Lecture 18. PGM Representation

COMP90051 Statistical Machine Learning

Semester 1, 2021
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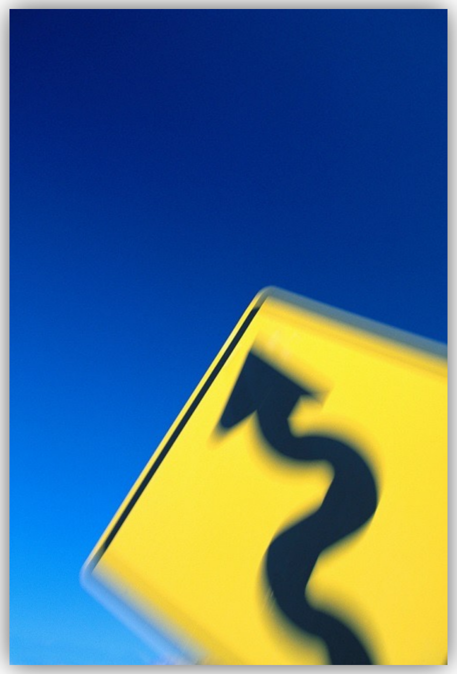
THE UNIVERSITY OF MELBOURNE

Next Lectures

- Representation of joint distributions
- Conditional/marginal independence
  * Directed vs undirected
- Probabilistic inference
  * Computing other distributions from joint
- Statistical inference
  * Learn parameters from (missing) data
- Examples



This lecture

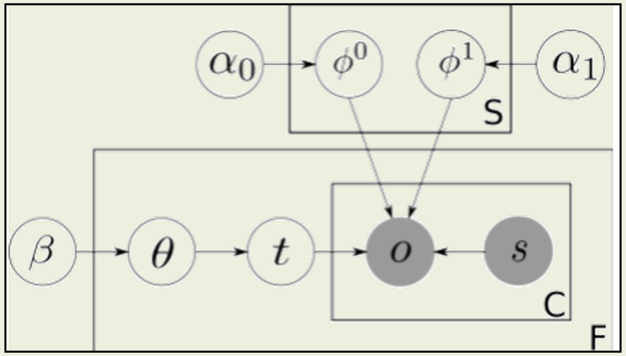
- (Directed) probabilistic graphical models
  * Motivations: applications, unifies algorithms
  * Motivation: ideal tool for Bayesians
  * Independence lowers computational/model complexity
    - Conditional independence
  * PGMs: compact representation of factorised joints
- Undirected PGMs and conversion from D-PGMs
- Example PGMs, applications

Probabilistic Graphical Models

Marriage of graph theory and probability theory.
Tool of choice for Bayesian statistical learning.

We'll stick with easier discrete case,
ideas generalise to continuous.

Motivation by practical importance



- **Many applications**
  - Phylogenetic trees
  - Pedigrees, Linkage analysis
  - Error-control codes
  - Speech recognition
  - Document topic models
  - Probabilistic parsing
  - Image segmentation
  - …
- **discovered algorithms**
  - HMMs
  - Kalman filters
  - Mixture models
  - LDA
  - MRFs
  - CRF
  - Logistic, linear regression
  - …

Motivation by way of comparison

Bayesian statistical learning

- Model joint distribution of X's,Y and parameter r.v.'s
  - "Priors": marginals on parameters
- Training: update prior to posterior using observed data
- Prediction: output posterior, or some function of it (MAP)

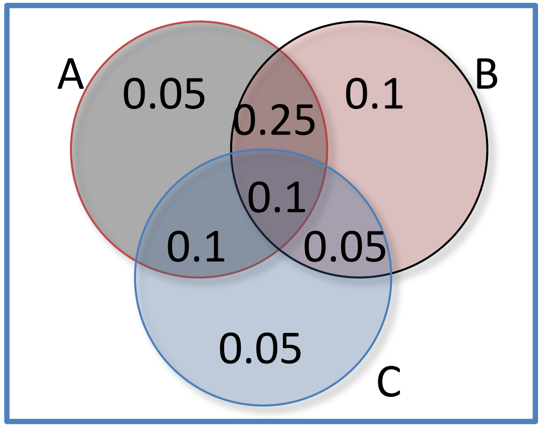
PGMs aka "Bayes Nets"

