Selected Topics of Pervasive Computing

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Overview and Structure

Intro

30.10.2013	Organisational
30.10.3013	Introduction
06.11.2013	Classification methods (Basic recognition, Bayesian, Non-parametric)
13.11.2013	Classification methods (Linear discriminant, Neural networks)
20.11.2013	_
27.11.2013	_
04.12.2013	_
11.12.2013	Classification methods (Sequential, Stochastic)
18.12.2013	Activity Recognition (Basics, Applications, Algorithms, Metrics)
08.01.2014	Security from noisy data (Basics, Entity, F. Commitment, F. Extractors)
15.01.2014	Security from noisy data (Error correcting codes, PUFs, Applications)
22.01.2014	Context prediction (Algorithms, Applications)
29.01.2014	Networked Objects (Sensors and sensor networks, body area networks)
05.02.2014	Internet of Things (Sensors and Technology, vision and risks)

Outline

Intro

Recognition of patterns

Bayesian decision theory

Non-parametric techniques

Linear discriminant functions

Neural networks

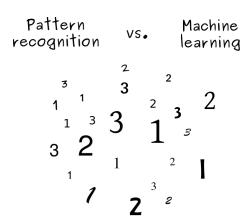
Sequential data

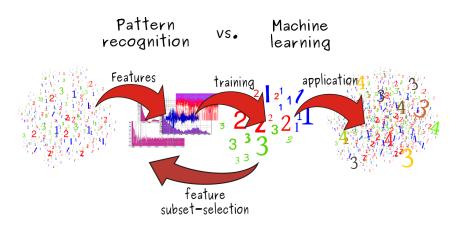
Stochastic methods

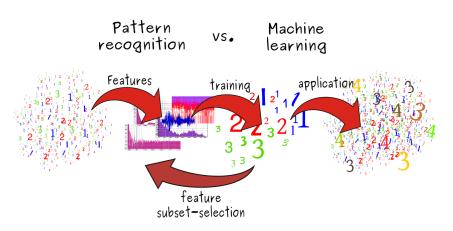
Pattern recognition

Machine VS. learning

Bayesian







- Mapping of features onto classes by using prior knowledge
- What are characteristic features?
- Which approaches are suitable to obtain these features?



Data sampling

- Record <u>sufficient</u> training data
 - Annotated! (Ground-truth)
 - Multiple subjects
 - Various environmental conditions (time of day, weather, ...)



Data sampling

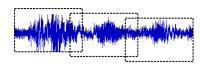
- Record <u>sufficient</u> training data
 - Annotated! (Ground-truth)
 - Multiple subjects
 - Various environmental conditions (time of day, weather, ...)

Example

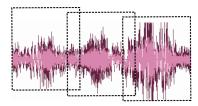
- Electric supply data over 15 years covers 5000 days but only 15 christmas days
- Especially critical events like accidents (e.g. plane, car, earthquake) are scarce



Feature subset-selection



- Pre-process data
 - Framing
 - Normalisation



Feature subset-selection

Intro

Domain knowledge?

-> better set of ad-hoc features

Features commensurate?

-> normalise

Pruning of input required?

 if no, create disjunctive features or weithted sums of features

Independent features?

-> construct conjunctive features or products of features

Is the data noisy?

-> detect outlier examples

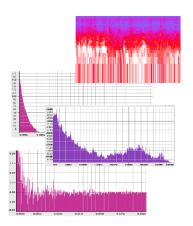
Do you know what to do first?

-> If not, use a linear predictor

- Pre-process data
 - Framing
 - Normalisation

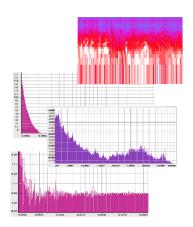
Feature extraction

- Identify meaningful features
 - remove irrelevant/redundant features



Feature extraction

- Identify meaningful features
 - remove irrelevant/redundant features
- Features can be contradictory!



Feature subset-selection

Simple ranking of features with correlation coefficients

Example: Pearson Correlation Coefficient

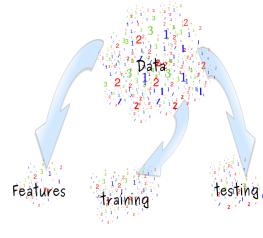
$$\varrho(X,Y) = \frac{\operatorname{Cov}(X,Y)}{\sqrt{\operatorname{Var}(X)\operatorname{Var}(Y)}} \tag{1}$$

• Identifies linear relation between input variables x_i and an output y

Feature subset-selection

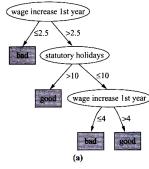
How to do reasonable feature selection

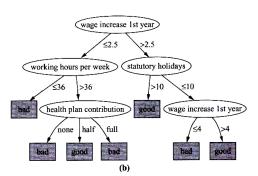
- Utilise dedicated test- and training- data-sets
- Pay attention that a single raw-data sample could not impact features in both these sets
- Don't train the features. on the training- or testdata-set



Intro

A decision tree classifier





Intro

Evaluation of classification performance

k-fold cross-validation

• Standard: k=10

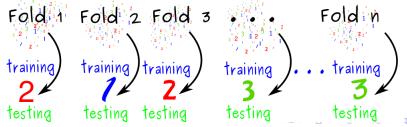


Intro

Evaluation of classification performance

Leave-one-out cross-validation

- n-fold cross validation where n is the number of instances in the data-set
- Each instance is left out once and the algorithm is trained on the remaining instances
- Performance of left-out instance (success/failure)

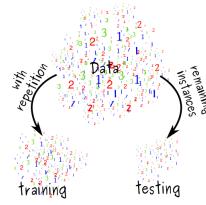


Evaluation of classification performance

0.632 Bootstrap

- Form training set by choosing n instances from the data-set with replacement
- All not picked instances are used for testing
- Probability to pick a specific instance:

$$1 - \left(1 - \frac{1}{n}\right)^n \approx 1 - e^{-1} \approx 0.632$$



Evaluation of classification performance

Classification accuracy

- Confusion matrices
- Precision
- Recall



	Classification									
	Aw	8	Po	Sb	S	Sr	St	recall		
Aw	.58	.09		.13	.11	.05	.04			
No	NOTICE SHOW	.872	.05	.014	.012	.034	.018			
To		.4	.59				.01			
Sb	.15	.22		.32	.04	.22	.05			
SI	.12	.11	.01	.06	.48	.08	.14			
Sr	.04	.15		.06	.01	.67	.07			
St	.03	.18	.01	.01	.24	.1	.43			
ргес	.630	.791	.686	.492	.511	.519	.518			

Evaluation of classification performance

Information score

Let C be the correct class of an instance and $\mathcal{P}(C)$, $\mathcal{P}'(C)$ be the prior and posterior probability of a classifier We define:¹

$$I_{i} = \begin{cases} -\log(\mathcal{P}(C)) + \log(\mathcal{P}'(C)) & \text{if } \mathcal{P}'(C) \ge \mathcal{P}(C) \\ -\log(1 - \mathcal{P}(C)) + \log(1 - \mathcal{P}'(C)) & \text{else} \end{cases}$$
(2)

The information score is then

$$IS = \frac{1}{n} \sum_{i=1}^{n} I_i \tag{3}$$

^{1.} Kononenko and I. Bratko: Information-Based Evaluation Criterion for Classifier's Performance, Machine

Training of the classifier

Evaluation of classification performance

Brier score

The Brier score is defined as

Brier =
$$\sum_{i=1}^{n} (t(x_i) - p(x_i))^2$$
 (4)

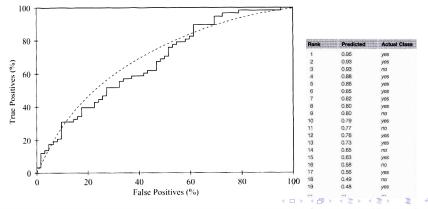
where

$$t(x_i) = \begin{cases} 1 & \text{if } x_i \text{ is the correct class} \\ 0 & \text{else} \end{cases}$$
 (5)

and $p(x_i)$ is the probability the classifier assigned to the class x_i .

