# BAYESIAN LEARNING - LECTURE 7

### Mattias Villani

Division of Statistics and Machine Learning
Department of Computer and Information Science
Linköping University

### LECTURE OVERVIEW

- ► Monte Carlo simulation and random number generation
- ► Gibbs sampling
- Data augmentation
  - ► Probit regression
  - Mixture models

# MONTE CARLO SAMPLING

▶ If  $\theta^{(1)}$ ,  $\theta^{(2)}$ , ....,  $\theta^{(N)}$  is an *iid* sequence from a distribution  $p(\theta)$ , then

$$\frac{1}{N} \sum_{t=1}^{N} \theta^{(t)} \rightarrow E(\theta)$$

$$\frac{1}{N} \sum_{t=1}^{N} g(\theta^{(t)}) \rightarrow E[g(\theta)]$$

where  $g(\theta)$  is some well-behaved function.

▶ Easy to compute **tail probabilities**  $Pr(\theta \le c)$  by letting

$$g(\theta) = I(\theta \le c)$$

and

$$\frac{1}{N} \sum_{t=1}^{N} g(\theta^{(t)}) = \frac{\# \theta \text{-draws smaller than } c}{N}.$$

# DIRECT SAMPLING BY THE INVERSE CDF METHOD

- ► How to simulate from a distribution?
- Let f(x) be the density function of a stochastic variable. CDF: F(x). Inverse CDF method:
  - 1. Generate u from the uniform distribution on [0, 1].
  - **2.** Compute  $x = F^{-1}(u)$ .
- ► Example 1: Exponential distribution:

$$u = F(x) = 1 - \exp(-\lambda x)$$

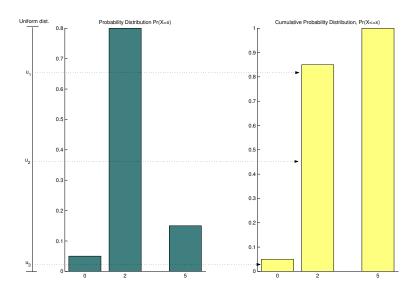
Inverting gives

$$x = -\ln(1-u)/\lambda$$

But 1 - u is also uniformly distributed on [0,1]. So:

▶ If  $x = -(\ln u)/\lambda$  where  $u \sim Unif(0,1)$ , then  $x \sim Expon(\lambda)$ .

# INVERSE CDF METHOD, DISCRETE CASE



# DIRECT SAMPLING BY THE INVERSE CDF METHOD

► Example 2: Cauchy distribution:

$$f(x) = \frac{1}{\pi} \frac{1}{1+x^2}$$

$$u = F(x) = \frac{1}{2} + \frac{1}{\pi} \arctan(x)$$

Inverting ...

$$x = \tan[\pi(u - 1/2)].$$

- We can also use relations between distribution to sample from distributions.
- ► Cauchy-example, cont. If y and z are independent N(0,1) variables, then  $z = \frac{y}{z} \sim Cauchy$ .
- Example: Chi-square. If  $x_1, ..., x_v \stackrel{iid}{\sim} N(0, 1)$ , then  $y = \sum_{i=1}^{v} x_i^2 \sim \chi_v^2$ .

# GIBBS SAMPLING

- Easily implemented methods for sampling from multivariate distributions,  $p(\theta_1, ..., \theta_k)$ .
- ► Requirements: Easily sampled full conditional posteriors:

  - $\triangleright p(\theta_k | \theta_1, \theta_2, ..., \theta_{k-1})$
- ▶ Started out in the early 80's in the image analysis literature.
- ► Gibbs sampling is a **special case of Metropolis-Hastings** (see Lecture 8)
- ► Metropolis-Hastings is a Markov Chain Monte Carlo (MCMC) algorithm.

