

CSC 412/2506:
Probabilistic Machine Learning
Week 3: Markov Random Fields/Exact Inference

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Today's lecture

Summary of the content:

- *Undirected* graphical models: Markov Random Fields (MRFs).
- Exact inference on graphical models
- Variable elimination

Some announcements:

- Assignment 1 is released September 22nd, due October 5th.
- TA office hours September 30th and October 2nd, 6-7PM, Pratt bldg. room 286.

Are DAGMs always useful?

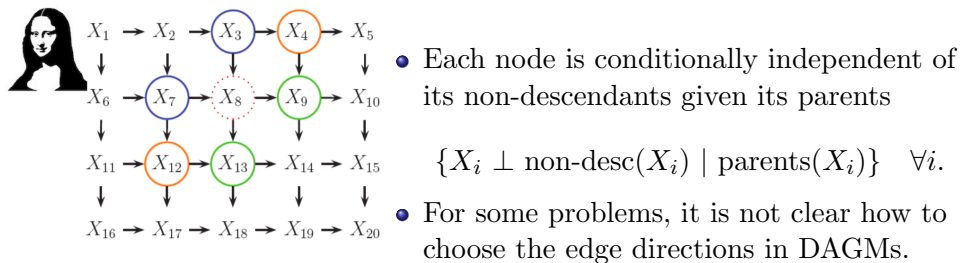


Figure : Causal MRF or a Markov mesh

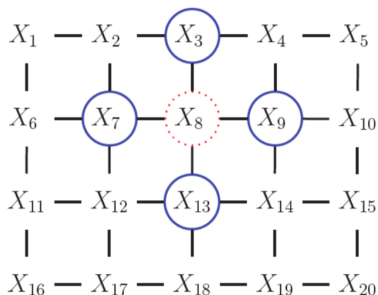
Markov blanket (mb): the set of nodes that makes X_i conditionally independent of all the other nodes.

In our example: $\text{mb}(X_8) = \{X_3, X_4, X_7, X_9, X_{12}, X_{13}\}$.

One would expect X_4 and X_{12} not to be in the Markov blanket $\text{mb}(X_8)$, especially given X_2 and X_{14} are not.

Markov Random Fields

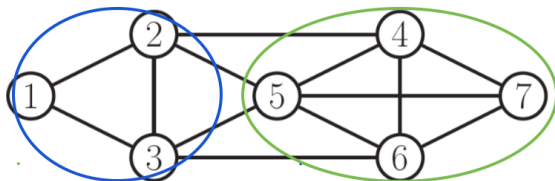
- Undirected graphical models (aka **Markov random fields (MRFs)**) are models with dependencies described by an undirected graph.
- The nodes in the graph represent random variables. However, in contrast to DAGMs, edges represent probabilistic interactions between neighbors (as opposed to conditional dependence).



Cliques

A **clique** is a subset of nodes such that every two vertices in the subset are connected by an edge.

A **maximal clique** is a clique that cannot be extended by including one more adjacent vertex.



Distributions Induced by MRFs

Let $\mathbf{x} = (x_1, \dots, x_m)$ be the set of all random variables in our graph G .

Let $\mathcal{C}$ be the set of all maximal cliques of G .

The distribution p of X factorizes with respect to G if

$$p(\mathbf{x}) \propto \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

for some nonnegative *potential* functions ψ_C , where $x_C = (x_i)_{i \in C}$.

The MRF on G represents the distributions that factorize wrt G .

The factored structure of the distribution makes it possible to more efficiently do the sums/integrals and is a form of dimension reduction.

Hammersley-Clifford Theorem

If $p(\mathbf{x}) > 0$ for all $\mathbf{x}$, the following statements are equivalent:

- p factorizes according to G , that is,

$$p(\mathbf{x}) \propto \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

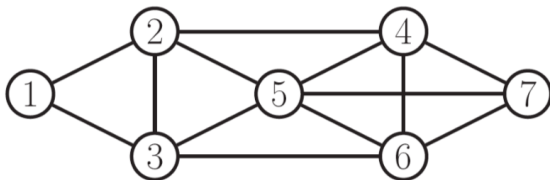
for some nonnegative potential functions ψ_C .

