Closing Session

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Understand your data

- Univariate data analysis
- Gaussian Distribution
- Relative Probability
- Bivariate data statistics
- Correlation (Pearson correlation)
- Spearman Rank (correlation)

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Symbolical Machine learning

- Decision Trees
  - ID3, greedy search with heuristic (*algorithm*)
  - Heuristic function: **Shannon Entropy**
    - What dies the formula indicate? How close the distribution is to uniform distribution

$$H = -\sum_{t}^{K} p(x_t) \cdot \log_2 p(x_t) = -\sum_{x \in X} p(x) \cdot \log_2 p(x).$$

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Model Evaluation

- Confusion Matrix for binary Classifier

true/actual/target

predicted		P	N	
	P	True Positives (TP)	False Positives (FP)	TP+FP
	N	False Negatives (FN)	True Negatives (TN)	FN+TN
		P=TP+FN	N=FP+TN	All=P+N

Recall/sensitivity
% of positive observations predicted as positive

$$Recall = \frac{TP}{P} = \frac{TP}{TP+FN}$$

Precision
% of positive observations among the observations predicted as positive

$$Precision = \frac{TP}{TP + FP}$$

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Balanced Measure

- Precision and Recall have to be simultaneously interpreted.
- We can combine both values with the *harmonic mean*

$$F = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$$

- Both values are evenly weighted.
- This measure is also called the balanced measure.

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Bayes' Rule

$$p(h_k|D) = \frac{p(D|h_k) \cdot p(h_k)}{p(D)} = \frac{p(D, h_k)}{p(D)}$$

- *$p(h_k)$ is called the* ***prior*** *(before)*
  - *For example, what is the probability of some illness in Portugal*
- *$p(D|h_k)$ is called* ***likelihood*** *and can can be easily estimated*
  - *For example, what is the probability that some illness generates some symptoms?*
  - *$p(D,h_k)$ is called* ***joint distribution***
- *$p(h_k|D)$ is called* ***posterior probability***

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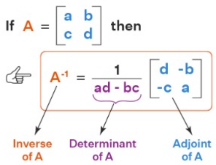
Bayesian optimal classifier: Multivariate Gaussian

Approximate a multivariate Gaussian distribution using the following points: $\{(-2,2)^T, (-1,3)^T, (0,1)^T, (-2,1)^T\}$

- $\mu = \frac{1}{4}\left(\begin{bmatrix}-2\\2\end{bmatrix} + \begin{bmatrix}-1\\3\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix} + \begin{bmatrix}-2\\1\end{bmatrix}\right) = \begin{bmatrix}-1.25\\1.75\end{bmatrix}$
- $c_{12} = c_{21} = \frac{(-2+1.25)(2-1.75)+(-1+1.25)(3-1.75)+(0+1.25)(1-175)+(-2+1.25)(1-1.75)}{3} = -0.83$
- $c_{11} = \frac{(-2+1.25)^2+(-1+1.25)^2+(0+1.25)^2+(-2+1.25)^2}{3} = 0.92$
- $c_{22} = \frac{(2-1.75)^2+(3-1.75)^2+(1-175)^2+(1-1.75)^2}{3} = 0.92$
- $\Sigma = \begin{pmatrix}c_{11} & c_{21}\\ c_{12} & c_{22}\end{pmatrix} = \begin{pmatrix}0.92 & -0.083\\ -0.083 & 0.92\end{pmatrix}$.
- $\Sigma^{-1} = \begin{pmatrix}1.1 & 0.1\\ 0.1 & 1.1\end{pmatrix}$. Det(Σ)=| Σ|=0.833Type equation here.



