Lecture 22. 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

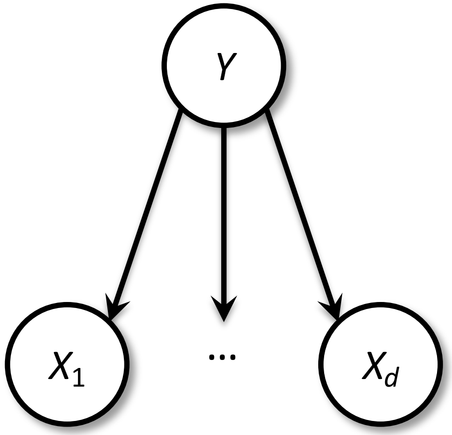
Probabilistic inference on PGMs

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

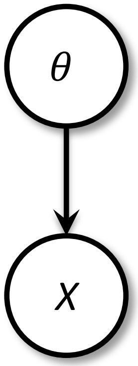
This deck: how to do it efficiently.

Two familiar examples

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



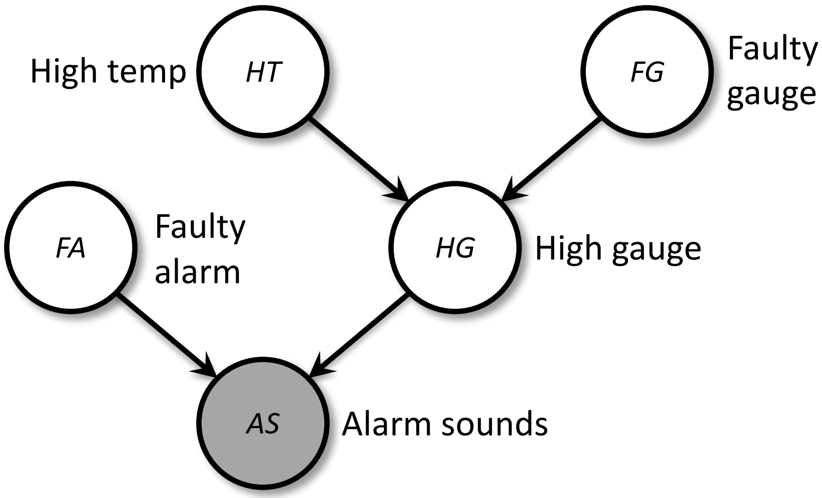
- Data $X|\theta \sim N(\theta, 1)$ with prior $\theta \sim N(0,1)$ (Bayesian)
  - Given observation $X = x$ update posterior
  - $\Pr(\theta|X) = \frac{\Pr(\theta, X)}{\Pr(X)} = \frac{\Pr(\theta, X)}{\sum_\theta \Pr(\theta, X)}$



- Joint + Bayes rule + marginalisation → anything

Nuclear power plant

In essence, the equation is saying: "To get the joint probability of a high temperature and the alarm sounding at a specific level t, sum up the probabilities over all possible scenarios of the faulty gauge, high gauge reading, and faulty alarm."



- **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*

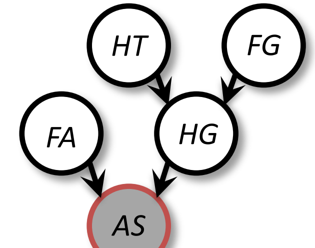
  $$= \sum_{FG} \sum_{HG} \sum_{FA} Pr(HT) Pr(HG|HT, FG) Pr(FG) Pr(AS=t|FA, HG) Pr(FA)$$

  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.)

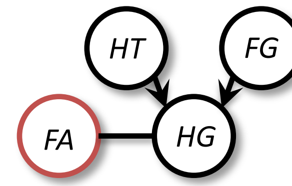


$= \Pr(HT)\sum_{FG}\Pr(FG)\sum_{HG}\Pr(HG|HT,FG)\sum_{FA}\Pr(FA)\Pr(AS=t|FA,HG)$

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

message

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

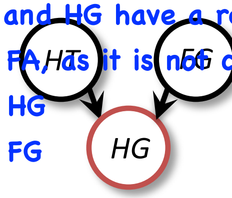


eliminate *FA*: multiplying 1x2 by 2x2

Process of Elimination

1. eliminate evidence node
2. make FA and HG have a relation: message left by eliminating AS
3. eliminate FA, as it is not connected to other nodes
4. eliminate HG
5. eliminate FG

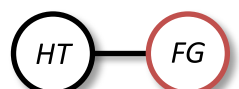
$= \Pr(HT)\sum_{FG}\Pr(FG)\sum_{HG}\Pr(HG|HT,FG)\, m_{FA}(HG)$



