COMPSCI 689
Lecture 18: Mixture Models

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Probabilistic Unsupervised Learning

- In probabilistic unsupervised learning, our goal is to model multivariate data $\mathbf{x} = [x_1, ..., x_D]$ generated by an unknown probabilistic process using a probabilistic model learned from a data set $\mathcal{D} = \{\mathbf{x}_n | 1 \leq n \leq N\}$.
- Since the data are vectors, we use vector-valued random variables to model them $\mathbf{X} = [X_1, ..., X_D]$.
- Each data dimension d takes values from a potentially different set $\mathcal{X}_d$. We have $\mathbf{x} \in \mathcal{X}$. $\mathcal{X} = \mathcal{X}_1 \times ... \times \mathcal{X}_D$.

Joint Distributions

- A probability distribution over the joint settings of multiple random variables is referred to as a *joint distribution*.
- When all dimensions of $\mathbf{x}$ are discrete, the joint distribution is represented by a *joint probability mass* function $P(\mathbf{X} = \mathbf{x}) = P(X_1 = x_1, ..., .X_D = x_d)$.
- When all dimensions of $\mathbf{x}$ are continuous, the joint distribution is represented by a *joint probability density* function $p(\mathbf{X} = \mathbf{x}) = p(X_1 = x_1, ..., .X_D = x_d)$.
- When the data are of mixed-type, we can still model them via a probability distribution consisting of both mass and density function components.

Product of Marginals

- The most basic way to construct a joint probability model over a vector of random variables $\mathbf{X}$ is to model the marginal distribution of each random variable. The joint distribution is then defined as the product of marginals.

$$P(\mathbf{X} = \mathbf{x}|\theta) = \prod_{d=1}^{D} P(X_d = x_d|\theta_d)$$

$$N(x_d; \mu_{d1}, \sigma^2_{d2})$$

$$p(\mathbf{X} = \mathbf{x}|\theta) = \prod_{d=1}^{D} p(X_d = x_d|\theta_d)$$

Mixture Models

- Mixture models are basic universal probability distribution models that only require a small change to the product of marginals.
- They are constructed by introducing a finite discrete *latent* random variable Z to the observed variables $\mathbf{X}$.
- Instead of using a product of marginals to model $\mathbf{X}$, we use a product of distributions conditioned on Z.
- The joint distribution of $\mathbf{X}$ and Z is given by:

$$P(\mathbf{X} = \mathbf{x}, Z = z|\theta) = P(Z = z|\pi) \prod_{d=1}^{D} P(X_d = x_d|Z = z, \phi_{dz})$$

Mixture Models

- The distribution of $\mathbf{X}$ is given by marginalization of the joint over the values of $z \in [1, ..., K]$:

$$P(\mathbf{X} = \mathbf{x}|\theta) = \sum_{z=1}^{K} P(Z = z|\pi) \prod_{d=1}^{D} P(X_d = x_d|Z = z, \phi_{dz})$$

- The construction above is shown for an $\mathbf{X}$ that is all discrete, but the same construction works for continuous $\mathbf{X}$ as well as for mixed-types.

Example: Binary Mixture

Suppose the data are binary. We have $x_d \in \{0, 1\}$ for $1 \leq d \leq D$. We construct a mixture distribution for these data as follows:

$$
\begin{aligned}
P(Z = z|\pi) &= \pi_z \\
P(X_d = x_d|Z = z, \phi_{dz}) &= \phi_{dz}^{x_d}(1 - \phi_{dz})^{1-x_d} \\
P(\mathbf{X} = \mathbf{x}|Z = z, \phi_z) &= \prod_{d=1}^{D} P(X_d = x_d|Z = z, \phi_{dz}) \\
P(\mathbf{X} = \mathbf{x}, Z = z|\pi, \phi_z) &= P(Z = z|\pi)P(\mathbf{X} = \mathbf{x}|Z = z, \phi_z) \\
&= \pi_z \cdot \prod_{d=1}^{D} \phi_{dz}^{x_d}(1 - \phi_{dz})^{1-x_d}
\end{aligned}
$$

Example: Binary Mixture

The mixture distribution over $\mathbf{X}$ is obtained by marginalizing the mixture indicator variable Z out of the model:

$$P(\mathbf{X} = \mathbf{x}|\pi, \phi) = \sum_{z=1}^{K} P(Z = z|\pi) P(\mathbf{X} = \mathbf{x}|Z = z, \phi_z)$$

$$= \sum_{z=1}^{K} \pi_z \cdot \prod_{d=1}^{D} \phi_{dz}^{x_d} (1 - \phi_{dz})^{1-x_d}$$

