

STA414: Statistical Methods for Machine Learning II

Lecture Notes

Yiliu Cao

May 3, 2024

Contents

1	Probabilistic models	2
1.1	An overview of probabilistic models	2
1.2	Statistical decision theory	3
2	Graphical Models	5
2.1	Introduction to graphical models	5
2.2	Directed Acyclic Graphical Models	6
2.3	Undirected Graphical Models	9
3	Exact Inference	12
3.1	Introduction to exact inference	12
3.2	Sum-product algorithm	14
4	Message passing	15
4.1	TrueSkill latent variable models	15
4.2	Message Passing	15
4.3	Belief Propagation on Trees	17
5	Monte Carlo Methods	18
6	Appendix	19
6.1	Example 1	19
6.2	Example 2	20
6.3	Derivations 1	21
6.4	Example 3	21

1 Probabilistic models

1.1 An overview of probabilistic models

We have the random vector $X = (X_1, X_2, \dots, X_n)$, and we want to compute the relationship between each random variable. The joint distribution is $p(x) = p(x_1, \dots, x_d)$. Denote the input data \mathbf{x} (high-dimensional), and output y (discrete or continuous). In general, we have two models:

Regression:

$$p(y|x) = \frac{p(x, y)}{p(x)} = \frac{p(x, y)}{\int p(x, y) dy}$$

Classification/Clustering:

$$p(c|x) = \frac{p(x, c)}{\sum_c p(x, c)}$$

Observed vs Unobserved random variables

Supervised classification(learning):

- We **KNOW** what to predict
- **Supervised Dataset:** $\{x^{(i)}, c^{(i)}\}_{i=1}^N \sim p(x, c)$
- The class labels are observed.

Unsupervised classification(learning):

- We do **NOT KNOW** what to predict
- **Unsupervised Dataset:** $\{x^{(i)}\}_{i=1}^N \sim p(x) = \sum_c p(x, c)$
- We only observe the inputs \mathbf{x}

In order to estimate the unknown distribution $p(x)$, we have few assumptions:

1. **IID Data:** we assume the samples $x^{(i)}$ are independent and identically distributed.
2. **Parametrized distribution:** $p(x|\theta)$ comes from a parametrized family $\mathcal{P} = \{p(x|\theta) : \theta \in \Theta\}$

Maximum Likelihood Estimation(MLE)

MLE is the method to estimate the parameters of an assume probability distribution, given some observed data. Technically, we can use MLE to estimate any parameters we want. More specifically:

- Let $x^{(i)} \sim p_* = p(x|\theta_*)$ for $i = 1, \dots, N$ be i.i.d. random variables.
- The joint of $\mathcal{D} = \{x^{(1)}, x^{(2)}, \dots, x^{(N)}\}$ is $p(\mathcal{D}|\theta_*) = \prod_i p(x^{(i)}|\theta_*)$.

- Assume we observe data \mathcal{D} and θ_* is unknown. The likelihood function is:

$$\mathcal{L}(\theta; \mathcal{D}) = p(\mathcal{D}|\theta) = \prod_{i=1}^N p(x^{(i)}|\theta)$$

- The log-likelihood function:

$$\ell(\theta; \mathcal{D}) = \log \mathcal{L}(\theta; \mathcal{D}) = \sum_{i=1}^N \log p(x^{(i)}|\theta)$$

Here is an example of MLE

Sufficient Statistics and Exponential Families

A **sufficient statistics** is a function of the data that conveys exactly the same information about the parameter as the entire data.

In addition, we can writing any exponential family member in the form:

$$p(x|\eta) = h(x) \exp\{\eta^\top T(x) - A(\eta)\}$$

where

$T(x)$: sufficient statistics

η : natural parameter

$A(\eta)$: log-partition function

$h(x)$: carrying measure

Moreover, let $X \sim p(x|\eta)$, then we have $E[T(X)] = A'(\eta)$

One example of exponential family

1.2 Statistical decision theory

Suppose we have an input vector x and the corresponding target, we want to predict the label given a new input. Notice that here we assume the output is the label/class which is discrete. However, the output can also be continuous (regression).

Intuitively, for a given new input x , we have:

$$p(\mathcal{C}_k|x) = \frac{p(x|\mathcal{C}_k)p(\mathcal{C}_k)}{p(x)}$$

We then pick the \mathcal{C}_k with the highest probability.

Decision Rule: Divide the input space to \mathcal{R}_1 & \mathcal{R}_2 such that all points in \mathcal{R}_k are assigned to class \mathcal{C}_k . We want to make mistakes as less as possible; equivalently, we want to minimize the **misclassification rate**.

For $k \in \{1, 2\}$:

$$p(\text{mistake}) = p(x \in \mathcal{R}_2, \mathcal{C}_1) + p(x \in \mathcal{R}_1, \mathcal{C}_2) = \int_{\mathcal{R}_1} p(x, \mathcal{C}_2) dx + \int_{\mathcal{R}_2} p(x, \mathcal{C}_1) dx \quad (1.1)$$

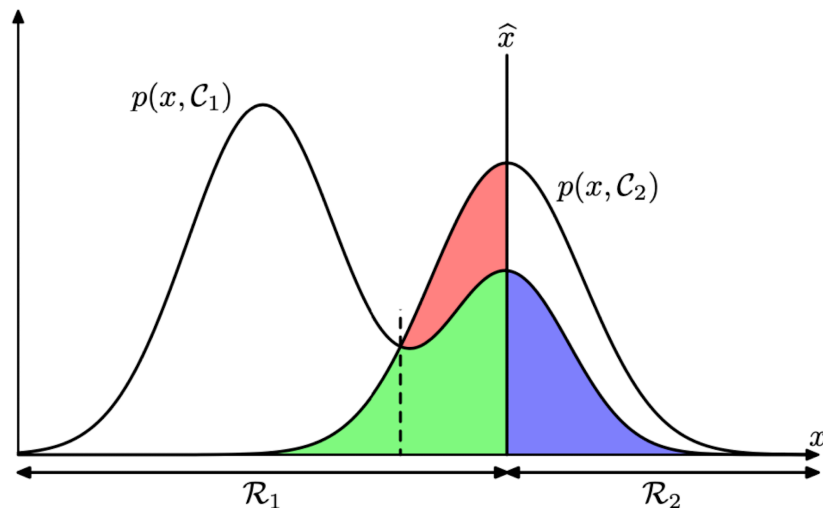


Figure 1.1: Misclassification Rate

1. **RedGreen regions:** inputs that belong to \mathcal{C}_2 but assigns to \mathcal{R}_1 as they are under $p(x, \mathcal{C}_2)$.
2. **Blue regions:** inputs that belong to \mathcal{C}_1 but assigns to \mathcal{R}_2 as they are under $p(x, \mathcal{C}_1)$
3. Therefore, for any data \mathbf{x} , if $p(x, \mathcal{C}_1) > p(x, \mathcal{C}_2)$, then we assign this point to \mathcal{C}_1 , vice-versa. Therefore, $\mathcal{R} = \{x : p(x, \mathcal{C}_1) > p(x, \mathcal{C}_2)\}$

We want to minimize the misclassification error rate \Rightarrow minimize the **loss**

Loss Function

Loss function measures the loss incurred by taking of any available decisions.

