## Advanced AI Techniques

## I. Bayesian Networks / 3. Parameter Learning with Missing Values

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## 1. Incomplete Data

## 2. Incomplete Data for Parameter Learning (EM algorithm)

## 3. An Example

Let $V$ be a set of variables. A complete case is a function

$$
c: V \rightarrow \bigcup_{v \in V} \operatorname{dom}(V)
$$

with $c(v) \in \operatorname{dom}(V)$ for all $v \in V$.

## A incomplete case (or a case with

 missing data) is a complete case $c$ for a subset $W \subseteq V$ of variables. We denote $\operatorname{var}(c):=W$ and say, the values of the variables $V \backslash W$ are missing or not observed.A data set $D \in \operatorname{dom}(V)^{*}$ that contains complete cases only, is called complete data; if it contains an incomplete case, it is called

## incomplete data.

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| case | $F$ | $L$ | $B$ | $D$ | $H$ |
| ---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 | 0 | 0 |
| 3 | 1 | 1 | 1 | 1 | 0 |
| 4 | 0 | 0 | 1 | 1 | 1 |
| 5 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | 0 | 0 | 1 | 1 |
| 8 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 1 | 1 | 1 |
| 10 | 1 | 1 | 0 | 1 | 1 |

Figure 1: Complete data for $V:=\{F, L, B, D, H\}$.

| case | $F$ | $L$ | $B$ | $D$ | $H$ |
| ---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | . | 0 | 0 | 0 | 0 |
| 3 | 1 | 1 | 1 | 1 | 0 |
| 4 | 0 | 0 | . | 1 | 1 |
| 5 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | . | 0 | . | 1 |
| 8 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 1 | 1 | 1 |
| 10 | 1 | 1 | . | 1 | 1 |

Figure 2: Incomplete data for marked by a dot.

Advanced AI Techniques / 1. Incomplete Data

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For each variable $v$, we can interpret its missing of values as new random variable $M_{v}$,

$$
M_{v}:= \begin{cases}1, & \text { if } v_{\mathrm{obs}}=. \\ 0, & \text { otherwise }\end{cases}
$$

called missing value indicator of $v$.

| case | F | $M_{F}$ | L | $M_{L}$ | B | $M_{B}$ | D | $M_{D}$ | H | $M_{H}$ |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | . | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 1 | 0 | 1 | 0 | 1 | 0 | 1 | 0 | 0 | 0 |
| 4 | 0 | 0 | 0 | 0 | . | 1 | 1 | 0 | 1 | 0 |
| 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | 0 | . | 1 | 0 | 0 | . | 1 | 1 | 0 |
| 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 1 | 0 |
| 10 | 1 | 0 | 1 | 0 | . | 1 | 1 | 0 | 1 | 0 |

Figure 3: Incomplete data for $V:=\{F, L, B, D, H\}$ and missing value indicators.

| case | $v_{\text {true }}$ | $v_{\text {observed }}$ |
| ---: | :---: | :---: |
| 1 | 1 | . |
| 2 | 2 | 2 |
| 3 | 2 | . |
| 4 | 4 | 4 |
| 5 | 3 | 3 |
| 6 | 2 | 2 |
| 7 | 1 | 1 |
| 8 | 4 | . |
| 9 | 3 | 3 |
| 10 | 2 | . |
| 11 | 1 | 1 |
| 12 | 3 | . |
| 13 | 4 | 4 |
| 14 | 2 | 2 |
| 15 | 2 | 2 |