# THE GIBBS SAMPLING ALGORITHM

```
A: Choose initial values \theta_2^{(0)}, \theta_3^{(0)}, ..., \theta_k^{(0)}.

B: B_1 Draw \theta_1^{(1)} from p(\theta_1|\theta_2^{(0)},\theta_3^{(0)},...,\theta_k^{(0)})

B_2 Draw \theta_2^{(1)} from p(\theta_2|\theta_1^{(1)},\theta_3^{(0)},...,\theta_k^{(0)})

:

B_n Draw \theta_k^{(1)} from p(\theta_n|\theta_1^{(1)},\theta_2^{(1)},...,\theta_{k-1}^{(1)})

C: Repeat Step B N times.
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# GIBBS SAMPLING, CONT.

► The Gibbs draws  $\theta^{(1)}$ ,  $\theta^{(2)}$ , ....,  $\theta^{(N)}$  are dependent (autocorrelated), but arithmetic means converge to expected values

$$\frac{1}{N} \sum_{t=1}^{N} \theta_{j}^{(t)} \rightarrow E(\theta_{j})$$

$$\frac{1}{N} \sum_{t=1}^{N} g(\theta^{(t)}) \rightarrow E[g(\theta)]$$

- $\bullet$   $\theta^{(1)}, ..., \theta^{(N)}$  converges in distribution to the target  $p(\theta)$ .
- $lackbox{ } heta_j^{(1)},..., heta_j^{(N)}$  converge to the marginal distribution of  $heta_j,\ p( heta_j).$
- ▶ Dependent draws → less efficient than iid sampling.
- Compare sampling from:
  - $\rightarrow x_t \stackrel{iid}{\sim} N(0, \sigma^2)$
  - $\star x_t = 0.9x_{t-1} + \varepsilon_t \text{ with } \varepsilon_t \stackrel{iid}{\sim} N(0, \sigma^2).$

# GIBBS SAMPLING MULTIVARIATE NORMAL

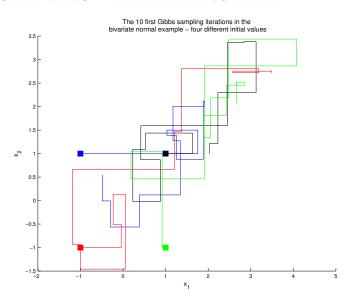
- ▶ Bivariate normal:
  - Joint distribution

$$\left(\begin{array}{c}\theta_1\\\theta_2\end{array}\right) \sim N_2\left[\left(\begin{array}{c}\mu_1\\\mu_2\end{array}\right), \left(\begin{array}{cc}1&\rho\\\rho&1\end{array}\right)\right]$$

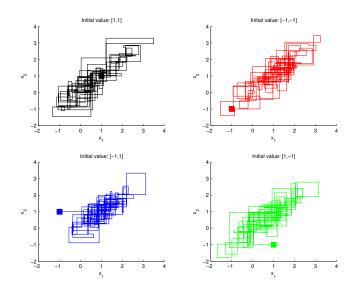
► Full conditional posteriors:

$$\begin{array}{lll} \theta_{1}|\theta_{2} & \sim & N[\mu_{1}+\rho(\theta_{2}-\mu_{2}),1-\rho^{2}] \\ \theta_{2}|\theta_{1} & \sim & N[\mu_{2}+\rho(\theta_{1}-\mu_{1}),1-\rho^{2}] \end{array}$$

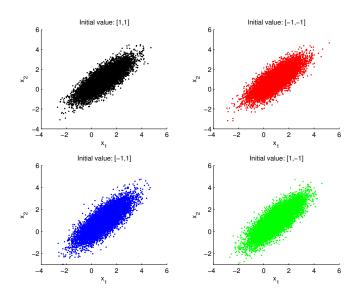
# GIBBS SAMPLING - BIVARIATE NORMAL



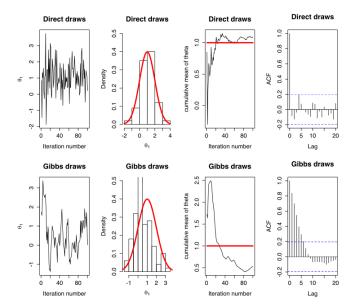
# GIBBS SAMPLING - BIVARIATE NORMAL



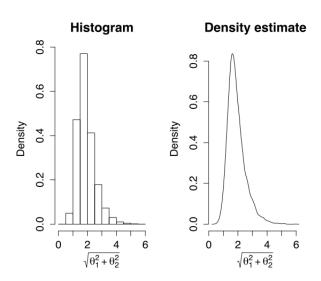
# GIBBS SAMPLING - BIVARIATE NORMAL



# DIRECT SAMPLING VS GIBBS SAMPLING



# Estimating the density of $g(\theta_1, \theta_2) = \sqrt{\theta_1^2 + \theta_2^2}$



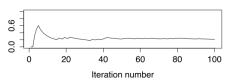
# ESTIMATING $Pr(\theta_1 > 0, \theta_2 > 0)$

▶ We can estimate a joint probability by counting:

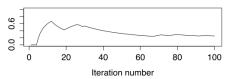
$$Pr(\theta_1 > 0, \theta_2 > 0) \approx N^{-1} \sum_{i=1}^{N} 1(\theta_1^{(i)} > 0, \theta_2^{i)} > 0)$$

.

#### **Direct draws**



#### Gibbs draws



# GIBBS SAMPLING FOR NORMAL MODEL WITH NON-CONJUGATE PRIOR

► Normal model with semi-conjugate prior

$$\mu \sim N(\mu_0, \tau_0^2)$$

$$\sigma^2 \sim Inv - \chi^2(\nu_0, \sigma_0^2)$$

Conditional posteriors

$$\mu|\sigma^{2}, x \sim N\left(\mu_{n}, \tau_{n}^{2}\right)$$

