

Probabilistic Graphical Models

Variable elimination

Siamak Ravanbakhsh

Fall 2019

Learning objective

- an intuition for inference in graphical models
- why is it difficult?
- exact inference by variable elimination

Probability query

marginalization

$$P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$$

Introducing **evidence** leads to *a similar* problem

$$P(X_1 = x_1 \mid X_m = x_m) = \frac{P(X_1 = x_1, X_m = x_m)}{P(X_m = x_m)}$$

Probability query

marginalization

$$P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$$

Introducing **evidence** leads to *a similar* problem

$$P(X_1 = x_1 \mid X_m = x_m) = \frac{P(X_1 = x_1, X_m = x_m)}{P(X_m = x_m)}$$

MAP inference changes sum to max $\mathbf{x}^* = \arg \max_{\mathbf{x}} P(\mathbf{X} = \mathbf{x})$

maximum a posteriori

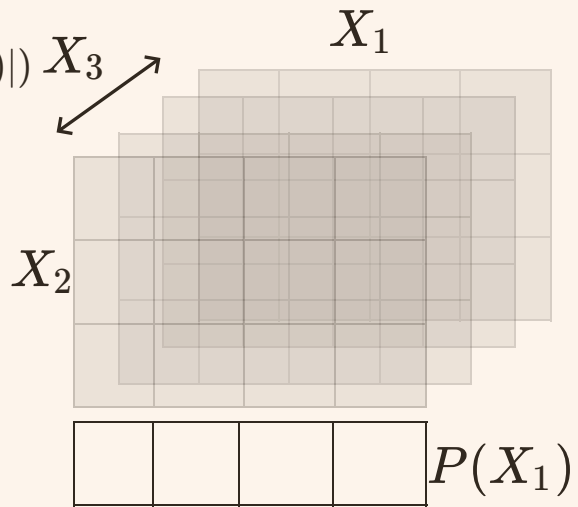
Probability query

marginalization $P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$

$n = 3$

representation: $\mathcal{O}(|Val(X_1) \times Val(X_2) \times Val(X_3)|)$

inference: $\mathcal{O}(|Val(X_1) \times Val(X_2) \times Val(X_3)|)$



Probability query

marginalization $P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$

complexity of **representation & inference** $\mathcal{O}(\prod_i |Val(X_i)|)$

- binary variables $\mathcal{O}(2^n)$

Probability query

marginalization $P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$

complexity of **representation & inference** $\mathcal{O}(\prod_i |Val(X_i)|)$

- binary variables $\mathcal{O}(2^n)$

can have a **compact representation** of P:

- Bayes-net or Markov net
 - e.g. $p(x) = \frac{1}{Z} \prod_{i=1}^{n-1} \phi_i(x_i, x_{i+1})$ has an $\mathcal{O}(n)$ representation

Probability query

marginalization $P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$

complexity of **representation & inference** $\mathcal{O}(\prod_i |Val(X_i)|)$

- binary variables $\mathcal{O}(2^n)$

can have a **compact representation** of P:

- Bayes-net or Markov net
 - e.g. $p(x) = \frac{1}{Z} \prod_{i=1}^{n-1} \phi_i(x_i, x_{i+1})$ has an $\mathcal{O}(n)$ representation

efficient inference ?

Complexity of inference

can we always avoid the exponential cost of inference? No!

can we at least guarantee a good approximation? No!

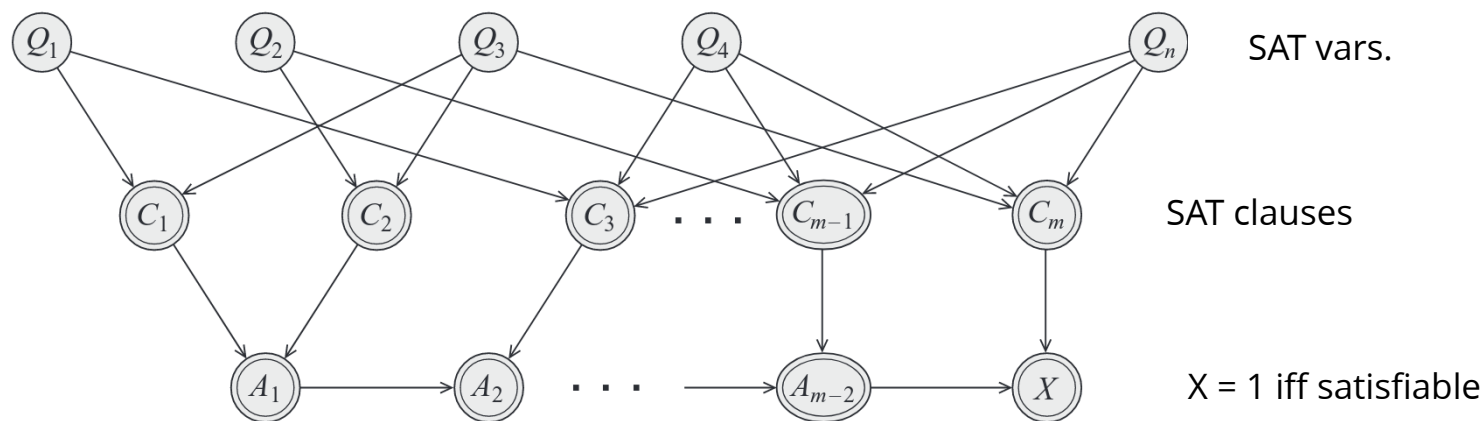
proof idea:

- reduce 3-SAT to inference in a graphical model
 - despite this, graphical models are used for combinatorial optimization (why?)

Complexity of inference: **proof**

given a BN, decide whether $P(X = x) > 0$ is **NP-complete**

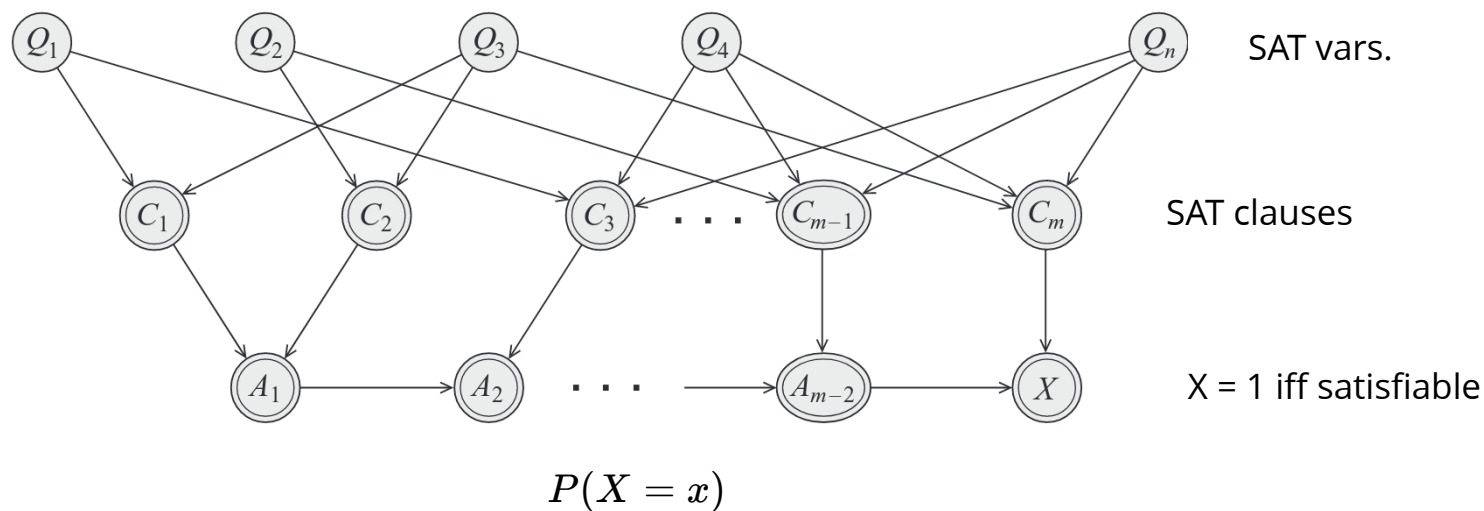
- belongs to **NP**
- **NP-hardness**: *answering this query \gg solving 3-SAT*



