# Machine Learning and Pervasive Computing 

Stephan Sigg<br>Georg－August－University Goettingen，Computer Networks

21．01．2015

4 ロ〉（白

## Overview and Structure

22.10.2014 Organisation
22.10.3014 Introduction (Def:: Machine learning, Supervised/Unsuperised, Examples)
29.10.2014 Machine Learning Basics (Toolchain, Features, Metrics, Rule-based)
05.11.2014 A simple Supervised learning algorithm
12.11.2014 Excursion: Avoiding local optima with random search
19.11.2014 -
26.11.2014 Bayesian learner
03.12.2014 -
10.12.2014 Decision tree learner
17.12.2014 k-nearest neighbour
07.01.2015 Support Vector Machines
14.01.2015 Artificial Neural Networks and Self Organizing Maps
21.01.2015 Hidden Markov models and Conditional random fields
28.01.2015 High dimensional data, Unsupervised learning
04.02.2015 Anomaly detection, Online learning, Recom. systems

## Outline

Markov chains

Hidden Markov Models
Evaluation
Deconding
Learning

Probabilistic Graphical Models

## 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) ${ }^{1}$

[^0]
## Markov chains

- 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 problems ${ }^{2}$


[^1]
## Markov chains

Independent trials of events

Dependent trials of events

## Markov chains

Independent trials of events

- Set of possible outcomes of a measurement $E_{i}$ associated with occurrence probability $p_{i}$
- Probability to observe sample sequence:
- $P\left\{\left(E_{1}, E_{2}, \ldots, E_{i}\right)\right\}=p_{1} p_{2} \cdots p_{i}$

Dependent trials of events

## Markov chains

Independent trials of events

- Set of possible outcomes of a measurement $E_{i}$ associated with occurrence probability $p_{i}$
- Probability to observe sample sequence:
- $P\left\{\left(E_{1}, E_{2}, \ldots, E_{i}\right)\right\}=p_{1} p_{2} \cdots p_{i}$

Dependent trials of events

- Probability to observe specific sequence $E_{1}, E_{2}, \ldots, E_{i}$ obtained by conditional probability:

$$
P\left(E_{i} \mid E_{1}, E_{2}, \ldots, E_{i-1}\right)
$$

## Markov chains

Independent random variables

Dependent random variables

## Markov chains

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

## Markov chains

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 $\frac{1}{4}$


## 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 $\left(E_{i}, E_{j}\right)$ has a conditional probability $p_{i j}$
- Additionally: Probability $a_{i}$ of the event $E_{i}$


## Markov chains

## Markov chain

A sequence of observations $E_{1}, E_{2}, \ldots$ is called a Markov chain if the probabilities of sample sequences are defined by

$$
P\left(E_{1}, E_{2}, \ldots, E_{i}\right)=a_{1} \cdot p_{12} \cdot p_{23} \cdots \cdot p_{(i-1) i}
$$

and fixed conditional probabilities $p_{i j}$ that the event $E_{i}$ is observed directly in advance of $E_{j}$.


## Markov chains

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)

## Markov chains

$p_{i j}^{k}$ denotes probability that $E_{j}$ is observed exactly $k$ observations after $E_{i}$ was observed.
Calculated as the sum of the probabilities for all possible paths $E_{i} E_{i_{1}} \cdots E_{i_{k-1}} E_{j}$ of length $k$
We already know

$$
p_{i j}^{1}=p_{i j}
$$

Consequently:

$$
\begin{aligned}
& p_{i j}^{2}=\sum_{\nu} p_{i \nu} \cdot p_{\nu j} \\
& p_{i j}^{3}=\sum_{\nu} p_{i \nu} \cdot p_{\nu j}^{2}
\end{aligned}
$$

## Markov chains

By mathematical induction:

