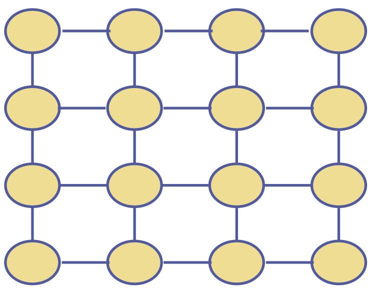
Machine Learning

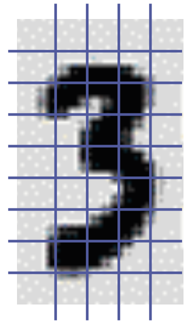
Topic 16

- Undirected Graphs
- Undirected Separation
- Inferring Marginals & Conditionals
- Moralization
- Junction Trees
- Triangulation

Undirected Graphs

- Separation is *much easier* for undirected graphs
- But, what are undirected graphs and why use them?
- Might be hard to call vars parent/child or cause/effect
- Example: Image pixels
- Each pixel is Bernoulli = {0,1}
- Where 0=dark, 1=bright

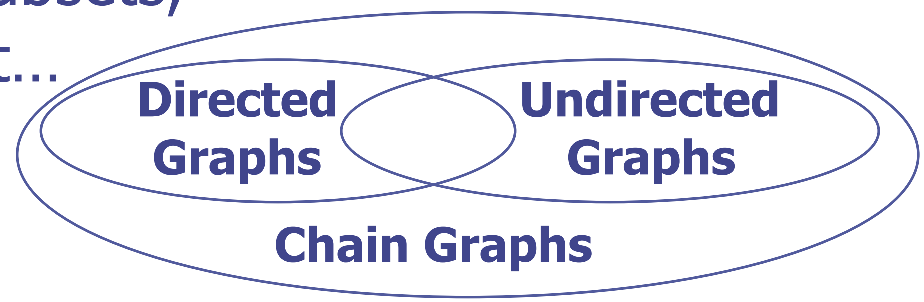




- Have probability over all pixels $p\left(x_{11},\ldots,x_{1M},\ldots,x_{M1},\ldots,x_{MM}\right)$
- Bright pixels have Bright neighbors
- Nearby pixels dependent, so connect with links
- Get a graphical model that looks like a grid
- But who is parent? No parents really, just probability
- Grid models are called Markov Random Fields
- Used in vision, physics (lattice, spin, or Ising models), etc.

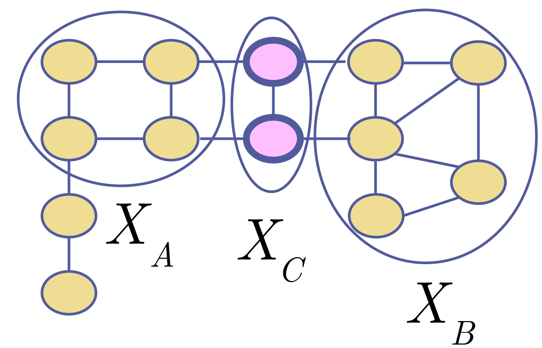
Undirected Graphs

- Undirected & directed not subsets,
- Chain Graphs are a superset…
- Some distributions behave as undirected graphs, some as directed, some as both

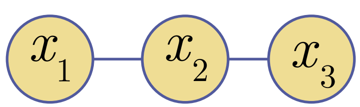


- Undirected graphs use the standard definition of separation:

  an undirected graph says that $p(x_1,\ldots,x_M)$ satisfies any statement $X_A \perp\!\!\!\perp X_B \mid X_C$ if no paths can go from X_A to X_B unless they go through X_C



- Thus, undirected graphs obey the general Markov property
- Recall the simple Markov property



$$x_1 \perp\!\!\!\perp x_3 \mid x_2 \Rightarrow p(x_1 \mid x_2, x_3) = p(x_1 \mid x_2)$$

Hammersley Clifford Theorem

Theorem[HC]: any distribution that obeys the Markov property

$$p\left(x_i \mid X_{U\setminus i}\right) = p\left(x_i \mid X_{Ne(i)}\right) \quad \forall\, i \in U$$

can be written as a product of terms over all maximal cliques

$$p\left(X_U\right) = p\left(x_1,\ldots,x_M\right) = \tfrac{1}{Z}\prod_{c\in C}\psi_c\left(X_c\right)$$

