Learning Bayesian Networks (part 1)

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Computer Scices 760
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Some of the slides in these lectures have been adapted/borrowed from materials developed by Tom Dietterich, Pedro Domingos, Tom Mitchell, David Page, and Jude Shavlik

Goals for the lecture

you should understand the following concepts

- the Bayesian network representation
- inference by enumeration
- the parameter learning task for Bayes nets
- the structure learning task for Bayes nets
- maximum likelihood estimation
- Laplace estimates
- *m*-estimates
- missing data in machine learning
    - hidden variables
    - missing at random
    - missing systematically
- the EM approach to imputing missing values in Bayes net parameter learning

Bayesian network example

- Consider the following 5 binary random variables:
  - *B* = a burglary occurs at your house
  - *E* = an earthquake occurs at your house
  - *A* = the alarm goes off
  - *J* = John calls to report the alarm
  - *M* = Mary calls to report the alarm

- Suppose we want to answer queries like what is $P(B \mid M, J)$?

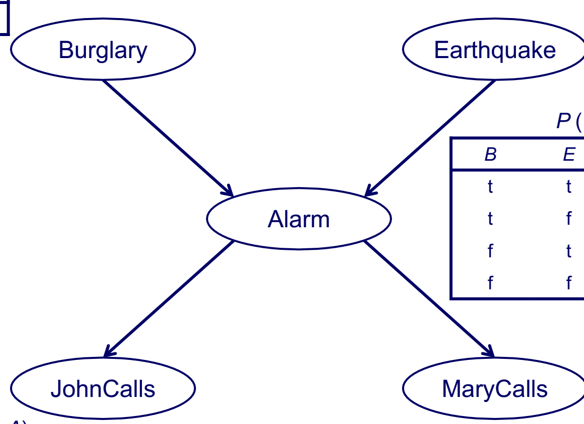
Bayesian network example

$P(B)$

t	f
0.001	0.999

$P(E)$

t	f
0.001	0.999



$P(A \mid B, E)$

B	*E*	t	f
t	t	0.95	0.05
t	f	0.94	0.06
f	t	0.29	0.71
f	f	0.001	0.999

$P(J \mid A)$

A	t	f
t	0.9	0.1
f	0.05	0.95

$P(M \mid A)$

A	t	f
t	0.7	0.3
f	0.01	0.99

Bayesian networks

- a BN consists of a Directed Acyclic Graph (DAG) and a set of conditional probability distributions
- in the DAG
  - each node denotes random a variable
  - each edge from X to Y represents that X *directly influences* Y
  - formally: each variable X is independent of its non-descendants given its parents
- each node X has a *conditional probability distribution* (CPD) representing $P(X \mid Parents(X))$

Bayesian networks

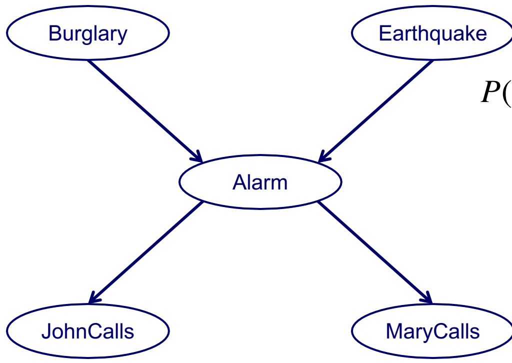
- using the chain rule, a joint probability distribution can be expressed as

$$P(X_1, \ldots, X_n) = \mathrm{P}(X_1)\prod_{i=2}^{n} P(X_i \mid X_1, \ldots, X_{i-1})$$

- a BN provides a compact representation of a joint probability distribution

$$P(X_1, \ldots, X_n) = \prod_{i=1}^{n} P(X_i \mid Parents(X_i))$$

Bayesian networks

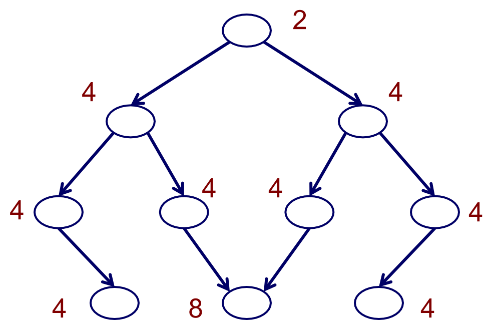


$$P(B,E,A,J,M) = P(B) \times P(E) \times P(A \mid B,E) \times P(J \mid A) \times P(M \mid A)$$

- a standard representation of the joint distribution for the Alarm example has $2^5 = 32$ parameters
- the BN representation of this distribution has 20 parameters

Bayesian networks

- consider a case with 10 binary random variables
- How many parameters does a BN with the following graph structure have?



