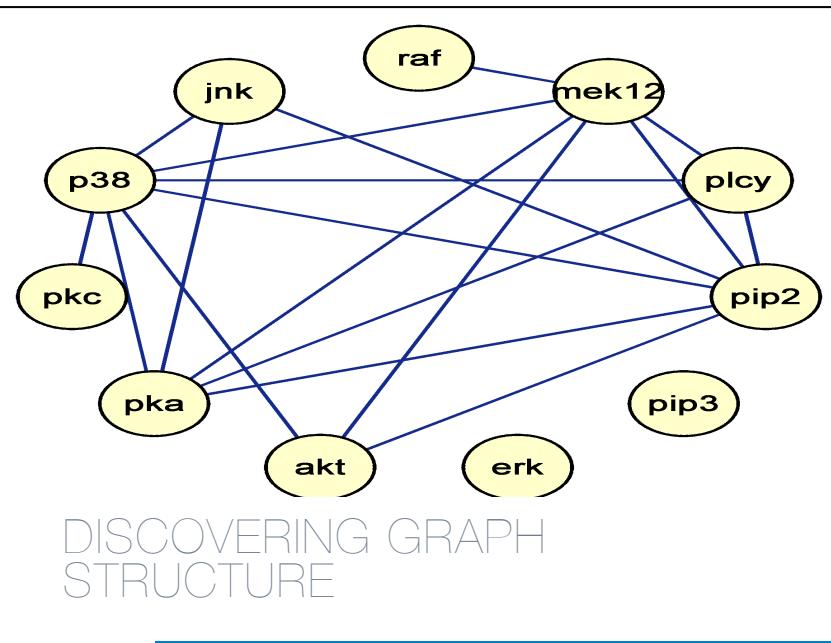




Royal Institute of  
Technology

# MACHINE LEARNING 2 – DGM, CH 10

## Lecture 2



Royal Institute of  
Technology

# SciLifeLab

Computational Biology

Machine Learning – a main tool

Jens Lagergren



## K-MEANS

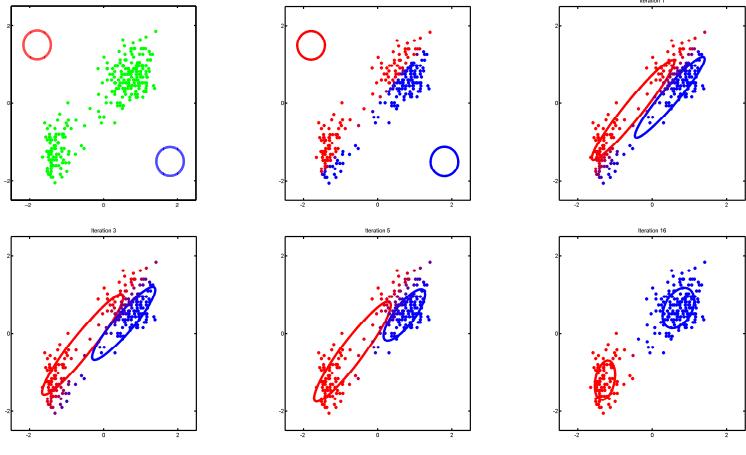
- ★ Data vectors  $D = \{x_1, \dots, x_N\}$
- ★ Randomly selected classes  $Z_1, \dots, Z_N$
- ★ Iteratively do

$$\mu_c = \frac{1}{N_c} \sum_{n:z_n=c} x_n, \quad \text{where } N_c = |\{n : z_n = c\}|$$