For discrete case

we denote L_{ij} as the (i, j) element of the loss matrix. We want to minimize the expected loss

Therefore:

$$\begin{aligned}\mathbb{E}[L] &= \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(x, \mathcal{C}_k) dx \\ &= \sum_j \int_{\mathcal{R}_j} \sum_k L_{kj} p(x, \mathcal{C}_k) dx\end{aligned}$$

Define $g_j(x) = \sum_k L_{kj} p(x, \mathcal{C}_k)$. Notice that $g_j(x) \geq 0$ and

$$\mathbb{E}[L] = \sum_j \int_{\mathcal{R}_j} g_j(x) dx$$

Thus, minimizing $\mathbb{E}[L]$ is equivalent to choosing

$$\mathcal{R}_j = \{x : g_j(x) < g_i(x) \text{ for all } i \neq j\} \quad (1.2)$$

$$\Rightarrow \mathcal{R}_j = \left\{ x : \sum_k L_{kj} p(\mathcal{C}_k | x) < \sum_k L_{ki} p(\mathcal{C}_k | x) \text{ for all } i \neq j \right\} \quad (1.3)$$

For regression

- Consider the input/target (x, t) , where t is continuous and the joint density is $p(x, t)$
- The regression function is $y(x)$
- The loss function is $L(y(x), t) = (y(x) - t)^2$

Therefore the expected loss will be:

$$\begin{aligned} \mathbb{E}[L] &= \iint L(y(x), t) p(x, t) dx dt \\ &= \iint (y(x) - \mathbb{E}[t | x])^2 p(x, t) dx dt + \iint (\mathbb{E}[t | x] - t)^2 p(x, t) dx dt \end{aligned}$$

Full derivations here

The second term is the conditional variance of $t|x$ and does not depend on $y(x)$ and hence the expected loss is minimized when $y(x) = \mathbb{E}[t|x]$. Therefore, we can see that the loss function will change the decision rule significantly; however, we can always reject the option or not making a decision.

2 Graphical Models

2.1 Introduction to graphical models

Remember our goal is to specify the joint distribution N random variables $p(x_1, \dots, x_N) = p(x)$. If we assume each x_i is binary such that $x_i \in \{0, 1\}$, then we need $2^N - 1$ parameters to specify $p(x)$. For example, $p(x_1 = 0, x_2 = 0, \dots, x_N = 0)$ or $p(x_1 = 1, x_2 = 0, \dots, x_N = 0)$.

Equivalently, we can specify the joint distribution $p(x)$ as:

$$\begin{aligned} p(x_1, x_2, \dots, x_N) &= \prod_{j=1}^N p(x_j | x_1, x_2, \dots, x_{j-1}) \\ &= p(x_1 | x_0) p(x_2 | x_1, x_0) \dots \end{aligned}$$

Thus total number of parameters is $1 + 2 + 4 + \dots + 2^{N-1} = 2^N - 1$

We can see that it requires a huge number of parameters to specify the joint distribution. We want to draw relationships between variables.

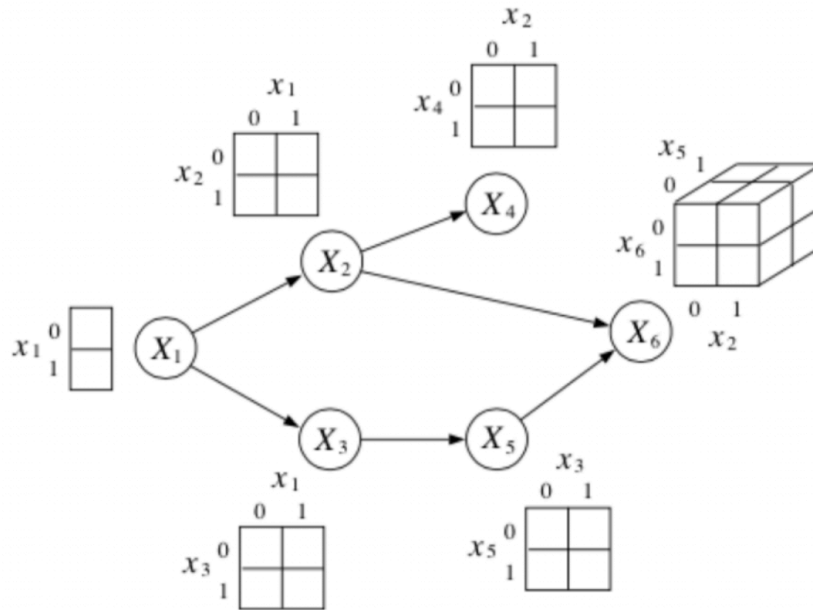


Figure 2.1: An example of conditional probability tables(CPT)

Condition independence

For three random variables x_A, x_B, x_C , if x_A, x_B are conditionally independent given x_C , then we write $x_A \perp x_B \mid x_C$. The following conditions are equivalent:

- $x_A \perp x_B \mid x_C$
- $p(x_A, x_B \mid x_C) = p(x_A \mid x_C)p(x_B \mid x_C)$
- $p(x_A \mid x_B, x_C) = p(x_A \mid x_C)$
- $p(x_B \mid x_A, x_C) = p(x_B \mid x_C)$

2.2 Directed Acyclic Graphical Models

A directed cyclic graphical model encode a particular form of factorization of the joint distribution. The form of factorization is various.

Figure 2 shows an example of conditional probability. From the graph, we only need $2^1 * 4 + 2^0 + 2^2 = 13 < 2^6 - 1$ parameters.

D-separation: If C d-separates A and B , then $x_A \perp x_B \mid x_C \forall a \in A, b \in B$

Bayes ball algorithm

Bayes ball determines the conditional independence/dependence in a DAG (I personally found this part most ambiguous). There are three fundamental Bayes ball algorithms which are causal chain, common cause and explaining away. For each one, we will under it intuitively by drawing a story.