$$N(\mathbf{x}|\boldsymbol{\mu},\Sigma) = \frac{1}{(2\pi)^{2/2}\sqrt{0.083}} exp\left(-\frac{1}{2}\left(\begin{bmatrix}x_1\\x_2\end{bmatrix} - \begin{bmatrix}-1.25\\1.75\end{bmatrix}\right)^T \begin{bmatrix}1.1 & 0.1\\0.1 & 1.1\end{bmatrix}\left(\begin{bmatrix}x_1\\x_2\end{bmatrix} - \begin{bmatrix}-1.25\\1.75\end{bmatrix}\right)\right)$$

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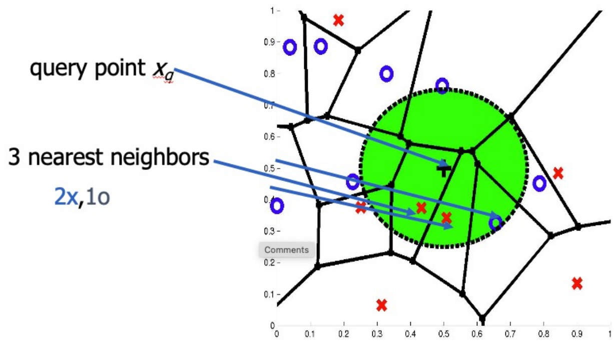
K Nearest Neighbour

- The cost of the learning process is *0*, all the cost is in the computation of the prediction
- This kind learning is also known as *lazy learning*

3-Nearest Neighbors



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Error Functions

- **Error Mnimization**

$$E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{\eta=1}^{N} (t_\eta - y(\mathbf{x}_\eta, \mathbf{w}))^2 = \frac{1}{2} \cdot \|\mathbf{t} - \mathbf{y}\|^2$$

$$E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{\eta=1}^{N} \left(t_\eta - \mathbf{w}^T \cdot \mathbf{x}_\eta)\right)^2 = \frac{1}{2} \cdot \sum_{\eta=1}^{N} \left(t_\eta - \mathbf{x}_\eta^T \cdot \mathbf{w})\right)^2$$

$$E(\mathbf{w}) = \frac{1}{2} \cdot \|\mathbf{t} - X \cdot \mathbf{w}\|^2 = \frac{1}{2} \cdot (\mathbf{t} - X \cdot \mathbf{w})^T (\mathbf{t} - X \cdot \mathbf{w})$$

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Least-Squares Estimation

We set the gradient of $E(\mathbf{w})$ to zero with the gradient operator

$$\nabla = \left[\frac{\partial}{\partial w_1}, \frac{\partial}{\partial w_2}, \cdots, \frac{\partial}{\partial w_D}\right]^T$$

$$\nabla E(\mathbf{w}) = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \cdots, \frac{\partial E}{\partial w_D}\right]^T$$

$$\nabla E(\mathbf{w}) = \nabla \left(\frac{1}{2} \cdot (\mathbf{t} - X \cdot \mathbf{w})^T \cdot (\mathbf{t} - X \cdot \mathbf{w})\right) = 0$$

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With

$$\Phi_{\eta,j} = \phi_j(\mathbf{x}_\eta)$$

- Dimensions change since the dimension are not determined by the dimension of the vector **x** which is D
- The number of the is M-1

$$\begin{pmatrix} y_1 \\ \vdots \\ y_\eta \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} 1 & \phi_{1,1} & \phi_{1,2} & \cdots & \phi_{1,M-1} \\ 1 & \phi_{2,1} & \phi_{2,2} & \cdots & \phi_{2,M-1} \\ \vdots & \vdots & \ddots & \vdots & \\ 1 & \phi_{N,1} & \phi_{N,2} & \cdots & \phi_{N,M-1} \end{pmatrix} \cdot \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_j \\ \vdots \\ w_{M-1} \end{pmatrix}$$

with $\Phi^\dagger$ is Moore-Penrose or the pseudo-inverse of Φ as before with

$$\Phi^\dagger = \left(\Phi^T \cdot \Phi\right)^{-1} \cdot \Phi^T$$

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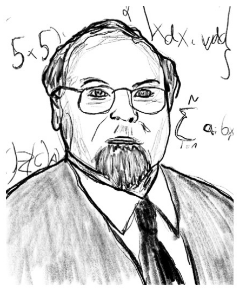
Quadratic Function