Clique: a subset of nodes that are all pair-wise adjacent

Maximal clique: cannot add more variables and still be a clique

Each c is a maximal clique of variables X_c in the graph

C is the set of all maximal cliques

Undirected Graph Functions

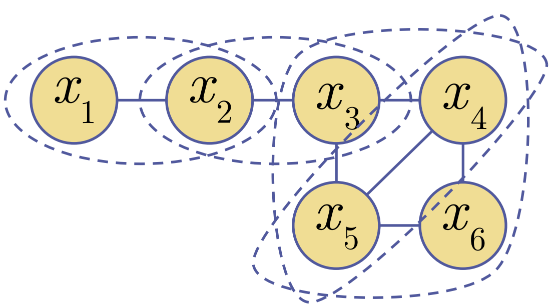
- Probability for undirected factorizes as a product of small non-negative Potential Functions over cliques in the graph

$$\boxed{p(X) = p(x_1,\ldots,x_M) = \tfrac{1}{Z}\prod_{c\in C}\psi_c(X_c)}$$

- Normalizing term $Z = \sum_X \prod_{c\in C}\psi_c(X_c)$ makes p(X) sum to 1
- Potentials ψ are non-negative un-normalized functions over cliques (subgroups of fully inter-connected variables)

- Use only maximal cliques since small ψ absorb into larger ψ

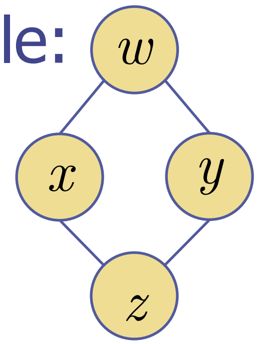
$$\psi(x_2,x_3)\psi(x_2) \to \psi(x_2,x_3) = \begin{bmatrix} 1 & 2 \\ 5 & 0 \end{bmatrix}$$



$$p(X) = \tfrac{1}{Z}\psi(x_1,x_2)\psi(x_2,x_3)\psi(x_3,x_4,x_5)\psi(x_4,x_5,x_6)$$

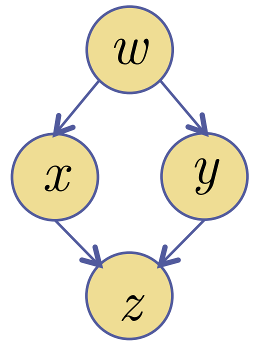
Undirected Separation Examples

- Example:



$$x \perp\!\!\!\perp y \mid \{w, z\}$$

$$w \perp\!\!\!\perp z \mid \{x, y\}$$

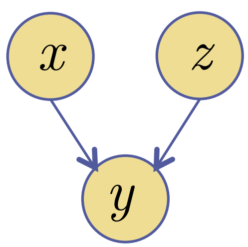


$$x \perp\!\!\!\perp y \mid \{w\}$$

$$x \not\perp\!\!\!\perp y \mid \{w, z\}$$

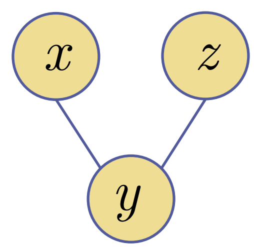
Directed can't do it!
Must be acyclic
Will have at least one
V structure and ball
goes through

- Example:



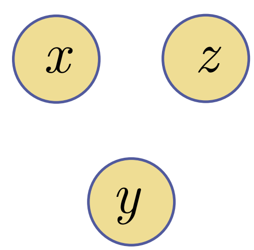
$$x \perp\!\!\!\perp z$$

$$x \not\perp\!\!\!\perp z \mid y$$



Undirected can't do it!

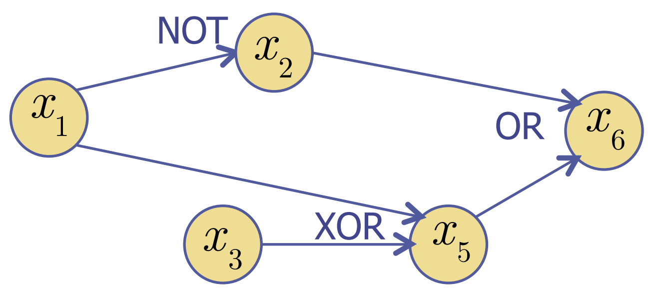
$$x \perp\!\!\!\perp z \mid y$$

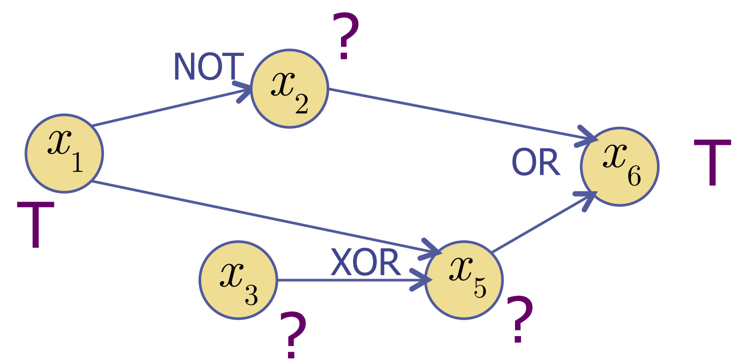


$$x \perp\!\!\!\perp z$$

Logical Inference

- Classic logic network: nodes are binary
- Arrows represent AND, OR, XOR, NAND, NOR, NOT etc.
- Inference: given observed binary variables, predict others