= 42

- How many parameters does the standard table representation of the joint distribution have?

= 1024

Advantages of the Bayesian network representation

- Captures independence and conditional independence where they exist
- Encodes the relevant portion of the full joint among variables where dependencies exist
- Uses a graphical representation which lends insight into the complexity of inference

The inference task in Bayesian networks

Given: values for some variables in the network (*evidence*), and a set of *query* variables

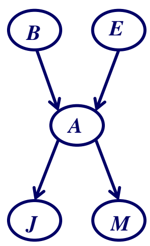
Do: compute the posterior distribution over the query variables

- variables that are neither evidence variables nor query variables are *hidden* variables
- the BN representation is flexible enough that any set can be the evidence variables and any set can be the query variables

Inference by enumeration

- let a denote A=true, and $\neg a$ denote A=false
- suppose we're given the query: $P(b \mid j, m)$

  "probability the house is being burglarized given that John and Mary both called"
- from the graph structure we can first compute:



$$P(b,j,m) = \sum_{e,\neg e}\sum_{a,\neg a} P(b)P(E)P(A \mid b,E)P(j \mid A)P(m \mid A)$$

sum over possible values for E and A variables ($e, \neg e, a, \neg a$)

Inference by enumeration

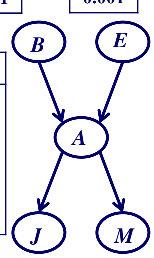
$$P(b,j,m) = \sum_{e,\neg e}\sum_{a,\neg a} P(b)P(E)P(A \mid b,E)P(j \mid A)P(m \mid A)$$

$$= P(b)\sum_{e,\neg e}\sum_{a,\neg a} P(E)P(A \mid b,E)P(j \mid A)P(m \mid A)$$

P(B)
0.001

P(E)
0.001

B	E	P(A)
t	t	0.95
t	f	0.94
f	t	0.29
f	f	0.001



A	P(J)
t	0.9
f	0.05

A	P(M)
t	0.7
f	0.01

$$\begin{array}{lr} \quad\;\; B \qquad\quad E \qquad\;\; A \qquad J \qquad M & \\ = 0.001 \times (0.001 \times 0.95 \times 0.9 \times\ 0.7 + & e, a \\ \qquad\qquad\;\; 0.001 \times 0.05 \times 0.05 \times 0.01 + & e, \neg a \\ \qquad\qquad\;\; 0.999 \times 0.94 \times 0.9 \times\ 0.7 + & \neg e, a \\ \qquad\qquad\;\; 0.999 \times 0.06 \times 0.05 \times 0.01) & \neg e, \neg a \end{array}$$

Inference by enumeration

- now do equivalent calculation for $P(\neg b,\ j, m)$
- and determine $P(b \mid j, m)$

$$P(b \mid j,m) = \frac{P(b,j,m)}{P(j,m)} = \frac{P(b,j,m)}{P(b,j,m) + P(\neg b,j,m)}$$

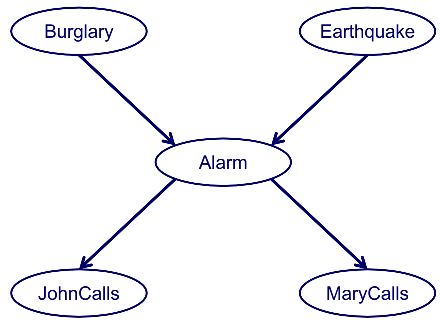
Comments on BN inference

- *inference by enumeration* is an *exact* method (i.e. it computes the exact answer to a given query)
- it requires summing over a joint distribution whose size is exponential in the number of variables
- in many cases we can do exact inference efficiently in large networks
  - key insight: save computation by pushing sums inward
- in general, the Bayes net inference problem is NP-hard
- there are also methods for approximate inference – these get an answer which is “close”
- in general, the approximate inference problem is NP-hard also, but approximate methods work well for many real-world problems

