Royal Institute of Technology

STATISTICAL METHODS IN CS, CH 10

Lecture 5

LAST LECTURE

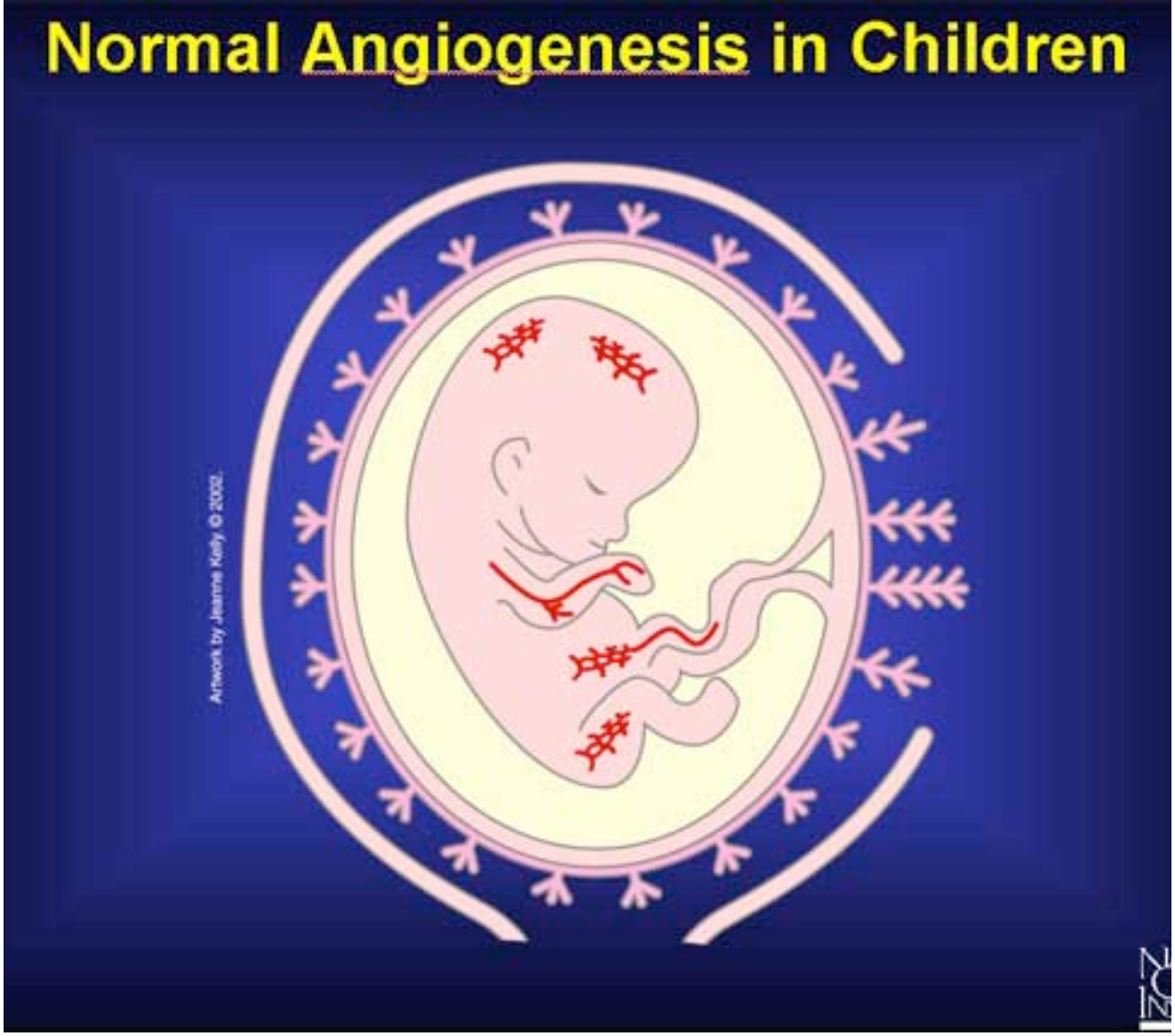
- The Bayesian approach
- How to analyse and use the posterior
- Empirical Bayes
- Cancer incidents - sharing parameters

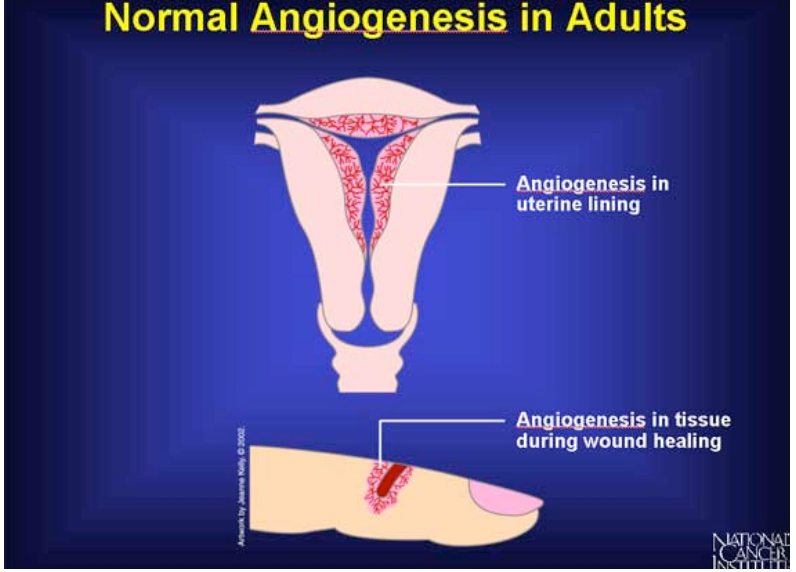
THIS LECTURE

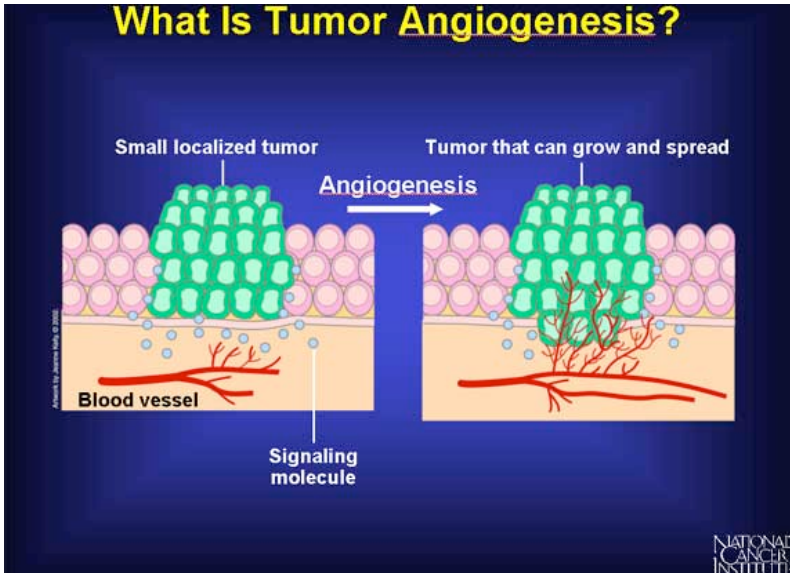
- DGMs
- Basic example
- Computing the likelihood
- Factorizing (decomposing) the likelihood
- A decomposable prior
- Categorical CPDs - easy to get a posterior

REPRESENTING AND WORKING WITH DISTRIBUTIONS

- For all but the smallest n, the explicit representation of the joint distribution is *unmanageable from every perspective*.
  - Computationally, it is very *expensive to manipulate* and generally *too large to store* in memory.
  - Cognitively, it is *impossible to acquire so many numbers* from a human expert; moreover, the numbers are very small and *do not correspond to events that people can reasonably contemplate*.
  - Statistically, if we want to learn the distribution from data, we would *need ridiculously large amounts of data to estimate* this many parameters robustly.
- These problems were the *main barrier* to the adoption of probabilistic methods for expert systems *until the development of the methodologies we now will consider.*







ABERRATION DEPENDENCIES - EX. ANGIOGENESIS

SOMATIC EVOLUTION

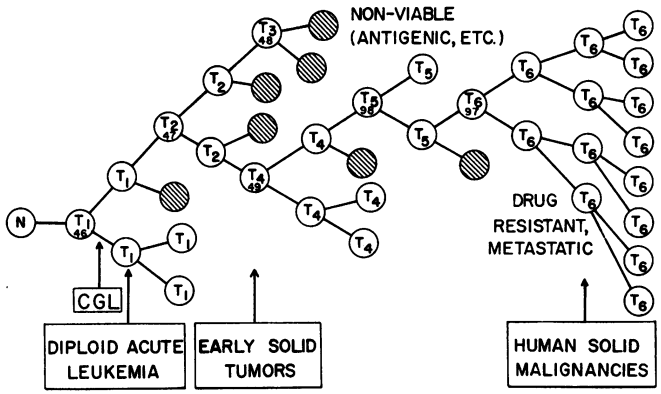
The Clonal Evolution of Tumor Cell Populations

Acquired genetic lability permits stepwise selection of variant sublines and underlies tumor progression.

