Probabilistic Graphical Models

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1 Graphical Representations

1.1 Factors

Definition 1.1. Let $X_1, X_2, \cdots, X_k$ be a set of random variables, then a **factor** ϕ is a mapping from values of these random variables to $\mathbb{R}$.

$$\phi : Val(X_1, X_2, \cdots, X_k) \to \mathbb{R} \tag{1}$$

The set of random variables $\{X_1, X_2, \cdots, X_k\}$ is defined as the **scope** of ϕ.

Remark 1.1. In principle, a factor can take any value in $\mathbb{R}$. However, in practice, we restrict our considerations to factors with positive ranges only.

Definition 1.2. Let ϕ_1 and ϕ_2 be two factors with scopes $\{A, B\}$ and $\{B, C\}$. Then the **factor product** $\phi_1 \times \phi_2$ is a factor with scope $\{A, B, C\}$ defined as

$$\phi_1 \cdot \phi_2(a, b, c) = \phi_1(a, b) \cdot \phi_2(b, c) \tag{2}$$

Definition 1.3. Let ϕ be a factor with scope $\{A, B, C\}$, then **marginalizing** C **from** ϕ results in a factor ϕ' with scope $\{A, B\}$ defined as the following:

$$\phi'(a, b) = \sum_{c \in Val(C)} \phi(a, b, c) \tag{3}$$

Definition 1.4. The **factor reduction** operation restricts $\phi(A, B, C)$ to take only a specific value

of $C = c$, and results in a factor ϕ' with scope $\{A, B\}$.

$$\phi'(a, b) = \phi(a, b, c) \tag{4}$$

1.2 Semantics and Factorization

Definition 1.5. A **Bayesian network** consists of (i) a directed acyclic graph (DAG) G whose nodes correspond to random variables $X_1, \cdots, X_n$ (ii) and a conditional probability distribution $P(X_i|Par_G(X_i))$ for each node X_i. The joint distribution is defined as the factorization

$$P(X_1, \cdots, X_n) = \prod_{i=1}^{n} P(X_i|\text{Par}_G(X_i)) \tag{5}$$

Definition 1.6. Let G be a graph over $X_1, \cdots, X_n$, then the joint probability P **factorizes** over G if and only if

$$P(X_1, \cdots, X_n) = \prod_{i=1}^{n} P(X_i|\text{Par}_G(X_i)) \tag{6}$$

1.3 Pass of Influences in Bayesian Networks

Definition 1.7. A path $X_1 - \cdots - X_k$ in Bayesian network G is **active** if there is no explaining-away structure $X_{i-1} \to X_i \leftarrow X_{i+1}$ in it.

Definition 1.8. Let $Z \subseteq V_G$ be a set of random variables in the Bayesian network, then a path $X_1 - \cdots - X_k$ in G is **active conditioned on** Z if

1. for all explaining-away structure $X_{i-1} \to X_i \leftarrow X_{i+1}$ in the path, X_i or some decedents of X_i are in Z,

2. and no other node in the path is in Z.

Definition 1.9. Let $X, Y, Z \subseteq V_G$, if there is no path from X to Y is active conditioned on Z, then X and Y are **d-separated** by Z in graph G denoted as $\text{d-sep}_G(X, Y|Z)$.

1.4 Independencies and Factorizations

Definition 1.10. Let X, Y, Z be random variables with distribution P, then $X \perp\!\!\!\perp Y$ if and only if $P(X, Y) = P(X)P(Y)$, $X \perp\!\!\!\perp Y|Z$ if and only if $P(X, Y|Z) = P(X|Z)P(Y|Z)$.

