Module 8: Part III: Gibbs Sampling and Data Augmentation

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Announcements

- At the end of class today, if everyone could fill out the course evaluation, I would be really appreciative. (Check your email for this).
- Duke Undergraduate Machine Learning Day is Saturday March 23. You can register at http://dukeml.org/ and see the full schedule of events.
- If you're interested in doing an undergraduate thesis, poster presentations will be given by our seniors on Friday, March 29 at 3:30 – 4:30 PM, Brodhead Center Multipurpose Room, 068.
- DataFest is April 6 – 8 and you can register on the main statistical science page.
- I will hand back Midterm II next week in class. Overall, the exams were quite good. Well done:)

Agenda

- Two Component Mixture Model
- Latent Variable Allocation (Trick for Gibbs Sampling)
- Application to the Dutch Example

Data augmentation for auxiliary variables

- A commonly-used technique for designing MCMC samplers is to use *data augmentation*, also known as *auxiliary variables*.
- Introduce variable(s) Z that depends on the distribution of the existing variables in such a way that the resulting conditional distributions, with Z included, are easier to sample from and/or result in better mixing.
- Z's are latent/hidden variables that are introduced for the purpose of simplifying/improving the sampler.

Idea: Create Z's and throw them away at the end!

Goal: Sample from $p(x, y)$

Problem: We cannot sample from $p(x|y)$ and/or $p(y|x)$.

Solution:

1. Introduce a latent/hidden variable Z such that

   $$p(x|y, z), p(y|x, z), p(z|x, y)$$

   are easy to sample from.
2. Then construct a Gibbs sampler that will approximate samples from $p(x, y, z)$ using the full conditionals above.
3. The output of the three-stage Gibbs sampler is (X, Y, Z).

But, our main interest is sampling from $p(x, y)$. Thus, we just throw away the Z's and we will have samples (X, Y) from $p(x, y)$.

Dutch Example

Consider a data set on the heights of 695 Dutch women and 562 Dutch men.

Suppose we have the list of heights, but we don't know which data points are from women and which are from men.

Dutch Example

From Figure 1 can we still infer the distribution of female heights and male heights?

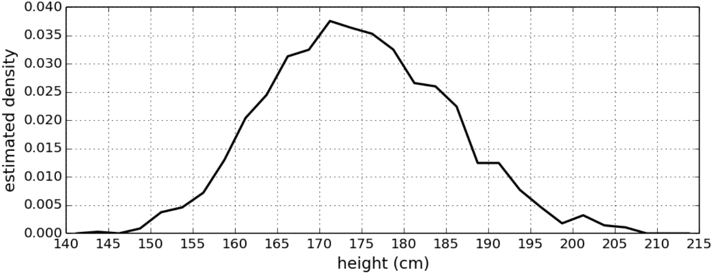


Figure 1: Heights of Dutch women and men, combined.

Surprisingly, the answer is yes!

Dutch example

What's the magic trick?

The reason is that this is a two-component mixture of Normals, and there is an (essentially) unique set of mixture parameters corresponding to any such distribution.

We'll get to details soon. Be patient!

Constructing a Gibbs sampler

To construct a Gibbs sampler for this situation:

- Common to introduce an auxiliary variable Z_i for each data point, indicating which mixture component it is drawn from.
- In this example, Z_i indicates whether subject i is female or male.
- This results in a Gibbs sampler that is easy to derive/implement.

Two-component mixture model

Let's assume that both mixture components (female and male) have the same precision, say λ, and that λ is fixed and known. Assume below that a, b, m, ℓ are known.

Then the usual two-component Normal mixture model is:

$$
\begin{align}
X_1, \ldots, X_n \mid \mu, \pi \ &\sim F(\mu, \pi) \tag{1}\\
\mu := (\mu_0, \mu_1) &\overset{iid}{\sim} \mathcal{N}(m, \ell^{-1}) \tag{2}\\
\pi &\sim \text{Beta}(a, b), \tag{3}
\end{align}
$$

Remark: π is the prior probability that a subject comes from component 1.

where $F(\mu, \pi)$ is the distribution with p.d.f.

$$f(x|\mu, \pi) = (1-\pi)\mathcal{N}(x \mid \mu_0, \lambda^{-1}) + \pi\mathcal{N}(x \mid \mu_1, \lambda^{-1})$$

and $\mu = (\mu_0, \mu_1)$.

