BML. 3. Intro to MCMC
From Gibbs to Hamilton

DataLab CSIC

Brief description

1. presented key methods in Bayesian inference and basic models and faced ‘severe’ computational problems quite rapidly (beta-binomial, logistic regression)

2. overviewed Bayesian computational strategies

3. Will focus on MCMC (Markov chain Monte Carlo): Gibbs, Metropolis, Hybrid, Hamiltonian.

Other stuff, including SG-MCMC later on

Computational problems in Bayesian analysis

Computing the posterior

$$f(\theta|x) = \frac{f(x|\theta)\, f(\theta)}{f(x)} = \frac{f(x|\theta)\, f(\theta)}{\int f(x|\theta)\, f(\theta)\, d\theta} \propto f(x|\theta)\, f(\theta)$$

Computing posterior expectations

$$\int h(\theta)\, f(\theta|x)\, d\theta$$

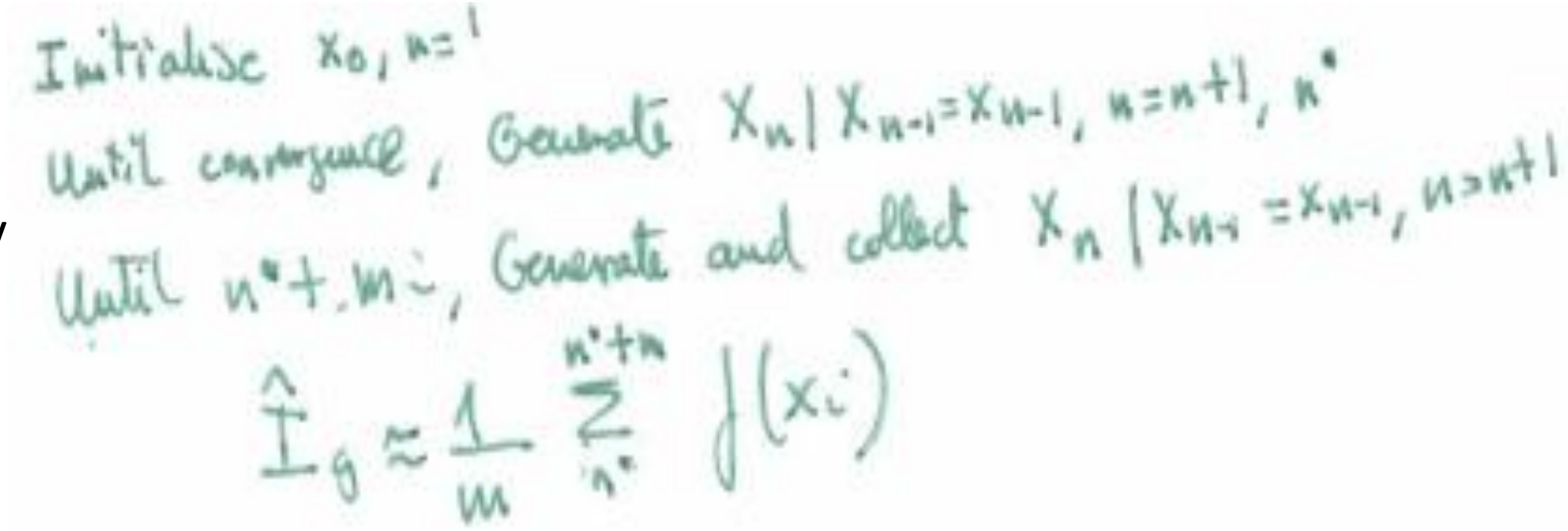
$$\frac{1}{N} \sum_{i=1}^{n} h(\theta_i) \qquad \theta_i \sim f(\theta|x)$$

General idea MCMC

Markov chain X_n with same state space as target and convergent to target distribution g

$X_n \xrightarrow{d} g$

Strategy



a. Gibbs sampling

Sources

French and DRI (2000) Ch 7

DRI et al (2010) Ch4

BDA3 (2015) Ch11, 12

Hoff (2009) Ch 6,7

Labs

3.1 Gibbs

Basic, Re-usable,Paralel chains

Multivariate normal

Normal-gamma inverse

Generic Gibbs sampler

$$X = (X_1, \cdots, X_p) \sim \pi$$

Sample from $X_s \mid X_{-s} = (X_1, \cdots, X_{s-1}, X_{s+1}, \cdots, X_p)$

Initialize $X_1^0, \cdots, X_p^0$, $i = 1$

Iterate

Sample $X_1^i \sim X_1 \mid X_2^{i-1}, \cdots, X_p^{i-1}$

Sample $X_2^i \sim X_2 \mid X_1^i, X_3^{i-1}, \cdots, X_p^{i-1}$

...

Sample $X_p^i \sim X_p \mid X_1^i, X_2^i, \cdots, X_p^{i-1}$

$i := i+1$

Important Gibbs sampling examples

Purpose

Through several important examples reinforce Gibb sampling concept

Motivation

Model and prior

Posterior conditionals

Gibbs sampler

Use

(Many implemented in labs)

Sampling the bi-variate normal

Simple example to recall approach

Model. Bivariate normal with unknown means. Variances 1. Known correlation ϱ

1 observation

Prior. Uniform

Use. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

Auxiliary result (eg Handbook of the Normal Distribution)

$$\theta \mid \mu, \Sigma \sim N(\mu, \Sigma) \qquad f(\theta) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\theta-\mu)' \Sigma^{-1} (\theta-\mu)\right)$$

$$C = I - \left[\operatorname{diag}(\Sigma^{-1})\right]^{-1} \Sigma^{-1}$$

$$\theta_i \mid \theta_j, j \neq i \sim N\left(\mu_i + \sum_{j \neq i} c_{ij} (\theta_j - \mu_j), \left((\Sigma^{-1})_{ii}\right)^{-1}\right)$$

Sampling the bi-variate normal. Model and posterior

$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\,\pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)'\,\Sigma^{-1}(y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)'\,\Sigma^{-1}(\theta-y)\right)$$

$$\theta | y \sim N(y, \Sigma)$$

Sampling the bi-variate normal. Gibbs sampler

$$\theta_1 | \theta_2, y \sim N(y_1 + \rho(\theta_2 - y_2), 1 - \rho^2)$$
$$\theta_2 | \theta_1, y \sim N(y_2 + \rho(\theta_1 - y_1), 1 - \rho^2)$$

θ_2^0 ARBITRARY, $i = 1$

UNTIL CONVERGENCE

$$\theta_1^i \sim N(y_1 + \rho(\theta_2^{i-1} - y_2), 1 - \rho^2)$$
$$\theta_2^i \sim N(y_2 + \rho(\theta_1^i - y_1), 1 - \rho^2)$$
$$i = i + 1$$

Sampling the bi-variate normal. Answers

$$\hat{E}(\theta_1 | y) = \frac{1}{K} \sum_{i=1}^{K} \theta_1^{M+i}$$

$$\hat{E}(\theta_1 \theta_2 | y) = \frac{1}{K} \sum_{i=1}^{K} \left(\theta_1^{M+i} \theta_2^{M+i} \right)$$

$$Pr(\theta_1 \in A | y) = \frac{\#\{ \theta_1^{M+i} \in A \}}{K}$$

Inference for normal-gamma

A very important example. Analytic solution available. Serves as benchmark

Model. Normal with unknown mean and variance. Prior normal-gamma.

Use. Quartiles of mean, Interval of probability 0.7, Test null that mean is bigger than 0

https://en.wikipedia.org/wiki/Inverse-gamma_distribution

https://en.wikipedia.org/wiki/Normal-inverse-gamma_distribution

Inference for normal-gamma. Model

$$x_1, \dots, x_n \mid \theta, \sigma^2 \sim N(\theta, \sigma^2)$$

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

$$\frac{1}{\sigma^2} = \tilde{\sigma}^2 \sim Ga\left(\frac{\nu_0}{2}, \frac{\nu_0 \sigma_0^2}{2}\right)$$

$$p(\theta, \sigma^2) = p(\theta)\, p(\sigma^2)$$

$$p(\theta \mid \sigma^2, x_1, \dots, x_n) \sim N(\mu_n, \tau_n^2)$$

$$\mu_n(\tilde{\sigma}^2) = \frac{\frac{1}{\tau_0^2}\mu_0 + \frac{n}{\sigma^2}\bar{x}}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}}$$

$$\tau_n(\tilde{\sigma}^2) = \frac{1}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}}$$

Inference for normal-gamma. Conditional

$$p(\tilde{\sigma}^2 \mid \theta, x_1, \dots, x_n) \propto p(x_1, \dots, x_n, \theta, \tilde{\sigma}^2) = p(x_1, \dots, x_n \mid \theta, \tilde{\sigma}^2)\, p(\theta \mid \tilde{\sigma}^2)\, p(\tilde{\sigma}^2)$$

$$= p(x_1, \dots, x_n \mid \theta, \tilde{\sigma}^2)\, p(\theta)\, p(\tilde{\sigma}^2) \propto p(x_1, \dots, x_n \mid \theta, \tilde{\sigma}^2)\, p(\tilde{\sigma}^2)$$

$$\propto (\tilde{\sigma}^2)^{n/2} \exp\left(-\tilde{\sigma}^2 \sum_{i=1}^{n} (x_i - \theta)^2/2\right) (\tilde{\sigma}^2)^{\nu_0/2 - 1} \exp\left(-\tilde{\sigma}^2 \nu_0 \sigma_0^2/2\right)$$

$$= (\tilde{\sigma}^2)^{(\nu_0 + n)/2 - 1} \exp\left\{-\tilde{\sigma}^2 \left[\nu_0 \sigma_0^2 + \sum (x_i - \theta)^2\right]/2\right\}$$

$$\tilde{\sigma}^2 \mid x_1, \dots, x_n \sim \mathrm{Ga}\left(\frac{\nu_n}{2}, \frac{\nu_n \sigma_n^2(\theta)}{2}\right)$$

$$\nu_n = \nu_0 + n \qquad s_n^2(\theta) := \frac{\sum (x_i - \theta)^2}{2}$$

$$\sigma_n^2(\theta) = \frac{1}{\nu_n} \left[\nu_0 \sigma_0^2 + n s_n^2(\theta)\right]$$

Inference for normal-gamma. Sampler

$\tilde{\sigma}^{2(0)}$ ARBITRARY, $i = 1$

UNTIL CONVERGENCE

$$\theta_i \sim N\left(\mu_n\left(\tilde{\sigma}^{2(i-1)}\right), \tau_n\left(\tilde{\sigma}^{2(i-1)}\right)\right)$$

$$\tilde{\sigma}^{2(i)} \sim Ga\left(\nu_n/2, \frac{\nu_n \sigma_n^2(\theta_i)}{2}\right)$$

$i = i+1$

Inference for normal-gamma. Answers

$\theta^s = \text{SORT}(\theta_i)_M^{K+M}$

MEDIAN $= \theta^s_{M/2}$ ...

LB $= \theta^s_{[0.16M]}$

UB $= \theta^s_{[0.65M]}$

PROB $= \#\{\theta_i \geq 0\} / K$

IF (PROB $\geq$ 0.5) ACCEPT

ELSE

REJECT

ENDIF

Inference for a mixture of exponentials

An example with mixtures. Very important in modern statistics and machine learning, e.g. Latent Dirichlet allocation. Used in clustering, density estimation,… Also introduces latent variables.

Model. Mixture of k exponentials, gamma priors. Dirichlet-multinomial on labels.

