Lecture 20. Inference on PGMs

COMP90051 Statistical Machine Learning

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This lecture

- Probabilistic inference: computing (conditional) marginals from joint distributions
  - Needed to learn (posterior update) in Bayesian ML
  - Exact inference: Elimination algorithm
  - Approximate inference: Sampling
- Statistical inference: Parameter estimation
  - Fully observed case: Factors decompose under MLE
  - Latent variables: Motivates the EM algorithm

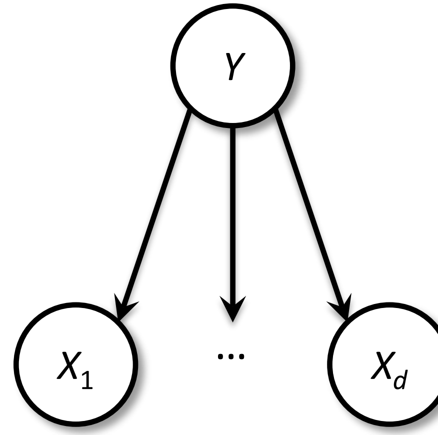
Probabilistic inference on PGMs

Computing marginal and conditional distributions from the joint of a PGM using Bayes rule and marginalisation.

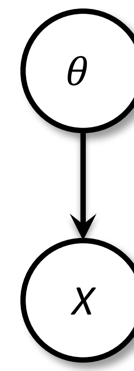
This deck: how to do it efficiently.

Two familiar examples

- Naïve Bayes (frequentist/Bayesian)
  - Chooses most likely class given data
  - $\Pr(Y|X_1,\dots,X_d) = \frac{\Pr(Y,X_1,\dots,X_d)}{\Pr(X_1,\dots,X_d)} = \frac{\Pr(Y,X_1,\dots,X_d)}{\sum_y \Pr(Y=y,X_1,\dots,X_d)}$

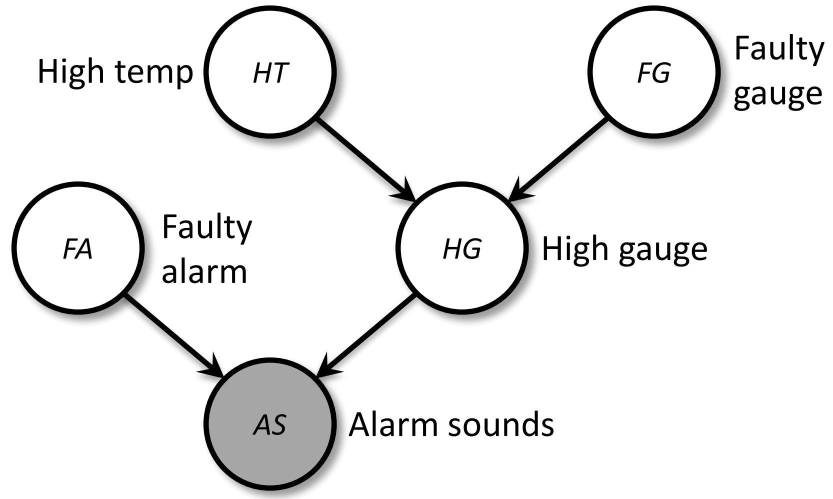


- Data $X|\theta \sim N(\theta,1)$ with prior $\theta \sim N(0,1)$ (Bayesian)
  - Given observation $X = x$ update posterior
  - $\Pr(\theta|X) = \frac{\Pr(\theta,X)}{\Pr(X)} = \frac{\Pr(\theta,X)}{\sum_\theta \Pr(\theta,X)}$



- Joint + Bayes rule + marginalisation → anything

Nuclear power plant



- **Alarm sounds**; meltdown?!
- $\Pr(HT|AS=t) = \frac{\Pr(HT, AS{=}t)}{\Pr(AS{=}t)}$

$$= \frac{\sum_{FG,\,HG,\,FA} \Pr(AS{=}t, FA, HG, FG, HT)}{\sum_{FG,\,HG,\,FA,\,HT'} \Pr(AS{=}t, FA, HR, FG, HT')}$$