The parameter learning task

- Given: a set of training instances, the graph structure of a BN

B	E	A	J	M
f	f	f	t	f
f	t	f	f	f
f	f	t	f	t
		…		



- Do: infer the parameters of the CPDs

The structure learning task

- Given: a set of training instances

B	E	A	J	M
f	f	f	t	f
f	t	f	f	f
f	f	t	f	t
		…		

- Do: infer the graph structure (and perhaps the parameters of the CPDs too)

Parameter learning and maximum likelihood estimation

- *maximum likelihood estimation* (MLE)
  - given a model structure (e.g. a Bayes net graph) G and a set of data D
  - set the model parameters θ to maximize $P(D \mid G, \theta)$

- i.e. make the data D look as likely as possible under the model $P(D \mid G, \theta)$

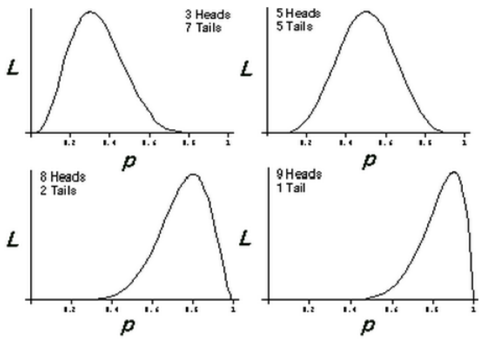
Maximum likelihood estimation

consider trying to estimate the parameter θ (probability of heads) of a biased coin from a sequence of flips

$$\boldsymbol{x} = \{1,1,1,0,1,0,0,1,0,1\}$$

the likelihood function for θ is given by:

$$L(\theta : x_1, \ldots, x_n) = \theta^{x_1}(1-\theta)^{1-x_1} \cdots \theta^{x_n}(1-\theta)^{1-x_n}$$
$$= \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}$$



for h heads in n flips
the MLE is h/n

MLE in a Bayes net

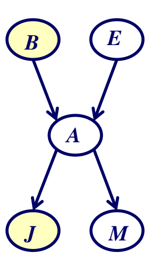
$$L(\theta : D, G) = P(D \mid G, \theta) = \prod_{d \in D} P(x_1^{(d)}, x_2^{(d)}, \ldots, x_n^{(d)})$$

$$= \prod_{d \in D} \prod_i P(x_i^{(d)} \mid Parents(x_i^{(d)}))$$

$$= \prod_i \underbrace{\left(\prod_{d \in D} P(x_i^{(d)} \mid Parents(x_i^{(d)})) \right)}_{\text{independent parameter learning problem for each CPD}}$$

Maximum likelihood estimation

now consider estimating the CPD parameters for B and J in the alarm network given the following data set



B	E	A	J	M
f	f	f	t	f
f	t	f	f	f
f	f	f	t	t
t	f	f	f	t
f	f	t	t	f
f	f	t	f	t
f	f	t	t	t
f	f	t	t	t

$$P(b) = \frac{1}{8} = 0.125$$

$$P(\neg b) = \frac{7}{8} = 0.875$$

$$P(j \mid a) = \frac{3}{4} = 0.75$$

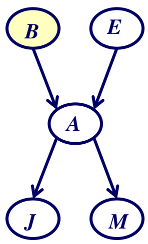
$$P(\neg j \mid a) = \frac{1}{4} = 0.25$$

$$P(j \mid \neg a) = \frac{2}{4} = 0.5$$

$$P(\neg j \mid \neg a) = \frac{2}{4} = 0.5$$

Maximum likelihood estimation

suppose instead, our data set was this…



B	E	A	J	M
f	f	f	t	f
f	t	f	f	f
f	f	f	t	t
f	f	f	f	t
f	f	t	t	f
f	f	t	f	t
f	f	t	t	t
f	f	t	t	t

$$\boxed{P(b) = \frac{0}{8} = 0}$$

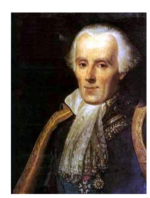
$$P(\neg b) = \frac{8}{8} = 1$$

do we really want to set this to 0?

