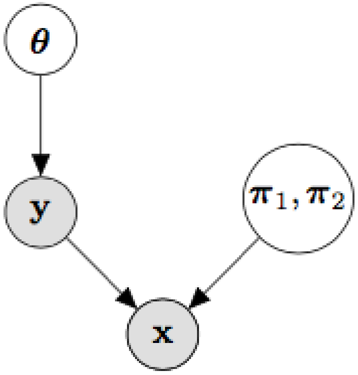
CS 181 Spring 2017 Section 8
Mixture Modeling and EM
Solution

1 Graphical Models

We can represent a large class of probabilistic models within the framework of *directed graphical models*. A directed graphical model is a visual representation that shows the conditional relationships between parameters, latent variables, and observed variables, and provides a language for factorizing a joint distribution.

Exercise 1. *Use the following graphical model to factorize the joint distribution* $p(\mathbf{x}, \mathbf{y} | \theta, \boldsymbol{\pi}_1, \boldsymbol{\pi}_2)$*. Which of the models we have studied in this class does this graphical model represent?*



Solution. $p(\mathbf{x}, \mathbf{y} | \theta, \boldsymbol{\pi}_1, \boldsymbol{\pi}_2) = p(\mathbf{y}|\theta) p(\mathbf{x}|\mathbf{y}, \boldsymbol{\pi}_1, \boldsymbol{\pi}_2)$. This is the graphical representation of the Naive Bayes algorithm we saw earlier in the class. □

2 Mixture Models

A *mixture model* is a type of probabilistic model for unsupervised learning. The basic idea is the following: we assume that our data is generated by first sampling a category from some predefined set, and then sampling an observation within that category. That is, we sample a latent variable $\mathbf{z}$ according to a categorical distribution $p(\mathbf{z} = C_k; \boldsymbol{\theta}) = \theta_k$, and then sample an observation $\mathbf{x}$ from some distribution $p(\mathbf{x}|\mathbf{z})$.

Mixture models are very useful for modeling *latent variables*, i.e., variables that aren't directly observed at training time, but are still part of the data generation process. For example, we can cluster data by fitting a mixture model, and then determining the most likely latent class for each data point. Unfortunately, training mixture models cannot be done simply in closed form. Instead we need to use a form of approximate maximum-likelihood estimation called *expectation maximization*.

3 Expectation Maximization

Expectation maximization is a general technique for maximum-likelihood estimation used primarily for models with latent variables. While we talk primarily here about mixture models, EM is often used for a variety of other models.

Consider a generative mixture model consisting of a latent variable $\mathbf{z}$ from a distribution $p(\mathbf{z}; \mathbf{w})$ and an observed variable $\mathbf{x}$, such that we draw $\mathbf{x}$ from a distribution $p(\mathbf{x}|\mathbf{z}; \mathbf{w})$ for some vector of parameters $\mathbf{w}$.

We have 2 goals: first, to compute the MLE for $\mathbf{w}$, i.e. the value of $\mathbf{w}$ that maximizes $p(\mathbf{x}; \mathbf{w})$, and second, to estimate the latent variable $\mathbf{z}$ corresponding to a particular $\mathbf{x}$, which in this case means maximize the distribution $p(\mathbf{z}|\mathbf{x}; \mathbf{w})$. The latter goal is easy once we have an estimate of the MLE for $\boldsymbol{\theta}$, because we can apply Bayes rule:

$$p(\mathbf{z}|\mathbf{x}; \mathbf{w}) \propto p(\mathbf{x}|\mathbf{z}; \mathbf{w}) p(\mathbf{z}; \mathbf{w}) \tag{1}$$

So all we need to do is build a model for the generative process ($p(\mathbf{x}|\mathbf{z}; \mathbf{w})$ and $p(\mathbf{z}; \mathbf{w})$), and determine out how to calculate the MLE.