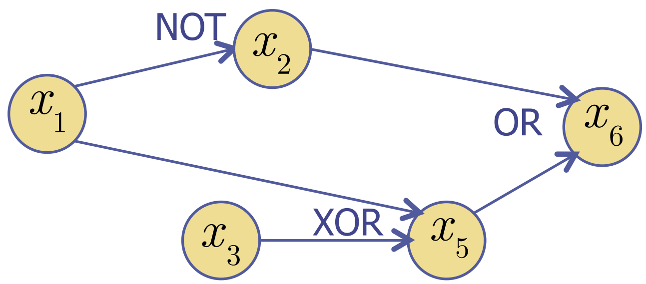




- Problems: uncertainty, conflicts and inconsistency
- Could get x_3=T and x_3=F following two different paths
- We need a way to enforce consistency and combine conflicting statements via probabilities and Bayes rule!

Probabilistic Inference

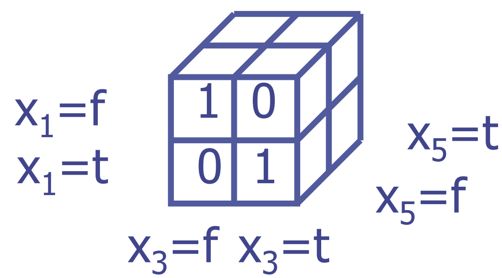
- Replace logic network with Bayesian network
- Tables represent AND, OR, XOR, NAND, NOR, NOT etc.
- Probabilistic Inference: given observed binary variables, predict marginals over others



NOT

	x_3=f	x_3=t
x_1=f	0	1
x_1=t	1	0

XOR



- Can also have soft versions of the functions

soft NOT

	x_3=f	x_3=t
x_1=f	.1	.9
x_1=t	.9	.1

Probabilistic Inference

- Two types of inference with a probability distribution:

$$p(X) = p(x_1, \ldots, x_M) \;\; with\ queries\ X_F \subseteq X \;\; given\ \ evidence\ X_E \subseteq X$$

- Marginal Inference:

$$p(X_F | X_E) = p(X_F, X_E) \big/ p(X_E) = \sum_{X \setminus X_F \cup X_E} p(X) \Big/ \sum_{X \setminus X_E} p(X)$$

or... $p(x_i | X_E) \;\; \forall \; x_i \in X_F$

- Maximum a posteriori (MAP) inference:

$$\arg\max_{X_F} \; p(X_F | X_E)$$

...for now we focus on marginal inference

Traditional Marginal Inference

- Marginal inference problem: given graph and probability function $p(X) = p(x_1, \ldots, x_M)$ for any subsets of variables find

$$p(X_F | X_E) = {p(X_F, X_E)} \Big/ {p(X_E)}$$

- So, we basically compute both marginals and divide
- But finding marginals can take exponential work!
- A problem for both directed & undirected graphs:

$$p(x_j, x_k) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_M} \prod_{i=1}^{M} p(x_i | \pi_i)$$
$$p(x_j, x_k) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_M} \tfrac{1}{Z} \prod_{c \in C} \psi_c(X_c)$$

- Graphs gave efficient storage, learning, Bayes Ball…
- Graphs can also be used to perform efficient inference!
- Junction Tree Algorithm: method to efficiently find marginals

Traditional Marginal Inference

- Example: brute force inference on a directed graph…
- Given a directed graph structure & *filled-in* CPTs
- We would like to efficiently compute arbitrary marginals
- Or we would like to compute arbitrary conditionals

$$p(X) = p(x_1)\,p(x_2 \mid x_1)\,p(x_3 \mid x_1)\,p(x_4 \mid x_2)\,p(x_5 \mid x_3)\,p(x_6 \mid x_2, x_5)$$

$$p(x_1, x_3) = p(x_1)\,p(x_3 \mid x_1)$$

$$p(x_1, x_6) = \sum_{x_2, x_3, x_4, x_5} p(x_1)\,p(x_2 \mid x_1)\,p(x_3 \mid x_1)\,p(x_4 \mid x_2)\,p(x_5 \mid x_3)\,p(x_6 \mid x_2, x_5)$$

$$p(x_1 \mid x_6) = \sum\nolimits_{x_2, x_3, x_4, x_5} p(X) \Big/ \sum\nolimits_{x_1, x_2, x_3, x_4, x_5} p(X)$$

