CSC412/2506 Winter 2020: Probabilistic Learning and Reasoning

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1 Introduction

2 Probabilistic Models

Definition 2.1. Given an i.i.d. dataset $\mathcal{D}$, the log-likelihood of θ is defined as

$$\ell(\theta; \mathcal{D}) = \sum_{i=1}^{N} \log p(x^{(i)}|\theta) \tag{2.1}$$

Definition 2.2. A **statistic** is a deterministic function of a set of random variables.

Definition 2.3. $T(X)$ is a **sufficient statistic** for random variable X if

$$T(x^{(1)}) = T(x^{(2)}) \implies L(\theta; x^{(1)}) = L(\theta; x^{(2)}) \quad \forall \theta \tag{2.2}$$

equivalently,

$$P(\theta|T(X)) = P(\theta|X) \tag{2.3}$$

3 Directed Graphical Models

3.1 Decision Theory

3.2 Latent Variables

Complete data case Let $\mathcal{D} = \{x^{(i)}, y^{(i)}\}_{i=1}^{N}$ denote the dataset, then

$$\ell(\theta; \mathcal{D}) = \sum_{i=1}^{N} \log p\left(x^{(i)}, y^{(i)}|\theta\right) \tag{3.1}$$

Partially observed dataset Let

$$\mathcal{D}^c = \{(x^{(i)}, y^{(i)}) : i \in \mathcal{C}\} \subseteq \mathcal{D} \tag{3.2}$$

denote the part of dataset with observed labels, and let

$$\mathcal{D}^m = \{(x^{(i)}) : i \in \mathcal{M}\} \subseteq \mathcal{D} \tag{3.3}$$

denote the set of observations without labels. Note that $\mathcal{C} \cup \mathcal{M} = \{1, 2, \cdots, N\}$.
Then the log likelihood is

$$\ell(\theta; \mathcal{D}) = \sum_{c \in \mathcal{C}} \log p\left(x^c, y^c|\theta\right) + \sum_{m \in \mathcal{M}} \log p\left(x^m|\theta\right) \tag{3.4}$$

$$= \sum_{c \in \mathcal{C}} \log p\left(x^c, y^c|\theta\right) + \sum_{m \in \mathcal{M}} \log \sum_{y} p\left(x^m, y|\theta\right) \tag{3.5}$$

Inference with Latent Variables Let z denote the latent variable, then

$$p(y|x) = \sum_z p(y|x,z)p(z) \tag{3.6}$$

3.3 Mixture Models

Inference using mixture models Let $\Theta = \{\theta_z\} \cup \{\theta_1, \theta_2, \cdots, \theta_K\}$. Where θ_z quantifies the distribution of z, and θ_k for each $k \in \{1, 2, \cdots, K\}$ denote the set of parameters describing $p(x|z = k)$.

$$p(x|\Theta) = \sum_{k=1}^{K} p(x, z = k|\Theta) \tag{3.7}$$

$$= \sum_{k=1}^{K} p(z = k|\Theta)p(x|z = k, \Theta) \tag{3.8}$$

$$= \sum_{k=1}^{K} p\left(z = k|\theta_z\right) p\left(x|z = k, \theta_k\right) \tag{3.9}$$

Posterior probabilities / responsibilities

$$p\left(z = k|x, \theta_z\right) = \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{p(x|\Theta)} \tag{3.10}$$

$$= \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{\sum_j p(x, z = j|\Theta)} \tag{3.11}$$

$$= \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{\sum_j p\left(z = j|\theta_z\right) p\left(x|z = j, \theta_j\right)} \tag{3.12}$$

Gaussian mixture models

$$p(x|\theta) = \sum_k \alpha_k \mathcal{N}\left(x|\mu_k, \Sigma_k\right) \tag{3.13}$$

$$\log\left(x_1, x_2, \ldots, x_N\right)|\theta) = \sum_n \log \sum_k \alpha_k \mathcal{N}(x^{(n)}|\mu_k, \Sigma_k) \tag{3.14}$$

$$p(z = k|x, \theta) = \frac{\alpha_k \mathcal{N}\left(x|\mu_k, \Sigma_k\right)}{\sum_j \alpha_j \mathcal{N}\left(x|\mu_j, \Sigma_j\right)} \tag{3.15}$$

Mixtures of experts

$$p(y|x, \theta) = \sum_{k=1}^{K} p\left(z = k|x, \theta_z\right) p\left(y|z = k, x, \theta_K\right) \tag{3.16}$$

$$= \sum_{k=1}^{K} \alpha_k\left(x|\theta_z\right) p_k\left(y|x, \theta_k\right) \tag{3.17}$$

4 Exact Inference

Notation 4.1. Let X denote the set of all random variables in the model, and

1. X_E = The observed evidence;

2. X_F = The unobserved variable we want to infer;

3. $X_R = X - \{X_F, X_E\}$ = Remaining variables, extraneous to query.

