CSC 311: Introduction to Machine Learning

Tutorial 10 - EM Algorithm

University of Toronto, Fall 2020

Overview

- First, brief overview of Expectation-Maximization algorithm.
  - In the lecture we were using Gaussian Mixture Model fitted with Maximum Likelihood (ML) estimation.
- Today, practice with the E-M algorithm in an image completion task.
- We will use Mixture of Bernoullis fitted with Maximum a posteriori (MAP) estimation.
  - Learning the parameters
  - Posterior inference

The Generative Model

- We'll be working with the following generative model for data $\mathcal{D}$
- Assume a datapoint $\mathbf{x}$ is generated as follows:
  - Choose a cluster z from $\{1, \ldots, K\}$ such that $p(z = k) = \pi_k$
  - Given z, sample $\mathbf{x}$ from a probability distribution. (Earlier you saw Guassian $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_z, \mathbf{I})$, now we will work with Bernoulli(θ_z))
- Can also be written:

$$p(z = k) = \pi_k$$

$$p(\mathbf{x}|z = k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \mathbf{I})/\text{Bernoulli}(\theta_k)$$

Maximum Likelihood with Latent Variables

- How should we choose the parameters $\{\pi_k, \boldsymbol{\mu}_k\}_{k=1}^K$?
- Maximum likelihood principle: choose parameters to maximize likelihood of observed data
- We don't observe the cluster assignments z, we only see the data $\mathbf{x}$
- Given data $\mathcal{D} = \{\mathbf{x}^{(n)}\}_{n=1}^N$, choose parameters to maximize:

$$\log p(\mathcal{D}) = \sum_{n=1}^{N} \log p(\mathbf{x}^{(n)})$$

- We can find $p(\mathbf{x})$ by marginalizing out z:

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

Log-likelihood derivatives

$$\frac{\partial}{\partial\theta}\log p(x) = \frac{\partial}{\partial\theta}\log\sum_z p(x,z)$$

Log-likelihood derivatives

$$\frac{\partial}{\partial\theta}\log p(x) = \frac{\partial}{\partial\theta}\log\sum_z p(x,z)$$
$$= \frac{\frac{\partial}{\partial\theta}\sum_z p(x,z)}{\sum_{z'} p(x,z')}$$

Log-likelihood derivatives

$$
\begin{aligned}
\frac{\partial}{\partial \theta} \log p(x) &= \frac{\partial}{\partial \theta} \log \sum_z p(x, z) \\
&= \frac{\frac{\partial}{\partial \theta} \sum_z p(x, z)}{\sum_{z'} p(x, z')} \\
&= \frac{\sum_z \frac{\partial}{\partial \theta} p(x, z)}{\sum_{z'} p(x, z')}
\end{aligned}
$$

Log-likelihood derivatives

$$\begin{aligned}
\frac{\partial}{\partial\theta}\log p(x) &= \frac{\partial}{\partial\theta}\log\sum_z p(x,z) \\
&= \frac{\frac{\partial}{\partial\theta}\sum_z p(x,z)}{\sum_{z'} p(x,z')} \\
&= \frac{\sum_z \frac{\partial}{\partial\theta}p(x,z)}{\sum_{z'} p(x,z')} \\
&= \frac{\sum_z p(x,z)\frac{\partial}{\partial\theta}\log p(x,z)}{\sum_{z'} p(x,z')}
\end{aligned}$$

Log-likelihood derivatives

$$
\begin{aligned}
\frac{\partial}{\partial\theta}\log p(x) &= \frac{\partial}{\partial\theta}\log\sum_z p(x,z) \\
&= \frac{\frac{\partial}{\partial\theta}\sum_z p(x,z)}{\sum_{z'} p(x,z')} \\
&= \frac{\sum_z \frac{\partial}{\partial\theta}p(x,z)}{\sum_{z'} p(x,z')} \\
&= \frac{\sum_z p(x,z)\frac{\partial}{\partial\theta}\log p(x,z)}{\sum_{z'} p(x,z')} \\
&= \sum_z \left(\frac{p(x,z)}{\sum_{z'} p(x,z')}\frac{\partial}{\partial\theta}\log p(x,z)\right)
\end{aligned}
$$