3.1 Why EM?

Unfortunately calculating the MLE is often computationally intractable, because the log-likelihood is:

$$\log p(\mathbf{x}; \mathbf{w}) = \log \sum_{\mathbf{z} \in Z} p(\mathbf{x}, \mathbf{z}; \mathbf{w}) \tag{2}$$

We know the form of the model $p(\mathbf{x}, \mathbf{z}; \mathbf{w})$, but in general we don't know the likelihood $p(\mathbf{x}; \mathbf{w})$ in closed form. There is no closed form expression for the MLE because it is the log of a sum of expressions, which makes simplifying difficult. Note that we've assumed that our latent variable $\mathbf{z}$ takes on values in a discrete space Z (below, that space will be a set of class labels or clusters, and thus $Z = \{C_k\}_{k=1}^{c}$, and $\mathbf{z}$ is one-hot)— things get even more difficult in the continuous case (the sum becomes an integral, etc.).

3.2 Algorithm

Since finding the MLE directly is difficult, we will use an approximate iterative approach. This takes the following form: we approximate the MLE, approximate the distribution of the latent variables $\mathbf{z}$, and repeat until the approximation is very good. This makes the problem simpler, since we usually have good ways to find the MLE given the value of the $\mathbf{z}$, and to find the distribution of $\mathbf{z}$ given the MLE. In particular, if we know the value of $\mathbf{w}$, then the distribution of $\mathbf{z}$ is $p(\mathbf{z}|\mathbf{x};\mathbf{w})$. Additionally if we know the distribution of $\mathbf{z}$, then the expected complete data log-likelihood is tractable, since we are calculating:

$$\begin{aligned}
\mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}}\left[\sum_{i=1}^{n}\log p(\mathbf{x}_i,\mathbf{z}_i;\mathbf{w})\right] &= \mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}}\left[\sum_{i=1}^{n}(\log p(\mathbf{x}_i|\mathbf{z}_i;\mathbf{w})+\log p(\mathbf{z}_i;\mathbf{w}))\right] && (3)\\
&= \sum_{\mathbf{z}\in\mathcal{Z}} p(\mathbf{z}|\mathbf{x};\mathbf{w})\left[\sum_{i=1}^{n}(\log p(\mathbf{x}_i|\mathbf{z}_i;\mathbf{w})+\log p(\mathbf{z}_i;\mathbf{w}))\right] && (4)\\
&= \sum_{\mathbf{z}\in\mathcal{Z}} q(\mathbf{z})\left[\sum_{i=1}^{n}(\log p(\mathbf{x}_i|\mathbf{z}_i;\mathbf{w})+\log p(\mathbf{z}_i;\mathbf{w}))\right] && (5)
\end{aligned}$$

where $p(\mathbf{z}|\mathbf{x};\mathbf{w}) = q(\mathbf{z})$. So the steps of the algorithm are:

1. Initialize a $\mathbf{w}^{(0)}$ randomly (what are we trying to avoid in this initialization?).
2. Calculate the distribution $\mathbf{q}$ over $\mathbf{z}$:

$$q_{i,k} = p(\mathbf{z}_i = C_k|\mathbf{x}_i;\mathbf{w}^{(i)}) \propto p(\mathbf{x}_i|\mathbf{z}_i;\mathbf{w}^{(i)})p(\mathbf{z}_i;\mathbf{w}^{(i)}) \tag{6}$$

3. Choose the value of $\mathbf{w}^{(i+1)}$ that maximizes the expected complete data log likelihood (where the expectation is over the distribution calculated above):

$$\mathbf{w}^{(i+1)} = \underset{\mathbf{w}}{\operatorname{argmax}}\,\mathbb{E}_{\mathbf{q}}\left[\log p(\mathbf{x},\mathbf{z};\mathbf{w})\right] \tag{7}$$

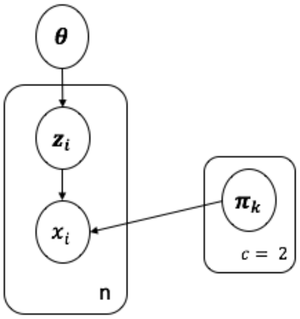
4. Go back to step 2 until the log likelihood estimate converges.