- Now we can define the quadratic function, minimising it is equivalent to maximising $\mathbf{w}_{MAP}(N)$

$$E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{\eta=1}^{N} (t_\eta - \mathbf{w}^T \cdot \mathbf{x}_\eta)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$



- We set the gradient of $E(\mathbf{w})$ to zero with the gradient operator

$$\nabla E(\mathbf{w}) = \nabla \left(\frac{1}{2} \cdot (\mathbf{t} - X \cdot \mathbf{w})^T \cdot (\mathbf{t} - X \cdot \mathbf{w}) + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w} \right) = 0$$

$$-2 \cdot X^T \cdot \mathbf{t} + 2 \cdot X^T \cdot X \cdot \mathbf{w} + 2 \cdot \lambda \cdot \mathbf{w} = 0$$

$$-X^T \cdot \mathbf{t} + X^T \cdot X \cdot \mathbf{w} + \lambda \cdot \mathbf{w} = 0$$

$$X^T \cdot \mathbf{t} = \left(X^T \cdot X + \lambda \cdot I \right) \cdot \mathbf{w}$$

$$\left(X^T \cdot X + \lambda \cdot I \right)^{-1} \cdot X^T \cdot \mathbf{t} = \mathbf{w}$$

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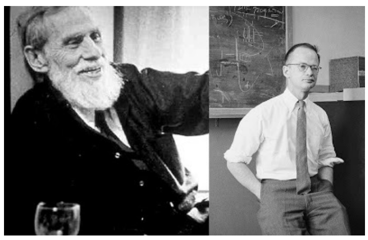
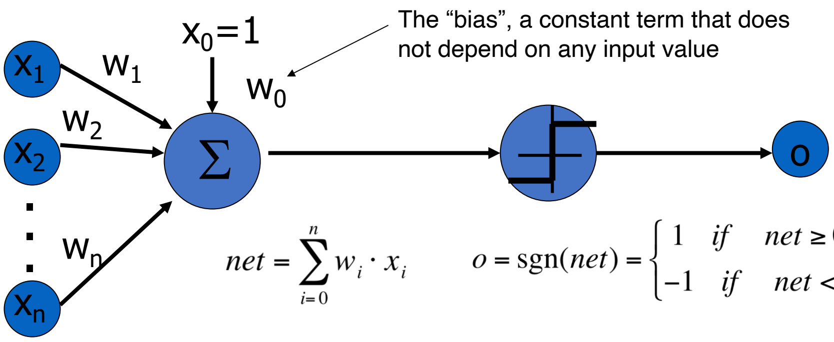
Perceptron (1957)



- Linear threshold unit (LTU)



$$net = \sum_{i=0}^{n} w_i \cdot x_i$$

$$o = \mathrm{sgn}(net) = \begin{cases} 1 & if \quad net \geq 0 \\ -1 & if \quad net < 0 \end{cases}$$

McCulloch-Pitts model of a neuron (1943)

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In this example a linearly separable training set is described by four vectors

$$\mathbf{x}_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \mathbf{x}_2 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \mathbf{x}_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \mathbf{x}_4 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and the corresponding targets

$$t_1 = -1, t_2 = 1, t_3 = 1, t_4 = -1.$$

The weights are initialized to 1 and the learning rate η for simplicity is set to 1 as well

$$w_0 = 1, w_1 = 1, w_2 = 1, \quad \eta = 1$$

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$$o_1 = sgn(1 \cdot 0 + 1 \cdot 0 + 1) = sgn(1) = 1; \quad \delta_1 = -2; \quad \mathbf{w} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix},$$

$$o_2 = sgn(1 \cdot 0 + 1 \cdot 2 - 1) = sgn(1) = 1; \quad \delta_2 = 0; \quad \mathbf{w} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix},$$

$$o_3 = sgn(1 \cdot 1 + 1 \cdot 1 - 1) = sgn(1) = 1; \quad \delta_3 = 0; \quad \mathbf{w} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix},$$

$$o_4 = sgn(1 \cdot 1 + 1 \cdot (-1) - 1) = sgn(-1) = -1; \quad \delta_4 = 0; \quad \mathbf{w} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}$$