- Numerator (denominator similar)

expanding out sums, joint *summing once over 2^5 table*

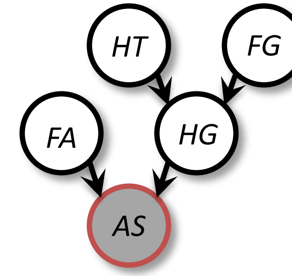
$$= \sum_{FG} \sum_{HG} \sum_{FA} \Pr(HT) \Pr(HG|HT, FG) \Pr(FG) \Pr(AS = t|FA, HG) \Pr(FA)$$

distributing the sums as far down as possible *summing over several smaller tables*

$$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT, FG) \sum_{FA} \Pr(FA) \Pr(AS = t|FA, HG)$$

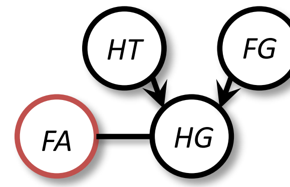
$f(X=a) = \sum_x f(X=x)\,\delta(x=a)$

Nuclear power plant (cont.)



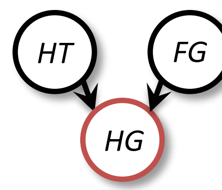
$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT,FG) \sum_{FA} \Pr(FA) \Pr(AS=t|FA,HG)$

eliminate *AS*: since *AS* observed, really a no-op



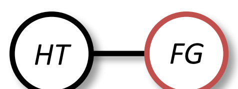
$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT,FG) \sum_{FA} \Pr(FA)\, m_{AS}(FA,HG)$

eliminate *FA*: multiplying 1x2 by 2x2



$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT,FG)\, m_{FA}(HG)$

eliminate *HG*: multiplying 2x2x2 by 2x1



$= \Pr(HT) \sum_{FG} \Pr(FG)\, m_{HG}(HT,FG)$

eliminate *FG*: multiplying 1x2 by 2x2

$= \Pr(HT)\, m_{FG}(HT)$

Multiplication of tables, followed by summing, is actually matrix multiplication

$m_{FA}(HG)=$

FA = f	*FA* = t
0.6	0.4

X

FA \ *HG*	f	t
f	1.0	0
t	0.8	0.2

Elimination algorithm

Eliminate (Graph G, Evidence nodes E, Query nodes Q)

1. Choose node ordering I such that Q appears last
2. Initialise empty list active
3. For each node X_i in G
   a) Append $\Pr(X_i \mid parents(X_i))$ to active

initialise

4. For each node X_i in E
   a) Append $\delta(X_i, x_i)$ to active

evidence

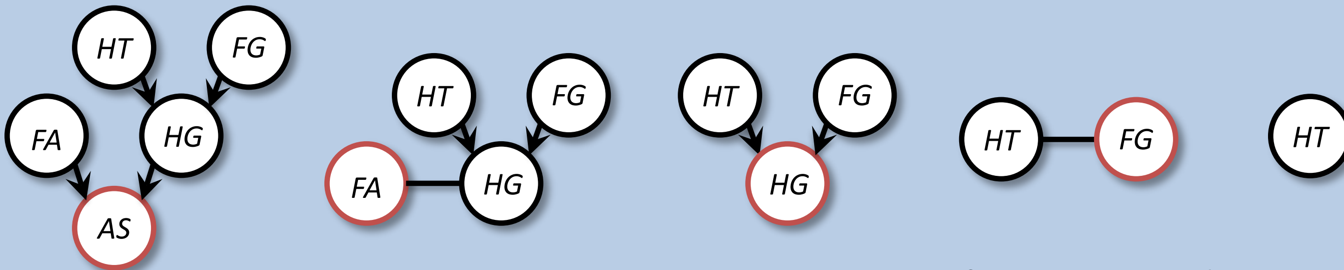
5. For each i in I
   a) potentials = Remove tables referencing X_i from active
   b) N_i = nodes other than X_i referenced by tables
   c) Table $\phi_i(X_i, X_{N_i})$ = product of tables
   d) Table $m_{i(X_{N_i})} = \sum_{X_i} \phi_i(X_i, X_{N_i})$
   e) Append $m_i(X_{N_i})$ to active

marginalise

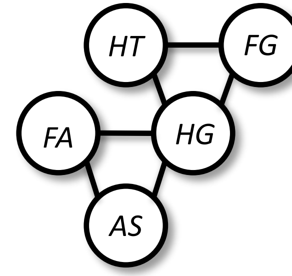
6. Return $\Pr(X_Q | X_E = x_E) = \phi_Q(X_Q) / \sum_{X_Q} \phi_Q(X_Q)$

normalise

Runtime of elimination algorithm



PGM after successive eliminations



"reconstructed" graph From process called ***moralisation***

- Each step of elimination
  - Removes a node
  - Connects node's remaining neighbours
    → forms a clique in the "reconstructed" graph
    (cliques are exactly r.v.'s involved in each sum)
- Time complexity exponential in largest clique