$$z_n = \operatorname{argmin}_c \|x_n - \mu_c\|_2$$

- ★ One step  $O(NKD)$ , can be improved

## EXAMPLE



## Expected complete: notation

$$\begin{aligned}
 \log p(\mathbf{x}_n | \boldsymbol{\theta}') &= \log \sum_{\mathbf{z}_n} p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}') \\
 &= \log \sum_{\mathbf{z}_n} p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta}) \frac{p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}')}{p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta})} \\
 &= \log E_{\mathbf{z}_n} \left( \frac{p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}')}{p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta})} \mid \mathbf{x}_n, \boldsymbol{\theta} \right) \\
 &\geq_{\text{Jensen}} E_{\mathbf{z}_n} \left( \log \frac{p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}')}{p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta})} \mid \mathbf{x}_n, \boldsymbol{\theta} \right) \\
 &= \sum_{\mathbf{z}_n} p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta}) \log \frac{p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}')}{p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta})} \\
 &= \sum_{\mathbf{z}_n} p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta}) \log p(\mathbf{x}_n, \mathbf{z}_n | \boldsymbol{\theta}') - \sum_{\mathbf{z}_n} p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta}) \log p(\mathbf{z}_n | \mathbf{x}_n, \boldsymbol{\theta}) \\
 &= Q_n(\boldsymbol{\theta}' ; \boldsymbol{\theta}) - R_n(\boldsymbol{\theta}; \boldsymbol{\theta})
 \end{aligned}$$

## CONDITIONING

$$p(x, y) = p(y)p(x|y) \quad \text{or} \quad p(x|y) = \frac{p(x, y)}{p(y)}$$

## INFERENCE – THE CHAIN RULE

$$p(\underbrace{\mathbf{x}_{[V]}}_{\mathbf{x}_1, \dots, \mathbf{x}_V}) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2) \cdots p(\mathbf{x}_V|\mathbf{x}_{[V-1]})$$

- \* Assuming binary r.v.,  $p(X_V | X_{[V-1]})$  has  $2^{V-1}$  parameters
- \* Total # parameters  $\sum_{1 \leq i \leq V} 2^{i-1} = 2^V - 1$

## CONDITIONAL INDEPENDENCE (MAY SAVE US)

- ★ X and Y are conditionally independent given Z iff

$$p(X, Y | Z) = P(X | Z) P(Y | Z)$$

- ★ Implies

$$p(X | Y, Z) = p(X, Y | Z) / p(Y | Z) = p(X | Z)$$

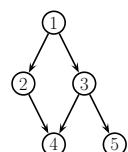
## EX. WHERE IND. OBVIOUSLY FACILITATES

$$p(\underbrace{\mathbf{x}_{[V]}}_{\mathbf{x}_1, \dots, \mathbf{x}_V}) = p(\mathbf{x}_1)p(\mathbf{x}_2 | \mathbf{x}_1)p(\mathbf{x}_3 | \mathbf{x}_1, \mathbf{x}_2) \cdots p(\mathbf{x}_V | \mathbf{x}_{[V-1]})$$

- ★ Assume first order Markov property  $\mathbf{x}_t \perp \mathbf{x}_{[t-2]} | \mathbf{x}_{t-1}$

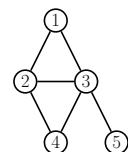
i.e., if time ordered, future independent of past given present

- ★ Then  $p(\mathbf{x}_{[V]}) = p(\mathbf{x}_1) \prod_{t=1}^{V-1} p(\mathbf{x}_{t+1} | \mathbf{x}_t)$



Directed graphical model

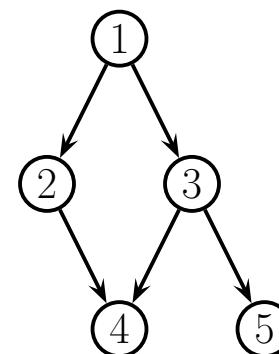
- DAG
- vertices r.v.s
- equipped with local CPDs



Undirected graphical model

- graph
- vertices r.v.s
- equipped with local “factors”

## GRAPHICAL MODELS



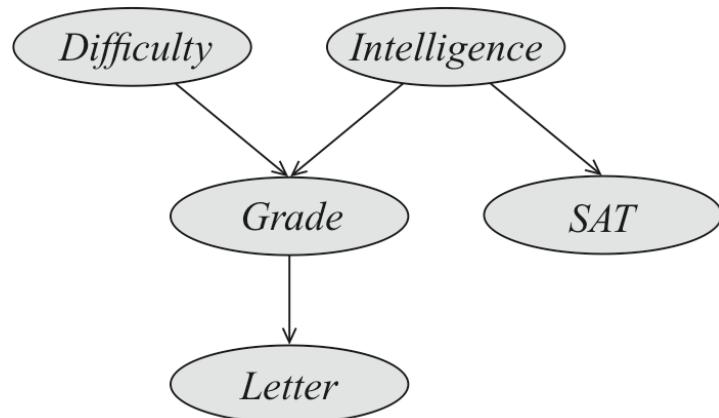
## DGM

- ★ What is the meaning of the underlying DAG? what is the semantics?

