Advanced AI Techniques

I. Bayesian Networks / 2. Parameter Learning (2/2)

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Complete and incomplete cases

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

$$c : V \to \bigcup_{v \in V} \mathrm{dom}(V)$$

with $c(v) \in \mathrm{dom}(V)$ 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 $\mathrm{var}(c) := W$ and say, the values of the variables $V \setminus W$ are **missing** or **not observed**.

A data set $D \in \mathrm{dom}(V)^*$ that contains complete cases only, is called **complete data**; if it contains an incomplete case, it is called **incomplete data**.

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 $V := \{F, L, B, D, H\}$. Missing values are marked by a dot.

Missing value indicators

For each variable v, we can interpret its missing of values as new random variable M_v,

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

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.

Types of missingness / MCAR

A variable $v \in V$ is called **missing completely at random** (MCAR), if the probability of a missing value is (unconditionally) independent of the (true, unobserved) value of v, i.e, if

$$I(M_v, v_{\text{true}})$$

(MCAR is also called **missing unconditionally at random**).

Example: think of an apparatus measuring the velocity v of wind that has a loose contact c. When the contact is closed, the measurement is recorded, otherwise it is skipped. If the contact c being closed does not depend on the velocity v of wind, v is MCAR.

If a variable is MCAR, for each value the probability of missing is the same, and, e.g., the sample mean of v_{obs} is an unbiased estimator for the expectation of v_{true}; here

case	v_{true}	v_{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.

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

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

$$I(M_v, v_{\text{true}} \mid W)$$

for some set of variables $W \subseteq V \setminus \{v\}$ (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,

case	v_{true}	v_{observed}	h
1	1	.	0
2	2	2	0
3	3	.	0
4	3	3	0
5	1	1	0
6	3	3	0
7	1	1	0
8	2	.	0
9	2	2	0
10	3	.	1
11	4	4	1
12	4	.	1
13	3	3	1
14	3	.	2
15	4	4	2
16	4	.	2
17	5	5	2
18	3	.	2
19	5	.	2
20	3	3	2
21	4	.	2
22	5	.	2

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

then v is missing at random (conditionally on h).

Types of missingness / MAR

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:

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

case	v_{true}	v_{observed}	h
1	1	.	0
2	2	2	0
3	3	.	0
4	3	3	0
5	1	1	0
6	3	3	0
7	1	1	0
8	2	.	0
9	2	2	0
10	3	.	1
11	4	4	1
12	4	.	1
13	3	3	1
14	3	.	2
15	4	4	2
16	4	.	2
17	5	5	2
18	3	.	2
19	5	.	2
20	3	3	2
21	4	.	2
22	5	.	2

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

Types of missingness / missing systematically

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	v_{true}	v_{observed}
1	1	.
2	1	1
3	2	.
4	3	.
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_{true}	I_{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.

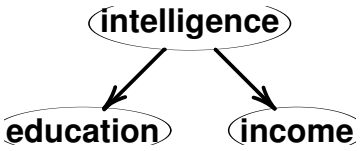


Figure 8: Suggested dependency of variables I, E, and C.

types of missingness

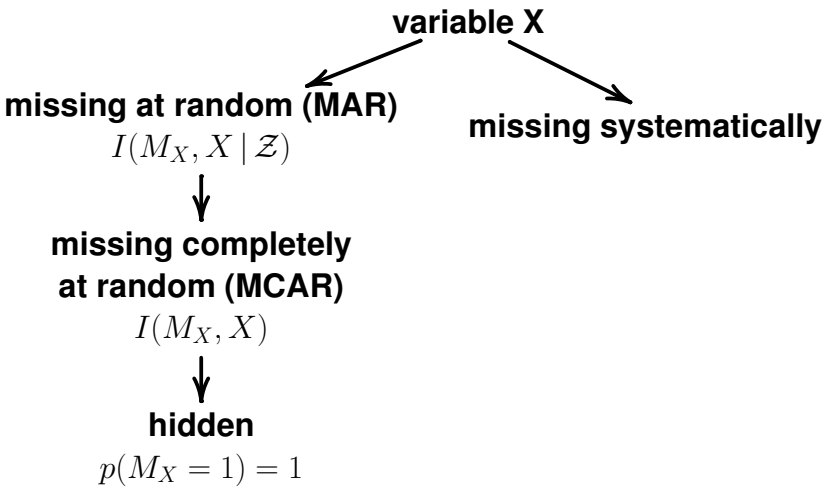


Figure 9: Types of missingness.

MAR/MCAR terminology stems from [LR87].

complete case analysis

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

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

If D is MCAR, estimations based on the subsample D_{compl} are unbiased for D_{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

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).

20 variables the probability of a case to be complete is

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

for 50 variables it is ≈ 0.08, i.e., most cases are deleted.

available case analysis

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 ($W = \text{fam}(v)$), use only complete cases of $D|_W$

$$(D|_W)_{\text{compl}} = \{d \in D|_W \mid d \text{ is complete}\}$$

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

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).

completions

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

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

is called a **completion of** d.