Maximum a posteriori (MAP*)* estimation

- instead of estimating parameters strictly from the data, we could start with some <u>prior belief</u> for each

- for example, we could use *Laplace estimates*



$$P(X = x) = \frac{n_x + 1}{\sum_{v \in \text{Values}(X)} (n_v + 1)}$$

pseudocounts

- where n_v represents the number of occurrences of value v

Maximum a posteriori estimation

a more general form: *m-estimates*

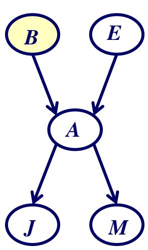
$$P(X=x) = \frac{n_x + p_x m}{\left(\sum_{v \in \text{Values}(X)} n_v\right) + m}$$

prior probability of value x

number of "virtual" instances

M-estimates example

now let's estimate parameters for B using $m=4$ and $p_b=0.25$



B	E	A	J	M
f	f	f	t	f
f	t	f	f	f
f	f	f	t	t
f	f	f	f	t
f	f	t	t	f
f	f	t	f	t
f	f	t	t	t
f	f	t	t	t

$$P(b) = \frac{0 + 0.25 \times 4}{8+4} = \frac{1}{12} = 0.08 \qquad P(\neg b) = \frac{8 + 0.75 \times 4}{8+4} = \frac{11}{12} = 0.92$$

Missing data

- Commonly in machine learning tasks, some feature values are missing
- some variables may not be observable (i.e. *hidden*) even for training instances
- values for some variables may be *missing at random*: what caused the data to be missing does not depend on the missing data itself
  - e.g. someone accidentally skips a question on an questionnaire
  - e.g. a sensor fails to record a value due to a power blip
- values for some variables may be *missing systematically*: the probability of value being missing depends on the value
  - e.g. a medical test result is missing because a doctor was fairly sure of a diagnosis given earlier test results
  - e.g. the graded exams that go missing on the way home from school are those with poor scores

Missing data

- hidden variables; values *missing at random*
  - these are the cases we'll focus on
  - one solution: try impute the values
- values *missing systematically*
  - may be sensible to represent "*missing*" as an explicit feature value

Imputing missing data with EM

Given:

- data set with some missing values
- model structure, initial model parameters

Repeat until convergence

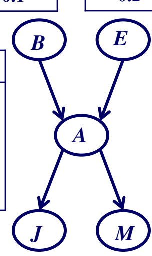
- *Expectation* (E) step: using current model, compute expectation over missing values
- *Maximization* (M) step: update model parameters with those that maximize probability of the data (MLE or MAP)

example: EM for parameter learning

suppose we're given the following initial BN and training set

P(B)
0.1

P(E)
0.2



B	E	P(A)
t	t	0.9
t	f	0.6
f	t	0.3
f	f	0.2

A	P(J)
t	0.9
f	0.2

A	P(M)
t	0.8
f	0.1

B	E	A	J	M
f	f	?	f	f
f	f	?	t	f
t	f	?	t	t
f	f	?	f	t
f	t	?	t	f
f	f	?	f	t
t	t	?	t	t
f	f	?	f	f
f	f	?	t	f
f	f	?	f	t

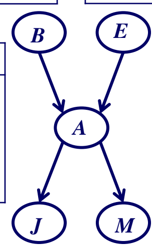
example: E-step

$P(a \mid \neg b, \neg e, \neg j, \neg m)$

$P(\neg a \mid \neg b, \neg e, \neg j, \neg m)$

P(B)
0.1

P(E)
0.2



B	*E*	*P(A)*
t	t	0.9
t	f	0.6
f	t	0.3
f	f	0.2

A	*P(J)*
t	0.9
f	0.2

A	*P(M)*
t	0.8
f	0.1

B	*E*	*A*	*J*	*M*
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f:0.8	t	f
t	f	t:0.98 f: 0.02	t	t
f	f	t: 0.2 f: 0.8	f	t
f	t	t: 0.3 f: 0.7	t	f
f	f	t:0.2 f: 0.8	f	t
t	t	t: 0.997 f: 0.003	t	t
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f: 0.8	t	f
f	f	t: 0.2 f: 0.8	f	t