3.3 Example 1 - Coins

Consider a setup where we have 2 biased coins. We generate data by picking between the two coins with another biased coin, and then flip the chosen coin to generate a new data point x_i. We wish to do inference on the parameters of the coins, but the only data we're given is the outcomes of the flips.

Here, we have a very clear choice of $\mathbf{z}_i$: a value that indicates whether the ith coin flip was from the first or second coins. To keep parity with the lecture, which essentially uses the same model for the mixture of multinomials, we'll let the variable $\mathbf{z}_i$ be a one-hot vector (of size 2) indicating which coin it came from. Also, we'll denote the vector of probabilities for the coin used to choose between coins as $\boldsymbol{\theta} \in \mathbb{R}^2$, where θ_1 is the probability we'll pick the first coin, and θ_2 the second. Finally, we'll use $\boldsymbol{\pi}_1, \boldsymbol{\pi}_2 \in \mathbb{R}^2$ to denote the biases for each coin, where $\boldsymbol{\pi}_1$ is the vector of probabilities for coin 1, etc. This is exactly the same setup as in class for a mixture of multinomials except we only have two multinomials here (coins 1 and 2) and they have 2 outcomes (heads or tails). We let $\mathbf{w} := \{\boldsymbol{\theta}, \boldsymbol{\pi}\}$.

Exercise 2. *Draw a graphical model that represents this generative process.*



Solution.

□

First we note that we can calculate $\mathbf{q}_i$ from $\mathbf{w}^{(i)}$ by writing:

$$\begin{aligned}
\mathbf{q}_i &= \begin{bmatrix} p(\mathbf{z}_i = C_1 | \mathbf{x}_i; \mathbf{w}^{(i)}) \\ p(\mathbf{z}_i = C_2 | \mathbf{x}_i; \mathbf{w}^{(i)}) \end{bmatrix} && (8)\\
&\propto \begin{bmatrix} p(\mathbf{x}_i | \mathbf{z}_i = C_1; \mathbf{w}^{(i)}) p(\mathbf{z}_i = C_1; \mathbf{w}^{(i)}) \\ p(\mathbf{x}_i | \mathbf{z}_i = C_2; \mathbf{w}^{(i)}) p(\mathbf{z}_i = C_2; \mathbf{w}^{(i)}) \end{bmatrix} && (9)\\
&\propto \begin{bmatrix} (\pi_{11})^{x_1} (\pi_{12})^{x_2} \theta_1 \\ (\pi_{21})^{x_1} (\pi_{22})^{x_2} \theta_2 \end{bmatrix} && (10)
\end{aligned}$$

We also have the data log-likelihood as

$$\begin{aligned}
\log p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w}) &= \log p(\mathbf{x}_i | \mathbf{z}; \mathbf{w}) p(\mathbf{z}; \mathbf{w}) && (11)\\
&= \log \prod_{k=1}^{c=2} \left(\theta_k \prod_{j=1}^{2} \pi_{kj}^{x_{ij}} \right)^{z_{ik}} && (12)\\
&= z_{i1} \left(\log \theta_1 + x_{i1} \log \pi_{11} + x_{i2} \log \pi_{12} \right) && (13)\\
&+ z_{i2} \left(\log \theta_2 + x_{i1} \log \pi_{21} + x_{i2} \log \pi_{22} \right) && (14)\\
\log p(\mathbf{x}, \mathbf{z}; \mathbf{w}) &= \sum_{i=1}^{n} \log p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w}) && (15)
\end{aligned}$$