Complexity of inference: **proof**

given a BN, decide whether $P(X = x) > 0$ is **NP-complete**

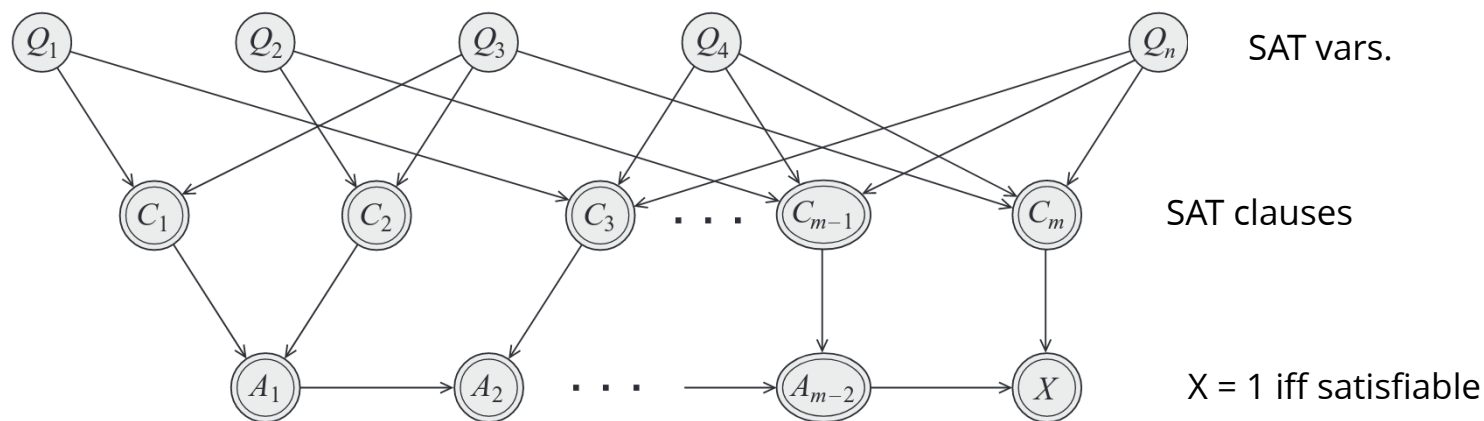
- belongs to **NP**
- **NP-hardness**: *answering this query \gg solving 3-SAT*



Complexity of inference: **proof**

given a BN, decide whether $P(X = x) > 0$ is **NP-complete**

- belongs to **NP**
- **NP-hardness**: *answering this query \gg solving 3-SAT*



given a BN, calculating $P(X = x)$ is **#P-complete**

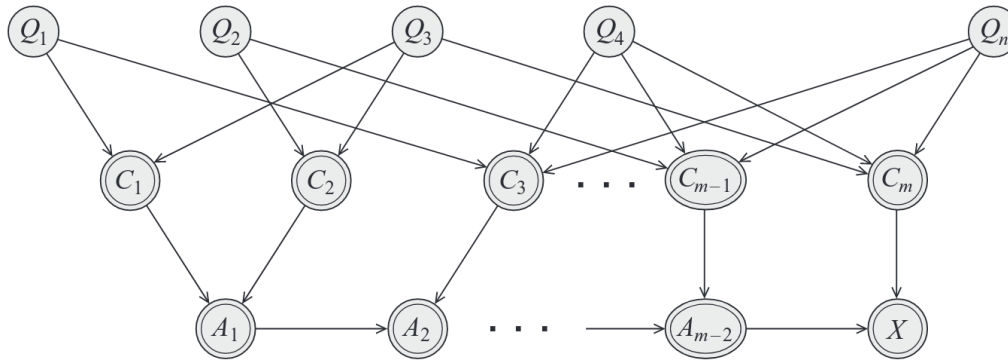
Complexity of **approximate** inference

given a BN, approximating $P(X = x)$ with a *relative error* ϵ is **NP-hard**

Proof: $\rho > 0 \Leftrightarrow P(X = 1) > 0$

$$\frac{\rho}{1+\epsilon} \leq P(X = x) \leq \rho(1 + \epsilon)$$

our approximation



Complexity of **approximate** inference

given a BN, approximating $P(X = x \mid E = e)$ with an *absolute error* ϵ

for any $0 < \epsilon < \frac{1}{2}$ is **NP-hard**

$$\rho(1 - \epsilon) \leq P(X = x) \leq \rho(1 + \epsilon)$$

Complexity of **approximate** inference

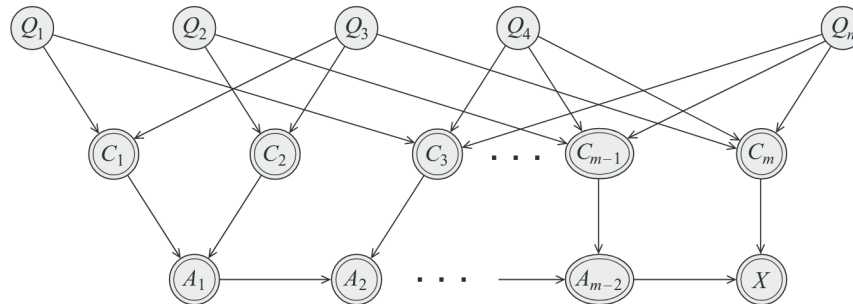
given a BN, approximating $P(X = x \mid E = e)$ with an *absolute error* ϵ

for any $0 < \epsilon < \frac{1}{2}$ is **NP-hard**

$$\rho(1 - \epsilon) \leq P(X = x) \leq \rho(1 + \epsilon)$$

Proof:

- *sequentially* fix $q_i^* = \arg \max_q P(Q_i = q \mid (Q_1, \dots, Q_{i-1}) = (q_1^* \dots q_{i-1}^*), X = 1)$
- either $q_i^0 > \frac{1}{2}$ or $q_i^1 > \frac{1}{2}$
- since $\epsilon < \frac{1}{2}$ this leads to a solution



so far...

- reduce the **representation-cost** using a graph structure
- **inference-cost** is in the worst case exponential
- can we reduce it using the graph structure?

Probability query: **example**

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{i=1}^{n-1} \phi_i(x_i, x_{i+1}) \quad \textcircled{x_1} \dots \textcircled{} \textcircled{} \textcircled{} \dots \textcircled{x_n}$$

$$\text{Val}(X_i) = \{1, \dots, d\} \forall i$$

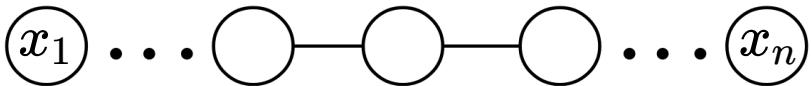
$p(x_n)$?

Take 1:

- calculate n -dim. array $p(\mathbf{x})$
- marginalize it $p(x_n) = \sum_{-x_n} p(\mathbf{x})$

$\mathcal{O}(d^n)$

Inference: example

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{i=1}^{n-1} \phi_i(x_i, x_{i+1})$$


$p(x_n)?$

Take 2:

- calculate $\tilde{p}(x_n) = \sum_{x_1} \dots \sum_{x_{n-1}} \phi_1(x_1, x_2) \dots \phi_{n-1}(x_{n-1}, x_n)$
 - without building $p(\mathbf{x})$
- normalize it $p(x_n) = \tilde{p}(x_n) / (\sum_{x_n} \tilde{p}(x_n))$
- **idea:** use the **distributive law:** $\underbrace{ab + ac}_{3 \text{ operations}} = \underbrace{a(b + c)}_{2 \text{ operations}}$

Inference and the **distributive law**

distributive law

$$\underline{ab + ac} = a(\underline{b + c})$$

3 operations 2 operations

save computation by **factoring** the operations

in disguise $\sum_{x,y} f(x,y)g(y,z) = \sum_y g(y,z) \sum_x f(x,y)$

- assuming $|Val(X)| = |Val(Y)| = |Val(Z)| = d$
- **complexity**: from $\mathcal{O}(d^3)$ to $\mathcal{O}(d^2)$

Inference: back to example

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{i=1}^{n-1} \phi_i(\mathbf{x}_i, \mathbf{x}_{i+1}) \quad \textcircled{\mathbf{x}_1} \dots \textcircled{\phantom{\mathbf{x}_i}} \textcircled{\phantom{\mathbf{x}_i}} \textcircled{\phantom{\mathbf{x}_i}} \dots \textcircled{\mathbf{x}_n}$$