Use. Predictive distribution, group for first observation

https://en.wikipedia.org/wiki/Multinomial_distribution

https://en.wikipedia.org/wiki/Dirichlet_distribution

https://en.wikipedia.org/wiki/Latent_Dirichlet_allocation

Inference for a mixture of exponentials

Model

$$t = (t_1, \dots, t_{n_t})$$

$$f(t|\theta) = q_1 \mu_1 \exp(-\mu_1 t) + \dots + q_K \mu_K \exp(-\mu_K t)$$

$$\theta = (q_1, \mu_1, \dots, q_K, \mu_K) \qquad \sum_{i=1}^{K} q_i = 1 \qquad q_i > 0$$

$$\mu_i \sim Ga(a_i, p_i) \qquad q \sim D(\alpha_1, \dots, \alpha_K) \qquad \alpha_i > 0$$

Inference for a mixture of exponentials

Latent variables

$$t_j \longrightarrow z_j = (z_{1j}, \dots, z_{Kj})$$

$$z_j \mid q, \mu \sim M_K(1; q_1, \dots, q_K)$$

$$\sum z_{ij} = 1 \qquad z_{ij} \in \{0, 1\}$$

$$t_j \mid z_j, q, \mu \sim \mathcal{E}\left(\prod_{i=1}^{k} \mu_i^{z_{ij}}\right)$$

Inference for a mixture of exponentials

Posterior conditionals

$$z_j \mid t_j, q, \mu \sim M_K\left(1; \frac{q_1 \mu_1 \exp(-\mu_1 t_j)}{\sum q_i \mu_i \exp(-\mu_i t_j)}; \ldots; \frac{q_K \mu_K \exp(-\mu_K t_j)}{\sum q_i \mu_i \exp(-\mu_i t_j)}\right) j = \ldots n$$

$$\mu_j \mid t, z \sim g\left(a_j + \sum_{i=1}^{n} z_{ji} t_i,\ p_j + \sum_{i=1}^{n} z_{ji}\right),\ j = 1, \ldots, K$$

$$q \mid t, z \sim D\left(\alpha_1 + \sum_{i=1}^{n} z_{1i}, \ldots, \alpha_K + \sum_{i=1}^{n} z_{Ki}\right)$$

Inference for a mixture of exponentials

Gibbs sampler

μ^0, z^0 ARBITRARY

UNTIL CONVERGENCE

$$z_j^{i+1} \sim z_j \mid t_j, q^i, \mu^i, \quad j = 1, \dots, n_s$$

$$q^{i+1} \sim q \mid t, z^{i+1}$$

$$\mu_j^{i+1} \sim \mu_j \mid t, z^{i+1}, \quad j = 1, \dots, k$$

$$i = i + 1$$

Inference for a mixture of exponentials

Answers

$$R(t_1 \in h) = \frac{\#\{z_1^i = h\}}{K}$$

FOR $i = 1$ TO K

$$\tau_i \sim \sum_{j=1}^{K} q_j^{M+i} \, \mathrm{Exp}\left(\mu_j^{M+i}\right)$$

Inference for normal multivariate

Again ultra-important. Bread and butter of multivariate analysis

Model. Multivariate normal (means and covariance matrix). Normal-Wishart prior

Use. Expected value of maximum, Probability that product of means is bigger than 4

https://en.wikipedia.org/wiki/Wishart_distribution

Inference for normal multivariate

Model

$$Y_1, \dots, Y_n \sim MN(\theta, \Sigma)$$

$$\theta \sim N(\mu_0, \Lambda_0)$$

$$\Sigma^{-1} \sim WISH(\nu_0, S_0^{-1})$$

$$E(\Sigma^{-1}) = \nu_0 S_0^{-1}$$

$$E(\Sigma) = \frac{1}{\nu_0 - p - 1} S_0$$

Inference for normal multivariate

Posterior conditionals

$$\theta \mid Y_1, \dots, Y_n, \Sigma \sim N(\mu_n, \Lambda_n)$$

$$\Lambda_n = (\Lambda_0^{-1} + n\Sigma^{-1})^{-1}$$

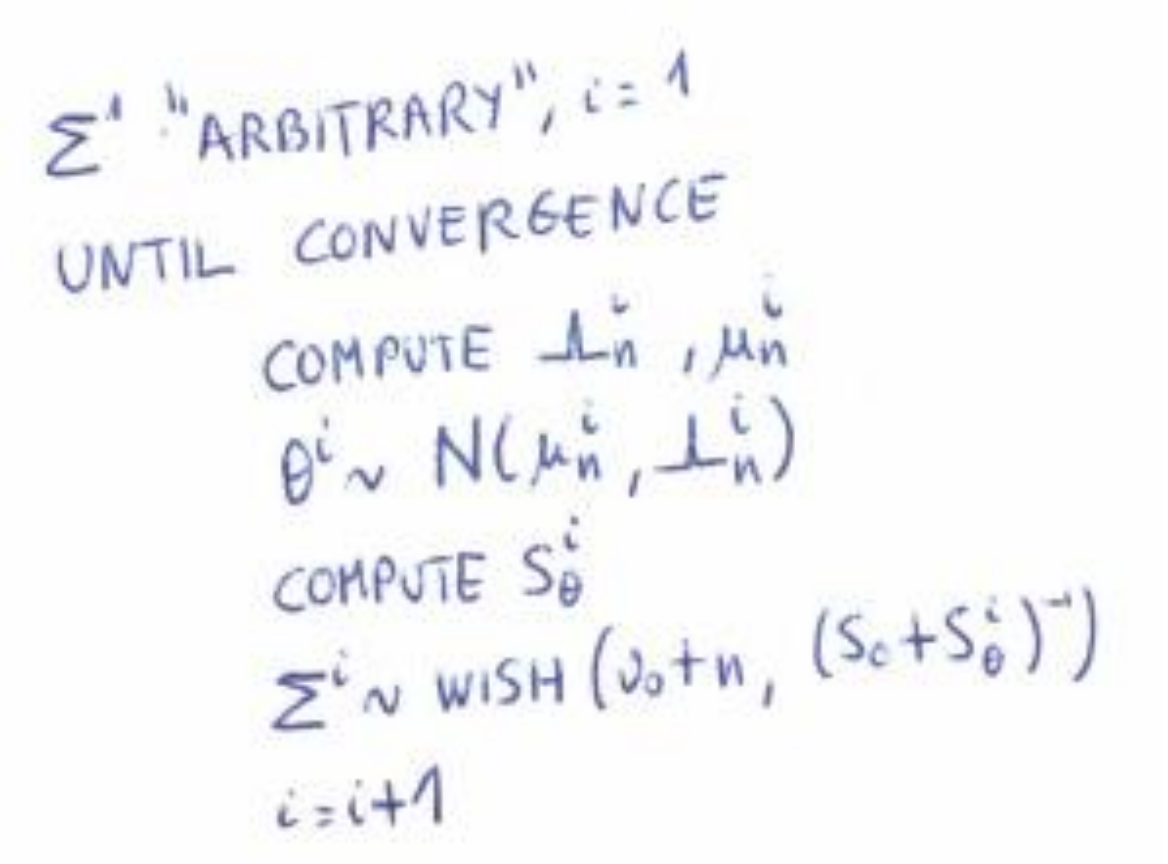
$$\mu_n = \Lambda_n^{-1}(\Lambda_0^{-1}\mu_0 + n\Sigma^{-1}\bar{Y})$$

$$\Sigma \mid Y_1, \dots, Y_n, \theta \sim \text{WISH}(\nu_0 + n, (S_0 + S_\theta)^{-1})$$

$$S_\theta = \sum_{i=1}^{n} (Y_i - \theta)(Y_i - \theta)^t$$

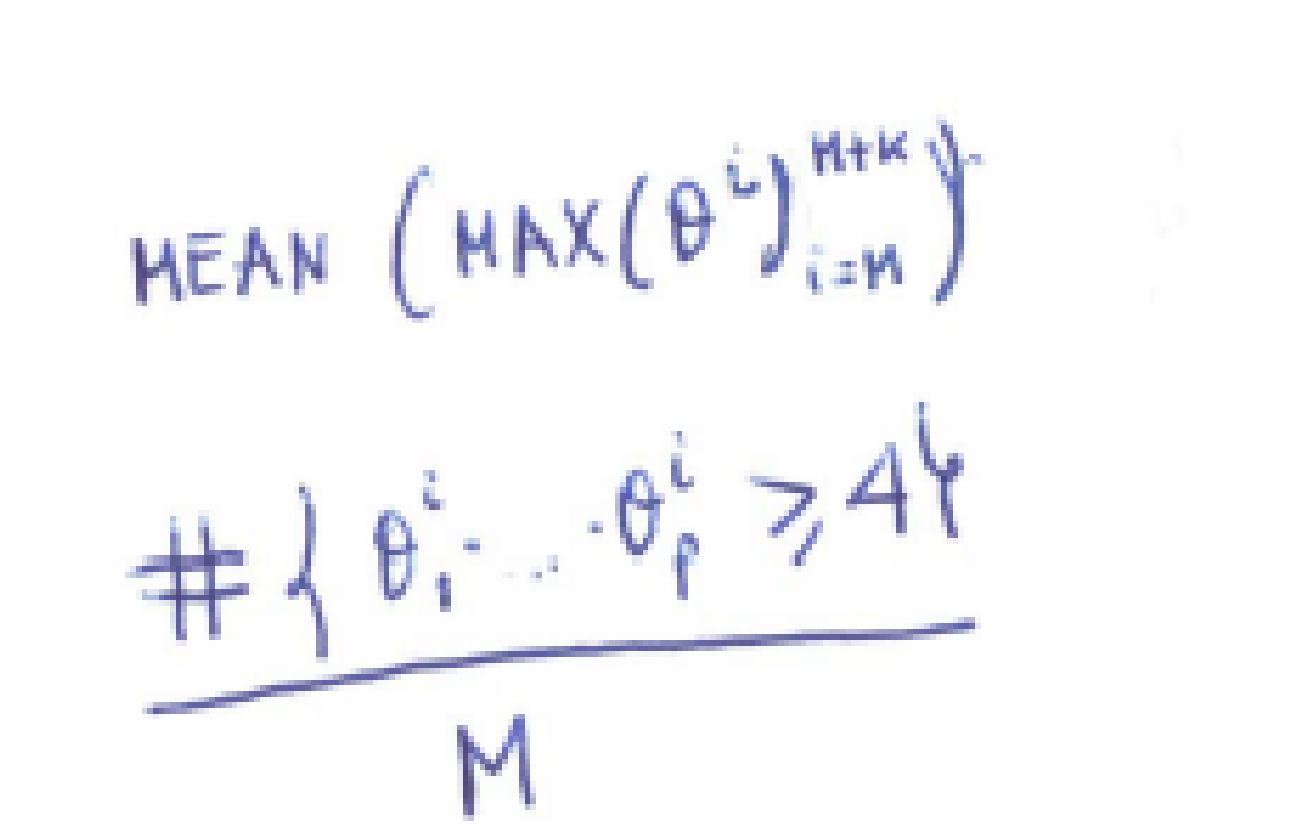
Inference for normal multivariate

Gibbs sampler



Inference for normal multivariate

Answers



Gibbs sampling theory

Recall

1. Choose initial values $(\theta_2^0, \ldots, \theta_k^0)$. $i = 1$

2. Until convergence is detected, iterate through
   - Generate $\theta_1^i \sim \theta_1 | \theta_2^{i-1}, .., \theta_k^{i-1}$
   - Generate $\theta_2^i \sim \theta_2 | \theta_1^i, \theta_3^{i-1}, ..., \theta_k^{i-1}$
   - ...
   - Generate $\theta_k^i \sim \theta_k | \theta_1^i, ..., \theta_{k-1}^i$.
   - $i = i + 1$