The workshop gives an example about this, the conclusion is that the best elimination strategy is not add any extra edge between nodes.

- Different elimination orderings produce different cliques
  - Treewidth: minimum over orderings of the largest clique
  - Best possible time complexity is exponential in the treewidth e.g. $O(2^{tw})$

Mini Summary

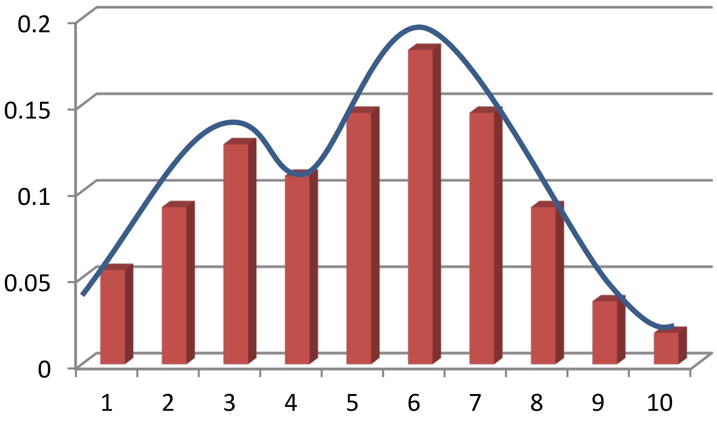
(Exact) probabilistic inference on PGMs

- What? Marginalise out variables, Condition
- Why? Example: Bayesian posterior updates!
- How? The elimination algorithm
- How long? Time exponential in treewidth

Next time: Approximate PGM probabilistic inference

Probabilistic inference by simulation

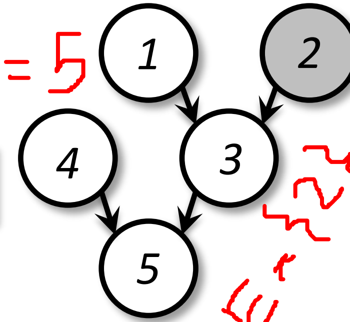
- Exact probabilistic inference can be expensive/impossible
  - Integration may not have analytical solution!
- Can we approximate numerically?
- Idea: sampling methods
  - Approximate **distribution** by **histogram of a sample**
  - We can't trivially sample: (1) only know desired distribution up to a (normalising) constant (2) naïve sampling approaches are inefficient in high dimensions.



https://www.youtube.com/watch?v=ER3DDBFzH2g

Gibbs sampling

$d=5$



Divide and conquer: Sampling single variable at a time.

- Given: D-PGM on d random variables
  Given: evidence values $\mathbf{x}_E$ over variables $E \subset \{1, \ldots, d\}$
  Goal: many approximately independent samples from joint conditioned on $\mathbf{x}_E$

