## Syllabus

Fri. 27.10. (1) 0. Introduction
A. Supervised Learning: Linear Models \& Fundamentals

Fri. 3.11. (2) A. 1 Linear Regression
Fri. 10.11. (3) A. 2 Linear Classification
Fri. 17.11. (4) A. 3 Regularization
Fri. 24.11. (5) A. 4 High-dimensional Data
B. Supervised Learning: Nonlinear Models

Fri. 1.12. (6) B. 1 Nearest-Neighbor Models
Fri. 8.12. (7) B. 4 Support Vector Machines
Fri. 15.12. (8) B. 3 Decision Trees
Fri. 22.12. (9) B. 2 Neural Networks

- Christmas Break -

Fri. 12.1. (10) B. 5 A First Look at Bayesian and Markov Networks

## C. Unsupervised Learning

Fri. 19.1. (11) C. 1 Clustering
Fri. 26.1. (12) C. 2 Dimensionality Reduction
Fri. 2.2. (13) C. 3 Frequent Pattern Mining
Fri. 9.2. (14) Q\&A
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Machine Learning

## Outline

1. Introduction
2. Examples
3. Inference
4. Learning

## Outline

## 1. Introduction

## 2. Examples

## 3. Inference

## 4. Learning

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## Machine Learning

## Joint Distribution

$x_{1}$ : the sun shines

$$
\left.\left.\begin{array}{l}
p\left(x_{1}=\text { false }\right)=0.25 \\
p\left(x_{1}=\text { true }\right)=0.75
\end{array}\right\} \equiv p\left(x_{1}\right)=\left\lvert\, \begin{array}{ll}
\text { false } & \text { true } \\
\begin{array}{ll}
0.25 & 0.75
\end{array}=(0.25,0.75) \text { ) } n=0
\end{array}\right.\right\}
$$

## Joint Distribution

$x_{1}$ : the sun shines

$$
\left.\left.\begin{array}{l}
p\left(x_{1}=\text { false }\right)=0.25 \\
p\left(x_{1}=\text { true }\right)=0.75
\end{array}\right\} \equiv p\left(x_{1}\right)=\begin{array}{ll}
\text { false } & \text { true } \\
\begin{array}{ll}
0.25 & 0.75
\end{array}=(0.25,0.75) \text { ) }
\end{array}\right\}
$$

$x_{2}$ : it rains

$$
\left.\begin{array}{l}
p\left(x_{2}=\text { false }\right)=0.67 \\
p\left(x_{2}=\text { true }\right)=0.33
\end{array}\right\} \equiv p\left(x_{2}\right)=\left\lvert\, \begin{array}{ll}
\text { false } & \text { true } \\
\hline 0.67 & 0.33
\end{array}=(0.67,0.33)\right.
$$

## Joint Distribution

$x_{1}$ : the sun shines

$$
\left.\left.\begin{array}{l}
p\left(x_{1}=\text { false }\right)=0.25 \\
p\left(x_{1}=\text { true }\right)=0.75
\end{array}\right\} \equiv p\left(x_{1}\right)=\left\lvert\, \begin{array}{ll}
\text { false } & \text { true } \\
\begin{array}{ll}
0.25 & 0.75
\end{array}=(0.25,0.75) \text { ) } n=(0)
\end{array}\right.\right\}
$$

$x_{2}$ : it rains

$$
\left.\begin{array}{l}
p\left(x_{2}=\text { false }\right)=0.67 \\
p\left(x_{2}=\text { true }\right)=0.33
\end{array}\right\} \equiv p\left(x_{2}\right)=\left\lvert\, \begin{array}{ll}
\text { false } & \text { true } \\
\hline 0.67 \quad 0.33
\end{array}=(0.67,0.33)\right.
$$

joint distribution:

$$
\left.\begin{array}{ll}
p\left(x_{1}=\text { false }, x_{2}=\text { false }\right) & =0.07 \\
p\left(x_{1}=\text { false }, x_{2}=\text { true }\right) & =0.18 \\
p\left(x_{1}=\text { true }, x_{2}=\text { false }\right) & =0.6 \\
p\left(x_{1}=\text { true }, x_{2}=\text { true }\right) & =0.15
\end{array}\right\} \equiv
$$