Evaluation of classification performance

Area under the receiver operated characteristic (ROC) curve (AUC)



Pattern recognition and classification

Data mining frameworks

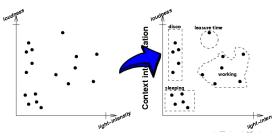
- Orange Data Mining (http://orange.biolab.si/)
- Weka Data Mining (http://www.cs.waikato.ac.nz/ml/weka/)





Pattern recognition and classification

- From features to context
 - Measure available data on features
 - Context reasoning by appropriate method
 - Syntactical (rule based e.g. RuleML)
 - Bayesian classifier
 - Non-parametric
 - Linear discriminant
 - Neural networks
 - Sequential
 - Stochastic



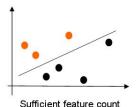
Pattern recognition and classification

- Allocation of sensor value by defined function
 - Correlation of various data sources
 - Several methods possible simple approaches
 - Template matching
 - Minimum distance methods
 - 'Integrated' feature extraction
 - Nearest Neighbour
 - Neural Networks
- Problem

Intro

- Measured raw data might not allow to derive all features required
- Therefore often combination of sensors





Pattern recognition and classification

- Methods Syntactical (Rule based)
 - Idea: Description of Situation by formal Symbols and Rules
 - Description of a (agreed on?) world view
 - Example: RuleML
- Comment
 - Pro:
 - Combination of rules and identification of loops and impossible conditions feasible

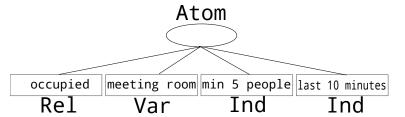
Contra:

- Very complex with more elaborate situations
- Extension or merge of rule sets typically not possible without contradictions

Pattern recognition and classification

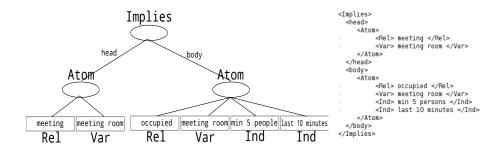
- Rule Markup Language: Language for publishing and sharing rules
- Hierarchy of rule-sub-languages (XML, RDF, XSLT, OWL)
- Example:

Intro

 A meeting room was occupied by min 5 people for the last 10 minutes. 

Pattern recognition and classification

- Also conditions can be modelled
 - A Meeting is taking place in a meeting room when it was occupied by min 5 people for the last 10 minutes.

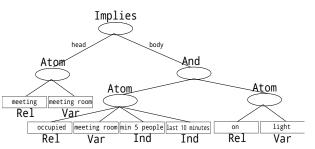


Recognition Bayesian Non-parametric Linear discriminant NN Sequential Stochastic

Pattern recognition and classification

Intro

- Logical combination of conditions
 - A Meeting is taking place in a meeting room when it was occupied by min 5 people for the last 10 minutes and the light is on.



<Implies> <head> <Atom> <Rel> meeting </Rel> <Var> meeting room </Var> </Atom> </head> <body> <And> <Atom> <Rel> on </Rel> <Var> light </Var> </Atom> <Atom> <Rel> occupied </Rel> <Var> meeting room </Var> <Ind> min 5 persons </Ind> <Ind> last 10 minutes </Ind> </Atom> </And> </body> </Implies>

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Recognition of patterns

Patterns can be described by a sufficient number of rules

Samples are inaccurate

Tremendous amount of rules to model all variations of one class

Therefore: Consider machine learning approaches



Recognition of patterns

Training set $x_1 \dots x_N$ of a large number of N samples is utilised

Classes $t_1 \dots t_N$ of all samples in this set known in advance

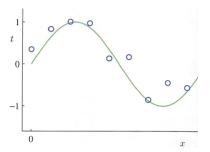
Machine learning algorithm computes a function y(x) and generates a new target t^{\prime}

Polynomial curve fitting

Example

A curve shall be approximated by a machine learning approach

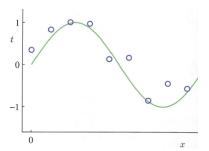
Sample points are created for the function $\sin(2\pi x) + \mathcal{N}$ where \mathcal{N} is a random noise value



Polynomial curve fitting

We will try to fit the data points into a polynomial function:

$$y(x, \overrightarrow{w}) = w_0 + w_1 x + w_2 x^2 + \dots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$



We will try to fit the data points into a polynomial function:

$$y(x, \overrightarrow{w}) = w_0 + w_1 x + w_2 x^2 + \dots + w_M x^M = \sum_{j=0}^M w_j x^j$$

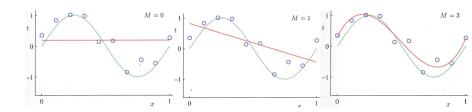
This can be obtained by minimising an error function that measures the misfit between $y(x, \overrightarrow{w})$ and the training data set:

$$E(\overrightarrow{w}) = \frac{1}{2} \sum_{i=1}^{N} \left[y(x_i, \overrightarrow{w}) - t_i \right]^2$$

 $E(\overrightarrow{w})$ is non-negative and zero if and only if all points are covered by the function

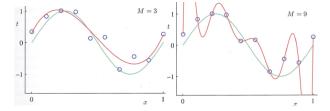
One problem is the right choice of the dimension M

When M is too small, the approximation accuracy might be bad



However, when M becomes too big, the resulting polynomial will cross all points exactly

When M reaches the count of samples in the training data set, it is always possible to create a polynomial of order M that contains all values in the data set exactly.