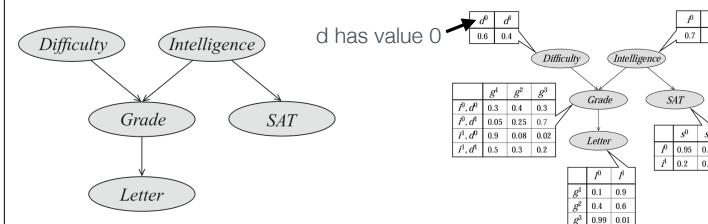
- ★ What does a DGM mean? what is the semantics?

- ★ Which DGMs represent a given distribution?

## EXTENDED STUDENT EXAMPLE



## RELATION DGM - DISTRIBUTIONS



## BERNOULLI & BINOMIAL

$$\text{Ber}(x|\theta) = \begin{cases} \theta & \text{if } x = 1 \\ 1 - \theta & \text{if } x = 0 \end{cases} \quad \text{Bin}(k|n, \theta) = \binom{n}{k} \theta^k (1 - \theta)^{n-k}$$

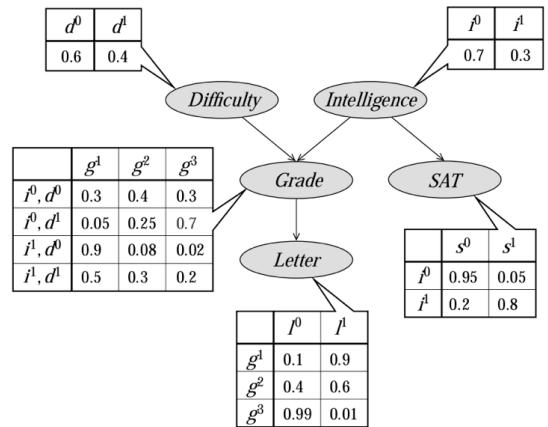
- ★ One or several (unordered) coin tosses

## CATEGORICAL & MULTINOMIAL

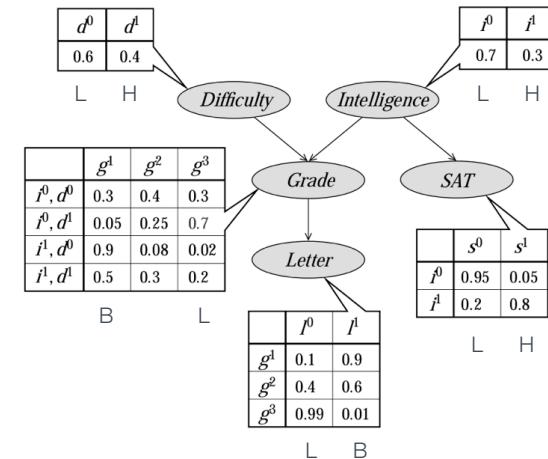
$$\text{Cat}(x|\boldsymbol{\theta}) = \theta_x \quad \text{Mul}(\mathbf{x}|n, \boldsymbol{\theta}) = \binom{n}{x_1, \dots, x_K} \prod_{k=1}^K \theta_k^{x_k}$$