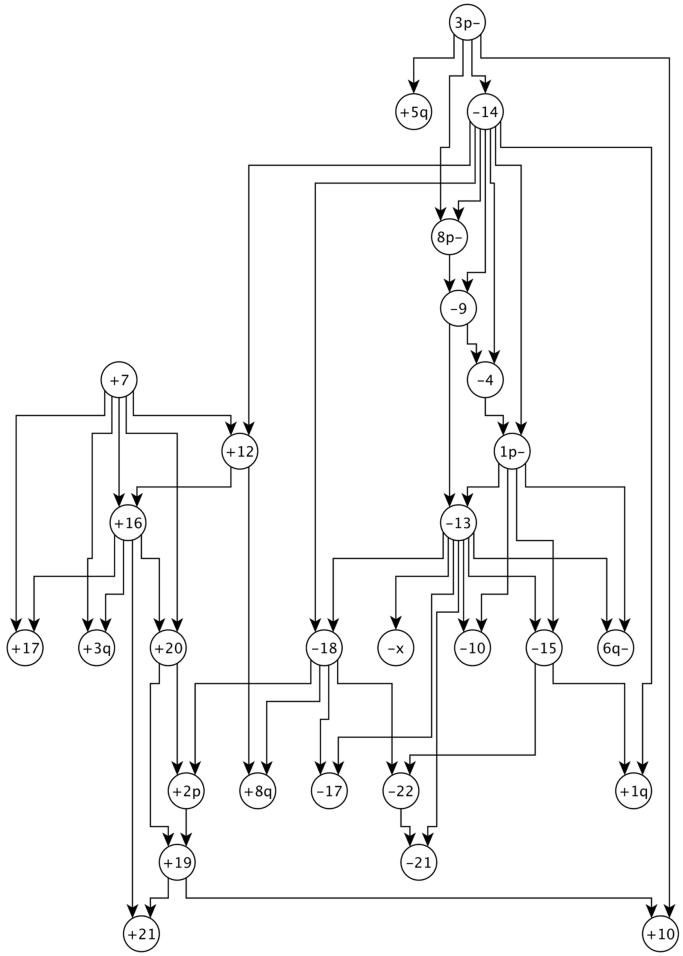
Peter C. Nowell

The author is professor of pathology, School of Medicine, University of Pennsylvania, Philadelphia 19174.

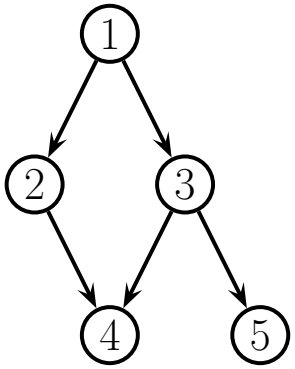
1 OCTOBER 1976 SCIENCE, VOL. 194



Oncogenetic network

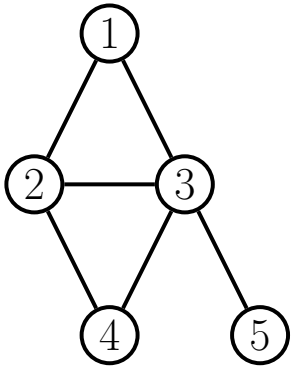


GRAPHICAL MODELS



Directed graphical model

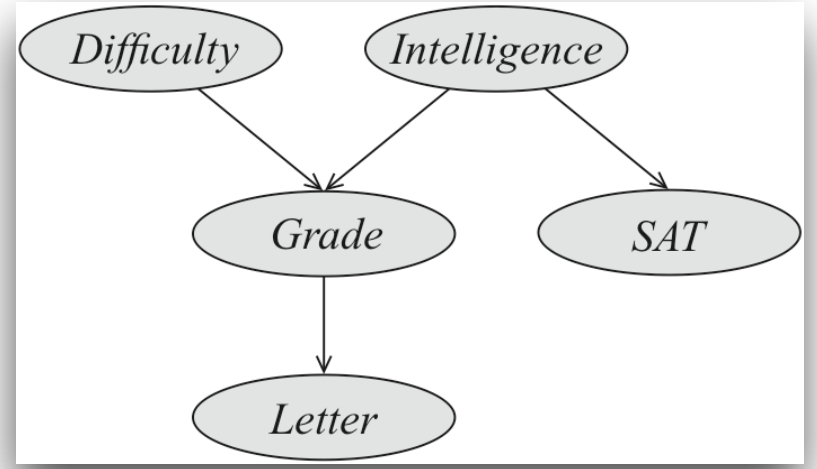
- DAG
- vertices r.v.s
- equipped with local CPDs
- allows causal like dependencies



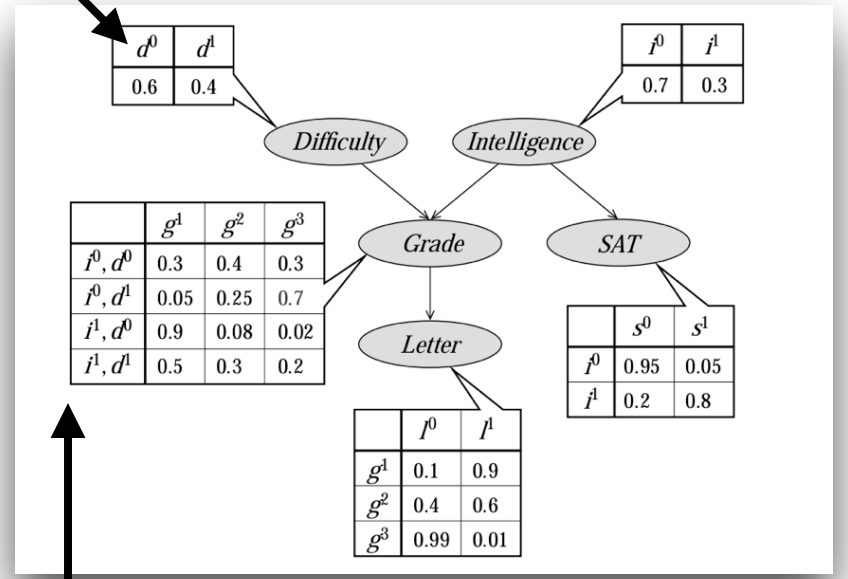
Undirected graphical model - Markov Random Fields

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

DGM - GRAPH AND CPDS VS JOINT



d has value 0

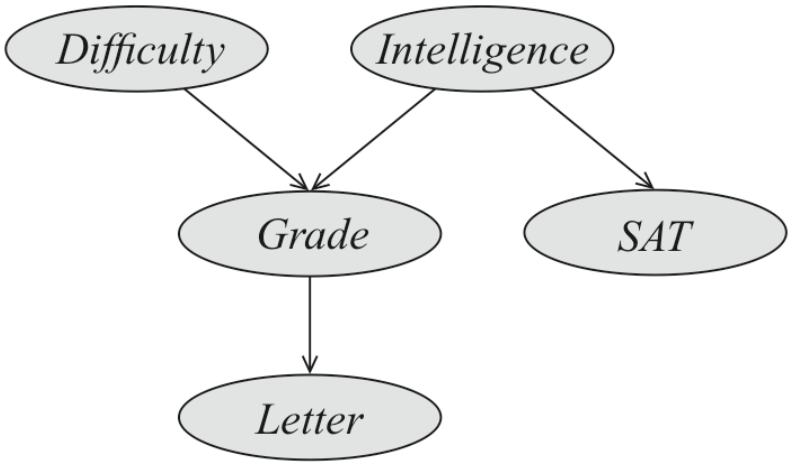


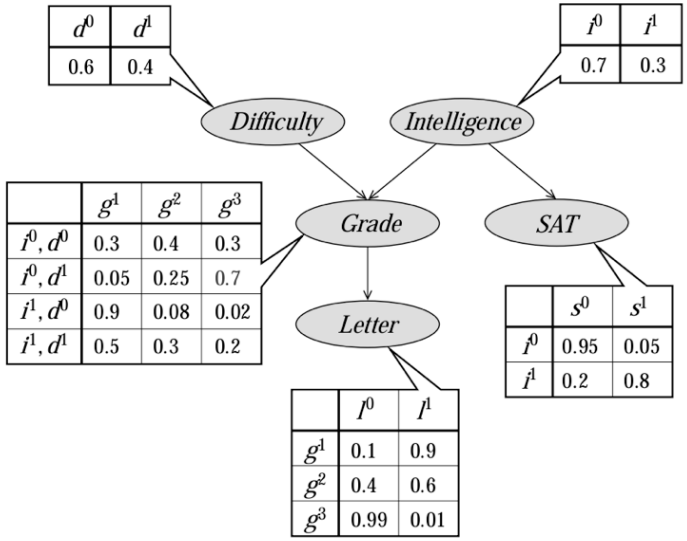
CPD

P(D,I,G,S,L)