For additional epochs, the weights do not change

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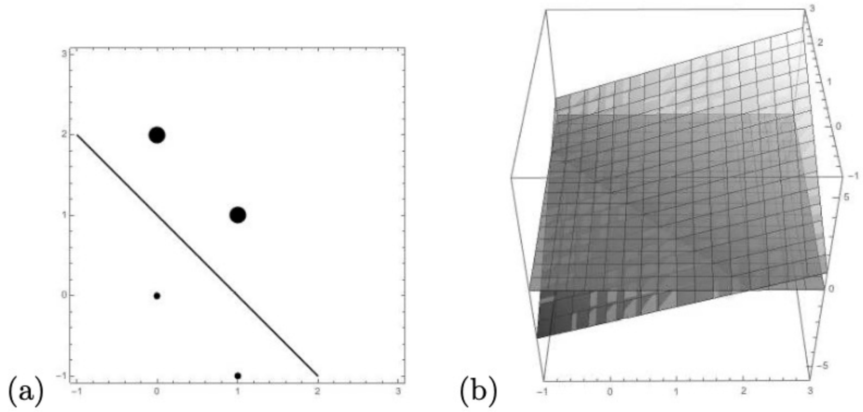

(a) The two classes 1 (indicated by a big point) and −1 (indicated a small point) are separated by the line $-1+x_1+x_2 = 0$. (b) The hyperplane $-1+x_1+x_2 = y$ defines the line for y = 0.

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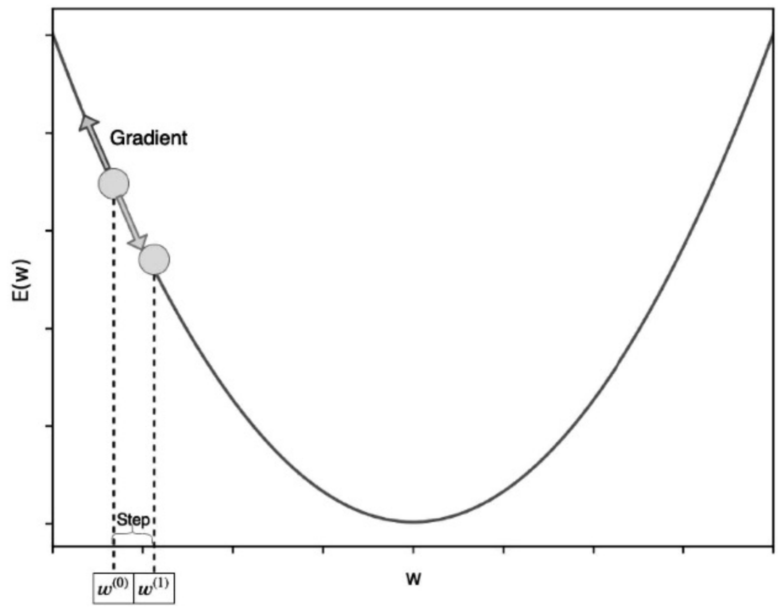

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Continuous activation functions - Squared Error