A probability distribution

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

with

$$\bar{d}^{\downarrow \mathrm{var}(d)} = \mathrm{epd}_d$$

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

$$\bar{d}_1 := (2, 1, 0, 1, 1)$$
$$\bar{d}_2 := (2, 2, 0, 1, 0)$$

etc. are possible completions, but

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

is not.

Assume $dom(v) := \{0, 1, 2\}$ for all $v \in V$. The potential

$$\bar{d} : \mathrm{dom}(V) \to [0,1]$$
$$(x_v)_{v \in V} \mapsto \begin{cases} \frac{1}{9}, & \text{if } x_F = 2, x_B = 0, \\ & \text{and } x_D = 1 \\ 0, & \text{otherwise} \end{cases}$$

is the uniform distribution of completions of d.

learning from "fuzzy cases"

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

find $(p_v)_{v \in V} s.t.\ p(D)$ is maximal,

where p denotes the JPD build from $(p_v)_{v \in V}$. Here,

$$p(D) := \prod_{q \in D} \prod_{v \in V} \prod_{x \in \text{dom}(\text{fam}(v))} (p_v(x))^{q^{\downarrow \text{fam}(v)}(x)}$$

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

$$p_v(x|y) := \frac{\sum_{q \in D} q^{\downarrow \text{fam}(v)}(x, y)}{\sum_{q \in D} q^{\downarrow \text{pa}(v)}(y)}$$

(if there is a $q \in D$ with $q^{\downarrow \text{pa}(v)} > 0$, otherwise $p_v(x|y)$ can be choosen arbitrarily – $p(D)$ does not depend on it).

Maximum likelihood estimates

If D is incomplete data, in general we are looking for

(i) distributions of completions $\bar{D}$ and

(ii) vertex potentials $(p_v)_{v \in V}$,

that are

(i) compatible, i.e.,

$$\bar{d} = \text{infer}_{(p_v)_{v \in V}}(d)$$

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 $(p_v)_{v \in V}$, is maximal:

$$p((p_v)_{v \in V}, \bar{D}_{\text{true}}) := \prod_{\bar{d} \in \bar{D}} \prod_{v \in V} \prod_{x \in \text{dom}(\text{fam}(v))} (p_v(x))^{\bar{d}^{\downarrow \text{fam}(v)}(x)}$$

(with the usual constraints that $\text{Im} p_v \subseteq [0, 1]$ and $\sum_{y \in \text{dom}(\text{pa}(v))} p_v(x|y) = 1$ for all $v \in V$ and $x \in \text{dom}(v)$).

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.

Example

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	.

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	α_4
4	0	1	$1-\alpha_4$
5,6	1	0	$2\,\alpha_5$
5,6	0	0	$2\,(1-\alpha_5)$
10	1	1	β_{10}
10	1	0	$1-\beta_{10}$

$$\begin{aligned}\theta =& p(A=1)\\ \eta_1 =& p(B=1\,|\,A=1)\\ \eta_2 =& p(B=1\,|\,A=0)\end{aligned}$$

$$\begin{aligned}p(D) =& \theta^{4+\alpha_4+2\,\alpha_5}\,(1-\theta)^{3+(1-\alpha_4)+2\,(1-\alpha_5)}\,\eta_1^{1+\alpha_4+\beta_{10}}\,(1-\eta_1)^{2+2\,\alpha_5+(1-\beta_{10})}\\ &\cdot\,\eta_2^{2+(1-\alpha_4)}\,(1-\eta_2)^{1+2\,(1-\alpha_5)}\end{aligned}$$

Optimization Problem (2/3)

From parameters

$$\begin{aligned}\theta =& p(A=1)\\ \eta_1 =& p(B=1\,|\,A=1)\\ \eta_2 =& p(B=1\,|\,A=0)\end{aligned}$$

we can compute distributions of completions:

$$\alpha_4 = p(A=1\,|\,B=1) = \frac{p(B=1\,|\,A=1)\,p(A=1)}{\sum_{a\in A} p(B=1\,|\,A=a)\,p(A=a)} = \frac{\theta\,\eta_1}{\theta\,\eta_1+(1-\theta)\,\eta_2}$$

$$\alpha_5 = p(A=1\,|\,B=0) = \frac{p(B=0\,|\,A=1)\,p(A=1)}{\sum_{a\in A} p(B=0\,|\,A=a)\,p(A=a)} = \frac{\theta\,(1-\eta_1)}{\theta\,(1-\eta_1)+(1-\theta)\,(1-\eta_2)}$$

$$\beta_{10} = p(B=1\,|\,A=1) = \eta_1$$

Optimization Problem (3/3)