Proposition 1.1. Let X, Y, Z be random variables with distribution P, then $X \perp\!\!\!\perp Y$ if and only if $P(X, Y)$ factorizes as the following

$$P(X, Y) \propto \phi_1(X)\phi_1(Y) \tag{7}$$

and $X \perp\!\!\!\perp Y|Z$ if and only if $P(X, Y, Z)$ factorizes as

$$P(X, Y, Z) \propto \phi_1(X, Z)\phi_1(Y, Z) \tag{8}$$

Proof. Relation (7) follows the definition immediately. Suppose $X \perp\!\!\!\perp Y|Z$, then

$$\begin{aligned}
& P(X, Y|Z) = P(X|Z)P(Y|Z) && (9)\\
\iff\ & P(X, Y, Z) = P(X|Z)P(Y|Z)P(Z) && (10)\\
& P(X, Y, Z) \propto P(X|Z)P(Z)P(Y|Z)P(Z) && (11)\\
& = P(X, Z)P(Y, Z) && (12)\\
& = \phi_1(X, Z)\phi_1(Y, Z) && (13)
\end{aligned}$$

■

Theorem 1.1 (Factorization $\implies$ Independence)**.** If P factorizes over G, and d-sep$_G(X, Y|Z)$ then P satisfies $(X \perp\!\!\!\perp Y|Z)$.

Theorem 1.2 (Causal Markov Condition)**.** For any random variable X_i in the Bayesian network, X_i is d-separated from all its non-descendants by $\text{Par}_G(X_i)$.

Corollary 1.1. If P factorizes over G, then in P, any variable is independent of its non-descendants given its parents.

Definition 1.11. Let $\mathcal{I}(G)$ denote the collection of independencies implicitly encoded by d-separations in graph G,

$$\mathcal{I}(G) := \{(X \perp\!\!\!\perp Y|Z) : X, Y, Z \in V \ s.t. \ \text{d-sep}_G(X, Y|Z)\} \tag{14}$$

If a distribution P over V satisfies all independencies in $\mathcal{I}(G)$, then we say that G is an **I-map** (independency map) of P.

That is, the I-map of distribution P is a graphical representation of all (and probably more) independencies of P.

Example 1.1. Let P be a probability distribution and let G be an I-map for P. Let $\mathcal{I}(P)$ and $\mathcal{I}(G)$ denote sets of independencies in P and G. Suppose G is a I-map of P, then all independencies encoded in G are satisfied by P, therefore,

$$\mathcal{I}(G) \subseteq \mathcal{I}(P) \tag{15}$$

Example 1.2. The I-map can be used for two graphs as well. G_1 is a I-map of G_1 if $\mathcal{I}(G_1) \subseteq \mathcal{I}(G_2)$. That is, G_1 is an I-map of G_2 if it does not make independence assumptions that are not true in G_2.

Theorem 1.3 (Independence $\Longrightarrow$ Factorization)**.** If G is an I-map for P, that is, P adheres all independencies encoded in G, then P factorizes over G.

1.5 Template Models

Definition 1.12. A **template variable** $X(U_1, \cdots, U_k)$ is instantiated (duplicated) multiple times in a graph. **Template models** are languages that specify how ground variables (i.e., instantiations of template variables) inherit dependency model from template.

Notation 1.1. Let $X^{(t)}$ denote the variable at time $t\Delta$, where Δ is the time granularity in the discrete timeline. Let $X^{(t:t')} = \{X^{(t)}, ^{(t+1)}, \cdots, X^{(t')}\}$ denote the set of variables over a period of time.

Definition 1.13. A Bayesian network is said to satisfy the **Markov assumption** if

$$X^{(t+1)} \perp\!\!\!\perp X^{(0:t-1)} | X^{(t)} \tag{16}$$

When Markov assumption holds, we may express the joint distribution of all X as

$$P(X^{(0:T)}) = P(X^{(0)}) \prod_{t=0}^{T-1} P(X^{(t+1)} | X^{(t)}) \tag{17}$$

Definition 1.14. A series of random variables $X^{(0)}, X^{(1)}, \cdots, X^{(T)}$ satisfies the **time invariance**

assumption if there exists a template probability model $P(X'|X)$ such that for all t,

$$P(X^{(t+1)}|X^{(t)}) = P(X'|X) \tag{18}$$

Definition 1.15. A **2-time-slice Bayesian network** (2TNB) over $X_1, \cdots, X_n$ (that is, n random variables for each time step) is specified as a Bayesian network fragment such that

- The nodes include $X'_1, \cdots, X'_n$ and a subset of $X_1, \cdots, X_n$,
- and only the nodes $X'_n, \cdots, X'_n$ have parents and a conditional probability distribution.

