

COMP 424 - Artificial Intelligence

Lecture 17: Learning Bayesian Networks

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Readings: R&N Ch 20

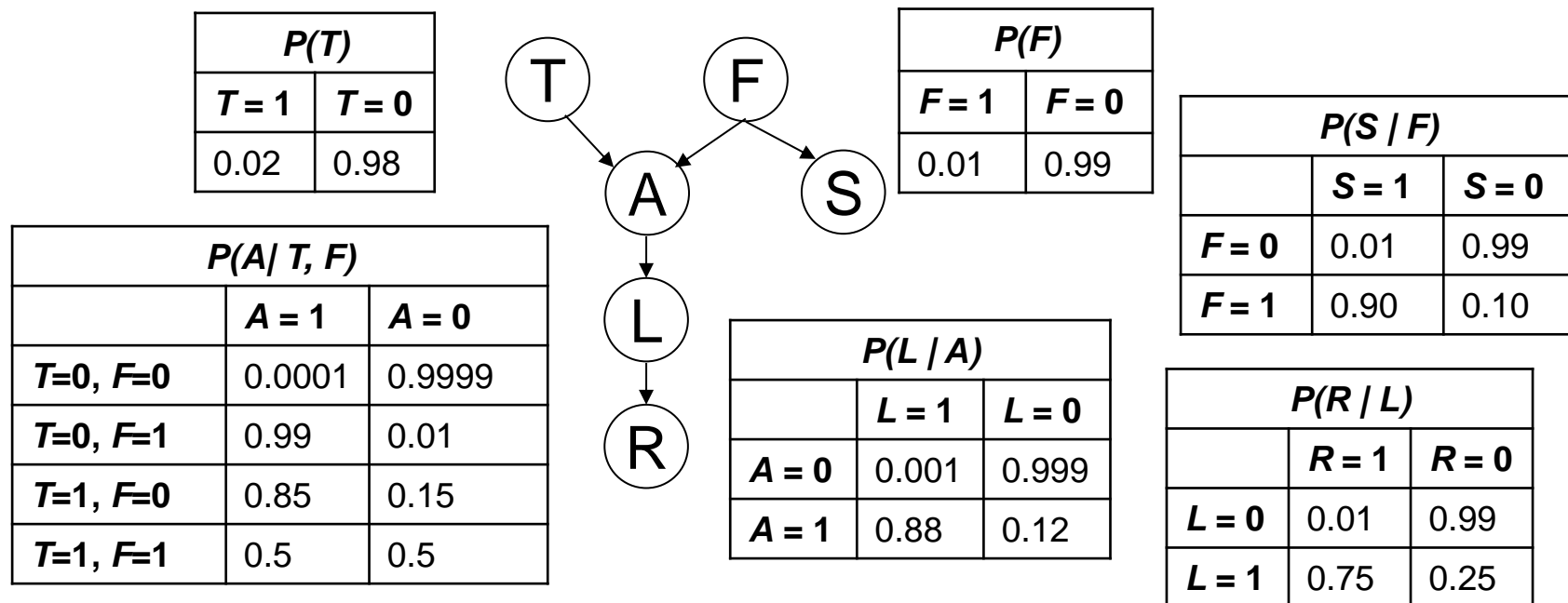
Review: Inference in Bayes nets

- Bayes nets encode information about conditional independence between variables.

$$P(x_1, x_2, \dots, x_n) = \prod_{i=1}^n P(x_i | \text{parents}(X_i))$$

- **Variable elimination** algorithm gives us dynamic programming approach for inferences in Bayes.
- Complexity of inference depends a lot on network's structure.
 - Inference is efficient (poly-time) for tree-structured networks.
 - In worse-case, inference is NP-complete.
- Can leverage DAG structure to facilitate inference.

Constructing Belief Nets: CPDs



Where do these numbers come from?

Parameter Estimation

Option 1: Ask an expert

- Use experts to select Bayes net structure and parameters
 - Experts are often scarce and expensive.
 - Experts can be inconsistent.
 - Experts can be non-existent!

Option 2: Estimate parameters from data

- Estimate how the world works by observing samples!

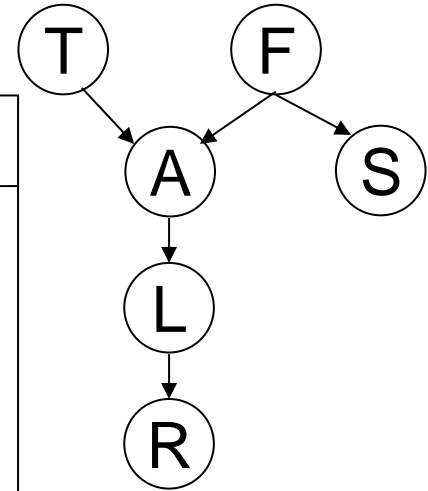
Outline

- Learning with complete data
 - Supervised learning
 - Maximum likelihood estimation
 - Laplace smoothing
- Learning with incomplete data
 - Expectation maximization

Learning in Bayesian networks

- Given **data** in the form of instances:

Tampering	Fire	Smoke	Alarm	Leaving	Report
No	No	No	No	No	No
No	Yes	Yes	Yes	Yes	No
...