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

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

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

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
4. For each node X_i in E
   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
   d) Table $m_i(X_{N_i}) = \sum_{X_i} \phi_i(X_i, X_{N_i})$ largest clique
   e) Append $m_i(X_{N_i})$ to active
6. Return $\Pr(X_Q | X_E = x_E) = \phi_Q(X_Q) / \sum_{X_Q} \phi_Q(X_Q)$

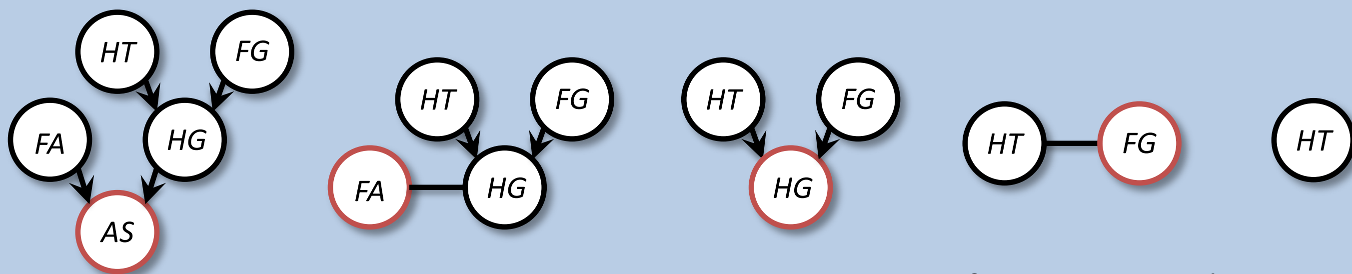
initialise

evidence

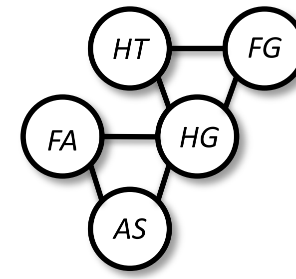
marginalise

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)

For instance, if the largest clique has size k, the time complexity could be O(2^k)

- 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

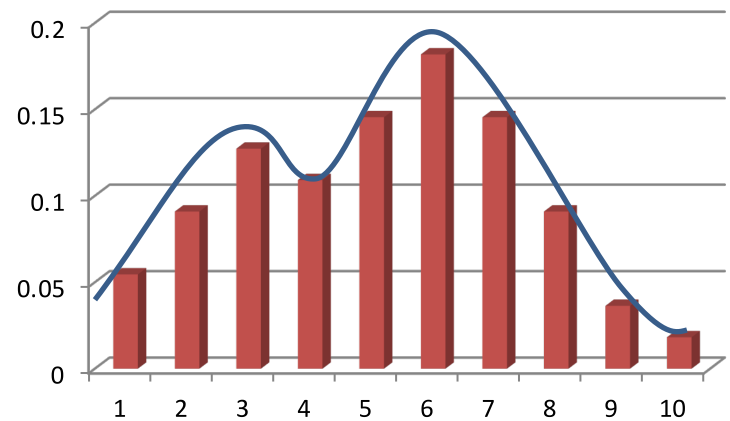
  naive way: consider whole table? ❌
  ✅: use elimination algorithm
- How long? Time exponential in treewidth

  2^5 -> 2^3 in our example

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.

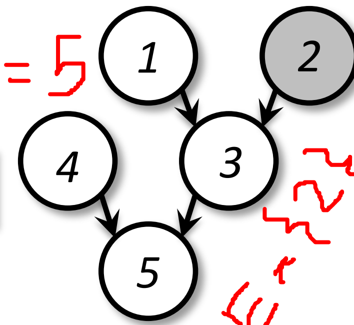


we want to obtain P(HT)
can we just simulate it? we can use the simulated node to get the distribution / or just use it. because in the end, we want to simulated it. cuz in the end we will perform the sampling
we want to directly sample from the query node

Gibbs sampling

evidence node

$d=5$



Divide and conquer: Sampling single variable at a time.

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

randomly pick up point

1. Initialise with a starting $\mathbf{X}^{(0)} = \left(X_1^{(0)}, \dots, X_d^{(0)}\right)$ with $\mathbf{X}_E^{(0)} = \mathbf{x}_E$

evidence node, give true sample value

2. Repeat many times

1,3,4,5: non-evidence node (randome pickup)

   a) Pick non-evidence node X_j uniformly at random
   b) Sample single node $X_j' \sim p\left(X_j | X_1^{(i-1)}, \dots, X_{j-1}^{(i-1)}, X_{j+1}^{(i-1)}, \dots, X_d^{(i-1)}\right)$

   sample from conditional distribution: because it is direct PGM

   c) Save entire joint sample $\mathbf{X}^{(i)} = \left(X_1^{(i-1)}, \dots, X_{j-1}^{(i-1)}, X_j', X_{j+1}^{(i-1)}, \dots, X_d^{(i-1)}\right)$