- ★ One or several (unordered) coin tosses

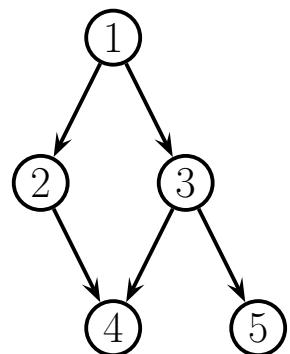
## EXTENDED STUDENT EXAMPLE



## EXTENDED STUDENT EXAMPLE

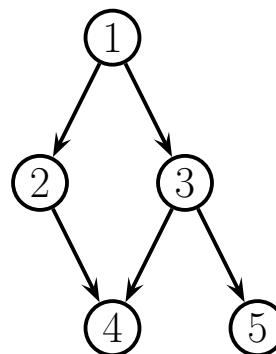


B - better  
H - higher  
L - less



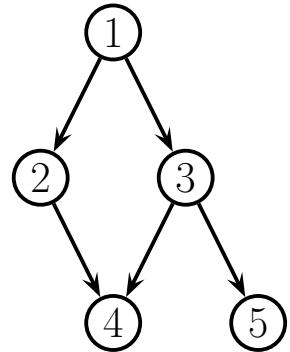
## TERMINOLOGY

- ★ Parent
- ★ Child
- ★ Family
- ★ Root
- ★ Leaf
- ★ Neighbors



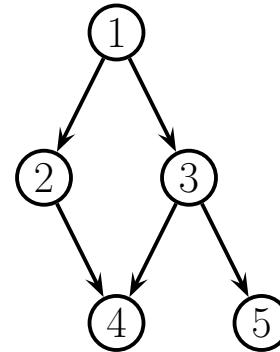
## TERMINOLOGY

- ★ Degree (in and out)
- ★ Cycle (directed or not)
- ★ Directed Acyclic Graph (DAG)
- ★ Topological order (parents < child)
- ★ Path (directed or not)
- ★ Ancestors



## TERMINOLOGY

- ★ Tree
- ★ Polytree – directed tree with multiple parents for some vertices
- ★ Forest
- ★ Subgraph
- ★ Clique
- ★ Maximal clique



## ORDERED MARKOV PROPERTY

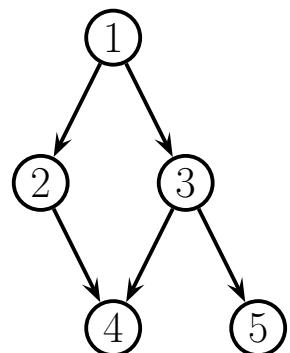
- ★ The ordered Markov Property

$$\mathbf{x}_t \perp \mathbf{x}_{V \setminus \text{desc}(t)} | \mathbf{x}_{\text{pa}(t)}$$

- ★ In this case

$$\begin{aligned} p(\mathbf{x}_{[5]}) &= p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2) \\ &\quad p(\mathbf{x}_4|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)p(\mathbf{x}_5|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) \\ &= p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1) \\ &\quad p(\mathbf{x}_4|\mathbf{x}_2, \mathbf{x}_3)p(\mathbf{x}_5|\mathbf{x}_3) \end{aligned}$$

1 2 3 4 5



## ORDERED MARKOV PROPERTY

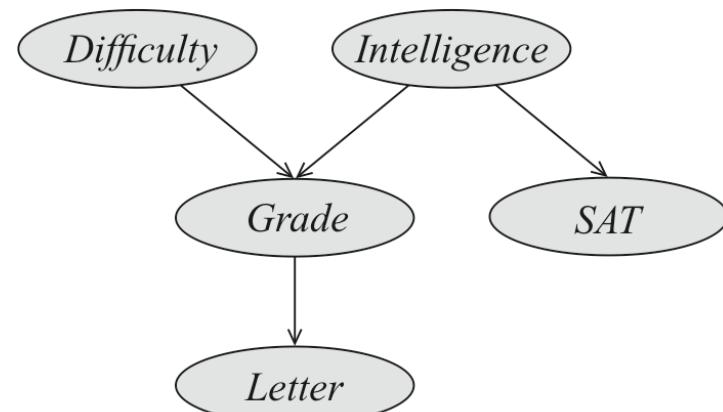
- ★ The ordered Markov Property

$$\mathbf{x}_t \perp \mathbf{x}_{V \setminus \text{desc}(t)} | \mathbf{x}_{\text{pa}(t)}$$