Take 2:

- objective $\tilde{p}(\mathbf{x}_m) = \sum_{x_1} \dots \sum_{x_{n-1}} \phi_1(\mathbf{x}_1, \mathbf{x}_2) \dots \phi_{n-1}(\mathbf{x}_{n-1}, \mathbf{x}_n)$
- ***systematically apply the factorization:***

$$\tilde{p}(\mathbf{x}_m) = \sum_{x_{n-1}} \phi_{n-1}(\mathbf{x}_{n-1}, \mathbf{x}_n) \sum_{x_{n-2}} \phi_{n-2}(\mathbf{x}_{n-2}, \mathbf{x}_{n-1}) \dots \sum_{x_1} \phi_1(\mathbf{x}_1, \mathbf{x}_2)$$

- complexity is $\mathcal{O}(nd^2)$ instead of $\mathcal{O}(d^n)$

Inference: example 2

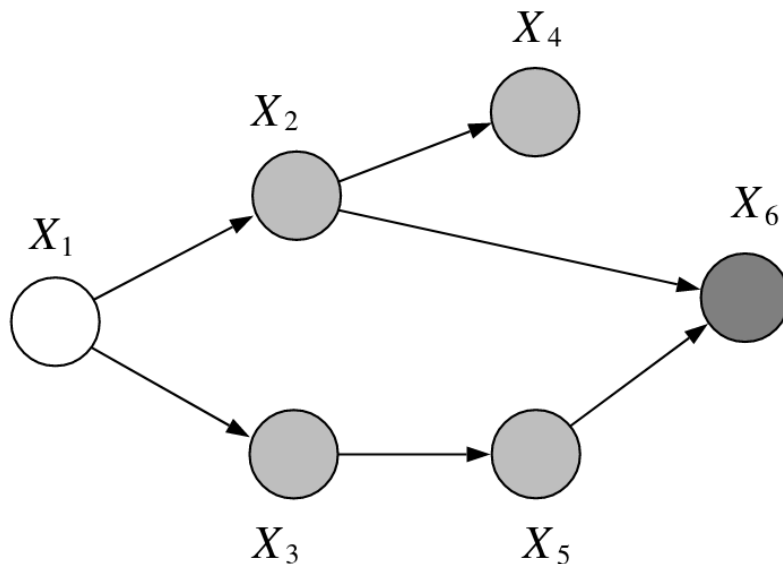
$$\text{Objective: } p(x_1 | \bar{x}_6) = \frac{p(x_1, \bar{x}_6)}{p(\bar{x}_6)}$$



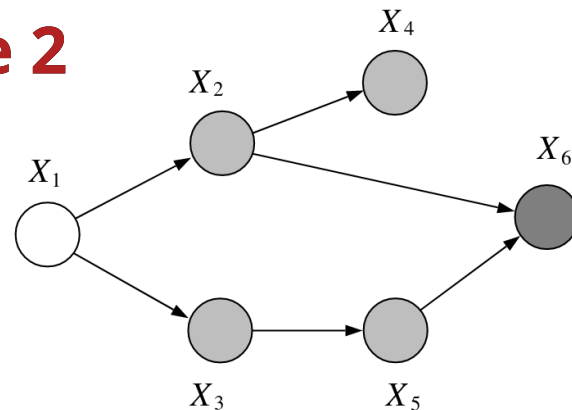
another way to write $P(X_1 | X_6 = \bar{x}_6)$
(used in Jordan's textbook)

- calculate the numerator
- denominator is then easy


$$p(\bar{x}_6) = \sum_{x_1} p(x_1, \bar{x}_6)$$



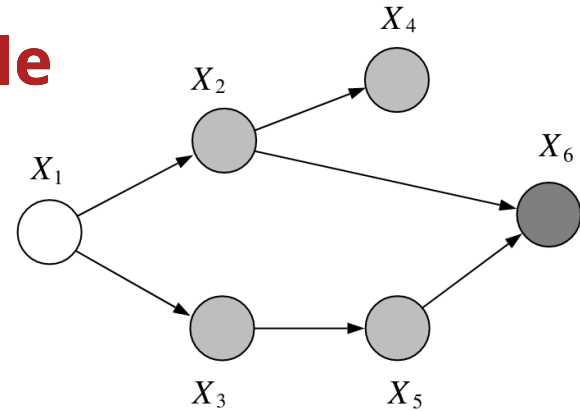
Inference: example 2



$$\begin{aligned}
 p(x_1, \bar{x}_6) &= \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} p(x_1) p(x_2 | x_1) p(x_3 | x_1) p(x_4 | x_2) p(x_5 | x_3) p(\bar{x}_6 | x_2, x_5) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) \sum_{x_4} p(x_4 | x_2) \sum_{x_5} p(x_5 | x_3) p(\bar{x}_6 | x_2, x_5) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) \sum_{x_4} p(x_4 | x_2) m_5(x_2, x_3)
 \end{aligned}$$

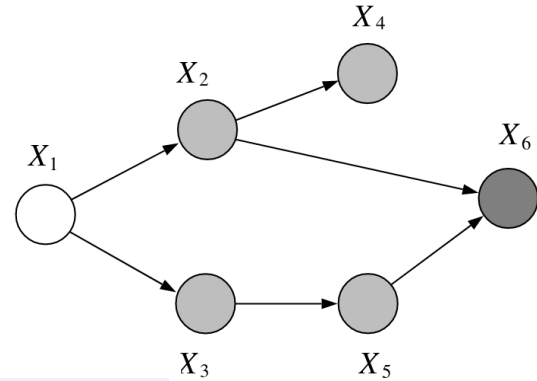

 $\mathcal{O}(d^3)$

Inference: example



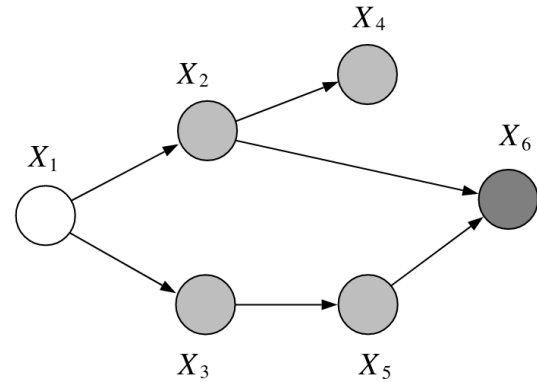
$$\begin{aligned}
 p(\mathbf{x}_1, \bar{\mathbf{x}}_6) &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) \sum_{x_4} p(x_4 | x_2) m_5(x_2, x_3) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) m_5(x_2, x_3) \sum_{x_4} p(x_4 | x_2) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) m_4(x_2) \sum_{x_3} p(x_3 | x_1) m_5(x_2, x_3).
 \end{aligned}
 \quad \Bigg| \quad \mathcal{O}(d^2)$$

Inference: example



$$\begin{aligned}
 p(\mathbf{x}_1, \bar{\mathbf{x}}_6) &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) \sum_{x_4} p(x_4 | x_2) m_5(x_2, x_3) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) \sum_{x_3} p(x_3 | x_1) m_5(x_2, x_3) \sum_{x_4} p(x_4 | x_2) \quad \text{is constant} \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) m_4(x_2) \sum_{x_3} p(x_3 | x_1) m_5(x_2, x_3) \quad \Big| \mathcal{O}(d^3) \\
 &= p(x_1) \sum_{x_2} p(x_2 | x_1) m_4(x_2) m_3(x_1, x_2) \quad \Big| \mathcal{O}(d^2) \\
 &= p(x_1) m_2(x_1).
 \end{aligned}$$