## Joint Distribution

$x_{1}$ : the sun shines

$$
\left.\begin{array}{l}
p\left(x_{1}=\text { false }\right)=0.25 \\
p\left(x_{1}=\text { true }\right)=0.75
\end{array}\right\} \equiv p\left(x_{1}\right)=\begin{array}{|ll}
\text { false } & \text { true } \\
\begin{array}{ll}
0.25 & 0.75
\end{array}=(0.25,0.75)
\end{array}
$$

$x_{2}$ : it rains

$$
\left.\begin{array}{l}
p\left(x_{2}=\text { false }\right)=0.67 \\
p\left(x_{2}=\text { true }\right)=0.33
\end{array}\right\} \equiv p\left(x_{2}\right)=\left\lvert\, \begin{array}{ll}
\text { false } & \text { true } \\
\hline 0.67 & 0.33
\end{array}=(0.67,0.33)\right.
$$

joint distribution:

$$
=\left(\begin{array}{ll}
0.07 & 0.18 \\
0.6 & 0.15
\end{array}\right)
$$

Machine Learning

## Independence

for two variables:

$$
p(x, y)=p(x) \cdot p(y)
$$

for two variable subsets:

$$
p\left(x_{1}, x_{2}, \ldots, x_{M}\right)=p\left(x_{l}\right) \cdot p\left(x_{J}\right), \quad I, J \subseteq\{1, \ldots, M\}, I \cap J=\emptyset
$$

Note: $x_{I}:=\left\{x_{m_{1}}, x_{m_{2}}, \ldots, x_{m_{K}}\right\}$ for $I:=\left\{m_{1}, m_{2}, \ldots, m_{K}\right\}$.

## Independence

for two variables:

$$
p(x, y)=p(x) \cdot p(y)
$$

for two variable subsets:

$$
p\left(x_{1}, x_{2}, \ldots, x_{M}\right)=p\left(x_{I}\right) \cdot p\left(x_{J}\right), \quad I, J \subseteq\{1, \ldots, M\}, I \cap J=\emptyset
$$

## Examples:

$\left(\begin{array}{ll}0.07 & 0.18 \\ 0.6 & 0.15\end{array}\right)$
not independent
$\left(\begin{array}{ll}0.17 & 0.08 \\ 0.5 & 0.25\end{array}\right)$
independent

Note: $x_{I}:=\left\{x_{m_{1}}, x_{m_{2}}, \ldots, x_{m_{K}}\right\}$ for $I:=\left\{m_{1}, m_{2}, \ldots, m_{K}\right\}$.
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## Chain Rule

$$
\begin{aligned}
p\left(x_{1}, x_{2}, \ldots, x_{M}\right)= & p\left(x_{1}\right) \\
& \cdot p\left(x_{2} \mid x_{1}\right) \\
& \cdot p\left(x_{3} \mid x_{1}, x_{2}\right) \\
& \vdots \\
& \cdot p\left(x_{M} \mid x_{1}, x_{2}, \ldots, x_{M-1}\right)
\end{aligned}
$$

## Chain Rule

$$
\begin{aligned}
p\left(x_{1}, x_{2}, \ldots, x_{M}\right)= & p\left(x_{1}\right) \\
& \cdot p\left(x_{2} \mid x_{1}\right) \\
& \cdot p\left(x_{3} \mid x_{1}, x_{2}\right) \\
& \vdots \\
& \cdot p\left(x_{M} \mid x_{1}, x_{2}, \ldots, x_{M-1}\right)
\end{aligned}
$$

## Examples:

$$
\left(\begin{array}{ll}
0.07 & 0.18 \\
0.6 & 0.15
\end{array}\right)=(0.25,0.75) \cdot\left(\begin{array}{ll}
0.28 & 0.72 \\
0.8 & 0.2
\end{array}\right)
$$

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## Machine Learning

## Chain Rule

$$
\begin{aligned}
p\left(x_{1}, x_{2}, \ldots, x_{M}\right)= & p\left(x_{1}\right) \\
& \cdot p\left(x_{2} \mid x_{1}\right) \\
& \cdot p\left(x_{3} \mid x_{1}, x_{2}\right) \\
& \vdots \\
& \cdot p\left(x_{M} \mid x_{1}, x_{2}, \ldots, x_{M-1}\right)
\end{aligned}
$$

## Examples:

$$
\left(\begin{array}{ll}
0.17 & 0.08 \\
0.5 & 0.25
\end{array}\right)=(0.25,0.75) \cdot\left(\begin{array}{ll}
0.67 & 0.33 \\
0.67 & 0.33
\end{array}\right)
$$