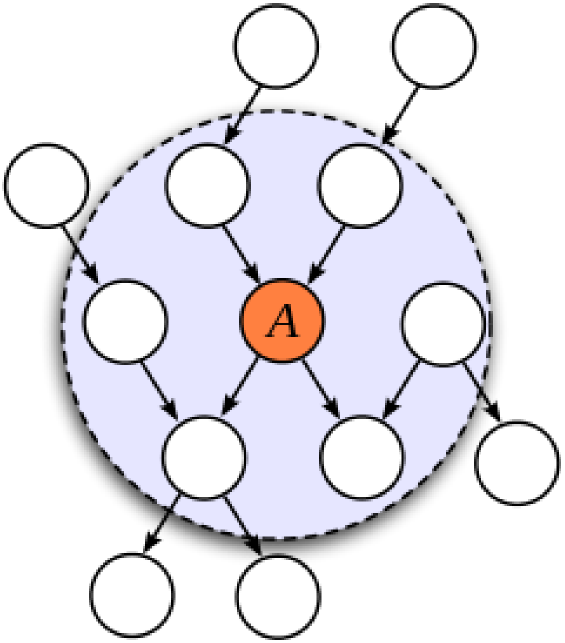
1. Initialise with a starting $\mathbf{X}^{(0)} = \left(X_1^{(0)}, \ldots, X_d^{(0)}\right)$ with $\mathbf{X}_E^{(0)} = \mathbf{x}_E$
2. Repeat many times
   a) Pick non-evidence node X_j uniformly at random
   b) Sample single node $X_j' \sim p\left(X_j | X_1^{(i-1)}, \ldots, X_{j-1}^{(i-1)}, X_{j+1}^{(i-1)}, \ldots, X_d^{(i-1)}\right)$
   c) Save entire joint sample $\mathbf{X}^{(i)} = \left(X_1^{(i-1)}, \ldots, X_{j-1}^{(i-1)}, X_j', X_{j+1}^{(i-1)}, \ldots, X_d^{(i-1)}\right)$

- Exercise: Why always $\mathbf{X}_E^{(i)} = \mathbf{x}_E$?

- Need not update nodes in random order, e.g. parents first order
  But do need to be able to sample from conditionals (e.g. conjugacy)

Markov blanket

- Intuition: all the nodes that you directly depend on. *Not just your parents/children!*
- Consider node X_i in D-PGM on nodes $N = \{1, \ldots, d\}$
- Markov blanket $\mathrm{MB}(i)$ of X_i:
  - Nodes $B \subseteq N \backslash \{i\}$ such that…
  - X_i independent of $\mathbf{X}_{\bar{B}\backslash\{i\}}$ given $\mathbf{X}_B$
  - $p(X_i \mid X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_d) = p\big(X_i \mid \mathrm{MB}(X_i)\big)$
- In D-PGM Markov blanket is:
  - Parents of i, children of i, parents of children of i
  - $p\big(X_i \mid \mathrm{MB}(X_i)\big) \propto p\big(X_i | X_{\pi_i}\big) \prod_{k:i\in\pi_k} p\big(X_k | X_{\pi_k}\big)$



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Markov Chain Monte Carlo (MCMC)

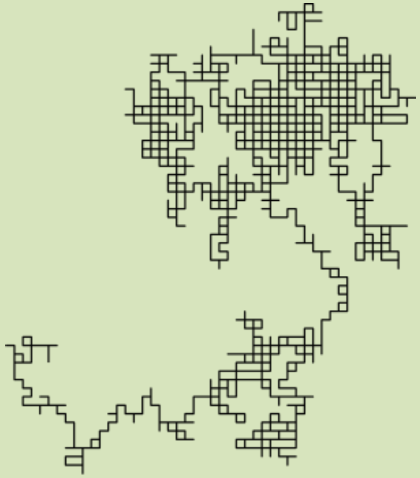
- Gibbs sampling produces a chain of samples $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots$ *approximating* draws from $p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$

- How good an approximation? Independent draws possible?

- Samples form a Markov chain: Each $\mathbf{X}^{(i)}$ depends only $\mathbf{X}^{(i-1)}$
  * States are all possible values taken by joint samples
  * Initial distribution $\mathbf{p}_0$ of state $\mathbf{X}^{(0)}$ given by initialisation process
  * Transition probability matrix $\mathbf{T}$ given by PGM conditional probabilities
  * Combines to: distribution $\mathbf{p}_i = (\mathbf{T})^i \mathbf{p}_0$ of state $\mathbf{X}^{(i)}$.

- Burn in: Run Gibbs long enough and $\mathbf{X}^{(i)} \sim p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$
  * "Limiting distribution" $\lim_{i \to \infty} \mathbf{p}_i$ is $p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$ under condition that no entry of $\mathbf{T}$ is zero ("ergodicity" – may not always hold)
  * Solution: throw away first few thousand samples

- Thinning: Want saved full samples to be independent
  * Neighbouring $\mathbf{X}^{(i)}, \mathbf{X}^{(i+1)}$ are highly correlated. Intuition why?
  * Solution: only keep every 100 or so samples



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Initialising Gibbs: Forward Sampling

- Set all evidence nodes to observed values
- Remaining nodes, parent-first order
  - Node has no parents? Sample from its D-PGM marginal
  - Sample node given previously sampled parents
- However Markov chain theory tells us MCMC converges irrespective of initial sample's distribution
  - The limiting distribution – the "equilibrium distribution" – is a property of the transition matrix (the PGM's joint) not the initial distribution

Now what??

