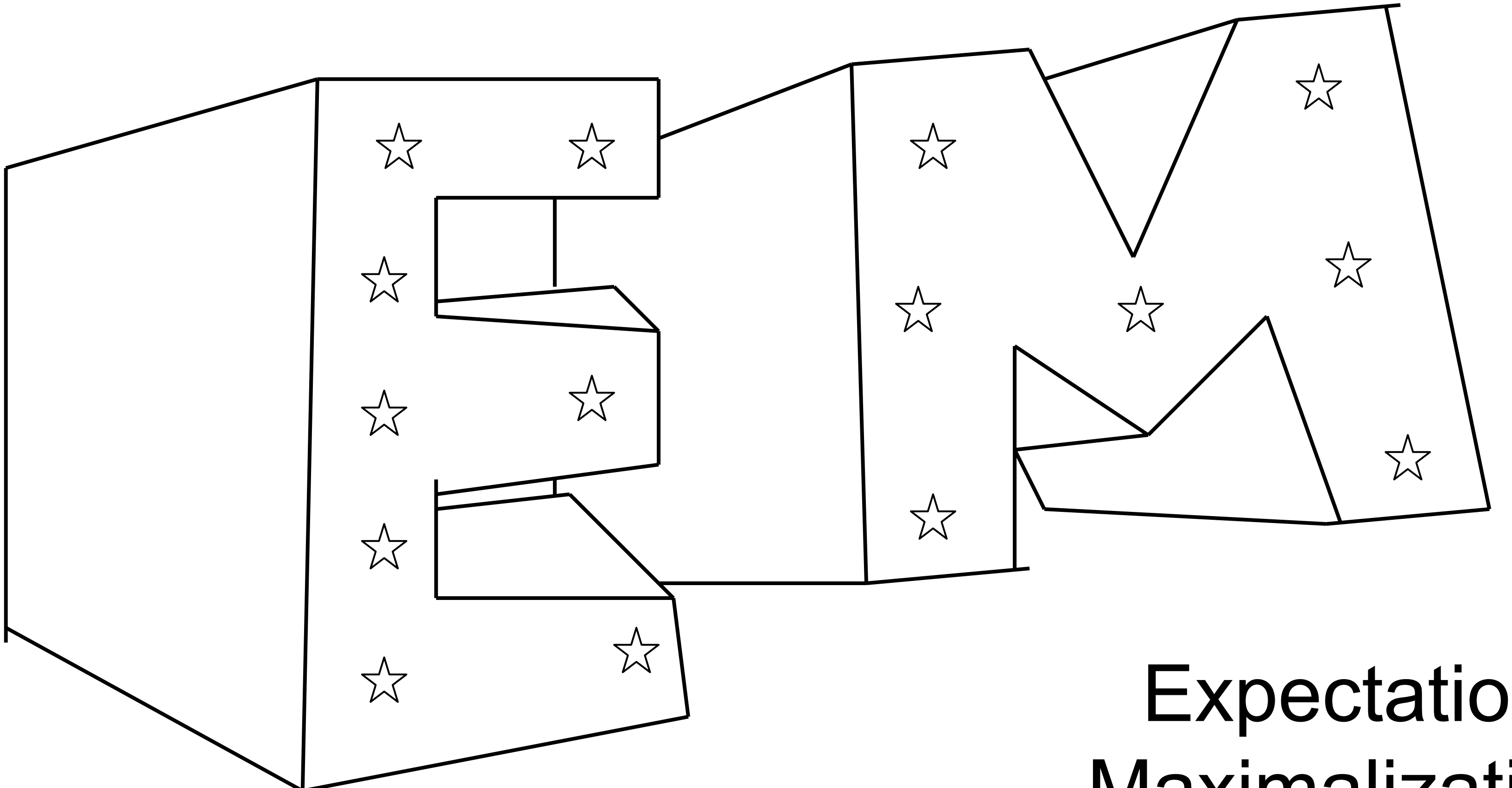


Expectation
Maximalization

The E.M. Algorithm

- We'll get back to unsupervised learning soon.
- But now we'll look at an even simpler case with hidden information.
- The EM algorithm
  - An excellent way of doing unsupervised clustering.
  - Many, many other uses, including inference of Hidden Markov Models.