## Conditional Independence

two variables $x, y$ are independent conditionally on variable $z$ :

$$
\begin{aligned}
x \perp y \mid z: \Leftrightarrow p(x, y \mid z)= & p(x \mid z) \\
& \cdot p(y \mid z)
\end{aligned}
$$

two variable sets are independent conditionally on variables $z_{1}, \ldots, z_{K}$ :

$$
\begin{aligned}
\left\{x_{1}, \ldots, x_{l}\right\} \perp\left\{y_{1}, \ldots, y_{J}\right\} \mid\left\{z_{1}, \ldots, z_{K}\right\}: \Leftrightarrow & \\
\qquad p\left(x_{1}, \ldots, x_{l}, y_{1}, \ldots, y_{J} \mid z_{1}, \ldots, z_{K}\right)= & p\left(x_{1}, \ldots, x_{I} \mid z_{1}, \ldots, z_{K}\right) \\
& \cdot p\left(y_{1}, \ldots, y_{J} \mid z_{1}, \ldots, z_{K}\right)
\end{aligned}
$$

## Conditional Independence / Example

Example:

$$
\begin{array}{r}
x_{n} \perp\left\{x_{1}, \ldots, x_{n-1}\right\} \mid x_{n-1} \quad \forall n \text { (Markov property) } \\
\rightsquigarrow p\left(x_{1}, \ldots, x_{N}\right)=p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{2}\right) \cdots p\left(x_{M} \mid x_{M-1}\right)
\end{array}
$$

## Graphical Models

- represent joint distributions of variables by graphs
- by directed graphs: Bayesian networks
- by undirected graphs: Markov networks
- by mixed directed/undirected graphs.
- nodes represent random variables
- absent edges represent conditional independence


## Directed Graph Terminology

- directed graph: $G:=(V, E), E \subseteq V \times V$
- $V$ set called nodes / vertices
- $E$ called edges, $(v, w) \in E$ edge from $v$ to $w$.
- adjacency matrix $A \in\{0,1\}^{N \times N}$

$$
A_{v, w}:=\delta((v, w) \in E), \quad v, w \in\{1, \ldots, N\}, N:=|V|
$$

- parents: $\operatorname{pa}(v):=\{w \in V \mid(w, v) \in E\}$
- children: $\operatorname{ch}(v):=\{w \in V \mid(v, w) \in E\}$
- neighbors: $\operatorname{nbr}(v):=\operatorname{pa}(v) \cup \mathrm{ch}(v)$
- family: fam $(v):=\mathrm{pa}(v) \cup\{v\}$
- root: $v$ without parents.
- leaf: $v$ without children.

Note: $\delta(P):=1$ if proposition $P$ is true, $:=0$ otherwise.

[Murphy, 2012, fig. 10.1a

## Directed Graph Terminology

- path: $p \in V^{*}:\left(p_{i}, p_{i+1}\right) \in E$ for all $i$.
- $p=\left(p_{1}, \ldots, p_{M}\right), p_{m} \in V$
- length $|p|:=M$
- starts at $p_{1}$
- ends at $p_{M}$
- paths $G^{*}:=\left\{p \in V^{*}\left|\left(p_{i}, p_{i+1}\right) \in E \quad \forall i=1, \ldots,|p|-1\right\}\right.$.
- $v \rightsquigarrow w$ : exists path from $v$ to $w$, i.e., $p \in G^{*}: p_{1}=v, p_{|p|}=w$.
- ancestors: $\operatorname{anc}(v):=\{w \in V \mid w \rightsquigarrow v\}$
- descendants: $\operatorname{desc}(v):=\{w \in V \mid v \rightsquigarrow w\}$
- in-degree $|\mathrm{pa}(\mathrm{v})|$
- out-degree $|c h(v)|$
- degree $|\operatorname{nbr}(v)|$

[Murphy, 2012, fig. 10.1a

Note: $V^{*}:=\bigcup_{M \in \mathbb{N}} V^{M}$ finite $V$-sequences.

## Directed Graph Terminology

- cycle/loop at $v: v \rightsquigarrow v$
- self loop: $(v, v) \in E$
- directed acyclic graph / DAG: directed graph without cycles.
- topological ordering: directed graph without cycles.
- numbering of the nodes s.t. all nodes have lower number than their children.
- exists for DAGs.