- Create a complete Bayes net!
 - Parameter estimation:** Given a graph structure, compute the Conditional Probability Distributions (CPDs). *Do this today!*
 - Structure learning:** Figure out the graph structure as well as the numbers in the CPDs. *Much harder to do!*

Parameter estimation with complete data

- Given:
 - A Bayes network structure G
 - A choice of representation for the CPDs: $P(X_i \mid \text{Parents}(X_i))$
- Goal:
 - Learn the CPD in each node, such that the network is “closest” to the probability distributions that generated the data.
- For simplicity, assume all random variables in graph are binary.

Solving a Detective Mystery

- Your friend just flipped a coin 10 times:
H, T, H, H, H, T, H, H, H, T (7 heads out of 10 tosses)
- They then mixed the coin up with a bunch of other coins. You know the biases of the coins. Which one did they flip?

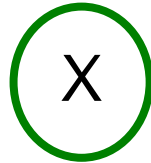


Coin toss example

- Your friend just flipped a coin 10 times:
H, T, H, H, H, T, H, H, H, T (7 heads out of 10 tosses)
- Which coin did they flip? The one with $P(H) =$
 - 0.2
 - 0.5
 - 0.7
 - 0.9
- Which of these values is possible? Probable? Likely?

A network with one node

- Can model as a one-node Bayesian network, $X=\{head, tail\}$.



- Let $P(X) = \theta$ be the (unknown) probability of landing on *head*.
- In this case, X is a **Bernoulli** random variable.
- Given sequence of tosses x_1, \dots, x_m , how can we estimate $P(X)$?

Statistical parameter fitting

- Given instances x_1, \dots, x_m that are **independently identically distributed (i.i.d.)**.
 - Set of possible values for each variable in each instance is known.
 - Each instance is obtained **independently** of the other instances.
 - Each instance is **sampled from the same distribution**.
- **The learning problem:**

Find a set of parameters θ such that the data can be summarized by a probability $P(x_j \mid \theta)$

 - θ depends on the family of probability distributions we consider (e.g. Bernoulli: $\theta = \{p\}$, Gaussian: $\theta = \{\mu, \sigma^2\}$, etc.).

How good is a parameter set?

- It depends on how likely it is to generate the observed data.
- Let D be the data set (all the instances).
- The **likelihood** of parameter set θ given data set D is defined as:

$$L(\theta \mid D) = P(D \mid \theta)$$

- If the **instances are i.i.d.** we have:

$$L(\theta \mid D) = P(D \mid \theta) = P(x_1, x_2, \dots, x_m \mid \theta) = \prod_{j=1:m} P(x_j \mid \theta)$$

Example: Coin tossing

- Suppose you see the following data: $D = H, T, H, T, T$

Recall $\theta = \text{Pr}(\text{Coin lands on Head})$

- What is the likelihood of this sequence for parameter θ ?

$$L(\theta \mid D) = \theta (1 - \theta) \theta (1 - \theta) (1 - \theta)$$

- Likelihood has a familiar form:

$$L(\theta \mid D) = \theta^{N(H)} (1 - \theta)^{N(T)}$$

where $N(H)$ and $N(T)$ are numbers of heads and tails observed.

Sufficient statistics

- To compute the likelihood in the coin tossing example, we only need to know $N(H)$ and $N(T)$ (number of heads and tails), not the full dataset.
- Here $N(H)$ and $N(T)$ are sufficient statistics for this probabilistic model (Bernoulli distribution).
 - A sufficient statistic of the data is a function of the data that summarizes enough information to compute the likelihood.
- Formally, $s(D)$ is a sufficient statistic if, for any two datasets D and D' :

$$s(D) = s(D') \quad \Rightarrow \quad L(\theta|D) = L(\theta|D')$$

Maximum likelihood estimation (MLE)

- Choose parameters that maximize the likelihood function.
- We want to maximize:

$$L(\theta \mid D) = \prod_{j=1:m} P(x_j \mid \theta)$$

- This is a product and products are hard to maximize!
- Instead, we can maximize:

$$\log L(\theta \mid D) = \sum_{j=1:m} \log P(x_j \mid \theta)$$

- To maximize, take the derivatives of this function with respect to θ and set them to 0 (calculus!).

MLE applied to the Bernoulli model

- The likelihood is:

$$L(\theta \mid D) = \theta^{N(H)} (1 - \theta)^{N(T)}$$

- The log-likelihood is:

$$\log L(\theta \mid D) = N(H) \log \theta + N(T) \log (1 - \theta)$$

- Take the derivative of the log-likelihood and set it to 0:

$$d \log L(\theta \mid D) / d\theta = N(H) / \theta - N(T) / (1 - \theta) = 0$$

- Solving this gives:

$$\theta = N(H) / (N(H) + N(T))$$

- This is a nice, intuitive answer – it is simply the proportion of times the coin comes up heads!