Figure 4: Data with a variable $v$ MCAR. Missing values are stroken through.
unbiased estimator for the expectation of $v_{\text {true }}$; here

$$
\begin{aligned}
\hat{\mu}\left(v_{\text {obs }}\right) & =\frac{1}{10}(2 \cdot 1+4 \cdot 3+2 \cdot 3+2 \cdot 4) \\
& =\frac{1}{15}(3 \cdot 1+6 \cdot 3+3 \cdot 3+3 \cdot 4)=\hat{\mu}\left(v_{\text {true }}\right)
\end{aligned}
$$

the probability of missing is the same, and, e.g., the sample mean of $v_{\text {obs }}$ is an
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Advanced AI Techniques / 1. Incomplete Data
Types of missingness / MAR
A variable $v \in V$ is called missing at random (MAR), if the probability of a missing value is conditionally independent of the (true, unobserved) value of $v$, i.e, if

$$
I\left(M_{v}, v_{\text {true }} \mid W\right)
$$

for some set of variables $W \subseteq V \backslash\{v\}$ (MAR is also called missing conditionally at random).

Example: think of an apparatus measuring the velocity $v$ of wind. If we measure wind velocities at three different heights $h=0,1,2$ and say the apparatus has problems with height not recording
$1 / 3$ of cases at height 0 ,
$1 / 2$ of cases at height 1 ,
$2 / 3$ of cases at height 2 ,


Figure 5: Data with a variable $v$ MAR (conditionally on $h$ ).
then $v$ is missing at random (conditionally on $h$ ).

If $v$ depends on variables in $W$, then, e.g., the sample mean is not an unbiased estimator, but the weighted mean w.r.t. $W$ has to be used; here:

$$
\begin{aligned}
& \sum_{h=0}^{2} \hat{\mu}(v \mid H=h) p(H=h) \\
&= 2 \cdot \frac{9}{22}+3.5 \cdot \frac{4}{22}+4 \cdot \frac{9}{22} \\
& \neq \frac{1}{11} \sum_{\substack{i=1, \ldots, 22 \\
v_{i} \neq .}} v_{i} \\
&= 2 \cdot \frac{6}{11}+3.5 \cdot \frac{2}{11}+4 \cdot \frac{3}{11}
\end{aligned}
$$



Figure 5: Data with a variable $v$ MAR (conditionally on $h$ ).

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Types of missingness / missing systematically UNIVERSITAAT FREIBURG
A variable $v \in V$ is called missing systematically (or not at random), if the probability of a missing value does depend on its (unobserved, true) value.

Example: if the apparatus has problems measuring high velocities and say, e.g., misses
$1 / 3$ of all measurements of $v=1$, $1 / 2$ of all measurements of $v=2$, $2 / 3$ of all measurements of $v=3$,
i.e., the probability of a missing value does depend on the velocity, $v$ is missing systematically.

| case | * | $\sim$ |
| :---: | :---: | :---: |
| 1 | 1 |  |
| 2 | 1 | 1 |
| 3 | 2 | - |
| 4 | B | . |
| 5 | 3 | 3 |
| 6 | 2 | 2 |
| 7 | 1 | 1 |
| 8 | 2 | . |
| 9 | 3 | . |
| 10 | 2 | 2 |

Figure 6: Data with a variable $v$ missing systematically.

Again, the sample mean is not unbiased; expectation can only be estimated if we have background knowledge about the probabilities of a missing value dependend on its true value.

Types of missingness / hidden variables

A variable $v \in V$ is called hidden, if the probability of a missing value is 1 , i.e., it is missing in all cases.

Example: say we want to measure intelligence $I$ of probands but cannot do this directly. We measure their level of education $E$ and their income $C$ instead. Then $I$ is hidden.

| case | $I_{\text {true }}$ | $I_{\text {obs }}$ | $E$ | $C$ |
| ---: | :---: | :---: | :---: | :---: |
| 1 | 1 | . | 0 | 0 |
| 2 | 2 | . | 1 | 2 |
| 3 | 2 | . | 2 | 1 |
| 4 | 2 | . | 2 | 2 |
| 5 | 1 | . | 0 | 2 |
| 6 | 2 | . | 2 | 0 |
| 7 | 1 | . | 1 | 2 |
| 8 | 0 | . | 2 | 1 |
| 9 | 1 | . | 2 | 2 |
| 10 | 2 | . | 2 | 1 |

Figure 7: Data with a hidden variable $I$.