- With our $\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(T)}$ in hand after running Gibbs for a while with burn-in and thinning…
- These form "i.i.d." sample of $p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$
- We can do heaps!
  a) Can approximate the distribution via a histogram of these samples (make bins, form counts).
  b) Marginalising out variables == Dropping components from samples
  c) Expectations: Estimating by sample mean of samples
- Posterior $p(\mathbf{w}|\mathbf{X}_{tr}, \mathbf{y}_{tr})$ combine (a) and (b)
  Mean posterior point estimate, combine with (c)

Mini Summary

Approximate probabilistic inference on PGMs

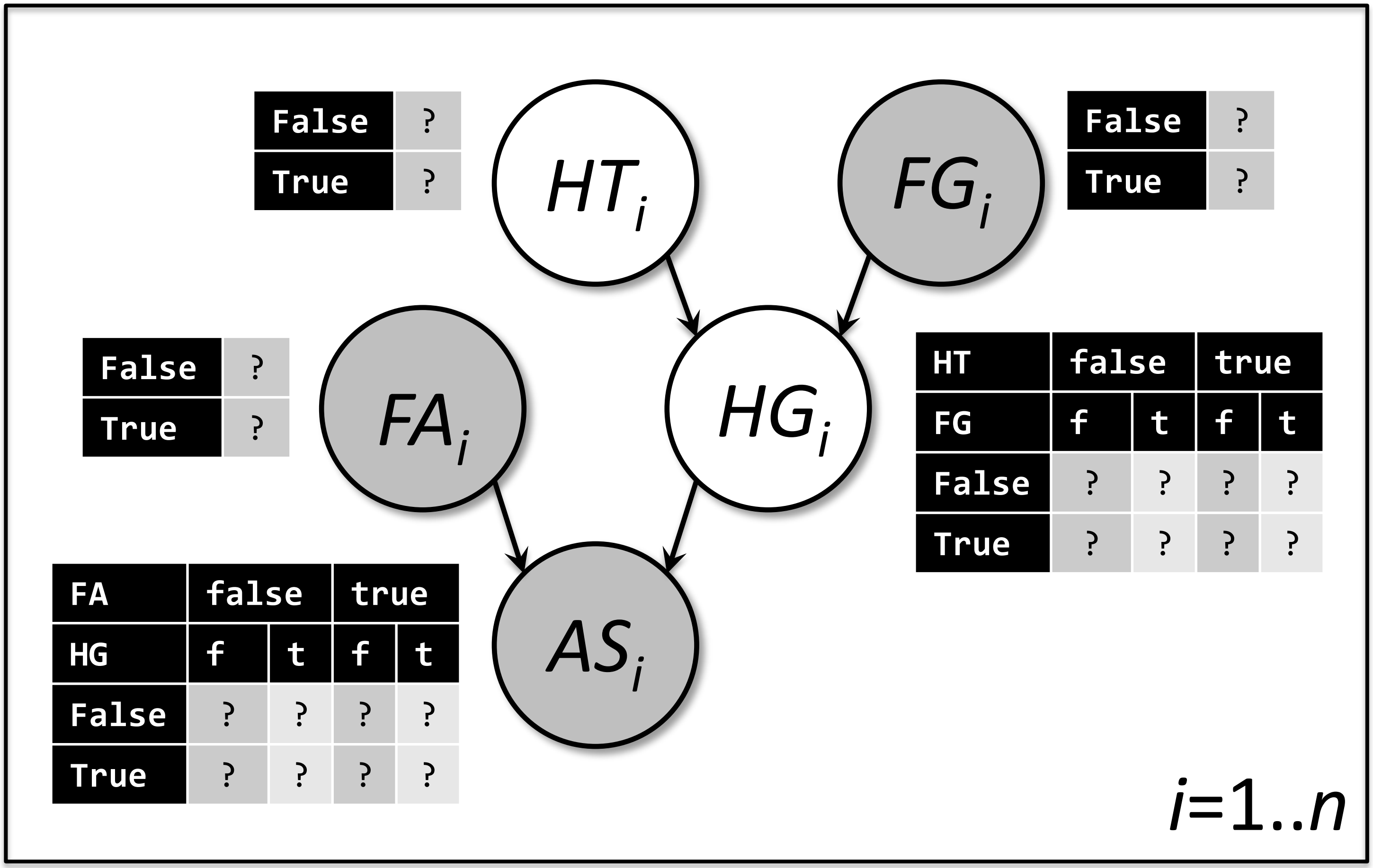
- Why? Summation/integration may be costly
- Why? Integration may be impossible analytically
- Briefly: Gibbs sampling