Convergence

Kernel $p_G(\theta^n, \theta^{n+1}) = \prod_{i=1}^{k} p(\theta_i^{n+1} \mid \theta_j^n, j > i; \theta_j^{n+1}, j < i).$

Proposition 43 *Suppose that* $D = \{\theta : p(\theta) > 0\}$ *is a product set,* $D = \prod_{i=1}^{k} D_i$. *Then:*

1. $p_{\theta_i}(\theta_i | \theta_j, j \neq i)$ *and* p_G *are well-defined for* $\theta \in D$.
2. p_G *is p-irreducible and aperiodic.*
3. p *is invariant with respect to* p_G.
4. $\theta^n \xrightarrow{w} \theta$

b. Metropolis Hastings algos

Brief description

The intro presented key methods in Bayesian inference and basic models and faced ‘severe’ computational problems quite rapidly (beta-binomial, logistic regression)

We have introduced MCMC and Gibbs sampling

We focus here on Metropolis-Hastings and hybrid samplers

More to be followed

Sources

French and DRI (2000) Ch 7
DRI et al (2010) Ch4
BDA3 (2015) Ch11, 12
Hoff (2009) Ch 6,7

Labs

3.2 Metropolis

Basic, Standard, MH

Multivariate normal

Linear regression (ecology)

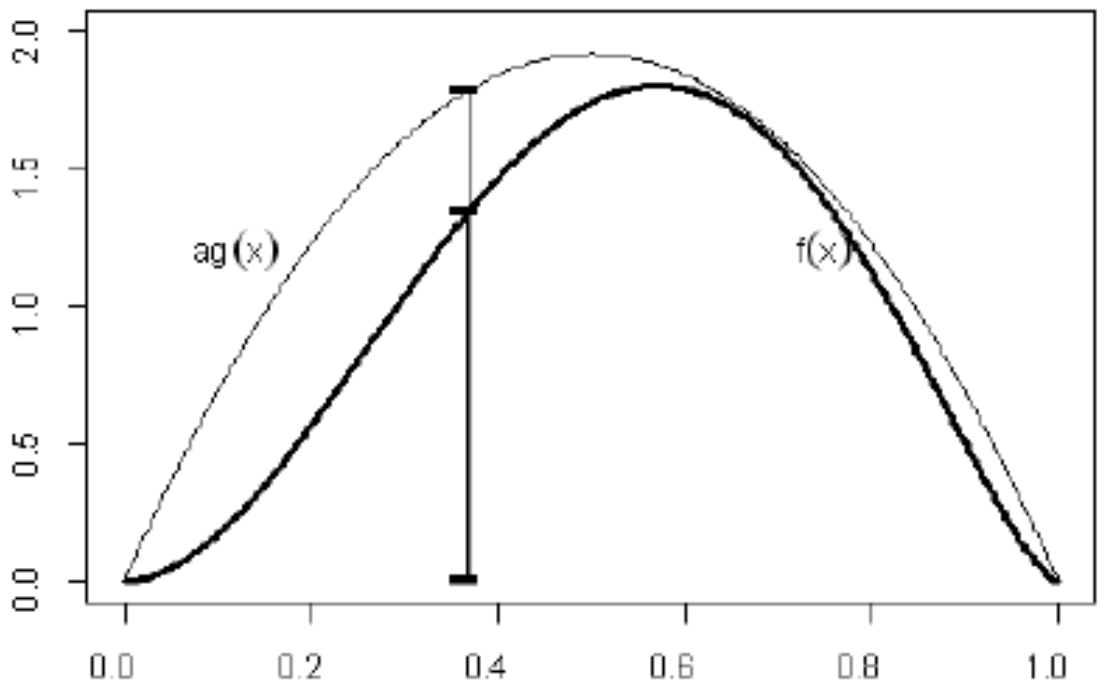
Poisson regression (ecology)

Understanding the Metropolis-Hastings algorithm

Recall: Acceptance-rejection sampling

TARGET DENSITY $\pi(x) = f(x)/K$, K possibly UNKNOWN

SAMPLING DENSITY $g(x)$: $f(x) \leq a g(x)$, $\forall x$



WHILE $U > f(x) / (a g(x))$

GENERATE $X \sim g$, $U \sim \mathcal{U}[0,1]$

OUTPUT X

$P(X \leq x \mid X \text{ ACCEPTED}) = F(x)$ (F cdf of X)

Metropolis-Hastings rationale I

Transition kernel of Markov chain $P(x, A)$

Invariant distribution $\Pi^*(dy) = \int P(x, dy)\, \Pi(x)\, dx$

n-th iterate $P^{(n)}(x, A) = \int P^{(n-1)}(x, dy)\, P(y, A)$

Metropolis-Hastings rationale II

Invariant distribution and reversibility. Suppose that for p kernel (x,y)

$$p(x, dy) = p(x,y)\,dy + r(x)\,\delta_x(dy)$$

$$p(x,x) = 0 \qquad \delta_x(dy) = \begin{cases} 1, & \text{if } x \in dy \\ 0, & \text{otherwise} \end{cases}$$

$$r(x) = 1 - \int p(x,y)\,dy$$

$$\pi(x)\,p(x,y) = \pi(y)\,p(y,x) \Rightarrow \pi \text{ invariant for } p(x,\cdot)$$

Metropolis-Hastings rationale III

Adjusting a candidate generating distribution

$q(x,y)$ CANDIDATE GENERATING DENSITY

SUPPOSE

$$\pi(x)\, q(x,y) > \pi(y)\, q(y,x)$$

INTRODUCE 'CORRECTION' PROBABILITY OF MOVE

$$\alpha(x,y) < 1$$

$$p_{MH}(x,y) \equiv q(x,y)\,\alpha(x,y) \qquad x \neq y$$

$$\pi(x)\, q(x,y)\,\alpha(x,y) = \pi(y)\, q(y,x)\,\alpha(y,x)$$

$$= \pi(y)\, q(y,x)$$

$$\Rightarrow \alpha(x,y) = \frac{\pi(y)\, q(y,x)}{\pi(x)\, q(x,y)}$$

Metropolis-Hastings rationale IV

Balance condition

$$\alpha(x,y) = \begin{cases} \min\left(\frac{\pi(y)\,q(y,x)}{\pi(x)\,q(x,y)}, 1\right), & \text{IF } \pi(x)\,q(x,y) > 0 \\ 1, & \text{OTHERWISE} \end{cases}$$

Observations

- Normalising constant not required
- If q symmetric, Metropolis

$$\alpha(x,y) = \min\left(\frac{\pi(y)}{\pi(x)}, 1\right)$$

Metropolis-Hastings algo

1. Choose initial values θ^0. $i = 0$

2. Until convergence is detected, iterate through

   . Generate a candidate $\theta^* \sim q(\theta|\theta^i)$.

   . If $p_\theta(\theta^i)q(\theta^i \mid \theta^*) > 0$, $\alpha(\theta^i, \theta^*) = \min\left(\frac{p_\theta(\theta^*)q(\theta^*|\theta^i)}{p_\theta(\theta^i)q(\theta^i|\theta^*)}, 1\right)$;

   . else, $\alpha(\theta^i, \theta^*) = 1$.

   . Do

$$\theta^{i+1} = \begin{cases} \theta^* & \text{with prob } \alpha(\theta^i, \theta^*), \\ \theta^i & \text{with prob } 1 - \alpha(\theta^i, \theta^*) \end{cases}$$

   . $i = i + 1$.

Metropolis-Hastings variants I

Random walk chain

$$q(x,y) = q_1(x-y)$$

$$y = x + z, \quad z \sim q_1 \quad \rightarrow \text{NORMAL} \quad \rightarrow t$$

Metropolis algorithm

$$\alpha(x,y) = \min\left(\frac{\pi(y)}{\pi(x)}, 1\right)$$

Independence chain

$$q(x,y) = q_2(y) \quad \rightarrow \text{NORMAL} \quad \rightarrow t$$

Metropolis-Hastings variants II

Exploiting form of target

$\pi(t) \propto \psi(t) h(t)$ h DENSITY, ψ UNIF. BOUND

$q(x,y) = h(y)$

$\alpha(x,y) = \min\left\{\frac{\psi(y)}{\psi(x)}, 1\right\}$

Acceptance rate not too high, not too low (23%). Tuning parameters

Examples

Sampling the bi-variate normal

Simple example to recall approach

Model. Bivariate normal with unknown means. Variances 1. Known correlation ϱ

1 observation

Prior. Uniform

Use. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

Sampling the bi-variate normal. Model and posterior

$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\,\pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)'\,\Sigma^{-1}(y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)'\,\Sigma^{-1}(\theta-y)\right)$$

$$\theta | y \sim N(y, \Sigma)$$

Sampling the bi-variate normal. Gibbs sampler

$$\theta_1 | \theta_2, y \sim N(y_1 + \rho(\theta_2 - y_2), 1 - \rho^2)$$
$$\theta_2 | \theta_1, y \sim N(y_2 + \rho(\theta_1 - y_1), 1 - \rho^2)$$

θ_2^0 ARBITRARY, $i = 1$

UNTIL CONVERGENCE

$$\theta_1^i \sim N(y_1 + \rho(\theta_2^{i-1} - y_2), 1 - \rho^2)$$
$$\theta_2^i \sim N(y_2 + \rho(\theta_1^i - y_1), 1 - \rho^2)$$
$$i = i + 1$$

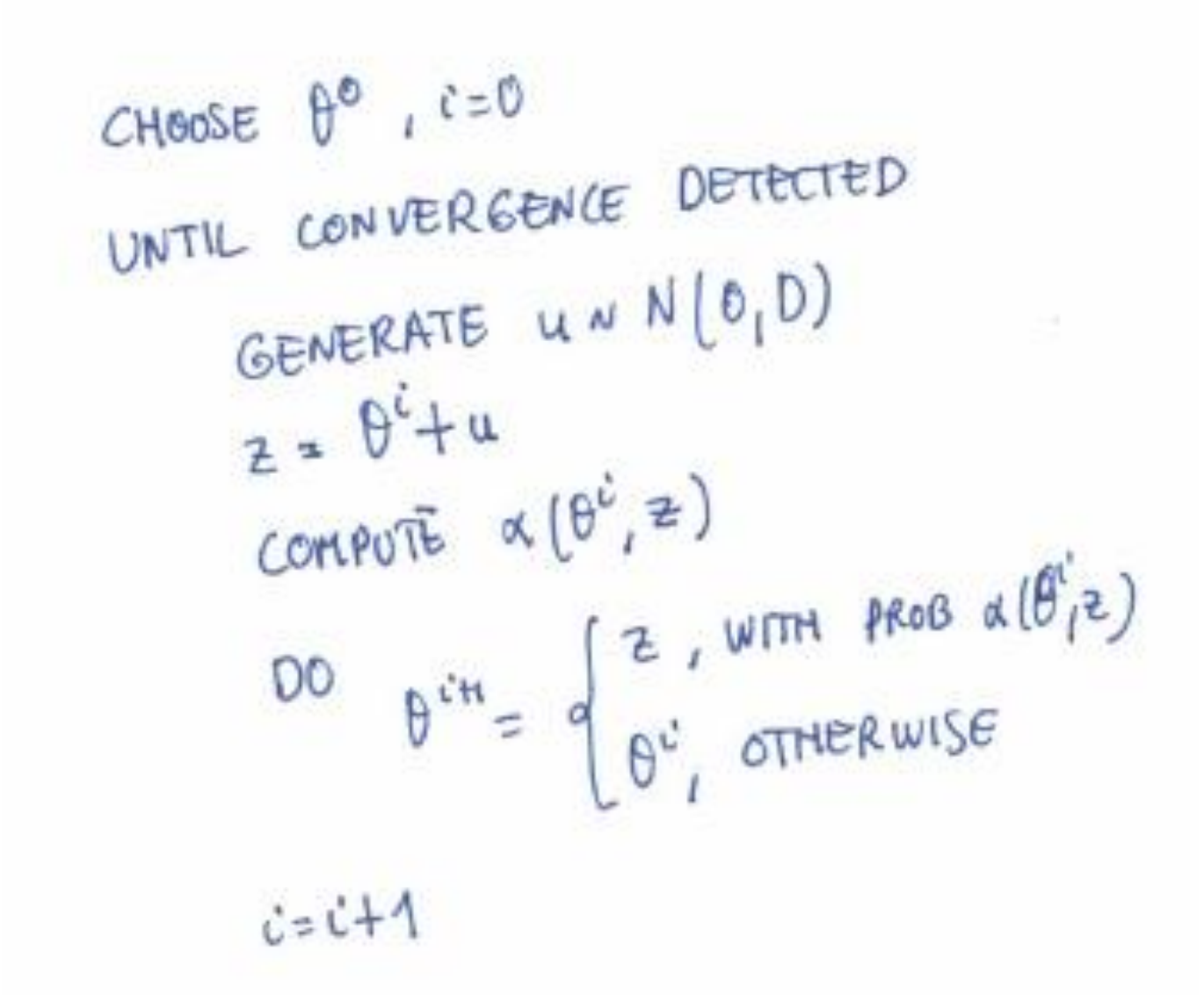
Sampling the bi-variate normal. Metropolis Hastings