- Efficient joint representation
  - Independence made explicit
  - Trade-off between expressiveness and need for data, easy to make
  - Easy for practitioners to model
- Algorithms to fit parameters, compute marginals, posterior

Everything Starts at the Joint Distribution

- All joint distributions on discrete r.v.'s can be represented as tables
- #rows grows exponentially with #r.v.'s
- Example: Truth Tables
  - *M* Boolean r.v.'s require 2^M-1 rows
  - Table assigns probability per row

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	?



The Good: What we can do with the joint

- **Probabilistic inference** from joint on r.v.'s
  - Computing any other distributions involving our r.v.'s
- Pattern: want a distribution, have joint; use: Bayes rule + marginalisation
- Example: **naïve Bayes classifier**
  - Predict class y of instance $\boldsymbol{x}$ by maximising

$$\Pr(Y=y|\boldsymbol{X}=\boldsymbol{x}) = \frac{\Pr(Y=y,\boldsymbol{X}=\boldsymbol{x})}{\Pr(\boldsymbol{X}=\boldsymbol{x})} = \frac{\Pr(Y=y,\boldsymbol{X}=\boldsymbol{x})}{\sum_y \Pr(\boldsymbol{X}=\boldsymbol{x},Y=y)}$$

Recall: *integration (over parameters)* continuous equivalent of sum (both referred to as marginalisation)

The Bad & Ugly: Tables *waaaaay* too large*!!*

- **The Bad**: Computational complexity
  - Tables have exponential number of rows in number of r.v.'s
  - Therefore → poor space & time to marginalise
- **The Ugly**: Model complexity
  - Way too flexible
  - Way too many parameters to fit
    → need lots of data OR will overfit
- Antidote: assume independence!

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	?

Example: You're late!

- Modeling a tardy lecturer. Boolean r.v.'s
  - T: Trevor teaches the class (vs. guest)
  - S: It is sunny (o.w. bad weather)
  - L: The lecturer arrives late (o.w. on time)
- Assume: Trevor sometimes delayed by bad weather; Trevor more likely late than other lecturers
  - $\Pr(S|T) = \Pr(S)$, $\Pr(S) = 0.3$ $\Pr(T) = 0.6$
- Lateness not independent on weather, lecturer
  - Need $\Pr(L|T = t, S = s)$ for all combinations

$\Pr(L = true \mid \ldots)$		T: False	T: True
S	False	0.1	0.2
	True	0.05	0.1

- Need just 6 parameters

$P(S)\,P(T)\,P(L|T,S)$

Independence: not a dirty word

Lazy Lecturer Model	Model details	# params
Our model with S, T independence	$\Pr(S,T)$ factors to $\Pr(S)\Pr(T)$	2
	$\Pr(L\|T,S)$ modelled in full	4
Assumption-free model	$\Pr(L,T,S)$ modelled in full	7

- Independence assumptions
  - Can be reasonable in light of domain expertise
  - Allow us to factor → Key to tractable models

Factoring Joint Distributions

- Chain Rule: for any ordering of r.v.'s can always factor:

$$\Pr(X_1, X_2, \ldots, X_k) = \prod_{i=1}^{k} \Pr(X_i | X_{i+1}, \ldots, X_k)$$

- Model's independence assumptions correspond to
  - Dropping conditioning r.v.'s in the factors!
  - Example unconditional indep.: $\Pr(X_1 | X_2) = \Pr(X_1)$
  - Example conditional indep.: $\Pr(X_1 | X_2, X_3) = \Pr(X_1 | X_2)$
- Example: independent r.v.'s $\Pr(X_1, \ldots, X_k) = \prod_{i=1}^{k} \Pr(X_i)$
- Simpler factors: speed up inference and avoid overfitting