Likelihood

The likelihood is

$$
\begin{aligned}
p(x_{1:n}|\mu,\pi) &= \prod_{i=1}^{n} f(x_i|\mu,\pi) \\
&= \prod_{i=1}^{n} \Big[(1-\pi)\mathcal{N}(x_i \mid \mu_0, \lambda^{-1}) + \pi\mathcal{N}(x_i \mid \mu_1, \lambda^{-1})\Big]
\end{aligned}
$$

which is a complicated function of μ and π, making the posterior difficult to sample from directly.

Latent allocation variables to the rescue!

Define an equivalent model that includes latent "allocation" variables $Z_1, \ldots, Z_n$.

These indicate which mixture component each data point comes from–that is, Z_i indicates whether subject i is female or male.

$$
\begin{align}
X_i \mid \mu, Z &\sim \mathcal{N}(\mu_{Z_i}, \lambda^{-1}) \text{ independently for } i = 1, \ldots, n. \tag{4}\\
Z_1, \ldots, Z_n \mid \mu, \pi &\overset{iid}{\sim} \text{Bernoulli}(\pi) \tag{5}\\
\mu = (\mu_0, \mu_1) &\overset{iid}{\sim} \mathcal{N}(m, \ell^{-1}) \tag{6}\\
\pi &\sim \text{Beta}(a, b) \tag{7}
\end{align}
$$

How can we check that the latent allocation model is equivalent to our original model?

Equivalence of both models

Recall

$$
\begin{aligned}
&X_i \mid \mu, Z \sim \mathcal{N}(\mu_{Z_i}, \lambda^{-1}) \text{ independently for } i = 1, \ldots, n.\\
&Z_1, \ldots, Z_n | \mu, \pi \overset{iid}{\sim} \text{Bernoulli}(\pi)\\
&\mu = (\mu_0, \mu_1) \overset{iid}{\sim} \mathcal{N}(m, \ell^{-1})\\
&\pi \sim \text{Beta}(a, b)
\end{aligned}
$$

This is equivalent to the model above, since

$$p(x_i|\mu,\pi) \tag{8}$$

$$= p(x_i|Z_i = 0, \mu, \pi)\mathbb{P}(Z_i = 0|\mu, \pi) + p(x_i|Z_i = 1, \mu, \pi)\mathbb{P}(Z_i = 1|\mu, \pi) \tag{9}$$

$$= (1-\pi)\mathcal{N}(x_i|\mu_0, \lambda^{-1}) + \pi\mathcal{N}(x_i|\mu_1, \lambda^{-1}) \tag{10}$$

$$= f(x_i|\mu, \pi), \tag{11}$$

Full conditionals

Recall

$$X_i \mid \mu, Z \sim \mathcal{N}(\mu_{Z_i}, \lambda^{-1}) \text{ independently for } i = 1, \ldots, n.$$

$$Z_1, \ldots, Z_n | \mu, \pi \overset{iid}{\sim} \text{Bernoulli}(\pi)$$

$$\mu = (\mu_0, \mu_1) \overset{iid}{\sim} \mathcal{N}(m, \ell^{-1})$$

$$\pi \sim \text{Beta}(a, b)$$

- $(\pi | \cdots)$ Given z, π is independent of everything else, so this reduces to a Beta–Bernoulli model, and we have

$$p(\pi | \mu, z, x) = p(\pi | z) = \text{Beta}(\pi \mid a + n_1,\ b + n_0)$$

where $n_k = \sum_{i=1}^{n} \mathbb{1}(z_i = k)$ for $k \in \{0, 1\}$.

That is, $n_o = \sum_{i=1}^{n} \mathbb{1}(z_i = 0)$; $n_1 = \sum_{i=1}^{n} \mathbb{1}(z_i = 1)$.