Next time: Statistical inference on PGMs

Statistical inference on PGMs

Learning from data – fitting probability tables to observations (eg as a frequentist; a ***Bayesian would just use probabilistic inference*** *to update prior to posterior)*

Have PGM, Some observations, No tables…



False	?
True	?

False	?
True	?

False	?
True	?

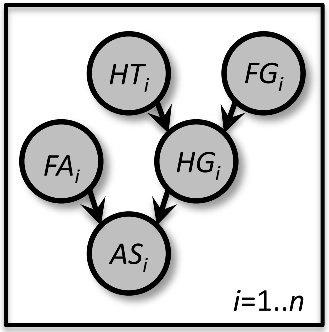
HT	false		true	
FG	f	t	f	t
False	?	?	?	?
True	?	?	?	?

FA	false		true	
HG	f	t	f	t
False	?	?	?	?
True	?	?	?	?

Fully-observed case is "easy"

- Max-Likelihood Estimator (MLE) says
  - If we observe *all* r.v.'s $\boldsymbol{X}$ in a PGM independently n times $\boldsymbol{x}_i$
  - Then maximise the *full* joint

$$\underset{\theta\in\Theta}{\arg\max} \prod_{i=1}^{n} \prod_j p\left(X^j = x_i^j | X^{parents(j)} = x_i{}^{parents(j)}\right)$$



