## MAT 653: Statistical Simulation

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# Gibbs Sampling

**Recall:** the block-wise Metropolis-Hastings. To sample from f(X,Y). We used two candidates:  $q_X(x|X,Y), q_Y(y|X,Y)$ .

1. Update X:

$$\begin{split} \gamma_X(X^*|X^{(s)},Y^{(s)}) &= \frac{f(X^*,Y^{(s)})}{f(X^{(s)},Y^{(s)})} \cdot \frac{q_X(X^{(s)}|X^{(s)},Y^{(s)})}{q_X(X^*|X^{(s)},Y^{(s)})} \\ &= \frac{f_{X|Y}(X^*|Y^{(s)})}{f_{X|Y}(X^{(s)}|Y^{(s)})} \cdot \frac{q_X(X^{(s)}|X^{(s)},Y^{(s)})}{q_X(X^*|X^{(s)},Y^{(s)})} \end{split}$$

Suppose we take  $q_X(x|X^{(s)},Y^{(s)})$  to be full condition distribution  $f_{X|Y}(x|Y^{(s)})$ , take  $q_Y(y|X^{(s)},Y^{(s)})$  to be full condition distribution  $f_{Y|X}(y|X^{(s)})$ , then

$$\gamma_X(X^*|X^{(s)},Y^{(s)}) = \frac{f(X^*,Y^{(s)})}{f(X^{(s)},Y^{(s)})} \cdot \frac{q_X(X^{(s)}|X^{(s)},Y^{(s)})}{q_X(X^*|X^{(s)},Y^{(s)})}$$

$$= \frac{f_{X|Y}(X^*|Y^{(s)})}{f_{X|Y}(X^{(s)}|Y^{(s)})} \cdot \frac{f_{X|Y}(X^{(s)}|Y^{(s)})}{f_{X|Y}(X^*|Y^{(s)})}$$

$$= 1$$

2. Update Y. Similar argument goes through if we use the full conditional distributions as our candidate transition densities.

**Definition:** Gibbs sampling is a special case of (blockwise) MH that take  $q_X(x|X_c, Y_c)$  to be  $f_{X|Y}(x|Y_c)$ , and take  $q_Y(y|X_c, Y_c)$  to be  $f_{Y|X}(y|X_c)$ , which then yield  $\gamma_X = \gamma_Y = 1$ . So following this sampling scheme, all proposals are automatically accepted.

Algorithm: Two stages Gibbs sampling

**Target:** f(X,Y), possibly unnormalized

Take  $x^{(0)}$ . For  $s = 1, 2, \dots$ , generate

- $Y^{(s)} \sim f_{Y|X}(\cdot|X^{(s-1)})$
- $X^{(s)} \sim f_{X|Y}(\cdot|Y^{(s)})$

Algorithm: Multi-stage Gibbs sampling

**Target:**  $f(X_1, X_2, \cdots, X_d)$ 

Starting Values:  $X^{(0)} = (X_1^{(0)}, X_2^{(0)}, \dots, X_d^{(0)})$ . Let  $f_j(X_j|X_{-j})$  denote the conditional density of  $X_j$  given all the rest components  $X_{-j} := \{X_i : i \neq j\}$ .

The algorithm generates  $X^{(s)}$  from  $X^{(s-1)}$  as follows:

(1) 
$$X_1^{(s)} \sim f_1(\cdot|X_2^{(s-1)}, \cdots, X_d^{(s-1)})$$
  
(2)  $X_2^{(s)} \sim f_2(\cdot|X_1^{(s)}, X_3^{(s-1)}, \cdots, X_d^{(s-1)})$   
 $\vdots$   
(d)  $X_d^{(s)} \sim f_d(\cdot|X_1^{(s)}, \cdots, X_{d-1}^{(s)})$ 

Repeat  $s \leftarrow s + 1$ .

Advantage: For high-dim problem, all the situation can be univariate and all probabilities are accepted.

#### Remark:

- The Gibbs sampler is a composition of MH moves with accept probability = 1. Each move is reversible, but the composition itself is not.
- Both (Blockwise) MH and Gibbs sampling have the target distribution as the invariant distribution (steady-state distribution).

### Example: Two-stage Gibbs sampling

$$f(x) \propto \frac{e^{-x^2/20}}{(1+(z_1-x)^2)(1+(z_2-x)^2)}, \quad z_1 = -4.3, z_2 = 5.2$$

Note that:  $\frac{1}{1+(z_i-x)^2} = \int_0^\infty e^{-w_i(1+(z_i-x)^2)} dw_i$ , then we can write

$$f(x, w_1, w_2) \propto e^{-x^2/20} \prod_{i=1}^{2} e^{-w_i(1+(z_i-x)^2)}$$

so f(x) is just the marginal pdf of  $f(x, w_1, w_2)$ .

Gibbs sampling:  $\vec{w} = (w_1, w_2)$ 

- $X^{(s)} \sim f_{X|\vec{w}}(\cdot|\vec{w}^{(s-1)})$
- $\vec{w} \sim f_{\vec{w}|X}(\cdot|X^{(s)})$

Here

$$f_{X|\vec{w}}(x|w_1, w_2) \overset{x}{\propto} e^{-\left(\sum w_i\right)x^2 + 2x \sum w_i z_i} \cdot e^{-x^2/20} \sim N\left(\frac{\sum w_i z_i}{\sum w_i + 1/20}, \frac{1}{2\left(\sum w_i + 1/20\right)}\right)$$
$$f_{\vec{w}|X}(w_1, w_2|x) \overset{\vec{w}}{\propto} e^{-w_1(1 + (z_1 - x)^2)} \cdot e^{-w_2(1 + (z_2 - x)^2)}$$

Note from the factorization above,  $w_1, w_2$  are independent given x, therefore,

$$f(w_1|X^{(s)}) \stackrel{w_1}{\propto} \text{exponential}(1 + (z_1 - X^{(s)})^2)$$
  
 $f(w_2|X^{(s)}) \stackrel{w_2}{\propto} \text{exponential}(1 + (z_2 - X^{(s)})^2)$ 

#### Multivariate Normal

Bivariate normal

$$(X,Y) \sim N\left(\begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \begin{pmatrix} \sigma_X^2 & \sigma_{XY} \\ \sigma_{XY} & \sigma_Y^2 \end{pmatrix}\right),$$

Let  $\rho = \frac{\sigma_{XY}}{\sigma_X\sigma_Y}$  be the correlation. It is a fact that

$$f_{X|Y}(x|y) \sim N(\mu_X + \rho \frac{\sigma_X}{\sigma_Y}(y - \mu_Y), \sigma_X^2(1 - \rho^2))$$

$$f_{Y|X}(y|x) \sim N(\mu_Y + \rho \frac{\sigma_Y}{\sigma_X}(x - \mu_X), \sigma_Y^2(1 - \rho^2))$$