Finally, if we have an estimate for $\mathbf{q}$, we also have

$$\begin{aligned}
\mathcal{L}_c &= \mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}} \left[\sum_{i=1}^{n} \log p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w}) \right] && (16) \\
&= \mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}} \left[\sum_{i=1}^{n} \log p(\mathbf{z}_i; \mathbf{w}) + \log p(\mathbf{x}_i | \mathbf{z}_i; \mathbf{w}) \right] && (17) \\
&= \sum_{i=1}^{n} \mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}} \left[\log p(\mathbf{z}_i; \mathbf{w}) + \log p(\mathbf{x}_i | \mathbf{z}_i; \mathbf{w}) \right] && (18) \\
&= \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \left(\log \theta_k + \sum_{j=1}^{2} x_{ij} \log \pi_{kj} \right) && (19) \\
&= \sum_{i=1}^{n} q_{i1} \left(\log \theta_1 + x_{i1} \log \pi_{11} + x_{i2} \log \pi_{12} \right) + q_{i2} \left(\log \theta_2 + x_{i1} \log \pi_{21} + x_{i2} \log \pi_{22} \right) && (20)
\end{aligned}$$

since $\mathbf{q}$ is just a pair of probabilities for each example. This gives us everything we need to use expectation-maximization. Let's walk through the steps:

1. Initialize $\mathbf{w}^{(0)}$ randomly.

2. Use $\mathbf{w}^{(i)}$ to calculate the vector of probabilities $\mathbf{q}_i$ for the distribution of each $\mathbf{z}_i$ (eqs. 8-10).

3. Calculate the approximate expected likelihood using $\mathbf{q}_i$ and $\mathbf{w}^{(i)}$ (eqs. 11-15). This step is not strictly necessary for calculating updates, but can be helpful for a variety of purposes, including debugging and testing convergence. Note that we need *both* $\mathbf{q}$ and $\mathbf{w}^{(i)}$ to get a value here.

4. Use $\mathbf{q}$ to calculate an updated set of parameters $\mathbf{w}^{(i+1)}$ by maximizing the expected likelihood as a function of $\mathbf{w}$ (eqs. 16-20). Note that here we do *not* use $\mathbf{w}^{(i)}$.

   During optimization we need to enforce that $\sum_k \theta_k = 1$ and that $\sum_j \pi_{kj} = 1$, so that the distributions parameterized by $\boldsymbol{\theta}$ and $\boldsymbol{\pi}$ valid. In general we want to use Langrange multipliers, but in this case we can substitute $\theta_2 = 1 - \theta_1$ and $\pi_{k2} = 1 - \pi_{k1}$:

$$\begin{aligned}
\mathcal{L}_c = \sum_{i=1}^{n} \; & q_{i1} \left(\log \theta_1 + x_{i1} \log \pi_{11} + x_{i2} \log(1 - \pi_{11}) \right) && (21) \\
& + q_{i2} \left(\log(1 - \theta_1) + x_{i1} \log \pi_{21} + x_{i2} \log(1 - \pi_{21}) \right) && (22)
\end{aligned}$$

And then optimize w.r.t. $\theta_1, \pi_{11}, \pi_{21}$:

$$\frac{\partial \mathcal{L}_c}{\partial \theta_1} = \sum_{i=1}^{n} \left(\frac{q_{i1}}{\theta_1} - \frac{q_{i2}}{1-\theta_1} \right) = 0 \tag{23}$$

$$\frac{\partial \mathcal{L}_c}{\partial \pi_{11}} = \sum_{i=1}^{n} q_{i1} \left(\frac{x_{i1}}{\pi_{11}} - \frac{x_{i2}}{1-\pi_{11}} \right) = 0 \tag{24}$$

$$\frac{\partial \mathcal{L}_c}{\partial \pi_{21}} = \sum_{i=1}^{n} q_{i2} \left(\frac{x_{i1}}{\pi_{21}} - \frac{x_{i2}}{1-\pi_{21}} \right) = 0 \tag{25}$$

From here we can solve for the optimal value of $\mathbf{w}$ (i.e. $\theta_1, \pi_{11}, \pi_{22}$), and set $\mathbf{w}^{(i+1)} = \operatorname{argmax}_{\mathbf{w}} \mathbb{E}_{\mathbf{z}|\mathbf{x};\mathbf{w}} \mathcal{L}_c$.