- **Global Markov Properties:** $X_A \perp\!\!\!\perp X_B \mid X_S$ if the sets A and B are *separated* by S in G (every path from A to B crosses S).

In particular,

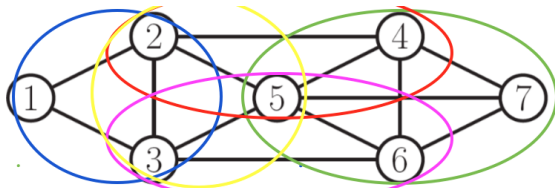
- If i, j are not connected by an edge then $X_i \perp\!\!\!\perp X_j \mid X_{\text{rest}}$.
- The Markov blanket of X_i is given by its neighbors in G .

Example:



- How many maximal cliques are there?
- What is the underlying factorization?
- What are the induced conditional independence statements?

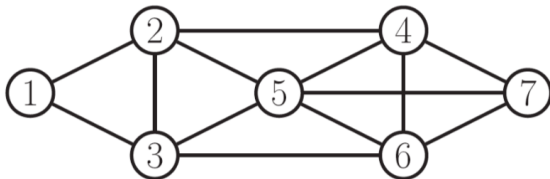
Example:



Lets see how to factorize the undirected graph of our running example:

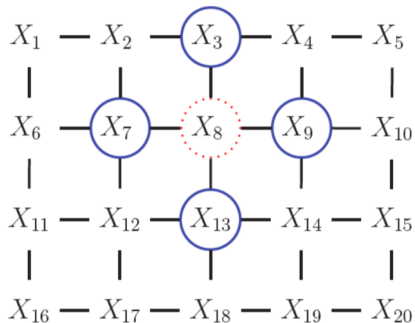
$$\begin{aligned} p(\mathbf{x}) \propto & \psi_{1,2,3}(x_1, x_2, x_3) \psi_{2,3,5}(x_2, x_3, x_5) \psi_{2,4,5}(x_2, x_4, x_5) \\ & \times \psi_{3,5,6}(x_3, x_5, x_6) \psi_{4,5,6,7}(x_4, x_5, x_6, x_7) \end{aligned}$$

Example:



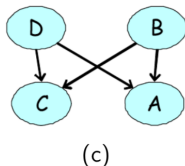
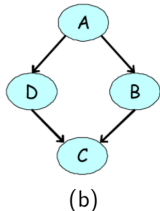
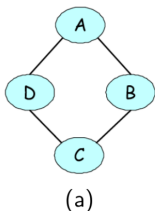
e.g. $(X_1, X_2) \perp (X_6, X_7) \mid (X_3, X_4, X_5)$
 $X_1 \perp X_5 \mid (X_2, X_3)$

Image MRF



Not all MRFs can be represented as DAGMs

Take the following MRF for example (a) and our attempts at encoding this as a DAGM (b, c).

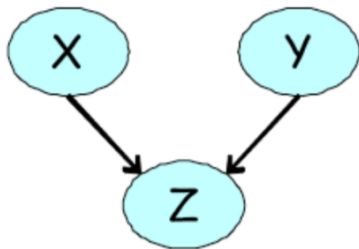


- Two conditional independencies in (a):
 - ▶ 1. $A \perp C | D, B$ 2. $B \perp D | A, C$
- In (b), we have the first independence, but not the second.
- In (c), we have the first independence, but not the second. Also, B and D are marginally independent.

Not all DAGMs can be represented as MRFs

Not all DAGMs can be represented as MRFs.

E.g. explaining away:



An undirected model is unable to capture the marginal independence, $X \perp Y$ that holds at the same time as $X \not\perp Y | Z$.