example: E-step

$$P(a \mid \neg b, \neg e, \neg j, \neg m) = \frac{P(\neg b, \neg e, a, \neg j, \neg m)}{P(\neg b, \neg e, a, \neg j, \neg m) + P(\neg b, \neg e, \neg a, \neg j, \neg m)}$$
$$= \frac{0.9 \times 0.8 \times 0.2 \times 0.1 \times 0.2}{0.9 \times 0.8 \times 0.2 \times 0.1 \times 0.2 \ + \ 0.9 \times 0.8 \times 0.8 \times 0.8 \times 0.9}$$
$$= \frac{0.00288}{.4176} = 0.0069$$

$$P(a \mid \neg b, \neg e, j, \neg m) = \frac{P(\neg b, \neg e, a, j, \neg m)}{P(\neg b, \neg e, a, j, \neg m) + P(\neg b, \neg e, \neg a, j, \neg m)}$$
$$= \frac{0.9 \times 0.8 \times 0.2 \times 0.9 \times 0.2}{0.9 \times 0.8 \times 0.2 \times 0.9 \times 0.2 \ + \ 0.9 \times 0.8 \times 0.8 \times 0.2 \times 0.9}$$
$$= \frac{0.02592}{.1296} = 0.2$$

$$P(a \mid b, \neg e, j, m) = \frac{P(b, \neg e, a, j, m)}{P(b, \neg e, a, j, m) + P(b, \neg e, \neg a, j, m)}$$
$$= \frac{0.1 \times 0.8 \times 0.6 \times 0.9 \times 0.8}{0.1 \times 0.8 \times 0.6 \times 0.9 \times 0.8 \ + \ 0.1 \times 0.8 \times 0.4 \times 0.2 \times 0.1}$$
$$= \frac{0.03456}{.0352} = 0.98$$

⋮

example: M-step

re-estimate probabilities using expected counts

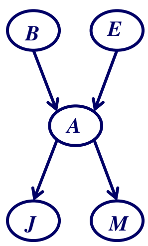
$$P(a \mid b,e) = \frac{E\#(a \wedge b \wedge e)}{E\#(b \wedge e)}$$

$$P(a \mid b,e) = \frac{0.997}{1}$$

$$P(a \mid b,\neg e) = \frac{0.98}{1}$$

$$P(a \mid \neg b,e) = \frac{0.3}{1}$$

$$P(a \mid \neg b,\neg e) = \frac{0.0069+0.2+0.2+0.2+0.0069+0.2+0.2}{7}$$



B	E	P(A)
t	t	0.997
t	f	0.98
f	t	0.3
f	f	0.145

re-estimate probabilities for $P(J \mid A)$ and $P(M \mid A)$ in same way

B	E	A	J	M
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f:0.8	t	f
t	f	t:0.98 f: 0.02	t	t
f	f	t: 0.2 f: 0.8	f	t
f	t	t: 0.3 f: 0.7	t	f
f	f	t:0.2 f: 0.8	f	t
t	t	t: 0.997 f: 0.003	t	t
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f: 0.8	t	f
f	f	t: 0.2 f: 0.8	f	t

example: M-step

re-estimate probabilities using expected counts

$$P(j \mid a) = \frac{E\#(a \wedge j)}{E\#(a)}$$

$$P(j \mid a) = \frac{0.2+0.98+0.3+0.997+0.2}{0.0069+0.2+0.98+0.2+0.3+0.2+0.997+0.0069+0.2+0.2}$$

$$P(j \mid \neg a) = \frac{0.8+0.02+0.7+0.003+0.8}{0.9931+0.8+0.02+0.8+0.7+0.8+0.003+0.9931+0.8+0.8}$$

denominator here is different from that in last slide, here is fraction of instances, because the number of A being true is not 100% but a fraction, e.g., 0.0069 in the 1st instance

B	E	A	J	M
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f:0.8	t	f
t	f	t:0.98 f: 0.02	t	t
f	f	t: 0.2 f: 0.8	f	t
f	t	t: 0.3 f: 0.7	t	f
f	f	t:0.2 f: 0.8	f	t
t	t	t: 0.997 f: 0.003	t	t
f	f	t: 0.0069 f: 0.9931	f	f
f	f	t:0.2 f: 0.8	t	f
f	f	t: 0.2 f: 0.8	f	t

Convergence of EM

- E and M steps are iterated until probabilities converge
- will converge to a maximum in the data likelihood (MLE or MAP)
- the maximum may be a local optimum, however
- the optimum found depends on starting conditions (initial estimated probability parameters)