1. Causal chain

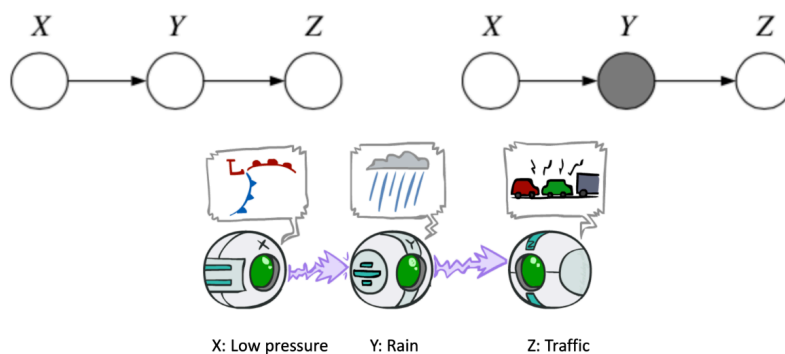


Figure 2.2: An illustration of causal chain

$$\begin{aligned}
 p(z \mid x, y) &= \frac{p(x, y, z)}{p(x, y)} \\
 &= \frac{p(x)p(y \mid x)p(z \mid y)}{p(x)p(y \mid x)} \\
 &= p(z \mid y) \\
 \Rightarrow X \text{ and } Z \text{ d-separated given } Y
 \end{aligned}$$

2. Common cause

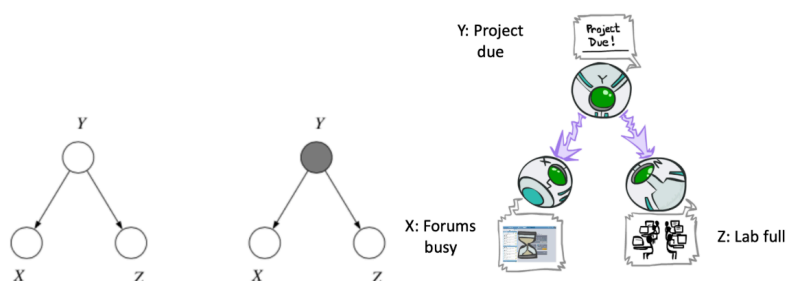


Figure 2.3: An illustration of common cause

$$\begin{aligned}
 p(x, z \mid y) &= \frac{p(x, y, z)}{p(y)} \\
 &= \frac{p(y)p(x \mid y)p(z \mid y)}{p(y)} \\
 &= p(x \mid y)p(z \mid y) \\
 \Rightarrow X \text{ and } Z \text{ d-separated given } Y
 \end{aligned}$$

3. Explaining away

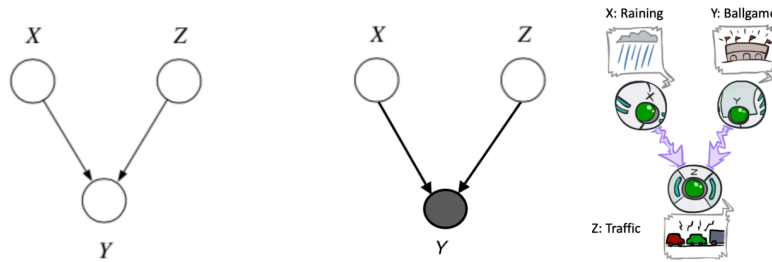


Figure 2.4: An illustration of explaining away

$$\begin{aligned}
 p(z \mid x, y) &= \frac{p(x)p(z)p(y \mid x, z)}{p(x)p(y \mid x)} \\
 &= \frac{p(z)p(y \mid x, z)}{p(y \mid x)} \neq p(z \mid y) \\
 \Rightarrow X \text{ and } Z \text{ are NOT d-separated given } Y
 \end{aligned}$$

In general, the Bayes ball works as follows:

1. Shade all nodes x_C (these are observed)
2. Place "balls" at each node in x_A (or x_B)
3. Let the "balls" "bounce" around according to some rules. If any of the balls reach any of the nodes in x_B from x_A then $x_A \not\perp x_B \mid x_C$. Otherwise $x_A \perp x_B \mid x_C$

Example

Question: Is $x_2 \perp x_3 \mid \{x_1, x_6\}$

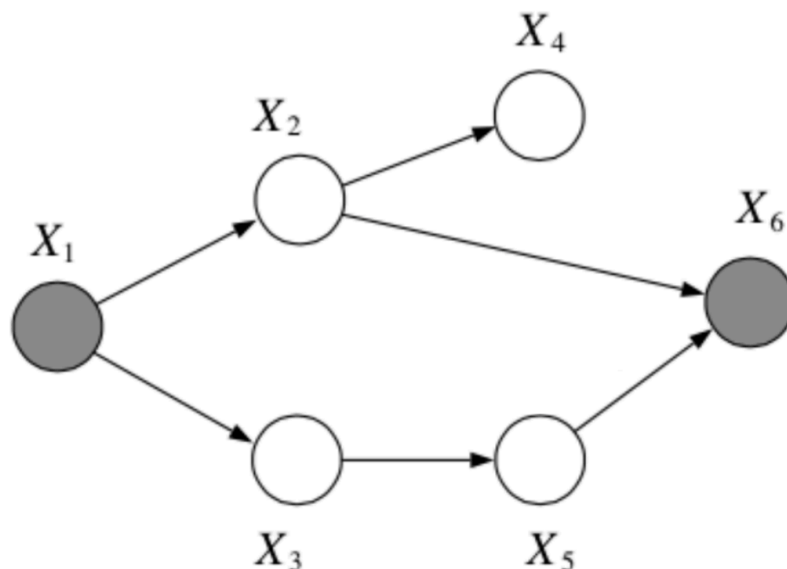


Figure 2.5: An illustration of explaining away

Answer: No. By Bayes ball algorithm, x_2 can travel to x_5 , and hence can travel to x_3 .

Moralization

Like I said, I personally do not like Bayes algorithm. Instead, another one called "moralization" is more straightforward and easier to use. We can follow the procedure:

1. **Draw the ancestral graph**

We only keep the ancestor of the mentioned nodes. That said, in the previous example, we only keep the ancestors of $\{x_2, x_3, x_1, x_6\}$. Hence we have the entire graph except the node x_4 . Note the ancestors includes **their parents, parents' parents etc.**

2. **"Moralize" the ancestral graph by "marrying" the parents**

If two nodes have the same children, such as x_2 and x_5 , then we draw a line between these two nodes.