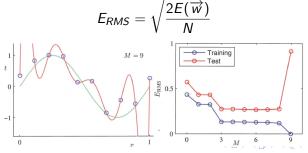


This event is called overfitting

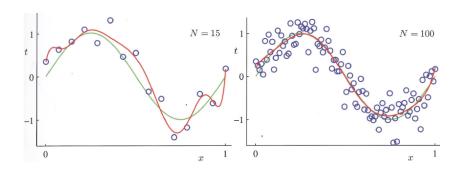
The polynomial now trained too well to the training data

It will therefore perform badly on another sample of test data for the same phenomenon

We visualise it by the Root of the Mean Square (RMS) of $E(\overrightarrow{w})$



With increasing number of data points, the problem of overfitting becomes less severe for a given value of M



One solution to cope with overfitting is regularisation

A penalty term is added to the error function

This term discourages the coefficients of \overrightarrow{w} from reaching large values

$$\overline{E}(\overrightarrow{w}) = \frac{1}{2} \sum_{i=1}^{N} \left[y(x_i, \overrightarrow{w}) - t_i \right]^2 + \frac{\lambda}{2} ||\overrightarrow{w}||^2$$

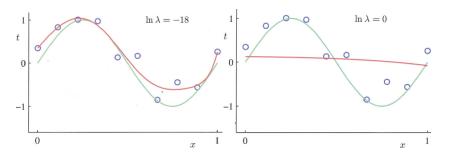
with

$$||\overrightarrow{w}||^2 = \overrightarrow{w}^T \overrightarrow{w} = w_0^2 + w_1^2 + \dots + w_M^2$$

NN

Polynomial curve fitting

Depending on the value of λ , overfitting is controlled



$$\overline{E}(\overrightarrow{w}) = \frac{1}{2} \sum_{i=1}^{N} \left[y(x_i, \overrightarrow{w}) - t_i \right]^2 + \frac{\lambda}{2} ||\overrightarrow{w}||^2$$

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Stochastic methods

Bayesian decision theory

With probability theory, the probability of events can be estimated by repeatedly generating events and counting their occurrences

When, however, an event only very seldom occurs or is hard to generate, other methods are required

Example:

Probability that the Arctic ice cap will have disappeared by the end of this century

In such cases, we would like to model uncertainty

In fact, it is possible to represent uncertainty by probability

Conditional probability

Conditional probability

The conditional probability of two events χ_1 and χ_2 with $P(\chi_2) > 0$ is denoted by $P(\chi_1|\chi_2)$ and is calculated by

$$P(\chi_1|\chi_2) = \frac{P(\chi_1 \cap \chi_2)}{P(\chi_2)}$$

 $P(\chi_1|\chi_2)$ describes the probability that event χ_2 occurs in the presence of event χ_2 .

Bayesian decision theory

With the notion of conditional probability we can express the effect of observed data $\overrightarrow{t} = t_1, \dots, t_N$ on a probability distribution of \overrightarrow{w} : $P(\overrightarrow{w})$.

Thomas Bayes described a way to evaluate the uncertainty of \overrightarrow{w} after observing \overrightarrow{t}

$$P(\overrightarrow{w}|\overrightarrow{t}) = \frac{P(\overrightarrow{t}|\overrightarrow{w})P(\overrightarrow{w})}{P(\overrightarrow{t})}$$

 $P(\overrightarrow{t}|\overrightarrow{w})$ expresses how probable a value for \overrightarrow{t} is given a fixed choice of \overrightarrow{w}

Bayesian decision theory

A principle difference between Bayesian viewpoint and frequentist viewpoint is that prior assumptions are provided

Example:

Consider a fair coin that scores heads in three consecutive tosses

Classical maximum likelihood estimate will predict head for future tosses with probability $\boldsymbol{1}$

Bayesian approach includes prior assumptions on the probability of events and would result in a less extreme conclusion



Bayesian curve fitting

In the curve fitting problem, we are given \overrightarrow{x} and \overrightarrow{t} together with a new sample x_{M+1}

The task is to find a good estimation of the value t_{M+1}

This means that we want to evaluate the predictive distribution

$$p(t_{M+1}|x_{M+1},\overrightarrow{x},\overrightarrow{t})$$

To account for measurement inaccuracies, typically a probability distribution (e.g. Gauss) is underlying the sample vector \overrightarrow{x}

Bayesian curve fitting

This means that we want to evaluate the predictive distribution

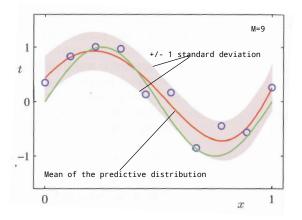
$$p(t_{M+1}|x_{M+1},\overrightarrow{x},\overrightarrow{t})$$

After consistent application of the sum and product rules of probability we can rewrite this as

$$p(t_{M+1}|x_{M+1},\overrightarrow{x},\overrightarrow{t}) = \int p(t_{M+1}|x_{M+1},\overrightarrow{w})p(\overrightarrow{w}|\overrightarrow{x},\overrightarrow{t})d\overrightarrow{w}$$

Bayesian curve fitting

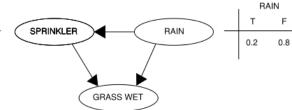
Intro



Example

Intro





CDACC WET

		GNASS WET	
SPRINKLER	RAIN	Т	F
F	F	0.0	1.0
F	Т	0.8	0.2
Т	F	0.9	0.1
Т	Т	0.99	0.01

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Histogram methods

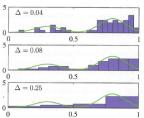
Alternative approach to function estimation: histogram methods

In general, the probability density of an event is estimated by dividing the range of N values into bins of size Δ_i

Then, count the number of observations that fall inside bin Δ_i

This is expressed as a normalised probability density

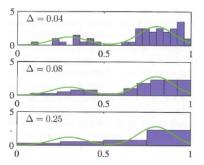
$$p_i = \frac{n_i}{N\Delta_i}$$



Histogram methods

Accuracy of the estimation is dependent on the width of the bins

Approach well suited for big data since the data items can be discarded once the histogram is created

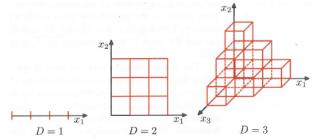


Histogram methods

Issues:

Due to the edges of the bins, the modelled distribution is characterised by discontinuities not present in the underlying distribution observed

The method does not scale well with increasing dimension (Curse of dimensionality)



Assume an unknown probability density $p(\cdot)$

We want to estimate the probability density $p(\overrightarrow{x})$ of \overrightarrow{x} in a \mathcal{D} -dimensional Euclidean space

We consider a small region \mathcal{R} around \overrightarrow{x} :

$$P = \int_{\mathcal{R}} p(\overrightarrow{x}) d\overrightarrow{x}$$

We utilise a data set of N observations

Each observation has a probability of P to fall inside $\mathcal R$

With the binomial distribution we can calculate the count K of points falling into \mathcal{R} :

$$Bin(K|N,P) = \frac{N!}{K!(N-K)!} P^K (1-P)^{N-K}$$

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With the binomial distribution we can calculate the count K of points falling into \mathcal{R} :

$$Bin(K|N,P) = \frac{N!}{K!(N-K)!} P^K (1-P)^{N-K}$$

For large N we can show

$$K \approx NP$$

With sufficiently small ${\mathcal R}$ we can also show for the volume V of ${\mathcal R}$

$$P \approx p(\overrightarrow{x})V$$

Therefore, we can estimate the density as

$$p(\overrightarrow{x}) = \frac{K}{NV}$$

We assume that ${\cal R}$ is a small hypercube

In order to count the number K of points that fall inside $\mathcal R$ we define

$$k(\overrightarrow{u}) = \begin{cases} 1, & |u_i| \leq \frac{1}{2}, & i = 1, \dots, D, \\ 0, & \text{otherwise} \end{cases}$$

This represents a unit cube centred around the origin

This function is an example of a kernel-function or Parzen window

$$k(\overrightarrow{u}) = \begin{cases} 1, & |u_i| \leq \frac{1}{2}, & i = 1, \dots, D, \\ 0, & \text{otherwise} \end{cases}$$