Note: Above we show the derivation of all steps of the algorithm, but in practice $\mathbf{w}^{(i+1)}$ has a closed form, so the steps of the algorithm are really just initialization, calculate the distribution $\mathbf{q}_i$ from $\mathbf{w}^{(i)}$, and then calculate $\mathbf{w}^{(i+1)}$ from $\mathbf{q}$. All the difficult work is in deriving the update equations. In more complicated models it can happen that $\mathbf{w}^{(i+1)}$ does not have a closed form, so instead we can do gradient descent to calculate the optimal value.

Exercise 3. *Derive the closed form updates for $\boldsymbol{\theta}^{(i)}, \boldsymbol{\pi}^{(i)}$ from the steps above.*

Solution. We use t to refer to the tth step to disambiguate from indexing over the data:

$$\theta_k^{(t)} \leftarrow \frac{\sum_{i=1}^{n} q_{ik}}{n}$$

$$\boldsymbol{\pi}_k^{(t)} \leftarrow \frac{\sum_{i=1}^{n} q_{ik} \mathbf{x}_i}{\sum_{i=1}^{n} \sum_{j=1}^{m} q_{ik} x_{ij}}$$

□

Once we have an estimate for the MLE, we can use it to do prediction of hidden states for a new incoming coin flip, using step 2 from above. So, given a new coin flip, we can predict whether it can from the first or the second coin. As you can imagine, this is a terrible process, since we get a single bit of information, and in particular it is impossible to tell the difference between having one coin with high probability at 0.5 (and another picked almost never with bias = 0.1 e.g.) and two equally likely coins with biases 0.4 and 0.6. This problem is due more to the data setup rather than the method, so let's try an easier problem:

Exercise 4. *Consider the following data generation process: the setup is the same as above, but instead of flipping the chosen coin once, we flip it 10 times before choosing a new coin.*

1. *Find an appropriate choice of latent variables $\mathbf{z}_i$ and calculate the distribution of $\mathbf{z}_i$ given the data $\mathbf{x}_{i,j}$ (where i iterates over the sets of 10 coin flips, and $j \in [1, 10]$) and an estimate for $\boldsymbol{\theta}$.*

2. *Find the expression for the expected complete data log-likelihood*
3. *Find the closed form update equations for $\boldsymbol{\theta}^{(i)}$, and compare them to the result from Exercise 1.*

Solution.

1. Here again we can use $\mathbf{z}_i$ to denote the 1-hot choice of the chosen coin, this time used for all 10 of the flips. The distribution of $\mathbf{z}_i$ is again proportional to the prior times the likelihood, which is:

   $$p(\mathbf{z}_i|\mathbf{x}_i, \mathbf{w}) \propto p(\mathbf{x}_i|\mathbf{z}_i, \mathbf{w}) \cdot p(\mathbf{z}_i|\mathbf{w}) = \prod_{k=1}^{c=2} \left(\prod_{j=1}^{10} \prod_{l=1}^{2} \pi_{kl}^{x_{ijl}} \right)^{z_{ik}} \cdot \prod_{k=1}^{c=2} \theta_k^{z_{ik}}$$

   where x_{ijl} is the indicator variable for the jth coin in the ith set of 10 being in class l (in this case, heads or tails).

2. The expected complete data loglikelihood is similar to the above case:

   $$\mathcal{L}_c = \sum_{i=1}^{n} \sum_{k=1}^{c=2} q_{ik} \left(\log \theta_k + \sum_{j=1}^{10} \sum_{l=1}^{2} x_{ijl} \log \pi_{kj} \right)$$

3. In fact, $\boldsymbol{\theta}$ satisfies the same expression as before, so the update is the same:

   $$\theta_k^{(t)} \leftarrow \frac{\sum_{i=1}^{n} q_{ik}}{n}$$

   The only thing that has changed here is the matrix $\mathbf{q}$. Remember that q_{ik} is proportional to the prior probability of choosing the coin, times the likelihood. Here the likelihood term is stronger (because we see more evidence per latent variable) so we can expect this estimate to be less noisy, and thus our estimation of θ is less noisy.

