# Lecture 21. 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

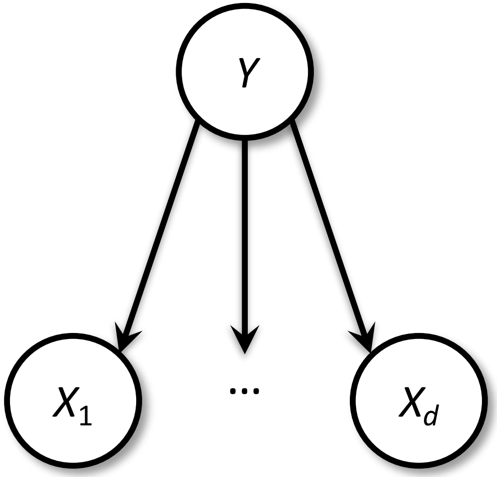
# Probabilistic inference on PGMs

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

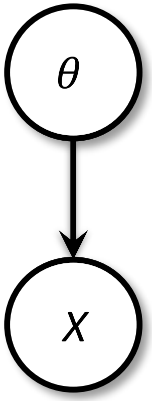
*This deck: how to do it efficiently.*

# Two familiar examples

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

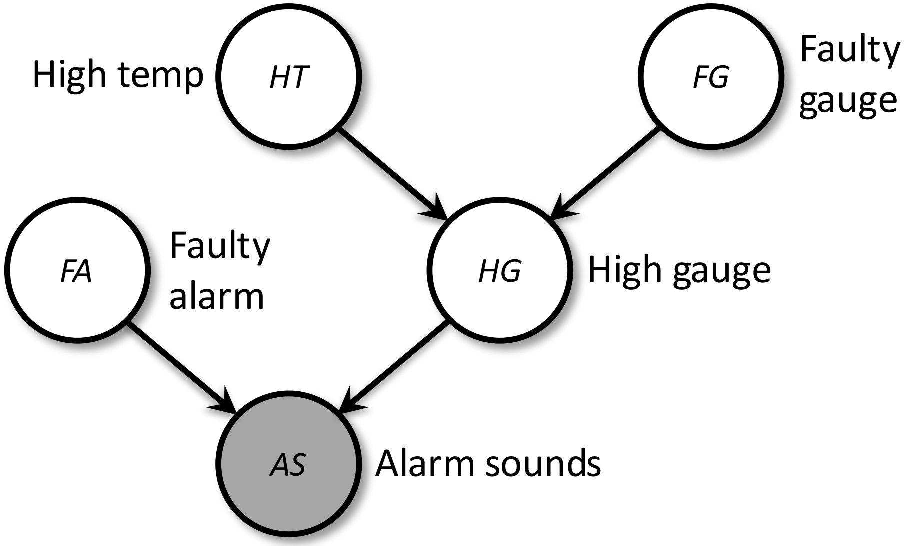


- Data $X|\theta \sim N(\theta, 1)$ with prior $\theta \sim N(0,1)$ (Bayesian)
  - Given observation $X = x$ update posterior
  - $\Pr(\theta|X) = \frac{\Pr(\theta, X)}{\Pr(X)} = \frac{\Pr(\theta, X)}{\sum_\theta \Pr(\theta, X)}$



- 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)

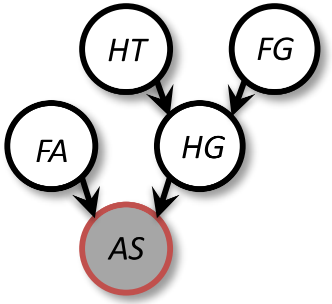
expanding out sums, joint *summing once over $2^5$ table*

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

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

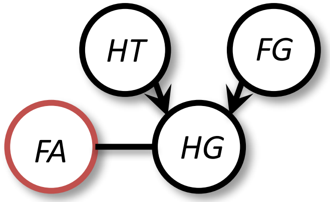
$$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT, FG) \sum_{FA} \Pr(FA) \Pr(AS=t|FA, HG)$$

# Nuclear power plant (cont.)



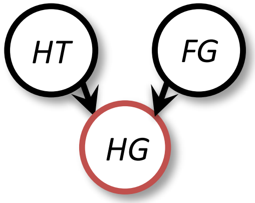
$= \Pr(HT)\sum_{FG}\Pr(FG)\sum_{HG}\Pr(HG|HT,FG)\sum_{FA}\Pr(FA)\,\Pr(AS=t|FA,HG)$

