Monte Carlo Methods — Why Do They Work? — Part III

In the previous two "Why Do They Work?" write-ups, I proved that the Metropolis algorithm worked and that the Metropolis-Hastings algorithm worked:

* https://brianhill.github.io/bayesian-statistics/resources/MonteCarloMethodsWhyDoTheyWork-I.nb.pdf
* https://brianhill.github.io/bayesian-statistics/resources/MonteCarloMethodsWhyDoTheyWork-II.nb.pdf

Both proofs required the Principle of Detailed Balance. Now we are going to prove that the Gibbs Sampling (GS) algorithm works, but all the hard work was actually in the second write-up, because Gibbs sampling is a special case of Metropolis-Hastings (and Metropolis is a special case of Metropolis-Hastings too).

To get going, and to leverage our previous write-up, we need to understand the relationship between Metropolis-Hastings and Gibbs sampling.

The Metropolis-Hastings and Gibbs Sampling Algorithms

The core of the Metropolis-Hastings algorithm (repeated *ad nauseam)* was:

Step 1: You are in bin i. You propose a random move from bin i to some other bin j. The probability of proposing the random move is denoted $g(j \mid i)$, which is read "g of j given i." (Note: If you want to recover Metropolis as a special case of Metropolis-Hastings, you put in that $g(i + 1 \mid i) = 0.5$ and $g(i - 1 \mid i) = 0.5$. In other words, you have 50% chance of moving to either of the nearest neighbors, and in Metropolis there is no chance of moving to anything but a nearest neighbor.)

Step 2: Compute the ***clamped*** appropriate ratio. The **clamped** appropriate ratio for going from $i \to j$ is $\min\left(\frac{p_j}{p_i}\ \frac{g(i \mid j)}{g(j \mid i)}, 1\right)$.

Step 3: Generate a random number between 0 and 1. If the number is less than clamped appropriate ratio, move to the proposed bin, and make a tally there. Otherwise stay in the current bin and make another tally in the current bin. Whatever bin you made the tally in is now the current bin, and you go back to step 1.

"Hold on to your papers, fellow scholars [apologies to Dr. Karoly Zsolnai-Feher]," here is what Gibbs sampling is:

You just choose $g(i \mid j) = p_i$.

Really, you have got to be kidding me. That is laughable and ridiculous. I'll get to why if you don't already see why. Anyway, let's see what happens to the clamped appropriate ratio:

We put $g(i \mid j) = p_i$ and $g(j \mid i) = p_j$ into the clamped appropriate ratio and you get:

$$\min\left(\frac{p_j}{p_i}\,\frac{g(i \mid j)}{g(j \mid i)}, 1\right) = \min\left(\frac{p_j}{p_i}\,\frac{p_i}{p_j}, 1\right) = \min(1, 1) = 1$$

The clamped appropriate ratio is always 1! So you always move. So let us summarize the Gibbs sampling algorithm (to be repeated *ad nauseam):*

Step 1: The current bin is bin i. You propose a random move from bin i to some other bin, bin j. The probability of the proposed random move to bin j is just p_j, where p_j is the probability distribution you are trying to sample.

Step 2: You accept the proposed move and make a tally in the proposed bin. The proposed bin is now the current bin, and you go back to step 1.

Now I'll say why it laughable and ridiculous:

The whole point of any Monte Carlo method is to generate a representative set of samples ***for a probability distribution that is hard to sample.*** The Gibbs sampling algorithm says to ***make the proposed move by drawing a representative sample from that very same probability distribution*** that you already had resigned yourself as being hard to sample. So it has "solved" the problem by requiring you to know the solution to the problem. ***This appears to be a circular solution with no benefit.***

The actual genius of the Gibbs sampling algorithm comes next.