Missing Data

A	B
1	1
1	1
0	0
0	0
0	0
0	H
0	1
1	0

- Given two variables, no independence relations
- Some data are missing
- Estimate parameters in joint distribution
- Data must be missing at random

Ignore it

A	B
1	1
1	1
0	0
0	0
0	0
0	H
0	1
1	0

Estimated Parameters

	~A	A
~B	3/7	1/7
B	1/7	2/7

	~A	A
~B	.429	.143
B	.143	.285

$$\begin{aligned}\log \Pr(D|M) &= \log(\Pr(D,H=0 \mid M) + \Pr(D,H=1 \mid M)) \\ &= 3\log .429 + 2\log .143 + 2\log .285 + \log(.429 + .143) \\ &= -9.498\end{aligned}$$

Fill in With Best Value

A	B
1	1
1	1
0	0
0	0
0	0
0	0
0	1
1	0

Estimated Parameters

	~A	A
~B	4/8	1/8
B	1/8	2/8

	~A	A
~B	.5	.125
B	.125	.25

$$\begin{aligned}\log \Pr(D|M) &= \log(\Pr(D, H=0 \mid M) + \Pr(D, H=1 \mid M)) \\ &= 3\log .5 + 2\log .125 + 2\log .25 + \log(.5 + .125) \\ &= -9.481\end{aligned}$$

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	H
0	1
1	0

Guess a distribution over A,B and compute a distribution over H

θ_0

	~A	A
~B	.25	.25
B	.25	.25

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	H
0	1
1	0

Guess a distribution over A,B and compute a distribution over H

θ_0

	~A	A
~B	.25	.25
B	.25	.25

$$
\begin{aligned}
\Pr(H|D,\theta_0) &= \Pr(H \mid D^6, \theta_0) \\
&= \Pr(B \mid \neg A, \theta_0) \\
&= \Pr(\neg A, B \mid \theta_0) / \Pr(\neg A \mid \theta_0) \\
&= .25 / 0.5 \\
&= 0.5
\end{aligned}
$$

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	0, 0.5 1, 0.5
0	1
1	0

Use distribution over H to compute better distribution over A,B

Maximum likelihood estimation using *expected counts*

θ_1

	~A	A
~B	3.5/8	1/8
B	1.5/8	2/8

	~A	A
~B	.4375	.125
B	.1875	.25

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	
0	1
1	0

Use new distribution over AB to get a better distribution over H

θ_1

	~A	A
~B	.4375	.125
B	.1875	.25

$$
\begin{aligned}
\Pr(H|D,\theta_1) &= \Pr(\neg A, B \mid \theta_1) / \Pr(\neg A \mid \theta_1) \\
&= .1875 / .625 \\
&= 0.3
\end{aligned}
$$

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	0, 0.7 1, 0.3
0	1
1	0

Use distribution over H to compute better distribution over A,B

θ_2

	~A	A
~B	3.7/8	1/8
B	1.3/8	2/8

	~A	A
~B	.4625	.125
B	.1625	.25

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	
0	1
1	0

Use new distribution over AB to get a better distribution over H

θ_2

	~A	A
~B	.4625	.125
B	.1625	.25

$$\Pr(H|D,\theta_2) = \Pr(\neg A, B \mid \theta_2) / \Pr(\neg A \mid \theta_2)$$
$$= .1625 / .625$$
$$= 0.26$$