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



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

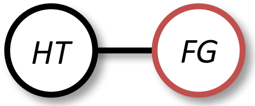
eliminate *FA*: multiplying 1x2 by 2x2



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

eliminate *HG*: multiplying 2x2x2 by 2x1

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



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

eliminate *FG*: multiplying 1x2 by 2x2

$$m_{FA}(HG) = \begin{array}{|c|c|} \hline \multicolumn{2}{|c|}{FA} \\ \hline f & t \\ \hline 0.6 & 0.4 \\ \hline \end{array} \;\text{X}\; \begin{array}{cc|c|c|} & & \multicolumn{2}{c|}{HG} \\ & & f & t \\ \hline FA & f & 1.0 & 0 \\ \hline & t & 0.8 & 0.2 \\ \hline \end{array}$$

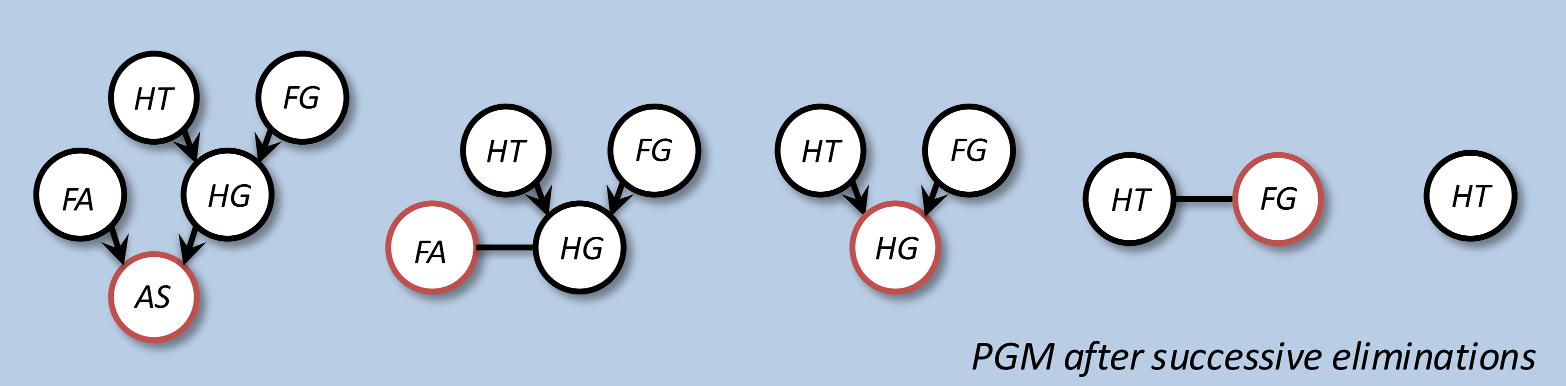
$= \Pr(HT)\,m_{FG}(HT)$

Useful trick: $f(X=a) = \sum_x f(X=x)\delta(x=a)$

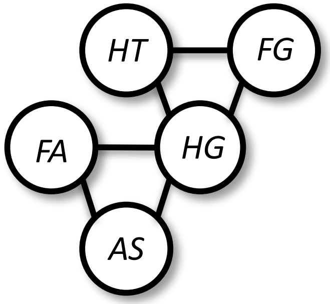
# Elimination algorithm

```
Eliminate (Graph $G$, Evidence nodes $E$, Query nodes $Q$)
1. Choose node ordering $I$ such that $Q$ appears last