$$z = \theta + u \qquad u \sim N(0, D)$$

$$\alpha(\theta, z) = \min\left\{ \frac{\exp\left(-\frac{1}{2}(z-\gamma)' \Sigma^{-1}(z-\gamma)\right)}{\exp\left(-\frac{1}{2}(\theta-\gamma)' \Sigma^{-1}(\theta-\gamma)\right)}, 1 \right\}$$

$$= \min\left\{ \frac{\exp\left(-\frac{1}{2}\left((z' \Sigma^{-1} z) - 2 z \Sigma^{-1} \gamma\right)\right)}{\exp\left(-\frac{1}{2}\left(\theta' \Sigma^{-1} \theta\right) - 2\theta \Sigma^{-1} \gamma\right)}, 1 \right\}$$

Sampling the bi-variate normal. Metropolis Hastings



Sampling the bi-variate normal. Answers....

$$\hat{E}(\theta_1 | y) = \frac{1}{K} \sum_{i=1}^{K} \theta_1^{M+i}$$

$$\hat{E}(\theta_1 \theta_2 | y) = \frac{1}{K} \sum_{i=1}^{K} \left(\theta_1^{M+i} \; \theta_2^{M+i} \right)$$

$$Pr(\theta_1 \in A | y) = \frac{\#\{ \theta_1^{M+i} \in A \}}{K}$$

Bayesian Probit Regression

$(x_i, y_i) \qquad y_i \in \{0, 1\}$

$$l(\beta | y) \propto \prod_{i=1}^{n} \phi(x^i \beta)^{y_i} (1 - \phi(x^i \beta))^{1-y_i}$$

WITH A FLAT PRIOR $\pi(\beta) \propto 1$

$$\pi(\beta | y) \propto \prod_{i=1}^{n} \phi(x^i \beta)^{y_i} (1 - \phi(x^i \beta))^{1-y_i}$$

M.H. RANDOM WALK $\tilde{\beta} \sim N(\beta_{t-1}, \tau^2 \hat{\Sigma})$

COMPUTE MLE $\hat{\beta}$, $\hat{\Sigma}$ ASYMPTOTIC COVARIANCE OF $\hat{\beta}$

Bayesian Probit Regression MH

$\beta_0 = \hat{\beta}, \; i = 1$

UNTIL CONVERGENCE

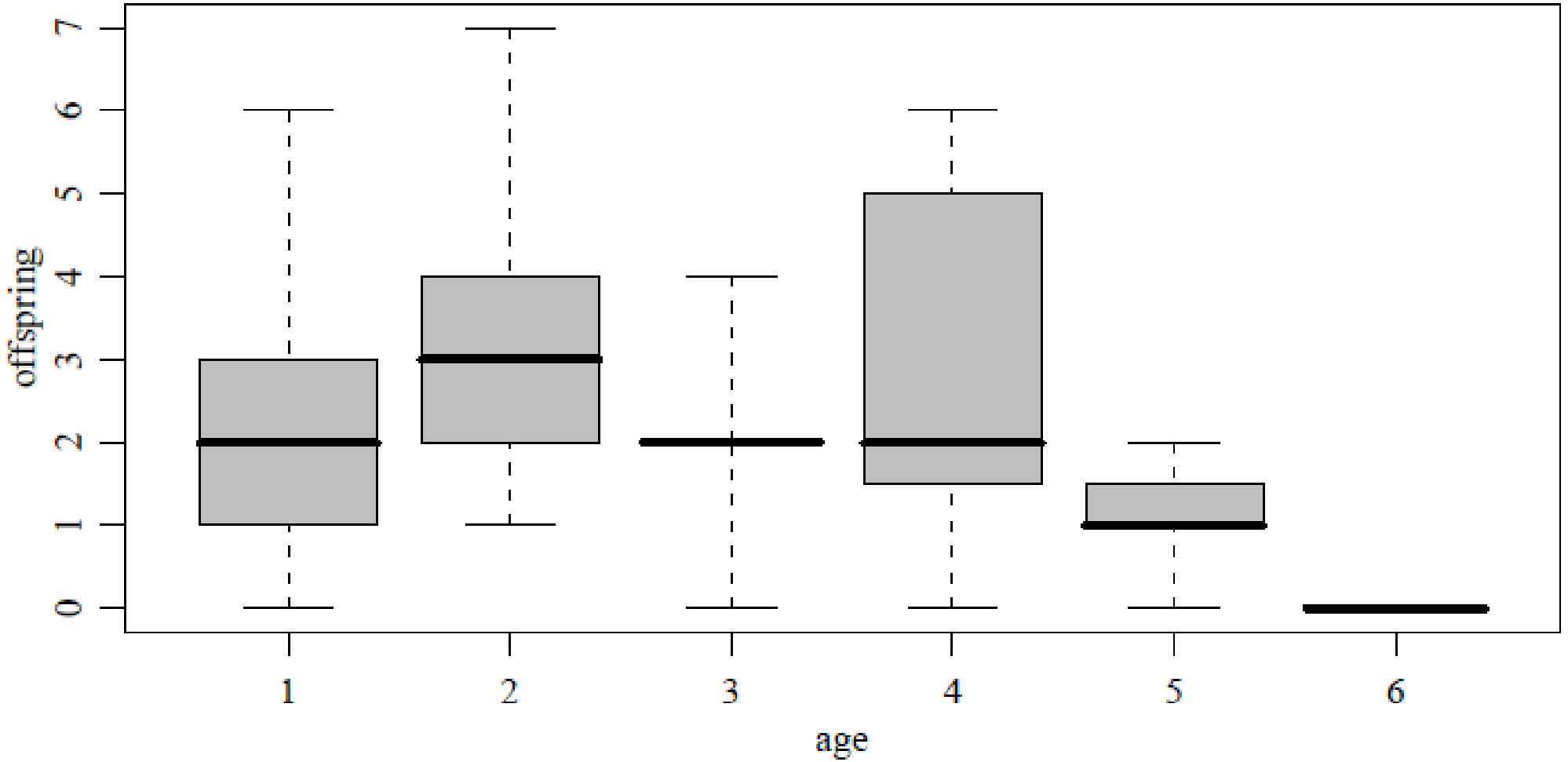
SAMPLE $\tilde{\beta} \sim N(\beta_{i-1}, \tau^2 \hat{\Sigma})$

COMPUTE $\alpha(\beta_{i-1}, \tilde{\beta}) = \min\left(1, \frac{\pi(\tilde{\beta}|y)}{\pi(\beta_{i-1}|y)}\right)$

$$\beta_{i+1} = \begin{cases} \tilde{\beta} & \text{WITH PROB } \alpha(\beta_{i-1}, \tilde{\beta}) \\ \beta_i, & \text{OTHERWISE} \end{cases}$$

$i = i + 1$

Bayesian Poisson Regression. Offspring of birds given age



Bayesian Poisson Regression

Offspring Y given age?? Per age?? Linear??

$$Y|x \sim \text{POISSON}(\theta_x)$$

$$\theta_x = \beta_1 + \beta_2 x + \beta_3 x^2 ??$$

$$\log \theta_x = \beta_1 + \beta_2 x + \beta_3 x^2$$

$$E(Y|x) = \exp(\beta_1 + \beta_2 x + \beta_3 x^2)$$

$$Y|x \sim \text{POISSON}(\exp(\beta^T x))$$

Bayesian Poisson Regression

Prior and posterior

$$\text{PRIOR} \quad \beta_i \sim N(0, 100)$$

$$\text{POSTERIOR} \propto \left[\prod_{i=1}^{3} N(\beta_i \mid 0, 100)\right] \left[\prod_{i=1}^{n} Po(y_i \mid \beta x)\right]$$

Acceptance probability in MH

$$\alpha(\beta, \hat{\beta}) = \min\left(\frac{\prod_{i=1}^{3} dnorm(\hat{\beta}_i, 0, 10)}{\prod_{i=1}^{3} dnorm(\beta_i, 0, 10)} \; \frac{\prod_{i=1}^{n} dpois(y_i, x_i \hat{\beta})}{\prod_{i=1}^{n} dpois(y_i, x_i \beta_i)} \; \frac{q(\hat{\beta}, \beta)}{q(\beta, \hat{\beta})}, 1\right)$$

MH theory

Recall

1. Choose initial values θ^0. $i = 0$

2. Until convergence is detected, iterate through
   - Generate a candidate $\theta^* \sim q(\theta|\theta^i)$.
   - If $p_\theta(\theta^i)q(\theta^i \mid \theta^*) > 0$, $\alpha(\theta^i, \theta^*) = \min\left(\frac{p_\theta(\theta^*)q(\theta^*|\theta^i)}{p_\theta(\theta^i)q(\theta^i|\theta^*)}, 1\right)$;
   - else, $\alpha(\theta^i, \theta^*) = 1$.
   - Do

$$\theta^{i+1} = \begin{cases} \theta^* & \text{with prob } \alpha(\theta^i, \theta^*), \\ \theta^i & \text{with prob } 1 - \alpha(\theta^i, \theta^*) \end{cases}$$

   - $i = i + 1$.

Convergence

Kernel $p_{MH}(\theta^n, \theta^{n+1}) = q(\theta^n, \theta^{n+1})\alpha(\theta^n, \theta^{n+1})$, if $\theta^n \neq \theta^{n+1}$, and $1 - \int q(\theta^n, z)\alpha(\theta^n, z)dz$, otherwise.