Inference: **example**



overall complexity $\mathcal{O}(d^3)$ instead of $\mathcal{O}(d^5)$

if we had built the 5d array of

$$p(x_1, x_2, x_3, x_4, x_5 \mid \bar{x}_6)$$

in the general case $\mathcal{O}(d^n)$

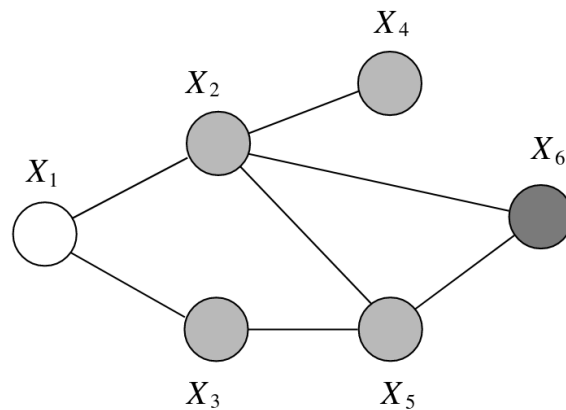
Inference: **example** (*undirected version*)

$$p(x_1, \bar{x}_6) = \frac{1}{Z} \sum_{x_2, \dots, x_5} \phi(x_1, x_2) \phi(x_1, x_3) \phi(x_2, x_3) \phi(x_3, x_5) \phi(x_2, x_5, x_6) \delta(x_6, \bar{x}_6)$$

using a delta-function for **conditioning**

$$\delta(x_6, \bar{x}_6) \triangleq \begin{cases} 1, & \text{if } x_6 = \bar{x}_6 \\ 0, & \text{otherwise} \end{cases}$$

add it as a local potential



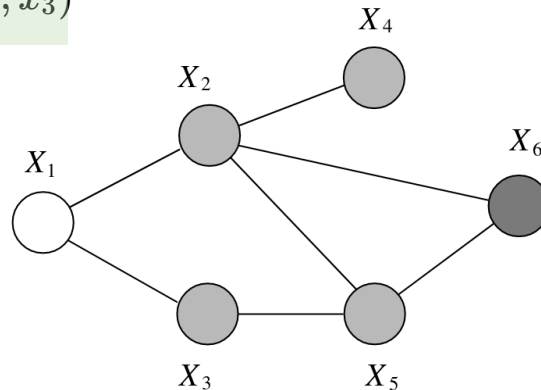
Inference: **example** (undirected version)

every step remains the same

$$\begin{aligned} p(x_1, \bar{x}_6) &= \frac{1}{Z} \sum_{x_2, \dots, x_5} \phi(x_1, x_2) \phi(x_1, x_3) \phi(x_2, x_3) \phi(x_3, x_5) \phi(x_2, x_5, x_6) \delta(x_6, \bar{x}_6) \\ &= \frac{1}{Z} \sum_{x_2, \dots, x_5} \phi(x_1, x_2) \phi(x_1, x_3) \phi(x_2, x_3) \phi(x_3, x_5) m_6(x_2, x_5) \\ &\quad \dots \\ &= \frac{1}{Z} \sum_{x_2} \phi(x_1, x_2) \dots, m_4(x_2) \sum_{x_3} \phi(x_1, x_3) m_5(x_2, x_3) \\ &= \frac{1}{Z} \sum_{x_2} \phi(x_1, x_2) \dots, m_4(x_2) m_3(x_1, x_2) \\ &= \frac{1}{Z} m_2(x_1) \end{aligned}$$

except: in Bayes-nets $Z=1$

- *at this point normalization is easy!*



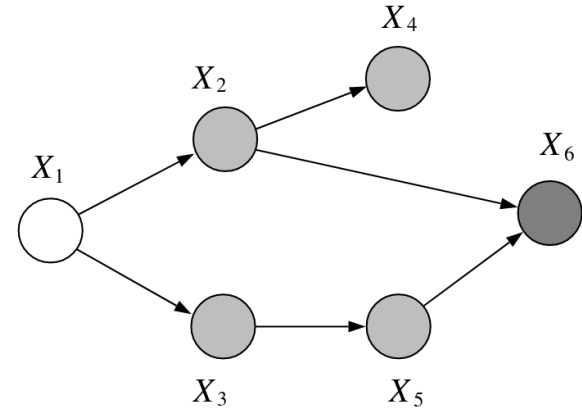
Variable elimination

- **input:** $\Phi^{t=0} = \{\phi_1, \dots, \phi_K\}$ a set of factors (e.g. CPDs)
- **output:** $\sum_{x_{i_1}, \dots, x_{i_m}} \prod_k \phi_k(\mathbf{D}_k)$
- go over x_{i_1}, \dots, x_{i_m} in **some order**:
 - collect all the **relevant factors**: $\Psi^t = \{\phi \in \Phi^t \mid x_{i_t} \in \text{Scope}[\phi]\}$
 - calculate their **product**: $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - **marginalize out** x_{i_t} : $\psi'_t = \sum_{x_{i_t}} \psi_t$
 - update the set of factors: $\Phi^t = \Phi^{t-1} - \Psi^t + \{\psi'_t\}$
- return the product of factors in $\Phi^{t=m}$

Variable elimination: **example**

- **input:** $\Phi^{t=0} = \{\phi_1, \dots, \phi_K\}$ a set of factors (e.g. CPDs)

$$\Phi^0 = \{p(x_2 | x_1), p(x_3 | x_1), p(\bar{x}_6 | x_2, x_5), p(x_4 | x_2), p(x_5 | x_3)\}$$



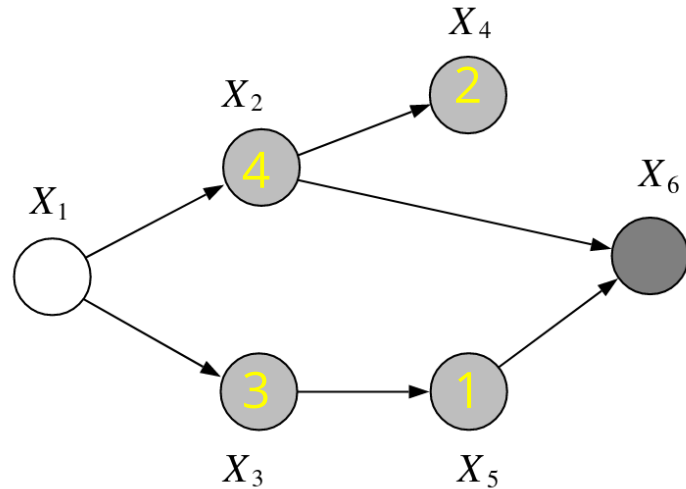
- **output:** $\sum_{x_{i_1}, \dots, x_{i_m}} \prod_k \phi_k(\mathbf{D}_k)$

$$p(x_1, \bar{x}_6) = \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} p(x_1) p(x_2 | x_1) p(x_3 | x_1) p(x_4 | x_2) p(x_5 | x_3) p(\bar{x}_6 | x_2, x_5)$$

Variable elimination: **example**

- go over x_{i_1}, \dots, x_{i_m} in **some order**:

x_5, x_4, x_3, x_2



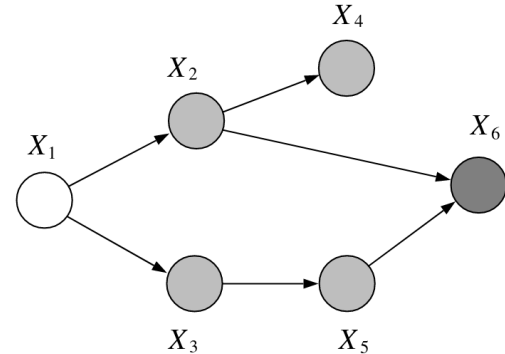
Variable elimination: **example**

- for x_5 :

- collect all the **relevant factors** $\Psi^t = \{\phi \in \Phi^t \mid x_{it} \in \text{Scope}[\phi]\}$
- calculate their **product** $\psi_t = \prod_{\phi \in \Psi^t} \phi$

$$\Psi^0 = \{p(\bar{x}_6 \mid x_2, x_5), p(x_5 \mid x_3)\}$$

$$\psi_t(x_2, x_3, x_5) = p(\bar{x}_6 \mid x_2, x_5)p(x_5 \mid x_3)$$



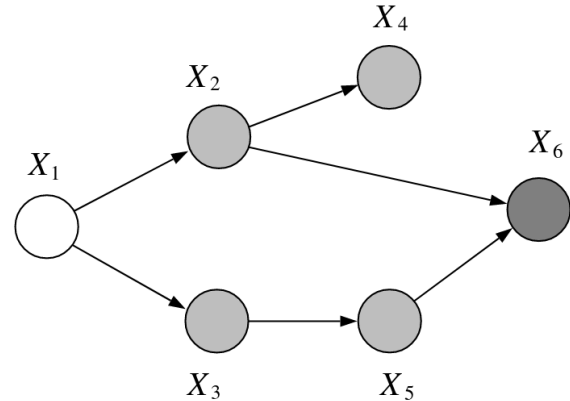
Variable elimination: **example**

- for x_5 :
 - collect all the relevant factors $\Psi^t = \{\phi \in \Phi^t \mid x_{it} \in \text{Scope}[\phi]\}$
 - calculate their product $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - **marginalize out x_5**