   subsititue to the new sample: we will use the sampled node to update our data

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

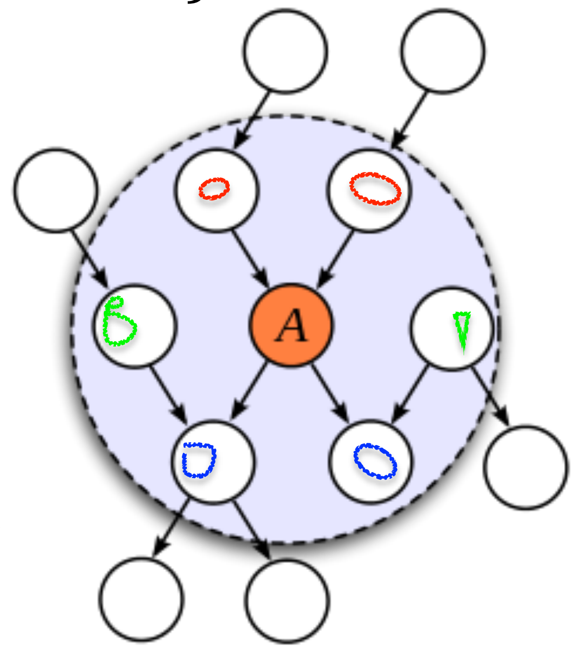
  E represnets the evidence nodes, their values are observed and fixed

- 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)

  conditional distribution is easier to obtain than joint dis

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 $B \subseteq N \setminus \{i\}$ such that…
  * X_i independent of $\mathbf{X}_{\bar{B}\setminus\{i\}}$ 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
  * $p\big(X_i \mid \mathrm{MB}(X_i)\big) \propto p\big(X_i \mid X_{\pi_i}\big) \prod_{k: i \in \pi_k} p\big(X_k \mid X_{\pi_k}\big)$



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if we find markov blanket: we find the conditional prob of Xi and we can use gibbs sampling

Markov Chain Monte Carlo (MCMC)

key advantage: we don't reject any sample in gibbs sampling

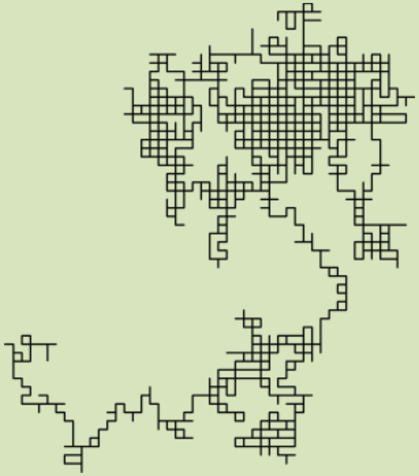
- Gibbs sampling produces a chain of samples $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots$ *approximating* draws from $p(\mathbf{X}_{\bar{E}} | \mathbf{X}_E = \mathbf{x}_E)$