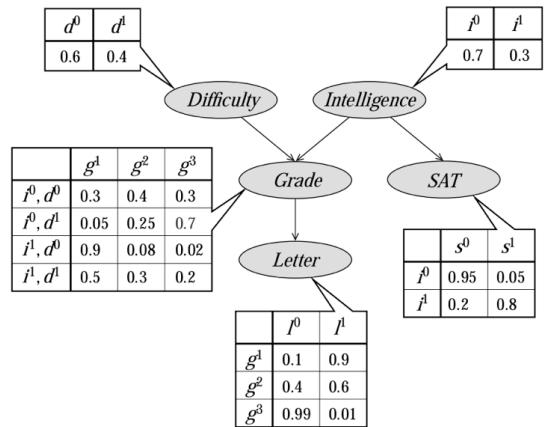
- ★ In general, if 1,...,V topological order, the likelihood is decomposable (factorizes)

$$p(\mathbf{x}_{[V]}|G) = \prod_{t=1}^V p(\mathbf{x}_t|\mathbf{x}_{\text{pa}(t)})$$

## EXTENDED STUDENT EXAMPLE



## EXTENDED STUDENT EXAMPLE



## AN EXAMPLE

Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = p(0, 1, 1, 1, 1 | \boldsymbol{\theta}) p(1, 1, 1, 0, 0 | \boldsymbol{\theta}) \\ p(1, 1, 0, 0, 1 | \boldsymbol{\theta}) p(1, 0, 0, 0, 0 | \boldsymbol{\theta}) \\ p(1, 1, 0, 0, 1 | \boldsymbol{\theta})$$

## AN EXAMPLE

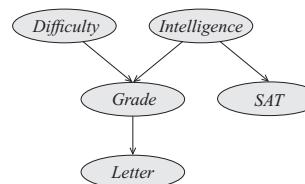
Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = p(0, 1, 1, 1, 1 | \boldsymbol{\theta}) p(1, 1, 1, 0, 0 | \boldsymbol{\theta}) \\ p(1, 1, 0, 0, 1 | \boldsymbol{\theta}) p(1, 0, 0, 0, 0 | \boldsymbol{\theta}) \\ p(1, 1, 0, 0, 1 | \boldsymbol{\theta}) \\ = p(D = (0, 1, 1, 1, 1) | \boldsymbol{\theta}_D) \dots$$

## AN EXAMPLE

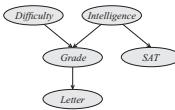
Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)



D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = p(D = (0, 1, 1, 1, 1) | \boldsymbol{\theta}_D) \\ p(I = (1, 1, 1, 0, 1) | \boldsymbol{\theta}_I) \\ p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S) \\ p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G) \\ p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE

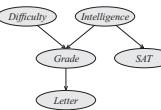


Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_D$	D=0	D=1
	2/5	3/5

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$\begin{aligned}
 L(\boldsymbol{\theta}; \mathcal{D}) &= p(D = (0, 1, 1, 1, 1) | \boldsymbol{\theta}_D) \\
 &\quad p(I = (1, 1, 1, 0, 1) | \boldsymbol{\theta}_I) \\
 &\quad p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S) \\
 &\quad p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G) \\
 &\quad p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)
 \end{aligned}$$



# AN EXAMPLE

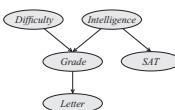
Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_D$	D=0	D=1
	2/5	3/5

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$\begin{aligned}
 L(\boldsymbol{\theta}; \mathcal{D}) &= \frac{2}{5} \left( \frac{3}{5} \right)^4 \\
 &\quad p(I = (1, 1, 1, 0, 1) | \boldsymbol{\theta}_I) \\
 &\quad p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S) \\
 &\quad p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G) \\
 &\quad p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)
 \end{aligned}$$

# AN EXAMPLE

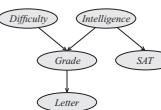


Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_I$	I=0	I=1
	1/4	3/4

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$\begin{aligned}
 L(\boldsymbol{\theta}; \mathcal{D}) &= \frac{2}{5} \left( \frac{3}{5} \right)^4 \\
 &\quad p(I = (1, 1, 1, 0, 1) | \boldsymbol{\theta}_I) \\
 &\quad p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S) \\
 &\quad p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G) \\
 &\quad p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)
 \end{aligned}$$



# AN EXAMPLE

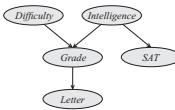
Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_I$	I=0	I=1
	1/4	3/4