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

and

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

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

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

## Markov chains



|  | Comex\| | ${ }_{\text {Conexx }}^{\text {Cr }}$ | ${ }_{\text {conex }}^{\text {cone }}$ |
| :---: | :---: | :---: | :---: |
| (conex | 0 | 0.3 | 0.7 |
| Comex | 0.5 | 0.2 | 0.3 |
| ${ }_{\text {comex }}$ | 0.1 | 0.5 | 0.4 |


|  | Conexx | ${ }_{\text {contex }}$ | comest |
| :---: | :---: | :---: | :---: |
| Contex | 0.22 | 0.41 | 0.37 |
| ${ }_{\text {conem }}^{\text {conex }}$ | 0.13 | 0.34 | 0.53 |
| ${ }_{\text {comex }}$ | 0.29 | 0.33 | 0.38 |


|  | Context <br> A | Context <br> B | Context <br> C |  |
| :---: | :---: | :---: | :---: | :---: |
| Context <br> A | 0.242 | 0.333 | 0.425 |  |
| Context <br> B | 0.223 | 0.372 | 0.405 |  |
| Context <br> C | 0.203 | 0.343 | 0.454 |  |
|  |  |  |  |  |

[^2]
## Outline

Markov chains

Hidden Markov Models
Evaluation
Deconding
Learning

Probabilistic Graphical Models

Machine Learning and Pervasive Computing

## Hidden Markov Models

Make a sequence of decisions for a process that is not directly observable ${ }^{3}$

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


[^3]
## Hidden Markov Models



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

## Hidden Markov Models



Probability to be in state $\omega_{j}(t)$ and emit symbol $v_{k}(t)$ :

$$
P\left(v_{k}(t) \mid \omega_{j}(t)\right)=b_{j k}
$$

Transition probabilities: $p_{i j}=P\left(\omega_{j}(t+1) \mid \omega_{i}(t)\right)$
Emission probability: $b_{j k}=P\left(v_{k}(t) \mid \omega_{j}(t)\right)$

## Hidden Markov Models

Central issues in hidden Markov models:
Evaluation problem Determine the probability that a particular sequence of visible symbols $V^{n}$ was generated by a given hidden Markov model
Decoding problem Determine the most likely sequence of hidden states $\omega^{n}$ that led to a specific sequence of observations $V^{n}$
Learning problem Given a set of training observations of visible symbols, determine the parameters $p_{i j}$ and $b_{j k}$ for a given HMM

## Hidden Markov Models - Evaluation problem

Probability that model produces a sequence $V^{n}$ :

$$
P\left(V^{n}\right)=\sum_{\bar{\omega}^{n}} P\left(V^{n} \mid \bar{\omega}^{n}\right) P\left(\bar{\omega}^{n}\right)
$$

Also:

$$
\begin{aligned}
P\left(\bar{\omega}^{n}\right) & =\prod_{t=1}^{n} P(\omega(t) \mid \omega(t-1)) \\
P\left(V^{n} \mid \bar{\omega}^{n}\right) & =\prod_{t=1}^{n} P(v(t) \mid \omega(t))
\end{aligned}
$$

Together:

$$
P\left(V^{n}\right)=\sum_{\bar{\omega}^{n}} \prod_{t=1}^{n} P(v(t) \mid \omega(t)) P(\omega(t) \mid \omega(t-1))
$$

## Hidden Markov Models - Evaluation problem

Probability that model produces a sequence $V^{n}$ :

$$
P\left(V^{n}\right)=\sum_{\bar{\omega}^{n}} \prod_{t=1}^{n} P(v(t) \mid \omega(t)) P(\omega(t) \mid \omega(t-1))
$$

Formally complex but straightforward
Naive computational complexity

- $\mathcal{O}\left(c^{n} n\right)$


## Hidden Markov Models - Evaluation problem

Probability that model produces a sequence $V^{n}$ :

$$
P\left(V^{n}\right)=\sum_{\bar{\omega}^{n}} \prod_{t=1}^{n} P(v(t) \mid \omega(t)) P(\omega(t) \mid \omega(t-1))
$$

Computationally less complex algorithm:

- Calculate $P\left(V^{n}\right)$ recursively
- $P(v(t) \mid \omega(t)) P(\omega(t) \mid \omega(t-1))$ involves only $v(t), \omega(t)$ and $\omega(t-1)$

$$
\alpha_{j}(t)= \begin{cases}0 & t=0 \text { and } j \neq \text { initial state } \\ 1 & t=0 \text { and } j=\text { initial state } \\ {\left[\sum_{i} \alpha_{i}(t-1) p_{i j}\right] b_{j k}} & \text { otherwise }\left(b_{j k} \text { leads to observed } v(t)\right)\end{cases}
$$