Figure 8: Suggested dependency of variables $I$, $E$, and $C$.

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Advanced AI Techniques / 1. Incomplete Data
types of missingness


Figure 9: Types of missingness.

MAR/MCAR terminology stems from [LR87].

The simplest scheme to learn from incomplete data $D$, e.g., the vertex potentials $\left(p_{v}\right)_{v \in V}$ of a Bayesian network, is complete case analysis (also called casewise deletion): use only complete cases

$$
D_{\text {compl }}:=\{d \in D \mid d \text { is complete }\}
$$

| case | $F$ | $L$ | $B$ | $D$ | $H$ |
| ---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | . | 0 | 0 | 0 | 0 |
| 3 | 1 | 1 | 1 | 1 | 0 |
| 4 | 0 | 0 | . | 1 | 1 |
| 5 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | . | 0 | . | 1 |
| 8 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 1 | 1 | 1 |
| 10 | 1 | 1 | . | 1 | 1 |

Figure 10: Incomplete data and data used in complete case analysis (highlighted).

If $D$ is MCAR, estimations based on the subsample $D_{\text {compl }}$ are unbiased for $D_{\text {true }}$.

But for higher-dimensional data (i.e., with a larger number of variables), complete cases might become rare.

Let each variable have a probability for missing values of 0.05 , then for 20 variables the probability of a case to be complete is

$$
(1-0.05)^{20} \approx 0.36
$$

for 50 variables it is $\approx 0.08$, i.e., most cases are deleted.

A higher case rate can be achieved by available case analysis. If a quantity has to be estimated based on a subset $W \subseteq V$ of variables, e.g., the vertext potential $p_{v}$ of a specific vertex $v \in V$ of a Bayesian network ( $W=\mathrm{fam}(v)$ ), use only complete cases of $\left.D\right|_{W}$
$\left(\left.D\right|_{W}\right)_{\text {compl }}=\left\{\left.d \in D\right|_{W} \mid d\right.$ is complete $\}$

| case | F | L | B | D | H |
| ---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | . | 0 | 0 | 0 | 0 |
| 3 | 1 | 1 | 1 | 1 | 0 |
| 4 | 0 | 0 | . | 1 | 1 |
| 5 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | . | 0 | . | 1 |
| 8 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 1 | 1 | 1 |
| 10 | 1 | 1 | . | 1 | 1 |

Figure 11: Incomplete data and data used in available case analysis for estimating the potential $p_{L}(L \mid F)$ (highlighted).

If $D$ is MCAR, estimations based on the subsample $\left(D_{W}\right)_{\text {compl }}$ are unbiased for $\left(D_{W}\right)_{\text {true }}$.

## 1. Incomplete Data

## 2. Incomplete Data for Parameter Learning (EM algorithm)

## 3. An Example

Let $V$ be a set of variables and $d$ be an incomplete case. A (complete) case $\bar{d}$ with

$$
\bar{d}(v)=d(v), \quad \forall v \in \operatorname{var}(d)
$$

is called a completion of $d$.
A probability distribution

$$
\bar{d}: \operatorname{dom}(V) \rightarrow[0,1]
$$

with

$$
\bar{d}^{\operatorname{var}(d)}=\mathrm{epd}_{d}
$$

is called a distribution of completions of $d$ (or a fuzzy completion of $d$ ).

Example If $V:=\{F, L, B, D, H\}$ and

$$
d:=(2, ., 0,1, .)
$$

an incomplete case, then

$$
\begin{aligned}
& \bar{d}_{1}:=(2,1,0,1,1) \\
& \bar{d}_{2}:=(2,2,0,1,0)
\end{aligned}
$$

etc. are possible completions, but

$$
e:=(1,1,0,1,1)
$$

is not.
Assume $\operatorname{dom}(v):=\{0,1,2\}$ for all $v \in V$. The potential
$\bar{d}: \operatorname{dom}(V) \rightarrow[0,1]$

$$
\left(x_{v}\right)_{v \in V} \mapsto\left\{\begin{array}{cc}
\frac{1}{9}, & \text { if } x_{F}=2, x_{B}=0 \\
\quad \text { and } x_{D}=1 \\
0, & \text { otherwise }
\end{array}\right.
$$

is the uniform distribution of completions of $d$.

