1,2} r^{(i)}(E^{(i)}(y) - E(y))^2$

Scalar

$$\dots = \frac{r^{(1)}r^{(2)}}{r} A^T (E^{(1)}(x) - E^{(2)}(x))^2 A = A^T S_B A$$

Fisher's criterion:

$$J_S(A) \equiv \frac{\hat{S}_B}{\hat{S}_W} = \frac{A^T S_B A}{A^T S_W A}$$

Maximizing the ratio of between-classes variance to within-class variance

Lagrange multiplier

$$J(a) \equiv a^T S_B a - \lambda(a^T S_W a - I)$$ →Maximize

Condition: $\hat{S}_W = I$

$$S_B a = \lambda S_W a$$

$$\Leftrightarrow S_W^{-1} S_B a = \lambda a$$

$$\Leftrightarrow \max\{J_S(a)\} = \lambda_1$$

The greatest eigenvalue of $S_W^{-1} S_B$

→ The eigenvector for the greatest eigenvalue of $S_W^{-1} S_B$ gives A that maximises Fisher's criterion