- CPT - table, i.e., categorical
- Gaussian

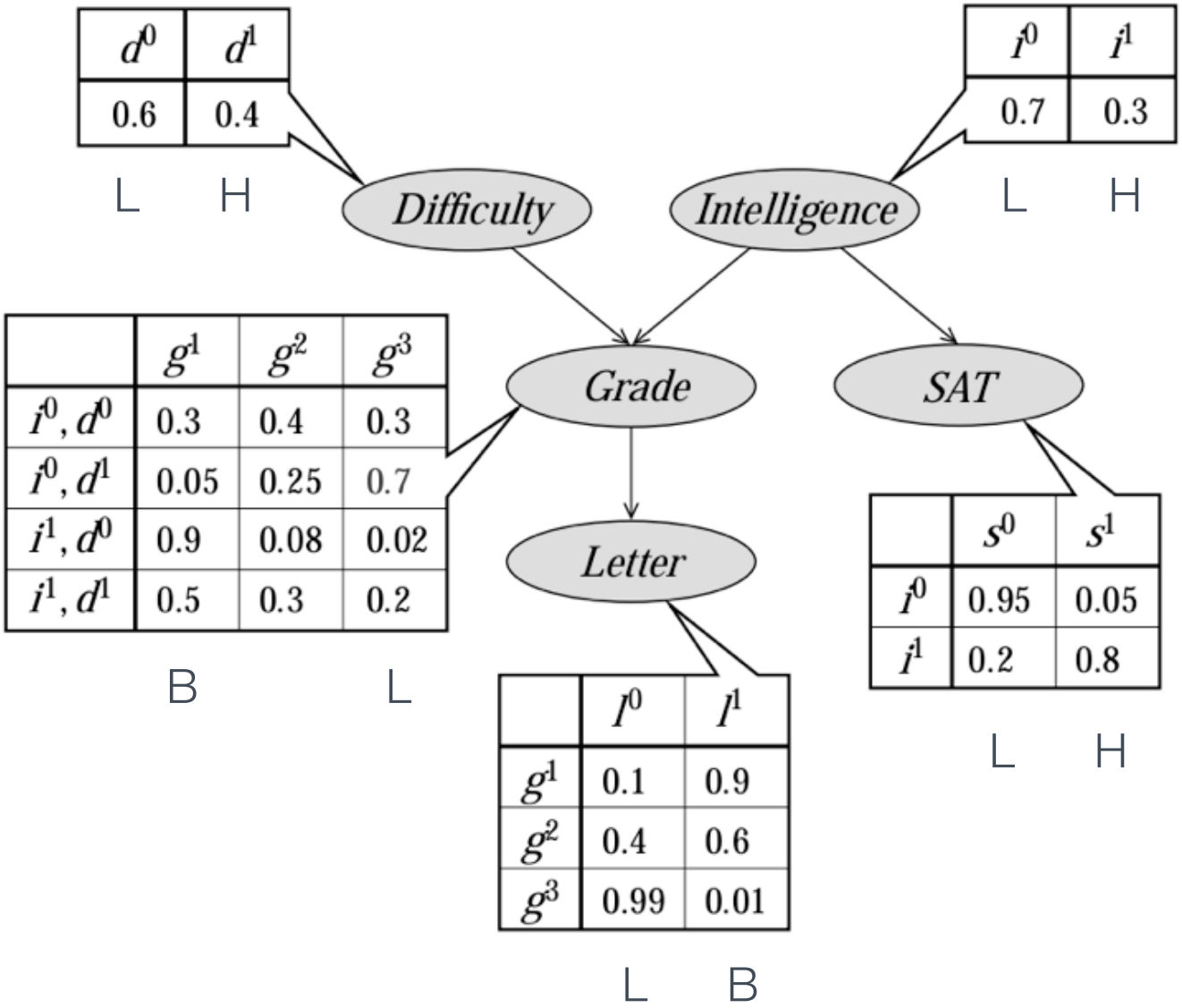
THREE LEVELS OF COMPUTATIONAL PROBLEMS





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

EXTENDED STUDENT-CATEGORICAL CPDS

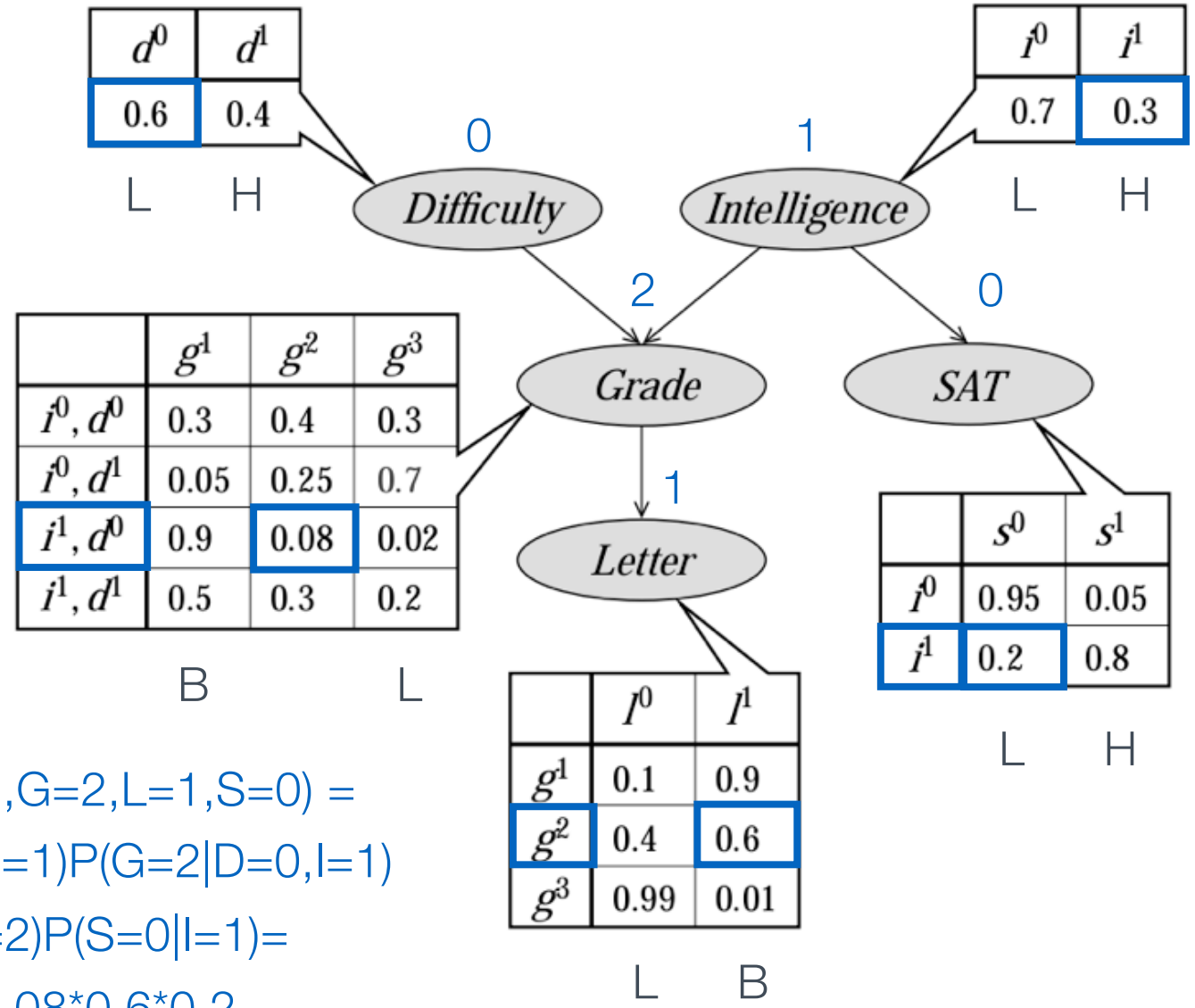


B - better

H - higher

L - less

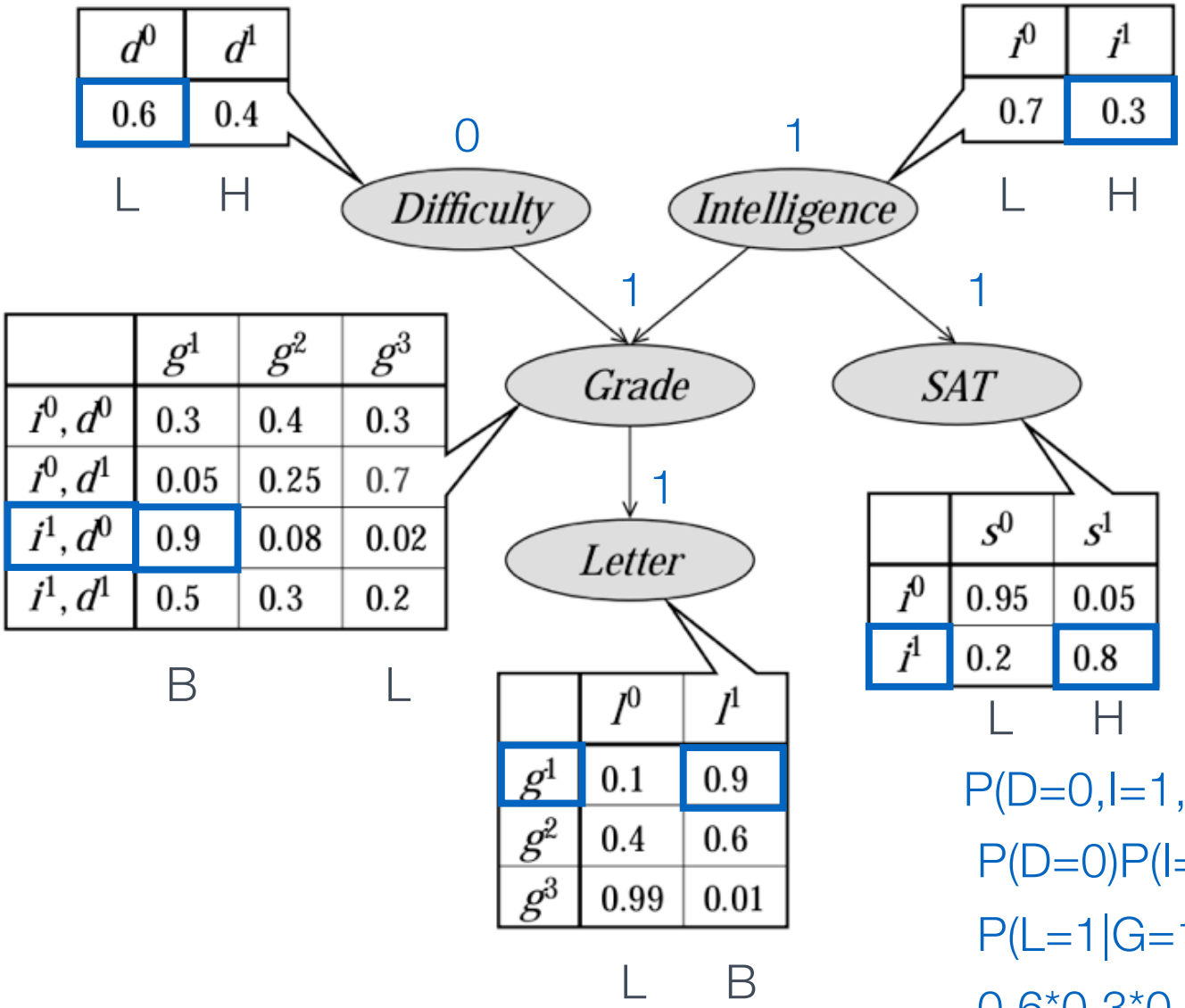
COMPLETE DATA



P(D=0,I=1,G=2,L=1,S=0) =
P(D=0)P(I=1)P(G=2|D=0,I=1)
P(L=1|G=2)P(S=0|I=1)=
0.6*0.3*0.08*0.6*0.2

B - better
H - higher
L - less

EXTENDED STUDENT EXAMPLE



P(D=0,I=1,G=1,L=1,S=1) =
P(D=0)P(I=1)P(G=1|D=0,I=1)
P(L=1|G=1)P(S=1|I=1)=
0.6*0.3*0.9*0.9*0.8