MRFs as Exponential Families

- Consider a parametric family of factorized distributions

$$p(\mathbf{x}|\theta) = \frac{1}{Z(\theta)} \prod_{C \in \mathcal{C}} \psi_C(x_C|\theta_C), \quad \theta = (\theta_C)_{C \in \mathcal{C}}.$$

- We can write this in an exponential form:

$$p(\mathbf{x}|\theta) = \exp \left\{ \sum_{C \in \mathcal{C}} \log \psi_C(x_C|\theta_C) - \underbrace{\log Z(\theta)}_{=A(\theta)} \right\}$$

- Suppose the potentials have a log-linear form

$$\log \psi_C(x_C|\theta_C) = \theta_C^\top \phi_C(x_C)$$

we get the exponential family

$$p(\mathbf{x}|\theta) = \exp \left\{ \sum_{C \in \mathcal{C}} \theta_C^\top \phi_C(x_C) - \underbrace{\log Z(\theta)}_{=A(\theta)} \right\}$$

MRFs as Exponential Families

Question: When $\log \psi_C(x_C|\theta_C) = \theta_C^\top \phi_C(x_C)$?

Finite discrete case:

- If X is finite discrete then x_C takes a finite number of values and so $\log \psi_C$ takes a finite number of values.
- Take θ_C as all these possible values, and let $\phi_C(x_C)$ is a vector 1 on the entry correspond to x_C and zeros otherwise.
- Then $\log \psi_C(x_C|\theta_C) = \theta_C^\top \phi_C(x_C)$ as required.

Multivariate Gaussian case will be covered later in the lecture.

We can find the expectation of the C -th feature

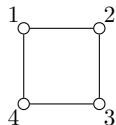
$$\frac{\partial \log Z(\theta)}{\partial \theta_C} = \mathbb{E}[\phi_C(X_C)].$$

Representing potentials

If the variables are finite discrete, we can represent the potential functions as tables of (non-negative) numbers.

e.f. consider a 4-cycle and binary random variables

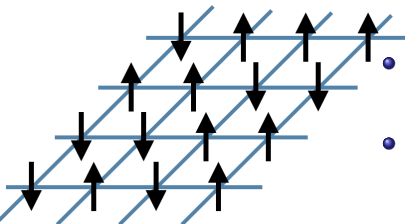
$$p(x_1, x_2, x_3, x_4) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \psi_{3,4}(x_3, x_4) \psi_{1,4}(x_1, x_4)$$



$\psi_{1,2}(x_1, x_2)$			$\psi_{2,3}(x_2, x_3)$			$\psi_{3,4}(x_3, x_4)$			$\psi_{1,4}(x_1, x_4)$		
x_1	x_2		x_2	x_3		x_3	x_4		x_1	x_4	
0	0	30	0	0	100	0	0	1	0	0	100
0	1	5	0	1	1	0	1	100	0	1	1
1	0	1	1	0	1	1	0	100	1	0	1
1	1	10	1	1	100	1	1	1	1	1	100

These potentials are not probabilities since we ignored the normalization constant!

Example: Ising model



- The Ising model is an MRF that is used to model magnets.
- The nodes variables are spins, i.e., we use $x_s \in \{-1, +1\}$.

- Define the pairwise **clique potentials** as

$$\psi_{st}(x_s, x_t) = e^{J_{st}x_sx_t}.$$

where J_{st} is the coupling strength between nodes s and t .

- $\psi_{st}(-1, -1) = \psi_{st}(1, 1) = e^{J_{st}}$; $\psi_{st}(-1, 1) = \psi_{st}(1, -1) = e^{-J_{st}}$
- If two nodes are not connected set $J_{st} = 0$.

Ising model

- We might want to add node potentials as well

$$\psi_s(x_s) = e^{b_s x_s}$$

- The overall distribution becomes

$$p(\mathbf{x}) \propto \prod_{s \sim t} \psi_{st}(x_s, x_t) \prod_s \psi_s(x_s) = \exp \left\{ \sum_{s \sim t} J_{st} x_s x_t + \sum_s b_s x_s \right\}.$$

- If $J_{st} > 0$ the model promotes same spins on neighboring spins.
- Hammersley-Clifford theorem: $J_{ij} = 0$ then $X_i \perp X_j | X_{\text{rest}}$.

