CS281 Section #7 Notes, v 1.1

Note: These notes are more of a lecture review than a collection of exercises.

1 Information Theory

Working at Bell Labs, Shannon tried to formalize communication mathematically. "The fundamental problem is that of reproducing at one point either exactly or approximately a message selected at another point" (*A Mathematical Theory of Communication*, 1948). Think in terms of sending a telegram:

- **information source**: telegram writer, wants to send a message.
- **encoder**: telegram machine, translates the message into a **code** for transmission
- **channel**: electrical wire connecting telegram machines, (often noisy) transmission medium
- **decoder**: telegram machine, tries to recover original message from the codes received

1.1 Entropy and related concepts

If a random variable X has K possible outcomes (e.g. the weather can only be rainy or sunny or cloudy), and the probability distribution is denoted by $p(X)$, then **entropy** is given by

$$H(X) = -\sum_k p(X=k)\log p(X=k) = -\mathbb{E}\big[\log p(x)\big].$$

Exercise: which distribution over K outcomes maximizes entropy? **Solution**: uniform distribution.

Entropy in statistical physics measures the orderlessness of a system. Entropy in info theory measures the uncertainty of a distribution, and information is the reduction of uncertainty. For continuous RVs:

$$H(X) = -\int_x p(x)\log p(x).$$

Conditional entropy of X conditioned on Y measures the *expected* uncertainty over X after a observing Y. $H(X|Y=y)$ is the uncertainty of X given a particular $Y=y$ but $H(X|Y)$ is an averages over all $Y=y$

$$H(X|Y) = \int_y p(x)H(X|Y=y) = -\int_x\int_y p(x,y)\log p(x|y) = -\mathbb{E}_{x,y}\log p(x|y)$$

Relative entropy, or **Kullback-Leibler divergence**, measures how different two distributions are

$$KL(p||q) = \int_x p(x)\log\frac{p(x)}{q(x)}.$$

Note that KL-divergence is not symmetric. That is, $KL(p||q) \neq KL(q||p)$. Another measure of the degree of difference between two distributions is the **Jensen-Shannon divergence**

$$JSD(p,q) = \frac{1}{2}KL(p||m) + \frac{1}{2}KL(q||m),$$

where $m = \frac{1}{2}(p+q)$.

Interpret $H(X)$ as the average number of bits needed to encode an outcome $x \sim p(X)$ using an optimal (minimum-length) coding scheme. **Cross entropy** $H_q(p)$ is the expected number of bits needed to encode outcomes $x \sim p(X)$ from distribution p using a scheme optimized for another distribution q

$$H(p, q) = H_q(p) = -\mathbb{E}_{p(X)}\big[\log q(X)\big] = H(p) + KL(p||q)$$

Now $KL(p||q)$ can be more concretely defined as the *increase in average bits* when switching from a coding scheme optimized for p to one optimized for q while continuing to send items from $p(X)$

Exercise: Show that the entropy of X is the average number of bits needed to encode an outcome under an optimal encoding scheme.
Solution: If you have K objects, you need $\log_2(K)$ bits to represent any one of the objects with a unique binary number. Using the optimal variable-length coding scheme (like Huffman Encoding), take the weighted average of the number of bits.

Mutual Information is a symmetric measurement that reflects how much information two distributions share

$$I(X; Y) = KL(p(X, Y)||p(X)p(Y)) = \int_x \int_y p(x, y) \log \frac{p(x, y)}{p(x)p(y)}$$

As a consequence of Jensen's inequality, which states that $f(\mathbb{E}[x]) \leq \mathbb{E}[f(x)]$ for convex f, mutual information is always non-negative. The mutual information is the *difference in uncertainty* $H(X) - H(X|Y)$. This is the amount of uncertainty of X explained by observing Y.

1.2 Some concepts in information geometry

To approximate a distribution p with another distribution q subject to some constraints, we choose q from a family of distributions Q and "project" p onto Q one of two ways

- **Information projection** (reverse) from p to Q is to find the q that minimizes $KL(q||p)$.
- **Moment projection** (forward) from p to Q is to find the q that minimizes $KL(p||q)$.

2 Latent Variables, Mixture Models, and EM

2.1 Latent Variables

A **latent variable** is one that is not observed at training time, but that is still part of the data generation process. Let $\{x_n\}$ be a set of observed variables and $\{z_n\}$ be a set of latent variables with joint density $p(z, x)$. The inference problem is to compute $p(z|x)$. We can write

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

but the **evidence** $p(x)$ can be intractable to compute

$$p(x) = \int p(z, x)dz$$

The evidence is needed to compute the conditional from the joint.