INFERENCE – THE CHAIN RULE

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

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

EX. WHERE IND. OBVIOUSLY FACILITATES

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

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

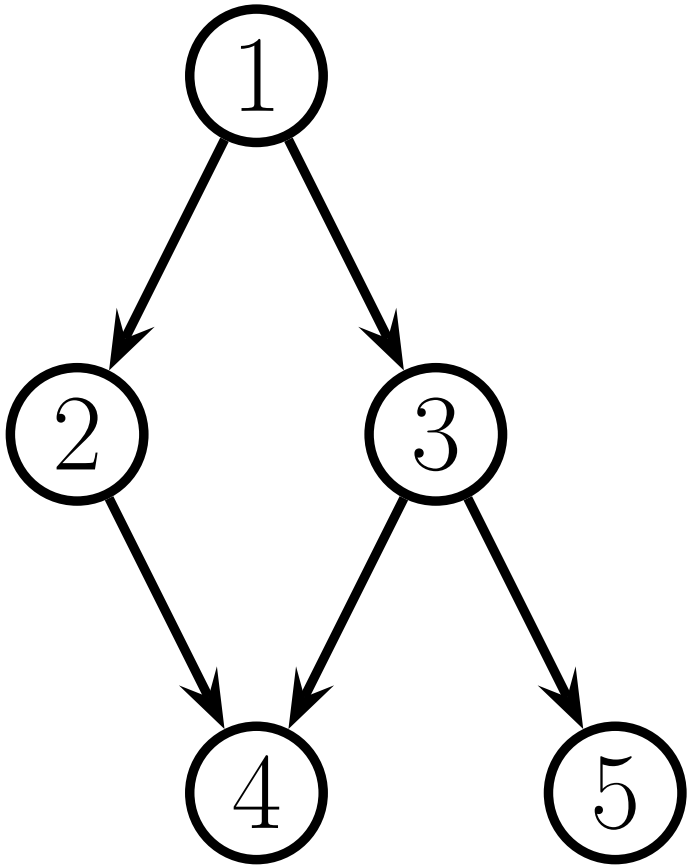
i.e., if time ordered, future independent of past given present

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

FACTORIZATION OVER G

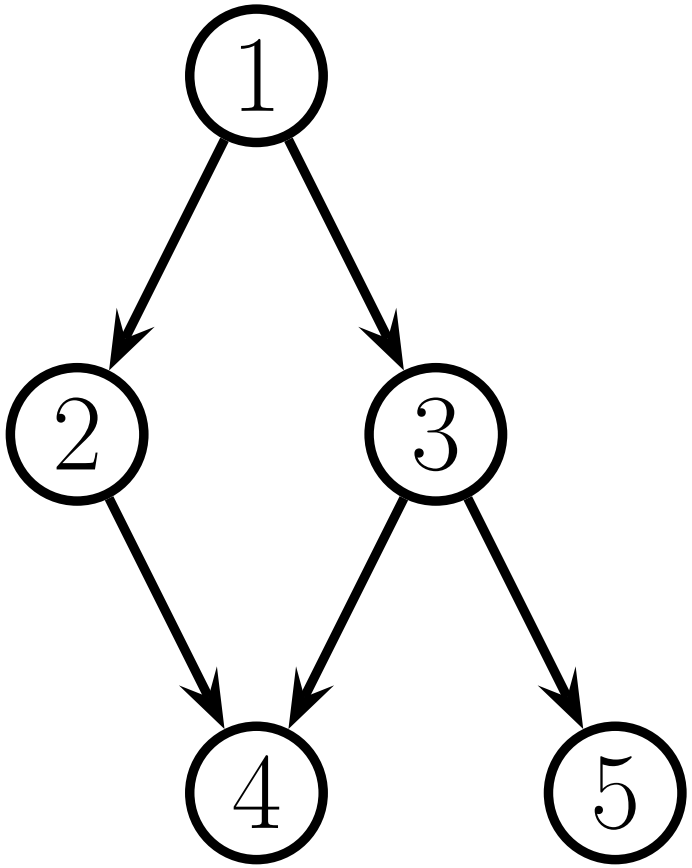
$$p(x_1, \ldots, x_N) = \prod_{n=1}^{N} p(x_n | \boldsymbol{x}_{\mathrm{pa}(x_n)})$$