Further, the 2TBN defines a conditional distribution

$$P(X'|X) = \prod_{i=1}^{n} P(X'_i|\text{Par}(X'_i)) \tag{19}$$

Definition 1.16. A **dynamic Bayesian network** (DNB) over $X_1, \cdots, X_n$ is defined by

- a 2TNB, $\text{BN}_{\rightarrow}$, over $X_1, \cdots, X_n$,
- and a Bayesian network, $\text{BN}^{(0)}$, over $X_1^{(0)}, \cdots, X_n^{(0)}$.

Definition 1.17. For a trajectory over $0, \cdots, T$, the **ground (unrolled) network** of a DNB is a model such that

- the dependency model for $X_1^{(0)}, \cdots, X_n^{(0)}$ is copied from $\text{BN}^{(0)}$,
- and the dependency model for $X_1^{(t)}, \cdots, X_n^{(t)}$ is copied from $\text{BN}_{\rightarrow}$.

1.6 Plate Models

We can use plate models to represent repetitions.

Example 1.3. Let $O_t \overset{i.i.d.}{\sim} \text{Bernoulli}(\theta)$, and $\{O_t\}_t$ is simply a set of coin tosses outcomes. Such scenario can be modelled as in Figure 1. Figure 2 illustrates an equivalent representation of this plate model.

Figure 1: A plate model for Bernoulli trails

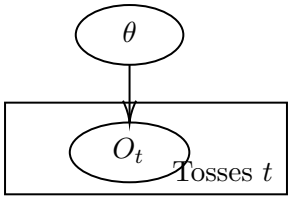
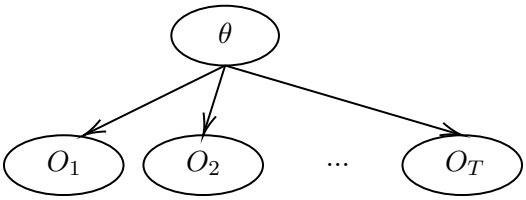


Figure 2: A plate model for Bernoulli trails



Remark 1.2. Parameters outside the plate are often omitted.

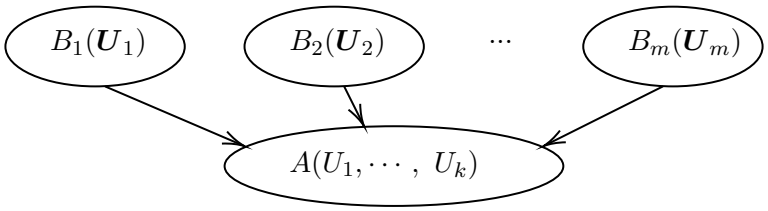
Example 1.4 (Nested Plate)**.**

Example 1.5 (Overlapping Plate)**.**

Example 1.6 (Collective Inference)**.**

Definition 1.18. A **plate dependency model** consists of a template variable $A(U_1, \cdots, U_k)$ and template parents $B_1(\mathbf{U}_1), \cdots, B_m(\mathbf{U}_m)$, where $\mathbf{U}_k \subseteq \{U_1, \cdots, U_k\}$. The conditional probability distribution in this model is $P(A|B_1, \cdots, B_m)$.

Figure 3: Plate dependency model



Definition 1.19. The concrete instantiation (**ground network**) of a plate dependency model consists of instantiations $u_1, \cdots, u_k$ of $U_1, \cdots, U_k$.

1.7 Local Structures

Definition 1.20. A **general conditional probability distribution** $P(X|Y_1, \cdots, Y_k)$ specifies distribution over X for each realization of $Y_1, \cdots, Y_k$. Any factor ϕ with scope $\{X, Y_1, \cdots, Y_K\}$

satisfying

$$\sum_x \phi(x, y_1, \cdots, y_k) = 1 \quad \forall y_1, \cdots, y_k \tag{20}$$

defines a valid general CPD.