3. **"Disorient" the graph**

Ignore the directions by replacing the arrows to edges.

4. **Delete the givens and their edges**

In the previous example, the givens are the x_1 and x_4 .

5. **Find the answer**

After we finished the step 1 to 4, we then justify whether the two nodes are connected or disconnected. If **connected**, then the two nodes are conditionally **dependent**. Otherwise **disconnected**, the two nodes are conditionally **independent**. In the previous example, we can easily find that x_2 and x_3 are d-separated by x_1 and x_6 .

Question: What about the marginal independence, such as $x_2 \perp x_3$?

Answer: We use the same way as above without step 4.

2.3 Undirected Graphical Models

The undirected graphical models are also called the **Markov random fields (MRFs)**. Compare to graphical models, we have no more directed edges; instead, the dependencies are now described as undirected graphs. Moreover, **Markov blanket** is the set of nodes that makes X_i conditionally independent of all other nodes. **Clique** is a subset of nodes that every two nodes are connected by an edge. **Maximal clique** a clique that can not be extended by including one more adjacent vertex.

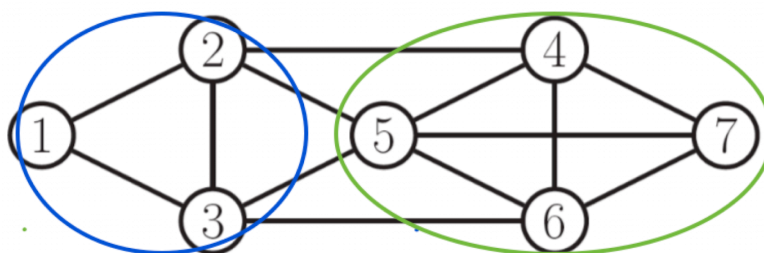


Figure 2.6: An example of Markov random fields: $\{1, 2, 3\}$ is a clique and $\{4, 5, 6, 7\}$ is a maximal clique

Distribution induced by MRFs

- Let $X = (X_1, \dots, X_m)$ 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

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

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

The density can be factorized to cliques is also called the **Hammersley-Clifford Theorem**.

Global markov properties: $X_A \perp X_B \mid X_S$ if the sets A and B are separated by S in G (every path from A to B has to pass S). Therefore, the joint distribution described on above is:

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

Not all DAGMs can be represented as MRFs. .

Relations between exponential families and MRFs

- Consider a parametric family of factorized distributions

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

- We can write this in an exponential form:

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

- Suppose the potentials have a log-linear form

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

we then get the exponential family

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

Question: When the potentials have a log-linear form?

Solution: Suppose we have the random vector x_1 and x_2 , and they are all binary. Then

there are four possible values of (x_1, x_2) : $(0, 0)$, $(1, 0)$, $(0, 1)$, $(1, 1)$. We take

$$\theta_{1,2} := \begin{bmatrix} \log \psi_{1,2}(0, 0) \\ \log \psi_{1,2}(0, 1) \\ \log \psi_{1,2}(1, 0) \\ \log \psi_{1,2}(1, 1) \end{bmatrix} \in \mathbb{R}^4$$

and let $\psi_{1,2}(x_1, x_2)$ be the function that satisfies

$$\begin{aligned} \phi_{1,2}(0, 0) &= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \phi_{1,2}(0, 1) = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \phi_{1,2}(1, 0) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \phi_{1,2}(1, 1) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}. \\ \Rightarrow \phi_{1,2}(x_1, x_2) &= \begin{bmatrix} (1-x_1)(1-x_2) \\ (1-x_1)x_2 \\ x_1(1-x_2) \\ x_1x_2 \end{bmatrix} \end{aligned}$$

We then have a linear form:

$$\log \psi_C(x_{12} \mid \theta_{12}) = \theta_{12}^\top \phi_{12}(x_{12})$$

Ising model

The Ising model is an example of MRFs, which is used to model magnets. It has a form of potential function:

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

Equivalently:

$$\begin{aligned} \psi_{st}(-1, -1) &= \psi_{st}(1, 1) = e^{J_{st}} \\ \psi_{st}(1, -1) &= \psi_{st}(-1, 1) = e^{-J_{st}} \\ \psi_{st}(x_s, x_t) &= 0 \text{ if the two nodes are not connected} \end{aligned}$$

In terms of the distribution in Ising model, we also include the node potential $\psi_s(x_s) = e^{b_sx_s}$:

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

Recall: Multivariate normal distribution

$X = (X_1, \dots, X_m) : \mu \in \mathbb{R}^m$ and Σ symmetric positive definite $m \times m$ matrix. Write $X \sim N_m(\mu, \Sigma)$ if the density of the vector X is

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

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

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

Intuitively, we can also visualize the conditional independencies between each variables (similar to Bayes ball). Just like the Ising model, here we can use concentration matrix K to represent the relationship between variables.

Conditional independence:

- $X_i \perp X_j$ if and only if $\Sigma_{ij} = 0$.
- $X_i \perp X_j \mid X_C$ 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:
 - $X_i \perp X_j \mid X_R$
 - $\Sigma_{ij} - \Sigma_{i,R} \Sigma_{R,R}^{-1} \Sigma_{R,j} = 0$
 - $(\Sigma^{-1})_{ij} = 0$

Hence we have the **Gaussian Graphical models**

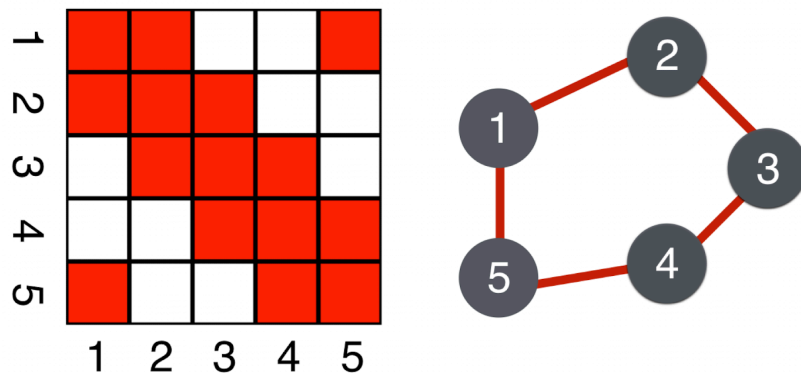


Figure 2.7: An example of Gaussian Graphical model

$K_{ij} = 0$ if and only if $X_i \perp X_j \mid X_{rest}$. For example, $X_1 \perp X_4 \mid X_{rest}$

3 Exact Inference

3.1 Introduction to exact inference

We want to explore the inference from the probabilistic graphical models. In notations, we have

- x_E represent the observed evidence
- x_F represent the unobserved variable we want to infer
- $x_R = x \setminus \{x_E, x_F\}$ represent the remaining variables

For the conditional probability $p(x_F | x_E)$, by Bayes theorem:

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

Moreover, we can also marginalize the extraneous variables to have the marginal joint distribution:

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

The below equation give us an intuition of exact inference, which is to marginalize other variables. However, when the number of variables increases, the order we marginalize will affect the computational cost. Hence we have to choose an appropriate **elimination order**. More specifically, we want to have the exact inference for one variable in DAGMs or MRFs.