p can be factorized over G if it can be expressed as above



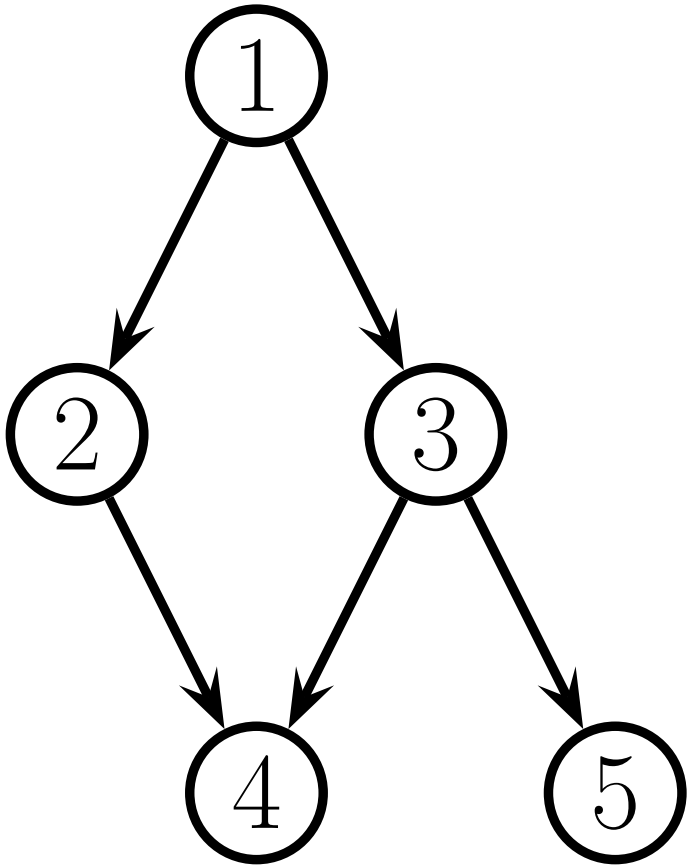
TERMINOLOGY

- ★ Parent
- ★ Child
- ★ Family
- ★ Root
- ★ Leaf
- ★Neighbor



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

CAT – NOTATION

- For a v ∈ [V],

  values $k \in [K_v]$

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

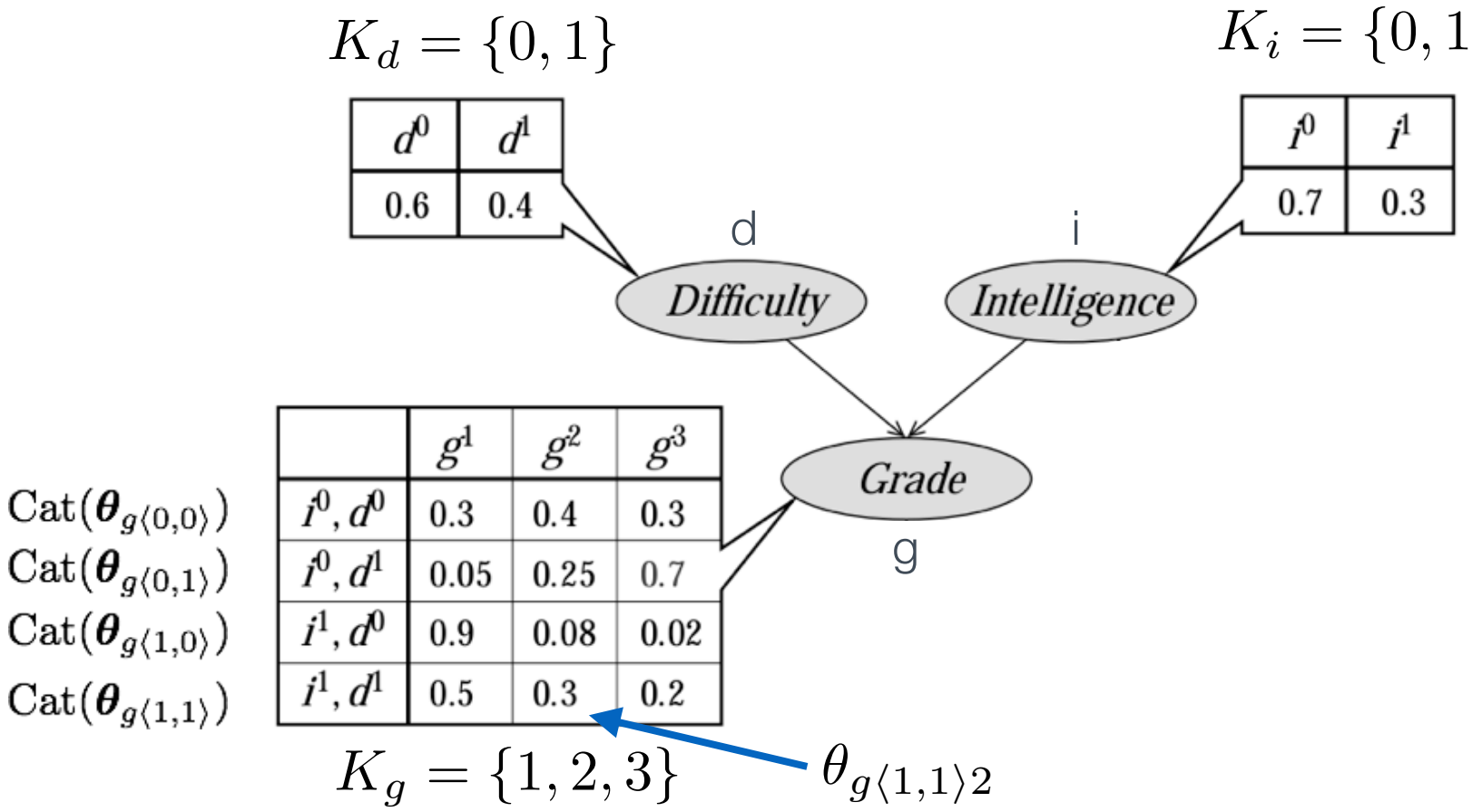
  Cartesian product

- Cat CPDs

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

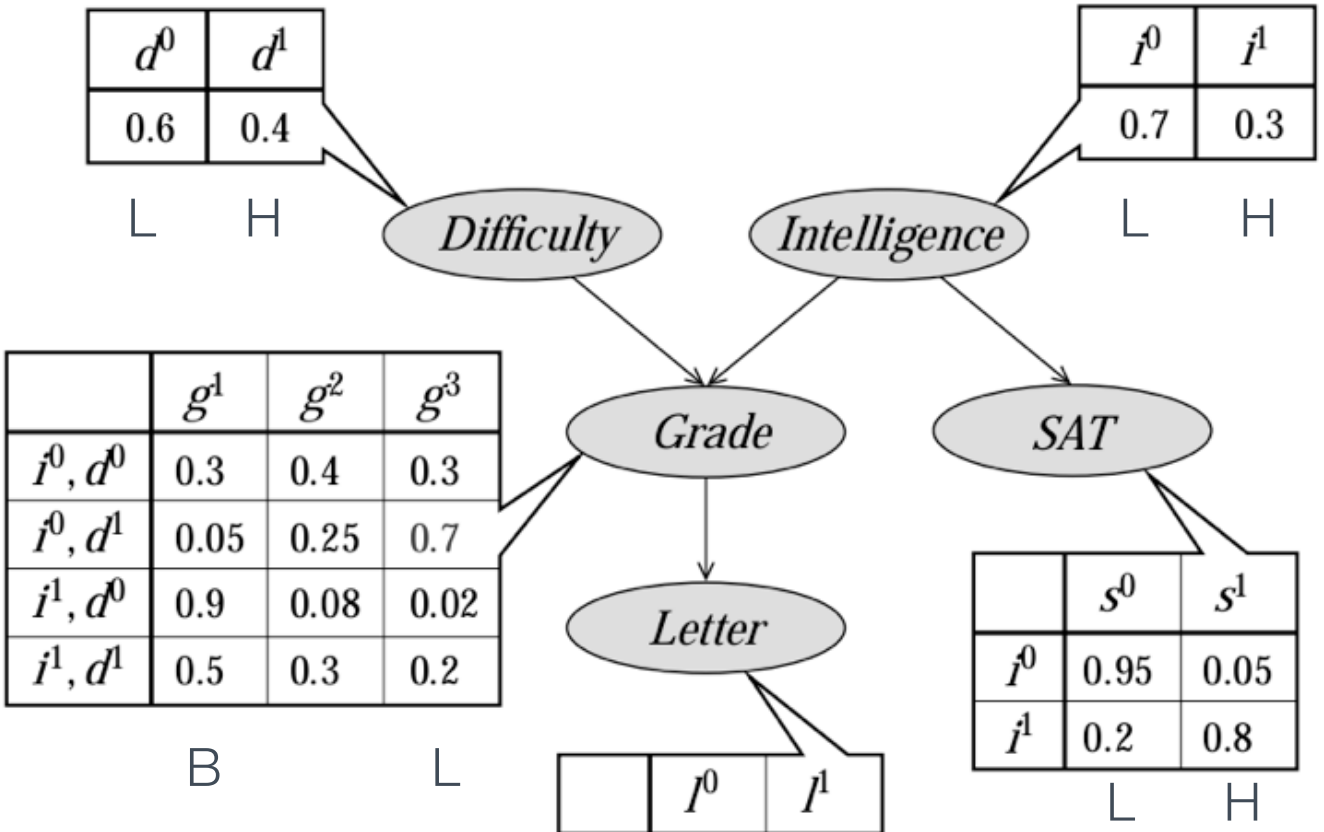
  and $\theta_{vck} = P(x_v = k | x_{\mathrm{pa}(v)} = c)$

NOTATION EXAMPLE



$$C_g = \prod_{s \in \text{pa}(g)} [K_s] = K_d \times K_i = \{\langle 0,0\rangle, \langle 0,1\rangle, \langle 1,0\rangle, \langle 1,1\rangle\}$$

EXTENDED STUDENT EXAMPLE



P(D=0,I=1,G=2,L=1,S=0) =
P(D=0)P(I=1)P(G=2|D=0,I=1)
P(L=1|G=2)P(S=0|I=1)=
0.6*0.3*0.08*0.6*0.2

P(D=0,I=1,G=1,L=1,S=1) =
P(D=0)P(I=1)P(G=1|D=0,I=1)
P(L=1|G=1)P(S=1|I=1)=
0.6*0.3*0.9*0.9*0.8

EXTENDED STUDENT EXAMPLE

$$P(D=0,I=1,G=2,L=1,S=0)\ P(D=0,I=1,G=1,L=1,S=0)$$
$$= P(D=0)P(I=1)P(G=1|D=0,I=1)\ P(L=1|G=1)P(S=1|I=1)$$
$$P(D=0)P(I=1)P(G=2|D=0,I=1)P(L=1|G=2)P(S=0|I=1)$$
$$= P(D=0)^2P(I=1)^2P(G=1|D=0,I=1)P(G=2|D=0,I=1)$$
$$P(L=1|G=1)P(L=1|G=2)P(S=1|I=1)P(S=0|I=1)$$

$$P(D=0,I=1,G=2,L=1,S=0) =$$
$$P(D=0)P(I=1)P(G=2|D=0,I=1)$$
$$P(L=1|G=2)P(S=0|I=1)=$$
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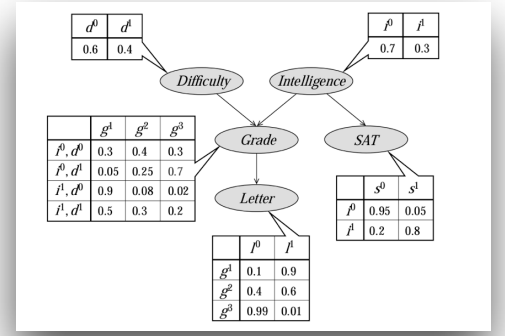
$$P(L=1|G=1)P(S=1|I=1)=$$
$$0.6*0.3*0.9*0.9*0.8$$

THE LIKELIHOOD FACTORIZES

★ Complete data

$$\mathcal{D} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$$

$$\boldsymbol{x}_n = \{\boldsymbol{x}_{n1}, \ldots, \boldsymbol{x}_{nV}\}$$



★ Likelihood

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

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

where D_v is values of v together with its parents and θ_v is v's CPD

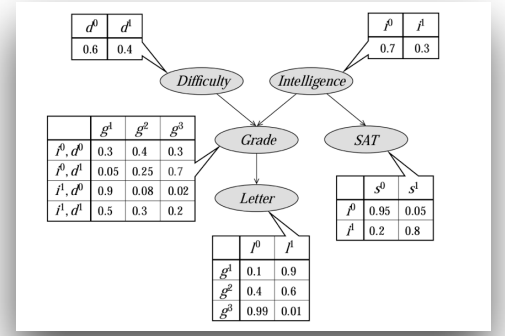
★ Called: decomposable likelihood (factorizes into family-factors)