Proposition 44 *The following hold:*

1. *If q is aperiodic, p_{MH} is aperiodic.*
2. *If q is p_{MH}-irreducible and $q(\theta^n, \theta^{n+1}) = 0$ iff $q(\theta^{n+1}, \theta^n) = 0$, p_{MH} is p_θ irreducible.*

Hybrid algos

Typical situation

Frequently

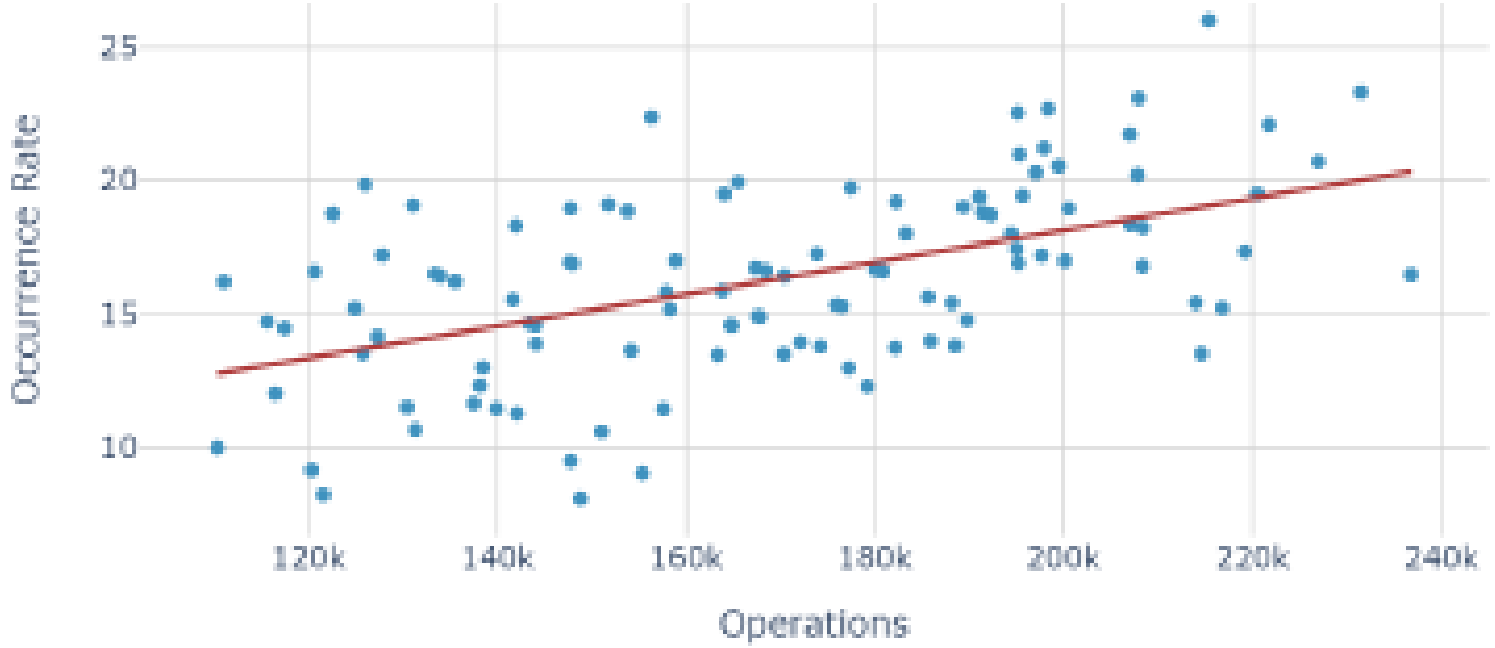
1. Some posterior conditionals available for efficient sampling
2. For others, just known up to a constant

Hybrid samplers

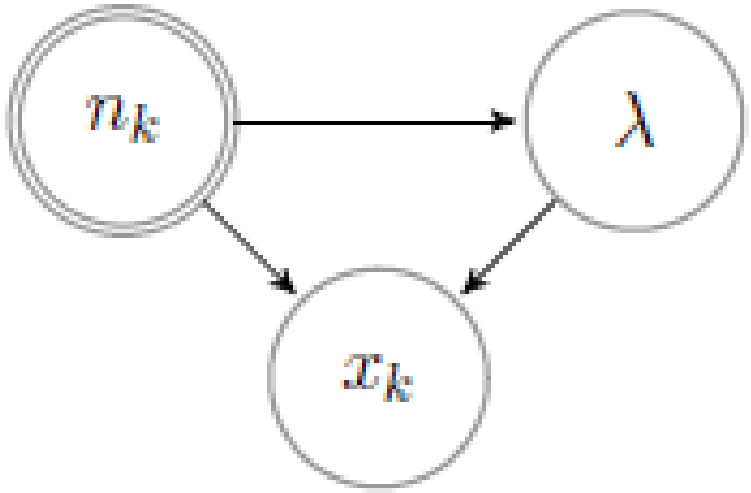
- Gibbs steps for type 1 conditionals
- MH steps for type 2 conditionals

Cse study: Aviation safety

Development of National Aviation Safety Plan. TCAS warnings



Aviation safety. Stress effect



$$x_k|\lambda, n_k \sim Po(\lambda n_k),$$

$$\lambda = an_k + b + \epsilon_k, \quad \epsilon_k \sim N(0, \sigma^2),$$

$$a \sim N(\mu_a, \sigma_a^2), \quad b \sim N(\mu_b, \sigma_b^2), \quad \sigma^2 \sim Inv\text{-}Gamma(\alpha, \beta)$$

Aviation safety. Stress effect

Posterior proportional to

$$\lambda^{\sum_{i=1}^{k-1} x_i} \sigma^{-3-2\alpha} \exp\left(-\lambda \sum_{i=1}^{k-1} n_i - \frac{(\lambda - a n_k - b)^2}{2\sigma^2} - \frac{(a-\mu_a)^2}{2\sigma_a^2} - \frac{(b-\mu_b)^2}{2\sigma_b^2} - \frac{\beta}{\sigma^2} \right)$$

Posterior conditionals

$$\begin{aligned}
p(a|\lambda, b, \sigma^2, D_k) &\sim N\left(a \,\middle|\, \frac{\sigma^2\mu_a + n_k\sigma_a^2(\lambda - b)}{\sigma^2 + n_k\sigma_a^2}, \frac{\sigma^2}{n_k^2 + \sigma^2/\sigma_a^2}\right), \\
p(b|\lambda, a, \sigma^2, D_k) &\sim N\left(b \,\middle|\, \frac{\sigma^2\mu_b + \sigma_b^2(\lambda - a n_k)}{\sigma^2 + \sigma_b^2}, \frac{1}{1/\sigma_b^2 + 1/\sigma^2}\right), \\
p(\sigma^2|\lambda, a, b, D_k) &\sim \textit{Inv-Gamma}\left(\sigma^2 \,\middle|\, \alpha + \frac{1}{2}, \beta + \frac{1}{2}(b + a n_k - \lambda)^2\right), \\
p(\lambda|a, b, \sigma^2, D_k) &\propto \lambda^{\sum x_i} \exp\left(-\frac{1}{2\sigma^2}\left(\lambda^2 - 2\lambda\left(a n_k + b - \sigma^2 \sum n_i\right)\right)\right).
\end{aligned}$$

Aviation safety. Stress effect algo

Algorithm 1: MCMC sampler for *Stress Effect* model

Set $a_0, b_0, \lambda_0, \sigma_0^2, j = 1$;

while *convergence not detected* **do**

Sample $\sigma_j^2 \sim \textit{Inv-Gamma}\left(\alpha + \frac{1}{2}, \beta + \frac{1}{2}(b_{j-1} + a_{j-1}n_k - \lambda_{j-1})^2\right)$;

Sample $b_j \sim N\left(\frac{\sigma_j^2\mu_b + \sigma_b^2(\lambda_{j-1} - a_{j-1}n_k)}{\sigma_j^2 + \sigma_b^2}, \frac{1}{1/\sigma_b^2 + 1/\sigma_j^2}\right)$;

Sample $a_j \sim N\left(\frac{\sigma_j^2\mu_a + n_k\sigma_a^2(\lambda_{j-1} - b_j)}{\sigma_j^2 + n_k\sigma_a^2}, \frac{\sigma_j^2}{n_k^2 + \sigma_j^2/\sigma_a^2}\right)$;

Sample $\lambda_j^* \sim q(\lambda_{j-1})$;

$Ga\left(1 + \sum_{i=1}^{k-1} x_i, \frac{\lambda}{2\sigma^2} + \sum_{i=1}^{k-1} n_i\right)$

Calculate $\alpha = \min\left(1, \frac{\pi(\lambda_j^*)}{\pi(\lambda_{j-1})}\frac{q(\lambda_{j-1})}{q(\lambda_j^*)}\right)$;

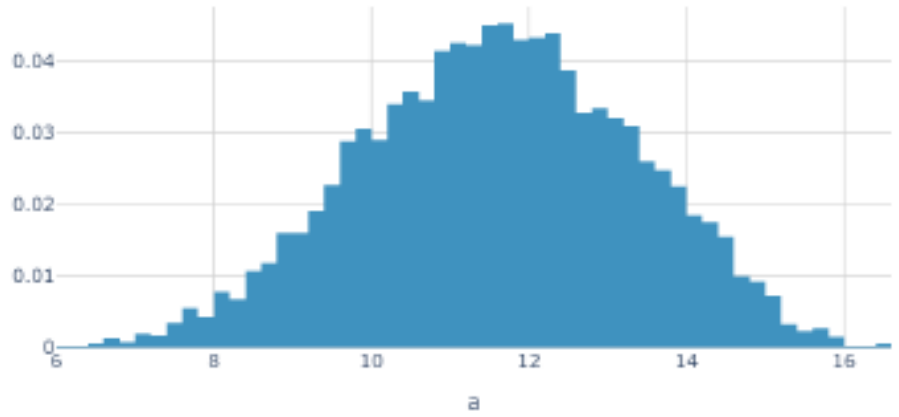
Do $\lambda_j = \begin{cases} \lambda_j^* & \text{with probability } \alpha \\ \lambda_{j-1} & \text{with probability } (1-\alpha) \end{cases}$;

$j \leftarrow j + 1$;

Aviation safety. Uses

$$Pr(x_k = z|D_k) = \iiint\!\!\!\int Pr(x_k = z|\lambda, n_k)\, p(\lambda|a, b, \sigma^2, D_k)\, p(a, b, \sigma^2|D_k)\, d\lambda\, da\, db\, d\sigma^2$$

$$\approx \frac{1}{N}\sum_{j=1}^{N} Pr(x_k = z|\lambda_j, n_k) = \frac{n_k^z}{N z!}\sum_{j=1}^{N} \exp(-\lambda_j n_k)\,(\lambda_j)^z\,,$$



Comments

Gibbs requires more analysis. Not always feasible

Metropolis requires less analysis. Not so fast. More automatic

Recall potentially severe autocorrelation problems, slow mixing, convergence,…

c. Hamiltonian Monte Carlo I

Brief description

We have introduced MCMC, Gibbs sampling and Metropolis-Hastings

We focus here on Hamiltonian Monte Carlo HMC

Sources

Sources:

- BDA3 (2015) 12.4 and 12.5
- Thomas and Tu. Learning HMC in R
- Betancourt. A conceptual intro to HMC
- Neal. MCMC using Hamiltonian dynamics

Labs

3.3 Hamiltonian MC

Multivariate normal

Hmclearn: Linear regression, Logistic regression (ecology)

Stan in later sessions!!