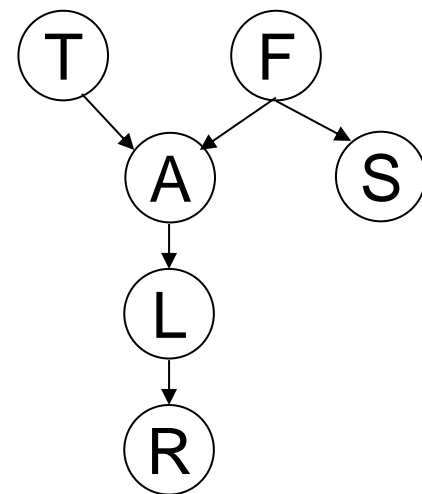
MLE applied to a categorical distribution

- Can show, with more calculus (including Lagrange multipliers – eek!), that the intuitive MLE answer generalizes to the case when there are k outcomes.
- Assume outcomes are $\{1, 2, \dots, k\}$, then parameters are $\theta = \{\theta_1, \theta_2, \dots, \theta_k\}$, where $\sum_i \theta_i = 1$
- In a data set of N samples,
$$\theta_i^{MLE} = N_i / N$$

Parameter estimation in a Bayes net

- Instances are of the form:

$$x_j = \langle t_j, f_j, a_j, s_j, l_j, r_j \rangle, j = 1, \dots, m$$



- What parameters are we trying to estimate?

$$\theta = \{ P(T), P(F), P(A|T,F), P(A|T,\neg F), P(A|\neg T,F), P(A|\neg T,\neg F), \\ P(S|F), P(S|\neg F), P(L|A), P(L|\neg A), P(R|L), P(R|\neg L) \}$$

i.e., Set of parameters in the conditional probability distributions

Alarm example

- Given m instances, how do we compute $P(A)$?

$$P(A) = (\# \text{ instances with } a_j = 1) / m$$

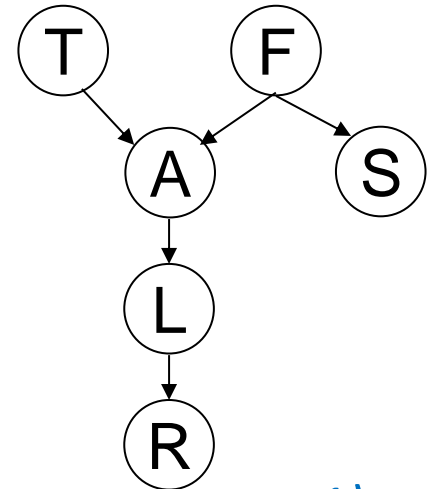
- How do we compute $P(L=1 \mid A=1)$?

$$P(L \mid A) = P(L, A) / P(A)$$

$$= (\# \text{ instances } l_j=1 \text{ and } a_j = 1) / (\# \text{ instances } a_j = 1)$$

- How do we compute $P(A=1 \mid T=1, F=0)$?

$$P(A \mid T, \neg F) = P(A, T, \neg F) / P(T, \neg F)$$



Parameter estimation for general Bayes nets

- Generalizing, for any Bayes net with variables X_1, \dots, X_n :

$$\begin{aligned} L(\theta \mid D) &= \prod_{j=1 \dots m} P(X_1(j), \dots, X_n(j) \mid \theta) && \text{from i.i.d.} \\ &= \prod_{j=1 \dots m} \prod_{i=1 \dots n} P(X_i(j) \mid \text{Parents}(X_i(j)), \theta) && \text{factorization} \\ &= \prod_{i=1 \dots n} \prod_{j=1 \dots m} P(X_i(j) \mid \text{Parents}(X_i(j)), \theta_i) && \text{simplification} \\ &= \prod_{i=1 \dots n} L(\theta_i \mid D) \end{aligned}$$

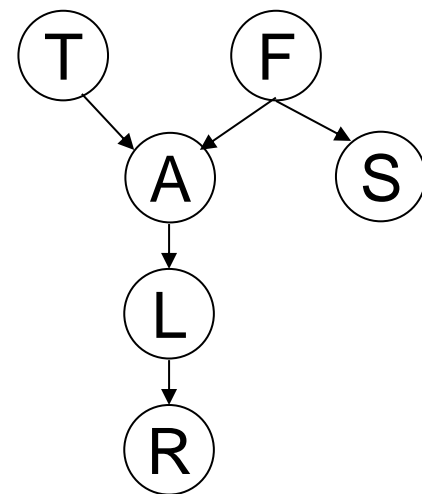
- The likelihood function **decomposes** according to the **structure of the network**, which creates independent estimation problems.

Coin tossing revisited

- Suppose you observed 3 coin tosses, and all come up with tails.
- What is the maximum predictor for θ ?
- Is this a good prediction?