$$\sigma^{2}|\mu, x \sim Inv - \chi^{2}\left(\nu_{n}, \frac{\nu_{0}\sigma_{0}^{2} + \sum_{i=1}^{n}\left(x_{i} - \mu\right)^{2}}{n + \nu_{0}}\right)$$

# GIBBS SAMPLING FOR AR PROCESSES

▶ AR(p) process

$$x_t = \mu + \phi_1(x_{t-1} - \mu) + \dots + \phi_p(x_{t-p} - \mu) + \varepsilon_t, \quad \varepsilon_t \stackrel{iid}{\sim} N(0, \sigma^2).$$

- ▶ Let  $\phi = (\phi_1, ..., \phi_p)'$ .
- ▶ Prior:
  - μ ~Normal
  - $\phi \sim$  Multivariate Normal
  - $\sigma^2 \sim \text{Scaled Inverse } \chi^2$ .
- ► The posterior can be simulated by Gibbs sampling:
  - $\nu | \mu | \phi, \sigma^2, x \sim \text{Normal}$

  - $\phi | \mu, \sigma^2, x \sim \text{Multivariate Normal}$   $\sigma^2 | \mu, \phi, x \sim \text{Scaled Inverse } \chi^2$

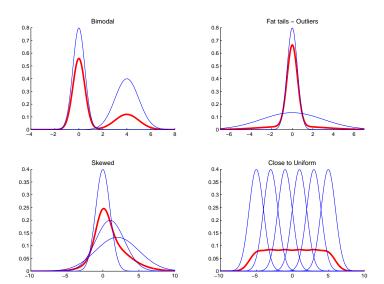
# DATA AUGMENTATION - MIXTURE DISTRIBUTIONS

- ▶ Let  $\phi(x|\mu,\sigma^2)$  denotes the PDF of a normal variable  $x \sim N(\mu,\sigma^2)$ .
- ► Two-component mixture of normals [MN(2)]

$$p(x) = \pi \cdot \phi(x|\mu_1, \sigma_1^2) + (1 - \pi) \cdot \phi(x|\mu_2, \sigma_2^2)$$

- ► Simulate from a MN(2):
  - ▶ Simulate an indicator  $I \in \{1, 2\}$ :  $I \sim \textit{Bern}(\pi)$ .
  - ▶ If I = 1, simulate x from  $N(\mu_1, \sigma_1^2)$ ▶ If I = 2, simulate x from  $N(\mu_2, \sigma_2^2)$ .

# **ILLUSTRATION OF MIXTURE DISTRIBUTIONS**



# MIXTURE DISTRIBUTIONS, CONT.

- ▶ Not easy to estimate directly the likelihood is a product of sums.
- Assume that we knew which of the two densities each observation came from.

$$I_i = \left\{ egin{array}{ll} 1 & \mbox{if } x_i \ \mbox{came from Density 1} \\ 2 & \mbox{if } x_i \ \mbox{came from Density 2} \end{array} 
ight. .$$

- Armed with knowledge of  $I_1, ..., I_n$  it is now easy to estimate  $\pi$ ,  $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$  by separating the sample according to the I's.
- ▶ But we do **not** know  $I_1, ..., I_n!$

# GIBBS SAMPLING FOR MIXTURE DISTRIBUTIONS

- ▶ Prior:  $\pi \sim Beta(\alpha_1, \alpha_2)$ . Conjugate prior for  $(\mu_j, \sigma_j^2)$ , see Lecture 5.
- ▶ Define:  $n_1 = \sum_{i=1}^{n} (I_i = 1)$  and  $n_2 = n n_1$ .
- ► Gibbs sampling:
  - $\blacksquare$   $\pi \mid \mathbf{I}, \mathbf{x} \sim Beta(\alpha_1 + n_1, \alpha_2 + n_2)$
  - $\sigma_1^2 \mid \mathbf{I}, \mathbf{x} \sim \mathit{Inv-}\chi^2(\nu_{n_1}, \sigma_{n_1}^2) \text{ and } \mu_1 \mid \mathbf{I}, \sigma_1^2, \mathbf{x} \sim \mathit{N}\left(\mu_{n_1}, \frac{\sigma_1^2}{\kappa_{n_1}^2}\right)$
  - $\qquad \qquad \sigma_2^2 \mid \mathbf{I}, \mathbf{x} \sim \mathit{Inv-}\chi^2(\nu_{n_2}, \sigma_{n_2}^2) \text{ and } \mu_2 | \mathbf{I}, \sigma_2^2, \mathbf{x} \sim \mathit{N}\left(\mu_{n_2}, \frac{\sigma_2^2}{\kappa_{n_2}}\right)$
  - ►  $I_i \mid \pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2, \mathbf{x} \sim Bern(\theta_i), i = 1, ..., n,$

$$\theta_i = \frac{(1-\pi)\phi(x_i; \mu_2, \sigma_2^2)}{\pi\phi(x_i; \mu_1, \sigma_1^2) + (1-\pi)\phi(x_i; \mu_2, \sigma_2^2)}.$$

