## COMP90051 Statistical Machine Learning

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22. PGM Probabilistic Inference


## 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
* $\operatorname{Pr}\left(Y \mid X_{1}, \ldots, X_{d}\right)=\frac{\operatorname{Pr}\left(Y, X_{1}, \ldots, X_{d}\right)}{\operatorname{Pr}\left(X_{1}, \ldots, X_{d}\right)}=\frac{\operatorname{Pr}\left(Y, X_{1}, \ldots, X_{d}\right)}{\sum_{y} \operatorname{Pr}\left(Y=y, X_{1}, \ldots, X_{d}\right)}$
- Data $X \mid \theta \sim N(\theta, 1)$ with prior $\theta \sim N(0,1)$ (Bayesian)
* Given observation $X=x$ update posterior
* $\operatorname{Pr}(\theta \mid X)=\frac{\operatorname{Pr}(\theta, X)}{\operatorname{Pr}(X)}=\frac{\operatorname{Pr}(\theta, X)}{\sum_{\theta} \operatorname{Pr}(\theta, X)}$
- Joint + Bayes rule + marginalisation $\rightarrow$ anything



## Nuclear power plant

- Alarm sounds; meltdown?!
- $\operatorname{Pr}(H T \mid A S=t)=\frac{\operatorname{Pr}(H T, A S=t)}{\operatorname{Pr}(A S=t)}$

$$
=\frac{\sum_{F G, H G, F A} \operatorname{Pr}(A S=t, F A, H G, F G, H T)}{\sum_{F G, H G, F A, H T^{\prime}} \operatorname{Pr}\left(A S=t, F A, H R, F G, H T^{\prime}\right)}
$$



- Numerator (denominator similar)
expanding out sums, joint summing once over $2^{5}$ table

$$
=\sum_{F G} \sum_{H G} \sum_{F A} \operatorname{Pr}(H T) \operatorname{Pr}(H G \mid H T, F G) \operatorname{Pr}(F G) \operatorname{Pr}(A S=t \mid F A, H G) \operatorname{Pr}(F A)
$$

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

$$
=\operatorname{Pr}(H T) \sum_{F G} \operatorname{Pr}(F G) \sum_{H G} \operatorname{Pr}(H G \mid H T, F G) \sum_{F A} \operatorname{Pr}(F A) \operatorname{Pr}(A S=t \mid F A, H G)
$$

## 

$=\operatorname{Pr}(H T) \sum_{F G} \operatorname{Pr}(F G) \sum_{H G} \operatorname{Pr}(H G \mid H T, F G) \sum_{F A} \operatorname{Pr}(F A) \operatorname{Pr}(A S=t \mid F A, H G)$ eliminate $A S$ : since $A S$ observed, really a no-op
$=\operatorname{Pr}(H T) \sum_{F G} \operatorname{Pr}(F G) \sum_{H G} \operatorname{Pr}(H G \mid H T, F G) \sum_{F A} \operatorname{Pr}(F A) m_{A S}(F A, H G)$ eliminate $F A$ : multiplying $1 \times 2$ by $2 \times 2$
$=\operatorname{Pr}(H T) \sum_{F G} \operatorname{Pr}(F G) \sum_{H G} \operatorname{Pr}(H G \mid H T, F G) m_{F A}(H G)$ eliminate $H$ : multiplying $2 \times 2 \times 2$ by $2 \times 1$


$$
F
$$

## Elimination algorithm

Green background = Slide just for fun!

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 $\operatorname{Pr}\left(X_{i} \mid \operatorname{parents}\left(X_{i}\right)\right)$ to active
4. For each node $X_{i}$ in $E$
a) Append $\delta\left(X_{i}, x_{i}\right)$ to active
5. For each $i$ in $I$
a) potentials $=$ Remove tables referencing $X_{i}$ from active
b) $\quad N_{i}=$ nodes other than $X_{i}$ referenced by tables
c) Table $\phi_{i}\left(X_{i}, X_{N_{i}}\right)=$ product of tables
d) Table $m_{i}\left(X_{N_{i}}\right)=\sum_{X_{i}} \phi_{i}\left(X_{i}, X_{N_{i}}\right)$
e) Append $m_{i}\left(X_{N_{i}}\right)$ to active
6. Return $\operatorname{Pr}\left(X_{Q} \mid X_{E}=x_{E}\right)=\phi_{Q}\left(X_{Q}\right) / \sum_{X_{Q}} \phi_{Q}\left(X_{Q}\right)$

## Runtime of elimination algorithm



- Each step of elimination
* Removes a node
* Connects node's remaining neighbours
$\rightarrow$ 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


## Probabilistic inference by simulation

- Exact probabilistic inference can be expensive/impossible
- Can we approximate numerically?
- Idea: sampling methods
* Cheaply sample from desired distribution
* Approximate distribution by histogram of samples



## Monte Carlo approx probabilistic inference

- Algorithm: sample once from joint

1. Order nodes' parents before children (topological order)
2. Repeat
a) For each node $X_{i}$
i. Index into $\operatorname{Pr}\left(X_{i} \mid\right.$ parents $\left.\left(X_{i}\right)\right)$ with parents' values
ii. Sample $X_{i}$ from this distribution
b) Together $\boldsymbol{X}=\left(X_{1}, \ldots, X_{d}\right)$ is a sample from the joint


- Algorithm: sampling from $\operatorname{Pr}\left(X_{Q} \mid X_{E}=x_{E}\right)$

1. Order nodes' parents before children
2. Initialise set $S$ empty; Repeat
3. Sample $\boldsymbol{X}$ from joint
4. If $X_{E}=x_{E}$ then add $X_{Q}$ to $S$
5. Return: Histogram of $S$, normalising counts via divide by $|S|$

- Sampling++: Importance weighting, Gibbs, Metropolis-Hastings


## Alternate forms of probabilistic inference

- Elimination algorithm produces single marginal
- Sum-product algorithm on trees
* $2 x$ cost, supplies all marginals
* Name: Marginalisation is just sum of product of tables
* "Identical" variants: Max-product, for MAP estimation
- In general these are message-passing algorithms
* Can generalise beyond trees (beyond scope): junction tree algorithm, loopy belief propagation
- Variational Bayes: approximation via optimisation


## 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