## Hidden Markov Models - Evaluation problem

Forward Algorithm
Computational complexity: $O\left(c^{2} n\right)$
Forward algorithm

$$
\begin{aligned}
& 1 \text { initialise } t \leftarrow 0, p_{i j}, b_{j k}, V^{n}, \alpha_{j}(0) \\
& 2 \quad \text { for } t \leftarrow t+1 \\
& 3 \\
& 4 \quad j \leftarrow 0 \\
& 5
\end{aligned} \quad \text { for } j \leftarrow j+1 .
$$

## Hidden Markov Models - Decoding problem

Given a sequence $V^{n}$, find most probable sequence of hidden states
Enumeration of every possible path will cost $O\left(c^{n}\right)$

- Not feasible


## Hidden Markov Models - Decoding problem

Given a sequence $V^{n}$, find most probable sequence of hidden states

```
Decoding algorithm
1 initialise: path }\leftarrow{},t\leftarrow
2 for t\leftarrowt+1
3 j
4 for }j\leftarrowj+
5 < < (t)\leftarrow b bk \mp@subsup{\sum}{i=1}{c}\mp@subsup{\alpha}{i}{}(t-1)\mp@subsup{p}{ij}{}
6 until j=c
7 j j}\leftarrow\operatorname{arg}\mp@subsup{\operatorname{max}}{j}{}\mp@subsup{\alpha}{j}{}(t
8 append }\mp@subsup{\omega}{\mp@subsup{j}{}{\prime}}{}\mathrm{ to path
9 until t=n
1 0 \text { return path}
11 end
```


## Hidden Markov Models - Decoding problem



Computational time of the decoding algorithm

- $O\left(c^{2} n\right)$


## Hidden Markov Models - Learning problem

Determine the model parameters $p_{i j}$ and $b_{j k}$

- Given: Training sample of observed values $V^{n}$

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


## Hidden Markov Models - Learning problem

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

$$
\beta_{i}(t)= \begin{cases}0 & t=n \text { and } \omega_{i}(t) \text { not final hidden state } \\ 1 & t=n \text { and } \omega_{i}(t) \text { final hidden state } \\ \sum_{j} \beta_{j}(t+1) p_{i j} b_{j k} & \text { otherwise }\left(b_{j k} \text { leads to } v(t+1)\right)\end{cases}
$$

## Hidden Markov Models - Learning problem

$\alpha_{i}(t)$ and $\beta_{i}(t)$ only estimates of their true values since transition probabilities $p_{i j}, b_{j k}$ unknown

Probability of transition between $\omega_{i}(t-1)$ and $\omega_{j}(t)$ can be estimated

- Provided that the model generated the entire training sequence $V^{n}$ by any path

$$
\gamma_{i j}(t)=\frac{\alpha(t-1) p_{i j} b_{j k} \beta_{j}(t)}{P\left(V^{n} \mid \Omega\right)}
$$

Probability that model generated sequence $V^{n}$ :

$$
P\left(V^{n} \mid \Omega\right)
$$

## Hidden Markov Models - Learning problem

Calculate improved estimate for $p_{i j}$ and $b_{j k}$

$$
\begin{gathered}
\overline{p_{i j}}=\frac{\sum_{t=1}^{n} \gamma_{i j}(t)}{\sum_{t=1}^{n} \sum_{k} \gamma_{i k}(t)} \\
\overline{b_{j k}}=\frac{\sum_{t=1, v(t)=v_{k}}^{n} \sum_{l} \gamma_{j l}(t)}{\sum_{t=1}^{n} \sum_{l} \gamma_{j l}(t)}
\end{gathered}
$$

Start with rough estimates of $p_{i j}$ and $b_{j k}$
Calculate improved estimates
Repeat until some convergence is reached