[Murphy, 2012, fig. 10.1a


## Bayesian Networks / Directed Graphical Models

A Bayesian network (aka directed graphical model) is a set of conditional probability distributions/densities (CPDs)

$$
p\left(x_{m} \mid x_{\operatorname{cttt}(m)}\right), \quad m \in\{1, \ldots, M\}
$$

s.t. the graph defined by

$$
\begin{aligned}
& V:=\{1, \ldots, M\} \\
& E:=\{(n, m) \mid m \in V, n \in \operatorname{ctxt}(m)\}, \quad \text { i.e., } \operatorname{pa}(m):=\operatorname{ctxt}(m)
\end{aligned}
$$

is a DAG.
A Bayesian network defines a factorization of the joint distribution

$$
p\left(x_{1}, \ldots, x_{M}\right)=\prod_{m=1}^{M} p\left(x_{m} \mid x_{\mathrm{pa}(m)}\right)
$$

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## Bayesian Networks / Example

 For the DAG below,$$
p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{1}\right) p\left(x_{4} \mid x_{2}, x_{3}\right) p\left(x_{5} \mid x_{3}\right)
$$


[Murphy, 2012, fig. 10.1a

## Bayesian Networks / Example

For the DAG below,

$$
p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{1}\right) p\left(x_{4} \mid x_{2}, x_{3}\right) p\left(x_{5} \mid x_{3}\right)
$$

If

- all variables are binary and
- all CPDs given as conditional probability tables (CPTs), then the BN is defined by the following 5 CPTs :


|  | $x_{1}$ |  |
| :--- | :--- | :--- |
| $x_{2}$ | 0 | 1 |
| 0 | $\cdots$ | $\cdots$ |
| 1 | $\cdots$ | $\cdots$ |


|  | $x_{1}$ |  |
| :--- | :--- | :--- |
| $x_{3}$ | 0 | 1 |
| 0 | $\cdots$ | $\cdots$ |
| 1 | $\cdots$ | $\cdots$ |


|  | $x_{2}$ | 0 |  | 1 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | $x_{3}$ | 0 | 1 | 0 | 1 |
| $x_{4}$ | 0 | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
|  | 1 | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |


|  | $x_{3}$ |  |
| :--- | :--- | :--- |
| $x_{5}$ | 0 | 1 |
| 0 | $\cdots$ | $\cdots$ |
| 1 | $\cdots$ | $\cdots$ |


[Murphy, 2012, fig. 10.1a

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Machine Learning

## Outline

## 1. Introduction

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## Naive Bayes Classifier

$$
\begin{aligned}
p\left(y, x_{1}, \ldots, x_{M}\right) & =p(y) p\left(x_{1} \mid y\right) p\left(x_{2} \mid y\right) \cdots p\left(x_{M} \mid y\right) \\
& =p(y) \prod_{m=1}^{M} p\left(x_{m} \mid y\right)
\end{aligned}
$$



Naive Bayes Classifier


Tree Augmented Naive Bayes
[Murphy, 2012, fig. 10.2]

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## Machine Learning

## Medical Diagnosis

- bipartite graph
- observed variables $x_{1}, \ldots, x_{M}$ (symptoms)
- hidden variables $z_{1}, \ldots, z_{K}$ (diseases / causes)

$$
p\left(x_{1}, \ldots, x_{M}, z_{1}, \ldots, z_{M}\right)=\prod_{k=1}^{K} p\left(z_{k}\right) \prod_{m=1}^{M} p\left(x_{m} \mid z_{\mathrm{pa}(m)}\right)
$$



Note: In the diagram $z$ is called $h$ and $x$ is called $v$.

## Markov Models

first order:

$$
\begin{aligned}
p\left(x_{1}, \ldots, x_{M}\right) & =p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{2}\right) \cdots p\left(x_{M} \mid x_{M-1}\right) \\
& =p\left(x_{1}\right) \prod_{m=1}^{M-1} p\left(x_{m+1} \mid x_{m}\right)
\end{aligned}
$$

## Markov Models / Second Order

second order:

$$
\begin{aligned}
p\left(x_{1}, \ldots, x_{M}\right) & =p\left(x_{1}, x_{2}\right) p\left(x_{3} \mid x_{1}, x_{2}\right) p\left(x_{4} \mid x_{2}, x_{3}\right) \cdots p\left(x_{M} \mid x_{M-2}, x_{M-1}\right) \\
& =p\left(x_{1}, x_{2}\right) \prod_{m=2}^{M-1} p\left(x_{m+1} \mid x_{m-1}, x_{m}\right)
\end{aligned}
$$