When the measured data point $\overrightarrow{x_n}$ lies inside a cube of side h centred around \overrightarrow{x} , we have

$$k\left(\frac{\overrightarrow{x}-\overrightarrow{x_n}}{h}\right)=1$$

The total count K of points that fall inside this cube is

$$K = \sum_{n=1}^{N} k \left(\frac{\overrightarrow{x} - \overrightarrow{x_n}}{h} \right)$$

The total count K of points that fall inside this cube is

$$K = \sum_{n=1}^{N} k \left(\frac{\overrightarrow{x} - \overrightarrow{x_n}}{h} \right)$$

When we substitute this in the density estimate derived above

$$p(\overrightarrow{x}) = \frac{K}{NV}$$

with volume $V = h^D$ we obtain the overall density estimate as

$$p(\overrightarrow{x}) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{h^{D}} \left(\frac{\overrightarrow{x} - \overrightarrow{x_{n}}}{h} \right)$$

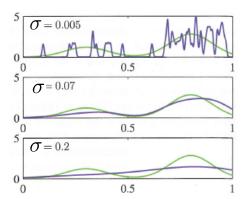
$$p(\overrightarrow{x}) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{h^{D}} \left(\frac{\overrightarrow{x} - \overrightarrow{x_{n}}}{h} \right)$$

Again, this density estimator suffers from artificial discontinuities (Due to the fixed boundaries of the cubes)

Problem can be overcome by choosing a smoother kernel function (A common choice is a Gaussian kernel with a standard deviation σ)

$$p(\overrightarrow{x}) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi\sigma^2)^{\frac{D}{2}}} e^{-\frac{||\overrightarrow{x} - \overrightarrow{x_n}||^2}{2\sigma^2}}$$

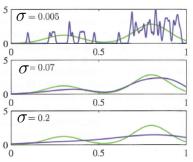
Density estimation for various values of σ



A problem with Parzen estimator methods is that the parameter governing the kernel width $(h \text{ or } \sigma)$ is fixed for all values \overrightarrow{x}

In regions with

...high density, a wide kernel might lead to over-smoothing ...low density, the same width may lead to noisy estimates



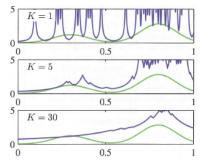
NN-methods address this by adapting width to data density

Parzen estimator methods fix V and determine K from the data Nearest neighbour methods fix K and choose V accordingly

Again, we consider a point \overrightarrow{x} and estimate the density $p(\overrightarrow{x})$

The radius of the sphere is increased until K data points (the nearest neighbours) are covered

The value K then controls the amount of smoothing Again, an optimum value for K exists



<u>Classification:</u> Apply KNN-density estimation for each class Assume data set of N points with N_k points in class C_k To classify sample \overrightarrow{x} , draw a sphere containing K points around \overrightarrow{x} Sphere can contain other points regardless of their class

Assume sphere has volume V and contains K_k points from C_k

Assume: Sphere of volume V contains K_k points from class C_k

We estimate the density of class C_k as

$$p(\overrightarrow{x}|C_k) = \frac{K_k}{N_k V}$$

The unconditional density is given as

$$p(\overrightarrow{x}) = \frac{K}{NV}$$

The probability to experience a class C_k is given as

$$p(C_k) = \frac{N_k}{N}$$

With Bayes theorem we can combine this to achieve

$$p(C_k|\overrightarrow{x}) = \frac{p(\overrightarrow{x}|C_k)p(C_k)}{p(\overrightarrow{x})} = \frac{K_k}{K}$$

$$p(C_k|\overrightarrow{x}) = \frac{p(\overrightarrow{x}|C_k)p(C_k)}{p(\overrightarrow{x})} = \frac{K_k}{K}$$

To minimise the probability of misclassification, assign \overrightarrow{x} to class with the largest probability

This corresponds to the largest value of

$$\frac{K_k}{K}$$

To classify a point, we identify the K nearest points

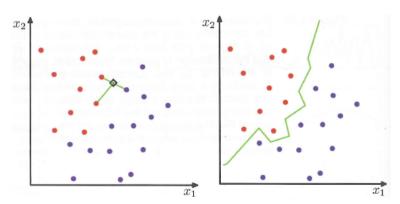
And assign the point to the class having most representatives in this set

Choice K = 1 is called nearest neighbour rule

For this choice, the error rate is never more than twice the minimum achievable error rate of an optimum classifier²

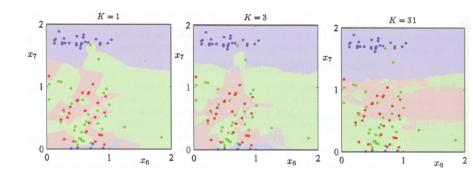
²T. Cover and P. Hart: Nearest neighbour pattern classification. IEEE Transactions on Information Theory, IT-11, 21-27, 1967

Classification of points by the K-nearest neighbour classifier



Nearest neighbour methods

Classification of points by the K-nearest neighbour classifier



Nearest neighbour methods

The KNN-method and the Parzen-method are not well suited for large data sets since they require the entire data set to be stored

Outline

Intro

Recognition of patterns

Bayesian decision theory

Non-parametric techniques

Linear discriminant functions

Neural networks

Sequential data

Stochastic methods

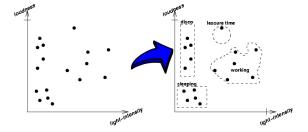
In classification we assign \overrightarrow{x} to one of K discrete classes C_k

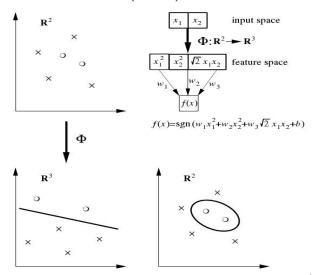
The input is divided by decision boundaries

Here we assume that decision boundaries are linear functions of \overrightarrow{x}

Data separable by linear decision surfaces are linear separable

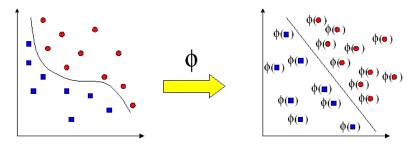
With high dimension, a set of two classes is always linear separable





SVM pre-processes data to represent patterns in a high dimension Dimension often much higher than original feature space

Then, insert hyperplane in order to separate the data



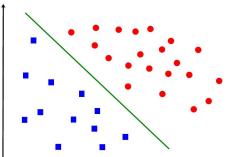
A pattern $\overrightarrow{x_k}$ is transformed to $\overrightarrow{y_k} = \varphi(\overrightarrow{x_k})$

Also, each $\overrightarrow{x_k}$ is associated with $z_k \in \{-1, 1\}$

A linear discriminant in an augmented \overrightarrow{y} space is $g(\overrightarrow{y}) = \overrightarrow{a}^t \overrightarrow{y}$

A separating hyperplane ensures for $y_0=1, a_0\geq 1$

$$z_k g(y_k) \geq 1$$

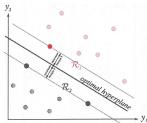


The goal for support vector machines is to find a separating hyperplane with the largest margin b to the outer points in all sets

$$\frac{z_k g(y_k)}{||\vec{a}||} \ge b, \ k = 1, \dots, n$$

If no such hyperplane exists, map all points into a higher dimensional space until such a plane exists