## Hidden Markov Models - Learning problem

Forward-Backward algorithm

| 1 | initialise $p_{i j}, b_{j k}, V^{n}$, convergence criterion $\Delta, t \leftarrow 0$ |
| :--- | :---: |
| 2 | do $t \leftarrow t+1$ |
| 3 | compute $\overline{p_{i j}(t)}$ |
| 4 | compute $\overline{b_{j k}(t)}$ |
| 5 | $p_{i j}(t) \leftarrow \overline{p_{i j}(t)}$ |
| 6 | $b_{j k}(t) \leftarrow \overline{b_{j k}(t)}$ |
| 7 | until $\max _{i, j, k}\left[p_{i j}(z)-p_{i j}(z-1), b_{j k}(t)-b_{j k}(t-1)\right]<\Delta$ |
| 8 | $($ renvergence achieved $)$ |
| 9 | end |

## Outline

Markov chains

Hidden Markov Models
Evaluation
Deconding
Learning

Probabilistic Graphical Models

## Probabilistic graphical models

Introduction

In the previous models, probabilistic inference was a prominent aspect.
We will now discuss probabilistic graphical models
Some of the classification approaches discussed earlier can be described by such models

## Probabilistic graphical models

## Introduction

In the previous models, probabilistic inference was a prominent aspect.
We will now discuss probabilistic graphical models
Some of the classification approaches discussed earlier can be described by such models

## Benefits of probabilistic graphical models

$\rightarrow$ Simple way to visualise the structure of a probabilistic model
$\rightarrow$ Insights into properties of the model, including conditional independence
$\rightarrow$ Graphical representation of complex computations required to perform inference and learning

## Probabilistic graphical models

Definition
A probabilistic graphical model comprises vertices connected by edges
Vertices represent random variables or groups of variables
Edges represent probabilistic relationships between variables


## Probabilistic graphical models

## Definition

A probabilistic graphical model comprises vertices connected by edges
Vertices represent random variables or groups of variables
Edges represent probabilistic relationships between variables


## Probabilistic graphical model

The graph captures the way in which the joint distribution over all of the random variables can be decomposed into a product of factors each depending only on a subset of variables

## Probabilistic graphical models



## Example

Consider an arbitrary joint distribution $\mathcal{P}[a, b, c]$.
We can then write

$$
\begin{aligned}
\mathcal{P}[a, b, c] & =\mathcal{P}[b \mid a, c] \mathcal{P}[a, c] \\
& =\mathcal{P}[b \mid a, c] \mathcal{P}[c \mid a] \mathcal{P}[a]
\end{aligned}
$$

## Probabilistic graphical models

## Example

Similarly we can define a joint distribution

$$
\mathcal{P}\left[x_{1}, \ldots, x_{n}\right]=\mathcal{P}\left[x_{n} \mid x_{1}, \ldots, x_{n-1}\right] \ldots \mathcal{P}\left[x_{2} \mid x_{1}\right] \mathcal{P}\left[x_{1}\right]
$$

## Probabilistic graphical models

## Example

Similarly we can define a joint distribution

$$
\mathcal{P}\left[x_{1}, \ldots, x_{n}\right]=\mathcal{P}\left[x_{n} \mid x_{1}, \ldots, x_{n-1}\right] \ldots \mathcal{P}\left[x_{2} \mid x_{1}\right] \mathcal{P}\left[x_{1}\right]
$$

These graphs are fully connected.
(One edge between every pair of nodes)

## Probabilistic graphical models

## Example

Similarly we can define a joint distribution

$$
\mathcal{P}\left[x_{1}, \ldots, x_{n}\right]=\mathcal{P}\left[x_{n} \mid x_{1}, \ldots, x_{n-1}\right] \ldots \mathcal{P}\left[x_{2} \mid x_{1}\right] \mathcal{P}\left[x_{1}\right]
$$

These graphs are fully connected.
(One edge between every pair of nodes)

The actual absence of links in the graph covers intersting information about the properties of the class of distributions represented

## Probabilistic graphical models

## Definition

A general distribution for a graph with $n$ nodes is

$$
\mathcal{P}[x]=\prod_{i=1}^{n} \mathcal{P}\left[x_{i} \mid \text { parents of vertex } x_{i}\right]
$$