High-Dimensional Probability Distributions

Back on Nov. 22, I launched the entire section on Monte Carlo Methods with my "Monte Carlo Methods Introduction" write-up:

* https://brianhill.github.io/bayesian-statistics/resources/MonteCarloMethodsIntroduction.nb.pdf

My example was a probability distribution that has 50 dimensions! It was the electoral college outcome. Now each state can only go one of two ways, so each axis was as simple as an axis can get. But still the total number of outcomes was 2^{50}. We did the math and saw that there is absolutely no way to exhaustively sample that space with any reasonable amount of computer time.

As a second example, I looked ahead to what will be our final example, which was a study of 106 babies vaccinated for Hepatitis B. For each baby, there are multiple blood samples, and the hepatitis

“titer” is measured in each blood sample. The blood sample data is going to be fitted by a slope and an intercept for each baby (in the study, they actually take the logarithm of the titer before doing the linear fit). So that is 212 parameters. There is no way you conclude an epidemiological paper by reporting 212 different numbers and error bars on each of them, so the authors introduced four more parameters that capture the distribution of those 212 parameters. So in total there are 216 parameters. The bottom line is that in this second example, you have a space with 216 parameters (instead of an electoral college with 50 states), and these are now continuous parameters (not just binary wins and losses). You can see that this is going to be a far worse probability distribution to sample than the electoral college problem, and that one was already practically impossible to exhaustively simple.

To summarize, we are motivated to study high-dimensional probability distributions with Monte Carlo methods because (a) they show up in interesting, real-world examples, and (b) they are impossible to exhaustively sample.

To study high-dimensional probability distributions, we need some new notation. Instead of bins labeled by an index i, the bins will now be labeled by D indices, i_1, i_2, i_3, ..., i_D. So the probability distribution we are trying to sample is now denoted:

$$p_{i_1\, i_2\, i_3 \ldots\, i_D}$$

The simplest case that has more than one-dimension would have $D = 2$, and the p's would look like:

$$p_{i_1\, i_2}$$

To make that even more concrete, we could have a really simple example in mind. How about the first axis represents whether a nodule that comes out of the potato harvester and is destined for the kitchen is a rock or a potato, and the second axis represents whether it is small, medium, or large. Then the six p’s would be:

$$p_{\text{rock small}}$$
$$p_{\text{rock medium}}$$
$$p_{\text{rock large}}$$
$$p_{\text{potato small}}$$
$$p_{\text{potato medium}}$$
$$p_{\text{potato large}}$$

Of course, the total of all 6 p’s has to add up to 1 (assuming there aren’t other things in the sack going to the kitchen, like rotten turnips).

Anyway, examples aside, it is for multi-dimensional probability distributions that Gibbs sampling has one more twist, why it is not just a circular solution with no benefit, and why it is in widespread use for sampling high-dimensional probability distributions.

Gibbs Sampling of High-Dimensional Probability Distributions

Our plan of attack has two parts: (1) We are going to move along only one axis at a time in the Gibbs sampling, and (2) assume that a substantial burden of calculating $p_{i_1\, i_2\, i_3 \ldots\, i_d}$ is simplified by the fact that along at least some of the axes, the p's factor.

1A. Conditional Movement

We introduce the idea of "conditional movement." Specifically, we are going to propose a movement that keeps the indices of all the axes the same, except for one of them. If we are in the bin with indices

$$i_1\, i_2 \ldots i_d \ldots\, i_D$$

we will propose a movement such that only the dth axis changes and the new dth index will be i_d'.

This is called "conditional movement" because we have the "condition" that all the other indices stay the same. We need a new set of p's that captures this idea, which we'll denote:

$$p_{i_d'|i_-}$$

You can read i_- as "all the i's except the dth one." You can read i_d' as the "proposed dth bin." You can read the whole expression as "the probability of moving to the proposed dth bin given that all the bins except the dth one stay the same." Also, "conditioned on" and "given" are synonyms, so you will sometimes see this read as "the probability of moving to the proposed dth bin conditioned on all the bins but the dth one staying the same."