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$\begin{aligned}
 L(\boldsymbol{\theta}; \mathcal{D}) &= \frac{2}{5} \left( \frac{3}{5} \right)^4 \frac{1}{4} \left( \frac{3}{4} \right)^4 \\
 &\quad p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S) \\
 &\quad p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G) \\
 &\quad p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)
 \end{aligned}$$

# AN EXAMPLE



Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_S$	$S=0$	$S=1$
I=0	1	0
I=1	1/6	5/6

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

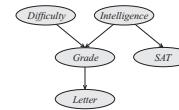
$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left( \frac{3}{5} \right)^4 \frac{1}{4} \left( \frac{3}{4} \right)^4$$

$$p(S = (1, 1, 0, 0, 0) | I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_S)$$

$$p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G)$$

$$p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE



Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_S$	$S=0$	$S=1$
I=0	1	0
I=1	1/6	5/6

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left( \frac{3}{5} \right)^4 \frac{1}{4} \left( \frac{3}{4} \right)^4 \left( \frac{1}{6} \right)^2 \left( \frac{5}{6} \right)^2$$

$$p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G)$$

$$p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE

Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

Less Better

$\theta_G$	$G=0$	$G=1$
D=0, I=0	1/2	1/2
D=1, I=0	3/5	2/5
D=0, I=1	1/10	9/10
D=1, I=1	2/5	3/5

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left( \frac{3}{5} \right)^4 \frac{1}{4} \left( \frac{3}{4} \right)^4 \left( \frac{1}{6} \right)^2 \left( \frac{5}{6} \right)^2$$

$$p(G = (1, 0, 0, 0, 0) | D = (0, 1, 1, 1, 1), I = (1, 1, 1, 0, 1), \boldsymbol{\theta}_G)$$

$$p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE

Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_G$	$G=0$	$G=1$
D=0, I=0	1/2	1/2
D=1, I=0	3/5	2/5
D=0, I=1	1/10	9/10
D=1, I=1	2/5	3/5

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left( \frac{3}{5} \right)^4 \frac{1}{4} \left( \frac{3}{4} \right)^4 \left( \frac{1}{6} \right)^2 \left( \frac{5}{6} \right)^2 \left( \frac{9}{10} \right) \left( \frac{2}{5} \right)^3 \left( \frac{3}{5} \right)^2$$

$$p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE

Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_L$	L=0	L=1
G=0	2/3	1/3
G=1	0	1

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left(\frac{3}{5}\right)^4 \frac{1}{4} \left(\frac{3}{4}\right)^4 \left(\frac{1}{6}\right)^2 \left(\frac{5}{6}\right)^2 \frac{9}{10} \left(\frac{2}{5}\right)^3 \frac{3}{5}$$

$$p(L = (1, 0, 1, 0, 1) | G = (1, 0, 0, 0, 0), \boldsymbol{\theta}_L)$$

# AN EXAMPLE

Difficulty (1 diff), Intelligence (1 int), Sat (1 good), Grade (1 good), Letter (1good)

$\theta_L$	L=0	L=1
G=0	2/3	1/3
G=1	0	1

D	I	S	G	L
0	1	1	1	1
1	1	1	0	0
1	1	0	0	1
1	0	0	0	0
1	1	0	0	1

$$L(\boldsymbol{\theta}; \mathcal{D}) = \frac{2}{5} \left(\frac{3}{5}\right)^4 \frac{1}{4} \left(\frac{3}{4}\right)^4 \left(\frac{1}{6}\right)^2 \left(\frac{5}{6}\right)^2 \frac{9}{10} \left(\frac{2}{5}\right)^3 \frac{3}{5} \left(\frac{2}{3}\right)^2 \left(\frac{1}{3}\right)^2$$