## Probabilistic graphical models

## Definition

A general distribution for a graph with $n$ nodes is

$$
\mathcal{P}[x]=\prod_{i=1}^{n} \mathcal{P}\left[x_{i} \mid \text { parents of vertex } x_{i}\right]
$$



Remark: Bayesian networks are represented in this way

## Probabilistic graphical models

Example: Bayesian Curve fitting

W Polynomial coefficients
$X=\left(x_{1}, \ldots, x_{n}\right)^{T}$ Input data
$Y=\left(y_{1}, \ldots, y_{n}\right)^{T}$ Observed data (Ground truth)
$\sigma^{2}$ Noise variance
$\alpha$ representation of the precision of the Gaussian prior over $W$

$$
\mathcal{P}[Y, W]=\mathcal{P}[W] \prod_{i=1}^{n} \mathcal{P}\left[y_{i} \mid W\right]
$$

(omitting deterministic parameters)

## Probabilistic graphical models

Example: Bayesian Curve fitting

W Polynomial coefficients
$X=\left(x_{1}, \ldots, x_{n}\right)^{T}$ Input data
$Y=\left(y_{1}, \ldots, y_{n}\right)^{T}$ Observed data (Ground truth)
$\sigma^{2}$ Noise variance
$\alpha$ representation of the precision of the Gaussian prior over $W$

$$
\mathcal{P}[Y, W]=\mathcal{P}[W] \prod_{i=1}^{n} \mathcal{P}\left[y_{i} \mid W\right]
$$

(omitting deterministic parameters)


## Probabilistic graphical models

## Example: Bayesian Curve fitting

$$
\mathcal{P}\left[Y, W \mid X, \alpha, \sigma^{2}\right]=\mathcal{P}[W \mid \alpha] \prod_{i=1}^{n} \mathcal{P}\left[y_{i} \mid W, x_{i}, \sigma^{2}\right]
$$



## Probabilistic graphical models

Prediction of $\bar{y}$ given the model and a new sample $\bar{x}$ as

$$
\mathcal{P}\left[\bar{y}, Y, W \mid \bar{x}, X, \alpha, \sigma^{2}\right]=\left[\prod_{i=1}^{n} \mathcal{P}\left[y_{i} \mid W, x_{i}, \sigma^{2}\right]\right] \mathcal{P}[W \mid \alpha] \mathcal{P}\left[\bar{y} \mid \bar{x}, W, \sigma^{2}\right]
$$



## Probabilistic graphical models

Prediction of $\bar{y}$ given the model and a new sample $\bar{x}$ as
$\mathcal{P}\left[\bar{y}, Y, W \mid \bar{x}, X, \alpha, \sigma^{2}\right]=\left[\prod_{i=1}^{n} \mathcal{P}\left[y_{i} \mid W, x_{i}, \sigma^{2}\right]\right] \mathcal{P}[W \mid \alpha] \mathcal{P}\left[\bar{y} \mid \bar{x}, W, \sigma^{2}\right]$
Sum rule of probability leads to predictive distribution for $\bar{y}$ :

$$
\mathcal{P}\left[\bar{y} \mid \bar{x}, X, \alpha, Y, \sigma^{2}\right] \propto \int \mathcal{P}\left[\bar{y}, Y, W \mid \bar{x}, X, \alpha, \sigma^{2}\right] d W
$$



## Probabilistic graphical models

Conditional independence between nodes of the graph
Consider variables $a, b$ and $c$ and assume the conditional distribution

$$
\mathcal{P}[a \mid b, c]=\mathcal{P}[a \mid c]
$$

Then: $a$ is conditionally independent of $b$ given $c$

## Probabilistic graphical models

Conditional independence between nodes of the graph
Consider variables $a, b$ and $c$ and assume the conditional distribution

$$
\mathcal{P}[a \mid b, c]=\mathcal{P}[a \mid c]
$$

Then: $a$ is conditionally independent of $b$ given $c$ Notation: $a \Perp b \mid c$

## Probabilistic graphical models

Conditional independence between nodes of the graph
Consider variables $a, b$ and $c$ and assume the conditional distribution

$$
\mathcal{P}[a \mid b, c]=\mathcal{P}[a \mid c]
$$

Then: $a$ is conditionally independent of $b$ given $c$ Notation: $a \Perp b \mid c$

Importance of conditional independence in probabilistic models
Conditional independence in probabilistic models for pattern recognition

- simplifies the structure of a model and
- the computations needed to perform inference and learning


## Probabilistic graphical models

Conditional independence between nodes of the graph

Conditional independence can be read directly from the graph!