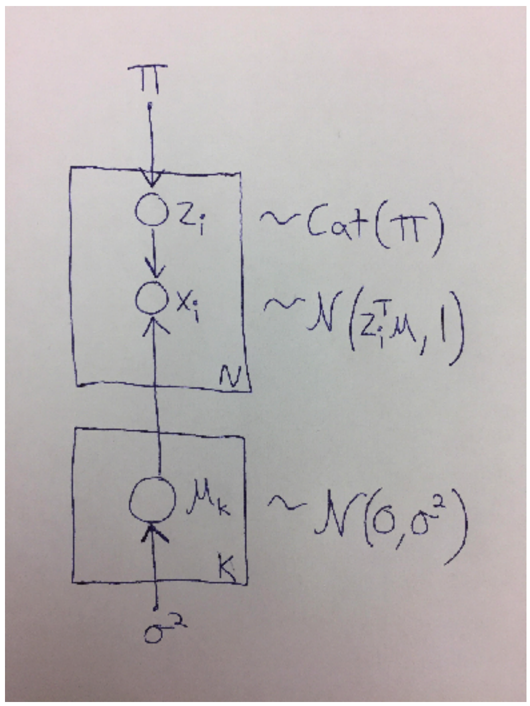
2.2 Bayesian Mixture of Gaussians

Note: Mixtures are much more general than Mixture of Gaussians

Consider a mixture of K unit-variance univariate Gaussians with means $\mu = \{\mu_1, ..., \mu_K\}$. The mean parameters are drawn independently from a common prior $p(\mu_k)$, for now assume $\mathcal{N}(0, \sigma^2)$ with given σ^2. To generate an observation x_i, first draw a cluster assignment z_i that indicates which latent cluster x_i comes from, drawn from $\text{Cat}(\pi)$. Then, draw x_i from $\mathcal{N}(z_i^\top \mu, 1)$ (z_i is one-hot and selects the proper μ_k).

$$\begin{aligned}\mu_k &\sim \mathcal{N}(0, \sigma^2)\\ z_i &\sim \text{Cat}(\pi)\\ x_i|z_i, \mu &\sim \mathcal{N}(z_i^\top \mu, 1)\end{aligned}$$

Exercise: Draw the DGM for this model
Solution:



The complete-data likelihood (given the current $\{z_n\}$ one-hot assignments) is

$$\log p(\{x_n\}, \{z_n\}|\pi, \{\mu\}) = \sum_n \sum_k z_{nk} \big[\log \pi_k + \log p(x_n|\mu_k) \big]$$

Integrating out over z^N assignments to get $p(x)$ is intractable.

2.3 Expectation Maximization

Consider a distribution over z so $q_{nk} = p(z_n = k|x_n, \pi, \mu)$. Don't worry about where it comes from for the moment. Then we can write **expected likelihood**

$$\mathbb{E}_{z\sim p(z_n|x_n \ldots)} \big[\log p(x_n, z_n|\pi, \mu) \big] = \sum_n \sum_k q_{nk} \log \pi_k + q_{nk} \log p(x_n|\mu_k)$$

Notice that we now have soft assignments. Using coordinate ascent, we can do the following:

1. **Expectation**: Compute $q_{nk} = p(z_n = k|x_n, \pi_k, \mu_k)$ using fixed parameters (this answers where $q_n k$ comes from... fixed parameters)

2. **Maximization**: Compute MLE of π and $\{\mu\}$ using q by maximizing the expected likelihood.

Initialize parameters randomly and then repeat the above steps until convergence of parameters.

For the **expectation** step, use

$$q_{nk} = p(z_n = k|x_n, \pi_k, \mu_k) \leftarrow \frac{\pi_k p(x_n|\mu_k)}{\sum_{k'} \pi_{k'} p(x_n|\mu_{k'})}$$

Notice that the expectation step is nothing different from what you would do if you were using an already-trained model to make predictions on test data.

For the **maximization** step, think of q_{nk} as "expected counts". Ask yourself what you would do in the fully-supervised Naive Bayes setting

$$\pi_k \leftarrow \frac{\sum_n q_{nk}}{\sum_n \sum_{k'} q_{nk'}}$$

The only difference is that all data points contribute to parameter updates for all latent classes. But, they are weighed by q_{nk}. Picture Q as an $N \times K$ grid. The numerator is a column sum for a particular k. Notice that the denominator sums to N because the row vector q_n sums to 1 across all K, and you sum across N.

