Computational Data Analysis

Machine Learning

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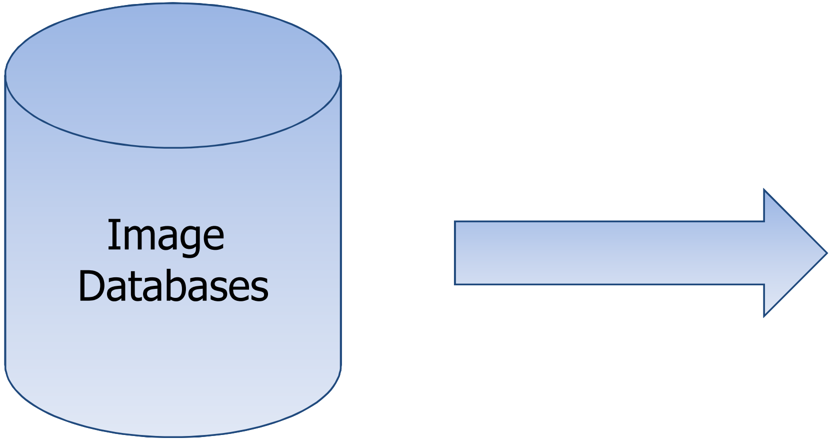
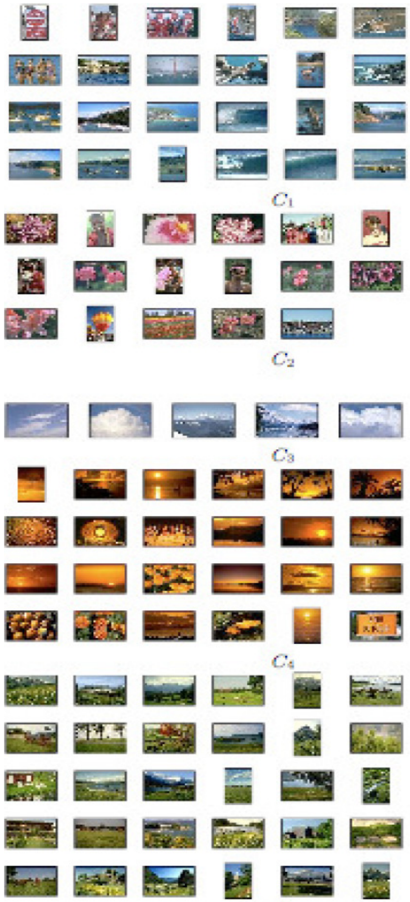
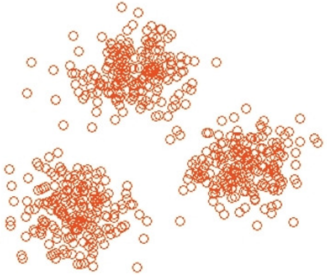
Dimensionality Reduction

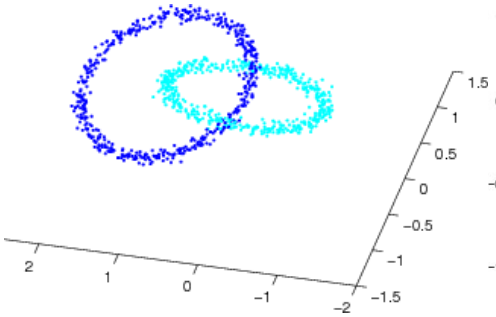
Principal Component Analysis

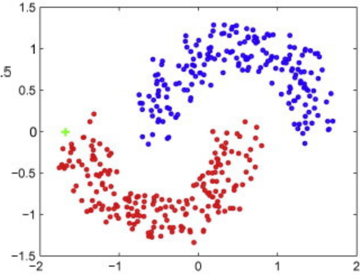




What are the relations between data points?