Mini Summary

- Joint distributions
- Probabilistic inference: Bayes rule & marginalisation
- Direct representation of joints
  - Probabilistic inference: Computationally costly
  - Statistical inference: Requires more data
- Factoring joints and conditional independence

Next: Directed probabilistic graphical models

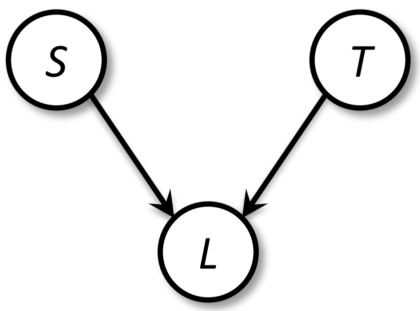
Directed PGM

- Nodes
- Edges (acyclic)

- Random variables
- Conditional dependence
  - Node table: $\Pr(child|parents)$
  - Child directly depends on parents
- Joint factorisation

$$\Pr(X_1, X_2, \dots, X_k) = \prod_{i=1}^{k} \Pr\left(X_i | X_j \in parents(X_i)\right)$$

Tardy Lecturer Example

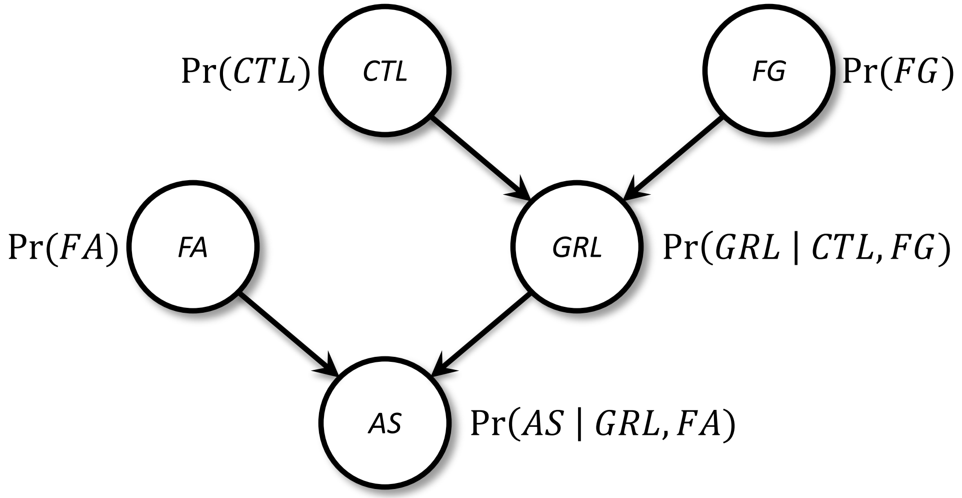


$\Pr(S)$ $\Pr(T)$

$\Pr(L|S,T)$

Example: Nuclear power plant

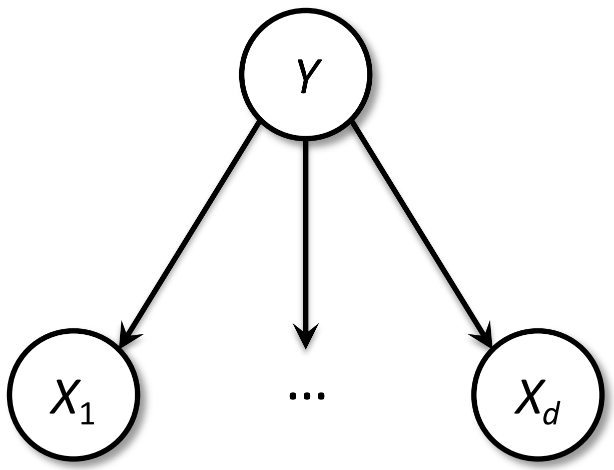
- Core temperature
  → Temperature Gauge
  → Alarm
- Model uncertainty in monitoring failure
  * GRL: gauge reads low
  * CTL: core temperature low
  * FG: faulty gauge
  * FA: faulty alarm
  * AS: alarm sounds
- PGMs to the rescue!