□

3.4 Example 2 - Gaussian Mixture Modeling

We covered this in class, but it's a good idea to go over some of the points in the derivation from class. Remember that the setup is that we have data $\mathbf{x}_i \in \mathbb{R}^m$ and a latent variable $\mathbf{z}_i$ (corresponding to the cluster that the point is drawn from) such that $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z} = C_k) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, where $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ are the mean and covariance of the kth cluster. The choice of cluster is drawn from a categorical distribution with probabilities $\boldsymbol{\theta} \in \mathbb{R}^c$. We are able to observe the data $\mathbf{x}_i$ and want to find the cluster centers and their covariances.

Following the same format as above, the steps of EM inference applied to this problem are:

1. Randomly initialize $\boldsymbol{\theta}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_k$.
2. Next, calculate the new distribution of each $\mathbf{z}_i$:

   $$q_{ik} = p(z_i = C_k|\mathbf{x}_i) \propto \theta_k \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{26}$$

   This is our new estimate of the distribution of $\mathbf{z}_i$ given the data and our estimate for $\boldsymbol{\theta}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_k$.
3. Find the expected complete data log-likelihood:

   $$\begin{aligned} \mathbb{E}_{\mathbf{Z}}\left[\mathcal{L}\right] &= \mathbb{E}_{\mathbf{Z}}[\sum_{i=1}^{n} \ln(p(\mathbf{x}_i, \mathbf{z}_i; \boldsymbol{\theta}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_k))] \qquad (27) \\ &= \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \ln \theta_k + q_{ik} \ln \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad (28) \end{aligned}$$

   and then optimize it for each of the parameters $\boldsymbol{\theta}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_k$. However, we need to be careful to remember constraints: since $\sum_k \theta_k = 1$, we must use Lagrange multipliers to optimize the parameters. We get the following update equations:

   $$\begin{aligned} \theta_k^{(i+1)} &= \frac{\sum_{i=1}^{n} q_{ik}}{n} \qquad (29) \\ \boldsymbol{\mu}_k^{(i+1)} &= \frac{\sum_{i=1}^{n} q_{ik}\mathbf{x}_i}{\sum_{i=1}^{n} q_{ik}} \qquad (30) \\ \boldsymbol{\Sigma}_k^{(i+1)} &= \frac{\sum_{i=1}^{n} q_{ik}(\mathbf{x}_i - \boldsymbol{\mu}_k^{(i+1)})(\mathbf{x}_i - \boldsymbol{\mu}_k^{(i+1)})^\top}{\sum_{i=1}^{n} q_{ik}} \qquad (31) \end{aligned}$$

4 Additional Practice

1. **Lightbulbs**

   Assume that the lifespan of a set of lightbulbs follows an exponential distribution with mean θ, where the pdf of the exponential is $f(t) = e^{-t/\theta}/\theta$. We run two experiments with n and m lightbulbs respectively to calculate θ. In the first experiment, we record the time until the lightbulbs have burned out as $x_1, \ldots, x_n$. Unfortunately while running the second experiment we forgot to check the room until time t, when r of the bulbs had already burnt out. We immediately stopped the experiment afterwards.

   (a) What is a natural choice for the hidden variables? How many of them do we need?

   (b) What form does the complete data log-likelihood take?

   Solution. A natural choice for the latent variable $\mathbf{z}$ is the vector of times $z_1, \ldots, z_m$ when the m bulbs in the second experiment failed, since that makes the distributions $p(r \mid \mathbf{z}; \theta)$ just a fixed value of $\#\{z_i < t\}$, and the form of $\mathbf{z}; \theta$ is convenient. □