THE LIKELIHOOD FACTORIZES

★ Complete data

$$\mathcal{D} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$$

$$\boldsymbol{x}_n = \{\boldsymbol{x}_{n1}, \ldots, \boldsymbol{x}_{nV}\}$$



★ Likelihood

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

where D_v is values of v together with its parents and θ_v is v's CPD

★ Each $p(\mathcal{D}_v|\boldsymbol{\theta}_v)$, i.e., here each $\boldsymbol{\theta}_{vc}$

can be maximized independently

MLE FOR CAT CPDS

★ Since $p(\mathcal{D}_v|\boldsymbol{\theta}_v)$, i.e., here each $\boldsymbol{\theta}_{vc}$

can be maximized independently

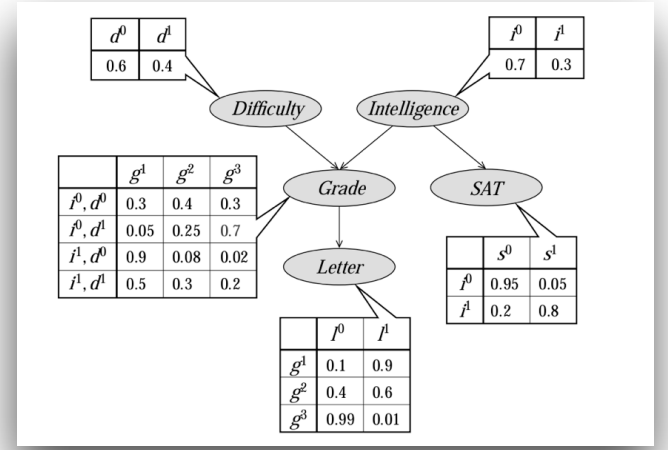
★ The MLE is

$$\boldsymbol{\theta}_{v\mathbf{c}k} = N_{v\mathbf{c}k}/N_{v\mathbf{c}}$$

★ where

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

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



BAYESIAN PARAMETER LEARNING

- ★ Decomposable prior

$$p(\boldsymbol{\theta}) = \prod_{v=1}^{V} p(\boldsymbol{\theta}_v) \qquad \text{where} \qquad \boldsymbol{\theta}_v = \{\boldsymbol{\theta}_{v\mathbf{c}}\}_{\mathbf{c} \in \mathbf{K}_{\mathrm{pa}(\mathbf{v})}}$$

- ★ Gives decomposable posterior

$$p(\boldsymbol{\theta}|\mathcal{D}) \propto p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}) = \prod_{v=1}^{V} p(\mathcal{D}_v|\boldsymbol{\theta}_v)p(\boldsymbol{\theta}_v)$$

POSTERIOR

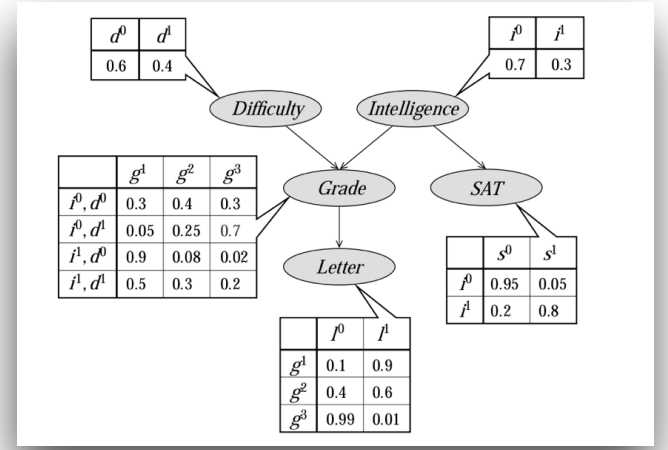
$$\boldsymbol{\theta}_v = \{\boldsymbol{\theta}_{v\mathbf{c}}\}_{\mathbf{c}\in\mathbf{K}_{\mathrm{pa}(\mathbf{v})}}$$

★ α_{vc} is a vector of hyperparameters, prior

$$\boldsymbol{\theta}_{v\mathbf{c}} \sim \mathrm{Dir}(\boldsymbol{\alpha}_{v\mathbf{c}})$$

★ The posterior is

$$\boldsymbol{\theta}_{v\mathbf{c}}|\mathcal{D} \sim \mathrm{Dir}(\boldsymbol{N}_{v\mathbf{c}} + \boldsymbol{\alpha}_{v\mathbf{c}})$$

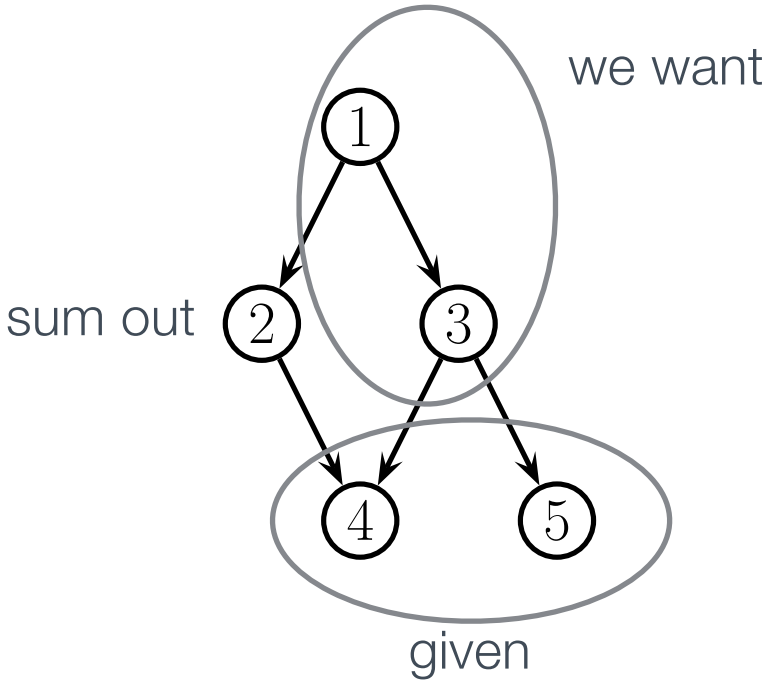


MARGINALIZE

X_1, X_3 two hidden variables that we want the marginal over

X_2 the other hidden variables

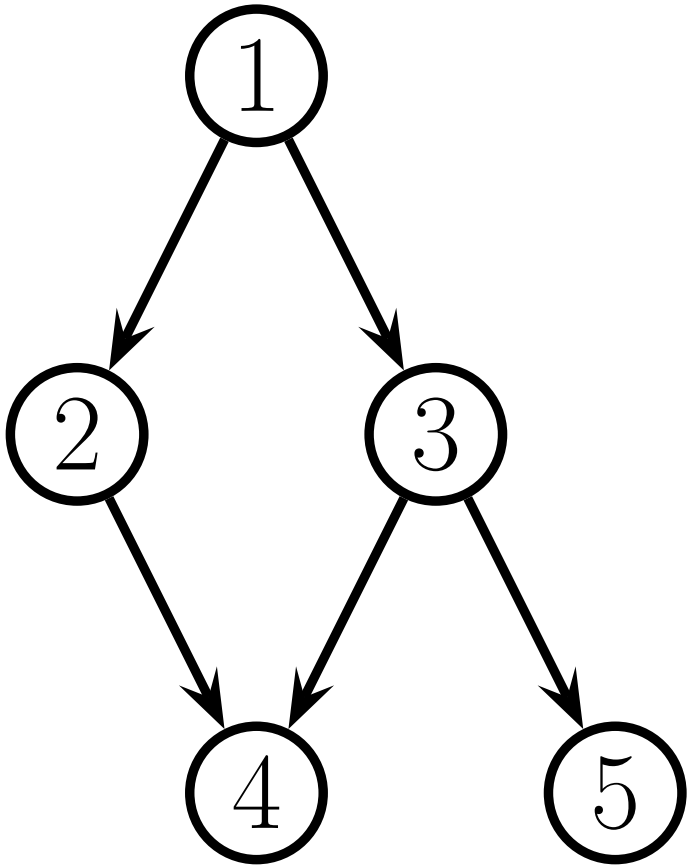
$x_e = \{x_4, x_5\}$ the visible variables



MARGINALIZE

$$p(\boldsymbol{X}_m|\boldsymbol{x}_e,\boldsymbol{\theta}) = \frac{\sum_{\boldsymbol{x}_{V\setminus(m\cup e)}} p(\boldsymbol{X}_m,\boldsymbol{x}_{V\setminus(m\cup e)},\boldsymbol{x}_e|\boldsymbol{\theta})}{\sum_{\boldsymbol{x}_{V\setminus e}} p(\boldsymbol{x}_{V\setminus e},\boldsymbol{x}_e|\boldsymbol{\theta})}$$

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



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?