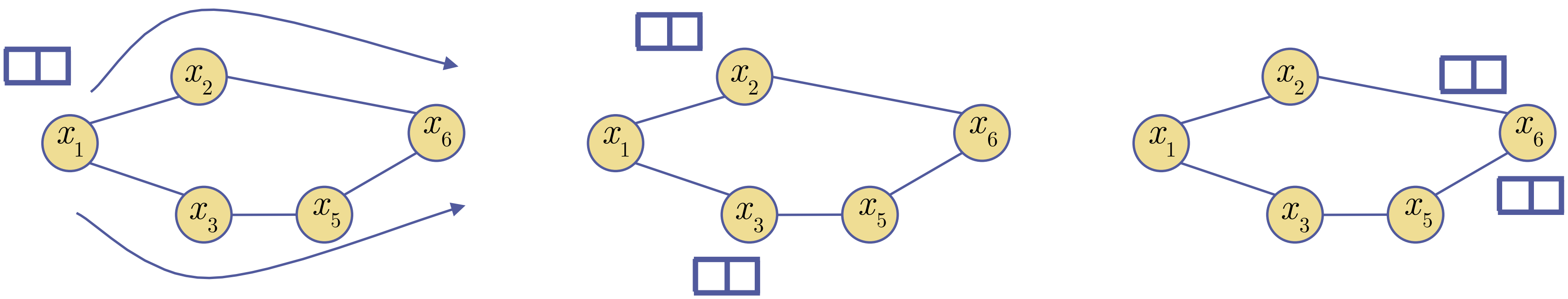
- For example, we may have some evidence, i.e. x_6=TRUE

$$p(x_1 \mid x_6 = TRUE) = \sum\nolimits_{x_2, x_3, x_4, x_5} p(X_{U \setminus 6}, x_6 = TRUE) \Big/ \sum\nolimits_{x_1, x_2, x_3, x_4, x_5} p(X_{U \setminus 6}, x_6 = TRUE)$$

- This is tedious & does not exploit the graph's efficiency

Efficient Marginals & Inference

- Another idea is to use some efficient graph algorithm
- Try sending messages (small tables) around the graph



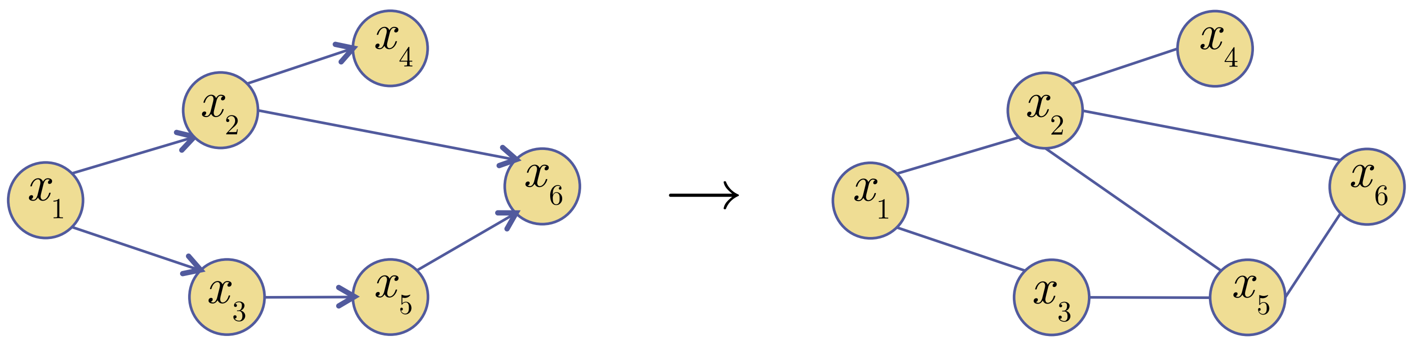
- Hopefully these somehow settle down and equal marginals

$$\hat{p}\left(x_1, x_6\right) = \sum_{x_2, x_3, x_4, x_5} p\left(X\right)$$

- AND marginals are self-consistent $\sum_{x_1} \hat{p}\left(x_1, x_6\right) = \sum_{x_2} \hat{p}\left(x_2, x_6\right)$
- Note: can't just return conditionals since they can be inconsistent $\sum_{x_1} \hat{p}\left(x_6 \mid x_1\right) \neq \sum_{x_2} \hat{p}\left(x_2 \mid x_6\right)$
- Junction Tree Algorithm must find consistent marginals