### GIBBS SAMPLING FOR MIXTURE DISTRIBUTIONS

► *K*-component mixture of normals

$$p(x) = \sum_{k=1}^{K} \pi_k \phi(x; \mu_k, \sigma_k^2),$$

where  $\sum_{k=1}^{K} \pi_k = 1$ .

- ▶ Multi-class indicators:  $I_i = k$  if observation i comes from density k.
- ► Gibbs sampling with
  - $(\pi_1, ..., \pi_K) \mid \mathbf{I}, \mathbf{x} \sim Dirichlet(\alpha_1 + n_1, \alpha_2 + n_2, ..., \alpha_K + n_K)$
  - $\sigma_k^2 \mid \mathbf{I}, \mathbf{x} \sim Inv \chi^2$  and  $\mu_k \mid \mathbf{I}, \sigma_k^2, \mathbf{x} \sim Normal$ , for k = 1, ..., K,
  - ▶  $I_i \mid \pi, \mu, \sigma^2, \mathbf{x} \sim Multinomial(\theta_{i1}, ..., \theta_{iK})$ , for i = 1, ..., n,

$$\theta_{ij} = \frac{\pi_j \phi(x_i; \mu_j, \sigma_j^2)}{\sum_{r=1}^k \pi_r \phi(x_i; \mu_r, \sigma_r^2)}.$$

► Gibbs sampling is very powerful for missing data problems. Semi-supervised learning.

# DATA AUGMENTATION - PROBIT REGRESSION

Probit model:

$$\Pr(y_i = 1 \mid x_i) = \Phi(x_i'\beta)$$

► Random utility formulation of the probit:

$$u_i \sim N(x_i'\beta, 1)$$
  
 $y_i = \begin{cases} 1 & \text{om } u_i > 0 \\ 0 & \text{om } u_i \leq 0 \end{cases}$ 

- ► Check:  $\Pr(y_i = 1 \mid x_i) = \Pr(u_i > 0) = 1 \Pr(u_i \le 0) = 1 \Pr(u_i x_i'\beta < -x_i'\beta) = 1 \Phi(-x_i'\beta) = \Phi(x_i'\beta).$
- ▶ If  $u = (u_1, ..., u_n)$  were observed, then  $\beta$  could be analyzed by traditional linear regression. But, u is **not observed**. Gibbs sampling to the rescue!

# GIBBS SAMPLING FOR THE PROBIT REGRESSION

- ► Simulate from joint posterior  $p(u, \beta|y)$  iterating between the **full** conditional posteriors:
  - ▶  $p(\beta|u,y)$ , which is multivariate normal (this is just a linear regression)
  - ▶  $p(u_i|\beta, y)$ , i = 1, ..., n.
- ▶ The full conditional posterior distribution of  $u_i$  is:

$$\begin{split} p(u_i|\beta,y) &\propto p(y_i|\beta,u_i)p(u_i|\beta) \\ &= \begin{cases} N(u_i|x_i'\beta,1) & \text{truncated to } u_i \in (-\infty,0] \text{ if } y_i = 0 \\ N(u_i|x_i'\beta,1) & \text{truncated to } u_i \in (0,\infty) \text{ if } y_i = 1 \end{cases} \end{split}$$

► Collect the  $\beta$ -draws. A histogram of these draws approximates  $p(\beta|y) = \int p(u, \beta|y) du$ .

# IMPROVING THE EFFICIENCY OF THE GIBBS SAMPLER

- ▶ *Efficient blocking*. Correlated parameters should ideally be included in the same updating block.
- ► *Reparametrization*. Convergence can improve dramatically in alternative parametrizations.
- ▶ Data augmentation. Bring in latent (unobserved) variables that make the full conditional posteriors more easily sampled (Probit, Mixture models etc). Downside: Typically increases the autocorrelation between draws.
- Parameter expansion. Introducing (non-sense) parameters in the model may break the dependence between the original parameters (Example probit).