Exercise: What is the $p(x|\mu_k)$ update?
Solution:

$$\mu_k \leftarrow \frac{\sum_n q_{nk}(x_n)}{\sum_n q_{nk}}$$

2.4 Understanding Intractability of $p(x)$

In class, we only talked about the cluster assignments z_n as latent. However, the parameters μ and π are also latent (that is, when we are performing inference on them and are not holding them fixed as we do in the Expectation step). We are generally interested in $p(\mu|x)$. How do we calculate that? Again we would need

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

But we are stuck with dependence on $p(x)$. See why this is hard. Assuming 3 latent classes:

$$p(\mu_1, \mu_2, \mu_3|x) = \frac{p(\mu_1, \mu_2, \mu_3, x)}{\int_{\mu_1} \int_{\mu_2} \int_{\mu_3} p(\mu_1, \mu_2, \mu_3, x)}$$

The numerator is easy

$$p(\mu_1, \mu_2, \mu_3, x) = p(\mu_1)p(\mu_2)p(\mu_3) \prod_{i=1}^{N} p(x_i|\mu_1, \mu_2, \mu_3)$$

where each likelihood term marginalizes out z_i

$$p(x_i|\mu_1, \mu_2, \mu_3) = \sum_{k=1}^{K} \pi_k p(x_i|\mu_k)$$

But consider the denominator

$$p(x) = \int_{\mu_1} \int_{\mu_2} \int_{\mu_3} p(\mu_1)p(\mu_2)p(\mu_3) \prod_{i=1}^{N} \sum_{k=1}^{K} \pi_k p(x_i|\mu_k)$$

Bring the summation outside of the integral

$$p(x) = \sum_{z} \int p(\mu_1)p(\mu_2)p(\mu_3) \prod_{i=1}^{N} p(x_i|\mu_{z_i})$$

Decompose by partitioning data according to z

$$p(x) = \sum_{z} \prod_{k=1}^{3} \left(\int_{\mu,k} p(\mu_k) \prod_{\{i:z_i=k\}} p(x_i|\mu_k) \right)$$

Exercise: Is each term within the large parenthesis computable? How many different assignments of the data must we consider for the whole expression?
Solution: Each term within the parenthesis is a Normal-Normal conjugate pair and is computable. However, there are 3^N assignments to consider. This problem requires **approximate inference**.

2.5 Looking ahead (only if extra time): the Evidence Lower Bound (ELBO)

As mentioned in the info theory lecture, we specify a distribution $q(z)$ to approximate $p(z|x)$ to avoid the calculation of

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

which requires the intractable $p(x)$. q is called the variational density. The optimal q^* is one that comes from a specified family Q of distributions that supports tractable inference such that

$$q^*(z) = \arg\min_{q(z) \in Q} KL(q(z)||p(z|x))$$

but how do we know if something is close to $p(z|x)$ if we don't know $p(z|x)$?

$$\begin{aligned} KL(q(z)||p(z|x)) &= \mathbb{E}[\log q(z)] - \mathbb{E}[\log p(z|x)] \\ &= \mathbb{E}[\log q(z)] - \mathbb{E}[\log p(z,x)] + \log p(x) \end{aligned}$$

Consider the following instead

$$elbo(q) = \mathbb{E}[\log p(z,x)] - \mathbb{E}[\log q(z)]$$

This is called the **evidence lower bound** (elbo). It's the negative of the KL divergence above, plus $\log p(x)$. The $\log p(x)$ term missing is only a constant with respect to $q(z)$. Maximizing the elbo is equivalent to minimizing the divergence. Rewriting gives

$$\begin{aligned} elbo(q) &= \mathbb{E}[\log p(z)] + \mathbb{E}[\log p(x|z)] - \mathbb{E}[\log q(z)] \\ &= \mathbb{E}[\log p(x|z)] - KL(q(z)||p(z)) \end{aligned}$$

It is called the evidence lower bound because

$$\log p(x) = KL(q(z)||p(z|x)) + elbo(q)$$

The bound follows from the fact that $KL(.) \geq 0$. This can be derived from Jensen's inequality.

Exercise Which values of z will this objective encourage $q(z)$ to place its mass on?

Solution The first term is an expected likelihood. It encourages densities that place their mass on configurations of the latent variables that explain the observed data. The second term is the negative divergence between the variational density and the prior. It encourages densities close to the prior.

3 References

1. CS281 Lectures on Info Theory and Mixture Models (2017), Sasha Rush

2. Bayesian Mixture Models and the Gibbs Sampler (2015), David M. Blei*

3. Variational Inference: A Review for Statisticians (2017), David M. Blei, Alp Kucukelbir, Jon D. McAuliffe*

* These notes borrow heavily from David Blei's tutorials. They are very good resources.