Junction Tree Algorithm

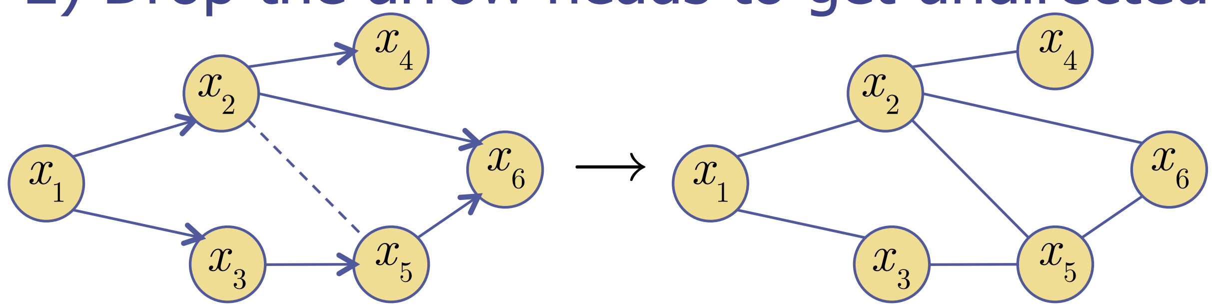
- An algorithm that achieves fast inference, by doing message passing on undirected graphs.
- We first convert a directed graph to an undirected one



- Then apply the efficient Junction Tree Algorithm:
  1) Moralization
  2) Introduce Evidence
  3) Triangulate
  4) Construct Junction Tree
  5) Propagate Probabilities (Junction Tree Algorithm)

Moralization

- Converts directed graph into undirected graph
- By moralization, marrying the parents:
  1) Connect nodes that have common children
  2) Drop the arrow heads to get undirected

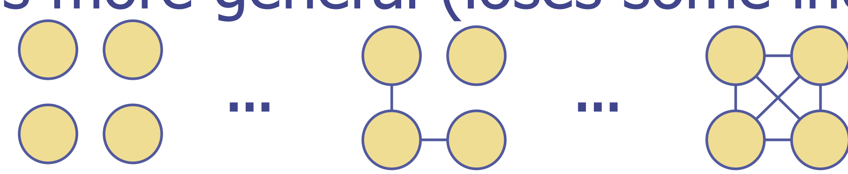


$$p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)p(x_5|x_3)p(x_6|x_2,x_5)$$
$$\rightarrow \tfrac{1}{Z}\psi(x_1,x_2)\psi(x_1,x_3)\psi(x_2,x_4)\psi(x_3,x_5)\psi(x_2,x_5,x_6)$$

$$p(x_1)p(x_2|x_1) \rightarrow \psi(x_1,x_2)$$
$$p(x_4|x_2) \rightarrow \psi(x_2,x_4)$$
$$Z \rightarrow 1$$

- Note: moralization resolves *coupling* due to marginalizing
- moral graph is more general (loses some independencies)

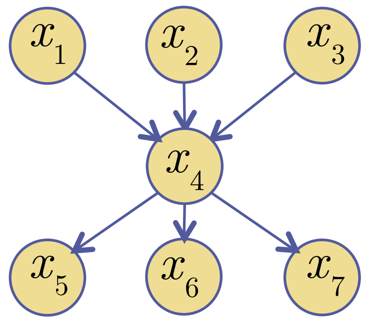
most specific



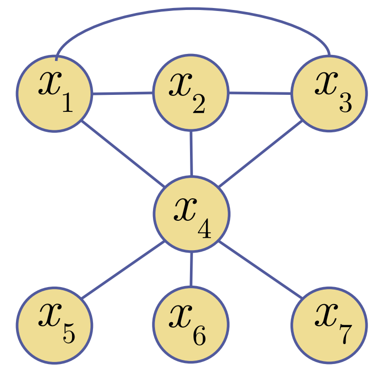
most general

Moralization

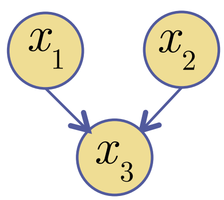
- More examples:



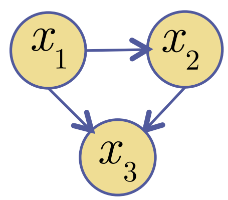
$\longrightarrow$



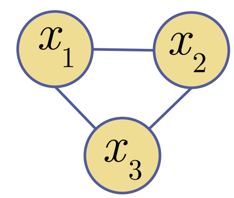
$$\longrightarrow \frac{1}{Z}\psi\left(x_1,x_2,x_3,x_4\right)\psi\left(x_4,x_5\right)\psi\left(x_4,x_6\right)\psi\left(x_4,x_7\right)$$



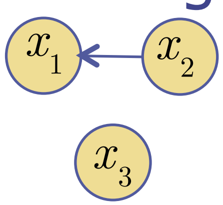
or



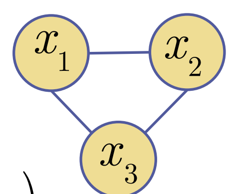
$\longrightarrow$



- More general graph less efficient but same inference:



$$p\left(x_1\right)=\sum_{x_2,x_3} p\left(x_1,x_2,x_3\right)$$
$$=\sum_{x_2,x_3} p\left(x_1 \mid x_2\right)p\left(x_2\right)p\left(x_3\right)$$
$$=\sum_{x_2} p\left(x_1 \mid x_2\right)p\left(x_2\right)$$