# THE LIKELIHOOD FACTORIZES

- ★ Complete data  $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$

$$\mathbf{x}_n = \{\mathbf{x}_{n1}, \dots, \mathbf{x}_{nV}\}$$

- ★ Likelihood

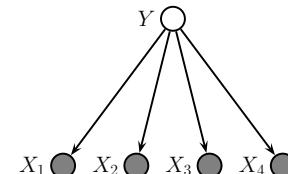
$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{n=1}^N p(\mathbf{x}_n|\boldsymbol{\theta}) = \prod_{n=1}^N \prod_{v=1}^V p(\mathbf{x}_{nv}|\mathbf{x}_{n,\text{pa}(v)}, \boldsymbol{\theta})$$

$$= \prod_{v=1}^V \prod_{n=1}^N p(\mathbf{x}_{nv}|\mathbf{x}_{n,\text{pa}(v)}, \boldsymbol{\theta}) = \prod_{v=1}^V p(\mathcal{D}_v|\boldsymbol{\theta}_v)$$

where  $D_v$  is values of  $v$  together with its parents and  $\theta_v$  is  $v$ 's CPD

- ★ Called: decomposable likelihood (factorizes into family-factors)

# SPECIAL CASE: NAIVE BAYES CLASSIFIER



$$p(\mathbf{x}, y) = p(y) \prod_{t=1}^4 p(x_t|y)$$

## SPECIAL CASE: LAYERED HIDDEN MARKOV MODEL (HMM)

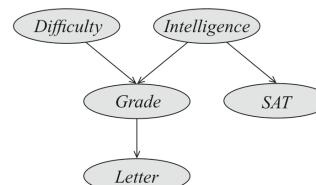
$$z_1 \rightarrow z_2 \rightarrow z_3 \cdots z_V$$

$\downarrow$        $\downarrow$        $\downarrow$        $\downarrow$

$$x_1 \quad x_2 \quad x_3 \quad x_V$$

- $Z_i$  hidden
- $X_i$  observable
- Hidden often not observable when training, never when applying

## THREE LEVELS OF COMPUTATIONAL PROBLEMS



$d^0$	$d^1$
0.6	0.4

$d^0, d^1$	$g^0$	$g^1$	$g^2$
0.3	0.4	0.3	
0.05	0.25	0.7	
0.9	0.08	0.02	
0.5	0.3	0.2	

$p$	$f$
0.7	0.3

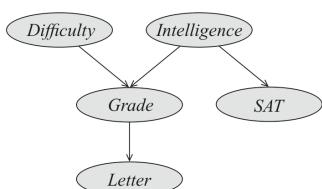
$p$	$s^0$	$s^1$
0.95	0.05	
0.2	0.2	0.8

$g^0$	$f$	$f$
0.1	0.9	
0.4	0.6	
0.99	0.01	

- Inference: given  $G$  and  $\theta$ , compute probabilities or marginalize
- Parameter learning: given  $G$  and  $D$ , learn  $\theta$
- Structure learning: given  $D$ , learn  $G$  and  $\theta$

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  - Parameter learning: given  $G$  and  $D$ , learn  $\theta$
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- Marginalize often hard
- Easy for observable data
- Hard unless trees, doable in practice for observable

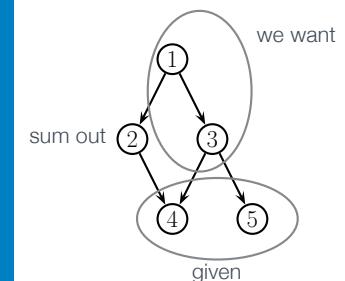
$X, X'$  two hidden variables

$X_h$  the other hidden variables

$X_v$  the visible variables

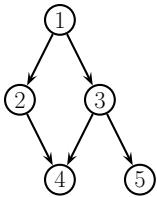
## MARGINALIZE

$$p(X = k, X' = k' | \mathbf{x}_v, \boldsymbol{\theta}) = \frac{p(X = k, X' = k', \mathbf{x}_v | \boldsymbol{\theta})}{P(\mathbf{x}_v | \boldsymbol{\theta})} = \frac{\sum_{x_h} p(X = k, X' = k', \mathbf{x}_h, \mathbf{x}_v | \boldsymbol{\theta})}{\sum_{x, x', x_h} p(x, x', \mathbf{x}_h, \mathbf{x}_v | \boldsymbol{\theta})}$$