A problem: Zero probabilities

- For problems with lots of variables, it is possible that not all possible values are seen in the data.
 - Especially for very rare events.
- What is the MLE for the corresponding parameters?
E.g. $\text{Prob}(\text{Heads})$ after seeing Tails times.
- **If a value is not seen, the corresponding MLE value for its parameters is 0.**

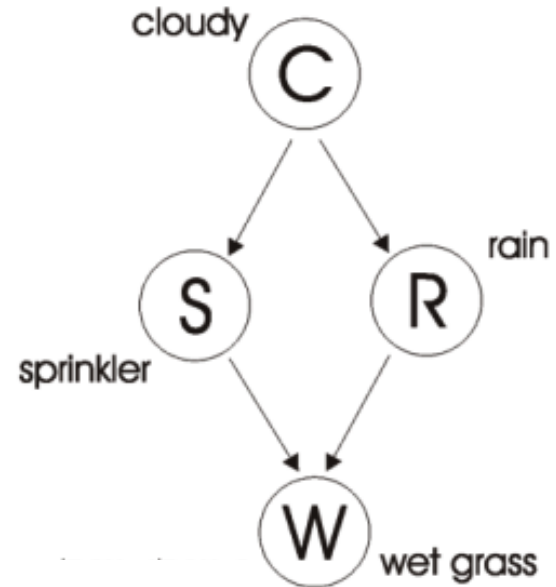


Laplace smoothing

- Instead of: $\theta = N(H) / (N(H) + N(T))$
- Use: $\theta = (N(H) + 1) / (N(H) + N(T) + 2)$
- Imagine that you have seen at least 1 instance of each type.
 - If you have no data, this estimate is: $\theta = 0.5$ +1 for Heads
+1 for Tails
 - With 3 tails, the estimate is: $\theta = 0.2$
 - With 98 tails, the estimate is: $\theta = 0.01$
- If θ is not a Bernoulli, the “+2” changes, e.g. for a categorical with k possible outcomes, add $+k$ in the denominator (and +1 for each possible outcome).

Exercise

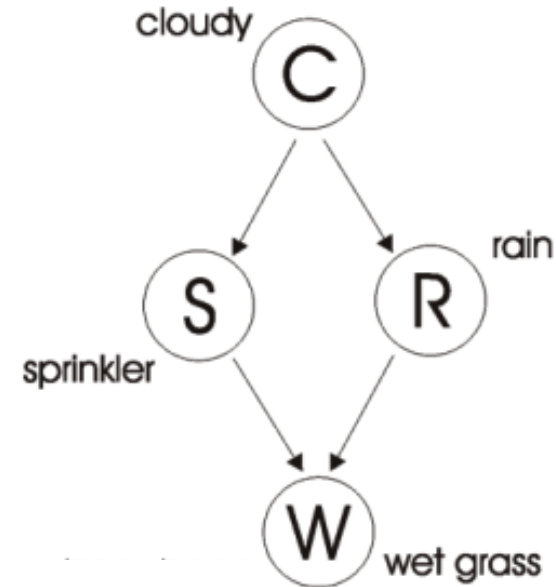
C	S	R	W
T	T	F	T
T	T	T	T
T	F	F	F
F	T	F	T
F	F	F	F



What is the MLE of this Bayes net?
The estimates after Laplace smoothing?

Answers: MLE

C	S	R	W
T	T	F	T
T	T	T	T
T	F	F	F
F	T	F	T
F	F	F	F



MLE:

$$P(C) = 3/5$$

$$P(S|C) = 2/3 \quad P(S|\sim C) = 1/2$$

$$P(R|C) = 1/3 \quad P(R|\sim C) = 0/2$$

$$P(W|S,R) = 1/1 \quad P(W|S,\sim R) = 2/2$$

$$P(W|\sim S,R) = 0/0 \quad P(W|\sim S,\sim R) = 0/2$$

Answers: Laplace Smoothing

C	S	R	W
T	T	F	T
T	T	T	T
T	F	F	F
F	T	F	T
F	F	F	F

Laplace:

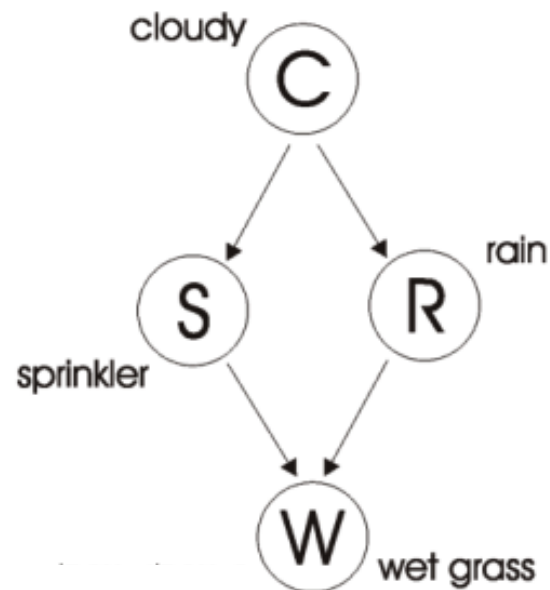
$$P(C) = 4/7$$

$$P(S|C) = 3/5 \quad P(S|\sim C) = 2/4$$

$$P(R|C) = 2/5 \quad P(R|\sim C) = 1/4$$

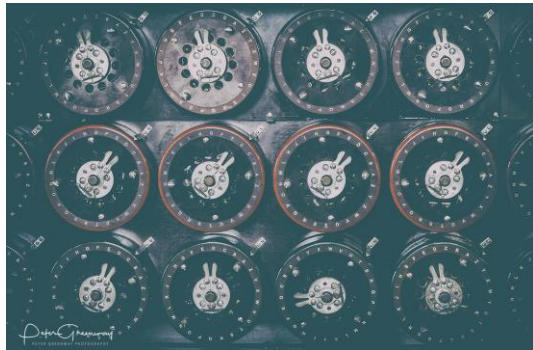
$$P(W|S,R) = 2/3 \quad P(W|S,\sim R) = 3/4$$