Advanced AI Techniques / 2. Incomplete Data for Parameter Learning (EM a learning from "fuzzy cases"

Given a bayesian network structure $G:=(V, E)$ on a set of variables $V$ and a "fuzzy data set" $D \in \operatorname{pdf}(V)^{*}$ of "fuzzy cases" (pdfs $q$ on $V$ ). Learning the parameters of the bayesian network from "fuzzy cases" $D$ means to find vertex potentials $\left(p_{v}\right)_{v \in V}$ s.t. the maximum likelihood criterion, i.e., the probability of the data given the bayesian network is maximal:
find $\left(p_{v}\right)_{v \in V} s . t . p(D)$ is maximal, where $p$ denotes the JPD build from $\left(p_{v}\right)_{v \in V}$. Here,

$$
\left.p(D):=\prod_{q \in D \in V \in V \in \operatorname{domem}(\tan (v)} \prod_{v}(x)\right)^{q^{\operatorname{timimp}()}(x)}
$$

Lemma 1. $p(D)$ is maximal iff

$$
p_{v}(x \mid y):=\frac{\sum_{q \in D} q^{\downarrow \operatorname{fam}(v)}(x, y)}{\sum_{q \in D} q^{\downarrow \operatorname{pa}(v)}(y)}
$$

(if there is a $q \in D$ with $q^{\lfloor\mathrm{pa}(v)}>0$, otherwise $p_{v}(x \mid y)$ can be choosen arbitrarily $-p(D)$ does not depend on it).

If $D$ is incomplete data, in general we are looking for
(i) distributions of completions $\bar{D}$ and
(ii) vertex potentials $\left(p_{v}\right)_{v \in V}$,
that are
(i) compatible, i.e.,

$$
\bar{d}=\operatorname{infer}_{\left(p_{v}\right)_{v \in V}}(d)
$$

for all $\bar{d} \in \bar{D}$ and s.t.
(ii) the probability, that the completed data $\bar{D}$ has been generated from the bayesian network specified by $\left(p_{v}\right)_{v \in V}$, is maximal:

$$
p\left(\left(p_{v}\right)_{v \in V}, \bar{D}\right):=\prod_{\bar{d} \in \bar{D}} \prod_{v \in V} \prod_{x \in \operatorname{dom}(\operatorname{fam}(v))}\left(p_{v}(x)\right)^{\bar{d}^{\downarrow \operatorname{tam}(v)}(x)}
$$

(with the usual constraints that $\operatorname{Im} p_{v} \subseteq[0,1]$ and $\sum_{y \in \operatorname{dom}(\mathrm{pa}(v))} p_{v}(x \mid y)=1$ for all $v \in V$ and $\left.x \in \operatorname{dom}(v)\right)$.

Advanced AI Techniques / 2. Incomplete Data for Parameter Learning (EM a
Maximum likelihood estimates

Unfortunately this is

- a non-linear,
- high-dimensional,
- for bayesian networks in general even non-convex optimization problem without closed form solution.

Any non-linear optimization algorithm (gradient descent, Newton-Raphson, BFGS, etc.) could be used to search local maxima of this probability function.

