

Class 14 Agenda: Markov Chains II

1 Questions/Lecture Recap

Any questions or reflections from the quiz or minilectures? (Definitions about Markov chains; stationary distributions; fundamental theorem of Markov chains; Markov Chain Monte Carlo)

2 Gibbs Sampling

In this group work, we'll explore a special case of MCMC, called "Gibbs Sampling" which arises in lots of applications.

Suppose that π is a joint distribution on X and Y . Suppose that it is hard to sample from π , but relatively easy to sample from $\pi(X|Y = y)$ or $\pi(Y|X = x)$ for any x, y in the support of X and Y respectively.

Consider the following way to set up a Markov chain $(X_0, Y_0), (X_1, Y_1), \dots$:

- Suppose $(X_t, Y_t) = (x, y)$.
- Draw $x' \sim \pi(X|Y = y)$.
- Draw $y' \sim \pi(Y|X = x')$.
- Set $(X_{t+1}, Y_{t+1}) = (x', y')$.

That is, we first condition on $Y = y$ and draw a new value x' for X , and then we condition on that value x' for X and draw a new value y' for Y .

Group work on next page...

Group Work

1. With the setup above, show that π is a stationary distribution for this Markov chain.

Hint: Recall that you want to show that for all x, y ,

$$\pi(x, y) = \sum_{x', y'} \pi(x', y') \Pr[(x', y') \rightarrow (x, y)]$$

(Why?)

Hint: Once you recall that you want to show the above, here are some steps to show that.

- Write down an expression for $\Pr[(x', y') \rightarrow (x, y)]$ in terms of $\pi(\cdot, \cdot)$, using the definition of Gibbs sampling.
 - You'll end up with some double-sums. Can you move those sums around productively?
2. Does the Fundamental Theorem of Markov Chains automatically apply in this setting? If not, what additional assumptions do you need to make?
 3. This procedure is called “Gibbs Sampling.” If it’s easy to sample from the marginal distributions, but difficult to sample from π itself, explain why the previous two parts (assuming your assumptions in the previous part are met) give us an algorithm to approximately sample from π . [Don’t worry about how efficient the algorithm is, and don’t overthink this part...].
 4. How would you generalize Gibbs sampling to more than two variables? Use your generalization to design an algorithm to sample a uniformly proper coloring of a random graph. Does this give the same Markov chain as the algorithm in the mini-lecture?
 5. Has anyone in your group encountered MCMC in general or Gibbs sampling in particular before? If so, in what context? If not, what else can you think of that Gibbs sampling or MCMC more generally might be useful for?

Group Work: Solutions

1. We want to show that $\pi = \pi \cdot P$, which is the same as showing

$$\pi(x, y) = \sum_{x', y'} \pi(x', y') \Pr[(x', y') \rightarrow (x, y)]$$

for all x, y . (This just follows from the definition of matrix multiplication). To see this, note that

$$\begin{aligned}
 \sum_{x', y'} \pi(x', y') \Pr[(x', y') \rightarrow (x, y)] &= \sum_{x', y'} \pi(x', y') \pi(x|y') \pi(y|x) \\
 &= \pi(y|x) \sum_{y'} \pi(x|y') \sum_{x'} \pi(x', y') \\
 &= \pi(y|x) \sum_{y'} \pi(x|y') \pi(y') \\
 &= \pi(y|x) \sum_{y'} \pi(x, y') \\
 &= \pi(y|x) \pi(x) \\
 &= \pi(x, y),
 \end{aligned}$$

as desired.

2. We need to check the following things:

- Aperiodic: check! There's a self-loop for any x, y with $\pi(x, y) > 0$. Indeed, the probability that we stay at x, y is $\pi(x|y) \cdot \pi(y|x) > 0$.
- Irreducible? Not necessarily! One way to envision what the requirement is is the following. Consider a bipartite graph, with x 's on the left and y 's on the right. There is an edge between x and y if $\pi(x, y) > 0$. Then we can view our states as edges of this graph. Two states are connected to each other (that is, we can get from one to the other in one step of our Markov chain) if the corresponding edges are incident. We need our underlying state graph to be connected, which is the same as saying that we need this bipartite graph to be connected.

Another way to say this is that if Π is a matrix with rows indexed by x 's and columns indexed by y 's, and $\Pi_{x,y} = \pi(x, y)$, then if we look at the non-zero pattern of Π , it should correspond to the adjacency matrix of a connected bipartite graph.

- Finite? Sure, as long as π has finite support.

3. The Fundamental Theorem of Markov Chains says that, eventually, $(X_t, Y_t) \rightarrow \pi$. Since we can efficiently sample from the marginals $\pi(X|Y)$ and $\pi(Y|X)$, we can efficiently step this Markov chain along. Of course, we don't yet know how large we need to take t to get close to π ... (that's next time!!)

4. There are two reasonable ways to think about generalizing to more than two variables, which differ only in what we call a "step" of the Markov chain. One way is to do the same thing we saw above, but iterate over all of the variables. Thus, all coordinates of X_t could change when going from X_t to X_{t+1} . Another way is to say

that we'll iterate through all of the variables in order, but also call the intermediate samples "steps" in our Markov chain. Yet another way would be to choose a variable and random, and update just that variable based on the conditional distribution. All of these can be found somewhere as a definition of "Gibbs Sampling."

Here's one way to do it, which gives us an algorithm that's close, but not quite the same, as the one we saw in the mini-lecture. We'll define a variable for the color of each vertex. We get this procedure:

- Start with an arbitrary proper coloring.
 - While True:
 - For each vertex v :
 - * Uncolor v .
 - * Choose a uniformly random color for v among all of the colors that are legitimate, and color v that color.
5. (Some discussion in class. Note that this question gets a bit away from the theory, and in particular you aren't responsible for this sort of thing for HW or the exam).