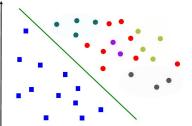
Support vectors satisfy $\cdot = b'$



Simple application to several classes by iterative approach:

```
belongs to class 1 or not?
belongs to class 2 or not?
...
```

Search for optimum mapping between input space and feature space complicated (no optimum approach known)



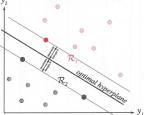
Simple learning approach to find the correct hyperplane:

Starting from an initial separating hyperplane

Find worst classified pattern (on the wrong side of the hyperplane)

Design a new hyperplane with this pattern as one of the support vectors

Iterate until all patterns are correctly classified



Outline

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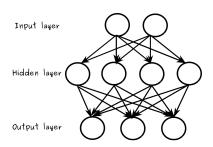
Stochastic methods

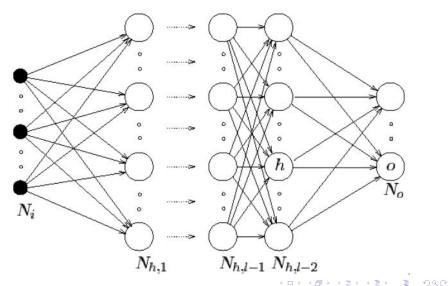
Learn mapping from input to output vector

Representation by edge-weighted graph

Distinction between

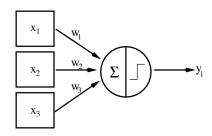
- Input neurons
- Output neurons
- Hidden nodes





Input neurons are only equipped with outgoing edges

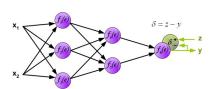
Hidden nodes 'fire' (output value 1) when weighted inputs exceed threshold function Θ

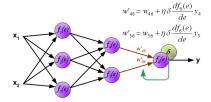


$$y_i = \begin{cases} 1, & \text{if } \sum_{i=1}^n x_i w_i \ge \Theta \\ 0, & \text{else.} \end{cases}$$

Learning with back-propagation (schematic): (Iterate until the error is sufficiently small)

- Choose a training-pair and copy it to the input layer
- Propagate it through the network
- Calculate error between computed and expected output
- Propagate the sum product of the weights back into the network in order to calculate the error in internal layers
- Adapt weights to the error



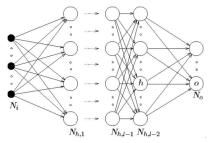


Single hidden layer sufficient to represent arbitrary multi-dimensional functions

Well suited for noisy input data

Implicit clustering of input data possible

Complex to extend network (e.g. add new features)



For the input layer, we construct M linear combinations of the input variables x_1, \ldots, x_D and weights w_1, \ldots, w_D

$$a_j = \sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

Each a; is transformed using a differentiable, non-linear activation function

$$z_j = h(a_j)$$

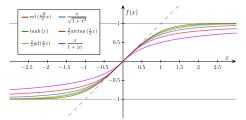
Input layer M linear combinations of x_1, \ldots, x_D and w_1, \ldots, w_D

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

Activation function: Differentiable, non-linear

$$z_j = h(a_j)$$

 $h(\cdot)$ function is usually a sigmoidal function or tanh



Values z_j are again linearly combined in hidden layers:

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

with k = 1, ..., K describing the total number of outputs

Again, these values are transformed using a sufficient transformation function σ to obtain the network outputs y_k

$$y_k = \sigma(a_k)$$

For multi-class problems, we use a function such as

$$\sigma(a) = \frac{1}{1 + e^{-a}}$$

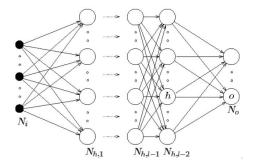
Combine these stages to achieve overall network function:

$$y_k(\overrightarrow{x}, \overrightarrow{w}) = \sigma \left(\sum_{j=1}^{M} w_{kj}^{(2)} h \left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)} \right) + w_{k0}^{(2)} \right)$$

(Multiple hidden layers are added analogously)

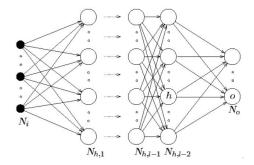
Activation functions of hidden units are linear \Rightarrow Always find equivalent network without hidden units

(Composition of successive linear transformations itself linear transformation)



Number of hidden units < number of input or output units \Rightarrow not all linear functions possible

(Information lost in dimensionality reduction at hidden units)



Neural networks are Universal approximators³ ⁴ ⁵ ⁶ ⁷ ⁸ ⁹ ¹⁰

⇒ 2-layer linear NN can approximate any continuous function

 $^{^3\}text{K}$. Funahashi: On the approximate realisation of continuous mappings by neural networks, Neural Networks, 2(3), 183-192, 1989 G. Cybenko: Approximation by superpositions of a sigmoidal function. Mathematics of control, signals and

systems, 2, 304-314, 1989

⁵K. Hornik, M. Sinchcombe, H. White: Multilayer feed-forward networks are universal approximators. Neural Networks, 2(5), 359-366, 1989

 $^{^6}$ N.E. Cotter: The stone-Weierstrass theorem and its application to neural networks. IEEE Transactions on Neural Networks 1(4), 290-295, 1990

 $^{^{7}\}mathrm{Y}$. Ito: Representation of functions by superpositions of a step or sigmoid function and their applications to neural network theory. Neural Networks 4(3), 385-394, 1991

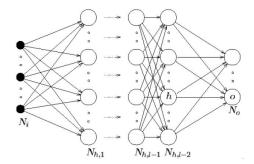
⁸K. Hornik: Approximation capabilities of multilayer feed forward networks: Neural Networks, 4(2), 251-257, 1991

 $^{^9\}mathrm{Y.V.}$ Kreinovich: Arbitrary non-linearity is sufficient to represent all functions by neural networks: a theorem. Neural Networks 4(3), 381-383, 1991

¹⁰ B.D. Riolev: Pattern Recognition and Neural Networks. Cambridge University Press, 1996.

Remaining issue in neural networks

- Find suitable parameters given a set of training data
- Several learning approaches have been proposed



Simple approach to determine network parameters: Minimise sum-of-squared error function

- Given a training set $\overrightarrow{x_n}$ with $n \in \{1, \dots, N\}$
- And corresponding target vectors $\overrightarrow{t_n}$
- Minimise the error function

$$E(\overrightarrow{w}) = \frac{1}{2} \sum_{n=1}^{N} (y(\overrightarrow{x_n}, \overrightarrow{w}) - \overrightarrow{t_n})^2$$

Neural networks – Classification

2 classes C_1 and C_2

We consider a network with a single output

$$y = \sigma(a) \equiv \frac{1}{1 + e^{-a}}$$

- Output interpreted as conditional probability $p(C_1|\overrightarrow{x})$
- Analogously, we have $p(\mathcal{C}_2|\overrightarrow{x}) = 1 p(\mathcal{C}_1|\overrightarrow{x})$

K classes C_1, \dots, C_K

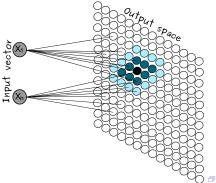
- Binary target variables $t_k \in \{0,1\}$
- Network outputs are interpreted as $y_k(\overrightarrow{X}, \overrightarrow{W}) = p(t_k = 1 | \overrightarrow{X})$

Proposed by Teuvo Kohonen¹¹

As a model of the self-organisation of neural connections

Maps high dimensional input to low dimensional output

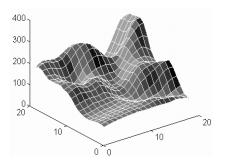
Based on neural network learning of the underlying mapping

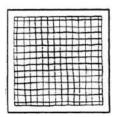


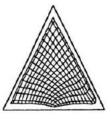
Present all points in a source space by points in a target space

Given a sequence of points in a sample space,

Create a mapping of these points into a target space that respects the neighbourhood relation in the sample space







SOM is a topology preserving lattice of predefined number of nodes Represents topology of elements in input space.