## Hidden Markov Models

- observed variables $x_{1}, \ldots, x_{M}$
- hidden variables $z_{1}, \ldots, z_{M}$

$$
p\left(x_{1}, \ldots, x_{M}, z_{1}, \ldots, z_{M}\right)=p\left(z_{1}\right) \prod_{m=1}^{M-1} p\left(z_{m+1} \mid z_{m}\right) \prod_{m=1}^{M} p\left(x_{m} \mid z_{m}\right)
$$

- transition model $p\left(z_{m+1} \mid z_{m}\right)$
- observation model $p\left(x_{m} \mid z_{m}\right)$

[Murphy, 2012, fig. 10.4]

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Machine Learning

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## The Probabilistic Inference Problem

Given

- a Bayesian network model $\theta:=G=(V, E)$,
- a query consisting of
- a set $X:=\left\{x_{1}, \ldots, x_{M}\right\} \subseteq V$ of predictor variables (aka observed, visible variables)
- with a value $v_{m}$ for each $x_{m}(m=1, \ldots, M)$ and
- a set $Y:=\left\{y_{1}, \ldots, y_{J}\right\} \subseteq V$ of target variables (aka query variables), with $X \cap Y=\emptyset$,
compute

$$
\begin{aligned}
& p(Y \mid X=v ; \theta):=p\left(y_{1}, \ldots, y_{J} \mid x_{1}=v_{1}, x_{2}=v_{2}, \ldots, x_{M}=v_{M} ; \theta\right) \\
= & \left(p\left(y_{1}=w_{1}, \ldots, y_{J}=w_{J} \mid x_{1}=v_{1}, x_{2}=v_{2}, \ldots, x_{M}=v_{M} ; \theta\right)\right)_{w_{1}, \ldots, w_{J}}
\end{aligned}
$$

Variables that are neither predictor variables nor target variables are called nuisance variables.

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## Inference Without Nuisance Variables

Without nuisance variables: $V=X \dot{\cup} Y$.

$$
p(Y \mid X=v ; \theta) \stackrel{\text { def }}{=} \frac{p(X=v, Y ; \theta)}{p(X=v ; \theta)}=\frac{p(X=v, Y ; \theta)}{\sum_{w} p(X=v, Y=w ; \theta)}
$$

- first, clamp predictors $X$ to their observed values $v$,
- then, normalize $p(X=v, Y ; \theta)$ to sum to 1 (over $Y$ ).
- $p(X=v ; \theta)$ likelihood of the data / probability of evidence is a constant.


## Inference With Nuisance Variables

Nuisance variables: $Z:=\left\{z_{1}, \ldots, z_{K}\right\}:=V \backslash(X \dot{\cup} Y)$.

1. add to target variables
2. answer resulting query without nuisance variables: $p(Y, Z \mid X)$.
3. marginalize out nuisance variables:

$$
p(Y \mid X=v ; \theta) \stackrel{\text { marginalization }}{=} \sum_{u} p(Y, Z=u \mid X=v ; \theta)
$$

Note: Summation over $u$ is over all possible values of variables $Z$.
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## Inference With Nuisance Variables

Nuisance variables: $Z:=\left\{z_{1}, \ldots, z_{K}\right\}:=V \backslash(X \dot{\cup} Y)$.

1. add to target variables
2. answer resulting query without nuisance variables: $p(Y, Z \mid X)$.
3. marginalize out nuisance variables:

$$
p(Y \mid X=v ; \theta) \stackrel{\text { marginalization }}{=} \sum_{u} p(Y, Z=u \mid X=v ; \theta)
$$

Caveat: This is a naive algorithm never used in practice. See BN lecture for practically useful BN inference algorithms.

Note: Summation over $u$ is over all possible values of variables $Z$.

## Complexity of Inference

- for simplicity assume
- all $M$ predictor variables are nominal with $L$ levels,
- all $K$ nuisance variables are nominal with $L$ levels,
- a single target variable: $Y=\{y\}, J=1$ also nominal with $L$ levels.
- without (Conditional) Independencies:
- full table $p$ requires $L^{M+K+1}-1$ cells storage.
- inference requires $O\left(L^{K+1}\right)$ operations.
- for each $Y=w$ sum over all $L^{K}$ many $Z=u$.
- with (Conditional) Independencies / Bayesian network:
- CPDs $p$ require $O\left((M+K+1) L^{\text {max indegree }+1}\right)$ cells storage.
- inference requires $O\left((K+1) L^{\text {treewidth }+1}\right)$ operations.
- treewidth=1 for a chain!