Fill in With Distribution

A	B
1	1
1	1
0	0
0	0
0	0
0	0, 0.74 1, 0.26
0	1
1	0

Use distribution over H to compute better distribution over A,B

θ_3

	~A	A
~B	3.74/8	1/8
B	1.26/8	2/8

	~A	A
~B	.4675	.125
B	.1575	.25

Increasing Log-Likelihood

θ_0

	~A	A
~B	.25	.25
B	.25	.25

$$\log \Pr(D \mid \theta_0) = -10.3972$$

θ_1

	~A	A
~B	.4375	.125
B	.1875	.25

$$\log \Pr(D \mid \theta_1) = -9.4760$$

θ_2

	~A	A
~B	.4625	.125
B	.1625	.25

$$\log \Pr(D \mid \theta_2) = -9.4524$$

θ_3

	~A	A
~B	.4675	.125
B	.1575	.25

$$\log \Pr(D \mid \theta_3) = -9.4514$$

Increasing Log-Likelihood

θ_0

	~A	A
~B	.25	.25
B	.25	.25

$$\log \Pr(D \mid \theta_0) = -10.3972$$

ignore: -9.498

best val: -9.481

θ_1

	~A	A
~B	.4375	.125
B	.1875	.25

$$\log \Pr(D \mid \theta_1) = -9.4760$$

θ_2

	~A	A
~B	.4625	.125
B	.1625	.25

$$\log \Pr(D \mid \theta_2) = -9.4524$$

θ_3

	~A	A
~B	.4675	.125
B	.1575	.25

$$\log \Pr(D \mid \theta_3) = -9.4514$$

Another (Simple) Example

Let events be "grades in a class"

w_1 = Gets an A $\quad$ $P(A) = ½$

w_2 = Gets a B $\quad$ $P(B) = \mu$

w_3 = Gets a C $\quad$ $P(C) = 2\mu$

w_4 = Gets a D $\quad$ $P(D) = ½-3\mu$

(Note $0 \leq \mu \leq 1/6$)

Assume we want to estimate μ from data. In a given class there were

a A's
b B's
c C's
d D's

What's the maximum likelihood estimate of μ given a,b,c,d ?

Simple Example - contd

Let events be “grades in a class”

w_1 = Gets an A	P(A) = ½
w_2 = Gets a B	P(B) = μ
w_3 = Gets a C	P(C) = 2μ
w_4 = Gets a D	P(D) = $½-3\mu$
	(Note $0 \le \mu \le 1/6$)

Assume we want to estimate μ from data. In a given class there were

a A’s
b B’s
c C’s
d D’s

What’s the maximum likelihood estimate of μ given a,b,c,d ?

Trivial Statistics

$P(A) = \frac{1}{2}$ $P(B) = \mu$ $P(C) = 2\mu$ $P(D) = \frac{1}{2}-3\mu$

$P(a,b,c,d \mid \mu) = K(\frac{1}{2})^{a}(\mu)^{b}(2\mu)^{c}(\frac{1}{2}-3\mu)^{d}$

$\log P(a,b,c,d \mid \mu) = \log K + a\log \frac{1}{2} + b\log \mu + c\log 2\mu + d\log (\frac{1}{2}-3\mu)$

$$\text{FOR MAX LIKE } \mu\text{, SET } \frac{\partial \text{LogP}}{\partial \mu} = 0$$

$$\frac{\partial \text{LogP}}{\partial \mu} = \frac{b}{\mu} + \frac{2c}{2\mu} - \frac{3d}{1/2 - 3\mu} = 0$$

$$\text{Gives max like } \mu = \frac{b+c}{6(b+c+d)}$$

So if class got

A	B	C	D
14	6	9	10

$$\text{Max like } \mu = \frac{1}{10}$$

Same Problem with Hidden Information

REMEMBER

$P(A) = ½$

$P(B) = \mu$

$P(C) = 2\mu$

$P(D) = ½-3\mu$

Someone tells us that

Number of High grades (A's + B's) = h

Number of C's = c

Number of D's = d

What is the max. like estimate of μ now?

Same Problem with Hidden Information

REMEMBER

P(A) = ½

P(B) = μ

P(C) = 2μ

P(D) = ½-3μ

Someone tells us that

Number of High grades (A's + B's) = *h*

Number of C's = *c*

Number of D's = *d*

What is the max. like estimate of μ now?

We can answer this question circularly:

EXPECTATION

If we know the value of μ we could compute the expected value of *a* and *b*

Since the ratio a:b should be the same as the ratio ½ : μ

$$a = \frac{\frac{1}{2}}{\frac{1}{2}+\mu}h \qquad b = \frac{\mu}{\frac{1}{2}+\mu}h$$

MAXIMIZATION

If we know the expected values of *a* and *b* we could compute the maximum likelihood value of μ

$$\mu = \frac{b+c}{6(b+c+d)}$$

E.M. for our Trivial Problem

REMEMBER

P(A) = ½

P(B) = μ

P(C) = 2μ

P(D) = ½-3μ

We begin with a guess for μ

We iterate between EXPECTATION and MAXIMALIZATION to improve our estimates of μ and *a* and *b*.