Let the following bayesian network structure and training data given.

| case | $A$ | $B$ |
| ---: | ---: | ---: |
| 1 | 0 | 0 |
| 2 | 0 | 1 |
| 3 | 0 | 1 |
| 4 | . | 1 |
| 5 | . | 0 |
| 6 | . | 0 |
| 7 | 1 | 0 |
| 8 | 1 | 0 |
| 9 | 1 | 1 |
| 10 | 1 | . |

## $A \longrightarrow B$

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Optimization Problem (1/3)

| case | $A$ | $B$ | weight |
| ---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 1 |
| 2 | 0 | 1 | 1 |
| 3 | 0 | 1 | 1 |
| 7 | 1 | 0 | 1 |
| 8 | 1 | 0 | 1 |
| 9 | 1 | 1 | 1 |
| 4 | 1 | 1 | $\alpha_{4}$ |
| 4 | 0 | 1 | $1-\alpha_{4}$ |
| 5,6 | 1 | 0 | $2 \alpha_{5}$ |
| 5,6 | 0 | 0 | $2\left(1-\alpha_{5}\right)$ |
| 10 | 1 | 1 | $\beta_{10}$ |
| 10 | 1 | 0 | $1-\beta_{10}$ |

$$
\begin{aligned}
\theta & =p(A=1) \\
\eta_{1} & =p(B=1 \mid A=1) \\
\eta_{2} & =p(B=1 \mid A=0)
\end{aligned}
$$

$$
\begin{aligned}
p(D)= & \theta^{4+\alpha_{4}+2 \alpha_{5}}(1-\theta)^{3+\left(1-\alpha_{4}\right)+2\left(1-\alpha_{5}\right)} \eta_{1}^{1+\alpha_{4}+\beta_{10}}\left(1-\eta_{1}\right)^{2+2 \alpha_{5}+\left(1-\beta_{10}\right)} \\
& \cdot \eta_{2}^{2+\left(1-\alpha_{4}\right)}\left(1-\eta_{2}\right)^{1+2\left(1-\alpha_{5}\right)}
\end{aligned}
$$

## From parameters

$$
\begin{aligned}
\theta & =p(A=1) \\
\eta_{1} & =p(B=1 \mid A=1) \\
\eta_{2} & =p(B=1 \mid A=0)
\end{aligned}
$$

we can compute distributions of completions:
$\alpha_{4}=p(A=1 \mid B=1)=\frac{p(B=1 \mid A=1) p(A=1)}{\sum_{a \in A} p(B=1 \mid A=a) p(A=a)}=\frac{\theta \eta_{1}}{\theta \eta_{1}+(1-\theta) \eta_{2}}$
$\alpha_{5}=p(A=1 \mid B=0)=\frac{p(B=0 \mid A=1) p(A=1)}{\sum_{a \in A} p(B=0 \mid A=a) p(A=a)}=\frac{\theta\left(1-\eta_{1}\right)}{\theta\left(1-\eta_{1}\right)+(1-\theta)\left(1-\eta_{2}\right)}$
$\beta_{10}=p(B=1 \mid A=1) \quad=\eta_{1}$

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Substituting $\alpha_{4}, \alpha_{5}$ and $\beta_{10}$ in $p(D)$, finally yields:

$$
\begin{aligned}
p(D)= & \theta^{4+\frac{\theta \eta_{1}}{\theta \eta_{1}+(1-\theta) \eta_{2}}+2 \frac{\theta\left(1-\eta_{1}\right)}{\theta\left(1-\eta_{1}\right)+(1-\theta)\left(1-\eta_{2}\right)}} \\
& \cdot(1-\theta)^{6-\frac{\theta \eta_{1}}{\theta \eta_{1}+(1-\theta) \eta_{2}}-2 \frac{\theta\left(1-\eta_{1}\right)}{\theta\left(1-\eta_{1}\right)+(1-\theta)\left(1-\eta_{2}\right)}} \\
& \cdot \eta_{1}^{1+\frac{\theta \eta_{1}}{\theta \eta_{1}+(1-\theta) \eta_{2}}+\eta_{1}} \\
& \cdot\left(1-\eta_{1}\right)^{3+2 \frac{\theta\left(1-\eta_{1}\right)}{\theta\left(1-\eta_{1}\right)+(1-\theta)\left(1-\eta_{2}\right)}-\eta_{1}} \\
& \cdot \eta_{2}^{3-\frac{\theta \eta_{1}}{\theta \eta_{1}+(1-\theta) \eta_{2}}} \\
& \cdot\left(1-\eta_{2}\right)^{3-2 \frac{\theta\left(1-\eta_{1}\right)}{\theta\left(1-\eta_{1}\right)+(1-\theta)\left(1-\eta_{2}\right)}}
\end{aligned}
$$

For bayesian networks a widely used technique to search local maxima of the probability function $p$ is
Expectation-Maximization (EM, in essence a gradient descent).