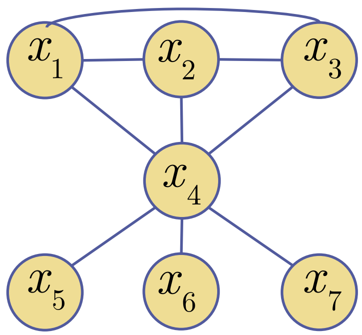


$$p\left(x_1\right)=\sum_{x_2,x_3} \frac{1}{Z}\psi\left(x_1,x_2,x_3\right)$$

same

Introducing Evidence

- Given moral graph, note what is observed $X_E \rightarrow \bar{X}_E$
  $$p\left(X_F \mid X_E = \bar{X}_E\right) \equiv p\left(X_F \mid \bar{X}_E\right)$$
- If we know this is *always* observed at $X_E \rightarrow \bar{X}_E$, simplify…
- Reduce the probability function since those X_E fixed
- Only keep probability function over remaining nodes X_F
- Only get marginals and conditionals with subsets of X_F



$$p\left(X\right) = \tfrac{1}{Z}\psi\left(x_1,x_2,x_3,x_4\right)\psi\left(x_4,x_5\right)\psi\left(x_4,x_6\right)\psi\left(x_4,x_7\right)$$

$$say\ X_E = \left\{x_3,x_4\right\} \rightarrow \bar{X}_E = \left\{\bar{x}_3,\bar{x}_4\right\}$$

Replace potential functions with slices

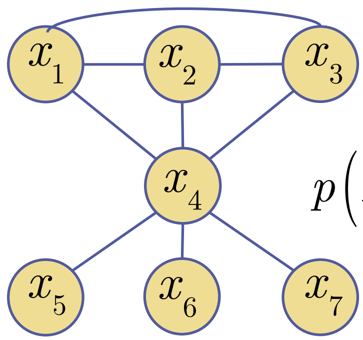
0.3	0.13
0.12	0.1

$$p\left(X_F \mid \bar{X}_E\right) \propto \tfrac{1}{Z}\psi\left(x_1,x_2,x_3=\bar{x}_3,x_4=\bar{x}_4\right)\psi\left(x_4=\bar{x}_4,x_5\right)\psi\left(x_4=\bar{x}_4,x_6\right)\psi\left(x_4=\bar{x}_4,x_7\right)$$
$$\propto \tfrac{1}{Z}\tilde{\psi}\left(x_1,x_2\right)\tilde{\psi}\left(x_5\right)\tilde{\psi}\left(x_6\right)\tilde{\psi}\left(x_7\right)$$

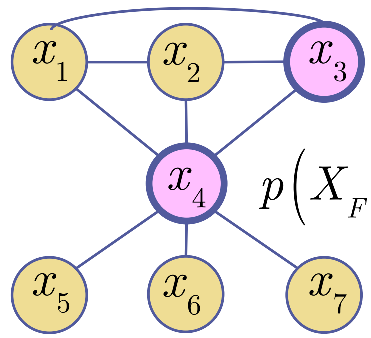
But, need to recompute different normalization Z…

Introducing Evidence

- Recall undirected separation, observing X_E separates others



$$p\left(X_F, X_E\right)$$



$$p\left(X_F \mid \bar{X}_E\right)$$

- But, need to recompute new normalization …

$$p\left(X_F \mid \bar{X}_E\right) \propto \frac{1}{Z} \tilde{\psi}\left(x_1, x_2\right) \tilde{\psi}\left(x_5\right) \tilde{\psi}\left(x_6\right) \tilde{\psi}\left(x_7\right)$$