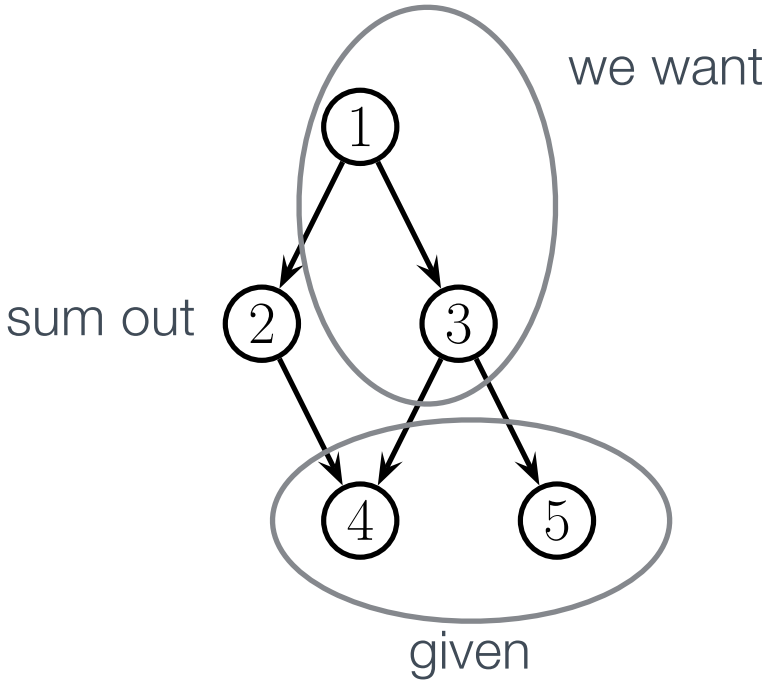
EXPECTED SUFFICIENT STATISTICS - ESS

X, X' two hidden variables

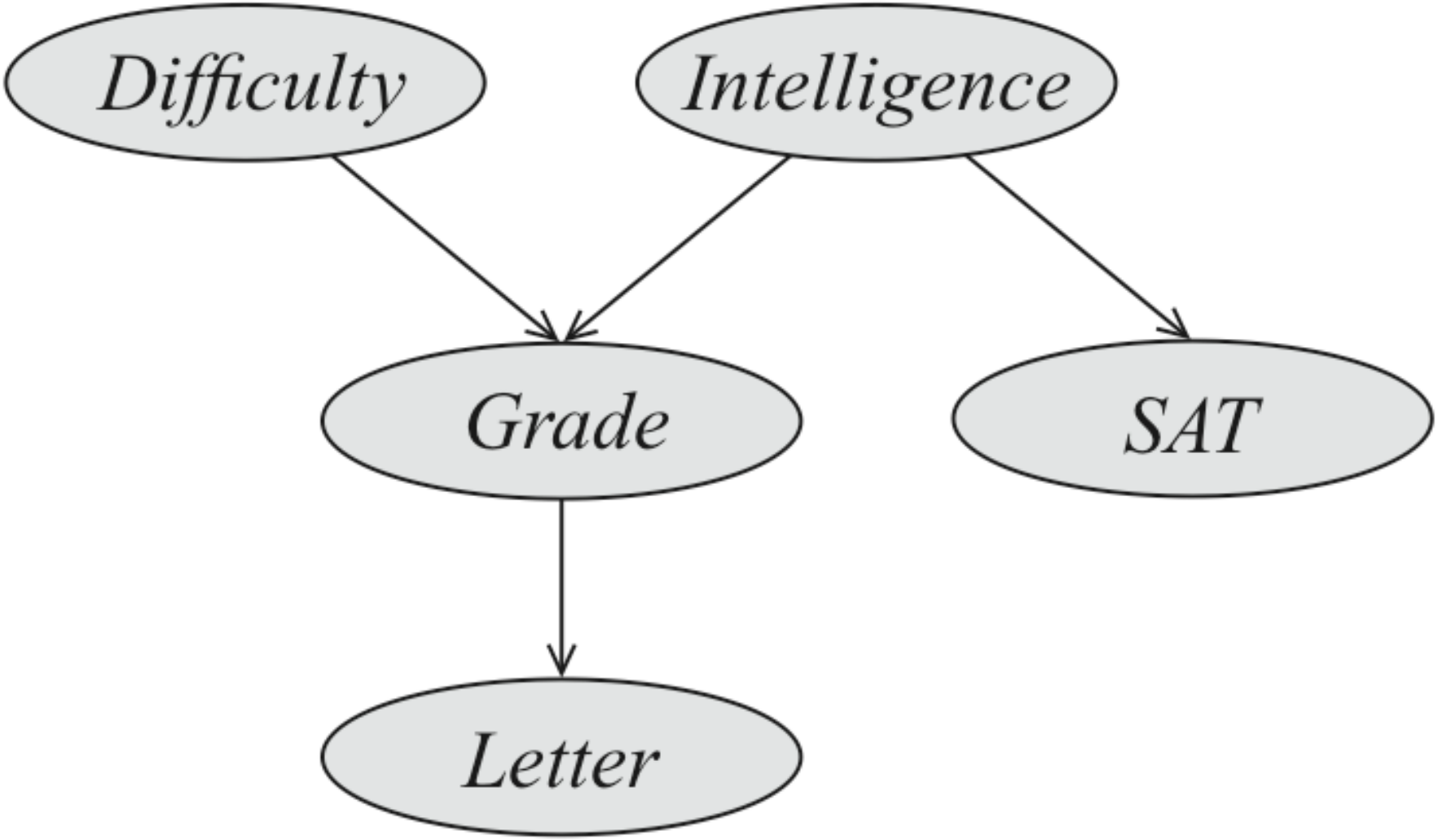
X_h the other hidden variables

X_v the visible variables

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



EXTENDED STUDENT EXAMPLE



INDEPENDENCE I-MAP

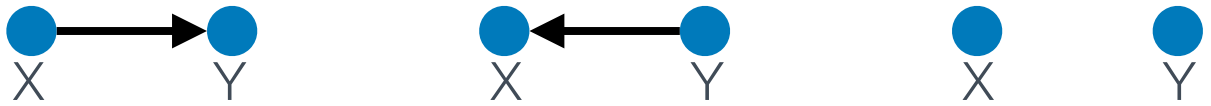
- I(G) (conditional) independences implied by G (not yet defined)
- I(P) (conditional) independences in the distribution P
- G I-map for P in I(G) ⊆ I(P)

p

X	Y	$P(X,Y)$
x^0	y^0	0.08
x^0	y^1	0.32
x^1	y^0	0.12
x^1	y^1	0.48

q

X	Y	$P(X,Y)$
x^0	y^0	0.4
x^0	y^1	0.3
x^1	y^0	0.2
x^1	y^1	0.1



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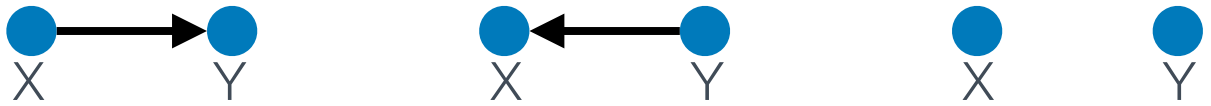
x^0	y^1	0.32
x^1	y^0	0.12
x^1	y^1	0.48

q

X	Y	$P(X,Y)$
x^0	y^0	0.4
x^0	y^1	0.3
x^1	y^0	0.2
x^1	y^1	0.1



- p: X and Y ind. ex. p(X=1) = 0.48 + 0.12 =0.6, p(Y=1) = 0.8, and p(X=1,Y=1) = 0.48
- q: X and Y are dependent

INDEPENDENCE I-MAP

- I(G) independences implied by G (not yet defined)
- I(P) independences in the distribution P
- G I-map for P in I(G) ⊆ I(P)

p

X	Y	$P(X,Y)$
x^0	y^0	0.08
x^0	y^1	0.32
x^1	y^0	0.12
x^1	y^1	0.48

q

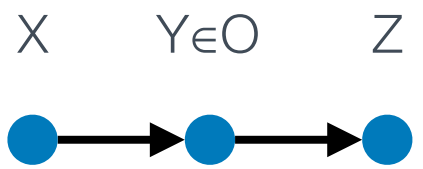
X	Y	$P(X,Y)$
x^0	y^0	0.4
x^0	y^1	0.3
x^1	y^0	0.2
x^1	y^1	0.1

- All three graphs are I-maps for p
- G_1 and G_2 are I-maps for q, but G_3 is not

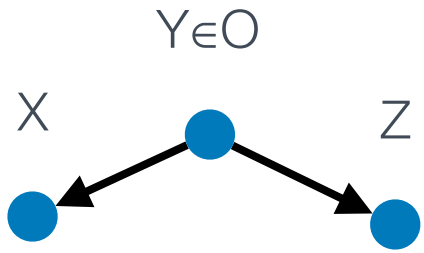
D-SEPARATION

★ A path is d-separated by O if it has

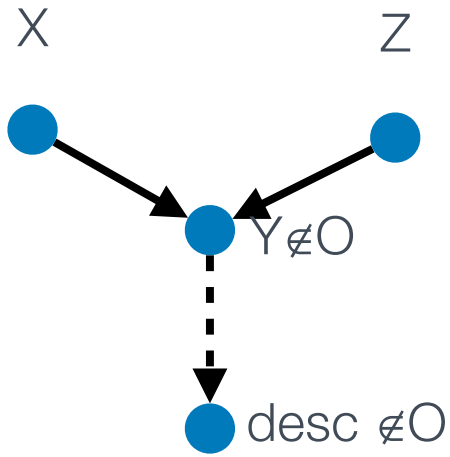
- a chain $X \rightarrow Y \rightarrow Z$ where $Y \in O$
- a fork $X \leftarrow Y \rightarrow Z$ where $Y \in O$
- a v-structure $X \rightarrow Y \leftarrow Z$ where $(Y \cup \text{desc}(Y)) \cap O = \varnothing$