Example: Binary Mixture

Given a vector $\mathbf{x}$, we can use probabilistic inference to infer the probability distribution over Z:

$$P(Z = z|\mathbf{X} = \mathbf{x}, \pi, \phi) = \frac{P(Z = z, \mathbf{X} = \mathbf{x}|\pi, \phi)}{P(\mathbf{X} = \mathbf{x}|\pi, \phi)}$$
$$= \frac{\pi_z \cdot \prod_{d=1}^{D} \phi_{dz}^{x_d}(1 - \phi_{dz})^{1-x_d}}{\sum_{z'=1}^{K} \pi_{z'} \cdot \prod_{d'=1}^{D} \phi_{d'z'}^{x_{d'}}(1 - \phi_{d'z'})^{1-x_{d'}}}$$

Note that when we have many dimensions, we need to be careful with this computation as both the numerator and denominator have the potential to underflow.

Example: Normal Mixture

Suppose the data x_d are real-valued for $1 \leq d \leq D$. We can model the data using a mixture where the component densities are conditional univariate normal distributions:

$$P(Z = z|\pi) = \pi_z$$

$$p(X_d = x_d|Z = z, \mu_{dz}, \sigma_{dz}) = \mathcal{N}(x_d; \mu_{dz}, \sigma^2_{dz})$$

$$p(\mathbf{x} = \mathbf{x}|Z = z, \mu_z, \sigma_z) = \prod_{d=1}^{D} \mathcal{N}(x_d; \mu_{dz}, \sigma^2_{dz})$$

$$P(\mathbf{X} = \mathbf{x}, Z = z|\pi, \mu, \sigma) = P(Z = z|\pi)p(\mathbf{x} = \mathbf{x}|Z = z, \mu_z, \sigma_z)$$

$$= \pi_z \cdot \prod_{d=1}^{D} \frac{1}{\sqrt{2\pi\sigma^2_{dz}}} \exp\left(-\frac{1}{2\sigma^2_{dz}}(x_d - \mu_{dz})^2\right)$$

Example: Normal Mixture

The mixture distribution over $\mathbf{X}$ is obtained by marginalizing the mixture indicator variable Z out of the model:

$$p(\mathbf{X} = \mathbf{x}|\pi, \mu, \sigma) = \sum_{z=1}^{K} P(Z = z|\pi) p(\mathbf{x} = \mathbf{x}|Z = z, \mu_z, \sigma_z)$$

$$= \sum_{z=1}^{K} \pi_z \cdot \prod_{d=1}^{D} \frac{1}{\sqrt{2\pi\sigma_{dz}^2}} \exp\left(-\frac{1}{2\sigma_{dz}^2}(x_d - \mu_{dz})^2\right)$$

$p(x = x_i|$:

$$p(x=n \mid z) = \prod_{d=1}^{D} \mathcal{N}(x_d; \mu_{dz}; \sigma_{dz}^2)$$

$$p(x=n, z=2 \mid \pi, \mu, \sigma) = p(z=2 \mid \pi) \; p(x=x \mid z, \mu_{2}, \sigma_{2})$$

$$= \sum_{z=1}^{K} \pi_2 \prod_{d=1}^{D} \frac{1}{\sqrt{2\pi}\sigma_{d2}^2} \exp\left(\frac{1}{2\sigma_{d2}^2}(x_d - \mu_{d2})^2\right)$$

$$p=(x=n \mid z=2) = \prod_{d=1}^{D} \mathcal{N}\left[x_d; \mu_{dz}, \sigma_{dz}^2\right)$$

$$p(x=n \mid z=?) = \frac{p(x_i \mid z)\, p(x_{-1} \mid z)}{\sqrt{2\pi\sigma_1^2 \times \cdots \sigma_{i-1}^2 \times \sigma_{i+1}^2 \times \cdots \sigma_D^2}}$$

$$\times \exp\left(\frac{-1}{2\sigma^2}\left(\left(\frac{x_1-\mu_1}{\sigma_1^2}\right) + \cdots + \frac{x_{i-1}-\mu_{i-1}}{\sigma_{i-1}^2}\right.\right.$$

$$+ \frac{r_{i+1} - \mu_{i+1}}{\sigma_{i+1}^2} + \cdots + \frac{x_d - \mu_d}{\sigma_d^2} \Big)$$