- 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

MCMC can start with any sample will always converge to the sample we desired

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

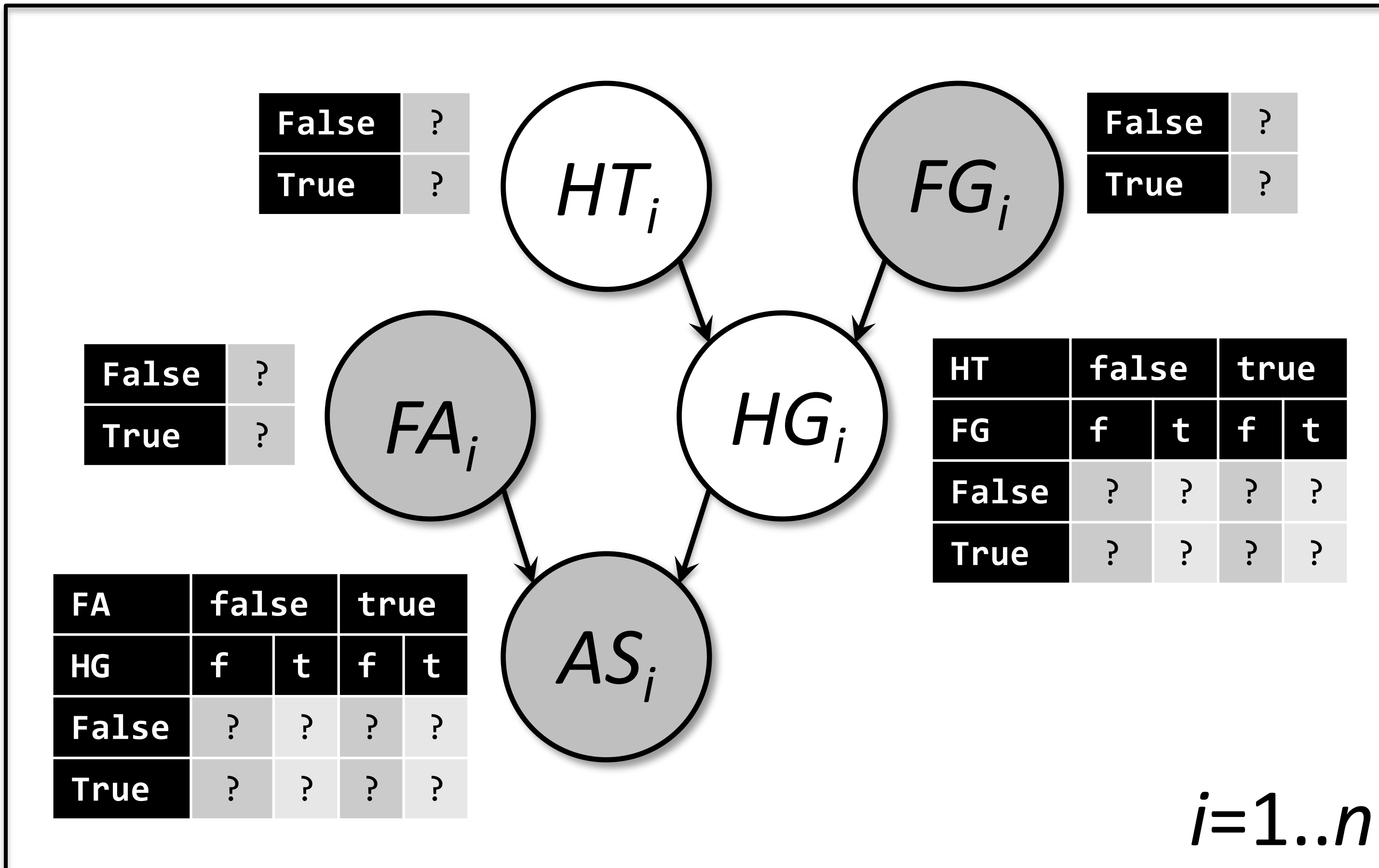
- Why? Summation/integration may be costly
- Why? Integration may be impossible analytically
- Briefly: Gibbs sampling

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	?

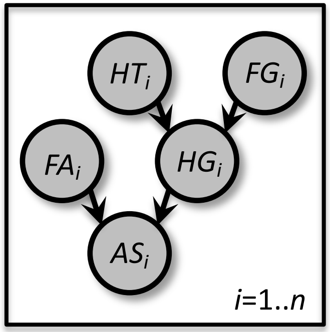
False	?
True	?

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

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

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

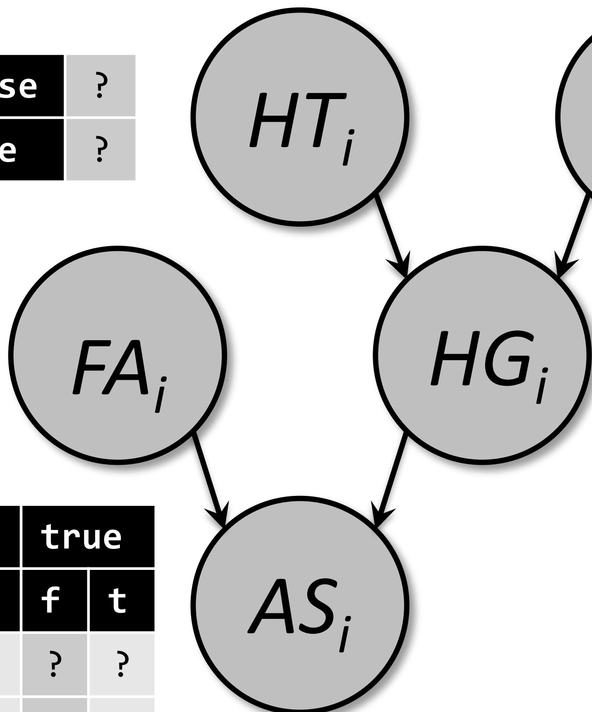
$$\arg\max_{\theta\in\Theta} \sum_{i=1}^{n} \sum_j \log p\left(X^j = x_i^j | X^{parents(j)} = x_i{}^{parents(j)}\right)$$

  - 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	?

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

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

false	?
true	?

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

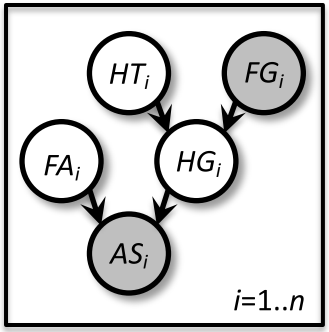
FA	false		true	
HG	f	t	f	t
false	?	?	?	?
true	?	?	?	?

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