# MARGINALIZE

$$p(\mathbf{x}_h | \mathbf{x}_v, \boldsymbol{\theta}) = \frac{p(\mathbf{x}_h, \mathbf{x}_v | \boldsymbol{\theta})}{P(\mathbf{x}_v | \boldsymbol{\theta})} = \frac{p(\mathbf{x}_h, \mathbf{x}_v | \boldsymbol{\theta})}{\sum_{x_h} p(\mathbf{x}_h, \mathbf{x}_v | \boldsymbol{\theta})}$$

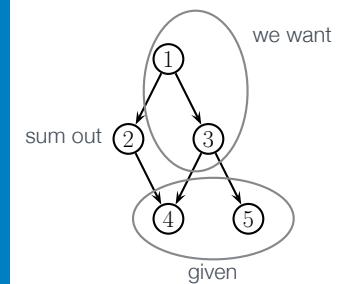


- The denominator contains a marginal likelihood
- Summing out V binary hidden variables –  $O(2^V)$
- K states –  $O(K^V)$

$X, X'$  two hidden variables  
 $X_h$  the other hidden variables  
 $X_v$  the visible variables

## EXPECTED SUFFICIENT STATISTICS - ESS

$$E[N_{k,k'}] = \sum_{\mathbf{x} \in \mathcal{D}} p(X = k, X' = k' | \mathbf{x}_v, \boldsymbol{\theta})$$



# LEARNING PARAMETERS (IN GENERAL)

★ "...Bayesian view, the parameters are unknown variables and should also be inferred"

★ Learning from complete data     $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$   
 $\mathbf{x}_n = \{\mathbf{x}_{n1}, \dots, \mathbf{x}_{nV}\}$

★ Likelihood

$$\begin{aligned} P(\mathcal{D} | \boldsymbol{\theta}) &= \prod_{n=1}^N P(\mathbf{x}_n | \boldsymbol{\theta}) = \prod_{n=1}^N \prod_{v=1}^V P(\mathbf{x}_{nv} | \mathbf{x}_{n, \text{pa}(v)}, \boldsymbol{\theta}) \\ &= \prod_{v=1}^V \prod_{n=1}^N P(\mathbf{x}_{nv} | \mathbf{x}_{n, \text{pa}(v)}, \boldsymbol{\theta}) = \prod_{v=1}^V P(\mathcal{D}_v | \boldsymbol{\theta}_v) \end{aligned}$$

where  $D_v$  is values of v together with its parents and  $\boldsymbol{\theta}_v$  is v's CPD

# CAT – NOTATION

★ For a  $v \in [V]$ ,

values     $k \in [K_v]$       Cartesian product

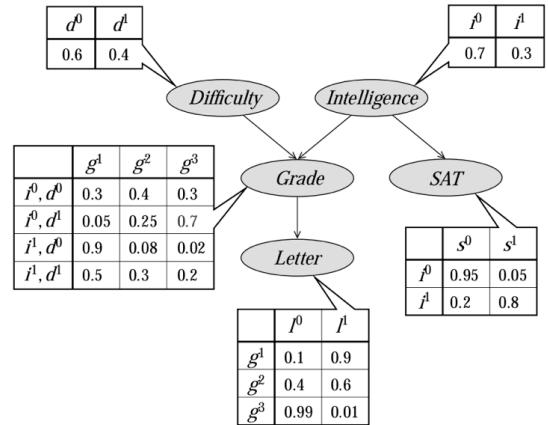
combined values     $c \in C_v = \prod_{s \in \text{pa}(v)} [K_s]$

★ Cat CPDs

where     $P(x_v | x_{\text{pa}(v)} = c) = \text{Cat}(\boldsymbol{\theta}_{vc})$

and     $\boldsymbol{\theta}_{vc} = P(x_v = k | x_{\text{pa}(v)} = c)$

## EXTENDED STUDENT EXAMPLE



## MLE FOR CAT CPDS

★ Each  $P(\mathcal{D}_v | \theta_v)$ , i.e., here each  $\theta_{vc}$

can be maximized independently

★ So, MLE is

$$\theta_{vc_k} = N_{vc_k} / N_{vc}$$

★ where

$$N_{vc_k} = \sum_{n=1}^N I(x_{nv} = k, x_{n,pa(v)} = \mathbf{c})$$

$$N_{vc} = \sum_{n=1}^N I(x_{n,pa(v)} = \mathbf{c})$$

c

THE END