NOTE: It is definitely not the case that $p_{i_d'|i_-}$ is the same as $p_{i_1\, i_2 \ldots\, i_d' \ldots\, i_D}$. But there is a relation:

$$p_{i_d'|i_-} = \frac{p_{i_1\, i_2 \ldots\, i_d' \ldots\, i_D}}{\sum_{i_d} p_{i_1\, i_2 \ldots\, i_d \ldots\, i_D}}$$

1B. The Principle of Detailed Balance

This is a new rule for movement, and you might be worried that our proof that it works still applies. Or to put it another way, this no longer seems like a specialization of Metropolis-Hastings as we originally claimed. But you can see that the proof definitely does still apply along the chosen axis. You bounce around on that axis using this rule, and you will properly sample that axis.

The leap of faith is that you can change up what axes you bounce around on, and over time you will build a sample of the multi-dimensional distribution that works along all axes.

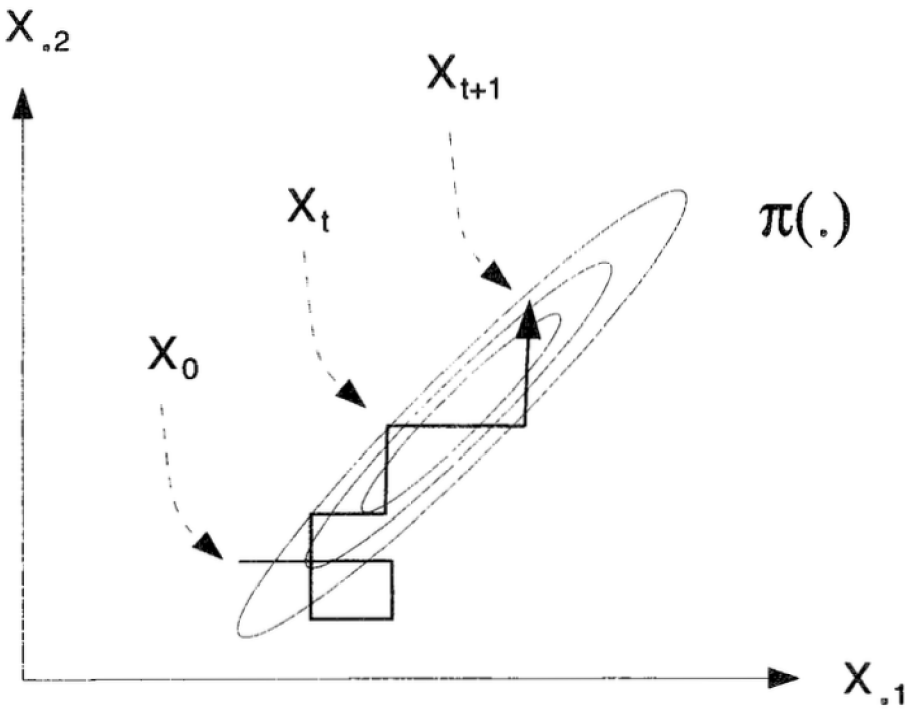
You can think of this as another detailed balance proof. Is it not the case, that along a given axis the tallies will settle down to the right ratios? And is it not the case that if we cycle through all the axes of movement enough times that along any given axis the tallies will settle down to the right ratios? So it must be the case that all the tallies along all the axes must settle down to the right ratios.

1C. Visualizing Gibbs Sampling

At this point in our study of Monte Carlo, we have left Donovan and Mickey behind, because I don't think their presentation particularly illuminates what I claim is a laughably simple method. For Gibbs sampling, I am instead using as my reference the first two chapters of the book edited by Gilks, Richardson, and Spiegelhalter. David Spiegelhalter is the author of BUGS. The other authors are also leaders in Markov Chain Monte Carlo analyses. On this web page, they have made a "Preview PDF" of most of the first two chapters of their book readily available:

* https://www.taylorfrancis.com/books/mono/10.1201/b14835

Here is their Figure 1.2 showing this axis-by-axis movement for the two-dimensional case:



The diagonal ellipses represent the region where the joint probability distribution is high. The meandering path consisting of straight-line movements in one axis and then the other represents movements such that the Gibbs sampling algorithm discovers and representatively samples the high probability region.