## Probabilistic graphical models

Conditional independence between nodes of the graph

Conditional independence can be read directly from the graph!

## Example

Assume a random experiment containing a biased and a fair coin.

Biased: $\mathcal{P}[$ head $]=0.8, \mathcal{P}[$ tail $]=0.2$
Fair: $\mathcal{P}[$ head $]=\mathcal{P}[$ tail $]=0.5$
The experiment consists of two steps:
(1) Choose which coin to toss

(2) Toss the coin twice

## Probabilistic graphical models

Conditional independence between nodes of the graph

Conditional independence can be read directly from the graph!

## Example

If we are ignorant of which coin we chose, the result of the first toss impacts our expectation of what we see in the second toss:
$\rightarrow$ e.g. if the first toss came out head, this will increase our expectation to see head also in
 the second toss

## Probabilistic graphical models

Conditional independence between nodes of the graph

Conditional independence can be read directly from the graph!

## Example

However, if we were given information about which coin we chose, the $x_{1}$ and $x_{2}$ independent.
$\rightarrow$ Since we know the distribution expected by both coins, knowledge of the outcome of $x_{1}$ does not change the expected outcome of $x_{2}$


## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\mathcal{P}[a, b, c]=\mathcal{P}[a \mid c] \mathcal{P}[b \mid c] \mathcal{P}[c]
$$

If none of the variables are observed, we can investigate whether $a$ and $b$ are independent by marginalizing both sides with respect to $c$ :

$$
\mathcal{P}[a, b]=\sum_{c} \mathcal{P}[a \mid c] \mathcal{P}[b \mid c] \mathcal{P}[c]
$$

Since this does not factorize into $\mathcal{P}[a] \mathcal{P}[b]$ in
 general, we conclude

$$
a \not \perp \quad b \mid \emptyset
$$

## Probabilistic graphical models

Conditional independence between nodes of the graph
If, however, $c$ is observed, we obtain

$$
\begin{aligned}
\mathcal{P}[a, b \mid c] & =\frac{\mathcal{P}[a, b, c]}{\mathcal{P}[c]} \\
& =\frac{\mathcal{P}[a \mid c] \mathcal{P}[b \mid c] \mathcal{P}[c]}{\mathcal{P}[c]} \\
& =\mathcal{P}[a \mid c] \mathcal{P}[b \mid c]
\end{aligned}
$$

And thus obtain the conditional independence property


$$
a \Perp b \mid c
$$

## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\mathcal{P}[a, b, c]=\mathcal{P}[a] \mathcal{P}[c \mid a] \mathcal{P}[b \mid c]
$$

Marginalizing over $c$ leads to

$$
\begin{aligned}
\mathcal{P}[a, b] & =\mathcal{P}[a] \sum_{c} \mathcal{P}[c \mid a] \mathcal{P}[b \mid c] \\
& =\mathcal{P}[a] \mathcal{P}[b \mid a]
\end{aligned}
$$

This does not factorize into $\mathcal{P}[a] \mathcal{P}[b]$ in general and therefore

$$
a \not \perp b \mid \emptyset
$$



## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\begin{aligned}
\mathcal{P}[a, b \mid c] & =\frac{\mathcal{P}[a, b, c]}{\mathcal{P}[c]} \\
& =\frac{\mathcal{P}[a] \mathcal{P}[c \mid a] \mathcal{P}[b \mid c]}{\mathcal{P}[c]} \\
& =\mathcal{P}[a \mid c] \mathcal{P}[b \mid c]
\end{aligned}
$$