Example 3.1.1. Suppose we have the simple chain for four variables A, B, C, D

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

where:

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

We want to compute the exact inference of D , $p(D)$ In the simple chain settings, we can express the joint distribution as:

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

If we choose an elimination order:

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

The above example give us an intuition that we can firstly marginalize the node with no children (C first). Equivalently, we start the nodes that comes early in the induced ordering of the DAG.

3.2 Sum-product algorithm

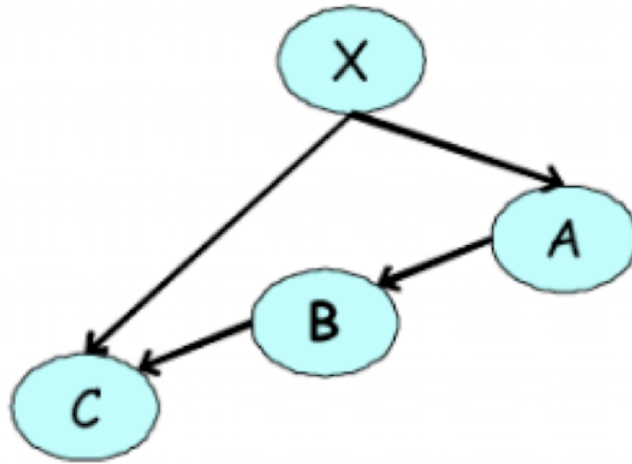


Figure 3.1: An example of Sum-product inference

Example 3.2.1.

To express the joint distribution, we introduce the nonnegative factors ψ :

$$\begin{aligned}
 p(A, B, C) &= \sum_X p(A, B, C, X) \\
 &= \sum_X p(X) p(A | X) p(B | A) p(C | B, X) \\
 &= \sum_X \psi_1(X) \psi_2(A, X) \psi_3(A, B) \psi_4(X, B, C) \\
 &= \psi_3(A, B) \sum_X \psi_1(X) \psi_2(A, X) \psi_4(X, B, C) \\
 &= \psi_3(A, B) \tau(A, B, C)
 \end{aligned}$$

We eventually end with a new factor τ and it is an example of how sum-product algorithm works.

In general, we compute the conditional distribution $p(x_F | x_E)$ using the **sum-product algorithm**. Denote \mathcal{F} as the set of potentials or factors.

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

For DAGMs, \mathcal{F} is $\{i\} \cup \text{parents}(i)$, \forall nodes i

For MRFs, \mathcal{F} is all maximal cliques.

We will see more about exact inference on message passing

4 Message passing

4.1 TrueSkill latent variable models

Latent variables are variables that can only be inferred indirectly through a mathematical model from other observable variables that can be directly observed or measured.

TrueSkill model is a player ranking system for competitive games. Our goal is to infer the skills of players in a competitive game, based on the results of the games. Hence, each player's skill is a **latent variable**, and we assume they are fixed. Moreover, we also assume each player's skill is independent such as independent Gaussian prior.

For each game, the probability that player i beats player j is

$$p(i \text{ beats } j) = \sigma(z_i - z_j), \text{ where}$$

$$\sigma(y) = \frac{1}{1 + \exp(-y)}$$

Hence the entire joint likelihood of players and games is:

$$\begin{aligned} p(z_1, z_2, \dots, z_N, \text{ game 1, game 2, .. game } T) \\ = \underbrace{\left[\prod_{i=1}^N p(z_i) \right]}_{\text{prior}} \underbrace{\left[\prod_{\text{games}} p(i \text{ beats } j \mid z_i, z_j) \right]}_{\text{likelihood}} \end{aligned}$$

However, it is hard to compute the posterior

$$\begin{aligned} p(z_1, z_2 \mid \text{ game 1, game 2, } \dots \text{ game } T) \\ = \int \dots \int p(z_1, z_2, z_3 \dots z_N \mid x) dz_3 \dots dz_N \end{aligned}$$

Message passing can help us to compute the posterior.

4.2 Message Passing

From the last section, we can see that determining an optimal elimination order is hard, and the resulting marginalization can be still costly. Therefore, we introduce the tress as any elimination ordering from leaves to the root is optimal.

Inference in trees

A graph is $G = (\mathcal{V}, \mathcal{E})$, where \mathcal{V} is vertices and \mathcal{E} is edges. A leaf in a tree is the nodes where it has only one neighbor. We can regard a tress as MRFs, with joint distribution:

$$p(x_1, x_2, \dots, x_n) = \underbrace{\frac{1}{Z}}_{\text{normalization}} \underbrace{\prod_{i \in \mathcal{V}} \psi(x_i)}_{\text{nodes}} \underbrace{\prod_{(i,j) \in \mathcal{E}} \psi_{ij}(x_i, x_j)}_{\text{edges}}$$

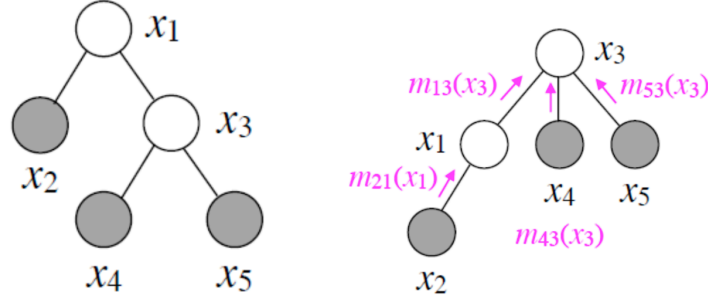


Figure 4.1: An example of tree and message passing

Example 4.2.1. Above shows a tree where $x_E = \{\bar{x}_2, \bar{x}_4, \bar{x}_5\}$, $x_R = x_1$. We want to compute $p(x_3 | x_E)$:

$$\begin{aligned} p(x_3 | x_E) &= \frac{p(x_3, x_E)}{\sum_{x'_3} p(x'_3, x_E)} \\ &= \frac{1}{Z_E} p(x_3, x_E) \end{aligned}$$

