Proof of Gibbs Sampling

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In the previous week, we introduced the Gibbs Sampling algorithm. In this notebook, we will prove that the Gibbs Sampling algorithm generates samples from the joint distribution of the variables of interest. Recall that the Gibbs sampling algorithm for sampling from a joint distribution $f_{X,Y}(X, Y)$ is as follows:

1. Start with some initial values X_0 and Y_0.
2. For $i = 1, 2, \dots, N$
    1. Sample $X_i \sim f_{X|Y}(\,\cdot\,|Y_{i-1})$.
    2. Sample $Y_i \sim f_{Y|X}(\,\cdot\,|X_i)$.
3. Return the (X_0, Y_0), (X_1, Y_1), ..., (X_N, Y_N).

The Gibbs sampling algorithm samples from a Markov Chain whose state space is the product space of the state spaces of the individual variables $\Omega = \Omega_X \times \Omega_Y$. The transition matrix of the Markov Chain in discrete case is given by

$$P\left(\begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} x' \\ y' \end{bmatrix}\right) = \mathbb{P}(X_{i+1} = x'|Y_i = y)\mathbb{P}(Y_{i+1} = y'|X_i = x').$$

In the continuous case, the transition *kernel* is given by

$$K\left(\begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} x' \\ y' \end{bmatrix}\right) = f_{X|Y}(x|y)f_{Y|X}(y|x').$$

Theorem 0.1. *The Gibbs sampling algorithm generates a Markov Chain with the transition matrix P as described above. The joint distribution $f_{X,Y}$ is a stationary distribution of the Markov Chain. Hence, if the Markov Chain converges to the stationary distribution, the samples generated by the Gibbs algorithm will be distributed according to $f_{X,Y}$.*

We'll provide a proof that Gibbs sampling generates samples from the joint distribution $f_{X,Y}$ in the discrete case. The proof for the continuous case is similar.

Proof

Ideally, we would have liked to show that the Gibbs MC is reversible with respect to the joint distribution $f_{X,Y}$. However, this is not the case. Instead, each step in Gibbs sampling is reversible with respect to the joint distribution.

Consider the following single-component Gibbs sampler whose single update step is as follows:

1. Sample $X_i \sim f_{X|Y}(\,\cdot\,|Y_{i-1})$.
2. Sample $Y_i \sim f_{Y|X}(\,\cdot\,|X_i)$.
3. Return (X_{i+1}, Y_i), (X_{i+1}, Y_{i+1}).

So that the samples generated are

$$\begin{bmatrix} X_0 \\ Y_0 \end{bmatrix} \to \begin{bmatrix} X_1 \\ Y_0 \end{bmatrix} \to \begin{bmatrix} X_1 \\ Y_1 \end{bmatrix} \to \begin{bmatrix} X_2 \\ Y_1 \end{bmatrix} \to \begin{bmatrix} X_2 \\ Y_2 \end{bmatrix} \to \dots .$$

This produces a non-homogeneous Markov chain whose transition probabilities are different for the even and odd steps. The transition matrix for the even steps (updating X) is given by

$$P_{\text{even}}\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} a' \\ b' \end{bmatrix}\right) = \begin{cases} f(a'|b) & \text{if } b = b' \\ 0 & \text{otherwise} \end{cases}$$

where $f(a'|b) = \mathbb{P}(X_i = a'|Y_{i-1} = b)$

and the transition matrix for the odd steps (updating Y) is given by

$$P_{\text{odd}}\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} a' \\ b' \end{bmatrix}\right) = \begin{cases} f(b'|a) & \text{if } a = a' \\ 0 & \text{otherwise.} \end{cases}$$

where $f(b'|a) = \mathbb{P}(Y_i = b'|X_i = a)$. Next we'll verify the detailed balance equations with respect to the distribution $f_{X,Y}$ for the even and odd steps.

Detailed balance for the even steps

The detailed balance equations for the even steps with respect to the joint distribution $f_{X,Y}$ are given by

$$\begin{aligned} & f(a,b)P_{\text{even}}\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} a' \\ b \end{bmatrix}\right) = f(a',b)P_{\text{even}}\left(\begin{bmatrix} a' \\ b \end{bmatrix}, \begin{bmatrix} a \\ b \end{bmatrix}\right) \\ \Leftarrow \quad & f(a,b)f(a'|b) = f(a',b)f(a|b) \\ \Leftarrow \quad & f(a,b)\frac{f(a',b)}{f(b)} = f(a',b)\frac{f(a,b)}{f(b)} \\ \Leftarrow \quad & f(a,b)f(a',b) = f(a',b)f(a,b). \end{aligned}$$

The last statement is true. When $b \neq b'$, the equation is trivially true. Hence, the detailed balance equations are satisfied for the even steps.

Detailed balance for the odd steps

The detailed balance equations for the odd steps with respect to the joint distribution $f_{X,Y}$ are given by

$$\begin{aligned} & f(a,b)P_{\text{odd}}\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} a \\ b' \end{bmatrix}\right) = f(a,b')P_{\text{odd}}\left(\begin{bmatrix} a \\ b' \end{bmatrix}, \begin{bmatrix} a \\ b \end{bmatrix}\right) \\ \Leftarrow \quad & f(a,b)f(b'|a) = f(a,b')f(b|a) \\ \Leftarrow \quad & f(a,b)\frac{f(a,b')}{f(a)} = f(a,b')\frac{f(a,b)}{f(a)} \\ \Leftarrow \quad & f(a,b)f(a,b') = f(a,b')f(a,b). \end{aligned}$$

The last statement is true. When $a \neq a'$, the equation is trivially true. Hence, the detailed balance equations are satisfied for the odd steps.

Conclusion

Using the detailed balance equations we get

$$f_{X,Y} = f_{X,Y}P_{\text{even}}f_{X,Y} = f_{X,Y}P_{\text{odd}} \implies f_{X,Y} = f_{X,Y}P_{\text{even}}P_{\text{odd}}.$$

But $P_{\text{even}}P_{\text{odd}} = P$ is the transition matrix of the Gibbs Markov Chain. Hence, the joint distribution $f_{X,Y}$ is a stationary distribution of the Gibbs Markov Chain.

Note the interesting algebraic structure of the proof. The detailed balance equations imply that P_{even} and P_{odd} are reversible with respect to the joint distribution $f_{X,Y}$. But $P = P_{\text{even}}P_{\text{odd}}$ is not reversible with respect to $f_{X,Y}$. However, $f_{X,Y}$ is stationary for P_{even} and P_{odd} separately, and hence for P. Thus stationarity is preserved under multiplication of transition matrices even if reversibility is not.

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