The model defines the joint distribution of all random variables:

$$p(X_E, X_F, X_R) \tag{4.1}$$

Definition 4.1. The joint distribution over evidence and subject of inference is

$$p\left(X_F, X_E\right) = \sum_{X_R} p\left(X_F, X_E, X_R\right) \tag{4.2}$$

Definition 4.2. The conditional probability distribution for inference given evidence is

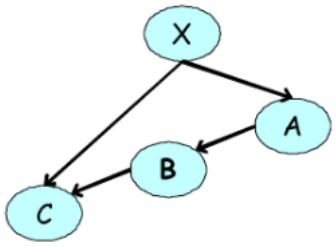
$$p\left(X_F | X_E\right) = \frac{p\left(X_F, X_E\right)}{p\left(X_E\right)} = \frac{p\left(X_F, X_E\right)}{\sum_{X_F} p\left(X_F, X_E\right)} \tag{4.3}$$

Definition 4.3. The distribution of evidence can be computed as

$$p\left(X_E\right) = \sum_{X_F, X_R} p\left(X_F, X_E, X_R\right) \tag{4.4}$$

4.1 Variable Elimination

4.2 Intermediate Factors



$$p(A, B, C) = \sum_X p(X)p(A|X)p(B|A)p(C|B, X) \tag{4.5}$$

$$= p(B|A) \underbrace{\sum_X p(X)p(A|X)p(C|B, X)}_{\text{unnormalized}} \tag{4.6}$$

Definition 4.4. A **factor** ϕ describes the local relation between random variables, meanwhile, $\int d\phi$ is not necessarily one.

Remark 4.1. Let $X_\ell \subseteq X$ be a group of local random variables, then $p(X_\ell)$ is automatically a factor $\phi(X_\ell)$.

$$p(A,B,C) = \sum_X \underbrace{p(X)p(A|X)p(B|A)p(C|B,X)}_{\text{from graphical representation}} \tag{4.7}$$

$$= \sum_X \underbrace{\phi(X)\phi(A,X)\phi(A,B)\phi(X,B,C)}_{\text{factor representation}} \tag{4.8}$$

$$= \phi(A,B) \sum_X \phi(X)\phi(A,X)\phi(X,B,C) \tag{4.9}$$

$$= \phi(A,B)\ \underbrace{\tau(A,B,C)}_{\text{another factor}} \tag{4.10}$$

4.3 Sum-Product Inference

Theorem 4.1. Consider a graphical model with random variables $X = Y \cup Z$. For an random variable Y in a directed or undirected model, $P(Y)$ can be computed using the **sum-product**

$$\tau(Y) = \sum_z \prod_{\phi \in \Phi} \phi(Scope[\phi] \cap Z, Scope[\phi] \cap Y) \tag{4.11}$$

where Φ is a set of factors.

Remark 4.2. For directed models,

$$\Phi = \{\phi_{x_i}\}_{i=1}^N = \{p\left(x_i|\text{ parents }(x_i)\right)\}_{i=1}^N \tag{4.12}$$

4.4 Complexity of Variable Elimination Ordering

Theorem 4.2. The complexity of the variable elimination algorithm is

$$\mathcal{O}(mk^{N_{max}}) \tag{4.13}$$

where

(i) m is the number of initial factors $|\Phi|$;

(ii) k is the number of states each random variable takes, assumed to be equal;

(iii) N_i is the number of random variables within each summation;

(iv) $N_{max} = \max_i N_i$.

5 Message passing, Hidden Markov Models, and Sampling

5.1 Message Passing (Computing All Marginals)

Notation 5.1. Let T denote the set of edges in a tree. For a node i, let $N(i)$ denote the set of its neighbours.

The factor of all random variables can be computed following

$$P\left(X_{1:n}\right)=\frac{1}{Z}\underbrace{\left[\prod_{i=1}^{n}\phi\left(x_i\right)\right]}_{\text{prior factors}}\underbrace{\prod_{(i,j)\in T}\phi_{i,j}\left(x_i,x_j\right)}_{\text{local factors}} \tag{5.1}$$

Definition 5.1. The **message** sent from variable j to $i \in N(j)$ is

$$m_{j\to i}\left(x_i\right)=\sum_{x_j}\left[\phi_j\left(x_j\right)\phi_{ij}\left(x_i,x_j\right)\prod_{k\in N(j)\neq i}m_{k\to j}\left(x_j\right)\right] \tag{5.2}$$

Algorithm 5.1 (Belief Propagation Algorithm)**.** Given a tree, inference on an arbitrary node $p(x_i)$ can be computed following:

1. Choose root r arbitrarily;
2. Pass messages from leaves to r;
3. Pass messages from r to leaves;
4. Compute inference

$$p\left(x_i\right)\propto\phi_i\left(x_i\right)\prod_{j\in N(i)}m_{j\to i}\left(x_i\right) \tag{5.3}$$

5.2 Markov Chains

Using chain rule of probability:

$$p\left(x_{1:T}\right)=\prod_{t=1}^{T}p\left(x_t|x_{t-1},\ldots,x_1\right) \tag{5.4}$$

Definition 5.2. A Markov chain is said to be **first-order** if

$$p\left(x_t|x_{1:t-1}\right)=p\left(x_t|x_{t-1}\right) \tag{5.5}$$

Simplification Therefore, for all first-order Markov chains, the full joint distribution can be reduced to

$$p\left(x_{1:T}\right)=\prod_{t=1}^{T}p\left(x_t|x_{t-1}\right) \tag{5.6}$$

Definition 5.3. A Markov chain is at m-order if

$$p\left(x_t|x_{1:t-1}\right)=p\left(x_t|x_{t-m:t-1}\right) \tag{5.7}$$

Definition 5.4. A Markov chain is said to be **homogenous** (i.e., stationary) if

$$p\left(x_t|x_{t-1}\right)=p\left(x_{t+k}|x_{t-1+k}\right)\quad\forall t,k \tag{5.8}$$

Parameterization Assume the random variable X_t takes k states, further suppose the chain is time homogenous. Then characterizing the transition probability

$$p(x_t|x_{t-1}, x_{t-2}, \cdots, x_{t-m}) \tag{5.9}$$

requires $(k-1)k^m$ parameters.

5.3 Hidden Markov Models

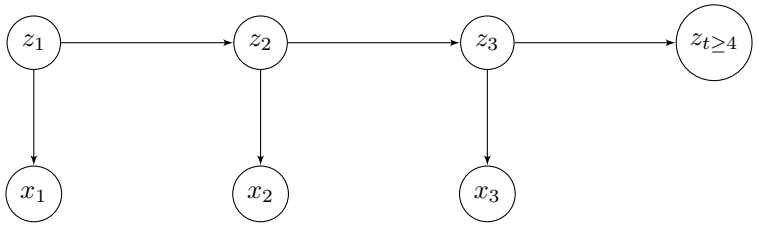


Figure 5.1: Hidden Markov Model

Joint distribution Following the conventional expansion

$$p(x_{1:T}, z_{1:T}) = p(z_1)\prod_{t=2}^{T} p(z_t|z_{t-1})\prod_{t=1}^{T} p(x_t|z_t) \tag{5.10}$$

Parameterization Assuming the HMM is homogenous with order 1, then the set of parameters Φ consists of

(i) Initial distribution of $p(z_1)$: $k-1$ parameters;

(ii) Transition distribution of $p(z_{t+1}|z_t)$: $(k-1)k$ parameters;

(iii) Emission distribution of $p(x_t|z_t)$: $(k-1)k$ parameters.

5.4 Forward-backward Algorithm

Smoothing compute posterior over past hidden state

$$p(z_\tau|x_{1:t}) \ s.t. \ 1 < \tau < t \tag{5.11}$$

Filtering compute posterior over current hidden state

$$p(z_t|x_{1:t}) \tag{5.12}$$

Prediction compute posterior over future hidden state

$$p(z_\tau|x_{1:t}) \ s.t. \ \tau > t \tag{5.13}$$

5.5 Procedure of Smoothing (Forward-backward Algorithm)

$$
\begin{aligned}
p(z_t|x_{1:T}) &\propto p(x_{1:T}, z_t) && (5.14)\\
&= p(z_t, x_{1:t})p(x_{t+1:T}|z_t, x_{1:t}) && (5.15)\\
&= p(z_t, x_{1:t})p(x_{t+1:T}|z_t) && (5.16)\\
&= p(z_t|x_{1:t})p(x_{1:t})p(x_{t+1:T}|z_t) && (5.17)\\
&\propto p(z_t|x_{1:t})p(x_{t+1:T}|z_t) && (5.18)
\end{aligned}
$$

Forward filtering (encoding) Define

$$\alpha_t(z_t) := p(z_t|x_{1:t}) \tag{5.19}$$

Then

$$
\begin{aligned}
p(z_t|x_{1:t}) &\propto p(z_t, x_{1:t}) && (5.20)\\
&= \sum_{z_{t-1}=1}^{k} p(z_{t-1}, z_t, x_{1:t}) && (5.21)\\
&= \sum_{z_{t-1}=1}^{k} p(x_t|z_{t-1}, z_t, x_{1:t-1})p(z_t|z_{t-1}, x_{1:t-1})p(z_{t-1}, x_{1:t-1}) && (5.22)\\
&= \sum_{z_{t-1}=1}^{k} p(x_t|z_t)p(z_t|z_{t-1})p(z_{t-1}, x_{1:t-1}) && (5.23)\\
&= p(x_t|z_t) \sum_{z_{t-1}=1}^{k} p(z_t|z_{t-1})p(z_{t-1}, x_{1:t-1}) && (5.24)\\
& && (5.25)
\end{aligned}
$$