$$\Psi^0 = \{p(\bar{x}_6 \mid x_2, x_5), p(x_5 \mid x_3)\}$$

$$\psi_t(x_2, x_3, x_5) = p(\bar{x}_6 \mid x_2, x_5)p(x_5 \mid x_3)$$

$$\psi'_t(x_2, x_3) = \sum_{x_5} \psi_t(x_2, x_3, x_5)$$



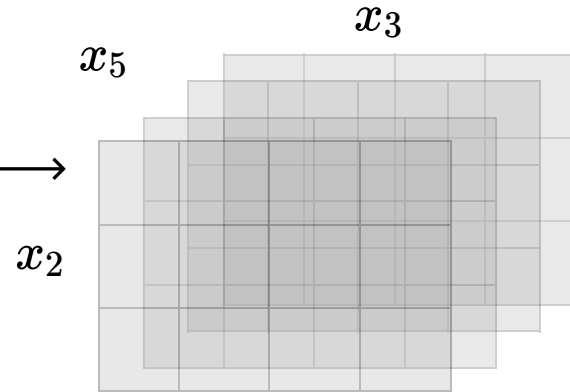
Variable elimination: **example**

- for x_5 :
 - collect all the relevant factors $\Psi^t = \{\phi \in \Phi^t \mid x_{it} \in \text{Scope}[\phi]\}$
 - calculate their product $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - **marginalize out x_5**

$$\Psi^0 = \{p(\bar{x}_6 \mid x_2, x_5), p(x_5 \mid x_3)\}$$

$$\psi_t(x_2, x_3, x_5) = p(\bar{x}_6 \mid x_2, x_5)p(x_5 \mid x_3) \longrightarrow$$

$$\psi'_t(x_2, x_3) = \sum_{x_5} \psi_t(x_2, x_3, x_5)$$



Variable elimination: **example**

- for x_5 :
 - collect all the relevant factors $\Psi^t = \{\phi \in \Phi^t \mid x_{i_t} \in \text{Scope}[\phi]\}$
 - calculate their product $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - marginalize out x_5
 - update the set of factors $\Phi^t = \Phi^{t-1} - \Psi^t + \{\psi'_t\}$

$$\psi'_t(x_2, x_3) = \sum_{x_5} \psi_t(x_2, x_3, x_5)$$

$$\Phi^0 = \{p(x_2 \mid x_1), p(x_3 \mid x_1), p(\bar{x}_6 \mid x_2, x_5), p(x_4 \mid x_2), p(x_5 \mid x_3)\}$$

↓

$$\Phi^1 = \{p(x_2 \mid x_1), p(x_3 \mid x_1), p(x_4 \mid x_2), \psi'_t(x_2, x_3)\}$$

Variable elimination: **example**

- for x_5 :
 - collect all the relevant factors $\Psi^t = \{\phi \in \Phi^t \mid x_{i_t} \in \text{Scope}[\phi]\}$
 - calculate their product $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - marginalize out x_5
 - update the set of factors $\Phi^t = \Phi^{t-1} - \Psi^t + \{\psi_t'\}$

$$\Phi^1 = \{p(x_2 \mid x_1), p(x_3 \mid x_1), p(x_4 \mid x_2), \psi_t'(2, 3)\}$$

repeat for x_4, x_3, x_2

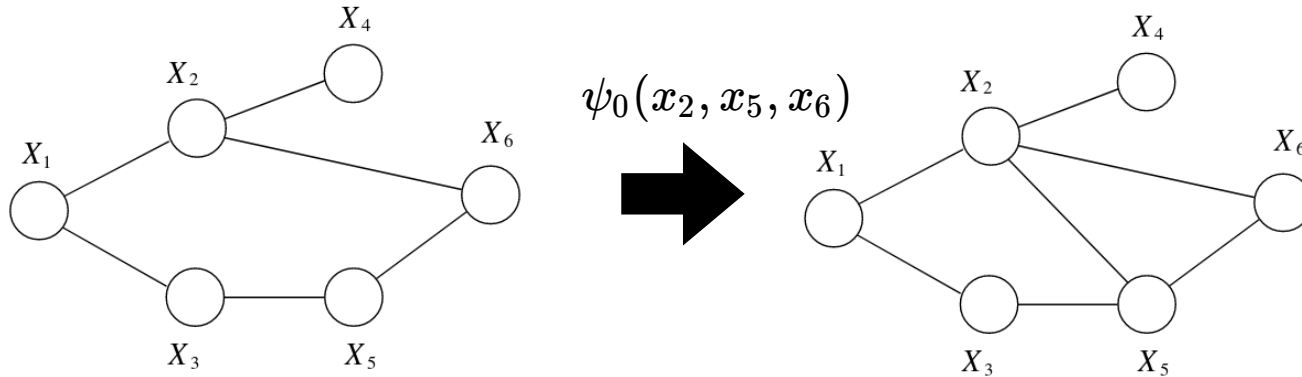
Variable elimination: **example**

calculating $p(x_1)$: **following the graph**

using the order **x_6, x_5, x_4, x_3, x_2**

$$\Phi^0 = \{p(x_2 | x_1), p(x_3 | x_1), p(x_6 | x_2, x_5), p(x_4 | x_2), p(x_5 | x_3)\}$$

t=1



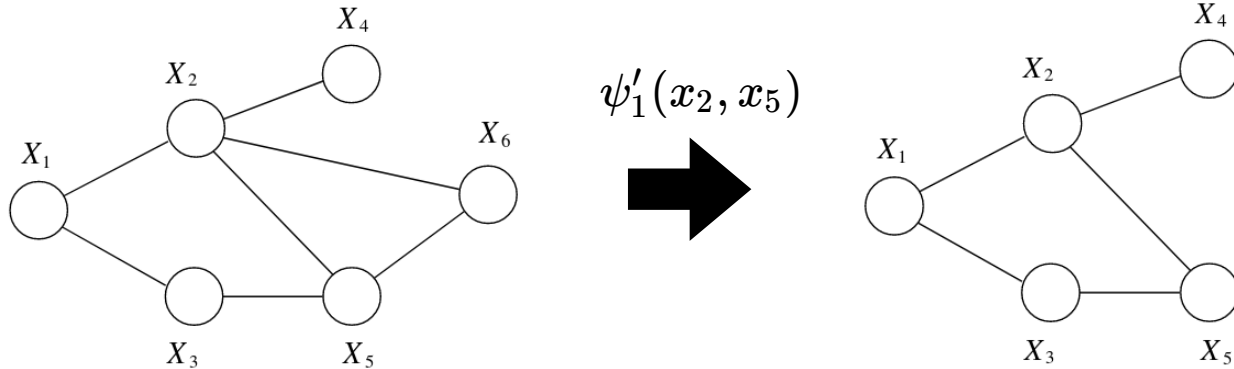
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^1 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_1(x_2, x_5), p(x_4 | x_2), p(x_5 | x_3)\}$$

t=1



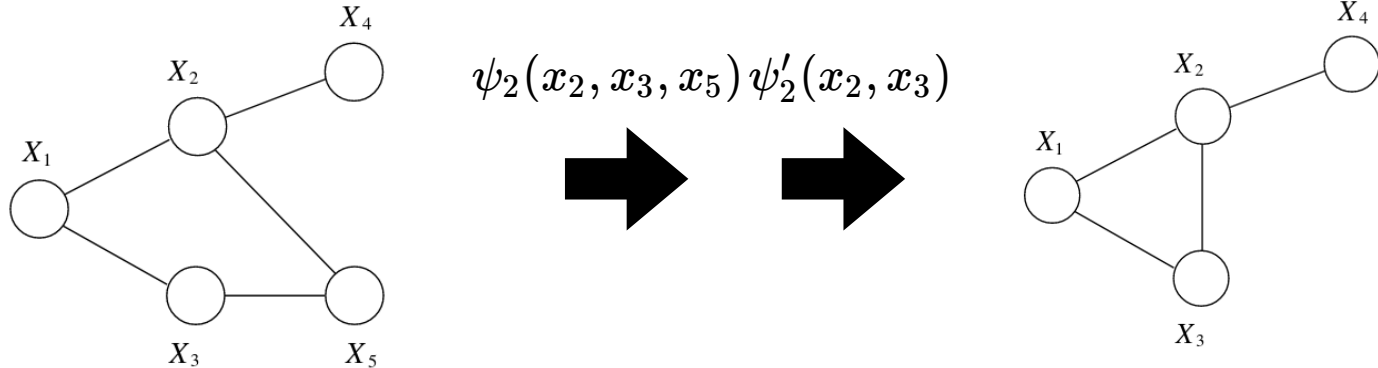
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^1 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_1(x_2, x_5), p(x_4 | x_2), p(x_5 | x_3)\}$$