At the beginning, $\left(p_{v}\right)_{v \in V}$ are initialized, e.g., by complete, by available case analysis, or at random.

Then one computes alternating expectation or E-step:

$$
\bar{d}:=\operatorname{infer}_{\left(p_{v}\right)_{v \in V}}(d), \quad \forall d \in D
$$

(forcing the compatibility constraint) and maximization or M-step:

$$
\left(p_{v}\right)_{v \in V} \text { with maximal } p\left(\left(p_{v}\right)_{v \in V}, \bar{D}\right)
$$

keeping $\bar{D}$ fixed.

The E-step is implemented using an inference algorithm, e.g., clustering [Lau95]. The variables with observed values are used as evidence, the variables with missing values form the target domain.

The M-step is implemented using lemma 2 :

$$
p_{v}(x \mid y):=\frac{\sum_{q \in D} q^{\lfloor\operatorname{tam}(v)}(x, y)}{\sum_{q \in D} q^{\lfloor\operatorname{pa}(v)}(y)}
$$

See [BKS97] and [FK03] for further optimizations aiming at faster convergence.

Advanced AI Techniques / 2. Incomplete Data for Parameter Learning (EM a

Let the following bayesian network structure and training data given.

|  |  |  |
| ---: | :---: | :---: |
| $A \longrightarrow$ | $B$ |  |
| case | $A$ | $B$ |
| 1 | 0 | 0 |
| 2 | 0 | 1 |
| 3 | 0 | 1 |
| 4 | . | 1 |
| 5 | . | 0 |
| 6 | . | 0 |
| 7 | 1 | 0 |
| 8 | 1 | 0 |
| 9 | 1 | 1 |
| 10 | 1 | . |

Using complete case analysis we estimate (1st M-step)

$$
p(A)=(0.5,0.5)
$$

and

$$
p(B \mid A)=\begin{array}{l|ll|}
A & 0 & 1 \\
\hline B=0 & 0.333 & 0.667 \\
1 & 0.667 & 0.333 \\
\hline
\end{array}
$$

Then we estimate the distributions of completions (1st E-step)

| case | $B$ | $p(A=0)$ | $p(A=1)$ |
| ---: | :---: | :---: | :---: |
| 4 | 1 | 0.667 | 0.333 |
| 5,6 | 0 | 0.333 | 0.667 |
| case | $A$ | $p(B=0)$ | $p(B=1)$ |
| 10 | 1 | 0.667 | 0.333 |

Advanced AI Techniques / 2. Incomplete Data for Parameter Learning (EM a example / second \& third step

From that we estimate (2nd M-step)

$$
p(A)=(0.433,0.567)
$$

and

$$
p(B \mid A)=\begin{array}{l|ll|}
A & 0 & 1 \\
\hline B=0 & 0.385 & 0.706 \\
1 & 0.615 & 0.294 \\
\hline
\end{array}
$$

Then we estimate the distributions of completions (2nd E-step)

| case | $B$ | $p(A=0)$ | $p(A=1)$ |
| ---: | :---: | :---: | :---: |
| 4 | 1 | 0.615 | 0.385 |
| 5,6 | 0 | 0.294 | 0.706 |
| case | $A$ | $p(B=0)$ | $p(B=1)$ |
| 10 | 1 | 0.706 | 0.294 |

From that we estimate (3rd M-step)

$$
p(A)=(0.420,0.580)
$$

and

$$
p(B \mid A)=\begin{array}{l|ll|}
A & 0 & 1 \\
\hline B=0 & 0.378 & 0.710 \\
1 & 0.622 & 0.290 \\
\hline
\end{array}
$$

etc.