Substituting α_4, α_5 and β_{10} in $p(D)$, finally yields:

$$\begin{aligned} p(D) =& \theta^{4+\frac{\theta\,\eta_1}{\theta\,\eta_1+(1-\theta)\eta_2}+2\,\frac{\theta\,(1-\eta_1)}{\theta\,(1-\eta_1)+(1-\theta)(1-\eta_2)}} \\ & \cdot (1-\theta)^{6-\frac{\theta\,\eta_1}{\theta\,\eta_1+(1-\theta)\eta_2}-2\,\frac{\theta\,(1-\eta_1)}{\theta\,(1-\eta_1)+(1-\theta)(1-\eta_2)}} \\ & \cdot \eta_1^{\,1+\frac{\theta\,\eta_1}{\theta\,\eta_1+(1-\theta)\eta_2}+\eta_1} \\ & \cdot (1-\eta_1)^{3+2\,\frac{\theta\,(1-\eta_1)}{\theta\,(1-\eta_1)+(1-\theta)(1-\eta_2)}-\eta_1} \\ & \cdot \eta_2^{\,3-\frac{\theta\,\eta_1}{\theta\,\eta_1+(1-\theta)\eta_2}} \\ & \cdot (1-\eta_2)^{3-2\,\frac{\theta\,(1-\eta_1)}{\theta\,(1-\eta_1)+(1-\theta)(1-\eta_2)}} \end{aligned}$$

EM algorithm

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, $(p_v)_{v\in V}$ are initialized, e.g., by complete, by available case analysis, or at random.

Then one computes alternating
expectation or E-step:

$$\bar{d} := \text{infer}_{(p_v)_{v\in V}}(d), \quad \forall d \in D$$

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

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

keeping $\bar{D}$ fixed.

EM algorithm

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.

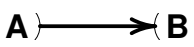
The M-step is implemented using lemma 2:

$$p_v(x|y) := \frac{\sum_{q \in D} q^{\downarrow \mathrm{fam}(v)}(x, y)}{\sum_{q \in D} q^{\downarrow \mathrm{pa}(v)}(y)}$$

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

Example

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	.

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

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

and

$$p(B|A) = \begin{array}{r|cc} A & 0 & 1 \\ \hline B = 0 & 0.33 & 0.67 \\ 1 & 0.67 & 0.33 \end{array}$$

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

case	B	p(A=0)	p(A=1)
4	1	0.67	0.33
5,6	0	0.33	0.67

case	A	p(B=0)	p(B=1)
10	1	0.67	0.33

example / second & third step

From that we estimate (2nd M-step)

$$p(A) = (0.44, 0.56)$$

and

$$p(B|A) = \begin{array}{r|cc} A & 0 & 1 \\ \hline B=0 & 0.38 & 0.62 \\ 1 & 0.71 & 0.29 \end{array}$$

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

case	B	p(A=0)	p(A=1)
4	1	0.62	0.38
5,6	0	0.29	0.71
case	A	p(B=0)	p(B=1)
10	1	0.71	0.29

From that we estimate (3rd M-step)

$$p(A) = (0.43, 0.57)$$

and

$$p(B|A) = \begin{array}{r|cc} A & 0 & 1 \\ \hline B=0 & 0.38 & 0.62 \\ 1 & 0.71 & 0.29 \end{array}$$

etc.

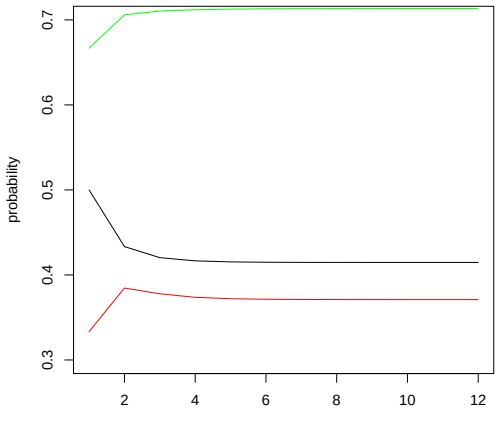


Figure 12: Convergence of the EM algorithm (black p(A=0), red p(B=0|A=0), green p(B=0|A=1)).

References

[BKS97] E. Bauer, D. Koller, and Y. Singer. Update rules for parameter estimation in Bayesian networks. In *Proceedings of the 13th Annual Conference on Uncertainty in AI (UAI)*, 1997.

[FK03] J. Fischer and K. Kersting. Scaled cgem: A fast accelerated em. In N. Lavrac, D. Gamberger, H. Blockeel, and L. Todorovski, editors, *Proceedings of the Fourteenth European Conference on Machine Learning (ECML-2003)*, pages 133–144, Cavtat, Croatia, 2003.

[Lau95] S. L. Lauritzen. The em algorithm for graphical association models with missing data. *Computational Statistics & Data Analysis*, 19:191–201, 1995.

[LR87] R. J. A. Little and D. B. Rubin. *Statistical analysis with missing data*. Wiley, New York, 1987.