t=2



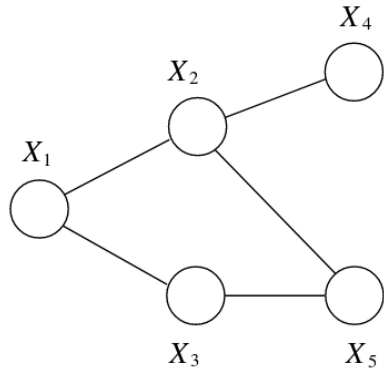
Variable elimination: **example**

calculating $p(x_1)$

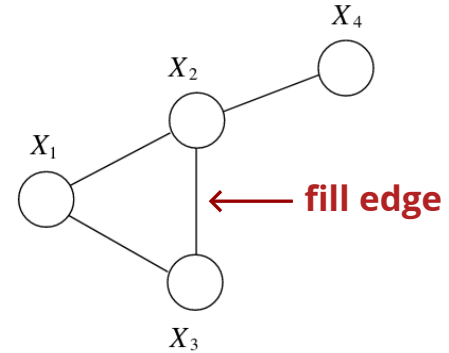
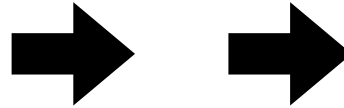
using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^2 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_2(x_2, x_3), p(x_4 | x_2)\}$$

t=2



$$\psi_2(x_2, x_3, x_5) \psi'_2(x_2, x_3)$$



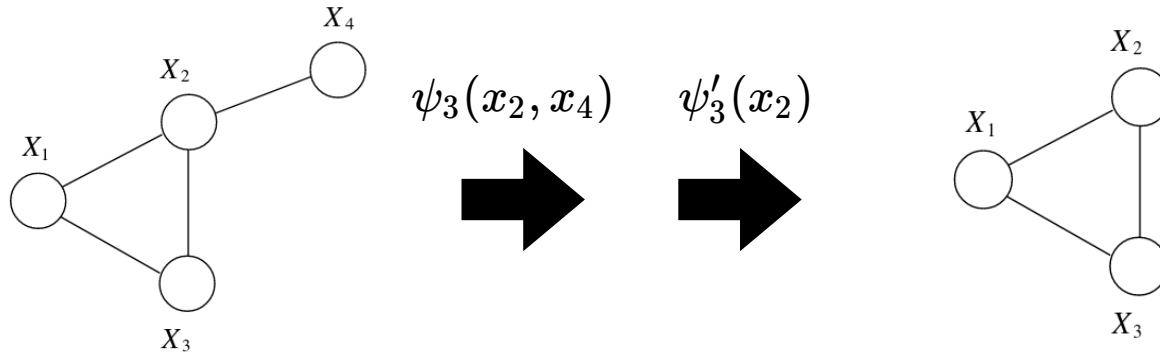
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^2 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_2(x_2, x_3), p(x_4 | x_2)\}$$

t=3



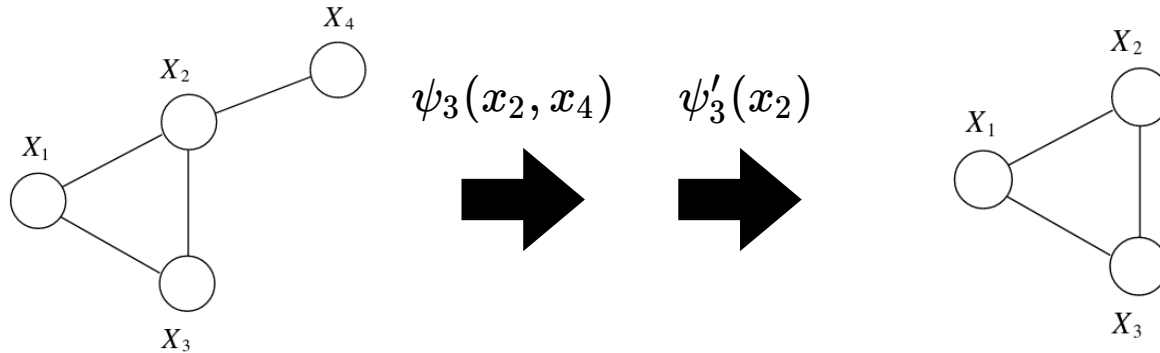
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^3 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_2(x_2, x_3), \psi'_3(x_2)\}$$

t=3



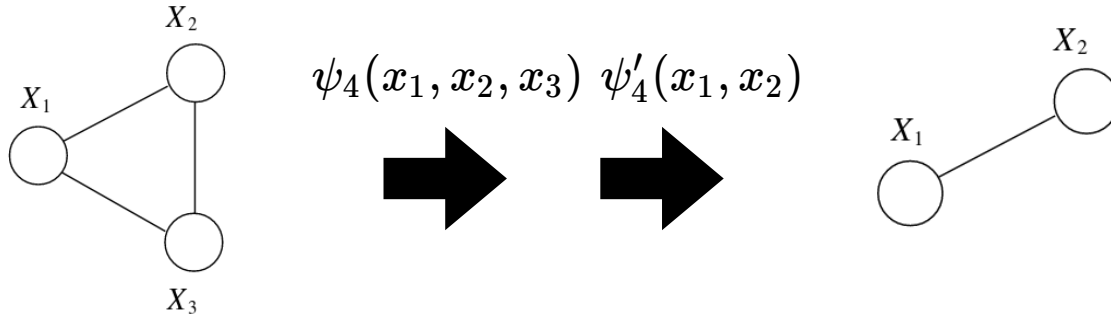
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^3 = \{p(x_2 | x_1), p(x_3 | x_1), \psi'_2(x_2, x_3), \psi'_3(x_2)\}$$

t=4



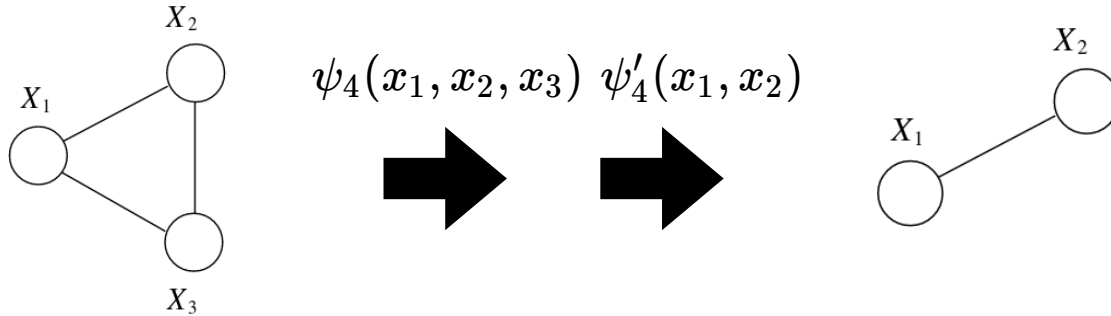
Variable elimination: **example**

calculating $p(x_1)$

using the order $x_6, x_5, x_4, \mathbf{x_3}, x_2$

$$\Phi^4 = \{p(x_2 | x_1), \psi'_3(x_2), \mathbf{\psi'_4(x_1, x_2)}\}$$

t=4



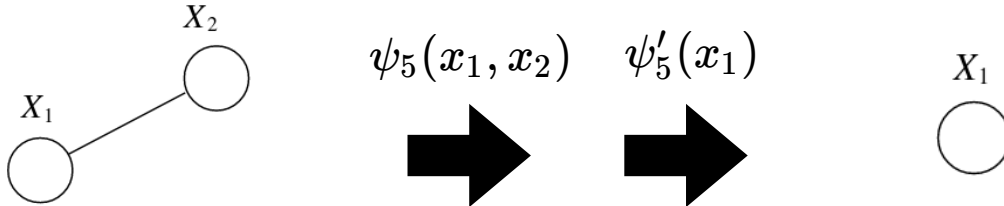
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^4 = \{p(x_2 | x_1), \psi'_3(x_2), \psi'_4(x_1, x_2)\}$$