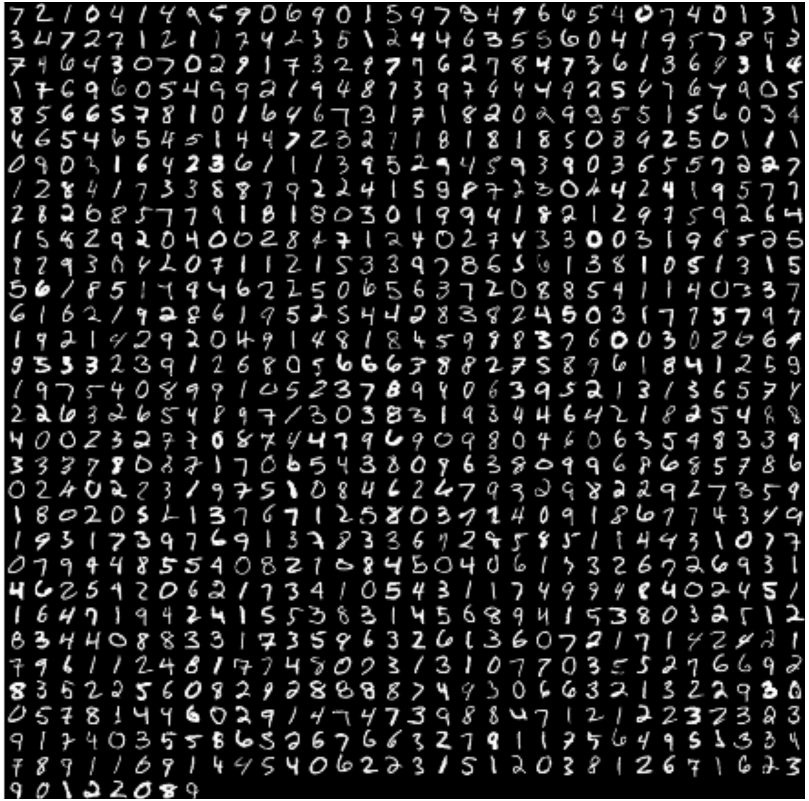


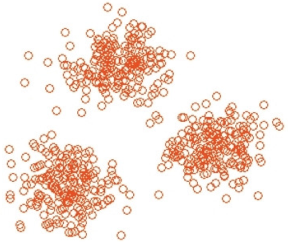


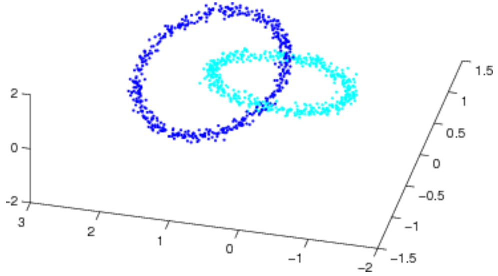


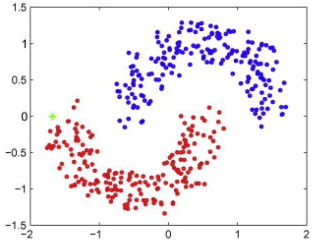
Handwritten digits

What are the relations between data points?





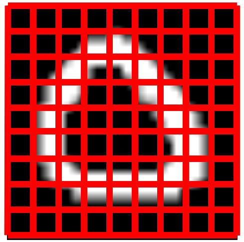




http://www.datawrangling.org/python-montage-code-for-displaying-arrays/

What is dimensionality reduction?

- The process of reducing the number of random variables under consideration
  - One can combine, transform or select variables
  - One can use linear or nonlinear operations



$$\begin{pmatrix}0\\0\\0\\1\\1\\1\\0\\0\\0\end{pmatrix}$$

vector in R^d

Original data point

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} \quad \xrightarrow{f(x): R^d \mapsto R^k} \quad z = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \end{pmatrix}$$

Reduced representation

$$k \ll d$$

Why dimensionality reduction and how to think

- The dimension-reduced data can be used for
  - Visualizing, exploring and understanding the data
  - Aggregating weak signals in the data
  - Cleaning the data
  - Speeding up subsequent learning task
  - Building simpler model later

- Key questions of a dimensionality reduction algorithm
  - What is the criterion for carrying out the reduction process?
  - What are the algorithm steps?

Principal component analysis

- Given m data points, $\{x^1, x^2, \dots x^m\} \in R^d$, with mean

- Step 1: Estimate the mean and covariance matrix from data

$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^i \quad and \quad C = \frac{1}{m}\sum_{i=1}^{m}(x^i - \mu)(x^i - \mu)^{\top}$$

"weights" to combine features: **Principal directions**

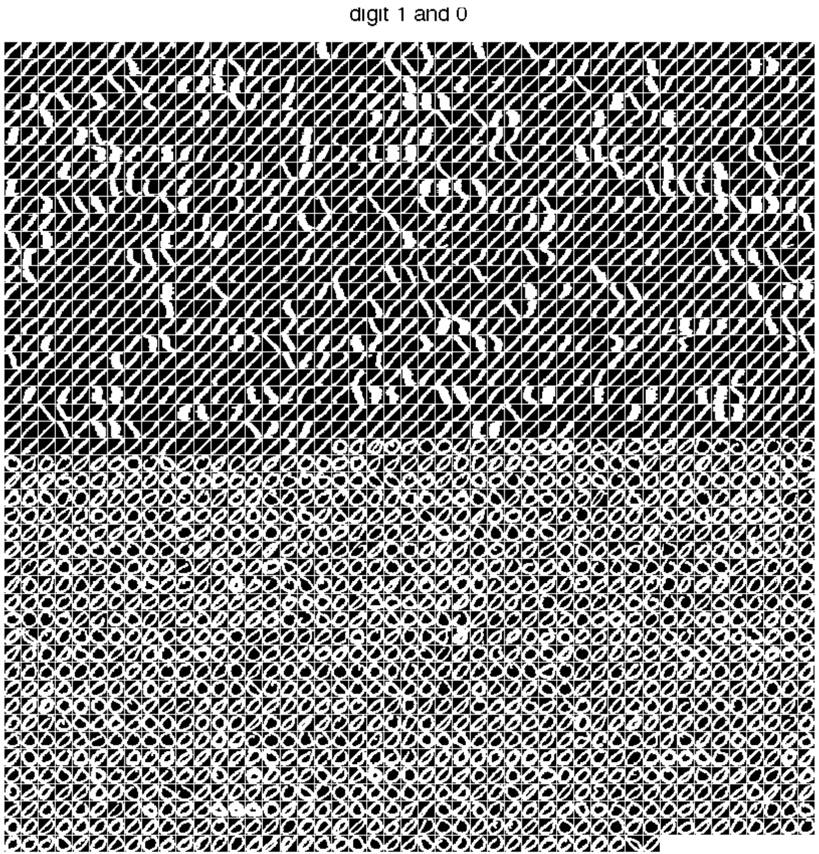
- Step 2: Take the eigenvectors $\boxed{w^1, w^2, \dots}$ of C corresponding to the largest eigenvalue λ_1, the second largest eigenvalue λ_2 …