Joint $\Pr(CTL, FG, FA, GRL, AS)$ given by

$$\Pr(AS|FA, GRL) \Pr(FA) \Pr(GRL|CTL, FG) \Pr(CTL) \Pr(FG)$$

Naïve Bayes



$Y \sim \text{Bernoulli}(\theta)$

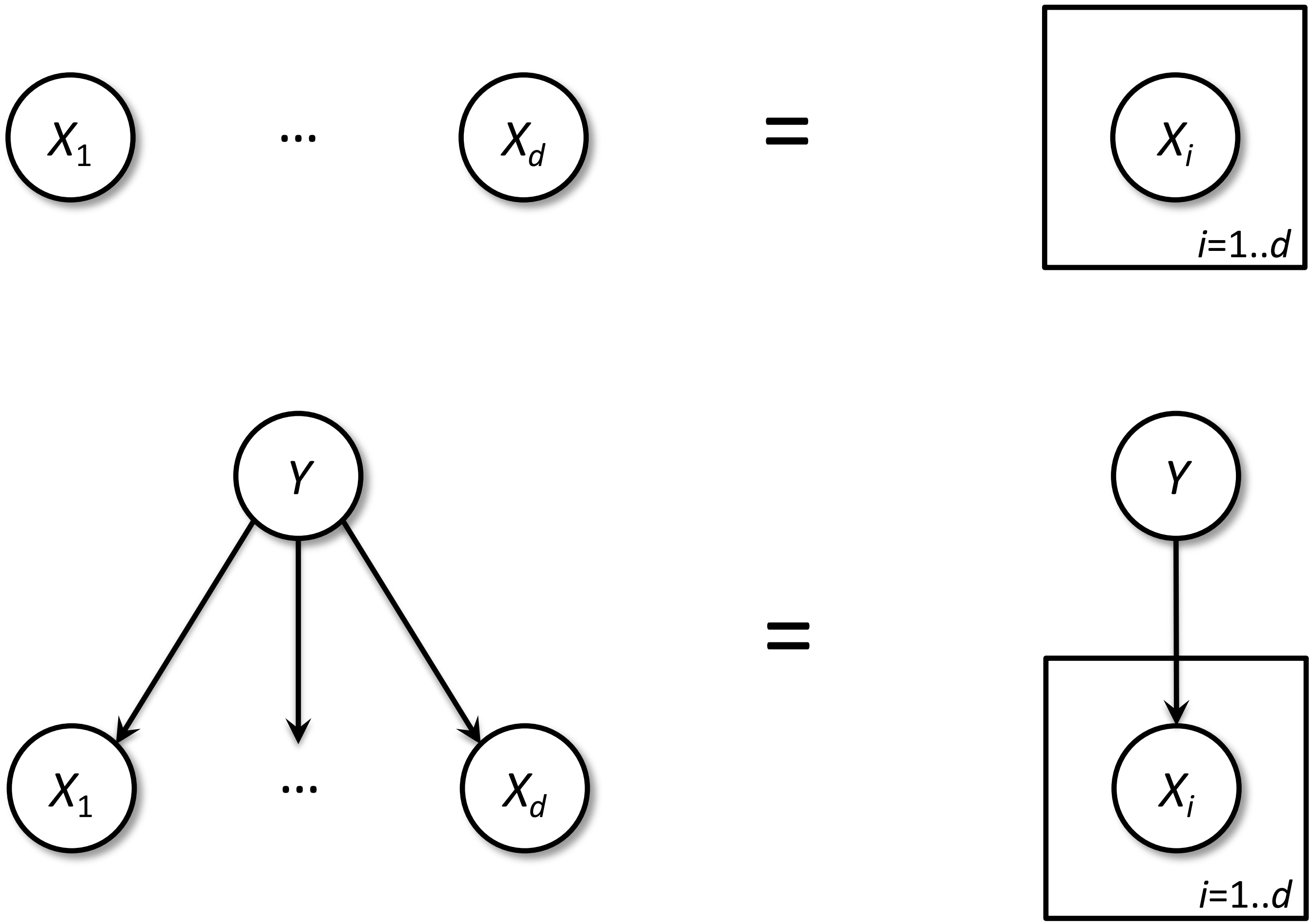
Aside: Bernoulli is just Binomial with count=1