Full conditionals

$$X_i \sim \mathcal{N}(\mu_{Z_i}, \lambda^{-1}) \text{ independently for } i = 1, \ldots, n.$$
$$Z_1, \ldots, Z_n | \mu, \pi \overset{iid}{\sim} \text{Bernoulli}(\pi)$$
$$\mu = (\mu_0, \mu_1) \overset{iid}{\sim} \mathcal{N}(m, \ell^{-1})$$
$$\pi \sim \text{Beta}(a, b)$$

- $(\mu | \cdots)$ Given z, we know which component each data point comes from. The model (conditionally on z) is just two independent Normal–Normal models, as we have seen before:

$$\boldsymbol{\mu}_0 | \mu_1, x, z, \pi \sim \mathcal{N}(M_0, L_0^{-1})$$
$$\boldsymbol{\mu}_1 | \mu_0, x, z, \pi \sim \mathcal{N}(M_1, L_1^{-1}), \text{where}$$

$$L_0 = \ell + n_0\lambda; L_1 = \ell + n_1\lambda$$
$$M_0 = \frac{\ell m + \lambda \sum_{i:z_i=0} x_i}{\ell + n_0\lambda}.$$

Full conditionals

- $(z|\cdots)$

$$
\begin{aligned}
p(z|\mu,\pi,x) \underset{z}{\propto} p(x,z,\pi,\mu) \underset{z}{\propto} p(x|z,\mu)p(z|\pi) \\
&= \prod_{i=1}^{n} \mathcal{N}(x_i|\mu_{z_i},\lambda^{-1})\,\text{Bernoulli}(z_i|\pi) \\
&= \prod_{i=1}^{n} \Big(\pi\mathcal{N}(x_i|\mu_1,\lambda^{-1})\Big)^{z_i}\Big((1-\pi)\mathcal{N}(x_i|\mu_0,\lambda^{-1})\Big)^{1-z_i} \\
&= \prod_{i=1}^{n} \alpha_{i,1}^{z_i}\alpha_{i,0}^{1-z_i} \\
&\underset{z}{\propto} \prod_{i=1}^{n} \text{Bernoulli}(z_i \mid \alpha_{i,1}/(\alpha_{i,0}+\alpha_{i,1}))
\end{aligned}
$$

where

$$
\begin{aligned}
\alpha_{i,0} &= (1-\pi)\mathcal{N}(x_i|\mu_0,\lambda^{-1}) \\
\alpha_{i,1} &= \pi\mathcal{N}(x_i|\mu_1,\lambda^{-1}).
\end{aligned}
$$

My Factory Settings!

We initialize the sampler at the same settings that we did when we looked at this application before. Let's review them below.

- $\lambda = 1/\sigma^2$ where $\sigma = 8$ cm ($\approx$ 3.1 inches) ($\sigma =$ standard deviation of the subject heights within each component)
- $a = 1$, $b = 1$ (Beta parameters, equivalent to prior "sample size" of 1 for each component)
- $m = 175$ cm ($\approx$ 68.9 inches) (mean of the prior on the component means)
- $\ell = 1/s^2$ where $s = 15$ cm ($\approx$ 6 inches) ($s =$ standard deviation of the prior on the component means)

My Factory Settings!

We initialize the sampler at the same settings that we did when we looked at this application before. Let's review them below.

- $\pi = 1/2$ (equal probability for each component)
- $z_1, \ldots, z_n$ sampled i.i.d. from Bernoulli$(1/2)$ (initial assignment to components chosen uniformly at random)
- $\mu_0 = \mu_1 = m$ (component means initialized to the mean of their prior)

Traceplots of the component means

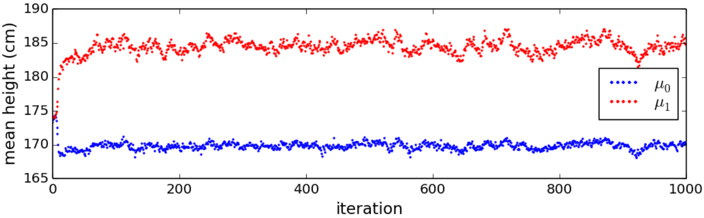


Figure 2: Traceplots of the component means, μ_0 and μ_1. The blue component quickly settles to have a mean of around 168–170 cm and the other (red) to a mean of around 182–186 cm.