Note: See the Bayesian networks lecture for BN inference algorithms.

## Outline

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## Learning Bayesian Networks

- parameter learning: given
- the structure of the network (graph G) and
- a regularization penalty $\operatorname{Reg}(\theta)$,
- data $x_{1}, \ldots, x_{N}$,
learn the CPDs $p$.

$$
\hat{\theta}:=\underset{\theta}{\arg \max } \sum_{n=1}^{N} \log p\left(x_{n} ; \theta\right)-\operatorname{Reg}(\theta)
$$

- structure learning: given
- data,
learn the structure $G$ and the CPDs $p$.


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## Bayesian Approach

- in the Bayesian approach, parameters are also considered to be random variables, thus,
- learning is just a special type of inference (with the parameters as targets)
- information about the distribution of the parameters before seeing the data is required (prior distribution $p(\theta)$ )
- parameter learning: given
- the structure of the network (graph G) and
- a prior distribution $p(\theta)$ of the parameters,
- data $x_{1}, \ldots, x_{N}$,
learn the CPDs $p$.

$$
\hat{\theta}:=\underset{\theta}{\arg \max } \sum_{n=1}^{N} \log p\left(x_{n} ; \theta\right)+\log p(\theta)
$$

## Plate Notation

- variables on plates are duplicated
- the number of copies is given in the lower right corner.
- an index is used to differentiate copies of the same variable.

Example 1: data $x_{1}, \ldots, x_{N}$ is independently identically distributed (iid)

[Murphy, 2012, fig. 10.7]
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## Plate Notation

- variables on plates are duplicated
- the number of copies is given in the lower right corner.
- an index is used to differentiate copies of the same variable.
- variables being in several plates will be duplicated for every combination, i.e., have several indices.
- for clarity, the index should be added to the plate (but often is omitted).
Example 2: Naive Bayes classifier.



## Learning from Complete Data

Likelihood decomposes w.r.t. graph structure:

$$
\begin{aligned}
p(\mathcal{D} \mid \theta): & =\prod_{n=1}^{N} p\left(x_{n} \mid \theta\right) \\
& =\prod_{n=1}^{N} \prod_{m=1}^{M} p\left(x_{n, m} \mid x_{n, \mathrm{pa}(m)}, \theta_{m}\right) \\
& =\prod_{m=1}^{M} \prod_{n=1}^{N} p\left(x_{n, m} \mid x_{n, \mathrm{pa}(m)}, \theta_{m}\right) \\
& =\prod_{m=1}^{M} p\left(\mathcal{D}_{m} \mid \theta_{m}\right)
\end{aligned}
$$

where $\theta_{m}$ are the parameters of $p\left(x_{m} \mid \mathrm{pa}(m)\right)$
Note: In Bayesian contexts, often $p(\ldots \mid \theta)$ is used instead of $p(\ldots ; \theta)$.

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## Learning from Complete Data

If the prior also factorizes,

$$
p(\theta)=\prod_{m=1}^{M} p\left(\theta_{m}\right)
$$

then the posterior factorizes as well

$$
p(\theta \mid \mathcal{D}) \propto p(\mathcal{D} \mid \theta) p(\theta)=\prod_{m=1}^{M} p\left(\mathcal{D}_{m} \mid \theta_{m}\right) p\left(\theta_{m}\right)
$$

and the parameters $\theta_{m}$ of each CPD can be estimated independently.

[^0]
## Learning from Complete Data / Dirichlet Prior

If

- all variables are nominal,
- variable $m$ has $L_{m}$ levels ( $m=1, \ldots, M$ ), and
- all CPDs are described by conditional probability tables (CPTs)

$$
\begin{aligned}
p\left(x_{m} \mid x_{\mathrm{pa}(m)}\right)= & \theta_{m, c, l}, \quad c:=x_{\mathrm{pa}(m)}, l:=x_{m} \\
& \text { with } \sum_{l=1}^{L} \theta_{m, c, l}=1, \quad \forall m, c
\end{aligned}
$$

a Dirichlet distribution for each row in the CPT

$$
\theta_{m, c, \cdot} \sim \operatorname{Dir}\left(\alpha_{m, c}\right), \quad \alpha_{m, c} \in\left(\mathbb{R}_{0}^{+}\right)^{L_{m}}
$$

is a useful prior.