For continuous activation function $\phi()$

$$o_k = \phi\left(\sum_{j=0}^{D} w_j \cdot x_{k,j}\right).$$

we can define as well the update rule for gradient decent with the differential

$$\frac{\partial E}{\partial w_j} = \sum_{k=1}^{N}(t_k - o_k) \cdot \frac{\partial}{\partial w_j}\left(t_k - \phi\left(\sum_{j=0}^{D} w_j \cdot x_{k,j}\right)\right)$$

$$\frac{\partial E}{\partial w_j} = \sum_{k=1}^{N}(t_k - o_k) \cdot \left(-\phi'\left(\sum_{j=0}^{D} w_j \cdot x_{k,j}\right) \cdot x_{k,j}\right)$$

$$\frac{\partial E}{\partial w_j} = -\sum_{k=1}^{N}(t_k - o_k) \cdot \phi'\left(\sum_{j=0}^{D} w_j \cdot x_{k,j}\right) \cdot x_{k,j}.$$

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- The **softmax function** is used in various multi class classification methods, such as multinomial logistic regression (also known as softmax regression) with the prediction

$$\sigma(net_{ks}) = \frac{\exp(net_{ks})}{\sum_{t=1}^{K} \exp(net_{kt})}$$

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Logistic Regression Algorithm

Given a training set (sample)

$$Data = \{(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2), \cdots, (\mathbf{x}_k, \mathbf{y}_k), \cdots, (\mathbf{x}_N, \mathbf{y}_N)\}$$

with $\mathbf{y}_k$ represented as vectors of dimension K. During the training each neuron is trained individually withs its target value y_{kt}

$$y_{kt} \in \{0, 1\}, \quad \sum_{t=1}^{K} y_{kt} = 1$$

the goal of the algorithm is to correctly classify the test set (population) into K classes $C_1 = 100\cdots$, $C_2 = 010\cdots$, $C_3 = 001\cdots$, $\cdots$

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Sigmoid Unit versus Logistic Regression

Sigmoid Unit is with target, should be positive (between zero and one):

$$\Delta w_j = \eta \cdot \alpha \cdot \sum_{k=1}^{N} (t_k - o_k) \; \sigma(net_{k,j}) \cdot (1 - \sigma(net_{k,j})) \; x_{k,j}$$

Logistic Regression is with target $t_k \in \{0, 1\}$

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

If we assume $\alpha = 1$ then the difference between sigmoid unit and the logistic regression that was derived by maximising the negative logarithm of the likelihood is

$$\sigma(net_{k,j}) \cdot (1 - \sigma(net_{k,j})) \geq 0$$

the step size in the direction of gradient. Does it mean that Sigmoid Unit converge faster?

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Linear Unit versus Logistic Regression

Target can be any value and can be solved by closed-form solution, by pseudo inverse

$$o_k = \sum_{j=0}^{D} w_j \cdot x_{k,j}$$

Target $t_k \in \{0,1\}$ cannot be solved by closed-form solution

$$o_k = \frac{1}{1 + e^{(-\alpha \cdot (\sum_{j=0}^{N} w_j \cdot x_{k,j}))}}$$

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

Logistic Regression as well as the sigmoid unit gives a better decision boundary.

For Sigmoid (Logistic) distant points from the decision boundary have the same impact

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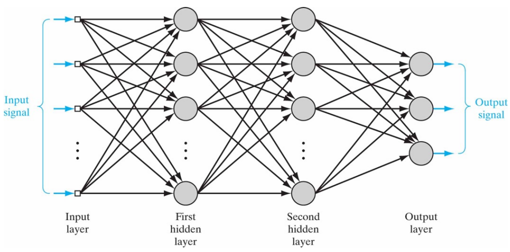
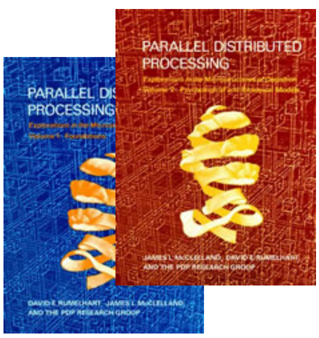
Back-propagation (1980)

- Back-propagation is a learning algorithm for multi-layer neural networks



Parallel Distributed Processing - Vol. 1
Foundations
David E. Rumelhart, James L. McClelland and the PDP Research Group

What makes people smarter than computers? These volumes by a pioneering neurocomputing.....