Define μ(t) the estimate of μ on the t'th iteration

b(t) the estimate of *b* on t'th iteration

$$\mu(0) = \text{initial guess}$$

$$b(t) = \frac{\mu(\mathrm{t})\, h}{1/2 + \mu(t)} = \mathrm{E}\left[b \mid \mu(t)\right]$$

E-step

$$\mu(t+1) = \frac{b(t) + c}{6\left(b(t) + c + d\right)}$$

$$= \text{max like est of } \mu \text{ given } b(t)$$

M-step

Continue iterating until converged.
Good news: Converging to local optimum is assured.
Bad news: "local" optimum.

E.M. Convergence

- Convergence proof based on fact that Prob(data | μ) must increase or remain same between each iteration [NOT OBVIOUS]
- But it can never exceed 1 [OBVIOUS]

So it must therefore converge [OBVIOUS]

In our example, suppose we had

$h = 20$

$c = 10$

$d = 10$

$\mu(0) = 0$

t	μ(t)	b(t)
0	0	0
1	0.0833	2.857
2	0.0937	3.158
3	0.0947	3.185
4	0.0948	3.187
5	0.0948	3.187
6	0.0948	3.187

Convergence is generally <u>linear</u>: error decreases by a constant factor each time step.

Recap

Maximum Likelihood Estimation

- We have data points $X_1, X_2, \ldots X_n$ drawn from some (finite or countable) set $\mathcal{X}$

- We have a parameter vector Θ

- We have a parameter space Ω

- We have a distribution $P(X \mid \Theta)$ for any $\Theta \in \Omega$, such that

$$\sum_{X \in \mathcal{X}} P(X \mid \Theta) = 1 \text{ and } P(X \mid \Theta) \geq 0 \text{ for all X}$$

- We assume that our data points $X_1, X_2, \ldots X_n$ are drawn at random (independently, identically distributed) from a distribution $P(X \mid \Theta^*)$ for some $\Theta^* \in \Omega$

Log-Likelihood

- We have data points $X_1, X_2, \ldots X_n$ drawn from some (finite or countable) set $\mathcal{X}$
- We have a parameter vector Θ, and a parameter space Ω
- We have a distribution $P(X \mid \Theta)$ for any $\Theta \in \Omega$
- The likelihood is

$$Likelihood(\Theta) = P(X_1, X_2, \ldots X_n \mid \Theta) = \prod_{i=1}^{n} P(X_i \mid \Theta)$$

- The log-likelihood is

$$L(\Theta) = \log Likelihood(\Theta) = \sum_{i=1}^{n} \log P(X_i \mid \Theta)$$

MLE: $$\Theta_{ML} = \text{argmax}_{\Theta \in \Omega} L(\Theta) = \text{argmax}_{\Theta \in \Omega} \sum_{i} \log P(X_i \mid \Theta)$$

Models with Hidden Variables: Formalization

- Now say we have two sets $\mathcal{X}$ and $\mathcal{Y}$, and a joint distribution $P(X, Y \mid \Theta)$

- If we had **fully observed data**, (X_i, Y_i) pairs, then

$$L(\Theta) = \sum_i \log P(X_i, Y_i \mid \Theta)$$

- If we have **partially observed data**, X_i examples, then

$$\begin{aligned} L(\Theta) &= \sum_i \log P(X_i \mid \Theta) \\ &= \sum_i \log \sum_{Y \in \mathcal{Y}} P(X_i, Y \mid \Theta) \end{aligned}$$

- The **EM (Expectation Maximization) algorithm** is a method for finding

$$\Theta_{ML} = \text{argmax}_\Theta \sum_i \log \sum_{Y \in \mathcal{Y}} P(X_i, Y \mid \Theta)$$

EM Formalization

- Let X be all *observed* variable values (over all examples)
- Let Z be all *unobserved* variable values
- Can't calculate MLE:

$$\theta \leftarrow \arg\max_{\theta} \log P(X, Z|\theta)$$

- EM seeks estimate:

$$\theta \leftarrow \arg\max_{\theta} E_{Z|X,\theta}[\log P(X, Z|\theta)]$$

Deriving the EM Algorithm

- Want to find θ to maximize $\Pr(D \mid \theta)$
- Instead, find θ, $\tilde{P}$ to maximize

$$g(\theta,\tilde{P}) = \sum_{H} \tilde{P}(H)\log(\Pr(D,H \mid \theta)/\tilde{P}(H))$$

$$= E_{\tilde{P}} \log \Pr(D,H \mid \theta) - \log \tilde{P}(H)$$

- Alternate between
  - holding θ fixed and optimizing $\tilde{P}$
  - holding $\tilde{P}$ fixed and optimizing θ
- g has same local and global optima as $\Pr(D \mid \theta)$