Express $p(x_3, x_E)$, we have

$$\begin{aligned} &= \sum_{x_1} \psi_1(x_1) \psi_2(\bar{x}_2) \psi_3(x_3) \psi_4(\bar{x}_4) \psi_5(\bar{x}_5) \psi_{12}(x_1, \bar{x}_2) \psi_{13}(x_1, x_3) \psi_{34}(x_3, \bar{x}_4) \psi_{35}(x_3, \bar{x}_5) \\ &= \frac{1}{Z_E} \underbrace{\psi_4(\bar{x}_4) \psi_{34}(x_3, \bar{x}_4)}_{m_{43}(x_3)} \underbrace{\psi_5(\bar{x}_5) \psi_{35}(x_3, \bar{x}_5)}_{m_{53}(x_3)} \psi_3(x_3) \sum_{x_1} \underbrace{\psi_1(x_1) \psi_{13}(x_1, x_3)}_{m_{13}(x_3)} \underbrace{\psi_2(\bar{x}_2) \psi_{12}(x_1, \bar{x}_2)}_{m_{21}(x_1)} \\ &= \frac{1}{Z_E} m_{43}(x_3) m_{53}(x_3) \psi_3(x_3) \underbrace{\sum_{x_1} \psi_1(x_1) \psi_{13}(x_1, x_3) m_{21}(x_1)}_{m_{13}(x_3)} \\ &= \frac{1}{Z_E} \psi_3(x_3) m_{43}(x_3) m_{53}(x_3) m_{13}(x_3) \\ &= \frac{\psi_3(x_3) m_{43}(x_3) m_{53}(x_3) m_{13}(x_3)}{\sum_{x'_3} \psi_3(x'_3) m_{43}(x'_3) m_{53}(x'_3) m_{13}(x'_3)} \end{aligned}$$

Sum-product algorithm

The above example shows how we can pass the message and eventually compute the conditional distribution. For each passed message such as $m_{43}(x_3)$, it uses the sum-product algorithm we introduced in the chapter of exact inference. To summarize, we have:

- If x_j **unobserved**, the message sent from variable j to $i \in N(j)$ is

$$m_{j \rightarrow i}(x_i) = \sum_{x_j} \psi_j(x_j) \psi_{ij}(x_i, x_j) \prod_{k \in N(j) \setminus i} m_{k \rightarrow j}(x_j)$$

- If x_j is **observed**, the message is

$$m_{j \rightarrow i}(x_i) = \psi_j(\bar{x}_j) \psi_{ij}(x_i, \bar{x}_j) \prod_{k \in N(j) \setminus i} m_{k \rightarrow j}(\bar{x}_j)$$

- Once the message passing stage is complete, we can compute our beliefs as

$$b(x_i) = p(x_i | x_E) \propto \psi_i(x_i) \prod_{j \in N(i)} m_{j \rightarrow i}(x_i).$$

4.3 Belief Propagation on Trees

The above algorithm shows how the message is passed from the leaves to the root. In a formal setting, we have four steps:

1. Choose the root r arbitrarily.
2. Pass the message from leaves to r .
3. **Pass the message from the root to the leafs.** Note that here we only pass the message from the root to the **unobserved** nodes.
4. Compute the beliefs/marginals for all unobserved nodes.

Example 4.3.1. We can still infer the previous example (image), and shows the complete belief propagation process. From Figure 4.1, our goal is to compute the beliefs

$$p(x_3 | \bar{x}_2, \bar{x}_4, \bar{x}_5)$$

and

$$p(x_1 | \bar{x}_2, \bar{x}_4, \bar{x}_5)$$

Step 1: Choose x_3 to be our root.

Step 2: Pass the message from leaves to x_3 .

$$\begin{aligned} m_{5 \rightarrow 3}(x_3) &= \psi_5(\bar{x}_5) \psi_{35}(x_3, \bar{x}_5) \\ m_{2 \rightarrow 1}(x_1) &= \psi_2(\bar{x}_2) \psi_{12}(x_1, \bar{x}_2) \\ m_{4 \rightarrow 3}(x_3) &= \psi_4(\bar{x}_4) \psi_{34}(x_3, \bar{x}_4) \\ m_{1 \rightarrow 3}(x_3) &= \sum_{x_1} \psi_1(x_1) \psi_{13}(x_1, x_3) m_{2 \rightarrow 1}(x_1) \end{aligned}$$

Step 3: Pass the message from the root to other unobserved nodes:

$$m_{3 \rightarrow 1}(x_1) = \sum_{x_3} \psi_3(x_3) \psi_{13}(x_1, x_3) m_{4 \rightarrow 3}(x_3) m_{5 \rightarrow 3}(x_3)$$

Step 4: Calculate the beliefs for x_1 and x_3 .

$$\begin{aligned} b(x_1) &\propto \psi_1(x_1) m_{2 \rightarrow 1}(x_1) m_{3 \rightarrow 1}(x_1) \\ b(x_3) &\propto \psi_3(x_3) m_{1 \rightarrow 3}(x_3) m_{4 \rightarrow 3}(x_3) m_{5 \rightarrow 3}(x_3) \end{aligned}$$

Loopy Belief Propagation

The inference we just introduced has limits that the graph (MRF) must be a tree. However, in most cases such as TrueSkill models, we do not have such prerequisites. What we do instead is to keep passing the message until convergence. This is called the Loopy Belief Propagation. It works as follows:

- Initialize all messages uniformly:

$$m_{i \rightarrow j}(x_j) = (1/k, \dots, 1/k)$$

where k is the number of states x_j can take.

- Keep running BP updates until **the messages** "converges":

$$m_{j \rightarrow i}(x_i) = \sum_{x_j} \psi_j(x_j) \psi_{ij}(x_i, x_j) \prod_{k \in N(j) \setminus i} m_{k \rightarrow j}(x_j)$$

and (sometimes) normalized for stability.

- It will generally not converge, but often works fine.
- Compute beliefs $b(x_i) \propto \psi_i(x_i) \prod_{j \in N(i)} m_{j \rightarrow i}(x_i)$.