$$P(W|\sim S,R) = 1/2 \quad P(W|\sim S,\sim R) = 1/4$$



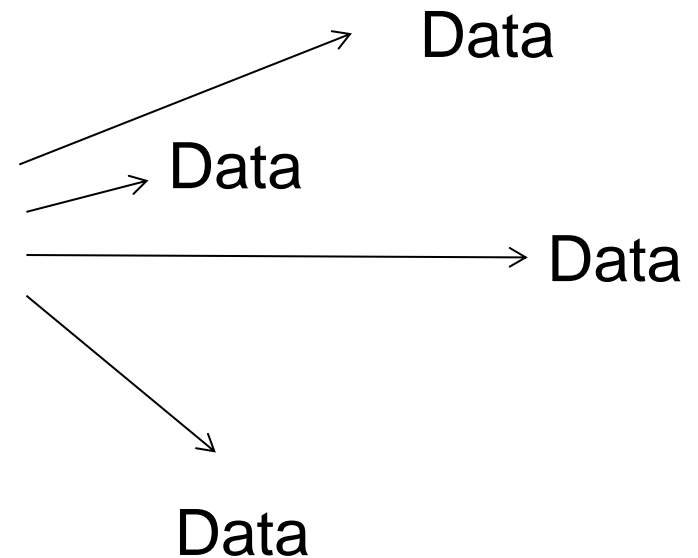
An Intuitive Analogy

- A Bayes net structure is like having a machine with many dials, which correspond to its parameters



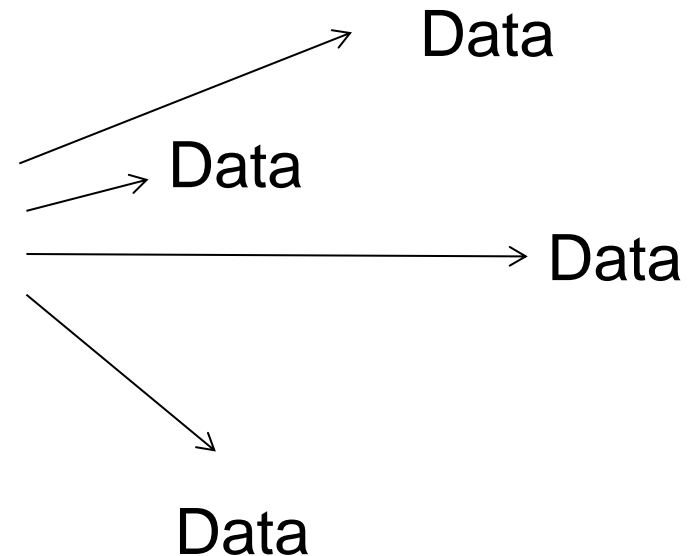
Learning

- We know that this machine was used to generate some observed samples, but we don't know what the dial settings were. Learning is to figure out the setting.



MLE vs Laplace

- MLE and Laplace are two alternative criteria to select the dial setting.
MLE: pick θ to maximize $P(D/\theta)$
Laplace: also care about generalization

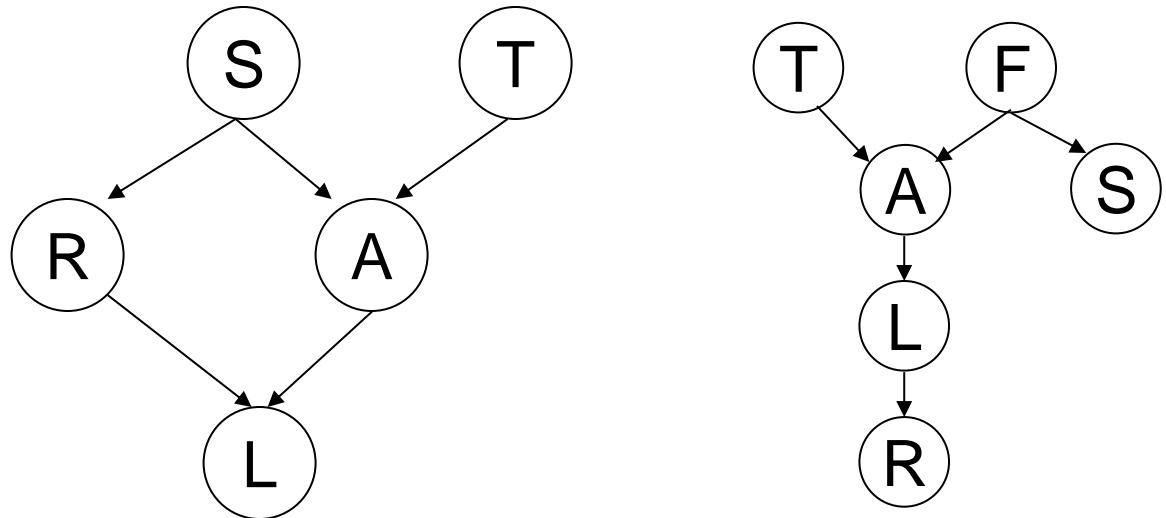


Summary of learning in Bayes Nets

- **Learning** is process of acquiring a model from a data set.
- In Bayes nets, we can learn the parameters of the networks (numbers in the CPDs) or its structure.
- The maximum likelihood principle says that parameters should make the observed data as likely as possible.
- Parameters can be found by taking the gradient of the likelihood function and setting it to 0.
- In the case of simple distributions, the solution is to use “empirical probabilities”, based on counting the data.