Therefore, we have the forward recursion:

$$\alpha_t(z_t) = p(x_t|z_t) \sum_{z_{t-1}=1}^{k} p(z_t|z_{t-1})\alpha_{t-1}(z_{t-1}) \tag{5.26}$$

$$\alpha_1(z_1) = p(x_1, z_1) \tag{5.27}$$

Backward filtering (decoding) Define

$$\beta_t(z_t) = p(x_{t+1:T}|z_t) \tag{5.28}$$

Then,

$$p(x_{t+1:T}|z_t) = \sum_{z_{k+1}=1}^{k} p(x_{t+1:T}, z_{t+1}|z_t) \tag{5.29}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+1}, x_{t+2:T}, z_{t+1}|z_t) \tag{5.30}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t, x_{t+1})p(x_{t+1}|z_t) \tag{5.31}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t, x_{t+1})p(x_{t+1}|z_t) \tag{5.32}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t)p(x_{t+1}|z_t) \tag{5.33}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}|z_t, z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) \tag{5.34}$$

$$= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}|z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) \tag{5.35}$$

$$= \sum_{z_{k+1}=1}^{k} \beta_{t+1}(z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) \tag{5.36}$$

5.6 Sampling

Problem 1 Generate samples

$$\{x^{(r)}\}_{r=1}^{R} \sim p(x) \tag{5.37}$$

Problem 2 Estimate expectations of functions $f(x)$ taking random variable $x \sim p(x)$.

$$\mathbb{E}_{x\sim p(x)} f(x) = \int f(x)p(x)\ dx \tag{5.38}$$

$$\approx \hat{E} = \frac{1}{N}\sum_{i=1}^{N} f(x^{(i)}) \tag{5.39}$$

Ancestral sampling sampling in a topological order. At each step, sample from any conditional distribution that you haven't visited yet, whose parents have all been sampled. This procedure will always start with the nodes that have no parents (i.e., a root).

Generating marginal samples for nodes $Y \subseteq X$:

(i) Construct $p(X) = \prod_{x_i \in X} p(x_i|\text{parent}[x_i])$;

(ii) Sample $(x_1, x_2, \cdots, x_N) \sim p(X)$;

(iii) Ignore $x_i \notin Y$.

Generating conditional samples for nodes $Y \subseteq Xt$ conditioned on $Z \subseteq X$:

Definition 5.5. The **simple Monte Carlo** estimator $\hat{\Phi}$ is defined as

$$\frac{1}{R}\sum_{r=1}^{R} f\left(x^{(r)}\right) = \hat{E} \approx E = \mathop{\mathbb{E}}_{x\sim p(x)}[f(x)] \tag{5.40}$$

Proposition 5.1. If the sample $\{x^{(r)}\}_{r=1}^{R}$ are generated from $p(x)$, then $\hat{E}$ is an unbiased estimator of E.

Proof.

$$\begin{aligned}
\mathbb{E}[\hat{E}]_{x\sim p\left(\{x^{(i)}\}_{r=1}^{R}\right)} &= \mathbb{E}\left[\frac{1}{R}\sum_{r=1}^{R} f\left(x^{(r)}\right)\right] && (5.41)\\
&= \frac{1}{R}\sum_{r=1}^{R}\mathbb{E}[f(x^{(r)})] && (5.42)\\
&= \frac{1}{R}\sum_{r=1}^{R}\mathbb{E}_{x\sim p(x)}[f(x)] && (5.43)\\
&= \frac{R}{R}\mathbb{E}_{x\sim p(x)}[f(x)] && (5.44)\\
&= E && (5.45)
\end{aligned}$$

■

Proposition 5.2. As the number of samples of R increases, the variance of $\hat{E}$ will decrease proportional to $\frac{1}{R}$.

Proof.

$$\begin{aligned}
Var[\hat{E}] &= Var[\frac{1}{R}\sum_{r=1}^{R} f(x^{(r)})] && (5.46)\\
&= \frac{1}{R^2}Var[\sum_{r=1}^{R} f(x^{(r)})] && (5.47)\\
&= \frac{1}{R^2}\sum_{r=1}^{R} Var[f(x^{(r)})] && (5.48)\\
&= \frac{1}{R^2}RVar[f(x)] && (5.49)\\
&= \frac{1}{R}Var[f(x)] && (5.50)
\end{aligned}$$

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