2. Factorization of the *p*'s

We now are going to remove a very substantial burden in sampling

$$p_{i_d'|i-} = \frac{p_{i_1 i_2 i_3 \ldots i_d' \ldots i_D}}{\sum_{i_d} p_{i_1 i_2 i_3 \ldots i_d \ldots i_D}}$$

by making an assumption. We are going to assume (at least along most axes), that the *p*'s factor. If there are just a few recalcitrant axes along which the *p*'s don't factor out of dozens or hundreds of axes along which they do factor, we will have vastly simplified the computational cost of sampling the $p_{i_d'|i-}$.

I could make some attempt to write this in all generality, but I think it is better if I just assume that the first five axes are the recalcitrant ones and the rest enjoy some factorization. That is, none of

$$p_{i_1'|i-} = \frac{p_{i_1' i_2 i_3 i_4 i_5 \ldots i_D}}{\sum_{i_1} p_{i_1 i_2 i_3 i_4 i_5 \ldots i_D}}$$

$$p_{i_2'|i-} = \frac{p_{i_1 i_2' i_3 i_4 i_5 \ldots i_D}}{\sum_{i_2} p_{i_1 i_2 i_3 i_4 i_5 \ldots i_D}}$$

$$p_{i_3'|i-} = \frac{p_{i_1 i_2 i_3' i_4 i_5 \ldots i_D}}{\sum_{i_3} p_{i_1 i_2 i_3 i_4 i_5 \ldots i_D}}$$

$$p_{i_4'|i-} = \frac{p_{i_1 i_2 i_3 i_4' i_5 \ldots i_D}}{\sum_{i_4} p_{i_1 i_2 i_3 i_4 i_5 \ldots i_D}}$$

$$p_{i_5'|i-} = \frac{p_{i_1 i_2 i_3 i_4 i_5' \ldots i_D}}{\sum_{i_5} p_{i_1 i_2 i_3 i_4 i_5 \ldots i_D}}$$

have any particularly simple expression. However, for all the rest:

$$p_{i_6'|i-} = \frac{p_{i_1 i_2 i_3 i_4 i_5 i_6' \ldots i_D}}{\sum_{i_6} p_{i_1 i_2 i_3 i_4 i_5 i_6 \ldots i_D}}$$

we are going to make a tremendously simplifying assumption.

Before I even state the simplifying assumption, so that you have the real problem in mind, recall the immunized babies study introduced back on Nov. 22nd. I discussed it in class, but I didn't write it up. If you remember the 106 babies, you'll remember that we need $106 \cdot 2 = 212$ parameters to do 106 linear fits to their respective titers. So the 6th and 7th axes are going to be the slope and intercept of the 1st baby's titer. The 8th and 9th axes are going to be the slope and intercept of the 2nd baby's titer. And so on and so on all the way out to the 216th and 217th axes, which are going to be the slope and intercept of the 106th baby's titer. Meanwhile, the first five axes, the ones that are recalcitrant, are going to be parameters in the distributions that characterize the distributions of all the slopes and the

intercepts plus one more parameter that characterizes the fundamental uncertainty in the titers. We will get way further into that as our case study, and frankly, if you are sick of theory, and just want to trust me on the factorization, and skip to seeing how it plays out in practice, you could go directly to the case study:

* https://brianhill.github.io/bayesian-statistics/resources/MonteCarloMethodsCaseStudy.nb.pdf

THE CASE STUDY IS THE MOTIVATION FOR SUFFERING THROUGH THE FACTORIZATION THAT FOLLOWS, AND ACTUALLY, IT IS STILL FORTHCOMING. I AM NOT SURE I HAVE THE FORTITUDE TO WRITE IT ALL OUT, ESPECIALLY SINCE MATHEMATICA JUST CRASHED AFTER I HAD WRITTEN OUT A BUNCH OF EQUATIONS REQUIRING A LOT OF TYPESETTING.