Hamiltonian MC. Basics

HMC. Pros and cons

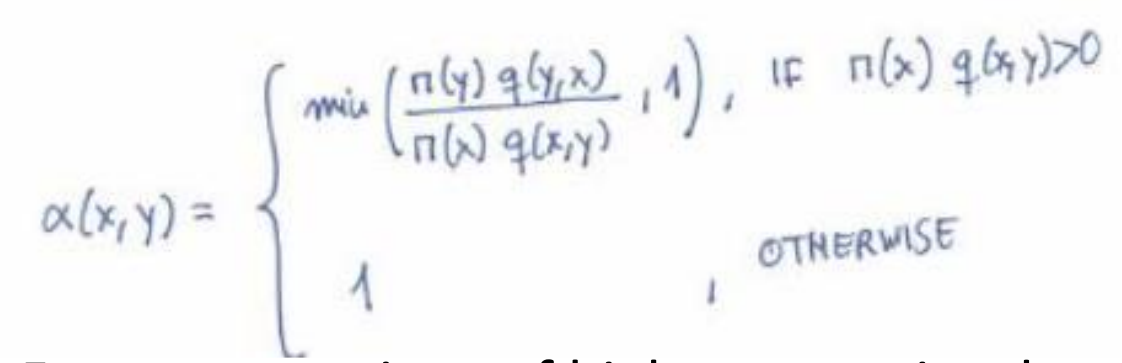
- Improved computational efficiency over MH et al (specially in high dimensional complex problems)

- Difficulties in implementation…. But Stan is available now: automates tuning of HMC parameters (and can be called from R and Python)
- But Stan a bit of a black box, hmclearn+this session before going through it

- Still insufficient for Bayesian analysis of deep learning models… soon

The drawback of MH

Balance condition in MH and M algos. Current x, proposed y



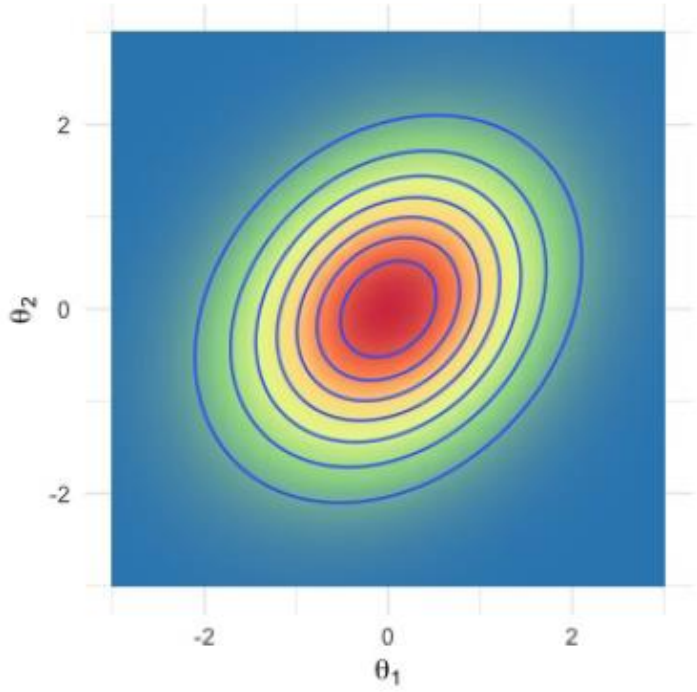
Frequents regions of higher posterior density. Sample from the right region

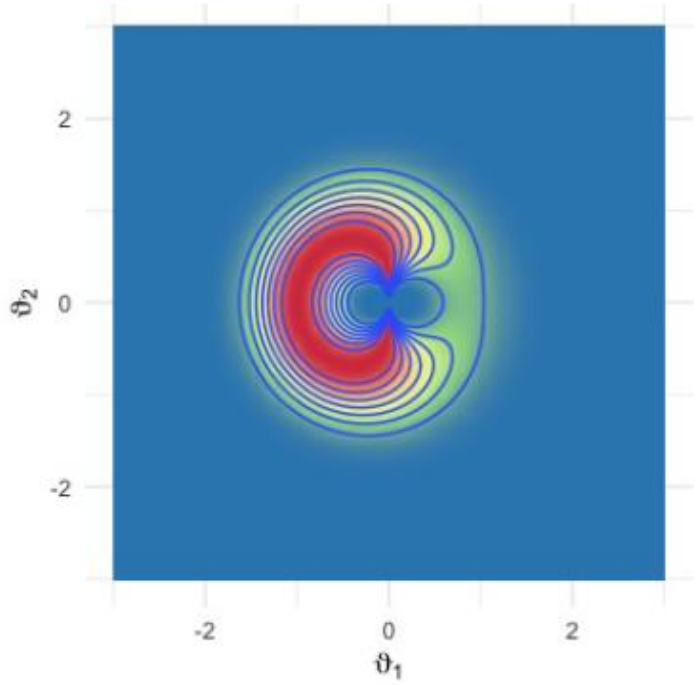
Ocasionally visits low density regions. Fully explore the sample space

As proposals are random, may take quite some time to get in HPD regions

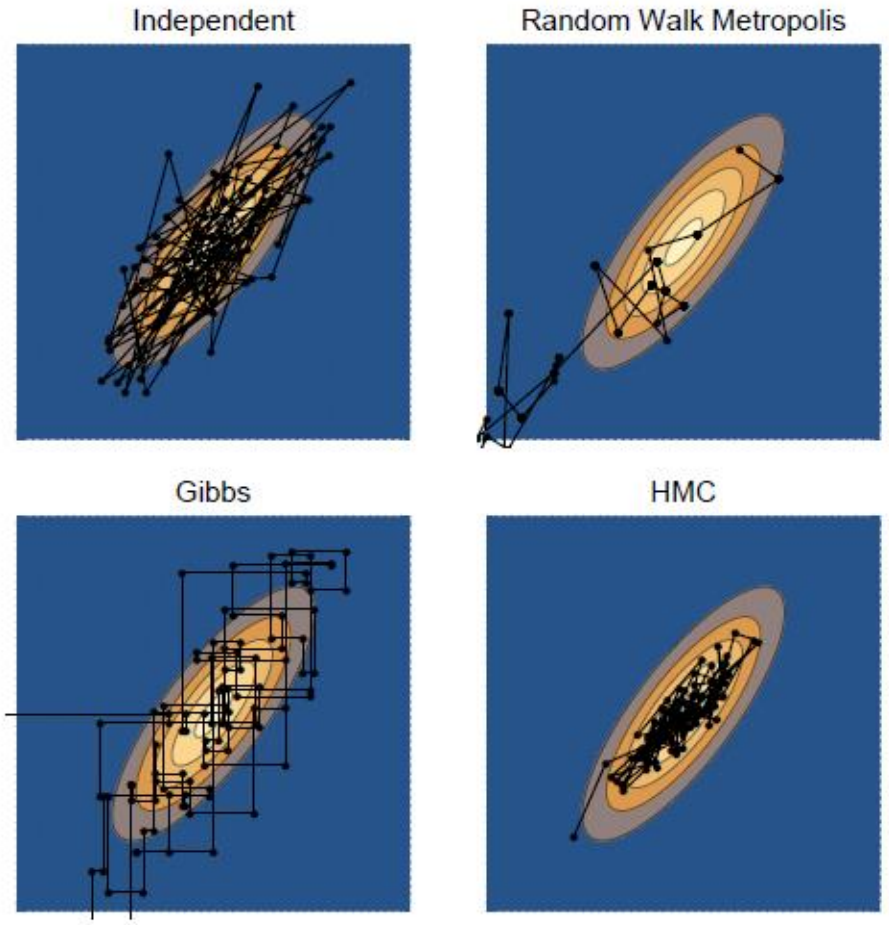
May get stuck

The drawback of MH





Comparing four MCMC algos



HMC. Qualitative description

- A guided proposal generation scheme

- Uses the gradient of log posterior to direct MC towards HPD regions:

A well-tuned HMC accepts proposals at much higher rate than MH

- But still samples the tails properly

HMC. Idea

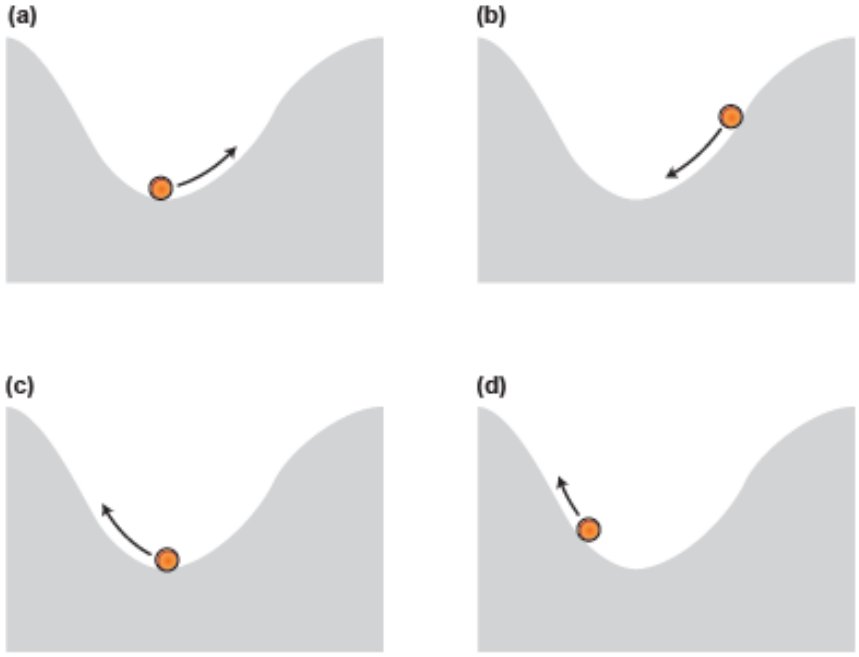
f is the posterior

-log (f) inverse bell-shaped

lower values reached guided by its gradient

In classical mechanics, exchanges between kinetic and potential energy dictate location through hamiltonian equations

(θ, p) horizontal and vertical positions. p is a momentum (auxiliary variable to actually simulate from θ) mass x velocity



Hamiltonian equations and MCMC

Target is posterior. Auxiliary momentum (same dimension)

$$\theta \sim f(\theta) \qquad \dim(\theta) = \dim(\rho)$$

Hamiltonian as potential + kinetic

$$H(\theta, \rho) = U(\theta) + K(\rho)$$

$$U(\theta) = -\log f(\theta) \qquad \rho \sim N(0, M)$$

$$H(\theta, \rho) = -\log f(\theta) + \frac{1}{2} \rho^T M^{-1} \rho$$

Hamiltonian equations

$$\left.\begin{aligned} \frac{d\rho}{dt} &= -\frac{\partial H(\theta,\rho)}{\partial \theta} = \nabla_\theta \log f(\theta) \\ \frac{d\theta}{dt} &= \frac{\partial H(\theta,\rho)}{\partial \rho} = M^{-1} \rho \end{aligned}\right\} (\theta, \rho)$$