What have we left out?

- Everything about choosing variables and structure learning!



- Search over model structures (i.e. adding, reversing, deleting arcs) to maximize $L(\theta_S, S \mid D) = P(D \mid \theta_S, S)$
- Need to trade-off between model complexity and data fidelity. Hard!

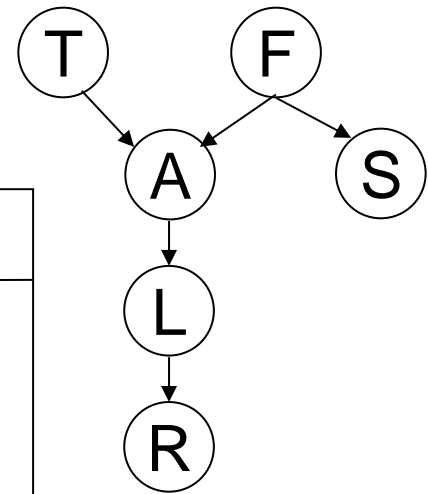
Summary of parameter estimation

- I.i.d. assumption
- Sufficient statistics
- Computing the maximum likelihood
- Laplace smoothing
- Extension to standard probability distributions (see textbook):
 - e.g., categorical, Gaussian, Poisson, exponential

Learning in Bayesian networks

- Given data in the form of instances:

Tampering	Fire	Smoke	Alarm	Leaving	Report
No	No	No	No	No	No
No	Yes	Yes	Yes	Yes	No
...

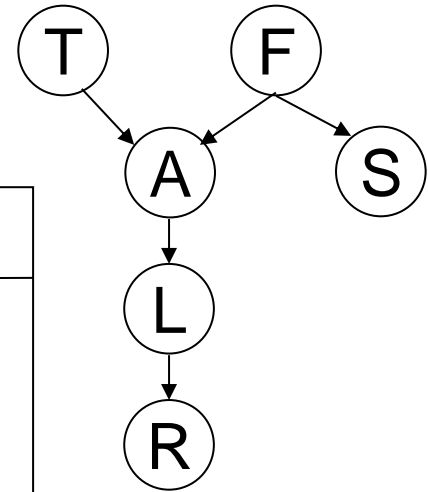


- Goal: Find parameters of the Bayes net.
- We discussed how to do this using maximum likelihood.

Learning in Bayesian networks

- **Plot twist:** Suppose some values are missing!

Tampering	Fire	Smoke	Alarm	Leaving	Report
?	No	No	No	No	No
No	Yes	Yes	Yes	?	No
...



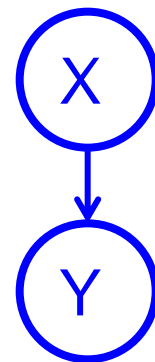
- Can we still use MLE?
 - How do we deal with the missing data?

Why do we get incomplete data?

- Some variables may not be assigned values in *some* instances.
 - E.g. not all patients undergo all medical tests.
- Some variables may not be observed in *any* of the data items.
 - E.g. viewer preferences for a show may depend on their metabolic cycle (what time they are awake) - which is not usually measured.
- **Problem:** the fact that a value is missing may be indicative of what the value actually is.
 - E.g. patient did not undergo X-ray because she had no bone problems; so X-ray would likely have come out negative.

Why missing values make life hard

- Consider a simple network $X \rightarrow Y$, and suppose we want to learn its parameters from samples $\langle x_1, y_1 \rangle, \dots, \langle x_m, y_m \rangle$.



- Which parameters do we need?

- Given all samples values, maximize log-likelihood of:

$$L(\theta_x, \theta_{Y|X=0}, \theta_{Y|X=1}) = (\theta_x)^{N1} (1-\theta_x)^{N0} (\theta_{Y|X=0})^{N01} (1-\theta_{Y|X=0})^{N00} (\theta_{Y|X=1})^{N11} (1-\theta_{Y|X=1})^{N10}$$

- Suppose now that x_1 is missing and $y_1=1$. What can we do?

Why missing values make life hard (2)

- We can consider both settings: $x_1=0$, $x_1=1$.
- For each setting we get a different likelihood.
- Overall likelihood combines both settings (weighted by probability of that setting).

$$L(\theta_X, \theta_{Y|X=0}, \theta_{Y|X=1}) = (1 - \theta_X) \Pr(<0, y_1>, <x_2, y_2>, \dots, <x_m, y_m> \mid \theta_X, \theta_{Y|X=0}, \theta_{Y|X=1}) + \theta_X \Pr(<1, y_1>, <x_2, y_2>, \dots, <x_m, y_m> \mid \theta_X, \theta_{Y|X=0}, \theta_{Y|X=1})$$

- **Problem:** If we have values missing for x_1 and x_2 , we have to consider all possible values for both instances! Etc.