Algorithm inherits self-organisation property

- Able to produce organisation starting from total disorder.
- Defines and preserves neighbourhood structure between nodes

Learning by two layer neural network



Intro

Input vector x_k : Wnk Output layer





When a pattern $\overrightarrow{\phi_i}$ is presented, each node (represented by outer neurons) in the target space computes its activation $\overrightarrow{\phi_i}$ \overrightarrow{w} .

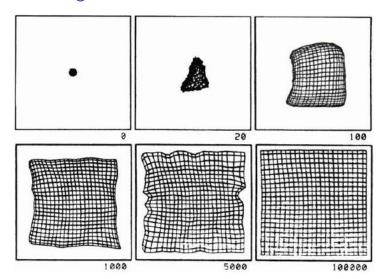
Most activated node y^* and weights to its neighbours are updated according to a learning rate $\rho(t)$

$$w_{ki}(t+1) = w_{ki}(t) +
ho(t)\Lambda(|y-y^*|)(\overrightarrow{\phi_i} - w_{ki}(t))$$

 $\Lambda(\cdot)$ defines a non-increasing neighbourhood function and $|y-y^*|$ describes the distance of nodes in the neighbourhood

SOM - Self organisation

Intro



SOM - Definition

Condensed definition of SOM from Cottrell et al. 12

Self organising maps

- Let $I = \{\overrightarrow{\eta_1}, \dots, \overrightarrow{\eta_{|S|}}\}$ be a set of km-dimensional vectors that are associated with nodes in a lattice.
- Neighbourhood structure provided by symmetrical neighbourhood function $d:I\times I\to \mathbb{R}$ which depends on the distance between two nodes $\overrightarrow{\eta_i}$ and $\overrightarrow{\eta_j}\in I$.
- State of the map at time t given by

$$\eta(t) = \left(\overrightarrow{\eta_1(t)}, \overrightarrow{\eta_2(t)}, \dots, \overrightarrow{\eta_{|S|}(t)}\right),$$

¹² M. Cottrell, J.C. Fort and G. Pages, *Theoretical aspects of the SOM algorithm*, Neurocomputing, pp. 119-138, vol 21, 1998.

Self organising map algorithm

The SOM algorithm is recursively defined by

$$\begin{array}{lcl} \emph{i}_{c}\left(\overrightarrow{v(t+1)},\overrightarrow{\eta(t)}\right) & = & \textit{argmin}\left\{\left\|\overrightarrow{v(t+1)}-\overrightarrow{\eta_{i}(t)}\right\|,\overrightarrow{\eta_{i}(t)}\in\eta(t)\right\},\\ \overrightarrow{\eta_{i}(t+1)} & = & \overrightarrow{\eta_{i}(t)}-\varepsilon_{t}d\left[\emph{i}_{c}\left(\overrightarrow{v(t+1)},\overrightarrow{\eta(t)}\right),\overrightarrow{\eta_{i}}\right]\\ & \cdot\left(\overrightarrow{\eta_{i}(t)}-\overrightarrow{v(t+1)}\right),\forall\overrightarrow{\eta_{i}}\in\emph{I}. \end{array}$$

In this formula, $i_c\left(\overrightarrow{v(t+1)},\overrightarrow{\eta(t)}\right)$ corresponds to the node in the network that is closest to the input vector.

Parameter ε_t controls the adaptability.

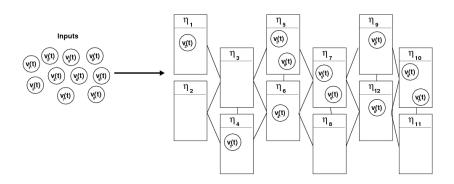
SOM – Operational principle

Inputs



Input values $v_i(t)$ are to be mapped onto the target space

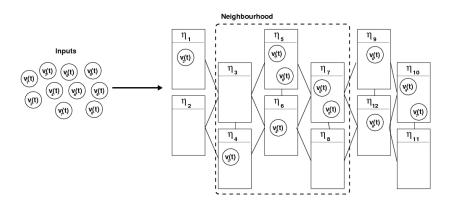
SOM – Operational principle



Node with the lowest distance is associated with the input value:

$$i_{c}\left(\overrightarrow{v(t+1)},\overrightarrow{\eta(t)}\right) = argmin\left\{\left\|\overrightarrow{v(t+1)} - \overrightarrow{\eta_{i}(t)}\right\|,\overrightarrow{\eta_{i}(t)} \in \eta(t)
ight\}$$

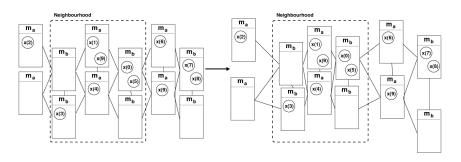
SOM – Operational principle



Nodes in the neighbourhood of the associated node are moved closer to the input value

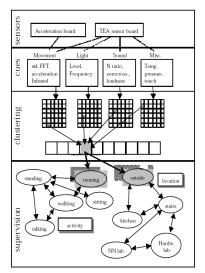


(NN)

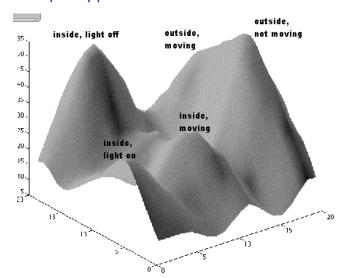


Nodes in the neighbourhood of the associated node are moved to the input value

$$\overline{\eta_{i}(t+1)} = \overline{\eta_{i}(t)} - \varepsilon_{t} d \left[i_{c} \left(\overline{v(t+1)}, \overline{\eta(t)} \right), \overline{\eta_{i}^{c}} \right] \\
\cdot \left(\overline{\eta_{i}(t)} - \overline{v(t+1)} \right), \forall \overline{\eta_{i}^{c}} \in I.$$



SOM - Example application: TEA



SOM – Remarks

SOM algorithm always converges¹³

Normalisation of input vectors might improve numerical accuracy

Not guaranteed that self-optimisation will always occur (Dependent on choice of parameters)

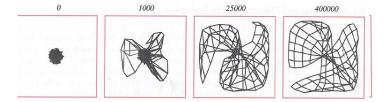
Difficult to set parameters of the model since SOM is not optimising any well-defined function¹⁴

If neighbourhood is chosen to be too small, the map will not be ordered globally

¹³Y. Cheng, Neural Computation, 9(8), 1997.