Hamiltonian equations through leapfrog

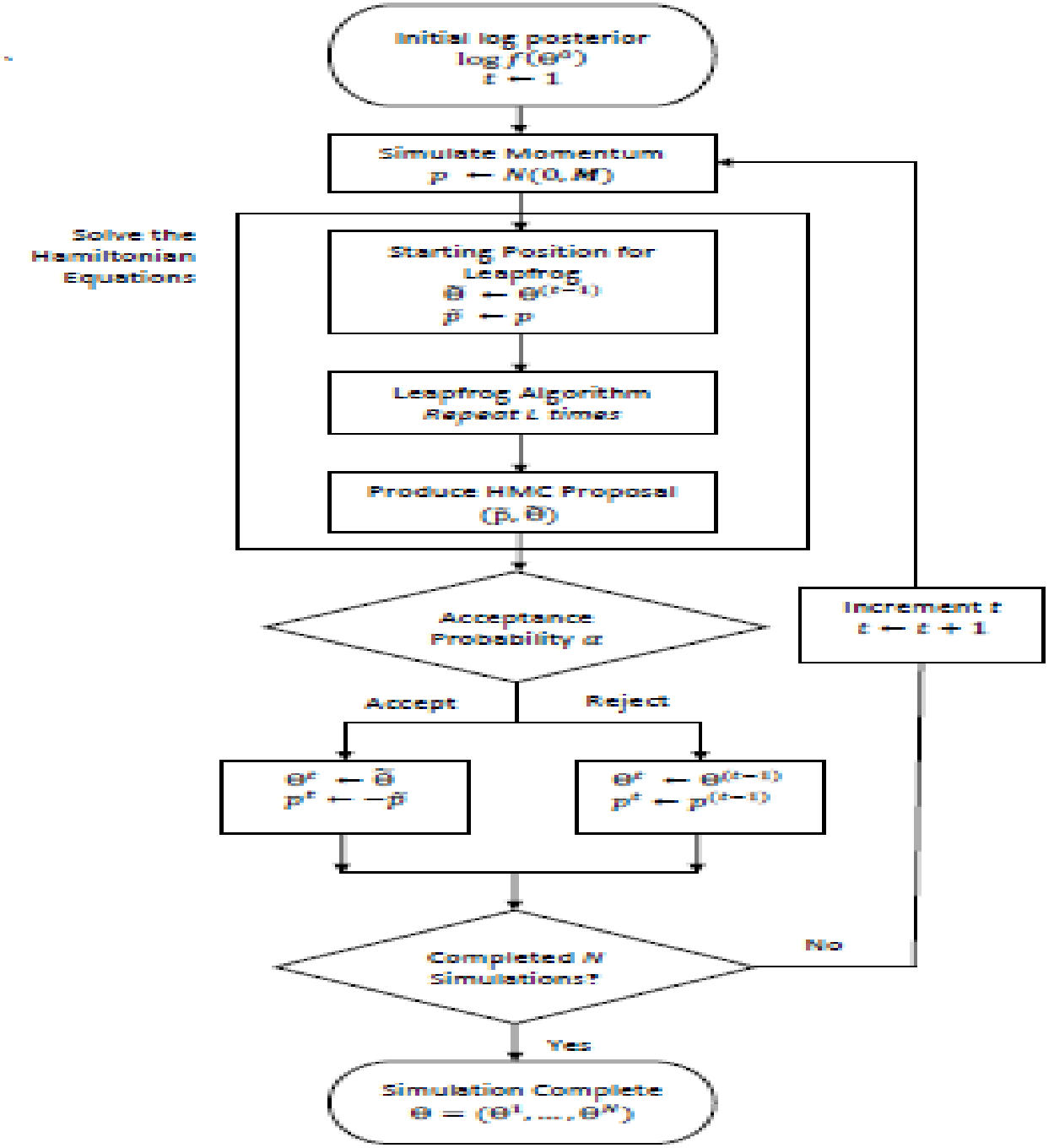
$$\frac{dp}{dt} = -\frac{\partial H(\theta,p)}{\partial \theta} = \nabla_\theta \log f(\theta) \qquad \frac{d\theta}{dt} = \frac{\partial H(\theta,p)}{\partial p} = M^{-1} p \quad \Big\} (\theta, p)$$

$$\mathbf{p}(t+\epsilon/2) = \mathbf{p}(t) + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}(t)),$$

$$\boldsymbol{\theta}(t+\epsilon) = \boldsymbol{\theta}(t) + \epsilon \mathbf{M}^{-1}\mathbf{p}(t+\epsilon/2),$$

$$\mathbf{p}(t+\epsilon) = \mathbf{p}(t+\epsilon/2) + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}(t+\epsilon)).$$

HMC. Algo I


Initial log posterior
$\log f(\theta^0)$
$t \leftarrow 1$
Simulate Momentum
$p \leftarrow N(0, M)$
Solve the Hamiltonian Equations
Starting Position for Leapfrog
$\bar{\theta} \leftarrow \theta^{(t-1)}$
$\bar{p} \leftarrow p$
Leapfrog Algorithm
Repeat L times
Produce HMC Proposal
$(\bar{p}, \bar{\theta})$
Acceptance Probability α
Increment t
$t \leftarrow t + 1$
Accept
Reject
$\theta^t \leftarrow \bar{\theta}$
$p^t \leftarrow -\bar{p}$
$\theta^t \leftarrow \theta^{(t-1)}$
$p^t \leftarrow p^{(t-1)}$
Completed N Simulations?
No
Yes
Simulation Complete
$\theta = (\theta^1, \ldots, \theta^N)$

HMC. Algo II

procedure HMC($\boldsymbol{\theta}^{(0)}, \log f(\boldsymbol{\theta}), \mathrm{M}, N, \epsilon, L$)

Calculate $\log f(\boldsymbol{\theta}^{(0)})$

for $t = 1, ..., N$ **do**

$\mathrm{p} \leftarrow N(0, \mathrm{M})$

$\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\mathrm{p}} \leftarrow \mathrm{p}$

for $i = 1, ..., L$ **do**

$\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}} \leftarrow \mathrm{Leapfrog}(\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}}, \epsilon, \mathrm{M})$

end for

$\alpha \leftarrow \min\left(1, \frac{\exp(\log f(\bar{\boldsymbol{\theta}}) - \frac{1}{2}\bar{\mathrm{p}}^T \mathrm{M}^{-1} \bar{\mathrm{p}})}{\exp(\log f(\boldsymbol{\theta}^{(t-1)}) - \frac{1}{2}\mathrm{p}^T \mathrm{M}^{-1} \mathrm{p})}\right)$

With probability α, $\boldsymbol{\theta}^{(t)} \leftarrow \bar{\boldsymbol{\theta}}$ and $\mathrm{p}^{(t)} \leftarrow -\bar{\mathrm{p}}$

end for

return $\boldsymbol{\theta}^{(1)}, ..., \boldsymbol{\theta}^{(N)}$

function LEAPFROG($\boldsymbol{\theta}^*, \mathrm{p}^*, \epsilon, \mathrm{M}$)

$\bar{\mathrm{p}} \leftarrow \mathrm{p}^* + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}^*)$

$\bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^* + \epsilon \mathrm{M}^{-1} \bar{\mathrm{p}}$

$\bar{\mathrm{p}} \leftarrow \bar{\mathrm{p}} + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\bar{\boldsymbol{\theta}})$

return $\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}}$

end function

end procedure

HMC Tuning

Step size. Small relative to parameter of interest

x Number of leapfrog steps. Large L.

Jointly acceptance rate of 65%

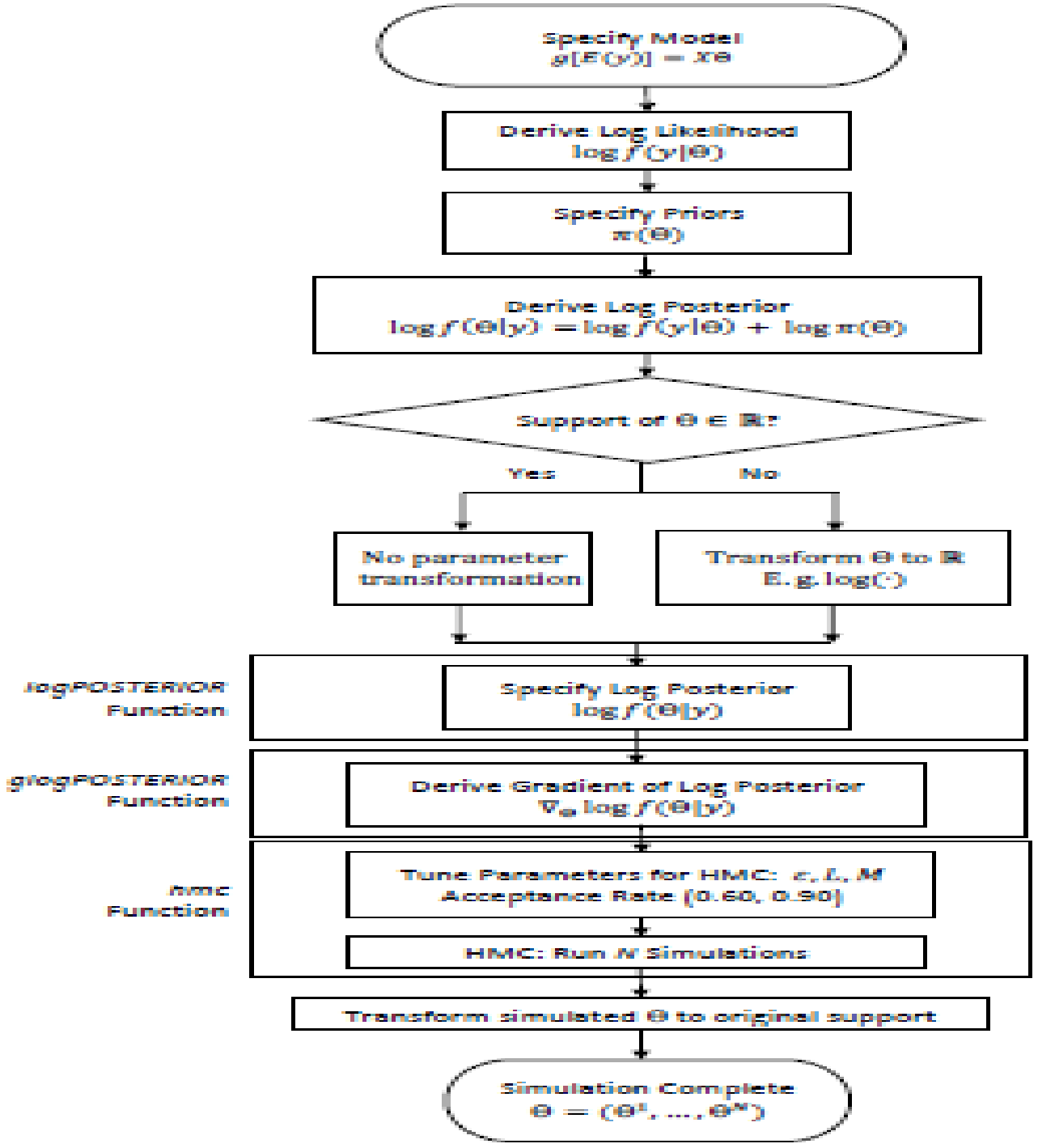
Examine for correlations

Adaptively select L as in No U-turn Sampler (NUTS) . To be seen with Stan

Covariance matrix M

Hamiltonian MC. Examples

Typical setup



Sampling the bi-variate normal

Simple example to recall approach

Model. Bivariate normal with unknown means. Variances 1. Known correlation ϱ

1 observation

Prior. Uniform

Use. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

Sampling the bi-variate normal. Model and posterior

$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\,\pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)'\,\Sigma^{-1}(y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)'\,\Sigma^{-1}(\theta-y)\right)$$

$$\theta | y \sim N(y, \Sigma)$$

Sampling the bi-variate normal. Gibbs sampler

$$\theta_1 | \theta_2, y \sim N(y_1 + \rho(\theta_2 - y_2), 1 - \rho^2)$$
$$\theta_2 | \theta_1, y \sim N(y_2 + \rho(\theta_1 - y_1), 1 - \rho^2)$$

θ_2^0 ARBITRARY, $i = 1$

UNTIL CONVERGENCE

$$\theta_1^i \sim N(y_1 + \rho(\theta_2^{i-1} - y_2), 1 - \rho^2)$$
$$\theta_2^i \sim N(y_2 + \rho(\theta_1^i - y_1), 1 - \rho^2)$$
$$i = i + 1$$