- Step 3: Compute reduced representation (principle components)

$$z^i = \begin{pmatrix} {w^1}^{\top}(x^i - \mu)/\sqrt{\lambda_1} \\ {w^2}^{\top}(x^i - \mu)/\sqrt{\lambda_2} \\ \vdots \end{pmatrix}$$

Good youtube on calculating eigenvectors and eigenvalue
https://www.youtube.com/watch?v=cHOsd2PhkqE

Run demo PCA_digits.m



Run demo PCA_leaf.m

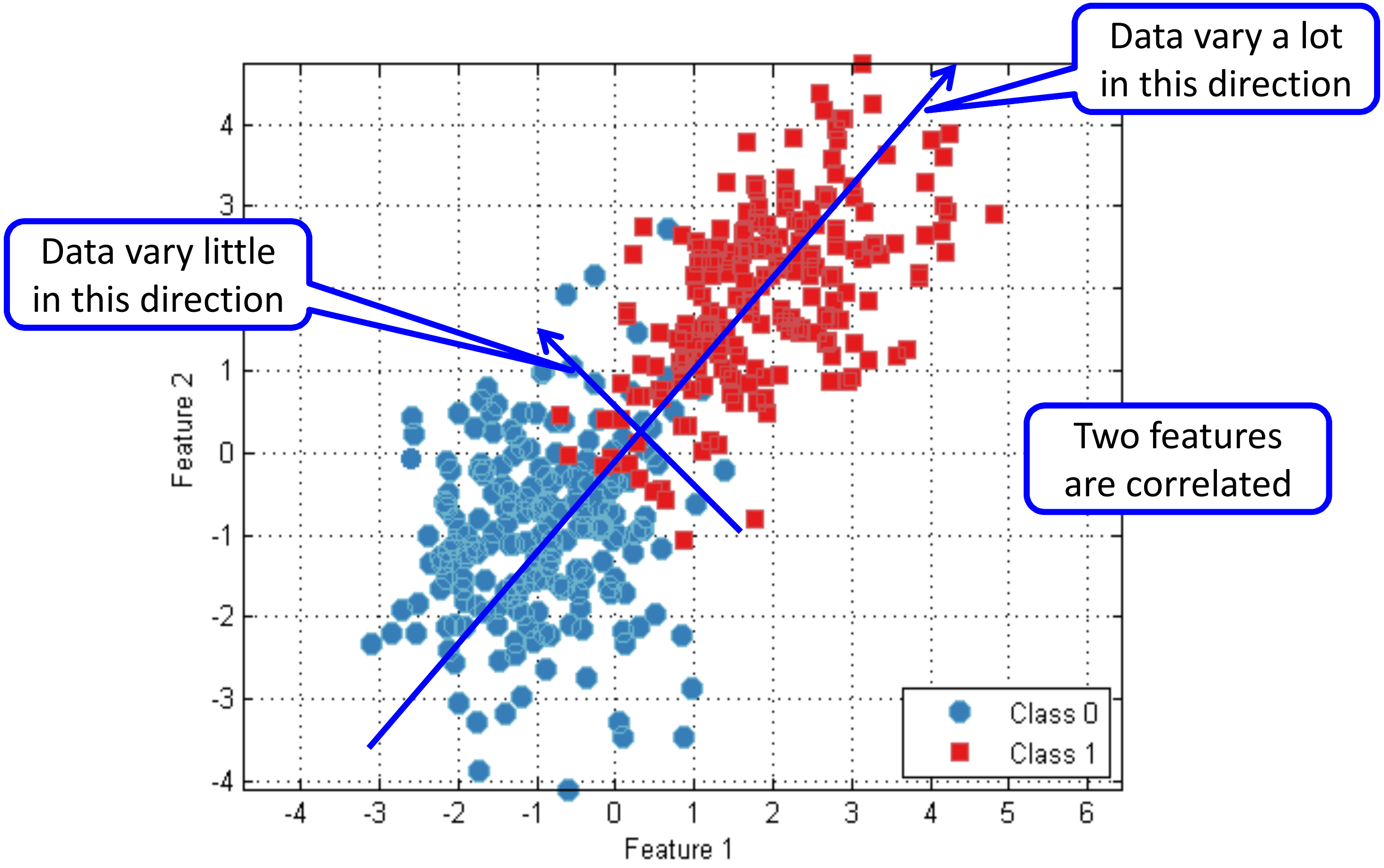
Use what criterion for reduction?

- There are many criteria (geometric based, information theory based, etc.)