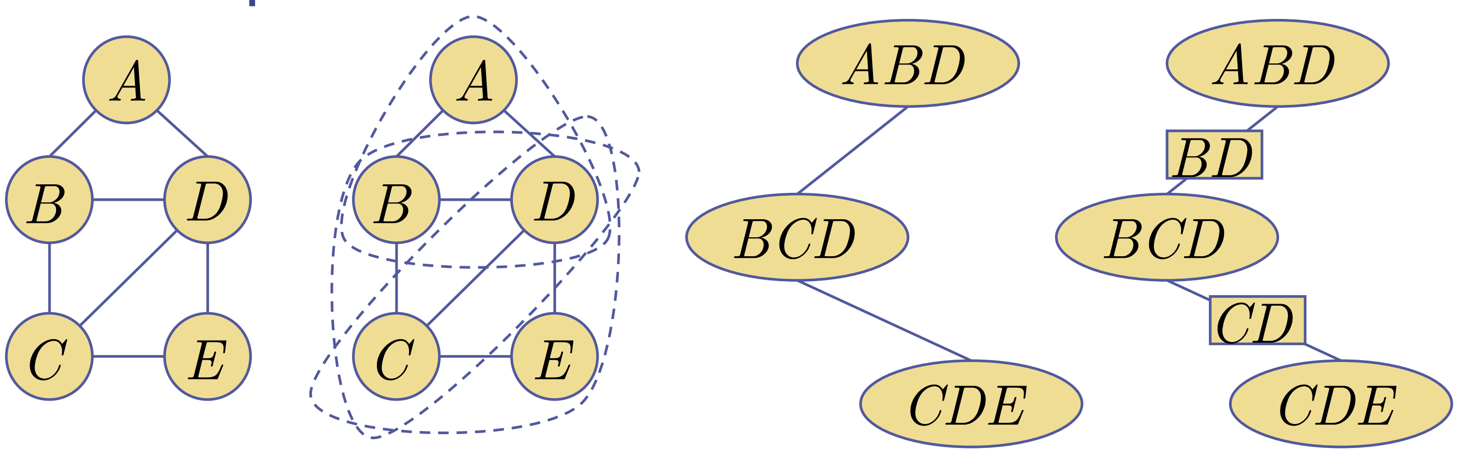
$$\tilde{p}\left(X_F\right) = \frac{1}{\tilde{Z}} \tilde{\psi}\left(x_1, x_2\right) \tilde{\psi}\left(x_5\right) \tilde{\psi}\left(x_6\right) \tilde{\psi}\left(x_7\right)$$

- Just avoid Z & normalize at the end when we are querying individual marginals and conditionals as subsets of X_F

$$\tilde{p}\left(x_2\right) = \frac{\sum_{x_1, x_5, x_6, x_7} \tilde{\psi}\left(x_1, x_2\right) \tilde{\psi}\left(x_5\right) \tilde{\psi}\left(x_6\right) \tilde{\psi}\left(x_7\right)}{\sum_{x_2} \sum_{x_1, x_5, x_6, x_7} \tilde{\psi}\left(x_1, x_2\right) \tilde{\psi}\left(x_5\right) \tilde{\psi}\left(x_6\right) \tilde{\psi}\left(x_7\right)}$$

Junction Trees

- Given moral graph want to build Junction Tree:
  - each node is a clique (ψ) of variables in moral graph
  - edges connect cliques of the potential functions
  - unique path between nodes & root node (tree)
  - between adjacent clique nodes, create separators (ϕ)
  - separator nodes contain intersection of variables



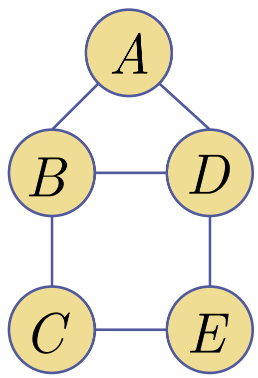
$$\psi(A,B,D)$$
$$\phi(B,D)$$
$$\psi(B,C,D)$$
$$\phi(C,D)$$
$$\psi(C,D,E)$$

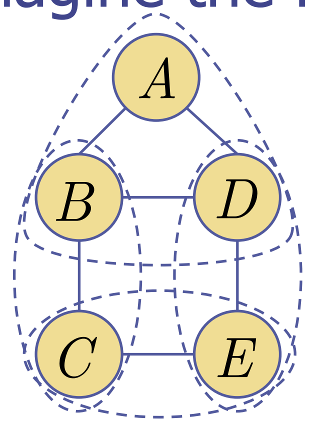
undirected **cliques** **clique tree** **junction tree**

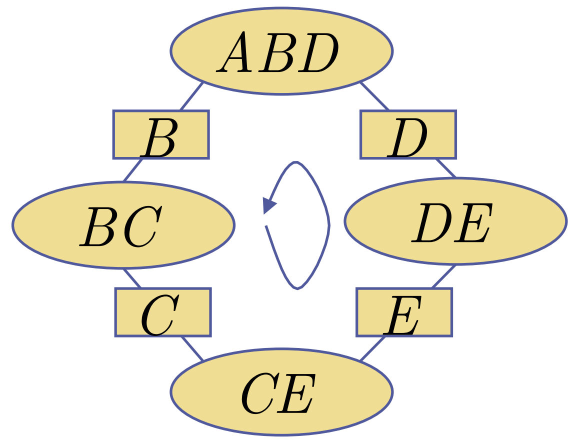
$$p(X) = \tfrac{1}{Z}\psi(A,B,D)\psi(B,C,D)\psi(C,D,E)$$