Log-likelihood derivatives

$$
\begin{aligned}
\frac{\partial}{\partial \theta} \log p(x) &= \frac{\partial}{\partial \theta} \log \sum_z p(x, z) \\
&= \frac{\frac{\partial}{\partial \theta} \sum_z p(x, z)}{\sum_{z'} p(x, z')} \\
&= \frac{\sum_z \frac{\partial}{\partial \theta} p(x, z)}{\sum_{z'} p(x, z')} \\
&= \frac{\sum_z p(x, z) \frac{\partial}{\partial \theta} \log p(x, z)}{\sum_{z'} p(x, z')} \\
&= \sum_z \left(\frac{p(x, z)}{\sum_{z'} p(x, z')} \frac{\partial}{\partial \theta} \log p(x, z) \right) \\
&= \sum_z p(z \mid x) \frac{\partial}{\partial \theta} \log p(x, z)
\end{aligned}
$$

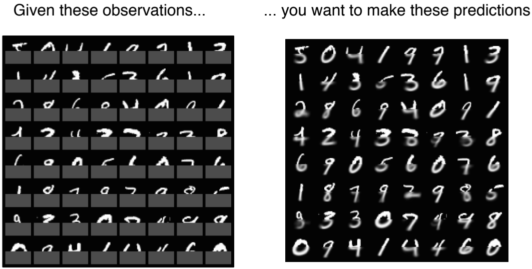
Expectation-Maximization algorithm

- The Expectation-Maximization algorithm alternates between two steps:
  1. E-step: Compute the posterior probabilities $r_k^{(n)} = p(z^{(n)} = k|\mathbf{x}^{(n)})$ given our current model - i.e. how much do we think a cluster is responsible for generating a datapoint.
  2. M-step: Use the equations on the last slide to update the parameters, assuming $r_k^{(n)}$ are held fixed- change the parameters of each distribution to maximize the probability that it would generate the data it is currently responsible for.

$$
\begin{aligned}
\frac{\partial}{\partial\theta}\log p(\mathcal{D}) &= \frac{\partial}{\partial\theta}\sum_{n=1}^{N}\log\sum_{k=1}^{K}p(z^{(n)}=k,\mathbf{x}^{(n)}) \\
&= \sum_{i=1}^{N}\sum_{k=1}^{K}p(z^{(n)}=k|\mathbf{x}^{(n)})\frac{\partial}{\partial\theta}\log p(x^{(n)},z^{(n)}) \\
&= \sum_{i=1}^{N}\sum_{k=1}^{K}r_k^{(i)}\left[\frac{\partial}{\partial\theta}\log\Pr(z^{(i)}=k)+\frac{\partial}{\partial\theta}\log p(\mathbf{x}^{(i)}\mid z^{(i)}=k)\right]
\end{aligned}
$$

Image Completion using Mixture of Bernoullis [1]

- A probabilistic model for the task of image completion.
- We observe the top half of an image of a handwritten digit, we would like to predict whats in the bottom half.



[1] Source

Mixture of Bernoullis model

- Our dataset is a set of 28×28 binary images represented as 784-dimensional binary vectors.
  - $N = 60{,}000$, the number of training cases. The training cases are indexed by i.
  - $D = 28 \times 28 = 784$, the dimension of each observation vector. The dimensions are indexed by j.
- Conditioned on the latent variable $z = k$, each pixel x_j is an independent Bernoulli random variable with parameter $\theta_{k,j}$:

$$
\begin{aligned}
p(\mathbf{x}^{(i)} \mid z = k) &= \prod_{j=1}^{D} p(x_j^{(i)} \mid z = k) \\
&= \prod_{j=1}^{D} \theta_{k,j}^{x_j^{(i)}} (1 - \theta_{k,j})^{1 - x_j^{(i)}}
\end{aligned}
$$

The Generative Process

This can be written out as the following generative process:

Sample z from a multinomial distribution $\boldsymbol{\pi}$.

For $j = 1, \ldots, D$:

Sample x_j from a Bernoulli distribution with parameter $\theta_{k,j}$, where k is the value of z.

It can also be written mathematically as:

$$z \sim \text{Multinomial}(\boldsymbol{\pi})$$
$$x_j \mid z = k \sim \text{Bernoulli}(\theta_{k,j})$$

Part 1: Learning the Parameters

- In the first step, well learn the parameters of the model given the responsibilities (M-step of the E-M algorithm).
- We want to use the MAP criterion instead of maximum likelihood (ML) to fit the Mixture of Bernoullis model.
  - The only difference is that we add a prior probability term to the ML objective function in the M-step.
  - ML objective function:

$$\sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \Pr(z^{(i)} = k) + \log p(\mathbf{x}^{(i)} \mid z^{(i)} = k) \right]$$

  - MAP objective function:

$$\sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \Pr(z^{(i)} = k) + \log p(\mathbf{x}^{(i)} \mid z^{(i)} = k) \right] + \log p(\boldsymbol{\pi}) + \log p(\boldsymbol{\Theta})$$