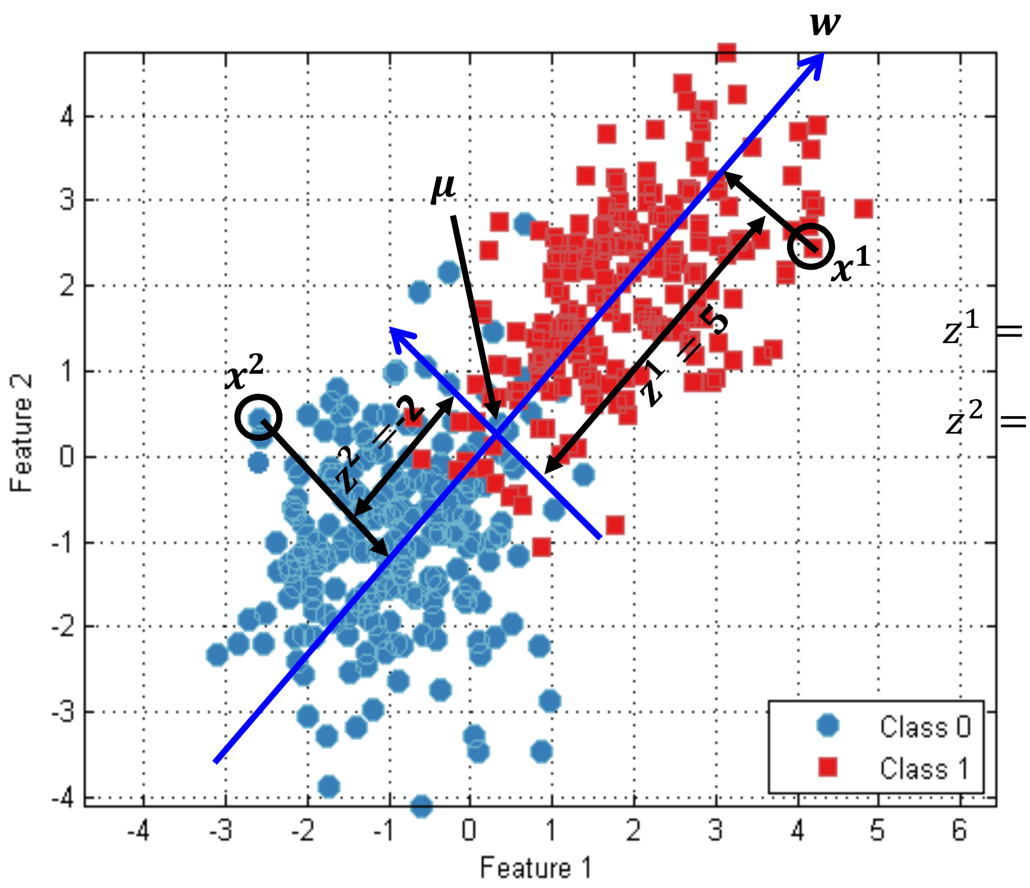
- One useful criterion: want to capture variation in data
  - variations are “signals” or information in the data
  - need to normalize each variables first

- In the process, also discover variables or dimensions highly correlated
  - represent highly related features
  - combine them to form a stronger signal
  - lead to simpler presentation

An example


Data vary a lot
in this direction
Data vary little
in this direction
Two features
are correlated
Feature 2
Feature 1
4
3
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4
5
6
Class 0
Class 1

Reduce to 1 dimension



$$z^1 = w^\top (x^1 - \mu)$$

$$z^2 = w^\top (x^2 - \mu)$$

How to formulate the problem

- Given m data points, $\{x^1, x^2, \dots x^m\} \in R^n$, with their mean $\mu = \frac{1}{m}\sum_{i=1}^{m} x^i$

- Find a direction $w \in R^n$ where $\|w\| \le 1$

- Such that the variance (or variation) of the data along direction w is maximized

$$\max_{w:\|w\|\le 1} \underbrace{\frac{1}{m}\sum_{i=1}^{m}\left(w^\top x^i - w^\top \mu\right)^2}_{\text{variance}}$$

Is it an easy optimization problem?

- Manipulate the objective with linear algebra

$$\frac{1}{m}\sum_{i=1}^{m}\left(w^{\top}x^{i}-w^{\top}\mu\right)^{2}$$

$$=\frac{1}{m}\sum_{i=1}^{m}(w^{\top}(x^{i}-\mu))^{2}$$

$$=\frac{1}{m}\sum_{i=1}^{m}w^{\top}\left(x^{i}-\mu\right)\left(x^{i}-\mu\right)^{\top}w$$

$$=w^{\top}\underbrace{\left(\frac{1}{m}\sum_{i=1}^{m}\left(x^{i}-\mu\right)\left(x^{i}-\mu\right)^{\top}\right)}_{\text{covariance matrix } C}w$$

Landscape of the optimization problem

- Suppose the data has two dimension ($n = 2$)