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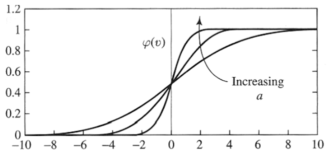
- We have to use a nonlinear differentiable activation function in **hidden units**
  - Examples:



$$f(x) = \sigma(x) = \frac{1}{1 + e^{(-\alpha \cdot x)}}$$

$$f^{'}(x) = \sigma^{'}(x) = \alpha \cdot \sigma(x) \cdot (1 - \sigma(x))$$

$$f(x) = \tanh(\alpha \cdot x)$$

$$f^{'}(x) = \alpha \cdot (1 - f(x)^2)$$

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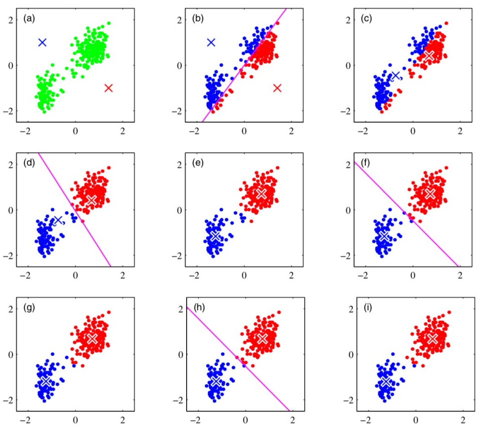
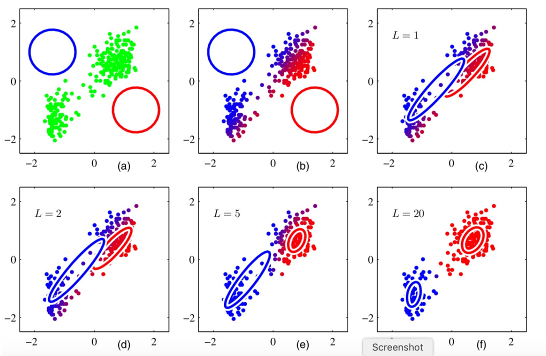
Clustering

- K-Means



EM: Expectation Maximization algorithm
(Bayes in E step)



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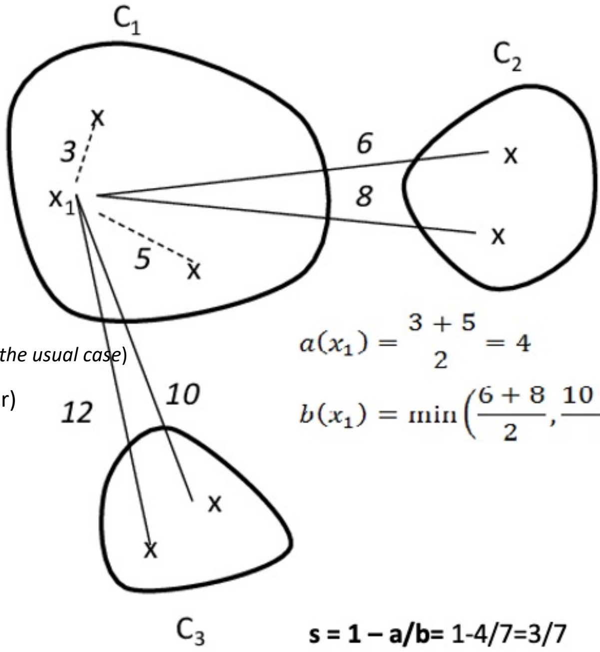
Validity index Silhouette



s = 1 – a/b if a < b, (*or s = b/a - 1 if a ≥ b, not the usual case*)

between -1 and 1 (the closer to 1 the better)