Multivariate Gaussians can express a graphical model

Univariate Gaussian: $f(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{1}{2\sigma^2}(x - \mu)^2)$.

Recall: Multivariate normal distribution, $X = (X_1, \dots, X_m)$:

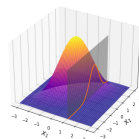
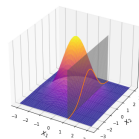
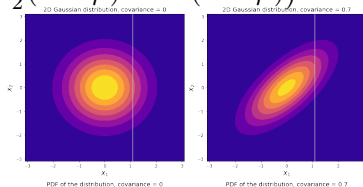
Let $\mu \in \mathbb{R}^m$ and Σ symmetric positive definite $m \times m$ matrix. We write $X \sim N_m(\mu, \Sigma)$ if the density of the vector X is

$$f(\mathbf{x}; \mu, \Sigma) = \frac{1}{(2\pi)^{m/2}} (\det \Sigma)^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu)\right).$$

Positive definite: $\forall \mathbf{u} \neq \mathbf{0} \quad \mathbf{u}^T \Sigma \mathbf{u} > 0$.

Moments:

- mean vector: $\mathbb{E}X = \mu$,
- covariance: $\text{var}(X) = \Sigma$.



Recall: Marginal and conditional distributions

Split X into two blocks $X = (X_A, X_B)$. Denote

$$\mu = (\mu_A, \mu_B) \quad \text{and} \quad \Sigma = \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}.$$

Marginal distribution

$$X_A \sim N(\mu_A, \Sigma_{AA})$$

Conditional distribution

$$X_A | X_B = x_B \sim N(\mu_A + \Sigma_{AB} \Sigma_{BB}^{-1} (x_B - \mu_B), \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA})$$

- Note that the conditional covariance does not depend on x_B .

Some other properties

Linear transformations:

$A \in \mathbb{R}^{m \times p}$ for $m \leq p$ and $X \sim N_p(\mu, \Sigma)$ then $AX \sim N_m(A\mu, A\Sigma A^T)$.

Conditional independence:

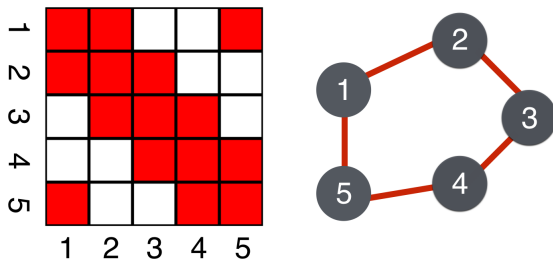
- $X_i \perp X_j$ if and only if $\Sigma_{ij} = 0$.
- $X_i \perp X_j | X_C$ if and only if $\Sigma_{ij} - \Sigma_{i,C} \Sigma_{C,C}^{-1} \Sigma_{C,j} = 0$
- Let $R = V \setminus \{i, j\}$. The following are equivalent:
 - ▶ $X_i \perp X_j | X_R$
 - ▶ $\Sigma_{ij} - \Sigma_{i,R} \Sigma_{R,R}^{-1} \Sigma_{R,j} = 0$
 - ▶ $(\Sigma^{-1})_{ij} = 0$

Gaussian Graphical models

Denote $K = \Sigma^{-1}$ then

$$p(\mathbf{x}|\mu, \Sigma) \propto \prod_s e^{-\frac{1}{2}K_{ss}(x_s-\mu_s)^2} \prod_{s < t} e^{-K_{st}(x_s-\mu_s)(x_t-\mu_t)}.$$

Important interpretation: $K_{ij} = 0$ if and only if $X_i \perp X_j | X_{\text{rest}}$.



Show that this is an exponential family.