- C is a diagonal matrix

$$C = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

- The optimization problem becomes

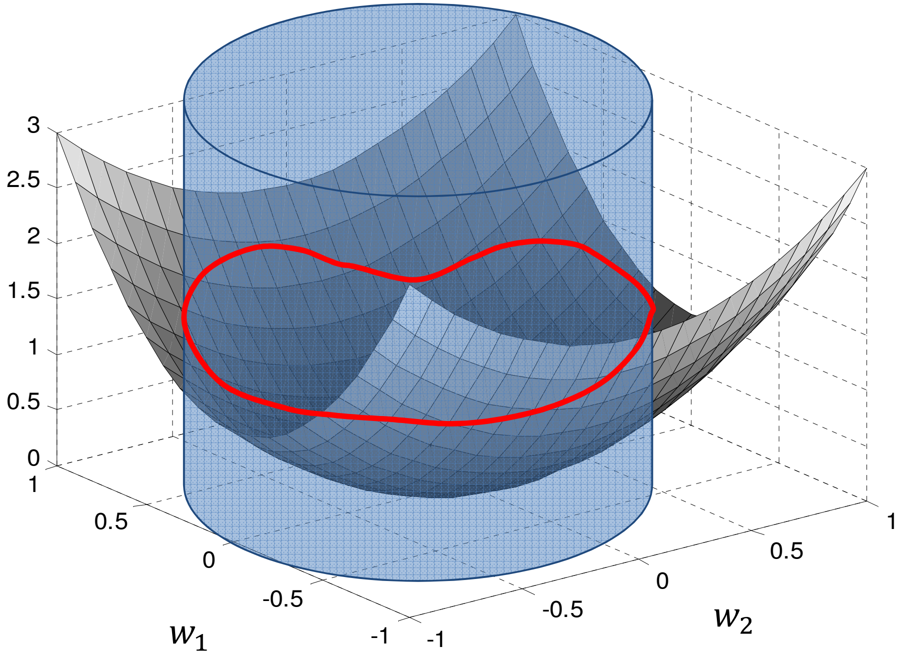
$$\max_{w:\|w\|\leq 1} w^\top C w$$

$$= \max_{w:\|w\|\leq 1} (w_1, w_2) \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$= \max_{w:\|w\|\leq 1} w_1^2 + 2w_2^2$$

Landscape of the optimization problem

- $f(w_1, w_2) = w_1^2 + 2w_2^2$



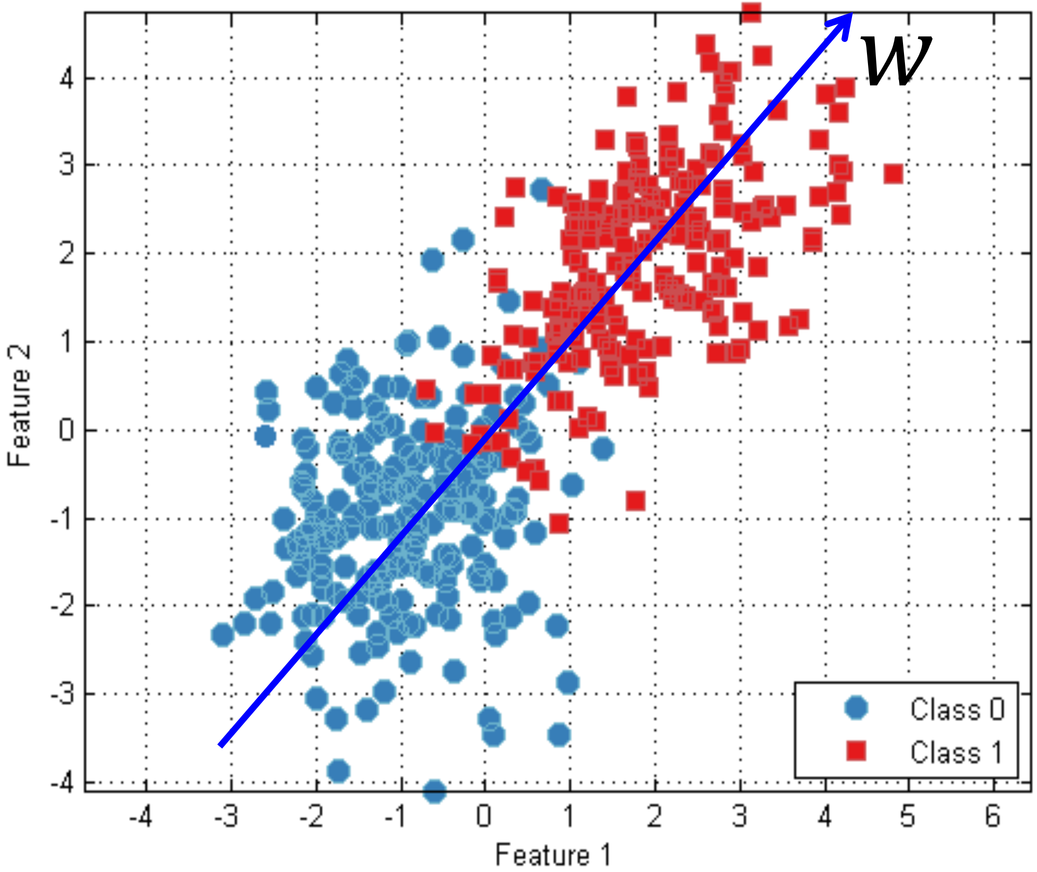
Eigen-value problem

- Eigen-value problem
  - Given a symmetric matrix $C \in R^{n \times n}$
  - Find a vector $w \in R^n$ and $\|w\| = 1$
  - Such that

$$Cw = \lambda w$$

- There will be multiple solution of $w^1, w^2, \ldots$ with different $\lambda_1, \lambda_2, \ldots$
  - They are ortho-normal: ${w^i}^\top w^i = 1, {w^i}^\top w^j = 0$