$X_j | Y \sim \text{Bernoulli}(\theta_{j,Y})$

$$\begin{aligned}
&\Pr(Y, X_1, \ldots, X_d) \\
&\quad = \Pr(X_1, \ldots, X_d, Y) \\
&\quad = \Pr(X_1|Y) \Pr(X_2|X_1, Y) \ldots \Pr(X_d|X_1, \ldots, X_{d-1}, Y) \Pr(Y) \\
&\quad = \Pr(X_1|Y) \Pr(X_2|Y) \ldots \Pr(X_d|Y) \Pr(Y)
\end{aligned}$$

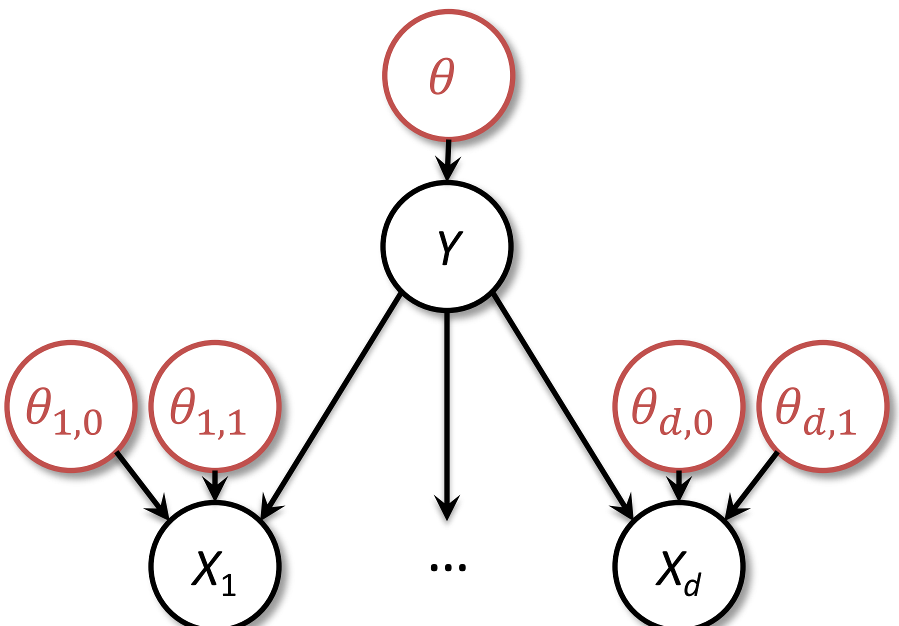
Prediction: predict label maximising $\Pr(Y|X_1, \ldots, X_d)$

Short-hand for repeats: Plate notation



PGMs: frequentist OR Bayesian…

- PGMs represent joints, which are central to Bayes
- Catch is that Bayesians add: node per parameters, with table being the parameter's prior



$Y \sim \text{Bernoulli}(\theta)$

$X_j|Y \sim \text{Bernoulli}(\theta_{j,Y})$

$\theta's \sim Beta$

Mini Summary

Directed probabilistic graphical models (D-PGMs)

- Definition as graph and conditionals
- Definition as joint distribution factorisation
- Plate notation
- Bayesian D-PGMs

Next: Undirected probabilistic graphical models

Undirected PGMs

Undirected variant of PGM, parameterised by arbitrary positive valued functions of the variables, and global normalisation.

