Astrostatistics: Tue 27 Feb 2017

https://github.com/CambridgeAstroStat/PartIII-Astrostatistics

- Lecture Demo Codes are online in directory lecture_codes/
- Example Class 2: Friday, Mar 2, **2:00pm**, MR 5
- Fitting Statistical Models to Astronomical Data
    - Markov Chain Monte Carlo
    - Refs: Not much in Ivezic, Ch 5, F&B Ch 3
    - Gelman et al. Bayesian Data Analysis (Ch 11 & 12)
    - Givens & Hoeting. “Computational Statistics” (Ch 7 & 8)
    - Roberts & Casella. “Monte Carlo Statistical Methods” (theory) (Ch 6 & 7)
    - Hogg & DFM, 2017 “Data analysis recipes: Using Markov Chain Monte Carlo.” https://arxiv.org/abs/1710.06068

Plan

- Last Time: M-H algorithm, Gibbs sampling
- Today:
    - Metropolis-within-Gibbs
    - Theoretical Justifications
- Next time? Gaussian Processes

Remarks on Multivariate Gaussians Properties

- Last time: Conditionals and Marginals of Multivariate Gaussians
- Last time: Building Jointly Multivariate Gaussians from Conditional and Marginals
- Dimensions of Covariance Matrices

What if you can't directly sample the posterior: $\theta_i \sim P(\theta\,|D)$?

$$\mathbb{E}[f(\boldsymbol{\theta})|\, D] = \int f(\boldsymbol{\theta}) P(\boldsymbol{\theta}|\, D)\, d\boldsymbol{\theta} \approx \frac{1}{m}\sum_{i=1}^{m} f(\boldsymbol{\theta}_i)$$

- Posterior simulation - Markov Chain Monte Carlo:
- Generate a correlated sequence (chain) of random variates (Monte Carlo) that (in a long run limit) are draws from the posterior distribution. The next value in the sequence only depends on the current values (Markov).
- Many degrees of freedom for user: choose to most efficiently generate *independent* samples

d-dim Metropolis Algorithm: Posterior $P(\theta \,|D)$, Symmetric Proposal/Jump dist'n $J(\theta^*|\, \theta) = J(\theta|\, \theta^*)$

1. Choose a random starting point θ_0
2. At step i = 1…N, propose a new parameter value $\theta^* \sim N(\theta_{i-1}, \mathbf{\Sigma_p})$. The proposal distr'n is $J(\theta^*|\, \theta_{i-1}) = N(\theta^*|\, \theta_{i-1}, \mathbf{\Sigma_p})$
3. Evaluate ratio of posteriors at proposed vs current values. $r = P(\theta^* \mid \mathbf{y}) / P(\theta_{i-1} \mid \mathbf{y})$.
4. Accept θ^* with probability min(r,1): $\theta_i = \theta^*$. If not accept, stay at same value $\theta_i = \theta_{i-1}$ for the next step & include in chain.
5. Repeat steps 2-4 until reach some measure of convergence (G-R) and gather enough independent samples to compute your inference (reduce Monte Carlo error)

Metropolis-Hastings Algorithm: More General Jumping Rule: $J(\theta^*|\theta_i)$ (Need not be symmetric - if symmetric you have the special case of Metropolis)

1. Choose a random starting point θ_0

2. At step i = 1…N, propose a new parameter value: $\theta^* \sim J(\theta^*|\theta_{i-1})$

3. Evaluate ratio of posteriors at proposed vs current values.
   $r = [P(\theta^* \mid \mathbf{y}) / J(\theta^*|\theta_{i-1})] / [P(\theta_{i-1} \mid \mathbf{y}) / J(\theta_{i-1}|\theta^*)]$

4. Accept θ^* with probability min(r,1): $\theta_i = \theta^*$. If not accept, stay at same value $\theta_i = \theta_{i-1}$ & include in chain.

5. Repeat steps 2-4 until reach some measure of convergence and gather enough samples to compute your inference

Gibbs Sampling

- Multi-dimensional sampling, when you can utilise the set of conditional posterior distributions.
- If joint posterior is $P(\theta, \phi | \boldsymbol{D})$
- And you can solve for tractable conditionals:

$$P(\theta | \phi, \boldsymbol{D})$$

$$P(\phi | \theta, \boldsymbol{D})$$

- Jump along one parameter-dimension at a time

d-dim Gibbs Sampler

$$\boldsymbol{\theta} = (\theta_1 \dots \theta_d) \qquad \boldsymbol{\theta}_{-j} \equiv (\theta_1, \dots \theta_{j-1}, \theta_{j+1} \dots \theta_d)$$

1. Choose a random starting point θ_0

2. At step i = 1…N, cycle through the d-parameters:
   For each j = 1… d, move jth parameter to $\theta_j \sim P(\theta_j | \boldsymbol{\theta}^{i-1}_{-j}, \boldsymbol{D})$ and always accept.