$$a(x_1) = \frac{3+5}{2} = 4$$

$$b(x_1) = \min\left(\frac{6+8}{2}, \frac{10+12}{2}\right) = 7$$

s = 1 – a/b= 1-4/7=3/7

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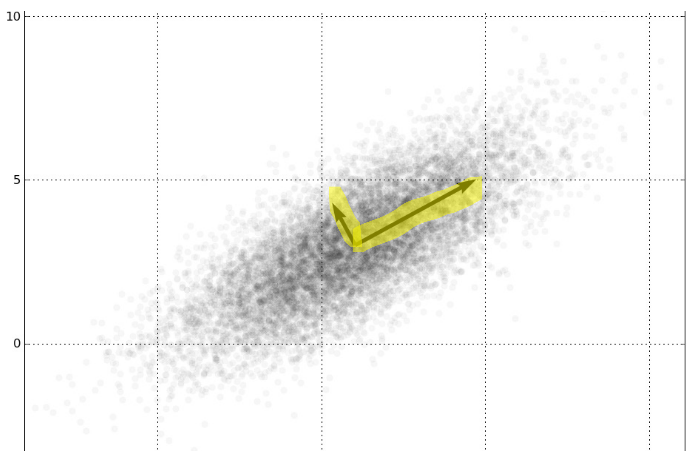
PCA



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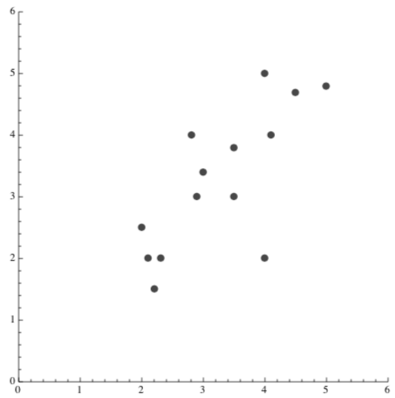
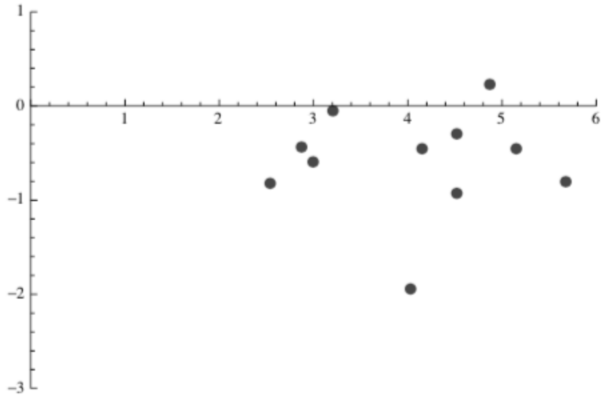
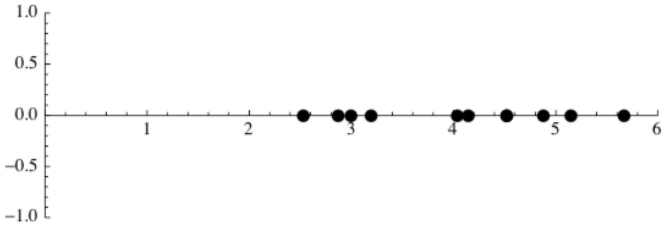




$$\mathbf{y} = U^\top \cdot \mathbf{x} = \begin{pmatrix} 0.611454 & 0.79128 \\ -0.79128 & 0.611454 \end{pmatrix} \cdot \mathbf{x},$$



$$\mathbf{z} = W^\top \cdot \mathbf{x} = \begin{pmatrix} 0.611454 & 0.79128 \end{pmatrix} \cdot \mathbf{x}$$

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Preparation:

- Practical Lectures
- Home works
- Prepare a **“cheat sheet”**

- Open Book Exam, Calculator
  - Careful: **Organize your knowledge**, you will have **no time** for search
- No ebook Reader, Computer, Smartphone, Smartwatch etc..

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