Part 1: Learning the Parameters (Prior Distribution)

- Use Beta distribution as the prior for $\mathbf{\Theta}$: Every entry is drawn independently from a beta distribution with parameters a and b:

$$p(\theta_{k,j}) \propto \theta_{k,j}^{a-1}(1-\theta_{k,j})^{b-1}$$

- Use Dirichlet distribution as the prior over mixing proportions $\boldsymbol{\pi}$:

$$p(\boldsymbol{\pi}) \propto \pi_1^{a_1-1}\pi_2^{a_2-1}\cdots\pi_K^{a_K-1}.$$

Part 1: Learning the Parameters

- Derive the M-step update rules for $\boldsymbol{\Theta}$ and $\boldsymbol{\pi}$ by setting the partial derivatives of the MAP objective function to zero.

$$J(\theta, \pi) = \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \Pr(z^{(i)} = k) + \log p(\mathbf{x}^{(i)} \mid z^{(i)} = k) \right] + \log p(\boldsymbol{\pi}) + \log p(\boldsymbol{\Theta})$$

$$\pi_k \leftarrow \ldots$$

$$\theta_{k,j} \leftarrow \ldots$$

Part 1: Learning the Parameters

$$J(\boldsymbol{\Theta}, \boldsymbol{\pi}) = \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \Pr(z^{(i)} = k) + \log p(\mathbf{x}^{(i)} \mid z^{(i)} = k) \right] + \log p(\boldsymbol{\pi}) + \log p(\boldsymbol{\Theta})$$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \pi_k + \sum_{j=1}^{D} x_j^{(i)} \log \theta_{k,j} + (1 - x_j^{(i)}) \log(1 - \theta_{k,j}) \right]$$
$$+ \sum_{k=1}^{K} (a_k - 1) \log \pi_k + \sum_{k=1}^{K} \sum_{j=1}^{D} [(a - 1) \log \theta_{k,j} + (b - 1) \log(1 - \theta_{k,j})] + C$$

Derivative wrt. $\theta_{k,j}$

$$J(\boldsymbol{\Theta}, \boldsymbol{\pi}) = \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \left[\log \pi_k + \sum_{j=1}^{D} x_j^{(i)} \log \theta_{k,j} + (1 - x_j^{(i)}) \log(1 - \theta_{k,j}) \right]$$
$$+ \sum_{k=1}^{K} (a_k - 1) \log \pi_k + \sum_{k=1}^{K} \sum_{j=1}^{D} [(a-1) \log \theta_{k,j} + (b-1) \log(1 - \theta_{k,j})] + C$$

- First we take derivative wrt. $\theta_{k,j}$:

$$\frac{\partial J}{\partial \theta_{k,j}} = \sum_{i=1}^{N} r_k^{(i)} \left[x_j^{(i)} \frac{1}{\theta_{k,j}} + (1 - x_j^{(i)}) \frac{1}{\theta_{k,j} - 1} \right] + (a-1) \frac{1}{\theta_{k,j}} + (b-1) \frac{1}{\theta_{k,j} - 1}$$
$$= \frac{1}{\theta_{k,j}} \left(\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) \right) + \frac{1}{\theta_{k,j} - 1} \left(\sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1 \right.$$

Derivative wrt. $\theta_{k,j}$

$$
\begin{aligned}
\frac{\partial J}{\partial \theta_{k,j}} &= \sum_{i=1}^{N} r_k^{(i)} \left[x_j^{(i)} \frac{1}{\theta_{k,j}} + (1 - x_j^{(i)}) \frac{1}{\theta_{k,j} - 1} \right] + (a-1)\frac{1}{\theta_{k,j}} + (b-1)\frac{1}{\theta_{k,j} - 1} \\
&= \frac{1}{\theta_{k,j}} \left(\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) \right) + \frac{1}{\theta_{k,j} - 1} \left(\sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1 \right.
\end{aligned}
$$

- Setting this to zero, and multiplying both sides by $\theta_{k,j}(\theta_{k,j} - 1)$ yields:

$$
0 = (\theta_{k,j} - 1) \left(\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) \right) + \theta_{k,j} \left(\sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1) \right)
$$

Derivative wrt. $\theta_{k,j}$

$$\frac{\partial J}{\partial \theta_{k,j}} = \sum_{i=1}^{N} r_k^{(i)} \left[x_j^{(i)} \frac{1}{\theta_{k,j}} + (1 - x_j^{(i)}) \frac{1}{\theta_{k,j} - 1} \right] + (a-1)\frac{1}{\theta_{k,j}} + (b-1)\frac{1}{\theta_{k,j} - 1}$$

$$= \frac{1}{\theta_{k,j}} \left(\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) \right) + \frac{1}{\theta_{k,j} - 1} \Bigg(\sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1$$