2. Initialise empty list active                                      initialise
3. For each node $X_i$ in $G$
   a) Append $\Pr(X_i \mid parents(X_i))$ to active
4. For each node $X_i$ in $E$                                        evidence
   a) Append $\delta(X_i, x_i)$ to active
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               marginalise
   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
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
- 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

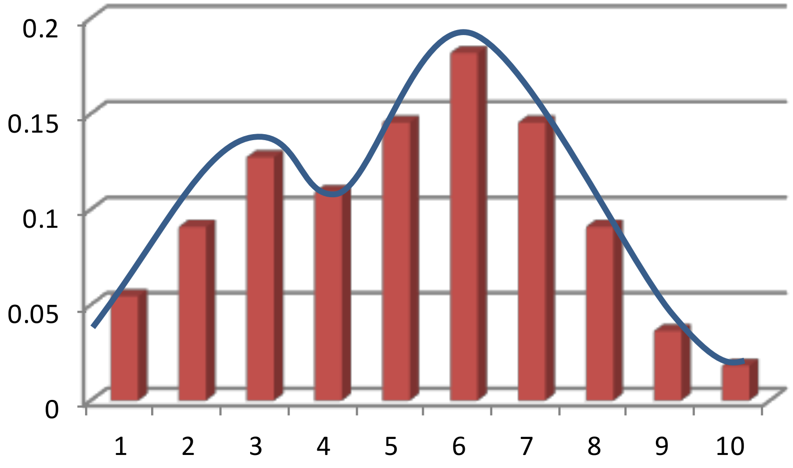
(Exact) probabilistic inference on PGMs

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

Next: Approximate PGM probabilistic inference

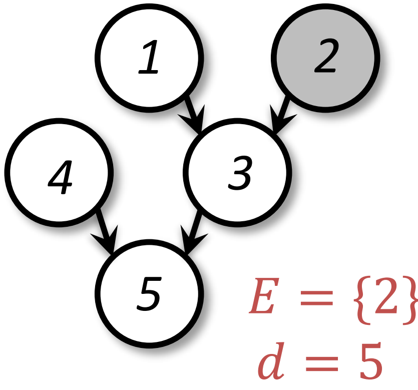
# Probabilistic inference by simulation

- 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.



# Gibbs sampling

Divide and conquer: Sampling single variable at a time.



$E = \{2\}$
$d = 5$

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