Inference as Conditional Distribution

- We explore inference in probabilistic graphical models (PGMs).
 - x_E = The observed evidence
 - x_F = The unobserved variable we want to infer
 - $x_R = \mathbf{x} - \{x_F, x_E\}$ = Remaining (extraneous) variables
- Focus on computing the conditional probability distribution

$$p(x_F|x_E) = \frac{p(x_F, x_E)}{p(x_E)} = \frac{p(x_F, x_E)}{\sum_{x_F} p(x_F, x_E)}$$

- for which, we marginalize out these extraneous variables, focusing on the joint distribution over evidence and subject of inference:

$$p(x_F, x_E) = \sum_{x_R} p(x_F, x_E, x_R)$$

Variable elimination

Order in which we marginalize affects the computational cost!

Our main tool is **variable elimination**:

- A simple and general **exact inference** algorithm in any probabilistic graphical model (DAGMs or MRFs).
- Computational complexity depends on the graph structure.
- Dynamic programming avoids enumerating all variable assignments.

Example: Simple chain

- Lets start with the example of a simple chain

$$A \rightarrow B \rightarrow C \rightarrow D$$

where we want to compute $p(D)$, with no evidence variables.

- We have

$$x_F = \{D\}, \quad x_E = \{\}, \quad x_R = \{A, B, C\}$$

- We saw last lecture that this graphical model describes the factorization of the joint distribution as:

$$p(A, B, C, D) = p(A)p(B|A)p(C|B)p(D|C)$$

- Assume each variable can take on k different values.

Example: Simple chain

- The goal is to compute the marginal $p(D)$:

$$p(D) = \sum_{A,B,C} p(A, B, C, D)$$

- However, if we do this sum naively, cost is exponential $O(k^{n=4})$:

$$\begin{aligned} p(D) &= \sum_{A,B,C} p(A, B, C, D) \\ &= \sum_C \sum_B \sum_A p(A)p(B|A)p(C|B)p(D|C) \end{aligned}$$

- Instead, choose an **elimination ordering**:

$$\begin{aligned} p(D) &= \sum_{C,B,A} p(A, B, C, D) \\ &= \sum_C p(D|C) \left(\sum_B p(C|B) \left(\sum_A p(A)p(B|A) \right) \right). \end{aligned}$$

Example: Simple chain

- This reduces the complexity by first computing terms that appear across the other sums.

$$p(D) = \sum_C p(D|C) \sum_B p(C|B) \sum_A p(A)p(B|A)$$

•

$$\begin{aligned} p(D) &= \sum_C p(D|C) \sum_B p(C|B) \sum_A p(A)p(B|A) \\ &= \sum_C p(D|C) \sum_B p(C|B)p(B) \\ &= \sum_C p(D|C)p(C) \end{aligned}$$

- The cost of performing inference on the chain in this manner is $\mathcal{O}(nk^2)$. In comparison, generating the full joint distribution and marginalizing over it has complexity $\mathcal{O}(k^n)$!

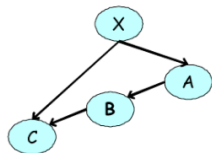
Best Elimination Ordering

- The complexity of variable elimination depends on the elimination ordering!
- Unfortunately, finding the best elimination ordering is NP-hard.

Intermediate Factors

The same algorithm both for DAGMs and MRFs:

- Introduce nonnegative **factors** ϕ (like for MRFs).
- e.g. in a simple DAG model:



$$\begin{aligned} p(A, B, C) &= \sum_X p(X)p(A|X)p(B|A)p(C|B, X) \\ &= \sum_X \phi_1(X)\phi_2(A, X)\phi_3(A, B)\phi_4(X, B, C) \\ &= \phi_3(A, B) \sum_X \phi_1(X)\phi_2(A, X)\phi_4(X, B, C) \\ &= \phi_3(A, B)\tau(A, B, C) \end{aligned}$$

- Marginalizing over X we introduce a new factor, denoted by τ .

Sum-Product Inference

- Abstractly, computing $p(x_F|x_E)$ is given by the **sum-product** algorithm:

$$p(x_F|x_E) \propto \tau(x_F, x_E) = \sum_{x_R} \prod_{C \in \mathcal{F}} \psi_C(x_C)$$

where $\mathcal{F}$ is a set of potentials or factors.