Max-product belief propagation

The main difference between the sum-product and max-product belief propagation is that we are now **maximizing** over x_j instead of summarizing them.

$$m_{j \rightarrow i}(x_i) = \max_{x_j} \psi_j(x_j) \psi_{ij}(x_i, x_j) \prod_{k \in N(j) \setminus i} m_{k \rightarrow j}(x_j)$$

Now the beliefs are called max-marginals:

$$\hat{b}(x_i) = \max_{x_i} p(x_i, x_{\setminus i}) \propto \psi_i(x_i) \prod_{j \in N(i)} m_{j \rightarrow i}(x_i).$$

MAP inference: take $\hat{x}_i := \arg \max_{x_i} \hat{b}(x_i)$ for all $i \notin E$.

Here is a numerical example of message passing.

5 Monte Carlo Methods

6 Appendix

6.1 Example 1

The Bernoulli Naïve Bayes model parameterized by θ and π defines the following joint probability of x and c ,

$$p(x, c | \theta, \pi) = p(c | \pi) p(x | c, \theta) = p(c | \pi) \prod_{j=1}^D p(x_j | c, \theta),$$

where $x_j | c, \theta \sim \text{Bernoulli}(\theta_{jc})$, i.e. $p(x_j | c, \theta) = \theta_{jc}^{x_j} (1 - \theta_{jc})^{1-x_j}$, and $c | \pi$ follows a simple categorical distribution, i.e. $p(c | \pi) = \pi_c$.

Solution:

For \mathbf{x}^1 , its likelihood function is:

$$L(\theta, \pi; x^1, c) = \prod_{c=1}^{10} [p(x^1, c | \theta, \pi)]^{1\{c^1=c\}} \quad (6.1)$$

$$= \prod_{c=1}^{10} \left[p(c | \pi) \prod_{j=1}^{784} p(x_j^1 | c, \theta) \right]^{1\{c^1=c\}} \quad (6.2)$$

$$= \prod_{c=1}^{10} \left[\pi_c \prod_{j=1}^{784} \theta_{jc}^{x_j^1} (1 - \theta_{jc})^{1-x_j^1} \right]^{1\{c^1=c\}} \quad (6.3)$$

Therefore, the joint likelihood function for $\mathbf{x}^1, \dots, \mathbf{x}^n$ is:

$$L(\theta, \pi) = \prod_{i=1}^n \prod_{c=1}^{10} \left[\pi_c \prod_{j=1}^{784} \theta_{jc}^{x_j^i} (1 - \theta_{jc})^{1-x_j^i} \right]^{1\{c^i=c\}} \quad (6.4)$$

$$\Rightarrow l(\theta, \pi) = \log \left(\prod_{i=1}^n \prod_{c=1}^{10} \left[\pi_c \prod_{j=1}^{784} \theta_{jc}^{x_j^i} (1 - \theta_{jc})^{1-x_j^i} \right]^{1\{c^i=c\}} \right) \quad (6.5)$$

$$= \sum_{i=1}^n \sum_{c=1}^{10} 1\{c^i = c\} \left\{ \log(\pi_c) + \sum_{j=1}^{784} [x_j^i \log(\theta_{jc}) + (1 - x_j^i) \log(1 - \theta_{jc})] \right\} \quad (6.6)$$

$$= \sum_{i=1}^n \sum_{c=1}^9 1\{c^i = c\} \left\{ \log(\pi_c) + \sum_{j=1}^{784} [x_j^i \log(\theta_{jc}) + (1 - x_j^i) \log(1 - \theta_{jc})] \right\} \quad (6.7)$$

$$+ \sum_{i=1}^n 1\{c^i = 10\} \left\{ \log(1 - \sum_{c=1}^9 \pi_c) + \sum_{j=1}^{784} [x_j^i \log(\theta_{j,10}) + (1 - x_j^i) \log(1 - \theta_{j,10})] \right\} \quad (6.8)$$

If we pick any $c \in [C]$ and $j \in [D]$:

$$\frac{\partial l(\theta, \pi)}{\partial \theta_{jc}} = \sum_{i=1}^n 1\{c^i = c\} \left(\frac{x_j^i}{\theta_{jc}} - \frac{1 - x_j^i}{1 - \theta_{jc}} \right) \quad (6.9)$$

Letting it equal to zero, we have:

$$\hat{\theta}_{jc} = \frac{\sum_{i=1}^n 1\{c^i = c\} x_j^i}{\sum_{i=1}^n 1\{c^i = c\}} \quad (6.10)$$

For π_c :

$$\frac{\partial l(\theta, \pi)}{\partial \pi_c} = \sum_{i=1}^n 1\{c^i = c\} \frac{1}{\pi_c} - \sum_{i=1}^n 1\{c^i = 10\} \frac{1}{1 - \sum_{c=1}^9 \pi_c} \quad (6.11)$$

Letting $n_c = \sum_{i=1}^n 1\{c^i = c\}$, when it equals to zero, we have:

$$n_c(1 - \sum_{c=1}^9 \hat{\pi}_c) = \hat{\pi}_c n_{10}, \quad \text{where } 1 \leq c \leq 9 \quad (6.12)$$

Summation on both sides over $1 \leq c \leq 9$, we have:

$$\sum_{c=1}^9 n_c(1 - \sum_{c=1}^9 \hat{\pi}_c) = \sum_{c=1}^9 \hat{\pi}_c n_{10} \quad (6.13)$$

$$\Rightarrow (n - n_{10})(1 - \sum_{c=1}^9 \hat{\pi}_c) = n_{10} \sum_{c=1}^9 \hat{\pi}_c \quad (6.14)$$

$$\sum_{c=1}^9 \hat{\pi}_c = \frac{n - n_{10}}{n} \quad (6.15)$$

Substituting back, we will have:

$$\hat{\pi}_c = \frac{n_c}{n}, \quad 1 \leq c \leq 9 \quad (6.16)$$

6.2 Example 2

We can write this distribution as an exponential family

$$p(x | \theta) = \theta^x (1 - \theta)^{1-x} \quad (6.17)$$

$$= \exp \{x \log(\theta) + (1 - x) \log(1 - \theta)\} \quad (6.18)$$

$$= \exp \left\{ x \log \left(\frac{\theta}{1 - \theta} \right) + \log(1 - \theta) \right\} \quad (6.19)$$

Here,

$$T(x) = x$$

$$\eta = \log \left(\frac{\theta}{1 - \theta} \right)$$

$$A(\eta) = \log(1 + e^\eta)$$

$$h(x) = 1$$

Notice that $A'(\eta) = \frac{e^\eta}{1+e^\eta} = \theta$ is the mean of $T(X) = X$ and $A''(\eta) = \frac{e^\eta}{(1+e^\eta)^2} = \theta(1 - \theta)$ is the variance of X .