And therefore

$$
a \Perp b \mid c
$$



## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\mathcal{P}[a, b, c]=\mathcal{P}[a] \mathcal{P}[b] \mathcal{P}[c \mid a, b]
$$

Marginalizing over $c$ leads to

$$
\mathcal{P}[a, b]=\mathcal{P}[a] \mathcal{P}[b]
$$

So, in this case, we obtain

$$
a \Perp b \mid \emptyset
$$



## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\begin{aligned}
\mathcal{P}[a, b \mid c] & =\frac{\mathcal{P}[a, b, c]}{\mathcal{P}[c]} \\
& =\frac{\mathcal{P}[a] \mathcal{P}[b] \mathcal{P}[c \mid a, b]}{\mathcal{P}[c]}
\end{aligned}
$$

Which does not in general factorize into $\mathcal{P}[a \mid c] \mathcal{P}[b \mid c]$ and so

$$
a \not \Perp b \mid c
$$

## Probabilistic graphical models

Conditional independence between nodes of the graph

$$
\begin{aligned}
\mathcal{P}[a, b \mid c] & =\frac{\mathcal{P}[a, b, c]}{\mathcal{P}[c]} \\
& =\frac{\mathcal{P}[a] \mathcal{P}[b] \mathcal{P}[c \mid a, b]}{\mathcal{P}[c]}
\end{aligned}
$$

Which does not in general factorize into $\mathcal{P}[a \mid c] \mathcal{P}[b \mid c]$ and so

$$
a \not \Perp b \mid c
$$

This rule applies also if, instead of $c$, any its descendants are observed!

## Probabilistic graphical models

Conditional independence between nodes of the graph

## D-separation

Consider a general directed graph in which $A, B$ and $C$ are arbitrary nonintersecting sets of nodes
$A$ is $d$-separated from $B$ by $C$ when all possible paths from $A$ to $B$ contain a node such that either
a) the node is in the set $C$ and the arrows meet head-to-tail or tail-to-tail
b) the node is not in the set $C$ nor any of its descendants and the arrows meet head-to-head

## Probabilistic graphical models

The concept of $d$-separation helps us to understand the probability distributions that are expressed by a particular graphical model:

## Probabilistic graphical models

The concept of $d$-separation helps us to understand the probability distributions that are expressed by a particular graphical model:

We have seen above that the joint distribution of a graph is given as its factorization:

$$
\mathcal{P}[x]=\prod_{i=1}^{n} \mathcal{P}\left[x_{i} \mid \text { parents of vertex } x_{i}\right]
$$

## Probabilistic graphical models

The concept of d-separation helps us to understand the probability distributions that are expressed by a particular graphical model:

We have seen above that the joint distribution of a graph is given as its factorization:

$$
\mathcal{P}[x]=\prod_{i=1}^{n} \mathcal{P}\left[x_{i} \mid \text { parents of vertex } x_{i}\right]
$$

The graph literally filters those distributions which can express it in terms of the factorization implied by the graph.


## Probabilistic graphical models

The concept of d-separation helps us to understand the probability distributions that are expressed by a particular graphical model:

We have seen above that the joint distribution of a graph is given as its factorization:

$$
\mathcal{P}[x]=\prod_{i=1}^{n} \mathcal{P}\left[x_{i} \mid \text { parents of vertex } x_{i}\right]
$$

The graph literally filters those distributions which can express it in terms of the factorization implied by the graph.

It can be shown that the set of distributions that pass the filter is precisely the set of distributions that fulfills the set of conditional independence properties defined by the d-separation property.

## Probabilistic graphical models

## Undirected graphical models

## Undirected graphical models

Also graphical models that are described by undirected graphs specify
a) a factorization
b) a set of conditional independence relations


## Probabilistic graphical models

Undirected graphical models
Assume three test of nodes $A, B$ and $C$ in such an undirected graph


## Probabilistic graphical models

Undirected graphical models
Assume three test of nodes $A, B$ and $C$ in such an undirected graph


## Conditional independence in undirected graphs

$A \Perp B \mid C$ if all paths between $A$ and $B$ contain an observed node from the set $C$
$A \not \Perp B \mid C$ if at least one path between $A$ and $B$ does not contain any observed node.