EM Algorithm

- Pick initial θ_0
- Loop until apparently converged
  - $\tilde{P}_{t+1}(H) = \Pr(H \mid D, \theta_t)$
  - $\theta_{t+1} = \arg\max_{\theta} E_{\tilde{P}_{t+1}} \log \Pr(D, H \mid \theta)$
- Monotonically increasing likelihood
- Convergence is hard to determine due to plateaus
- Problems with local optima

MLE for CPTs

- Each conditional probability table θ_i part of our parameters
- Given table, have pdf

$$p(x \mid \theta) = \prod_{i=1}^{n} p(x_i \mid \pi_i, \theta_i)$$

- Have M variables:

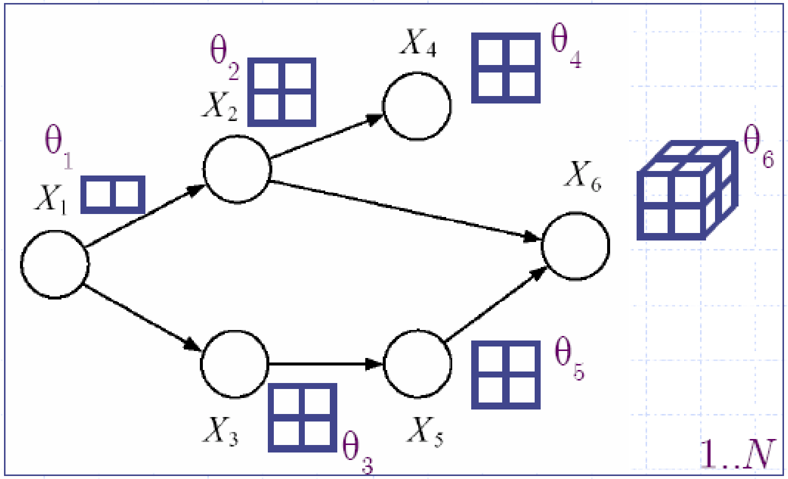
$$X_U = \{x_1, \ldots, x_M\}$$

- Have N x M dataset:

$$\mathcal{D} = \{X_{U,1}, \ldots, X_{U,N}\}$$

- Maximum likelihood:

$$\begin{aligned}
\theta^* &= \arg\max_\theta \log p(\mathcal{D} \mid \theta) \\
&= \arg\max_\theta \sum_{n=1}^{N} \log p(X_{U,n} \mid \theta) \\
&= \arg\max_\theta \sum_{n=1}^{N} \log \prod_{i=1}^{M} p(x_{i,n} \mid \pi_{i,n} \theta_i) \\
&= \arg\max_\theta \sum_{n=1}^{N} \sum_{i=1}^{M} \log p(x_{i,n} \mid \pi_{i,n} \theta_i)
\end{aligned}$$

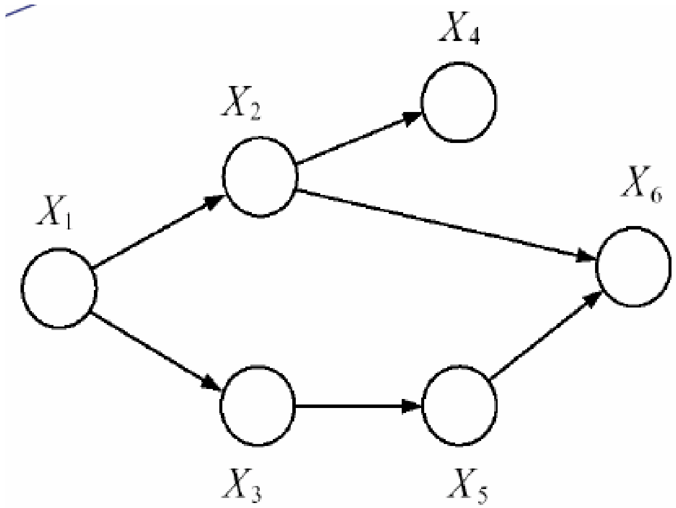


each θ_i appears independently, can do ML for each CPT alone! efficient storage + efficient learning