Recall we're not using the true assignments of subjects to components (we don't know whether they are male or female). Note that this is fairly close to the sample averages: 168.0 cm (5 feet 6.1 inches) for females, and 181.4 cm (5 feet 11.4 inches) for males.

Traceplots of the mixture weight, π

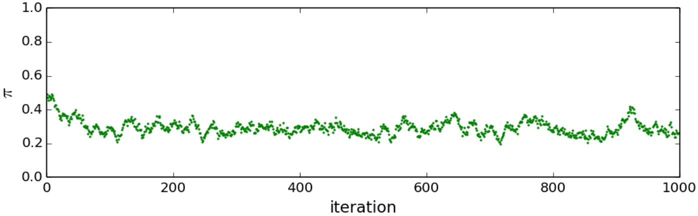


Figure 3: Traceplots of the mixture weight, π (prior probability that a subject comes from component 1).

The traceplot of π indicates that the sampler is exploring values of around 0.2 to 0.4—that is, the proportion of people coming from group 1 is around 0.2 to 0.4.

Looking at the actual labels (female and male), the empirical proportion of males is $562/(695 + 562) \approx 0.45$, so this is slight off.

How might we fix this in our model?

Back to the model

Recall

$$
\begin{aligned}
&X_i \mid \mu, Z \sim \mathcal{N}(\mu_{Z_i}, \lambda^{-1}) \text{ independently for } i = 1, \ldots, n. \\
&Z_1, \ldots, Z_n | \mu, \pi \overset{iid}{\sim} \text{Bernoulli}(\pi) \\
&\mu = (\mu_0, \mu_1) \overset{iid}{\sim} \mathcal{N}(m, \ell^{-1}) \\
&\pi \sim \text{Beta}(a, b),
\end{aligned}
$$

where a, b, m, ℓ are fixed.

Hint: Is it reasonable to think that we should have the same λ for the data? Consider

$$\lambda = (\lambda_0, \lambda_1)$$

How would you proceed next in a Bayesian hierarchical manner?

Histograms

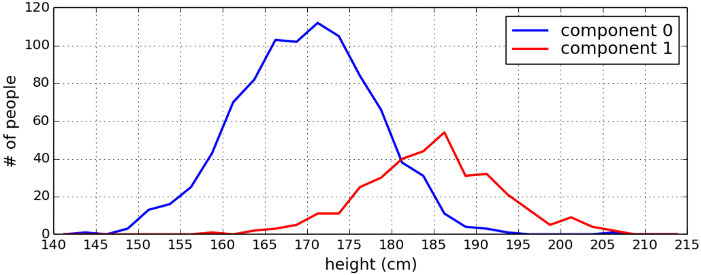


Figure 4: Histograms of the heights of subjects assigned to each component, according to $z_1, \ldots, z_n$, in a typical sample.

Question

Why are females assigned to component 0 and males assigned to component 1? Why not the other way around? Let's investigate this and see what happens if we look at another choice of starting values.

Traceplots of the component means

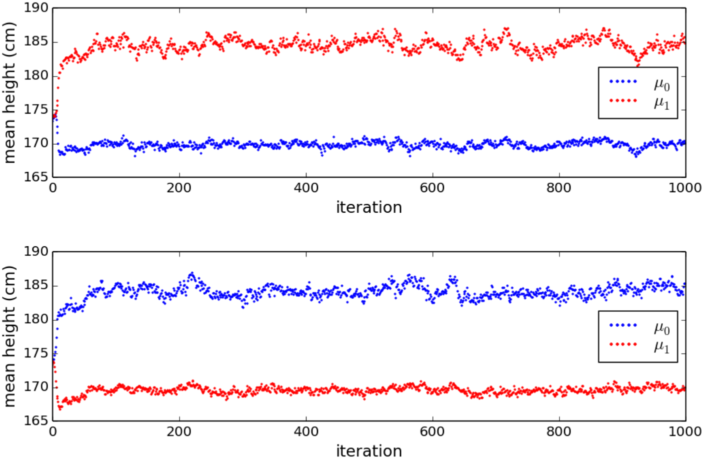


Figure 5: Traceplots of the component means, μ_0 and μ_1.