Missing at random assumption

- The probability that the value of X_i is missing is independent of its actual value, given the observed data.
- If this is not true, for variable X_i , we can introduce an additional Boolean variable, $X_i^{Observed}$ and satisfy the assumption.

Effects of missing data

Complete data

- Parameters of model can be estimated locally and independently.
- Log-likelihood has a unique maximum.
- Under certain assumptions, there is a nice closed-form solution for parameters.

Missing data

- Parameters cannot be estimated independently.
- Many local maxima. Maximizing likelihood becomes non-linear optimization problem.
- No closed-form solution.

Two solutions for maximizing likelihood

1. Gradient ascent: Use hill-climbing search through the space of parameters, following the gradient of the likelihood with respect to the parameters.

Gradient ascent

- **Basic idea:** Move parameters in the direction of the log-likelihood.
- Pros:
 - Flexible: allows different forms for the Conditional Prob. Distributions.
 - Easy to compute the gradient at any parameter setting.
 - Closely related to other learning methods (e.g., neural nets).
- Cons:
 - Solution needs to be projected on space of legal parameters (in our case, need to ensure that we get probability distributions.)
 - Sensitive to parameters (e.g., learning rate).
 - Slow!

Two solutions for maximizing likelihood

1. Gradient ascent: hill-climbing search through the space of parameters, following the gradient of the likelihood with respect to the parameters.
2. Expectation maximization: use the current parameter settings to construct a local approximation of the likelihood which is “nice” and can be optimized easily.

Expectation Maximization (EM)

- General purpose method for learning from incomplete data (not only Bayes nets), **whenever an underlying distribution is assumed.**
- Main idea: Alternate between two steps
 1. (**E-step**): For all the instances of missing data, we will “fantasize” how the data should look based on the current parameter setting.
 - This means we compute expected sufficient statistics.
 2. (**M-step**): Then maximize parameter setting, based on these statistics.

Outline of EM

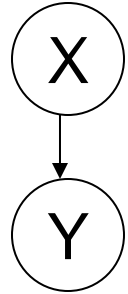
- **Initialization:**
 - Start with some initial parameter setting (e.g. $P(T)$, $P(F)$, $P(A/F, T)$, etc.).
 - These can be estimated from all complete data instances.
- **Repeat:**
 1. Expectation (E-step): Complete the data by assigning “values” to the missing items based on current parameter setting.
 2. Maximization (M-step): Compute the maximum likelihood parameter setting based on the completed data. This is what we did earlier this lecture.
- **Convergence:**
 - Nothing changes in E-step or M-step between 2 consecutive rounds.

EM in our example

- To start, guess the parameters of the network θ (using the known data):

E.g.

$$\theta_x = N_{x=1}(2:m) / (m-1)$$
$$\theta_{Y|x=0} = N_{Y=1,X=0}(2:m) / N_{X=0}(2:m)$$
$$\theta_{Y|x=1} = N_{Y=1,X=1}(2:m) / N_{X=1}(2:m)$$



- E-step:** Using initial θ , compute: $P(x_1=0 \mid y_1), P(x_1=1 \mid y_1)$
(Note that this step requires *exact inference* - so not cheap!)
Complete dataset with most likely value of x_1 .
Call new dataset D^* .
- M-step:** Compute new parameter vector θ , which maximizes the likelihood given the completed data: $L(\theta \mid D^*) = P(D^* \mid \theta)$
E.g.
$$\theta_x = N_{x=1} / m$$
$$\theta_{Y|x=0} = N_{Y=1,X=0} / N_{X=0}$$
$$\theta_{Y|x=1} = N_{Y=1,X=1} / N_{X=1}$$
- Repeat E-step and M-step until the parameter vector converges.**

Two version of the algorithm

- **Hard EM**: for each missing data point, assign the value that is most likely.

(This is the version we just saw.)

- **Soft EM**: for each missing data point, put a weight on each value, equal to its probability, and use the weights as counts.

(This is the most common version.)

Then these numbers are used as real counts, to provide a maximum likelihood estimate for θ .

Soft EM in our example

- To start, guess the parameters of the network θ (using the known data):

E.g.

$$\theta_x = N_{x=1}(2:m) / (m-1)$$

$$\theta_{y|x=0} = N_{y=1,x=0}(2:m) / N_{x=0}(2:m)$$

$$\theta_{y|x=1} = N_{y=1,x=1}(2:m) / N_{x=1}(2:m)$$

- E-step:** Using initial θ , compute: $w_0 = P(x_1=0 \mid y_1)$ $w_1 = P(x_1=1 \mid y_1)$

Now hypothesize two datasets:

$$D_0 = \langle w_0, y_1 \rangle, \langle x_2, y_2 \rangle, \dots, \langle x_m, y_m \rangle$$

$$D_1 = \langle w_1, y_1 \rangle, \langle x_2, y_2 \rangle, \dots, \langle x_m, y_m \rangle$$

- M-step:** Compute new parameter vector θ , which maximizes the expected likelihood given the completed data: $L(\theta \mid D^*) = w_0 P(D_0 \mid \theta) + w_1 P(D_1 \mid \theta)$

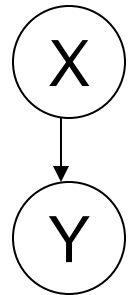
E.g.

$$\theta_x = (N_{x=1}(2:m) + w_1) / m$$

$$\theta_{y|x=0} = (N_{y=1,x=0}(2:m) + w_0) / (N_{x=0}(2:m) + w_0)$$

$$\theta_{y|x=1} = (N_{y=1,x=1}(2:m) + w_1) / (N_{x=1}(2:m) + w_1)$$

Repeat E and M steps!