Figure 12: Convergence ${ }^{\text {sen }} \mathrm{f} f$ the EM algorithm (black $p(A=1)$, red $p(B=1 \mid A=0)$, green $p(B=1 \mid A=1)$ ).

## 1. Incomplete Data

## 2. Incomplete Data for Parameter Learning (EM algorithm)

## 3. An Example

Definition 1. Let $\mathcal{V}$ be a set of variables and let $C \in \mathcal{V}$ be a variable called target variable.
The bayesian network structure on $\mathcal{V}$ defined by the set of edges

$$
E:=\{(C, X) \mid X \in \mathcal{V}, X \neq C\}
$$

is called naive bayesian network with target $C$.


Naive bayesian networks typically are used as classifiers for $C$ and thus called naive bayesian classifier.

A naive bayesian network encodes both,

- strong dependency assumptions:
there are no two variables that are independent, i.e.,

$$
\neg I(X, Y) \quad \forall X, Y
$$

- strong independency assumptions:
each pair of variables is conditionally independent given a very small set of variables:

$$
I(X, Y \mid C) \quad \forall X, Y \neq C
$$



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Learning a Naive Bayesian Network means to estimate

$$
p(C) \quad \text { and } \quad p\left(X_{i} \mid C\right)
$$

Inferencing in a Naive Bayesian Network means to compute

$$
p\left(C \mid X_{1}=x_{1}, \ldots, X_{n}=x_{n}\right)
$$

which is due to Bayes formula:

$$
\begin{aligned}
p\left(C \mid X_{1}=x_{1}, \ldots, X_{n}=x_{n}\right) & =\frac{p\left(X_{1}=x_{1}, \ldots, X_{n}=x_{n} \mid C\right) p(C)}{p\left(X_{1}=x_{1}, \ldots, X_{n}=x_{n}\right)} \\
& =\frac{\prod_{i} p\left(X_{i}=x_{i} \mid C\right) p(C)}{p\left(X_{1}=x_{1}, \ldots, X_{n}=x_{n}\right)} \\
& =\left(\prod_{i} p\left(X_{i}=x_{i} \mid C\right) p(C)\right)^{\mid C}
\end{aligned}
$$

Be careful,

$$
p\left(X_{1}=x_{1}, \ldots, X_{n}=x_{n}\right) \neq \prod_{i} p\left(X_{i}=x_{i}\right)
$$

in general and we do not have access to this probability easily.

The UCI mushroom data contains 23 attributes of 8124 different mushrooms.

edible: $\mathrm{e}=$ edible, $\mathrm{p}=$ poisonous
cap-shape: $b=b e l l, c=c o n i c a l, x=c o n v e x, f=f l a t, k=k n o b b e d, ~ s=s u n k e n ~$

Mushroom has missing values:

- in variable $X_{11}=$ stalk-root, starting at case 3985.


We want to learn target $C=$ edible based on all the other attributes, $X_{1}, \ldots, X_{22}=$ cap-shape, $\ldots$, habitat.
We split the dataset randomly in
7124 training cases plus 1000 test cases
class distribution:

| actual $=\mathrm{e}$ | 529 |
| ---: | ---: |
| p | 471 |

Accuracy of constant classifier (always predicts majority class e):

$$
\mathrm{acc}=0.529
$$



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Learning only from the 4942 complete cases (out of 7124), we are quite successful on the 702 complete test cases:
confusion matrix:

| predicted $=$ | $e$ | $p$ |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 433 | 3 |
| p | 0 | 266 |

$$
\text { acc }=0.9957
$$

But the classifier deterioriates dramatically, once evaluated on all 1000 cases, thereof 298 containing missing values:
confusion matrix:

| predicted $=$ | e | p |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 516 | 13 |
| p | 201 | 270 |