A.k.a. Markov Random Field.

Undirected vs directed

Undirected PGM

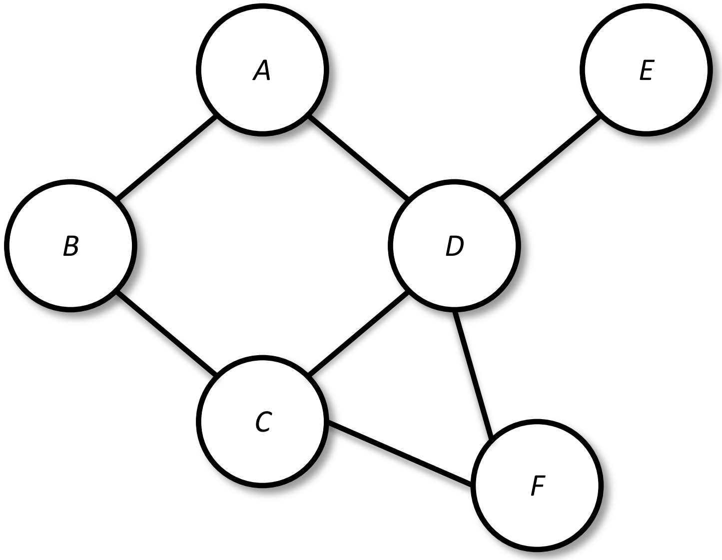
- Graph
  - Edges undirected
- Probability
  - Each node a r.v.
  - Each clique C has "factor" $\psi_C\left(X_j : j \in C\right) \geq 0$
  - Joint $\propto$ product of factors

Directed PGM

- Graph
  - Edged directed
- Probability
  - Each node a r.v.
  - Each node has conditional $p\left(X_i | X_j \in parents(X_i)\right)$
  - Joint $=$ product of cond'ls

Key difference = normalisation

Undirected PGM formulation



- Based on notion of
  - *Clique: a set of fully connected nodes (e.g., A-D, C-D, C-D-F)*
  - *Maximal clique: largest cliques in graph (not C-D, due to C-D-F)*
- Joint probability defined as

$$P(a,b,c,d,e,f) = \frac{1}{Z}\psi_1(a,b)\psi_2(b,c)\psi_3(a,d)\psi_4(d,c,f)\psi_5(d,e)$$

  - where each ψ is a positive function and Z is the normalising **'partition' function**

$$Z = \sum_{a,b,c,d,e,f} \psi_1(a,b)\psi_2(b,c)\psi_3(a,d)\psi_4(d,c,f)\psi_5(d,e)$$