Principal direction of the data



Variance of in the principal direction

- Principal direction w satisfies

$$Cw = \lambda w$$

- Variance in principal direction is

$$w^\top C w$$

$$= \lambda w^\top w$$

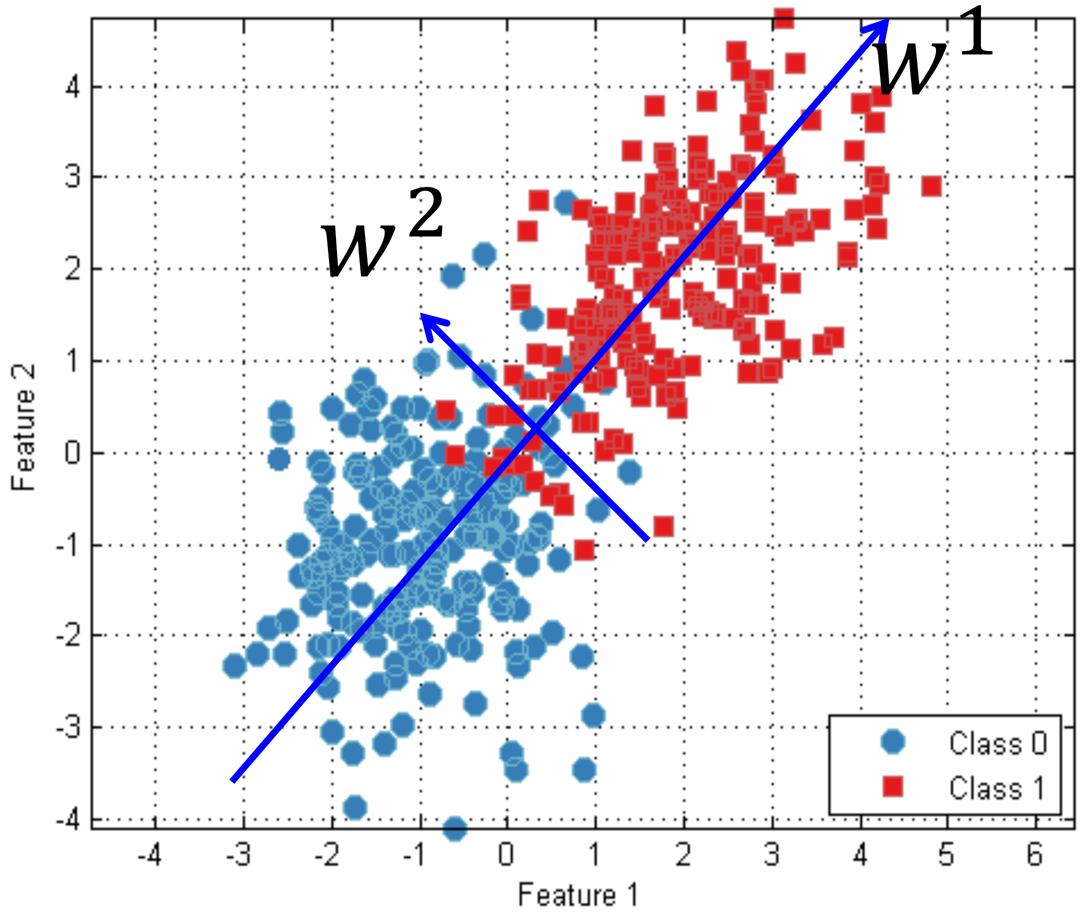
$$= \lambda$$

eigen-value

Find multiple principal directions

- Directions $w^1, w^2, \ldots$ which has
  - the largest variances
  - but are orthogonal to each other
- Take the eigenvectors $w^1, w^2, \ldots$ of C corresponding to
  - the largest eigenvalue λ_1,
  - the second largest eigenvalue λ_2
  - …

Principal direction of the data



Principal component analysis

- Given m data points, $\{x^1, x^2, \ldots x^m\} \in R^d$, with mean

- Step 1: Estimate the mean and covariance matrix from data

$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^i \quad and \quad C = \frac{1}{m}\sum_{i=1}^{m}(x^i - \mu)(x^i - \mu)^\top$$

Principal directions

- Step 2: Take the eigenvectors $w^1, w^2, \ldots$ of C corresponding to the largest eigenvalue λ_1, the second largest eigenvalue λ_2 …