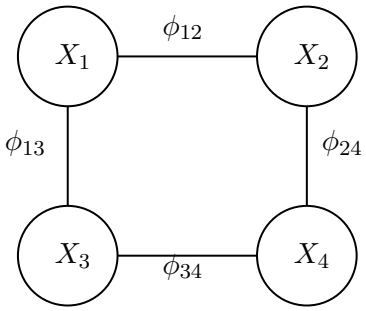
Definition 1.21 (Context-Specific Independence)**.** Let $P \in \Delta(\mathcal{X})$, let $X, Y \in \mathcal{X}$ and $\mathbf{Z}, \mathbf{C} \subseteq \mathcal{X}$. Let $\mathbf{c}$ be a realization of random variables $\mathbf{C}$. Then X is said to be independent from Y given Y in the context c, denoted as $(X \perp\!\!\!\perp_c Y|\mathbf{Z}, \mathbf{c})$, if

$$P(X, Y|\mathbf{Z}, \mathbf{c}) = P(X|\mathbf{Z}, \mathbf{c})P(Y|\mathbf{Z}, \mathbf{c}) \tag{21}$$

1.8 Pairwise Markov Networks

Definition 1.22. A **pairwise Markov network** is a undirected graph whose nodes are random variables $X_1, \cdots, X_n$ and each edge (X_i, X_j) is associated with a factor $\phi_{ij}(X_i, X_j)$.

Figure 4: A simple pairwise Markov network



1.9 General Gibbs Distributions

Definition 1.23. A **Gibbs distribution** over random variables $X_1, \cdots, X_n$ is specified by a set of general factors, $\Phi = \{\phi_i(D_i)\}_{i=1}^k$, where each $D_i \subseteq \{X_1, \cdots, X_n\}$. The corresponding unnormalized probability and partition function are

$$\tilde{P}_\Phi(X_1, \cdots, X_n) = \prod_{i=1}^k \phi_i(D_i) \tag{22}$$

$$Z_\Phi = \sum_{X_1, \cdots, X_n} \tilde{P}_\Phi(X_1, \cdots, X_n) \tag{23}$$

The probability distribution is

$$P_\Phi(X_1, \cdots, X_n) = \frac{\tilde{P}_\Phi(X_1, \cdots, X_n)}{Z_\Phi} \tag{24}$$

Definition 1.24. The **induced Markov network** of a set of factors $\Phi = \{\phi_i(D_i)\}_{i=1}^k$, where $D_i \subseteq \{X_1, \cdots, X_n\}$, denoted as H_Φ, is a network in which there is an edge between X_i and X_j whenever $\exists\ m \in [k]\ s.t.\ X_i, X_j \in D_m$.

Definition 1.25. A probability distribution P **factorizes** over a Markov network H if there exists $\Phi = \{\phi_1(D_1), \cdots, \phi_k(D_k)\}$ such that $P = P_\Phi$ and $H = H_\Phi$.

Remark 1.3. There can be multiple factorizations of a given Markov network.

Definition 1.26. A trail (path) $X_1 - \cdots - X_n$ in a Markov network is **active** given a set of nodes $\mathbf{Z}$ if no X_i is in $\mathbf{Z}$.

1.10 Conditional Random Fields

Definition 1.27 (CRF)**.** A **CRF representation** over random variables $X \cup Y$ consists of a set of factors $\Phi = \{\phi_1(D_1), \cdots, \phi_k(D_k)\}$, where $D_i \subseteq X \cup Y$.

The unnormalized probability and partition function are defined as

$$\tilde{P}(X, Y) = \prod_{i=1}^{k} \phi_i(D_i) \tag{25}$$

$$Z(X) = \sum_{Y} \tilde{P}(X, Y) \tag{26}$$

The conditional probability is therefore

$$P(Y|X) = \frac{1}{Z(X)} \tilde{P}(X, Y) \tag{27}$$

Remark 1.4. A CRF is parameterized the same as a Gibbs distribution, both of them are defined using factors. However, they are normalized differently, the partition function in CRF, $Z(X)$, depends on the particular realization of X, but Z_Φ depends on factors only.