Directed to undirected

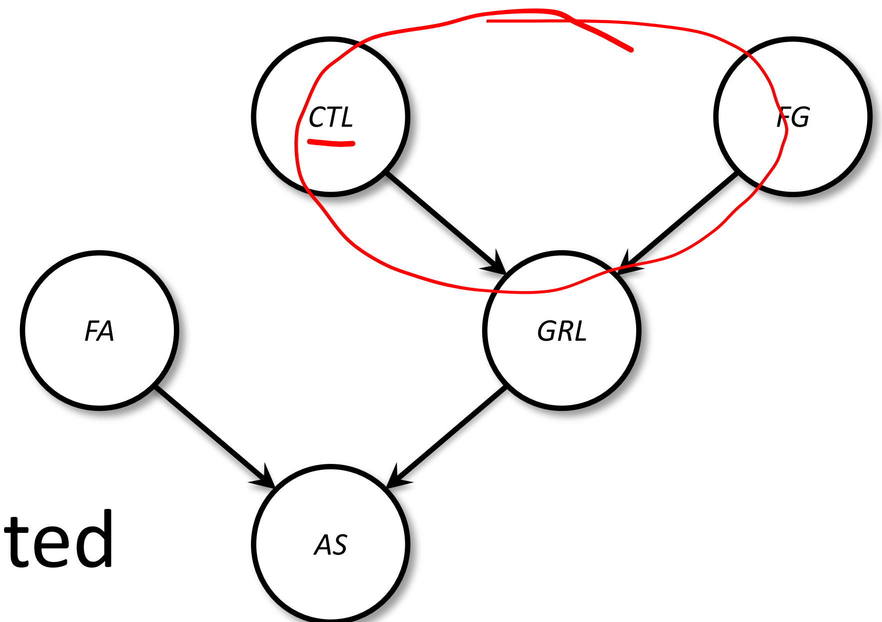
- Directed PGM formulated as

$$P(X_1, X_2, \ldots, X_k) = \prod_{i=1}^{k} Pr(X_i | X_{\pi_i})$$

where **π** indexes parents.

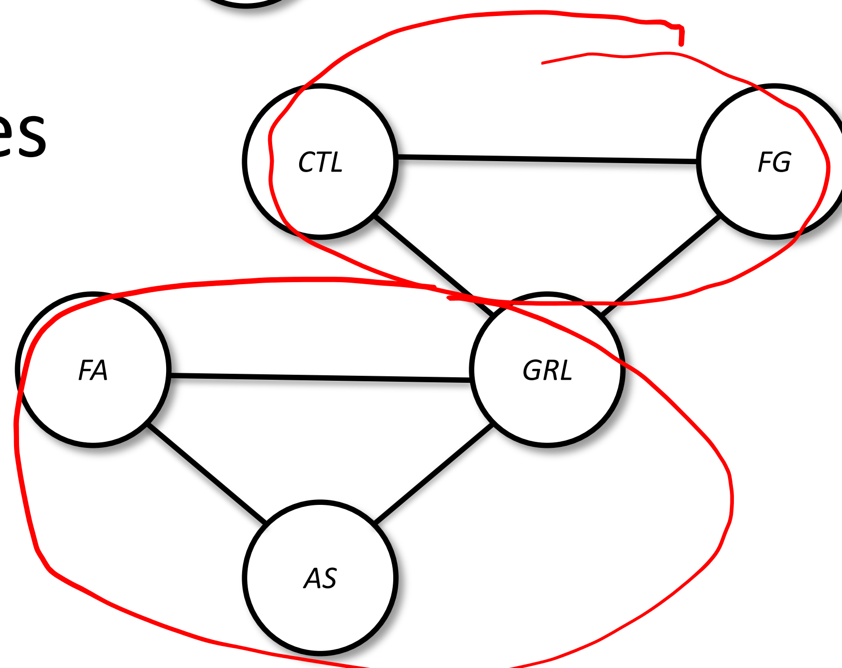
- Equivalent to U-PGM with
  - each conditional probability term is included in one factor function, ψ_c
  - clique structure links *groups of variables,* i.e., $\{\{X_i\} \cup X_{\pi_i}, \forall i\}$
  - normalisation term trivial, Z = 1

$P(GRL \mid CTL, FG)$



1. copy nodes
2. copy edges, undirected
3. 'moralise' parent nodes

$\psi(CTL, FG, GRL)$



Why U-PGM?

- Pros
  - generalisation of D-PGM
  - simpler means of modelling without the need for per-factor normalisation
  - general inference algorithms use U-PGM representation (supporting both types of PGM)
- Cons
  - (slightly) weaker independence
  - calculating global normalisation term (Z) intractable in general (but tractable for chains/trees, e.g., CRFs)

Mini Summary

Undirected probabilistic graphical models (U-PGMs)

- Definition
- Conversion to D-PGMs
- Pros/Cons over D-PGMs

Next: Examples and applications of PGMs
(deferred to lecture 19)

Summary

- Probabilistic graphical models
  - Motivation: applications, unifies algorithms
  - Motivation: ideal tool for Bayesians
  - Independence lowers computational/model complexity
  - PGMs: compact representation of factorised joints
  - U-PGMs

Next time: ~~elimination for probabilistic inference~~
Independence semantics + example PGMs, applications