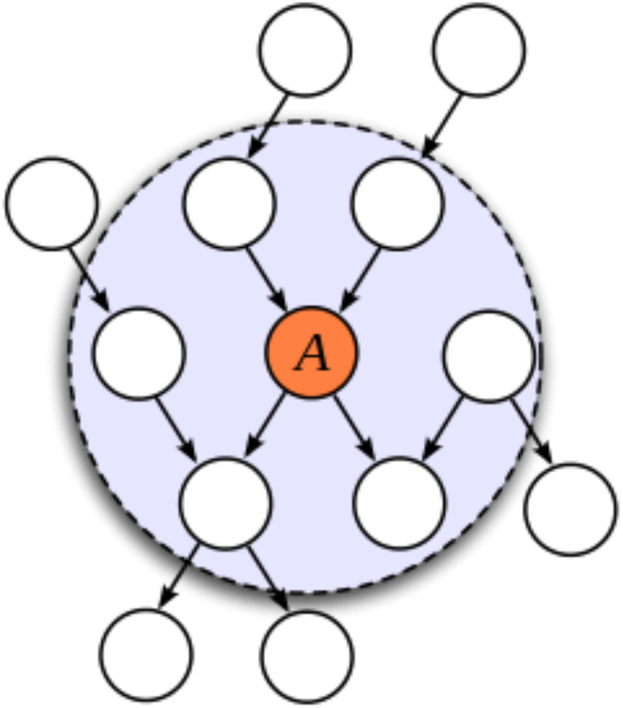
1. Initialise with a starting $\mathbf{X}^{(0)} = \left(X_1^{(0)}, \dots, X_d^{(0)}\right)$ with $\mathbf{X}_E^{(0)} = \mathbf{x}_E$
2. Repeat many times
   a) Pick non-evidence node $X_j$ uniformly at random
   b) Sample single node $X_j' \sim p\left(X_j | X_1^{(i-1)}, \dots, X_{j-1}^{(i-1)}, X_{j+1}^{(i-1)},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

- 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 $N = \{1, \dots, d\}$
- 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 $\mathbf{X}_B$
  - $p(X_i \mid X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d) = p\big(X_i \mid \mathrm{MB}(X_i)\big)$
- 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)

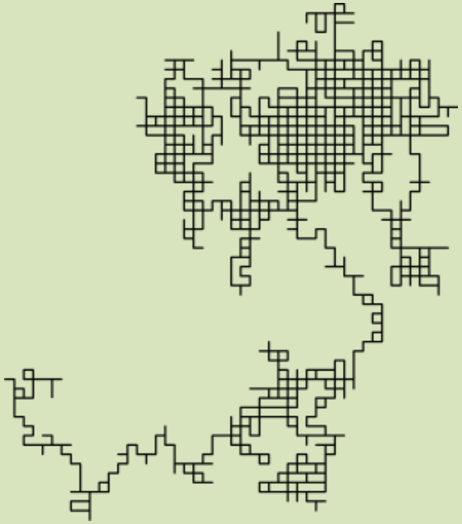
- Gibbs sampling produces a chain of samples $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots$ *approximating* draws from $p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$

- 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