## Probabilistic graphical models

## Factorization rule for undirected graphs

Two nodes $a$ and $b$ in a graph are conditionally independent (given all other nodes) if they are not connected by an edge
$\rightarrow$ Since there is no direct path between the nodes

## Probabilistic graphical models

## Factorization rule for undirected graphs

Two nodes $a$ and $b$ in a graph are conditionally independent (given all other nodes) if they are not connected by an edge
$\rightarrow$ Since there is no direct path between the nodes

Therefore, the joint distribution described by the graph is given by functions of the variables of the maximal cliques in the graph

## Probabilistic graphical models

## Factorization rule for undirected graphs

Two nodes $a$ and $b$ in a graph are conditionally independent (given all other nodes) if they are not connected by an edge
$\rightarrow$ Since there is no direct path between the nodes

Therefore, the joint distribution described by the graph is given by functions of the variables of the maximal cliques in the graph


## Probabilistic graphical models



The joint distribution is written as a product of potential functions $\phi_{C}\left(X_{C}\right)$ over the maximal cliques $X_{C}$ of the graph:

$$
\mathcal{P}[X]=\frac{1}{Z} \prod_{C} \phi_{C}\left(X_{C}\right)
$$

Here, $Z$ is a normalisation constant given by

$$
Z=\sum_{X} \prod_{C} \phi_{C}\left(X_{C}\right)
$$

to ensure that the distribution $\mathcal{P}[X]$ is correctly normalised.

## Probabilistic graphical models



The joint distribution is written as a product of potential functions $\phi_{C}\left(X_{C}\right)$ over the maximal cliques $X_{C}$ of the graph:

$$
\mathcal{P}[X]=\frac{1}{Z} \prod_{C} \phi_{C}\left(X_{C}\right)
$$

Here, $Z$ is a normalisation constant given by

$$
Z=\sum_{X} \prod_{C} \phi_{C}\left(X_{C}\right)
$$

## Gibbs distribution

to ensure that the distribution $\mathcal{P}[X]$ is correctly normalised.

## Probabilistic graphical models

Conditional random fields
Distinguishing between observed variables $X$ and target variables
$Y$, in the unnormalized measure

$$
\mathcal{P}[X, Y]=\prod_{C} \phi_{C}\left(X_{C}\right)
$$

we can define a conditional random field as

$$
\begin{aligned}
\mathcal{P}[Y \mid X] & =\frac{1}{Z(X)} \prod_{C} \phi_{C}\left(X_{C}\right) \\
Z(X) & =\sum_{X} \mathcal{P}[X, Y]
\end{aligned}
$$

## Probabilistic graphical models

## Conditional random fields

Distinguishing between observed variables $X$ and target variables
$Y$, in the unnormalized measure

$$
\mathcal{P}[X, Y]=\prod_{C} \phi_{C}\left(X_{C}\right)
$$

we can define a conditional random field as

$$
\begin{aligned}
\mathcal{P}[Y \mid X] & =\frac{1}{Z(X)} \prod_{C} \phi_{C}\left(X_{C}\right) \\
Z(X) & =\sum_{X} \mathcal{P}[X, Y]
\end{aligned}
$$

Compared to the Bayesian models represented in directed graphs, the CRF removes from the model any dependency between the input variables $x_{i}$

## Outline

Markov chains

Hidden Markov Models
Evaluation
Deconding
Learning

Probabilistic Graphical Models

## Questions?

Stephan Sigg<br>stephan.sigg@cs.uni-goettingen.de

## Literature

- C.M. Bishop: Pattern recognition and machine learning, Springer, 2007.
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001.



[^0]:    ${ }^{1}$ A. Kolmogorov, Anfangsgründe der Theorie der Markoffschen Ketten mit unendlich vielen möglichen Zuständen, 1936.

[^1]:    ${ }^{2}$ William Feller, An introduction to probability theory and its applications, Wiley, 1968.

[^2]:    Machine Learning and Pervasive Computing

[^3]:    ${ }^{3}$ Richard O. Duda, Peter E. Hart and David G. Stork, Pattern classification, Wiley interscience, 2001.