Example 1.7 (Logistic model as a CRF)**.** Let $X_1, \cdots, X_k$ denote the k random variables serve as features to generate the target variable Y. Figure 5 illustrates the logistic model as a Bayesian

network. For simplicity, assume X_i and Y are all binary. Define factors

$$\phi_i(X_i, Y) := \exp(w_i \mathbb{1}\{X_i = 1 \wedge Y = 1\}) = \exp(w_i X_i Y) \tag{28}$$

Therefore, the unnormalized probabilities are

$$\tilde{P}(Y = 0, X_i) = \prod_{i=1}^{k} \exp(w_i X_i 0) = 1 \tag{29}$$

$$\tilde{P}(Y = 1, X_i) = \prod_{i=1}^{k} \exp(w_i X_i) = \exp\left(\sum_{i=1}^{k} w_i X_i\right) \tag{30}$$

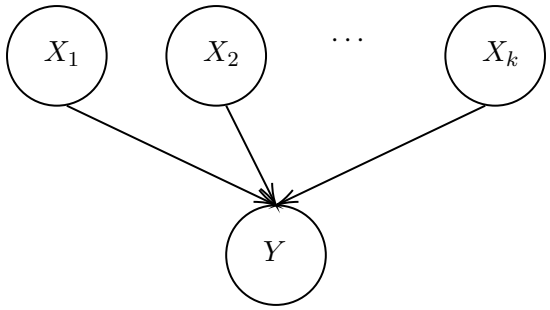
Then, the CPD can be expressed as

$$P(Y = 1 | X_1, \cdots, X_k) = \frac{\tilde{P}(Y = 1, X_i)}{\tilde{P}(Y = 0, X_i) + \tilde{P}(Y = 1, X_i)} \tag{31}$$

$$= \frac{\exp\left(\sum_{i=1}^{k} w_i X_i\right)}{1 + \exp\left(\sum_{i=1}^{k} w_i X_i\right)} \tag{32}$$

$$= \frac{1}{1 + \exp\left(-\sum_{i=1}^{k} w_i X_i\right)} = \sigma\left(\sum_{i=1}^{k} w_i X_i\right) \tag{33}$$

Figure 5: Logistic model as a Bayesian network



1.11 Independencies in Markov Networks

Definition 1.28. Two nodes X and Y in a Markov network H are **separated** given set of nodes Z if there is no active trail (path) in H between X and Y given Z. Denoted as $\text{sep}_H(X, Y|Z)$

Theorem 1.4. If distribution P factorizes over Markov network H, then P satisfies

$$\text{sep}_H(X, Y|Z) \implies X \perp\!\!\!\perp Y|Z \tag{34}$$

Proof. ■

Definition 1.29. Let $I(H)$ denote the collection of independencies induced by H:

$$\mathcal{I}(H) := \{(X \perp\!\!\!\perp Y|Z : \text{sep}_H(X, Y|Z)\} \tag{35}$$

If P satisfies $\mathcal{I}(H)$, then H is an **independency map** (I-map) of P.

Theorem 1.5. If P factorizes over H, then H is an I-map of P.

Proof. ■

Theorem 1.6 (Hammersley Clifford)**.** For a positive distribution P (i.e., $P(x) > 0$ for all x), if H is an I-map for P, then P factorizes over H.

Proof. ■

Remark 1.5. Let P be a distribution and let

$$\mathcal{I}(P) = \{(X \perp\!\!\!\perp Y|Z) : P \text{ satisfies } (X \perp\!\!\!\perp Y|Z)\} \tag{36}$$

denote the collection of independencies satisfied by P. As mentioned before, P factorizes over G implies G is an I-map for P, that is,

$$\mathcal{I}(G) \subseteq \mathcal{I}(P) \tag{37}$$

Note that the converse is not always true.