$$
\operatorname{acc}=0.786
$$

Diagnostics:

$$
p\left(X_{9}=b \mid C\right)=0
$$

as $X_{9}=b$ occurrs only with $X_{11}=.!$

For the whole dataset:

| $X_{9}=$ | b | e | g | h | k | n | o | p | r | u | w | y |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $M_{11}=$ false | 0 | 0 | 656 | 720 | 408 | 984 | 0 | 1384 | 24 | 480 | 966 | 22 |
| true | 1728 | 96 | 96 | 12 | 0 | 64 | 64 | 108 | 0 | 12 | 236 | 64 |

If we use available case analysis, this problem is fixed. confusion matrix:

| predicted $=$ | e | p |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 523 | 6 |
| p | 0 | 471 |

$$
\mathrm{acc}=0.994
$$

EM for predictor variables in Naive Bayesian Networks always converges to the available case estimates (easy exercise; compute the update formula).

Definition 2. mutual information of two random variables $X$ and $Y$ :

$$
\operatorname{MI}(X, Y):=\sum_{\substack{x \in \operatorname{dom} X, y \in \operatorname{dom} Y}} p(X=x, Y=y) \operatorname{lb} \frac{p(X=x, Y=y)}{p(X=x) p(Y=y)}
$$

| X | $\mathrm{MI}(X, C)$ | X | $\operatorname{MI}(X, C)$ |
| :---: | :---: | :---: | :---: |
| X1 | 0.04824 | X12 | 0.28484 |
| X2 | 0.02901 | X13 | 0.27076 |
| X3 | 0.03799 | X14 | 0.24917 |
| X4 | 0.19339 | X15 | 0.24022 |
| X5 | 0.90573 | X16 | 0.00000 |
| X6 | 0.01401 | X17 | 0.02358 |
| X7 | 0.10173 | X18 | 0.03863 |
| X8 | 0.23289 | X19 | 0.31982 |
| X9 | 0.41907 | X20 | 0.48174 |
| X10 | 0.00765 | X21 | 0.20188 |
| X11 | 0.09716 | X22 | 0.15877 |

If we use the 4 variables with highest mutual information only,

- X5 = odor
- X20 = spore-print-color
- X9 = gill-color
- X19 = ring-type
we still get very good results.
confusion matrix:

| predicted $=$ | e | p |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 529 | 0 |
| p | 6 | 465 |

$$
\mathrm{acc}=0.994
$$



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Advanced AI Techniques / 3. An Example


Fresh random split.
all variables:

acc $=.995$
$X_{5}, X_{9}, X_{19}$, and $X_{20}$ :

| predicted $=$ | e | p |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 544 | 0 |
| p | 8 | 447 |

acc $=.992$
$X_{1}, X_{2}, X_{3}$, and $X_{4}$ :

| predicted $=$ | e | p |
| ---: | ---: | ---: |
| actual $=\mathrm{e}$ | 419 | 126 |
| p | 101 | 354 |

acc $=.773$

Naive Bayesian Networks also could be used for cluster analysis.

The unknown cluster membership is modelled by a hidden variable $C$ called latent class.

EM algorithm is used to "learn" fuzzy cluster memberships.


Naive Bayesian Networks used this way are a specific instance of so called model-based clustering.

Each cluster contains "similar cases", i.e., cases that contain cooccurring patterns of values.

random

clustered

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Advanced AI Techniques / 3. An Example


- To learn parameters from data with missing values, sometimes simple heuristics as complete or available case analysis can be used.
- Alternatively, one can define a joint likelihood for distributions of completions and parameters.
- In general, this gives rise to a nonlinear optimization problem.
But for given distributions of completions, maximum
likelihood estimates can be computed analytically.
- To solve the ML optimization problem, one can employ the expectation maximization (EM) algorithm:
- parameters $\rightarrow$ completions (expectation; inference)
- completions $\rightarrow$ parameters (maximization; parameter learning)

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