t=5



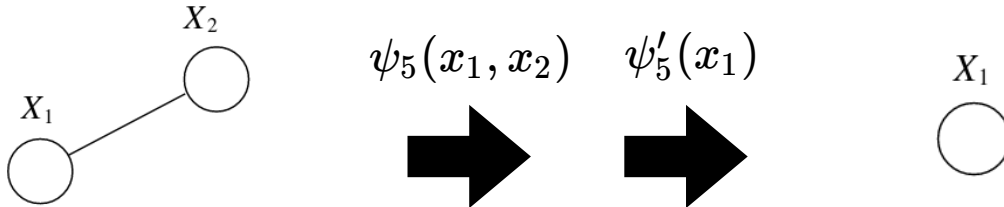
Variable elimination: **example**

calculating $p(x_1)$

using the order x_6, x_5, x_4, x_3, x_2

$$\Phi^5 = \{\psi'_5(x_1)\}$$

t=5



Variable elimination: **example**

$$p(x_1) = \frac{1}{Z} \sum_{x_2, \dots, x_6} \phi(x_1, x_2) \phi(x_1, x_3) \phi(x_2, x_3) \phi(x_3, x_5) \phi(x_2, x_5, x_6)$$

at final iteration: $\Phi^5 = \{\psi'_5(x_1)\}$

the **marginal** of interest $p(x_1) = \frac{1}{Z} \psi'_5(x_1)$ $\overset{X_1}{\bigcirc}$

One more elimination step: $\Phi^6 = \{\psi'_6(\emptyset) = Z\}$

- gives the **partition function** $Z = \sum_{x_1} \psi'_5(x_1)$

Complexity

- go over $\mathcal{X}_{i_1}, \dots, \mathcal{X}_{i_m}$ in some order:
 - collect all the relevant factors: $\Psi^t = \{\phi \in \Phi^t \mid x_{i_t} \in \text{Scope}[\phi]\}$
 - calculate their product: $\psi_t = \prod_{\phi \in \Psi^t} \phi$
 - marginalize out x_{i_t} : $\psi'_t = \sum_{x_{i_t}} \psi_t$
 - update the set of factors: $\Phi^t = \Phi^{t-1} - \Psi^t + \{\psi'_t\}$

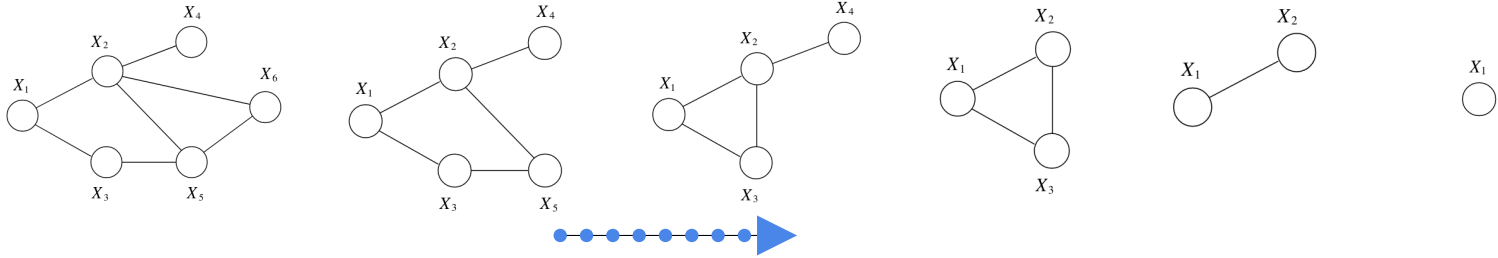
 **complexity:** number of vars in ψ_t : $\mathcal{O}(\max_t d^{|\text{Scope}[\psi_t]|})$

- depends on the **graph structure**

Induced graph

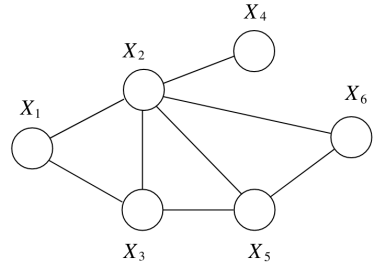
complexity of step t : number of vars in ψ_t $\mathcal{O}(d^{|\text{Scope}[\psi_t]|})$

- depends on the **graph structure**



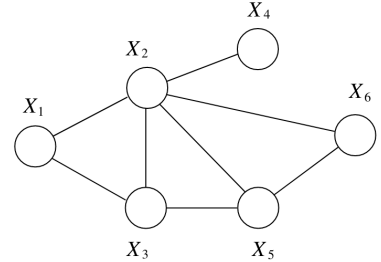
induced graph

- add edges created during the elimination
- maximal cliques correspond to $\psi_t \quad \forall t$



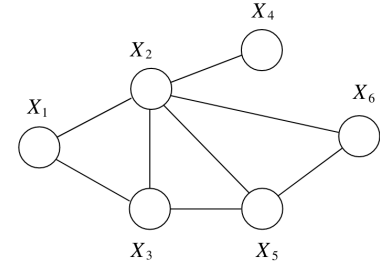
Induced graph

- maximal cliques correspond to some ψ_t **why?**
 - take one such clique - e.g., $\{X_2, X_3, X_5\}$
 - take the first to be eliminated - e.g., X_5
 - all the edges to X_5 exist **before** its elimination
 - therefore, removing X_5 will create a factor with $Scope[\psi_t] = \{X_2, X_3, X_5\}$



Induced graph

- maximal cliques correspond to some ψ_t **why?**
 - take one such clique - e.g., $\{X_2, X_3, X_5\}$
 - take the first to be eliminated - e.g., X_5
 - all the edges to X_5 exist **before** its elimination
 - therefore, removing X_5 will create a factor with $\text{Scope}[\psi_t] = \{X_2, X_3, X_5\}$



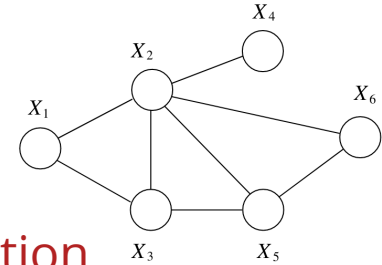
- the induced graph is **chordal** all the loops > 3 have a *chord*
 - a similar argument

Tree-width

maximal cliques correspond to ψ_t

cost of marginalizing ψ_t is $\mathcal{O}(d^{|\text{Scope}[\psi_t]|})$

largest clique dominates the **cost of variable elimination**



the tree-width

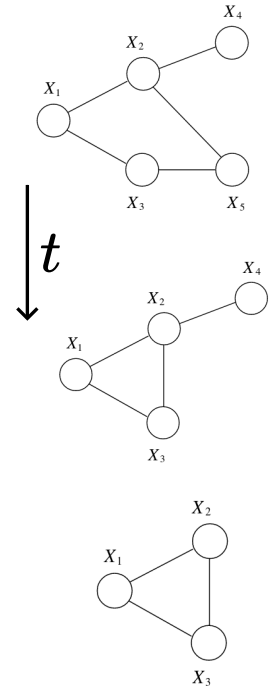
$$\min_{\text{orderings}} \max_{\psi_t} \text{scope}[\psi_t] - 1$$

- tree-width of a tree = 1
- **NP-hard** to calculate the tree-width
- use heuristics to find good orderings

Ordering heuristics

choose the next vertex to eliminate by:

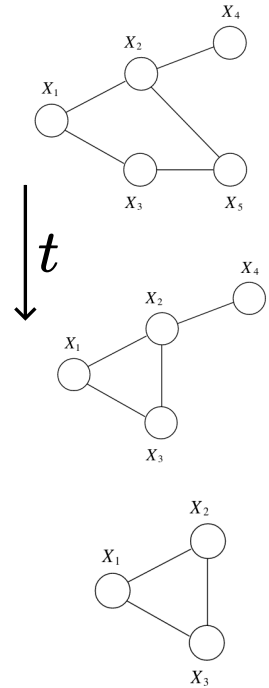
- minimizing the effect of the **created clique/factor**
 - **min-neighbours:** #neighbours in the current graph
 - **min-weight:** product of cardinality of neighbours