6.3 Derivations 1

We add and subtract $\mathbb{E}[t \mid x]$ and write

$$\begin{aligned}
 \mathbb{E}[L] &= \iint (y(x) - t)^2 p(x, t) dx dt \\
 &= \iint (y(x) - \mathbb{E}[t \mid x] + \mathbb{E}[t \mid x] - t)^2 p(x, t) dx dt \\
 &= \iint (y(x) - \mathbb{E}[t \mid x])^2 p(x, t) dx dt + \iint (\mathbb{E}[t \mid x] - t)^2 p(x, t) dx dt \\
 &\quad + 2 \iint (y(x) - \mathbb{E}[t \mid x])(\mathbb{E}[t \mid x] - t) p(x, t) dx dt
 \end{aligned}$$

The last term is zero since

$$\begin{aligned}
 &\iint (y(x) - \mathbb{E}[t \mid x])(\mathbb{E}[t \mid x] - t) p(x, t) dx dt \\
 &= \iint (y(x) - \mathbb{E}[t \mid x])(\mathbb{E}[t \mid x] - t) p(t \mid x) p(x) dx dt \\
 &= \int (y(x) - \mathbb{E}[t \mid x]) \underbrace{\left\{ \int (\mathbb{E}[t \mid x] - t) p(t \mid x) dt \right\}}_{=0} p(x) dx = 0
 \end{aligned}$$

6.4 Example 3

This shape of tree is from Figure 4.1. To have concrete numbers, suppose all variables are binary $\{0, 1\}$ and take $\psi_i(x_i) \equiv 1$ with

$$\psi_{12} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \psi_{13} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, \quad \psi_{34} = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}, \quad \psi_{35} = \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix}$$

We have

$$p(x_1, x_2, x_3, x_4, x_5) = \frac{1}{Z} \prod_{i=1}^5 \psi_i(x_i) \psi_{12}(x_1, x_2) \psi_{13}(x_1, x_3) \psi_{34}(x_3, x_4) \psi_{35}(x_3, x_5).$$

Since $x_E = \{x_2, x_4, x_5\}$, we can just fix the values of three variables: $\bar{x}_2 = 1, \bar{x}_4 = 1, \bar{x}_5 = 0$. Then

$$p(x_1, 1, x_3, 1, 0) = \frac{1}{Z} \psi_{12}(x_1, 1) \psi_{13}(x_1, x_3) \psi_{34}(x_3, 1) \psi_{35}(x_3, 0).$$

This gives

$$\begin{aligned}
 p(0, 1, 0, 1, 0) &= \frac{1}{Z} 2 \cdot 2 \cdot 1 \cdot 1 = \frac{4}{Z} \\
 p(0, 1, 1, 1, 0) &= \frac{1}{Z} 2 \cdot 1 \cdot 2 \cdot 1 = \frac{4}{Z} \\
 p(1, 1, 0, 1, 0) &= \frac{1}{Z} 1 \cdot 1 \cdot 1 \cdot 1 = \frac{1}{Z} \\
 p(1, 1, 1, 1, 0) &= \frac{1}{Z} 1 \cdot 2 \cdot 2 \cdot 1 = \frac{4}{Z}
 \end{aligned}$$

We can also compute the joint distribution:

$$\begin{aligned}
p(x_1, x_3 \mid x_2 = 1, x_4 = 1, x_5 = 0) &= \frac{p(x_1, 1, x_3, 1, 0)}{\sum_{x'_1, x'_3=0}^1 p(x'_1, 1, x'_3, 1, 0)} \\
&= \frac{\frac{1}{Z} \psi_{12}(x_1, 1) \psi_{13}(x_1, x_3) \psi_{34}(x_3, 1) \psi_{35}(x_3, 0)}{\frac{1}{Z}(4 + 4 + 1 + 4)} \\
&= \frac{\psi_{12}(x_1, 1) \psi_{13}(x_1, x_3) \psi_{34}(x_3, 1) \psi_{35}(x_3, 0)}{13} \\
&= \frac{1}{13} \begin{bmatrix} 4 & 4 \\ 1 & 4 \end{bmatrix}
\end{aligned}$$

For the message passing:

$$\begin{aligned}
m_{2 \rightarrow 1}(x_1) &= \psi_2(1) \psi_{12}(x_1, 1) = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \\
m_{4 \rightarrow 3}(x_3) &= \psi_4(1) \psi_{34}(x_3, 1) = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \\
m_{5 \rightarrow 3}(x_3) &= \psi_5(0) \psi_{35}(x_3, 0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}
\end{aligned}$$

Since x_3 is not observed we have

$$\begin{aligned}
m_{3 \rightarrow 1}(x_1) &= \sum_{x_3} \psi_3(x_3) \psi_{13}(x_1, x_3) m_{4 \rightarrow 3}(x_3) m_{5 \rightarrow 3}(x_3) \\
&= \psi_3(0) \psi_{13}(x_1, 0) m_{4 \rightarrow 3}(0) m_{5 \rightarrow 3}(0) + \psi_3(1) \psi_{13}(x_1, 1) m_{4 \rightarrow 3}(1) m_{5 \rightarrow 3}(1) \\
&= \begin{bmatrix} 4 \\ 5 \end{bmatrix}
\end{aligned}$$

From this we get

$$b(x_1) = p(x_1 \mid \bar{x}_2 = 1, \bar{x}_4 = 1, \bar{x}_5 = 0) \propto \psi_1(x_1) m_{2 \rightarrow 1}(x_1) m_{3 \rightarrow 1}(x_1) = \begin{bmatrix} 8 \\ 5 \end{bmatrix}$$

and so $p(x_1 = 1 \mid \bar{x}_2 = 1, \bar{x}_4 = 1, \bar{x}_5 = 0) = \frac{5}{13}$.

To compute $b(x_3) = p(x_3 \mid \bar{x}_2 = 1, \bar{x}_4 = 1, \bar{x}_5 = 0)$ we need to compute the message $m_{1 \rightarrow 3}$

$$m_{1 \rightarrow 3}(x_3) = \sum_{x_1} \psi_1(x_1) \psi_{13}(x_1, x_3) m_{2 \rightarrow 1}(x_1) = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

This gives

$$b(x_3) \propto \psi_3(x_3) m_{1 \rightarrow 3}(x_3) m_{4 \rightarrow 3}(x_3) m_{5 \rightarrow 3}(x_3) = \begin{bmatrix} 5 \\ 8 \end{bmatrix}$$

giving that $p(x_3 = 1 \mid \bar{x}_2 = 1, \bar{x}_4 = 1, \bar{x}_5 = 0) = \frac{8}{13}$.