$$p(x$$

$$p(x=x_i|z)\,p(x=x|z) = p(x=x_i)\,p(x_1=x_1|z)$$

$$p(x_i=x_i|z) = \frac{p(x=x|z)}{p(x=x_i|z)}$$

$$p(x_i=x_i|z) = \frac{p(x=x_i, z=z)}{p(z=z)}$$

$$p(x_i = x_{-i}, z = z) = \int p(z = z)\, p(x_{-i} = x_{-i} \mid z)$$

$$p(x_i = x_{-i}) = \int_z p(x_i = x_{-i}, z = z)\, dz$$

$$= \sum_z p(z = z \mid \pi) \prod_{d=1}^{D_i} f(x_{id}; \mu_{zd}, \sigma^2_{zd})$$

$$\therefore \sum_z p(z = z \mid \pi)$$

$$\frac{\frac{1}{\sqrt{(2\pi)^{D}\sigma_1^2\times\sigma_2^2\times\cdots\sigma_D^2}}\times\exp\left(\frac{-1}{2\sigma_1^2}(x_1-\mu_1)^2\right)\times\exp\left(\frac{-1}{2\sigma_1^2}(x_1-\mu_1)^2\right)\times\exp\left(\frac{-1}{\sum\sigma_D^2}(x_D-\mu_M)^2\right)}{\int\cdots\frac{1}{\sqrt{2\pi\sigma_1^2}}\exp\left(-\frac{1}{2}\sigma_1^2\frac{(x_1-\mu_1)^2}{}\right)}$$

$$p(z=z \mid x_i = x_i) = \frac{p(z=z)\; p(x_{-i} = x_{-i} \mid z)}{p(x_i = x_{-i})}$$

$$= \frac{p(z=z)}{\sum_z \pi_z \left(\prod_{d=1}^{D_{-i}} \frac{1}{\sqrt{2\pi\sigma_{dz}}} \exp\left(-\frac{1}{2\sigma_{dz}^2} (x - \mu_{dz})^2 \right) \right)}$$

$$p(x_i = x_i) = \int p(x_{-i} = x_{-i} \mid z=z)$$

$p(x=x, z=z) = p(z=z)\, p(x=x \mid z)$

$p(x=x_i, z=z) = p(x=x_i \mid z)$

$p(x=x_i, z=z) = \prod_{d=1}^{D} \mathcal{N}(x_d; \mu_{dz}, \sigma_{dz}^2)$

$p(x=x_i, z=z) =$

$$p(z=z \mid x_i) = \frac{p(x=x_i, z=z)}{p(x=x_i)}$$

$p(x=x, z=z) = p(z)\, p(x=x \mid z)$

$\Rightarrow p(x_i=x_i, z=z) = p(z)\, p(x_i=x_i \mid z)\, p(x_{\neg i}=x_{\neg i} \mid z)$

$$p(z=2 \mid x_{-i}) = \frac{p(x=x_{-i}, z=2)}{p(x_{-i}=x_{-i})}$$

$$p(x=x_i) = \int \underline{p(x=x_{-i}, x=x_i)}\, dx_{-i}$$

$$p(x=x_{-i}, x_2 x_i) \Big| \cdot \; p(x=x_i)$$

$$\downarrow$$

$$z=2$$

$$p(x=x_{-i} \mid \underline{x=x_i})$$

$$\downarrow$$

$$z=2$$

z = Number of data cases

Example: Normal Mixture

Given a vector $\mathbf{x}$, we can use probabilistic inference to infer the probability distribution over Z:

$$P(Z = z|\mathbf{X} = \mathbf{x}, \pi, \mu, \sigma) = \frac{P(Z = z, \mathbf{X} = \mathbf{x}|\pi, \mu, \sigma)}{p(\mathbf{X} = \mathbf{x}|\pi, \mu, \sigma)}$$

$$= \frac{\pi_z \cdot \prod_{d=1}^{D} \frac{1}{\sqrt{2\pi\sigma_{dz}^2}} \exp\left(-\frac{1}{2\sigma_{dz}^2}(x_d - \mu_{dz})^2\right)}{\sum_{z'=1}^{K} \pi_{z'} \cdot \prod_{d'=1}^{D} \frac{1}{\sqrt{2\pi\sigma_{d'z'}^2}} \exp\left(-\frac{1}{2\sigma_{d'z'}^2}(x_d - \mu_{d'z'})^2\right)}$$

Note that when we have many dimensions, we need to be careful with this computation as both the numerator and denominator have the potential to underflow or overflow.

Losses for Distributions

Unlike in supervised learning, there are few commonly used losses between distributions:

- Absolute Loss: $L_1(P_* \| P_\theta) = \mathbb{E}_{P_*(\mathbf{X})}\left[|P_*(\mathbf{x}) - P(\mathbf{x}|\theta)|\right]$
- Squared Loss: $L_2(P_* \| P_\theta) = \mathbb{E}_{P_*(\mathbf{X})}\left[(P_*(\mathbf{x}) - P(\mathbf{x}|\theta))^2\right]$
- KL Divergence: $KL(P_* \| P_\theta) = \mathbb{E}_{P_*(\mathbf{X})}\left[\log\left(\frac{P_*(\mathbf{x})}{P(\mathbf{x}|\theta)}\right)\right]$

Question: Which of these losses can we approximate using a sample of data $\mathcal{D} = \{\mathbf{x}_n\}_{1:N}$?