- Setting this to zero, and multiplying both sides by $\theta_{k,j}(\theta_{k,j} - 1)$ yields:

$$0 = (\theta_{k,j} - 1) \left(\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) \right) + \theta_{k,j} \left(\sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1) \right)$$

- This gives:

$$\theta_{k,j} = \frac{\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1)}{\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (a-1) + \sum_{i=1}^{N} [r_k^{(i)}] - \sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + (b-1)}$$

$$= \frac{\sum_{i=1}^{N} [r_k^{(i)} x_j^{(i)}] + a - 1}{\sum_{i=1}^{N} [r_k^{(i)}] + a + b - 2}$$

Derivative wrt. π_k

- Now we take derivative wrt. π_k.
- Note that it is a bit trickier because we need to account for the condition $\sum_{k=1}^{K} \pi_k = 1$.
- This can be done with the use of a Lagrange multiplier.
- Let $J_\lambda = J + \lambda(\sum_{k=1}^{K}[\pi_k] - 1)$

$$\frac{\partial J_\lambda}{\partial \pi_k} = \sum_{i=1}^{N} r_k^{(i)} \frac{1}{\pi_k} + (a_k - 1)\frac{1}{\pi_k} + \lambda$$

Derivative wrt. π_k

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- Note that it is a bit trickier because we need to account for the condition $\sum_{k=1}^{K} \pi_k = 1$.
- This can be done with the use of a Lagrange multiplier.
- Let $J_\lambda = J + \lambda(\sum_{k=1}^{K}[\pi_k] - 1)$

$$\frac{\partial J_\lambda}{\partial \pi_k} = \sum_{i=1}^{N} r_k^{(i)} \frac{1}{\pi_k} + (a_k - 1)\frac{1}{\pi_k} + \lambda$$

- Setting this to zero, we get:

$$\pi_k = \frac{(a_k - 1) + \sum_{i=1}^{N}[r_k^{(i)}]}{\lambda}$$

- Knowing that π_k sums to one, we obtain:

$$\pi_k = \frac{(a_k - 1) + \sum_{i=1}^{N}[r_k^{(i)}]}{\sum_{k=1}^{K}[(a_k - 1) + \sum_{i=1}^{N}[r_k^{(i)}]]} = \frac{(a_k - 1) + \sum_{i=1}^{N}[r_k^{(i)}]}{N + \sum_{k=1}^{K}(a_k - 1)}$$

- (We used $\sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} = \sum_{i=1}^{N} 1 = N$)

Part 2: Posterior inference

- We represent partial observations in terms of variables $m_j^{(i)}$, where $m_j^{(i)} = 1$ if the jth pixel of the ith image is observed, and 0 otherwise.
- Derive the posterior probability distribution $p(z \mid \mathbf{x}_{\text{obs}})$, where $\mathbf{x}_{\text{obs}}$ denotes the subset of the pixels which are observed.
- Using Bayes rule, we have:

$$\begin{aligned} p(z = k \mid x) &= \frac{p(x \mid z = k) p(z = k)}{p(x)} \\ &= \frac{\pi_k \prod_{j=1}^{D} \theta_{k,j}^{m_j x_j} (1 - \theta_{k,j}^{m_j (1 - x_j)})}{\sum_{l=1}^{K} \pi_l \prod_{j=1}^{D} \theta_{l,j}^{m_j x_j} (1 - \theta_{l,j}^{m_j (1 - x_j)})} \end{aligned}$$

Part 3: Posterior Predictive Mean

- Computes the posterior predictive means of the missing pixels given the observed ones.
- The posterior predictive distribution is:

$$p(x_2 \mid x_1) = \sum_z p(z \mid x_1) p(x_2 \mid z, x_1)$$

- Assume that the x_i values are conditionally independent given z.
- For instance, the pixels in one half of an image are clearly not independent of the pixels in the other half. But they are roughly independent, conditioned on a detailed description of everything going on in the image.
- So we have:

$$\begin{aligned}\mathbb{E}[p(x_{mis}|x_{obs})] &= \sum_{k=1}^{K} r_k p(x_{mis} = 1 \mid z = k) = \sum_{k=1}^{K} r_k \text{Bernoulli}(\theta_{k,mis}) \\ &= \sum_{k=1}^{K} r_k \theta_{k,mis}\end{aligned}$$

Questions?

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