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## Learning from Complete Data / Dirichlet Prior

Then the posterior $p\left(\theta_{m, c, .} \mid \mathcal{D}\right)$ is also Dirichlet:

$$
\begin{aligned}
\theta_{m, c, \cdot} \mid \mathcal{D} & \sim \operatorname{Dir}\left(\alpha_{m, c}+N_{m, c}\right) \\
N_{m, c, l} & :=\sum_{n=1}^{N} \delta\left(x_{n, m}=I, x_{n, \mathrm{pa}(m)=c}\right)
\end{aligned}
$$

with mean $\bar{\theta}_{m, c, l}=\frac{N_{m, c, l}+\alpha_{m, c, l}}{\sum_{l^{\prime}=1}^{L} N_{m, c, l^{\prime}}+\alpha_{m, c, l^{\prime}}}$

## Learning from Complete Data / Example

 graph structure: data:

| $x_{1}$ | $x_{2}$ | $x_{3}$ | $x_{4}$ | $x_{5}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | 1 | 1 |
| 1 | 1 | 0 | 1 | 0 |
| 0 | 1 | 1 | 0 | 0 |
| 0 | 1 | 1 | 1 | 0 |

prior:

$$
\begin{array}{r}
p\left(\theta_{m, c}\right):=\operatorname{Dir}(1,1) \\
\forall m, c
\end{array}
$$

learned parameters for CPT of $x_{4}(m=4)$ :


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Machine Learning

## Learning BN from Complete Data / Algorithm

learn-bn-params $\left(\mathcal{D}^{\text {train }}:=\left\{x_{1}, \ldots, x_{N}\right\} \subset \mathcal{X}_{1} \times \cdots \times \mathcal{X}_{M}, G, \alpha\right)$ :
for $n:=1: N$ : for $m:=1: M$ :
$\alpha_{m, \chi_{n, m}, \chi_{n, p(m)}}+=1$
return $\alpha$
where

- $\mathcal{X}_{m}:=\left\{1, \ldots, L_{m}\right\}$ discrete domains of variable $X_{m}$
(having $L_{m}$ different levels)
- $G$ is a DAG on $\{1, \ldots, M\}$
- $\left(\alpha_{m, l, c}\right)_{m=1: M, l=1: L_{m}, c \in \prod_{c \in \operatorname{pap}(m)} L_{c} \geq 0 \text { the Dirichlet prior of the parameters }}$


## Learning with Missing and/or Hidden Variables

Learning with

- missing values or
- hidden variables
is more complicated as
- the likelihood no longer factorizes and
- neither is convex.
$\rightsquigarrow$ use iterative approximation algorithms to find a local MAP or ML minimum.

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## Summary

- Bayesian Networks define a joint probability distribution by a factorization of conditional probability distributions (CPDs) $p\left(x_{n} \mid \mathrm{pa}\left(x_{n}\right)\right)$
- Conditions pa( $m$ ) form a DAG.
- For nominal variables, all CPDs can be represented as tables (CPTs).
- Storage complexity is $O\left(L^{\text {max indegree+1 }}\right)$ (instead of $O\left(L^{M}\right)$ ).
- Many model classes essentially are Bayesian networks:
- Naive Bayes classifier, Markov Models, Hidden Markov Models
- Inference in BN means to compute the (marginal joint) distribution of target variables given observed evidence of some predictor variables.
- A Bayesian network can answer queries for arbitrary targets (not just a predefined one as most predictive models).
- Nuisance variables (for a query) are variables neither observed nor used as targets.
- Inference with nuisance variables can be done efficiently for DAGs with small tree width.


## Summary (2/2)

- Learning BN has to distinguish between
- parameter learning: learn just the CPDs for a given graph, vs.
- structure learning: learn both, graph and CPDs.
- Parameter learning the maximum aposteriori (MAP) for BN with CPTs and Dirichlet prior can be done simply by counting the frequencies of families in the data.


## Further Readings

- [Murphy, 2012, chapter 10].


## References

Kevin P. Murphy. Machine Learning: A Probabilistic Perspective. The MIT Press, 2012.


[^0]:    Note: In Bayesian contexts, often $p(\ldots \mid \theta)$ is used instead of $p(\ldots ; \theta)$.