Traceplots of the mixture weight, π

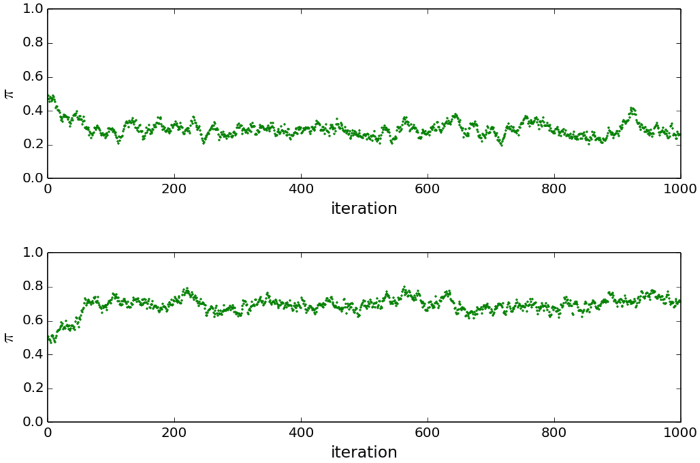
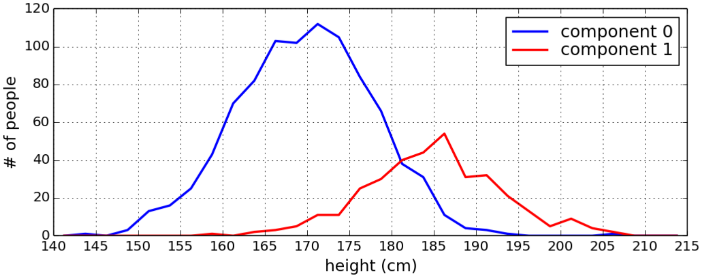
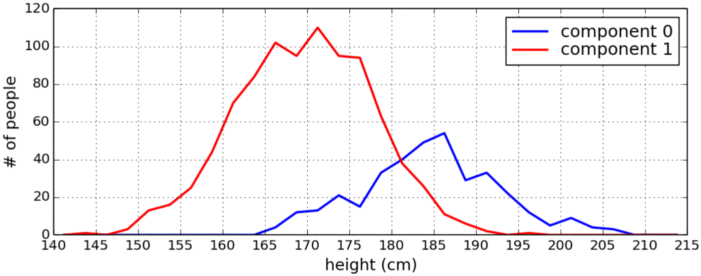


Figure 6: Traceplots of the mixture weight, π (prior probability that a subject comes from component 1).

Histograms



120
100
80
60
40
20
0
# of people
140
145
150
155
160
165
170
175
180
185
190
195
200
205
210
215
height (cm)
component 0
component 1



120
100
80
60
40
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0
# of people
140
145
150
155
160
165
170
175
180
185
190
195
200
205
210
215
height (cm)
component 0
component 1

Caution: watch out for modes

Example illustrates a big thing that can go wrong with MCMC (although fortunately, in this case, the results are still valid if interpreted correctly).

- Why are females assigned to component 0 and males assigned to component 1? Why not the other way around?
- In fact, the model is symmetric with respect to the two components, and thus the posterior is also symmetric.
- If we run the sampler multiple times (starting from the same initial values), sometimes it will settle on females as 0 and males as 1, and sometimes on females as 1 and males as 0 — see Figure 6.
- Roughly speaking, the posterior has two modes.
- If the sampler were behaving properly, it would move back and forth between these two modes.
- But it doesn't—it gets stuck in one and stays there.

Takeaways from Dutch Application

- This is a very common problem with mixture models.
- Fortunately, however, in the case of mixture models, the results are still valid if we interpret them correctly.
- Specifically, our inferences will be valid as long as we only consider quantities that are invariant with respect to permutations of the components (e.g. symmetry about the mean, others).
- To learn more about invariance and what quantities remain unchanged, see Theory of Point Estimation, Lehmann and Casella, Chapter 1 for a formal treatment. (For more advanced reading, see Chapter 3.) Feel free to see me in OH if you want to chat about this!