Optimizing KL Divergence

$$\min_\theta KL(P_*\|P_\theta) = \min_\theta \sum_{\mathbf{x}\in\mathcal{X}} P_*(\mathbf{x})\big(\log P_*(\mathbf{x}) - \log P(\mathbf{x}|\theta)\big)$$

$$= \min_\theta \sum_{\mathbf{x}\in\mathcal{X}} P_*(\mathbf{x}) \log P_*(\mathbf{x}) - \sum_{\mathbf{x}\in\mathcal{X}} P_*(\mathbf{x}) \log P(\mathbf{x}|\theta)$$

$$= \min_\theta - \sum_{\mathbf{x}\in\mathcal{X}} P_*(\mathbf{x}) \log P(\mathbf{x}|\theta)$$

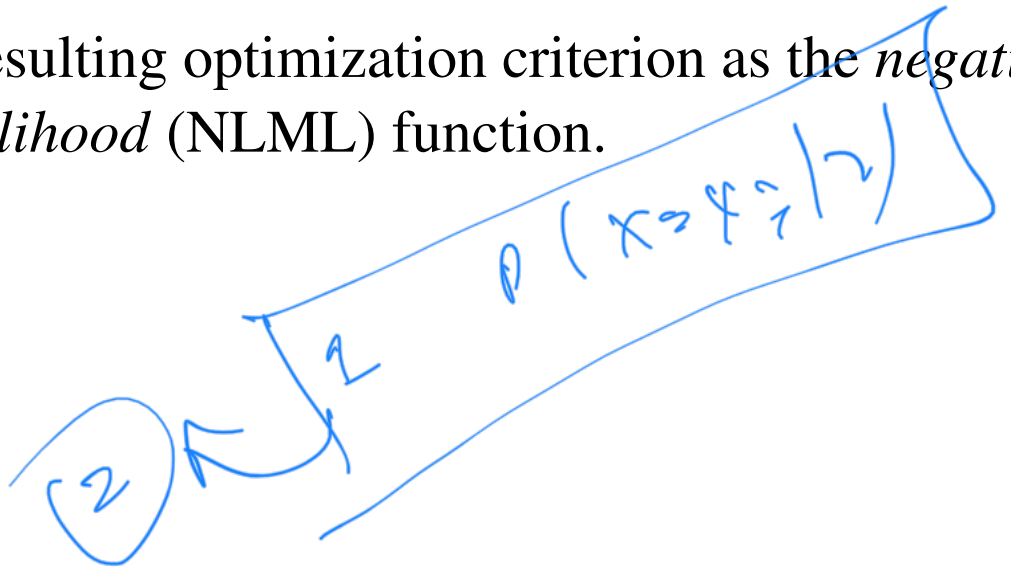
$$\approx \min_\theta -\frac{1}{N} \sum_{n=1}^{N} \log P(\mathbf{x}_n|\theta)$$

Optimization-Based Unsupervised Learning

- As we can see, selecting the value of θ that minimizes the NLL both makes the data the most likely and is a Monte Carlo approximation to selecting the value of θ that minimizes $KL(P_* \| P_\theta)$.
- The dominant approaches to optimization-based unsupervised learning of probabilistic models are thus maximum likelihood estimation and its penalized/regularized variants.

Learning for Mixture Models

- In a mixture model, the full joint distribution includes the data variables $\mathbf{X}$ and the latent mixture indicator variable Z.
- Since the mixture indicator variables Z are not observed, we need to marginalize them out of the model and then minimize the negative log likelihood of the marginalized distribution.
- We refer to the resulting optimization criterion as the *negative log marginal likelihood* (NLML) function.



Learning for Mixture Models

The negative log marginal likelihood for a generic mixture model is given below:

$$
\begin{aligned}
nlml(\mathcal{D}, \theta) &= -\sum_{n=1}^{N} \log P(\mathbf{x}_n|\theta) \\
&= -\sum_{n=1}^{N} \log \left(\sum_{z=1}^{K} P(Z = z|\pi) \prod_{d=1}^{D} P(X_d = x_{nd}|Z = z) \right)
\end{aligned}
$$

We can learn mixture models using direct negative log marginal likelihood minimization. Note that parameter transformations must be used to deal with constrained parameter spaces.