$$\textit{parents of child } i = pa_i = \pi_i$$

MLE for CPTs

PATIENT	FLU	FEVER	SINUS	TEMP	SWELL	HEAD
1	Y	Y	N	L	Y	Y
2	N	N	N	M	N	Y
3	Y	N	Y	H	Y	N
4	Y	N	Y	M	N	N



X_1 = FLU, X_2 = FEVER, X_3 =SINUS, X_4 = TEMP, X_5 = SWELL, X_6 = HEAD

Let: $\theta(x_i, \pi_i) = p(x_i \mid \pi_i, \theta_i)$

Note: $\sum_{x_i} \theta(x_i, \pi_i) = 1$

MLE: $\theta(x_i, \pi_i) = \dfrac{m(x_i, \pi_i)}{m(\pi_i)}$

	$x_1 = 0$	$x_1 = 1$	
$x_3 = 0$	1	1	$m(x_3, x_1)$
$x_3 = 1$	0	2	

1	3	$m(x_1)$

1	1/3	$p(x_3 \mid x_1)$
0	2/3	

EM for Bayesian Nets

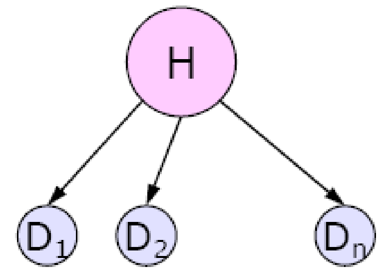
- D: observable variables
- H: values of hidden variables in each case
- Assume structure is known
- Goal: maximum likelihood estimation of CPTs

- Initialize CPTs to anything (with no 0's)
- Fill in the data set with distribution over values for hidden vars
- Estimate CPTs using expected counts

EM for BN Example

D_1	D_2	...	D_n	$\Pr(H^m \mid D^m, \theta_t)$
1	1		0	.9
0	1		0	.2
0	0		1	.1
1	0		1	.6
1	1		1	.2
1	1		1	.5
0	1		0	.3
0	0		0	.7
1	1		0	.2

Bayes net inference



$$E\#(H) = \sum_m \Pr(H^m \mid D^m, \theta_t) = 3.7$$

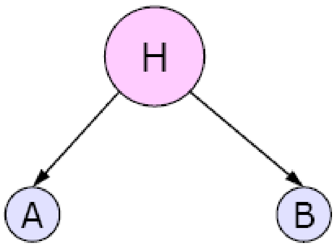
$$E\#(H \wedge D_2) = \sum_m \Pr(H^m \mid D^m, \theta_t) I(D_2^m) = .9 + .2 + .2 + .5 + .3 + .2 = 2.3$$

$$\Pr(D_2 | H) \approx 2.3 / 3.7 = .6216$$

Re-estimate θ

EM for BN: Worked Example

A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	
0	1	1	
1	0	1	
1	1	4	



$$\theta_1 = \Pr(H)$$

$$\theta_2 = \Pr(A \mid H)$$

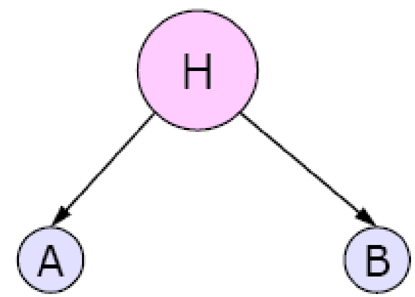
$$\theta_3 = \Pr(A \mid \neg H)$$

$$\theta_4 = \Pr(B \mid H)$$

$$\theta_5 = \Pr(B \mid \neg H)$$

EM for BN: Initial Model

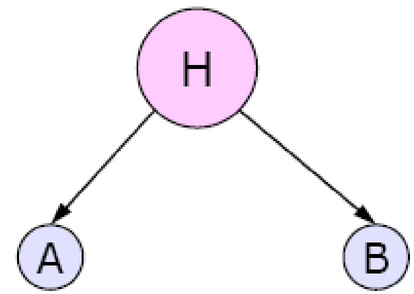
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	
0	1	1	
1	0	1	
1	1	4	



$$\Pr(H) = 0.4$$
$$\Pr(A|H) = 0.55$$
$$\Pr(A|\neg H) = 0.61$$
$$\Pr(B|H) = 0.43$$
$$\Pr(B|\neg H) = 0.52$$