- For DAGMs, $\mathcal{F}$ is given by the the sets of the form

$$\{i\} \cup \text{parents}(i) \quad \text{for all nodes } i.$$

- For MRFs, $\mathcal{F}$ is given by the set of maximal cliques.

Example



- This describes a factorization:

$$p(C, D, I, G, S, L, H, J) = p(C)p(D|C)p(I) \\ \times p(G|D, I)p(L|G)p(S|I)p(J|S, L)p(H|J, G)$$

We have

$$\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G\}\}$$

We are interested in the probability of getting a job, $p(J)$.

We perform exact inference as follows.

Example ($\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G\}\}$)

Elimination Ordering (generally, will be given in this course): $\prec \{C, D, I, H, G, S, L\}$

$$\begin{aligned}
 p(J) &= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \sum_I \psi(S, I) \psi(I) \sum_D \psi(G, D, I) \underbrace{\sum_C \psi(C) \psi(C, D)}_{\tau(D)} \\
 &= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \sum_I \psi(S, I) \psi(I) \underbrace{\sum_D \psi(G, D, I) \tau(D)}_{\tau(G, I)} \\
 &= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \underbrace{\sum_I \psi(S, I) \psi(I) \tau(G, I)}_{\tau(S, G)} \\
 &= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \tau(S, G) \underbrace{\sum_H \psi(H, G, J)}_{\tau(G, J)} \\
 &= \sum_L \sum_S \psi(J, L, S) \underbrace{\sum_G \psi(L, G) \tau(S, G) \tau(G, J)}_{\tau(J, L, S)} \\
 &= \sum_L \underbrace{\sum_S \psi(J, L, S) \tau(J, L, S)}_{\tau(J, L)} \\
 &= \underbrace{\sum_L \tau(J, L)}_{\tau(J)} \\
 &= \tau(J)
 \end{aligned}$$

Do we need to normalize the final τ ?

Complexity of Variable Elimination Ordering

- We discussed previously that variable elimination ordering determines the computational complexity. This is due to how many variables appear inside each sum.
- Different elimination orderings will involve different number of variables appearing inside each sum.
- The complexity of the VE algorithm is

$$O(mk^{N_{\max}})$$

where

- ▶ m is the number of initial factors.
- ▶ k is the number of states each random variable takes (assumed to be equal here).
- ▶ N_i is the number of random variables inside each sum $\sum_i$.
- ▶ $N_{\max} = \max_i N_i$ is the number of variables inside the largest sum.

Example

Elimination Ordering $\prec \{C, D, I, H, G, S, L\}$

- Here are all the initial factors:

$$\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G\}\}$$

$$\implies m = |\Phi| = 8$$

- Here are the sums, and the number of variables that appear in them

$$\begin{array}{ccc} \underbrace{\sum_C \psi(C) \psi(C, D)}_{N_C=2} & \underbrace{\sum_D \psi(G, D, I) \tau(D)}_{N_D=3} & \underbrace{\sum_I \psi(S, I) \psi(I) \tau(G, I)}_{N_I=3} \\ \underbrace{\sum_H \psi(H, G, J)}_{N_H=3} & \underbrace{\sum_G \psi(L, G) \tau(S, G) \tau(G, J)}_{N_G=4} & \underbrace{\sum_S \psi(J, L, S) \tau(J, L, S)}_{N_S=3} \\ \underbrace{\sum_L \tau(J, L)}_{N_L=2} & \implies \text{the largest sum is } N_G = 4. & \end{array}$$

- For simplicity, assume all variables take on k states. So the complexity of the variable elimination under this ordering is $O(8 \cdot k^4)$.

Undirected graphical models:

- MRFs are useful if there is no topological ordering in the graph.
- Cliques are key to parametrizing distributions induced by MRFs.
- Ising model and Gaussian graphical models are important examples.

Variable elimination:

- Variable elimination can be used for exact inference in PGMs.
- The ordering in variable elimination can significantly reduce the computational complexity.
- The overall complexity of the variable elimination algorithm can be computed.