 $^{^{14}}$ E. Erwin, K. Obermayer, K. Schulten: Self-organising maps: Ordering, convergence properties and energy functions. Biological Cybernetics, 67, 47-55, 1992 山 医水杨 医水黄 医多种

Problems of SOMs



Map created as target space might have several orientations

One part of the map might follow one orientation, while other parts are following other orientations

Outline

Intro

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Linear discriminant functions

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Stochastic methods



Sequential

Markov chains

Markov processes

- Intensively studied
- Major branch in the theory of stochastic processes

A. A. Markov (1856 – 1922)

Extended by A. Kolmogorov to chains of infinitely many states

 'Anfangsgründe der Theorie der Markoffschen Ketten mit unendlich vielen möglichen Zuständen' (1936) 15

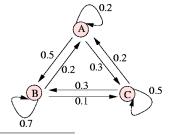
 $^{^{15}}$ A. Kolmogorov, $^{Anfangsgr\"{u}nde}$ der Theorie der Markoffschen Ketten mit unendlich vielen möglichen Zuständen, 1936.

- Theory applied to a variety of algorithmic problems
- Standard tool in many probabilistic applications

Intuitive graphical representation

Suitable for graphical illustration of stochastic processes

Popular for their simplicity and easy applicability to huge set of $\operatorname{problems}^{16}$



¹⁶ William Feller, An introduction to probability theory and its applications, Wiley, 1968.

Sequential

Viarkov chains Independent trials of events

Dependent trials of events

Independent trials of events

- Set of possible outcomes of a measurement E_i associated with occurrence probability p_i
- Probability to observe sample sequence:

•
$$P\{(E_1, E_2, \ldots, E_i)\} = p_1 p_2 \cdots p_i$$

Dependent trials of events

Independent trials of events

- Set of possible outcomes of a measurement E_i associated with occurrence probability p_i
- Probability to observe sample sequence:

•
$$P\{(E_1, E_2, \ldots, E_i)\} = p_1 p_2 \cdots p_i$$

Dependent trials of events

• Probability to observe specific sequence E_1, E_2, \ldots, E_i obtained by conditional probability:

$$P(E_i|E_1,E_2,...,E_{i-1})$$

In general:

$$P(E_i|E_1,E_2,\ldots,E_{i-1}) \neq P(E_i|E_2,E_1,E_3,E_4,\ldots,E_{i-1})$$

Independent random variables

Dependent random variables

Independent random variables

- Number of coin tosses until 'head' is observed
- Radioactive atoms always have same probability of decaying at next trial

Dependent random variables

Independent random variables

- Number of coin tosses until 'head' is observed
- Radioactive atoms always have same probability of decaying at next trial

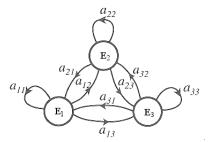
Dependent random variables

- Knowledge that no car has passed for five minutes increases expectation that it will come soon.
- Coin tossing:
 - Probability that the cumulative numbers of heads and tails will equalize at the second trial is $\frac{1}{2}$
 - Given that they did not, the probability that they equalize after two additional trials is only $\frac{1}{4}$

tro Recognition Bayesian Non-parametric Linear discriminant NN (Sequential) Stochastic

Markov property

In the theory of stochastic processes the described lack of memory is connected with the Markov property.



Outcome depends exclusively on outcome of directly preceding trial

- Every sequence (E_i, E_i) has a conditional probability p_{ij}
- Additionally: Probability a_i of the event E_i



Sequential

Markov chains

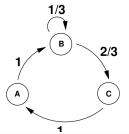
Markov chain

iviarkov chain

A sequence of observations E_1, E_2, \ldots is called a Markov chain if the probabilities of sample sequences are defined by

$$P(E_1, E_2, \ldots, E_i) = a_1 \cdot p_{12} \cdot p_{23} \cdot \cdots \cdot p_{(i-1)i}.$$

and fixed conditional probabilities p_{ij} that the event E_i is observed directly in advance of E_j .



Sequential

Described by probability a for initial distribution and matrix P of transition probabilities.

$$P = \left[\begin{array}{cccc} p_{11} & p_{12} & p_{13} & \cdots \\ p_{21} & p_{22} & p_{23} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array} \right]$$

P is called a stochastic matrix

(Square matrix with non-negative entries that sum to 1 in each row)

 p_{ii}^k denotes probability that E_i is observed exactly k observations after E; was observed.

Calculated as the sum of the probabilities for all possible paths $E_i E_{i_1} \cdots E_{i_{k-1}} E_i$ of length k

We already know

$$p_{ij}^1=p_{ij}$$

Consequently:

$$p_{ij}^2 = \sum_{\nu} p_{i\nu} \cdot p_{\nu j}$$

$$p_{ij}^3 = \sum_{\nu} p_{i\nu} \cdot p_{\nu j}^2$$

By mathematical induction:

$$p_{ij}^{n+1} = \sum_{\nu} p_{i\nu} \cdot p_{\nu j}^n$$

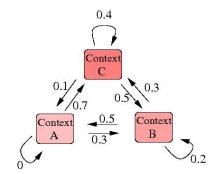
and

$$p_{ij}^{n+m} = \sum_{\nu} p_{i\nu}^m \cdot p_{\nu j}^n = \sum_{\nu} p_{i\nu}^n \cdot p_{\nu j}^m$$

Similar to matrix P we can create a matrix P^n that contains all p_{ii}^n p_{ii}^{n+1} obtained from P^{n+1} : Multiply row i of P with column j of P^n

Symbolically: $P^{n+m} = P^n P^m$.

$$P^{n} = \begin{vmatrix} p_{11}^{n} & p_{12}^{n} & p_{13}^{n} & \cdots \\ p_{21}^{n} & p_{22}^{n} & p_{23}^{n} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$



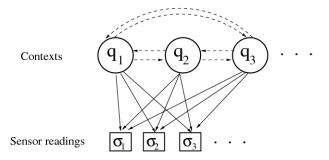
	Context A	Context B	Context C	
Context A	0	0.3	0.7	
Context B	0.5	0.2	0.3	
Context C	0.1	0.5	0.4	

	Context A	Context B	Context C	
Context A	0.22	0.41	0.37	
Context B	0.13	0.34	0.53	
Context C	0.29	0.33	0.38	
				Г

	Context A	Context B	Context C	
Context A	0.242	0.333	0.425	
Context B	0.223	0.372	0.405	
Context C	0.203	0.343	0.454	

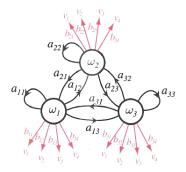
Make a sequence of decisions for a process that is not directly observable 17

Current states of the process might be impacted by prior states HMM often utilised in speech recognition or gesture recognition

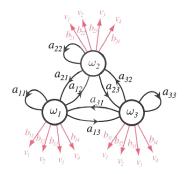


¹⁷ Richard O. Duda, Peter E. Hart and David G. Stork, Pattern classification, Wiley interscience, 2001.