Iteration 1: Fill in Data

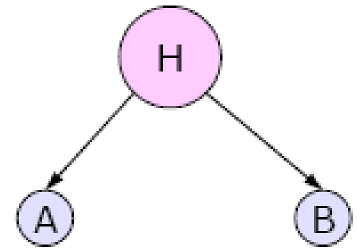
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.48
0	1	1	.39
1	0	1	.42
1	1	4	.33



$$\Pr(H) = 0.4$$
$$\Pr(A|H) = 0.55$$
$$\Pr(A|\neg H) = 0.61$$
$$\Pr(B|H) = 0.43$$
$$\Pr(B|\neg H) = 0.52$$

Iteration 1: Re-estimate Params

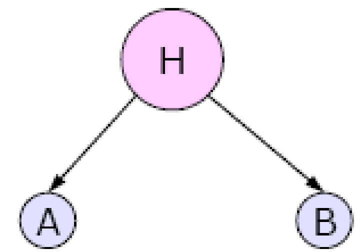
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.48
0	1	1	.39
1	0	1	.42
1	1	4	.33



$$\Pr(H) = 0.42$$
$$\Pr(A|H) = 0.35$$
$$\Pr(A|\neg H) = 0.46$$
$$\Pr(B|H) = 0.34$$
$$\Pr(B|\neg H) = 0.47$$

Iteration 2: Fill in Data

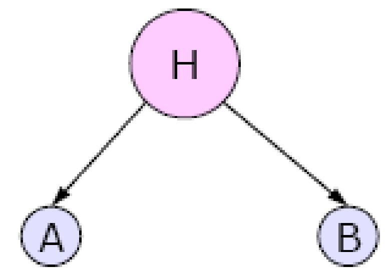
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.52
0	1	1	.39
1	0	1	.39
1	1	4	.28



$$\Pr(H) = 0.42$$
$$\Pr(A|H) = 0.35$$
$$\Pr(A|\neg H) = 0.46$$
$$\Pr(B|H) = 0.34$$
$$\Pr(B|\neg H) = 0.47$$

Iteration 2: Re-estimate Params

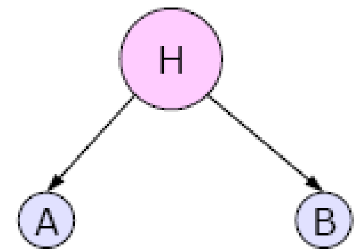
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.52
0	1	1	.39
1	0	1	.28
1	1	4	.28



$$\Pr(H) = 0.42$$
$$\Pr(A|H) = 0.31$$
$$\Pr(A|\neg H) = 0.50$$
$$\Pr(B|H) = 0.30$$
$$\Pr(B|\neg H) = 0.50$$

Iteration 5

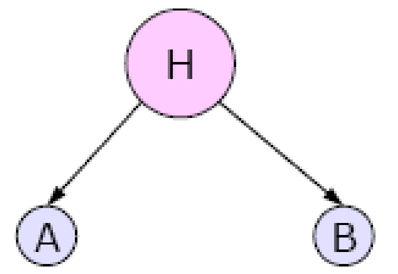
A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.79
0	1	1	.31
1	0	1	.31
1	1	4	.05



$$\Pr(H) = 0.46$$
$$\Pr(A|H) = 0.09$$
$$\Pr(A|\neg H) = 0.69$$
$$\Pr(B|H) = 0.09$$
$$\Pr(B|\neg H) = 0.69$$

Iteration 10

A	B	#	$\Pr(H^m \mid D^m, \theta_t)$
0	0	6	.971
0	1	1	.183
1	0	1	.183
1	1	4	.001



$$\Pr(H) = 0.52$$
$$\Pr(A \mid H) = 0.03$$
$$\Pr(A \mid \neg H) = 0.83$$
$$\Pr(B \mid H) = 0.03$$
$$\Pr(B \mid \neg H) = 0.83$$

Increasing Log-Likelihood