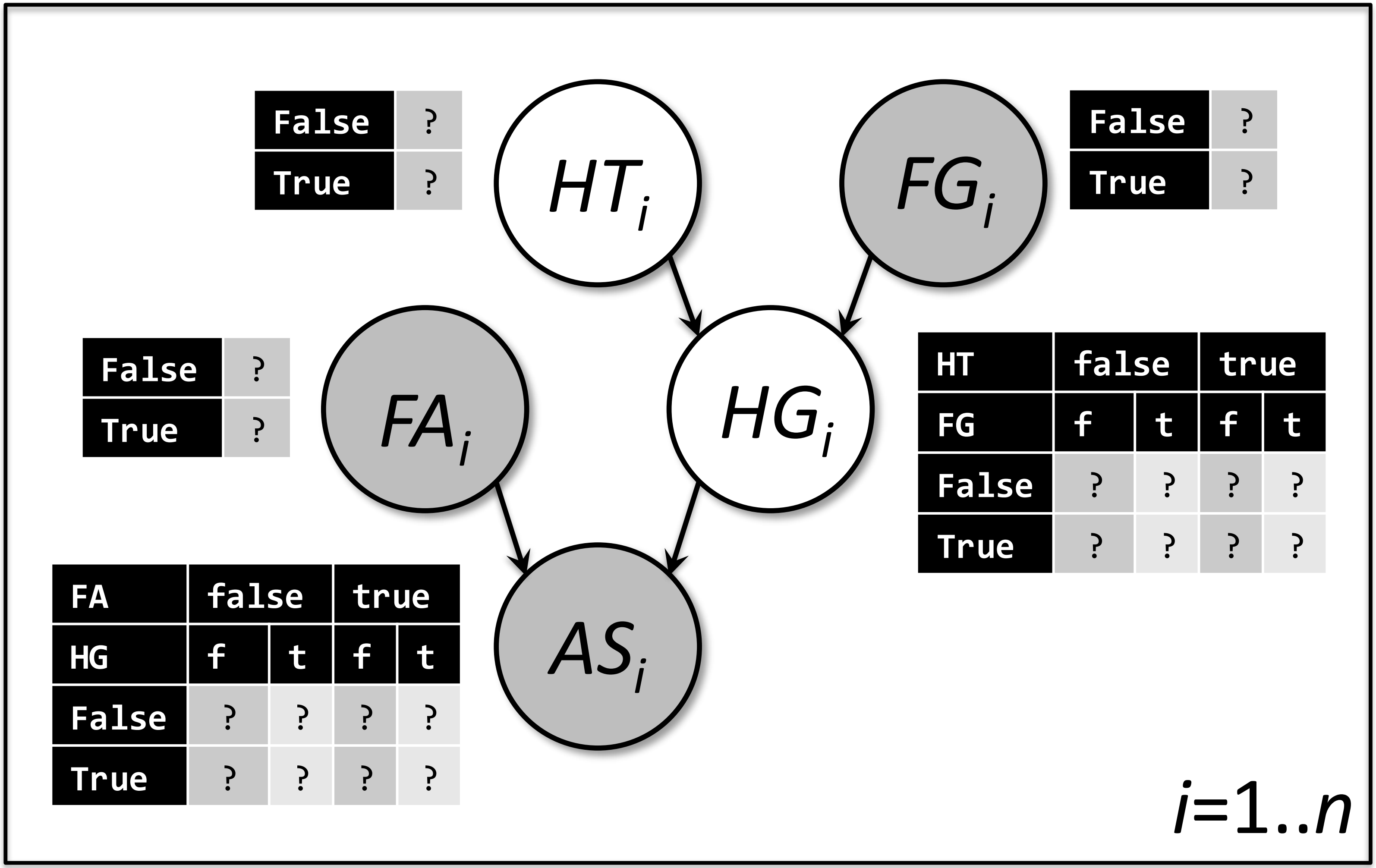
- Why? Summation/integration may be costly
- Why? Integration may be impossible analytically
- Briefly: Gibbs sampling

Next: 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 | ? |

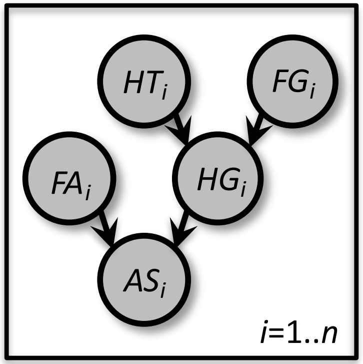
| HT | false |  | true |  |
|---|---|---|---|---|
| FG | f | t | f | t |
| False | ? | ? | ? | ? |
| True | ? | ? | ? | ? |

| 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

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

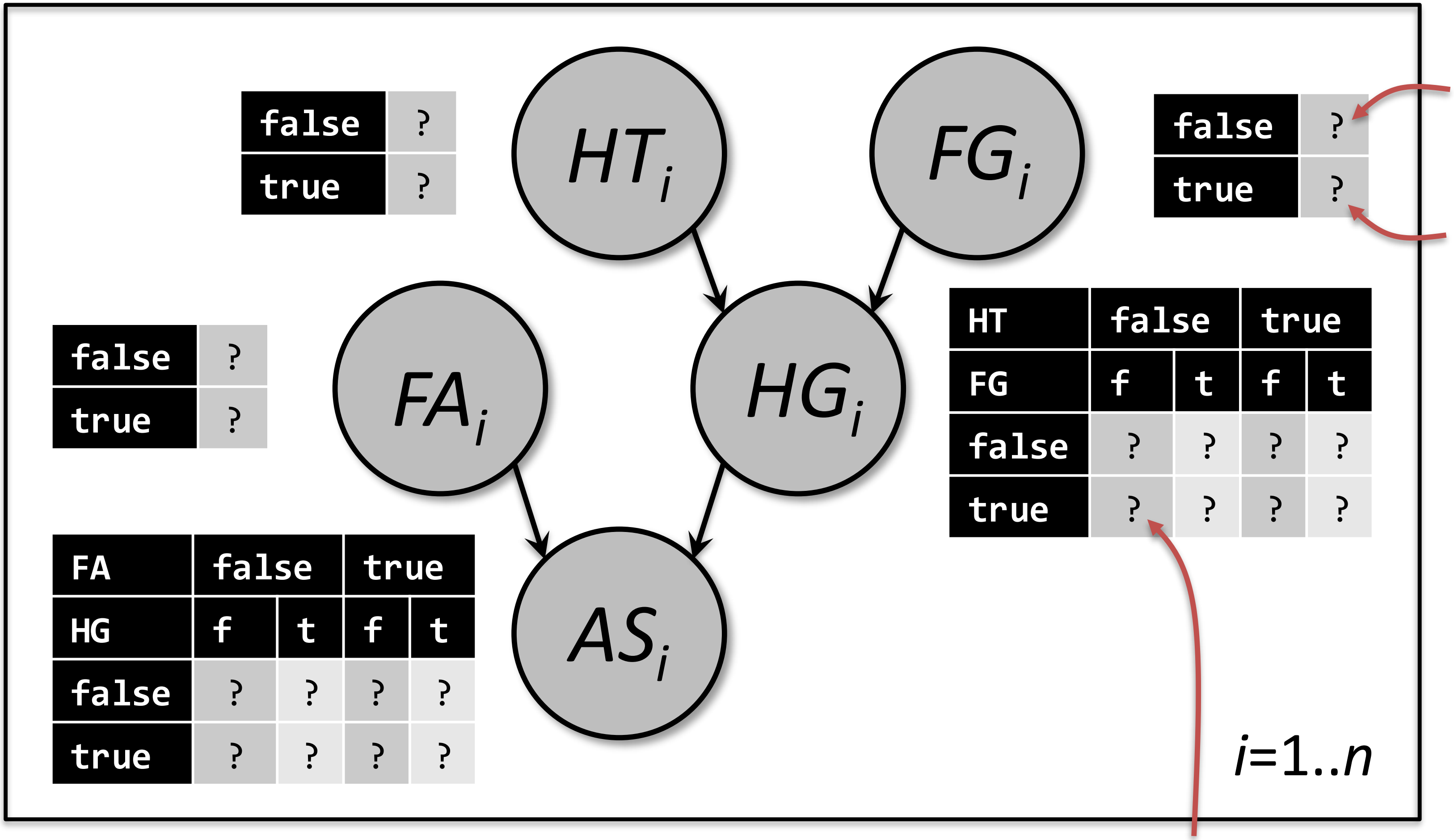


- Decomposes easily, leads to counts-based estimates
  - Maximise log-likelihood instead; becomes sum of logs

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

  - 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 | ? | ? | ? | ? |

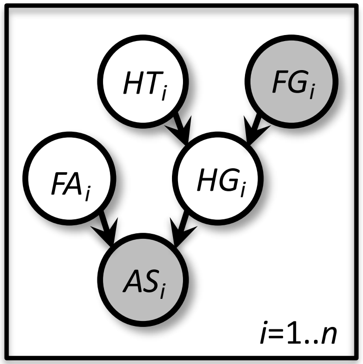
$$\frac{\#\{x_i|FG_i = false\}}{n}$$

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

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

# 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