Chain

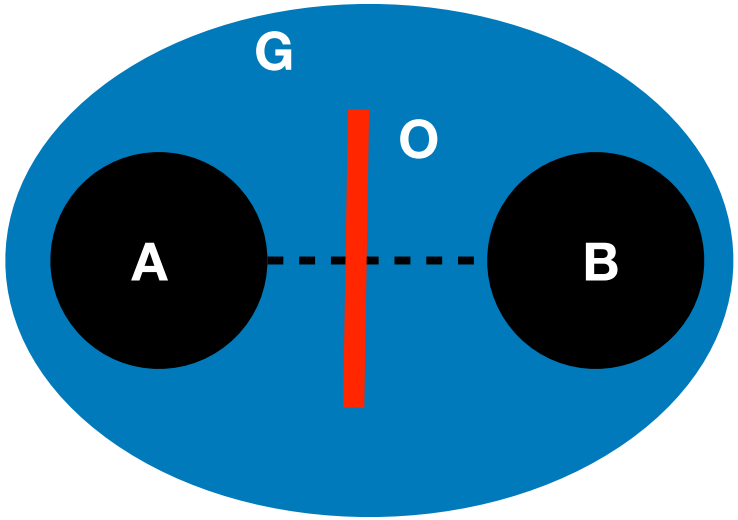


Fork



v-struct

D-SEPARATION SETS AND CI OF DAGS

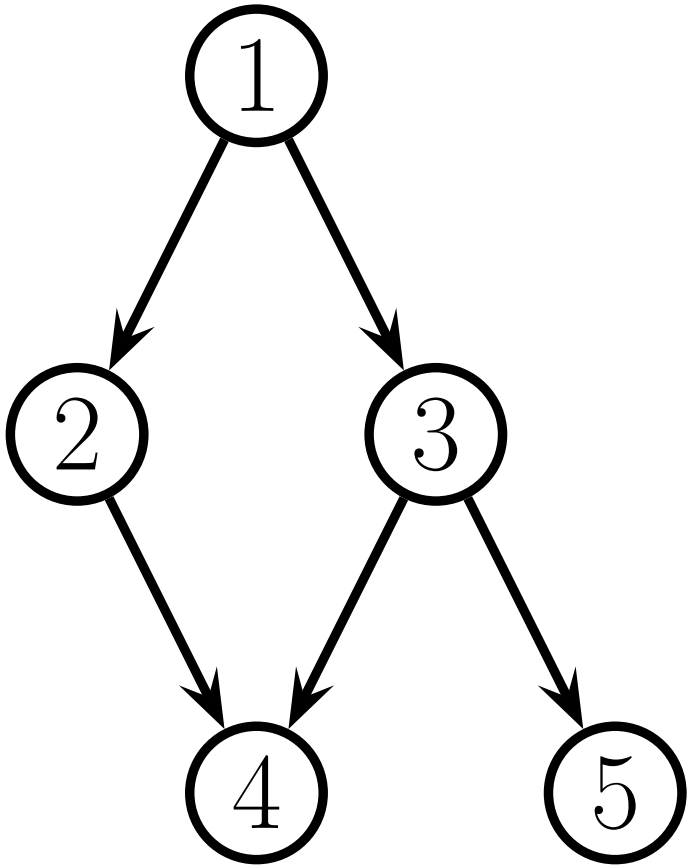


★ A is d-separated from B given O if every undirected path between A and B is d-separated by O

★ In a DAG G, global ind. def. by

$$\boldsymbol{x}_A \perp_G \boldsymbol{x}_B | \boldsymbol{x}_O$$

A is d-separated from B given O



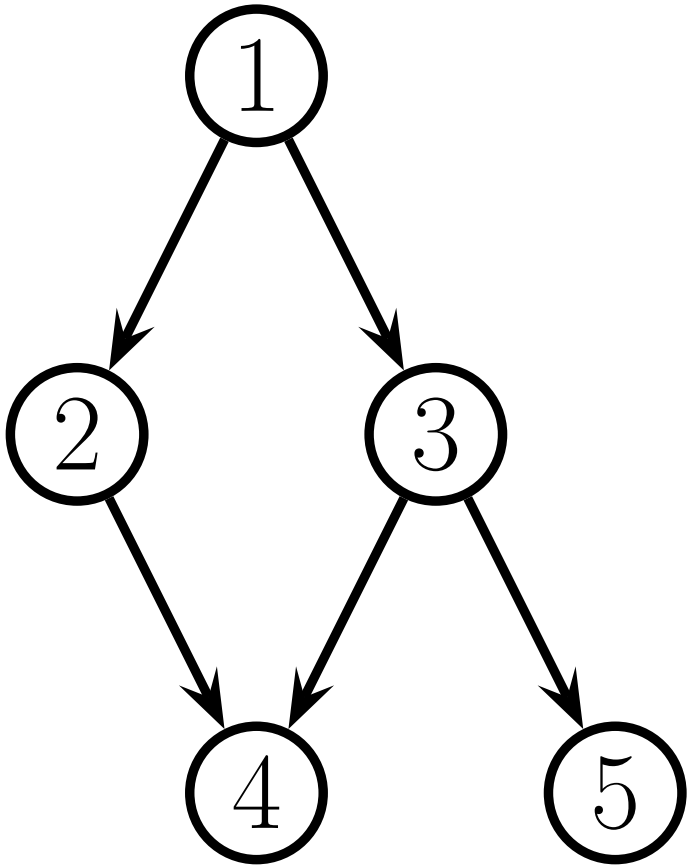
ORDERED MARKOV PROPERTY

★ The directed local Markov property.

$$\boldsymbol{x}_t \perp_G \boldsymbol{x}_{\mathrm{nd}(t)\setminus\mathrm{pa}(t)} | \boldsymbol{x}_{\mathrm{pa}(t)}$$

★ In this case

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



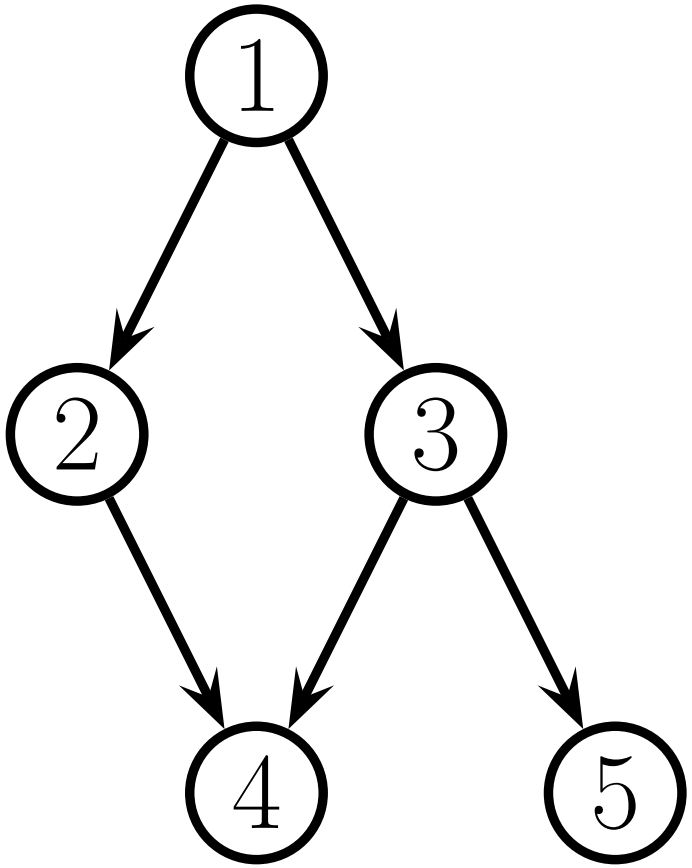
ORDERED MARKOV PROPERTY

★ The directed local Markov property.

$$\boldsymbol{x}_t \perp_G \boldsymbol{x}_{\mathrm{nd}(t)\setminus\mathrm{pa}(t)} | \boldsymbol{x}_{\mathrm{pa}(t)}$$

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

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



ORDERED MARKOV PROPERTY

★ The ordered Markov property.

$$\boldsymbol{x}_t \perp_G \boldsymbol{x}_{\mathrm{pred}(t)\setminus \mathrm{pa}(t)} | \boldsymbol{x}_{\mathrm{pa}(t)}$$

topological order

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

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

EQUIVALENCE OF INDEPENDENCE DEFINITIONS

- ★ Global (G): d-separation
- ★ Local (L):

$$\boldsymbol{x}_t \perp_G \boldsymbol{x}_{\mathrm{nd}(t)\setminus\mathrm{pa}(t)} | \boldsymbol{x}_{\mathrm{pa}(t)}$$

- ★ Ordered (O): $\boldsymbol{x}_t \perp_G \boldsymbol{x}_{\mathrm{pred}(t)\setminus\mathrm{pa}(t)} | \boldsymbol{x}_{\mathrm{pa}(t)}$

  where pred is according to a topological order

- ★ Factorized (F): can be family-factorized
- ★ Theorem: G ⇔ L ⇔ O ⇔ F

SOUNDNESS AND COMPLETENESS

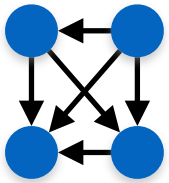
- Theorem

  If a distribution P factorizes according to G, then I(G) ⊆ I(P)

- Theorem

  If X and Y are not d-separated given Z in G, then X and Y are dependent given Z in some distribution P that factorize over G.

We cannot have all. Ex. clique and independent distribution



SKELETON AND EQUIVALENCE

- The skeleton is the underlying undirected graph
- Immorality is a pair of unmarried parents
- Theorem

  Let G_1 and G_2 be two graphs over X. Then G_1 and G_2 have the same skeleton and the same set of immoralities if and only if $I(G_1)=I(G_2)$

THE END