At every time step t the system is in an internal state $\omega(t)$ Additionally, we assume that it emits a (visible) symbol v(t)Only access to visible symbols and not to internal states



Probability to be in state $\omega_j(t)$ and emit symbol $v_k(t)$:

$$P(v_k(t)|\omega_i(t)) = b_{ik}$$

Transition probabilities: $p_{ij} = P(\omega_j(t+1)|\omega_i(t))$

Emission probability: $b_{ik} = P(v_k(t)|\omega_i(t))$



Central issues in hidden Markov models:

- Evaluation problem Determine the probability that a particular sequence of visible symbols V^T was generated by a given hidden Markov model
- Decoding problem Determine the most likely sequence of hidden states ω^T that led to a specific sequence of observations V^T
- Learning problem Given a set of training observations of visible symbols, determine the parameters p_{ii} and b_{ik} for a given HMM

Hidden Markov Models – Evaluation problem

Probability that model produces a sequence V^T :

$$P(V^T) = \sum_{\overline{\omega}^T} P(V^T | \overline{\omega}^T) P(\overline{\omega}^T)$$

Also:

$$P(\overline{\omega}^T) = \prod_{t=1}^{T} P(\omega(t)|\omega(t-1))$$

$$P(V^T|\overline{\omega}^T) = \prod_{t=1}^{T} P(v(t)|\omega(t))$$

Together:

$$P(V^T) = \sum_{t=1}^{T} \prod_{t=1}^{T} P(v(t)|\omega(t))P(\omega(t)|\omega(t-1))$$

Hidden Markov Models – Evaluation problem

Probability that model produces a sequence V^{I} :

$$P(V^{T}) = \sum_{\overline{\omega}^{T}} \prod_{t=1}^{T} P(v(t)|\omega(t)) P(\omega(t)|\omega(t-1))$$

Formally complex but straightforward

Naive computational complexity

•
$$\mathcal{O}(c^TT)$$

Hidden Markov Models - Evaluation problem

Probability that model produces a sequence V^T :

$$P(V^{T}) = \sum_{\overline{\omega}^{T}} \prod_{t=1}^{T} P(v(t)|\omega(t)) P(\omega(t)|\omega(t-1))$$

Computationally less complex algorithm:

- Calculate $P(V^T)$ recursively
- $P(v(t)|\omega(t))P(\omega(t)|\omega(t-1))$ involves only $v(t),\omega(t)$ and $\omega(t-1)$

$$lpha_j(t) = \left\{ egin{array}{ll} 0 & t = 0 ext{ and } j
eq ext{ initial state} \ 1 & t = 0 ext{ and } j = ext{ initial state} \ \left[\sum_j lpha_i(t-1) p_{ij} \right] b_{jk} & ext{ otherwise } _{(b_{jk} ext{ leads to observed }
u(t))} \end{array}
ight.$$

Hidden Markov Models - Evaluation problem

Forward Algorithm

Computational complexity: $O(c^2T)$

Forward algorithm

```
1 initialise t \leftarrow 0, p_{ij}, b_{jk}, V^T, \alpha_j(0)

2 for t \leftarrow t+1

3 j \leftarrow 0

4 for j \leftarrow j+1

5 \alpha_j(t) \leftarrow b_{jk} \sum_{i=1}^c \alpha_i(t-1)p_{ij}

6 until j=c

7 until t=T

8 return P(V^T) \leftarrow \alpha_j(T) for the final state

9 end
```

Sequential

Given a sequence V^T , find most probable sequence of hidden states Enumeration of every possible path will cost $O(c^T)$

Not feasible

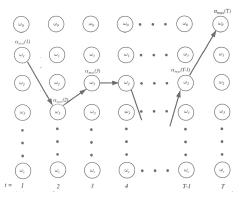
Hidden Markov Models – Decoding problem

Given a sequence V^T , find most probable sequence of hidden states

Decoding algorithm

```
initialise: path \leftarrow \{\}, t \leftarrow 0
         for t \leftarrow t + 1
             i \leftarrow 0;
              for i \leftarrow i + 1
4
                  \alpha_i(t) \leftarrow b_{ik} \sum_{i=1}^{c} \alpha_i(t-1) p_{ii}
6
             until i = c
             j' \leftarrow arg \max_i \alpha_i(t)
8
              append \omega_{i'} to path
9
         until t = T
     return path
11 end
```

Hidden Markov Models - Decoding problem



Computational time of the decoding algorithm

 $O(c^2T)$



Hidden Markov Models – Learning problem

Determine the model parameters p_{ii} and b_{ik}

• Given: Training sample of observed values V^T

No method known to obtain the optimal or most likely set of parameters from the data

- However, we can nearly always determine a good solution by the forward-backward algorithm
- General expectation maximisation algorithm
- Iteratively update weights in order to better explain the observed training sequences

Sequential

Probability that the model is in state $\omega_i(t)$ and will generate the remainder of the given target sequence:

$$\beta_i(t) = \left\{ \begin{array}{ll} 0 & t = T \text{ and } \omega_i(t) \text{ not final hidden state} \\ 1 & t = T \text{ and } \omega_i(t) \text{ final hidden state} \\ \sum_j \beta_j(t+1)p_{ij}b_{jk} & \text{otherwise } (b_{jk} \text{ leads to } v(t+1)) \end{array} \right.$$

Hidden Markov Models – Learning problem

 $\alpha_i(t)$ and $\beta_i(t)$ only estimates of their true values since transition probabilities p_{ii} , b_{ik} unknown

Probability of transition between $\omega_i(t-1)$ and $\omega_i(t)$ can be estimated

 Provided that the model generated the entire training sequence V^T by any path

$$\gamma_{ij}(t) = \frac{\alpha(t-1)p_{ij}b_{jk}\beta_j(t)}{P(V^T|\Omega)}$$

Probability that model generated sequence V^T :

$$P(V^T|\Omega)$$

Sequential

Hidden Markov Models – Learning problem

Calculate improved estimate for p_{ii} and b_{ik}

$$\overline{p_{ij}} = \frac{\sum_{t=1}^{T} \gamma_{ij}(t)}{\sum_{t=1}^{T} \sum_{k} \gamma_{ik}(t)}$$

$$\overline{b_{jk}} = \frac{\sum_{t=1, v(t)=v_k}^{I} \sum_{l} \gamma_{jl}(t)}{\sum_{t=1}^{T} \sum_{l} \gamma_{jl}(t)}$$

Start with rough estimates of p_{ij} and b_{jk}

Calculate improved estimates

Repeat until some convergence is reached

Hidden Markov Models - Learning problem

Forward-Backward algorithm

```
initialise p_{ii}, b_{ik}, V^T, convergence criterion \Delta, t \leftarrow 0
         do t \leftarrow t + 1
2
3
             compute p_{ii}(t)
             compute b_{ik}(t)
4
             p_{ii}(t) \leftarrow p_{ii}(t)
5
             b_{ik}(t) \leftarrow b_{ik}(t)
6
7
         until \max_{i,j,k}[p_{ii}(z)-p_{ii}(z-1),b_{ik}(t)-b_{ik}(t-1)] < \Delta
                           (convergence achieved)
8 return p_{ii} \leftarrow p_{ii}(t), b_{ik} \leftarrow b_{ik}(t)
9
  end
```

Outline

Intro

Recognition of patterns

Bayesian decision theory

Non-parametric techniques

Linear discriminant functions

Neural networks

Sequential data

Stochastic methods