Ordering heuristics

choose the next vertex to eliminate by:

- minimizing the effect of the **created clique/factor**
 - **min-neighbours:** #neighbours in the current graph
 - **min-weight:** product of cardinality of neighbours
- minimizing the effect of **fill edges**
 - **min-fill:** number of fill-edges after its elimination
 - **weighted min-fill:** edges are weighted by the product of the cardinality of the two vertices



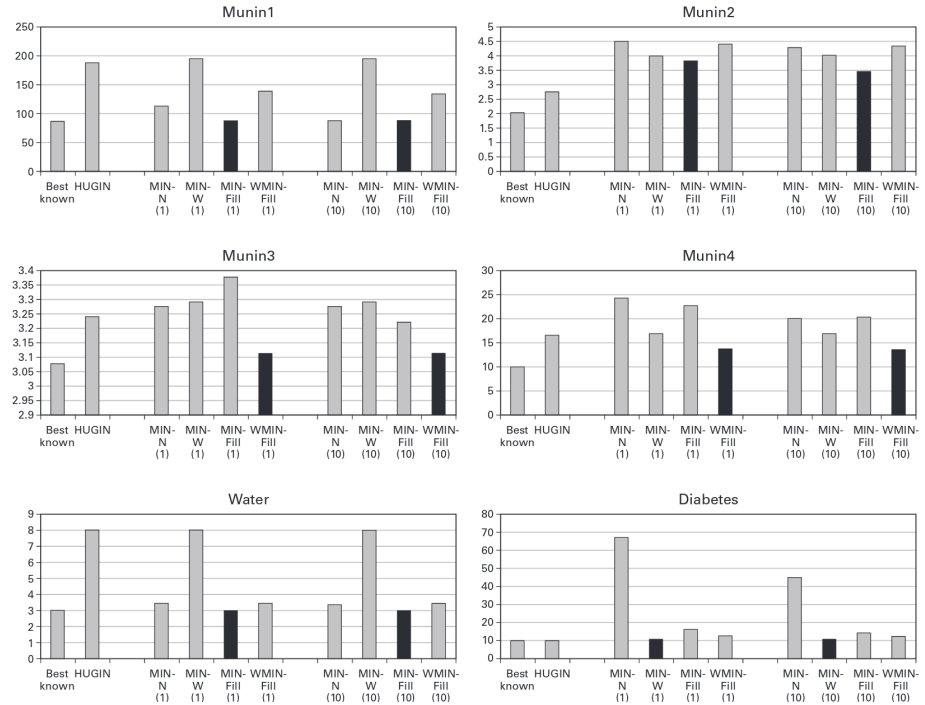
Ordering heuristics

minimizing the #fill edges tends to work better in practice

to minimize the cost one could:

- try different heuristics
- calculate the max-clique size
- pick the best ordering
- apply variable elimination

comparing the size of factors



Answering other queries

we saw variable elimination (VE) for **marginalization**

$$P(X_1) = \sum_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$$

Introducing **evidence** leads to *a similar* problem

$$P(X_1 \mid X_m = x_m) = \frac{P(X_1, X_m = x_m)}{P(X_m = x_m)}$$

- use VE to get $P(X_1, X_m = x_m)$
- marginalize this to get $P(X_m = x_m)$
- divide!

Answering other queries

we saw variable elimination (VE) for **marginalization**

$$P(X_1 = x_1) = \sum_{x_2, \dots, x_n} P(X_1 = x_1, X_2 = x_2, \dots, X_n = x_n)$$

MAP inference: sum \rightarrow max

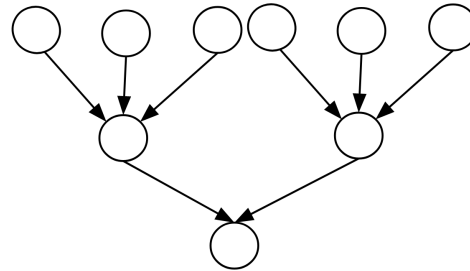
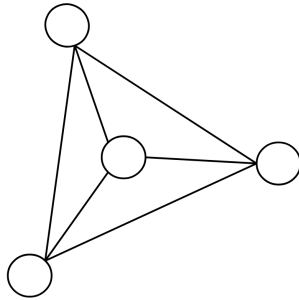
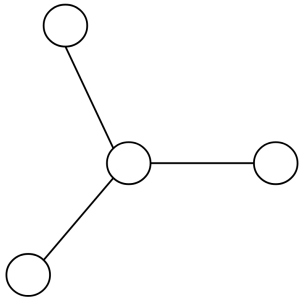
$$Q(X_1 = x_1) = \max_{x_2, \dots, x_n} P(X_1, X_2 = x_2, \dots, X_n = x_n)$$

- run VE with **maximization instead of summation**
- eliminating ALL the variables gives a single value $\max_{\mathbf{x}} P(\mathbf{X} = \mathbf{x})$
- we can also get the maximizing **assignment** as well (later!)

$$\arg \max_{\mathbf{x}} P(\mathbf{X} = \mathbf{x})$$

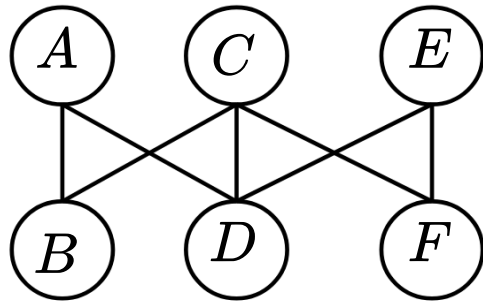
quiz: tree width

what is the tree-width in these graphical models?



quiz: induced graph

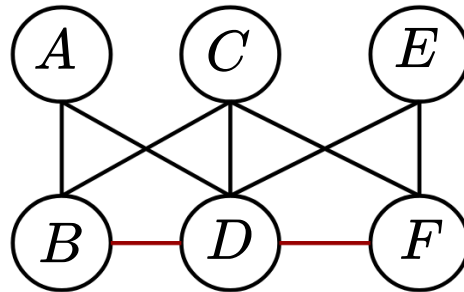
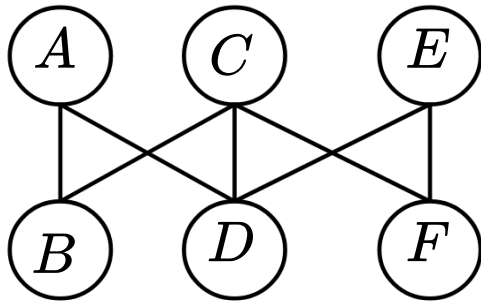
what are the fill-edges corresponding to the following elimination order? A, B, C, D, E, F



A	C	E
B	D	F

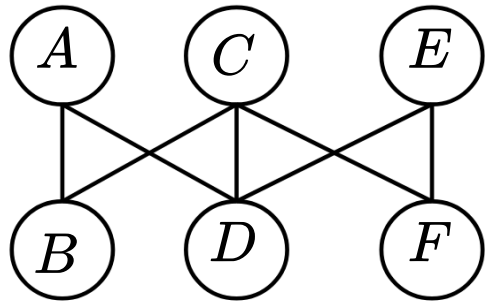
quiz: induced graph

what are the fill-edges corresponding to the following elimination order? A, B, C, D, E, F

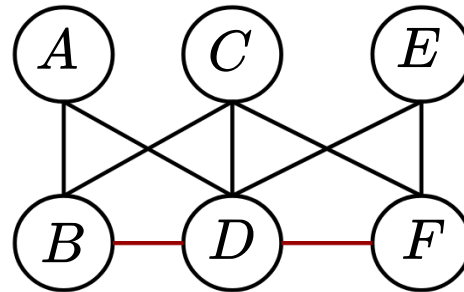


quiz: induced graph

what are the fill-edges corresponding to the following elimination order? A, B, C, D, E, F



is this graph chordal?



how about this one?

Summary

- inference in graphical models is **NP-hard**
 - even approximating it is **NP-hard**
- brute-force inference has an exponential cost
- use the **graph structure + distributive law**:
 - variable elimination algorithm
 - cost grows with the **tree-width** of the graph
 - **NP-hard** to calculate the tree-width / optimal ordering
 - use heuristics