Triangulation

- Problem: imagine the following undirected graph



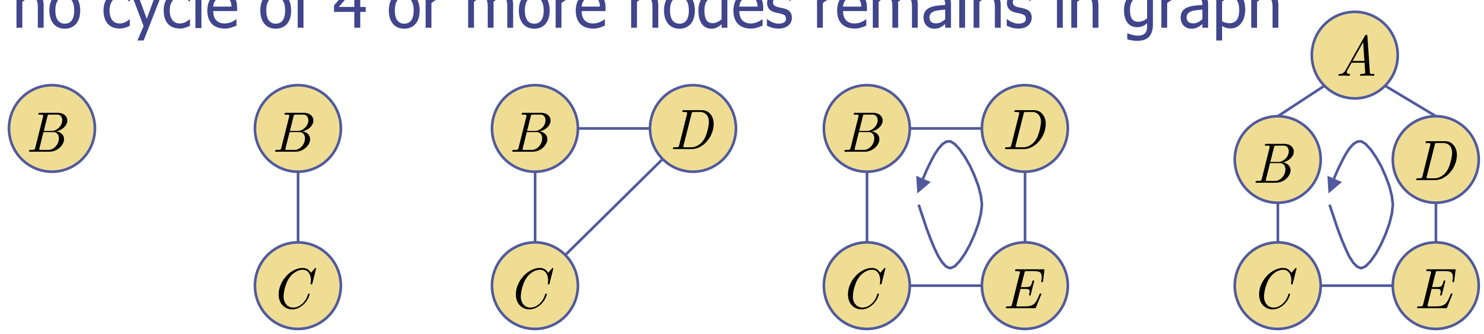




- Not a Tree!
- To ensure Junction Tree is a tree (no loops, etc.) before forming it must first Triangulate moral graph before finding the cliques…
- Triangulating gives more general graph (like moralization)
- Adds links to get rid of cycles or loops
- Triangulation: Connect nodes in moral graph until no chordless cycle of 4 or more nodes remains in the graph

Triangulation

- Triangulation: Connect nodes in moral graph such that no cycle of 4 or more nodes remains in graph

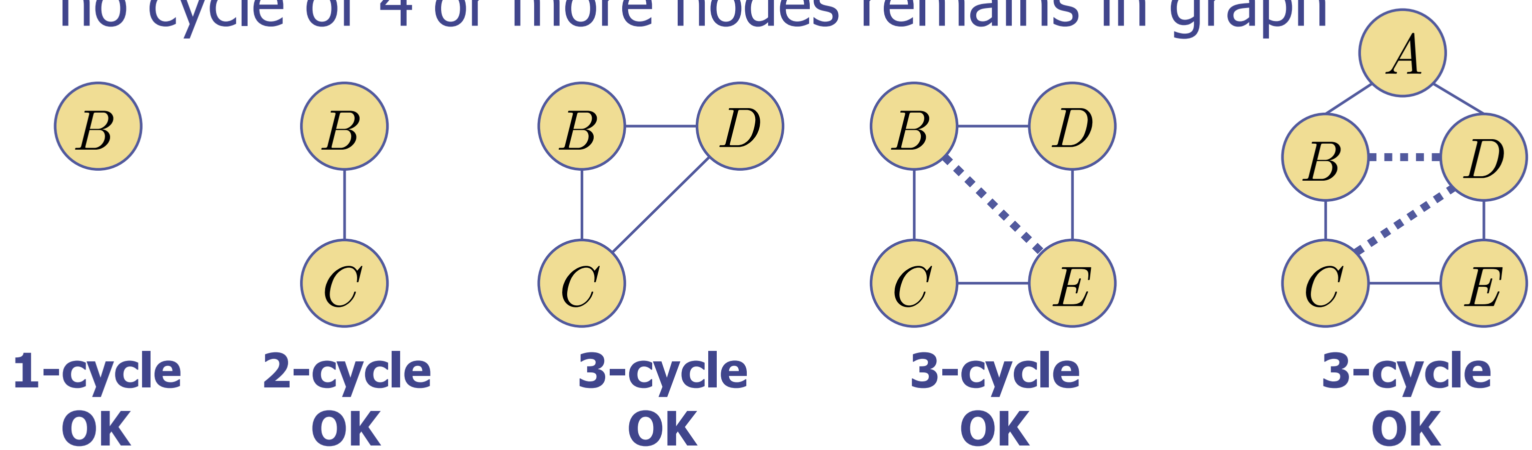


1-cycle OK **2-cycle OK** **3-cycle OK** **4-cycle BAD** **5-cycle BAD**

- So, *add links*, but many possible choices…
- HINT: Try to keep largest clique size small (makes junction tree algorithm more efficient)
- Sub-optimal triangulations of moral graph are Polynomial
- Triangulation that minimizes largest clique size is NP
- But, OK to use a suboptimal triangulation (slower JTA…)

Triangulation

- Triangulation: Connect nodes in moral graph such that no cycle of 4 or more nodes remains in graph



- So, *add links*, but many possible choices…
- HINT: Try to keep largest clique size small (makes junction tree algorithm more efficient)
- Sub-optimal triangulations of moral graph are Polynomial
- Triangulation that minimizes largest clique size is NP
- But, OK to use a suboptimal triangulation (slower JTA…)