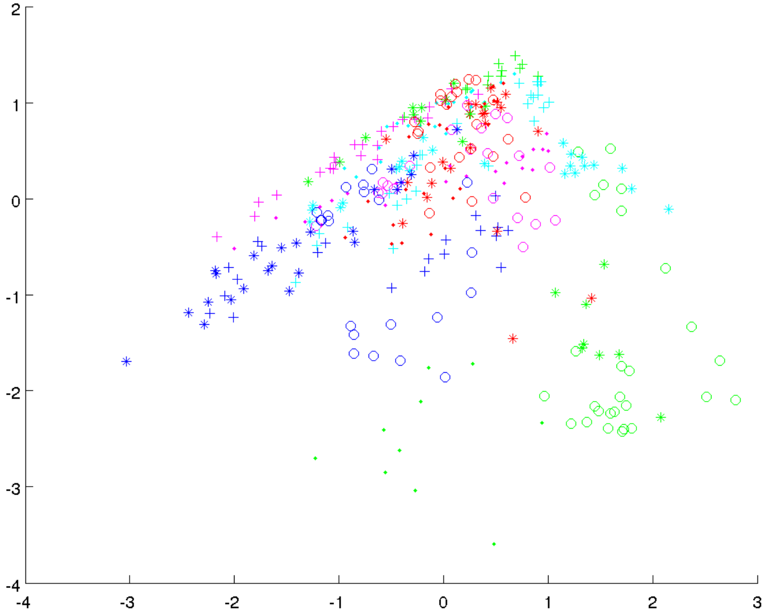
- Step 3: Compute reduced representation

$$z^i = \begin{pmatrix} {w^1}^\top (x^i - \mu)/\sqrt{\lambda_1} \\ {w^2}^\top (x^i - \mu)/\sqrt{\lambda_2} \\ \vdots \end{pmatrix}$$

Normalize by standard deviation

Look more into PCA_leaf.m

Interpreting the reduced representation



Principal direction:

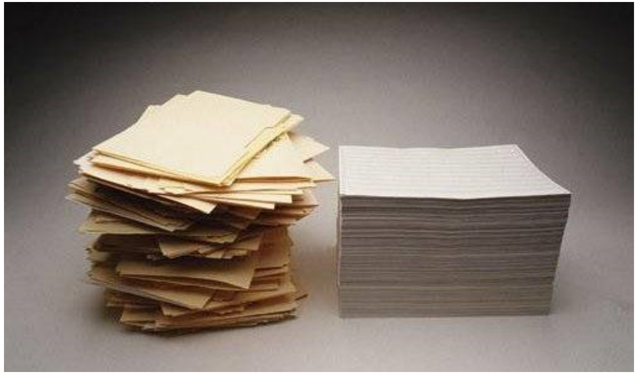
W =

0.0938	0.1924
0.1902	0.0253
0.2266	-0.1800
-0.1850	0.4084
-0.1600	0.3825
-0.2063	0.3488
0.1940	-0.4037
0.2150	-0.3566
-0.3723	-0.2001
-0.3657	-0.1974
-0.3602	-0.2037
-0.3175	-0.1886
-0.3056	-0.1243
-0.3482	-0.1829

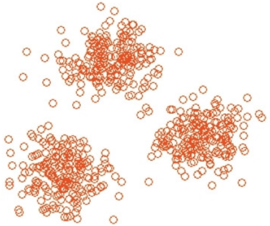
Shape features

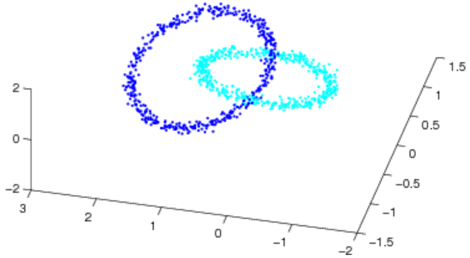
Texture features

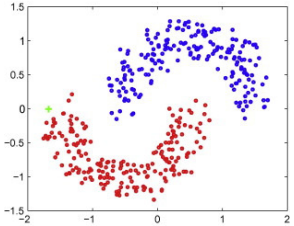
Documents collections



What are the relations between data points?