Comparison of hard EM and soft EM

- Soft EM does not commit to specific value for the missing item.
 - Instead, it considers all possible values, with some probability.
 - This is a pleasing property, given the uncertainty in the value.
- Complexity:
 - Hard EM requires computing most probable values.
 - Soft EM requires computing conditional probabilities for completing the missing values.
 - Same complexity: both require full probabilistic inference - which can be expensive!

Properties of EM

- Likelihood function is guaranteed to improve (or stay the same) with each iteration.
 - Algorithm can be stopped when no more improvement is achieved between iterations.
- EM is guaranteed to converge to a local optimum of the likelihood function.
 - Starting with different values of initial parameters is necessary (random re-starts, to avoid local optimum).
- EM is a widely used algorithm in practice!

A harder example

Suppose we have the simple Bayes net $A \rightarrow B \rightarrow C$, where each node is associated with a Bernoulli random variable. Further suppose we have the following sample data:

- (i) $A=1, B=?, C=1$
- (ii) $A=0, B=1, C=0$
- (iii) $A=1, B=0, C=0$
- (iv) $A=1, B=1, C=0$
- (v) $A=1, B=1, C=0$
- (vi) $A=0, B=0, C=?$

A harder example

Suppose we have the simple Bayes net $A \rightarrow B \rightarrow C$, where each node is associated with a Bernoulli random variable. Further suppose we have the following sample data:

- (i) $A=1, B=?, C=1$
- (ii) $A=0, B=1, C=0$
- (iii) $A=1, B=0, C=0$
- (iv) $A=1, B=1, C=0$
- (v) $A=1, B=1, C=0$
- (vi) $A=0, B=0, C=?$

$$\begin{aligned}
 w_{B_1=1} &= P(B_1 = 1 | A_1, C_1) \\
 &= P(B = 1 | A = 1, C = 1) \\
 &= \frac{P(A = 1, B = 1, C = 1)}{P(A = 1, C = 1)} \\
 &= \frac{P(A = 1, B = 1, C = 1)}{\sum_{b \in \{0,1\}} P(A = 1, C = 1, B = b)} \\
 &= \frac{\theta_A \theta_{B|A=1} \theta_{C|B=1}}{\theta_A \theta_{B|A=1} \theta_{C|B=1} + \theta_A (1 - \theta_{B|A=1}) \theta_{C|B=0}} \\
 &= \frac{(0.5)(0.5)(0.5)}{(0.5)(0.5)(0.5) + (0.5)(0.5)(0.5)} \\
 &= 0.5
 \end{aligned}$$

E-step

$$\begin{aligned}
 w_{B_1=0} &= P(B_1 = 0 | A_1, C_1) \\
 &= P(B = 0 | A = 1, C = 1) \\
 &= (1 - P(B = 1 | A = 1, C = 1)) \\
 &= (1 - w_{B_1=1}) \\
 &= 0.5
 \end{aligned}$$

$$\begin{aligned}
 w_{C_6=1} &= P(C_6 = 1 | A_6, B_6) \\
 &= P(C_6 = 1 | B_6) \quad \text{by conditional independence} \\
 &= P(C = 1 | B = 0) \\
 &= 0.5
 \end{aligned}$$

$$\begin{aligned}
 w_{C_6=0} &= (1 - w_{C_6=1}) \quad \text{same reasoning as } w_{B_1=0} = (1 - w_{B_1=1}) \\
 &= 0.5
 \end{aligned}$$

$$\begin{aligned}
 \theta_A^{ML} &= \frac{N_{A=1}(1:6)}{6} = \frac{4}{6} \approx 0.667 \\
 \theta_{B|A=1}^{ML} &= \frac{N_{B=1|A=1}(2:6) + w_{B_1=1}}{4} = \frac{2+0.5}{4} = 0.625 \\
 \theta_{B|A=0}^{ML} &= \frac{N_{B=1|A=0}(2:6)}{2} = \frac{1}{2} = 0.5 \\
 \theta_{C|B=1}^{ML} &= \frac{N_{C=1|B=1}(2:4) + w_{B_1=1}}{3 + w_{B_1=1}} = \frac{0.5}{3.5} \approx 0.143 \\
 \theta_{C|B=0}^{ML} &= \frac{N_{C=1|B=0}(2:4) + w_{B_1=0} + w_{C_6=1}}{2 + w_{B_1=0}} = \frac{0.5+0.5}{2.5} = 0.4
 \end{aligned}$$

M-step

And repeat...