Remark 1.6. A graph is said to be **sparser** if it encodes more independencies, and therefore fewer connections and parameters. Note that sparser graphs are more informative since they encode more independency assumptions.

Definition 1.30. Let P be a probability distribution, then a Bayesian network (or a Markov network) G is a **perfect map** if $\mathcal{I}(G) = \mathcal{I}(P)$. That is, G perfectly captures independencies in P.

Proposition 1.2. Perfect maps are not unique.

Proof. Let G_1 be the graph $X \to Y$ and G_2 be the graph $X \leftarrow Y$. Both $\mathcal{I}(G_1) = \mathcal{I}(G_2) = \varnothing$. Therefore, both G_1 and G_2 are I-maps for any distribution P. ■

Definition 1.31. Two graphs G_1 and G_2 over random variables $X_1, \cdots, X_n$ are **I-equivalent** if $\mathcal{I}(G_1) = \mathcal{I}(G_2)$. Many features of graphs are preserved within the same I-equivalence class.

1.12 Log-Linear Models

Definition 1.32. A **log-linear representation** of distribution consists of a set of features $\{f_j\}$ and corresponding scopes $\{D_j\}$. The unnormalized distribution is defined as

$$\tilde{P} = \exp\left(-\sum_j w_j f_j(D_j)\right) \tag{38}$$

$$= \sum_j \exp(-w_j f_j(D_j)) \tag{39}$$

The exact distribution can be computed using partition function as usual.

Example 1.8 (Metric MRFs)**.** For simplicity, suppose all random variables X_i take values from space V. Let $\mu : V \times V \to \mathbb{R}_+$ be a distance function satisfying

1. Reflexivity: $\mu(v, v) = 0$ for all $v \in V$,
2. Symmetry: $\mu(v_1, v_2) = \mu(v_2, v_1)$ for all $v_1, v_2 \in V$,
3. Triangle inequality: $\mu(v_1, v_2) \leq \mu(v_1, v_3) + \mu(v_3, v_2)$ for all $v_1, v_2, v_3 \in V$.

Define the feature function $f_{ij}(X_i, X_j) = \mu(X_i, X_j)$ and $w_{ij} > 0$. Using such metric, when more pairs (X_i, X_j) in the network are far away from each other, the probability assigned to this network is lower.

Example 1.9 (Shared Features)**.** We may specify a set of scopes $S(f_k)$ for each feature f_k. For example, if we want to apply feature f_k to all adjacent nodes, then

$$S(f_k) = \{\{X_i, X_j\} : X_i \text{ and } X_j \text{ are adjacent}\} \tag{40}$$

Applying the same weight w_k and feature constructor f_k on all scopes in $S(f_k)$, then summing them up gives the potential of feature k.

$$w_k \sum_{D \in S(f_k)} f_k(D) \tag{41}$$

The product of potentials from all features gives the unnormalized probability.

2 Inference

3 Learning

3.1 Learning Network Parameters

3.2 Learning Network Structure

Motivation We have discussed methods to estimate parameters given a network structure and dataset, however, ways to choose the structure remains uncovered. Specifically, given a dataset D, we have to choose one graph G as the skeleton of our model.

Compared with the graph representing the true data generating process, if the specified graph G contains less edges, G imposes more independence assumptions than necessary. In contrast, if the specified graph G has extra edges, then the redundant dependencies would require more parameters to be fitted using the limited dataset and leads to bad generalization.

To select the best structure G given dataset D, we can define a **scoring function** taking both G and D as arguments. Then the model selection problem turns into an optimization problem:

$$\text{Optimal } G^* := \underset{G \in \text{all models}}{\text{argmax}} \ \text{score}(G, D) \tag{42}$$

3.2.1 Likelihood Structure Scores

Definition 3.1. Likelihood structure score defines the compatibleness between a graph G and dataset D as

$$\text{score}_L(G; D) := \ell(G_{\hat{\theta}}; D) \tag{43}$$

Where $\hat{\theta}$ is the maximum likelihood estimations from of parameters in graph G from dataset D, and ℓ is the log-likelihood function.