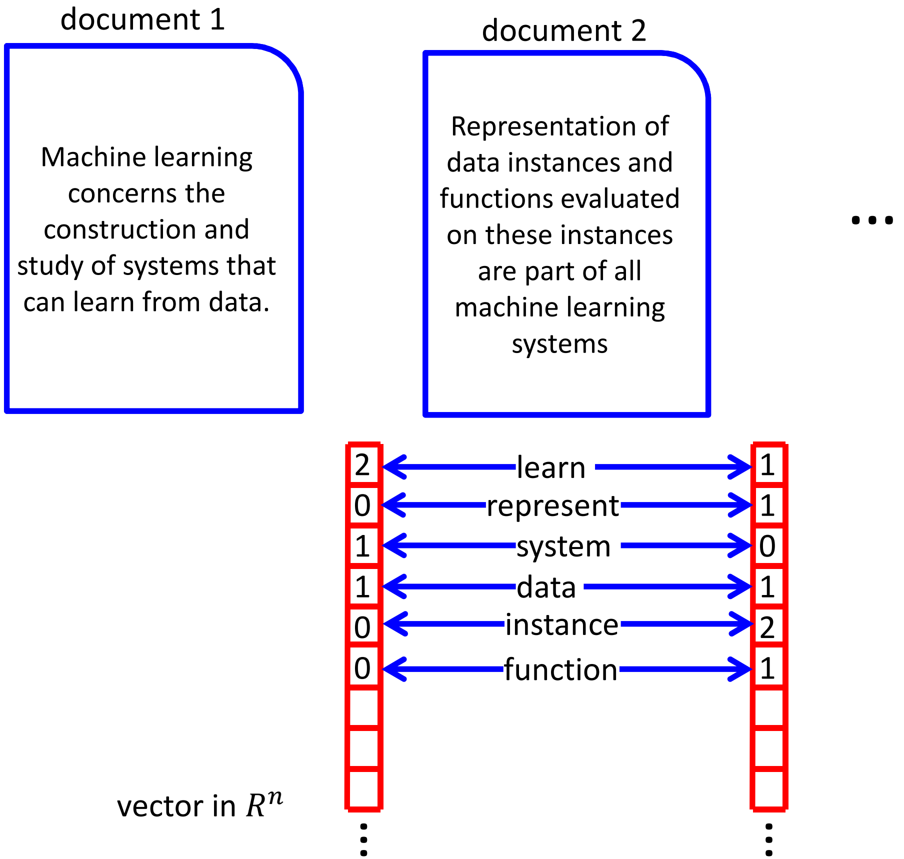






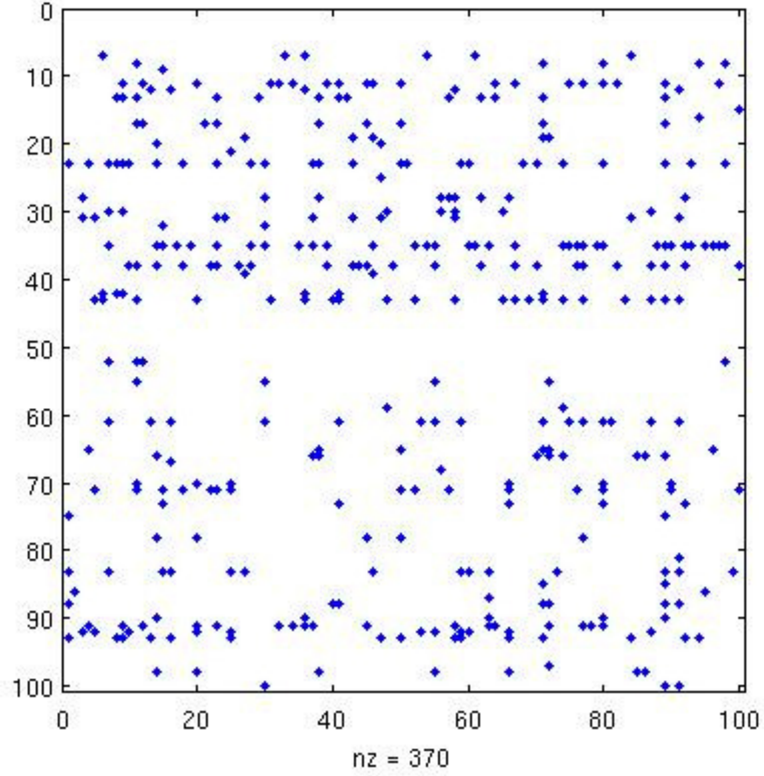
http://submitpapers.com/misc/docCollection.html

Bag of words representation



Experiments with 20 news groups

- Bag-of-words, or term-document matrix

$X =$ 

Singular Value Decomposition

- Singular value decomposition, known as SVD, is a factorization of a real matrix with applications in calculating pseudo-inverse, rank, solving linear equations, and many others.

- For a matrix $M \in \mathbb{R}^{m \times n}$ assume $n \leq m$
  - $M = U\Sigma V^\top$ where $U \in \mathbb{R}^{m \times m}$, $V^\top \in \mathbb{R}^{n \times n}$, $\Sigma \in \mathbb{R}^{m \times n}$

  - The m columns of U, and the n columns of V are called the left and right singular vectors of M. The diagonal elements of Σ, Σ_{ii} are known as the singular values of M.

  - Let v be the i^{th} column of V, and u be the i^{th} column of U, and σ be the i^{th} diagonal element of Σ

$$Mv = \sigma u \quad \text{and} \quad M^\top u = \sigma v$$

Singular Value Decomposition - II

- $M = [u_1 \quad u_2 \; \ldots \quad u_n] \begin{bmatrix} \Sigma_{11} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \Sigma_{mn} \end{bmatrix} [v_1 \quad v_2 \ldots \quad v_n]^\top$

  principal directions

  Scaling factor

  Projection in principal directions

- Singular value decomposition is related to eigenvalue decomposition
  - Suppose $M = [x_1 - \mu \quad x_2 - \mu \ldots \quad x_m - \mu] \in \mathbb{R}^{m \times n}$
  - Then covariance matrix is $C = \frac{1}{m} M M^\top$
  - Starting from singular vector pair
    - $M^\top u = \sigma v$
    - $\Rightarrow M M^\top u = \sigma M v$
    - $\Rightarrow M M^\top u = \sigma^2 u$
    - $\Rightarrow C u = \lambda u$


SUMMARY