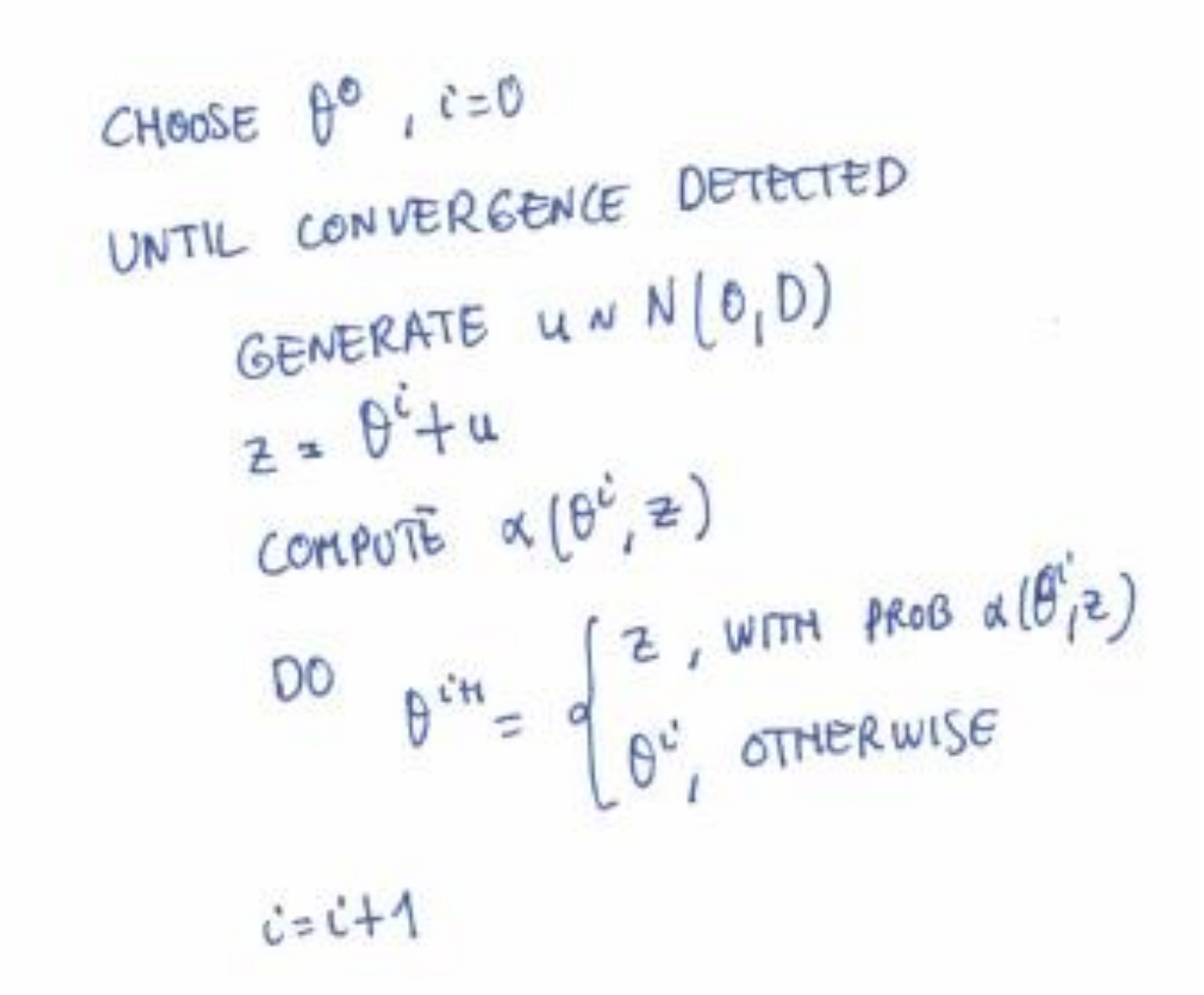
Sampling the bi-variate normal. Metropolis Hastings

$$\alpha(\theta, z) = \min\left\{ \frac{\exp\left(-\frac{1}{2}(z-\mu)' \Sigma^{-1} (z-\mu)\right)}{\exp\left(-\frac{1}{2}(\theta-\mu)' \Sigma^{-1} (\theta-\mu)\right)}, 1 \right\}$$

$$= \min\left\{ \frac{\exp\left(-\frac{1}{2}\left(z' \Sigma^{-1} z\right) - 2 z \Sigma^{-1} \mu\right)}{\exp\left(-\frac{1}{2}\left(\theta' \Sigma^{-1} \theta\right) - 2 \theta \Sigma^{-1} \mu\right)}, 1 \right\}$$

$$z = \theta + u \qquad u \sim N(0, D)$$

Sampling the bi-variate normal. Metropolis Hastings



Sampling the bi-variate normal. Hamiltonian MC

procedure HMC($\boldsymbol{\theta}^{(0)}, \log f(\boldsymbol{\theta}), \mathbf{M}, N, \epsilon, L$)
  Calculate $\log f(\boldsymbol{\theta}^{(0)})$
  for $t = 1, ..., N$ **do**
    $\mathbf{p} \leftarrow N(0, \mathbf{M})$
    $\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\mathbf{p}} \leftarrow \mathbf{p}$
    for $i = 1, ..., L$ **do**
      $\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}} \leftarrow \text{Leapfrog}(\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}}, \epsilon, \mathbf{M})$
    end for
    $\alpha \leftarrow \min\left(1, \frac{\exp(\log f(\bar{\boldsymbol{\theta}}) - \frac{1}{2}\bar{\mathbf{p}}^T\mathbf{M}^{-1}\bar{\mathbf{p}})}{\exp(\log f(\boldsymbol{\theta}^{(t-1)}) - \frac{1}{2}\mathbf{p}^T\mathbf{M}^{-1}\mathbf{p})}\right)$
    With probability α, $\boldsymbol{\theta}^{(t)} \leftarrow \bar{\boldsymbol{\theta}}$ and $\mathbf{p}^{(t)} \leftarrow -\bar{\mathbf{p}}$
  end for
  return $\boldsymbol{\theta}^{(1)}, ..., \boldsymbol{\theta}^{(N)}$
  function LEAPFROG($\boldsymbol{\theta}^*, \mathbf{p}^*, \epsilon, \mathbf{M}$)
    $\bar{\mathbf{p}} \leftarrow \mathbf{p}^* + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}^*)$
    $\bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^* + \epsilon\mathbf{M}^{-1}\bar{\mathbf{p}}$
    $\bar{\mathbf{p}} \leftarrow \bar{\mathbf{p}} + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\bar{\boldsymbol{\theta}})$
    return $\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}}$
  end function
end procedure

$\theta | y \sim N(y, \Sigma)$

$\log(f(\theta)) \propto -\frac{1}{2}(\theta - y)' \Sigma^{-1} (\theta - y)$

$-\log(f(\theta)) \propto \frac{1}{2}(\theta - y)' \Sigma^{-1} (\theta - y)$

$-\nabla_\theta (\log(f(\theta))) \propto (\theta - y)' \Sigma^{-1}$

Sampling the bi-variate normal. Hamiltonian MC. Bonus

$$H(\theta, p) = \frac{1}{2}(\theta - \gamma)^t \Sigma^{-1}(\theta - \gamma) + \frac{1}{2} p^t M^{-1} p$$

$$\frac{dp}{dt} = -\frac{\partial H(\theta, p)}{\partial \theta} = (\theta - \gamma)^t \Sigma^{-1}$$

$$\frac{d\theta}{dt} = \frac{\partial H(\theta, p)}{\partial p} = M^{-1} p$$

$$p(t + \tfrac{\varepsilon}{2}) = p(t) + \frac{\varepsilon}{2}(\gamma - \theta(t))^t \Sigma^{-1}$$

$$\theta(t + \varepsilon) = \theta(t) + \varepsilon M^{-1} p(t + \varepsilon/2)$$

$$p(t + \varepsilon) = p(t + \tfrac{\varepsilon}{2}) + \frac{\varepsilon}{2}(\gamma - \theta(t + \tfrac{\varepsilon}{2}))^t \Sigma^{-1}$$

Sampling the bi-variate normal. Answers (Whatever the method used)

$$\hat{E}(\theta_1 | y) = \frac{1}{K} \sum_{i=1}^{K} \theta_1^{M+i}$$

$$\hat{E}(\theta_1 \theta_2 | y) = \frac{1}{K} \sum_{i=1}^{K} \left(\theta_1^{M+i} \; \theta_2^{M+i} \right)$$

$$Pr(\theta_1 \in A | y) = \frac{\#\{ \theta_1^{M+i} \in A \}}{K}$$

Linear regression model

$$y_i = x_i^t \beta + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2) \quad i = 1, \dots, n$$

$$y = (y_1, \dots, y_n)$$

$$X = (x_1^t, \dots, x_n^t)$$

$$\log f(y \mid \beta, \sigma^2) \propto -n \log \sigma - \frac{1}{2\sigma^2} (y - X^t\beta)(y - X\beta)$$

Normal Prior for weights

$$f(\beta \mid \sigma_\beta^2) \propto \exp\left(-\frac{\beta^t \beta}{2\sigma_\beta^2}\right)$$

$$f(\sigma_\varepsilon^2 \mid a, b) = \frac{b^a}{\Gamma(a)} (\sigma_\varepsilon^2)^{-a-1} \exp\left(-\frac{b}{\sigma_\varepsilon^2}\right)$$

Inv-gamma prior for variance

$$\gamma = \log \sigma_\varepsilon^2 \qquad \sigma_\varepsilon^2 = e^\gamma$$

$$f(\gamma \mid a, b) = \frac{b^a}{\Gamma(a)} \exp\left(-a\gamma - \frac{b}{e^\gamma}\right)$$

$$\log\left(f(\gamma \mid a, b)\right) \propto -a\gamma - b e^{-\gamma}$$

Linear regression model

$$\log f(\beta, \sigma | y, X, \sigma_\beta^2, a, b) \propto -\left(\frac{n}{2} + a\right)\sigma - \frac{e^{-\sigma}}{2}(y - X\beta)^t(y - X\beta) - \frac{\beta^t\beta}{2\sigma_\beta^2} - be^{-\sigma}$$

$$\nabla_\beta \log f(\beta, \sigma | y, X, \sigma_\beta^2, a, b) \propto e^{-\sigma} X^T (y - X\beta) - \beta/\sigma_\beta^2$$

$$\nabla_\sigma \log f(\beta, \sigma | y, X, \sigma_\beta^2, a, b) \propto -\left(\frac{n}{2} + a\right) + \frac{e^{-\sigma}}{2}(y - X\beta)^T (y - X\beta) + be^{-\sigma}$$

Logistic regression model

$$P(y_i = 1 \mid x_i, \beta) = \frac{1}{1 + \exp(-x_i^t \beta)}$$

$$X = (x_1^t, \dots, x_n^t)^t \qquad \beta = (\beta_0, \dots, \beta_p)$$

$$\log f(y \mid X, \beta) = \beta^T X^T (y - 1_n) - 1_n^t \left(\log\left(1 + e^{-x_i \beta}\right)\right)_{n \times 1}$$

$$\beta \sim N(0, \sigma_\beta^2 I)$$

Logistic regression model

$$\log f(\beta \mid y, X, \sigma_\beta^2) \propto \beta^T X^T (y - 1_n) - 1_n^t \left(\log\left(1 + e^{-x_i^t \beta}\right) \right)_{n \times 1} - \frac{\beta^T \beta}{2\sigma_\beta^2}$$

$$\nabla_\beta \log f(\beta \mid y, X, \sigma_\beta^2) \propto X^T \left(y - 1_n + \left[\frac{e^{-x_i^t \beta}}{1 + e^{-x_i^t \beta}} \right]_{n \times 1} \right) - \beta / \sigma_\beta^2$$

Final comments

Final comments

Gibbs. Lots of hard prior work. Not always implementable. If so may work well.

Metropolis Hastings. Less prior work. Quite general. May work slowly.

Hamiltonian. Even less work. Quite general. Works more efficiently…. Yet suffers in large scale problems

More when introducing Stan

More when introducing SG-MCMC and Variational inference

See you in two weeks

introml@icmat.es for questions

Stuff at

https://datalab-icmat.github.io/courses_stats.html