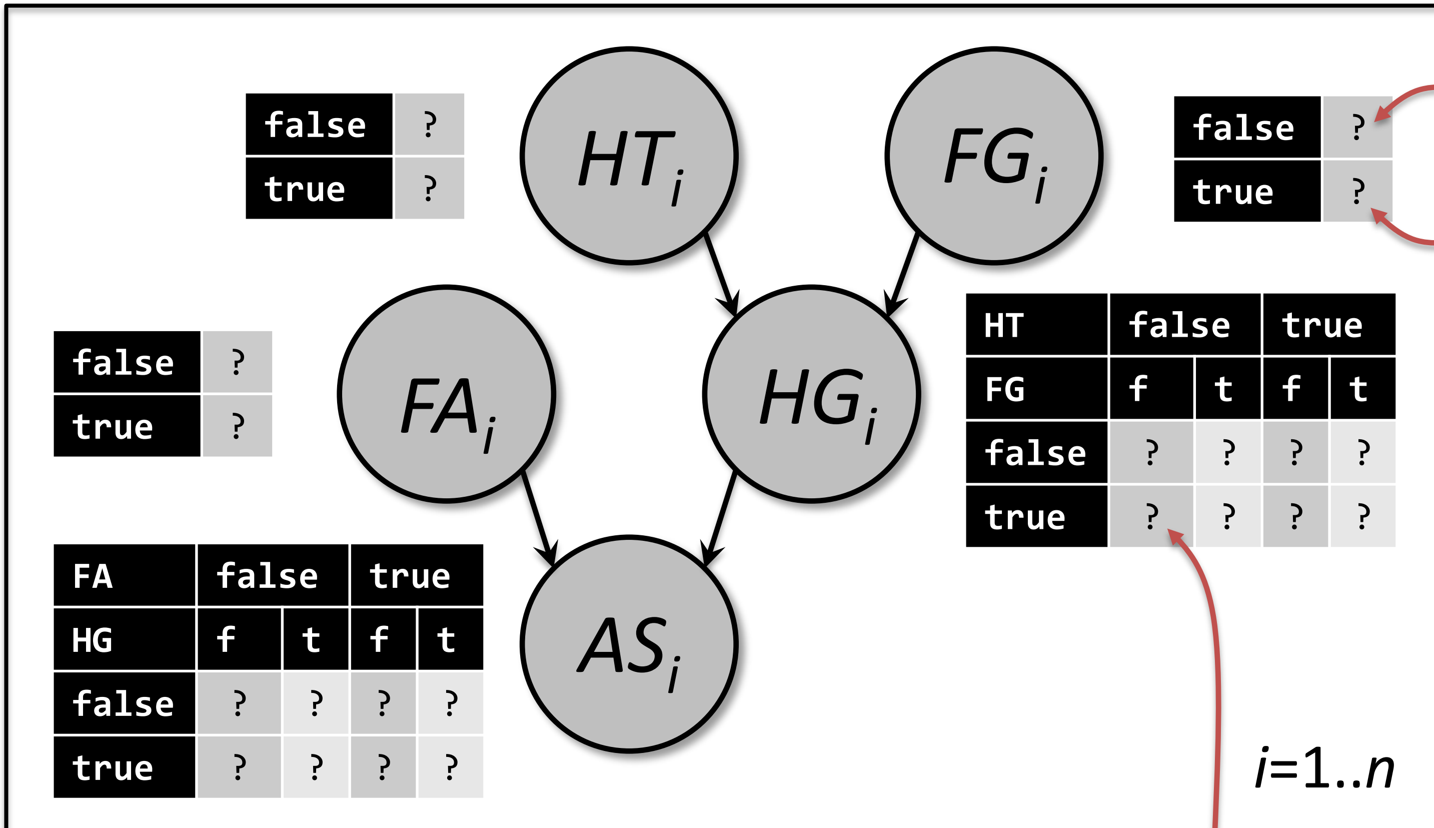
- Decomposes easily, leads to counts-based estimates
  - Maximise log-likelihood instead; becomes sum of logs

$$\underset{\theta\in\Theta}{\arg\max} \sum_{i=1}^{n} \sum_j \log p\left(X^j = x_i^j | X^{parents(j)} = x_i{}^{parents(j)}\right)$$

  - Big maximisation of all parameters together, decouples into small independent problems

- Example is training a naïve Bayes classifier

Example: Fully-observed case



false	?
true	?

false	?
true	?

false	?
true	?

HT	false		true	
FG	f	t	f	t
false	?	?	?	?
true	?	?	?	?

FA	false		true	
HG	f	t	f	t
false	?	?	?	?
true	?	?	?	?

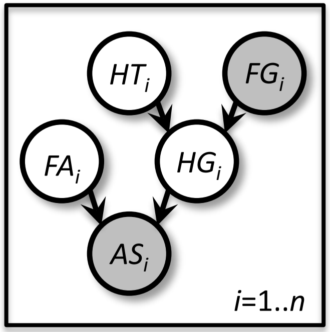
$$\frac{\#\{x_i|FG_i = false\}}{n}$$

$$\frac{\#\{x_i|FG_i = true\}}{n}$$

$$\frac{\#\{x_i|HG_i = true, HT_i = false, FG_i = false\}}{\#\{x_i|HT_i = false, FG_i = false\}}$$

Presence of unobserved variables trickier

- But most PGMs you'll encounter will have latent, or unobserved, variables



- What happens to the MLE?
  * Maximise likelihood of observed data only
  * Marginalise full joint to get to desired "partial" joint
  * $\arg\max_{\theta\in\Theta} \prod_{i=1}^{n} \sum_{\text{latent } j} \prod_j p\left(X^j = x_i{}^j | X^{parents(j)} = x_i{}^{parents(j)}\right)$
  * This won't decouple – oh-no's*!!*

→ Use EM algorithm!

Summary

- Probabilistic inference on PGMs
  - What is it and why do we care?
  - Elimination algorithm; complexity via cliques
  - Monte Carlo approaches as alternate to exact integration
- Statistical inference on PGMs
  - What is it and why do we care?
  - Straight MLE for fully-observed data
  - EM algorithm for mixed latent/observed data

Next time: deeper dive into HMMs and more