   The proposal distr'n is $J(\boldsymbol{\theta}^* | \boldsymbol{\theta}^{i-1}) = P(\theta_j | \, \boldsymbol{\theta}_{-j}, \boldsymbol{D})$

3. The Metropolis-Hastings ratio is always 1 (don't need to compute)

4. Always accept θ_j^*.

5. Repeat steps 2-4 until reach some measure of convergence (G-R) and gather enough independent samples to compute your inference (reduce Monte Carlo error)

Gibbs Sampling: Example (Gelman BDA Section 11.1)

Likelihood: $$\boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \sim N\left(\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right)$$ ρ known

Priors: $$P(\theta_1) = P(\theta_2) \propto 1$$

Posterior: $$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \Big| \boldsymbol{y} \sim N\left(\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right)$$

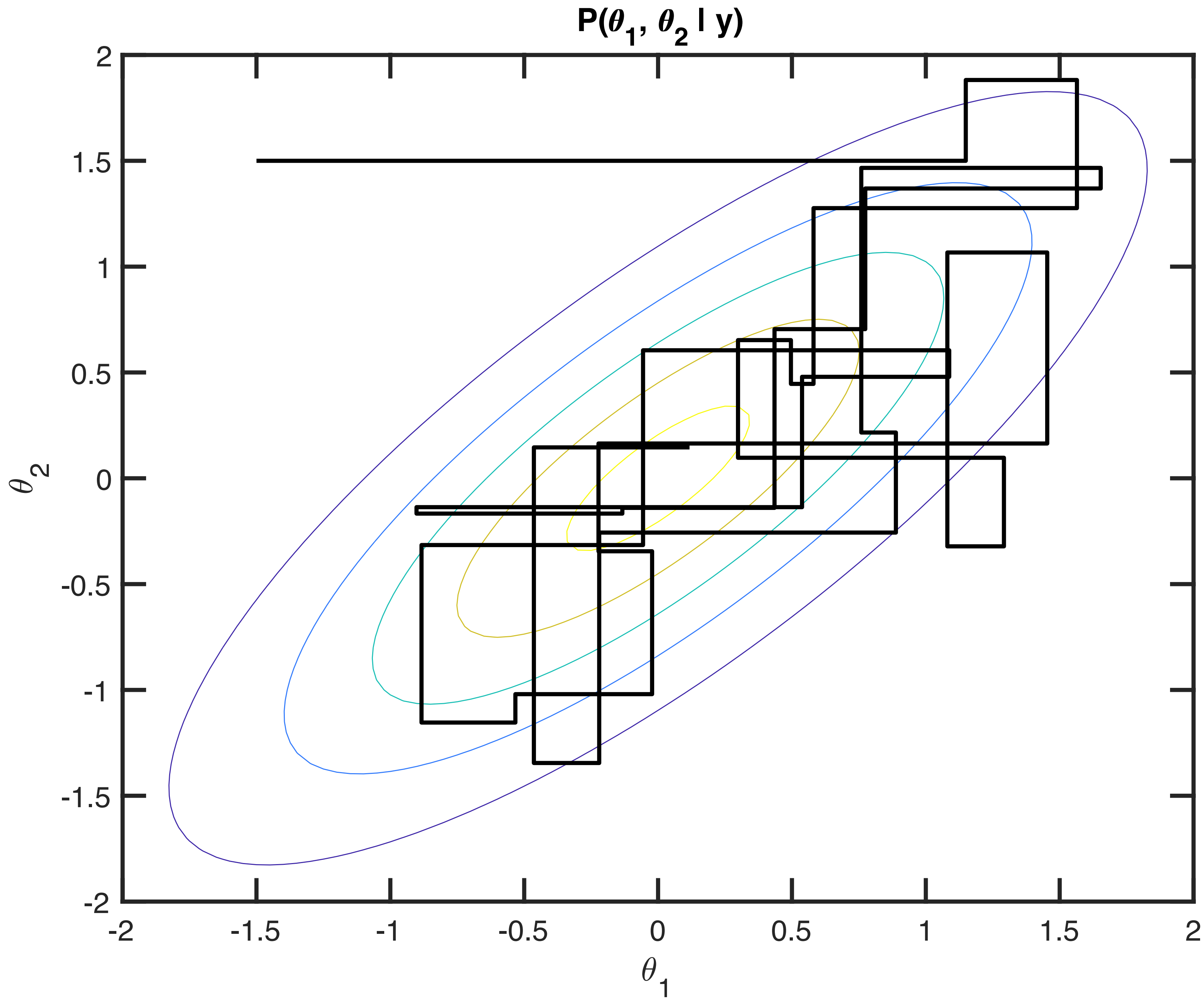
$$P(\boldsymbol{\theta}|y) = P(\theta_1|\theta_2, y)P(\theta_2|y) = P(\theta_2|\theta_1, y)P(\theta_1|y)$$

Conditional Posteriors:

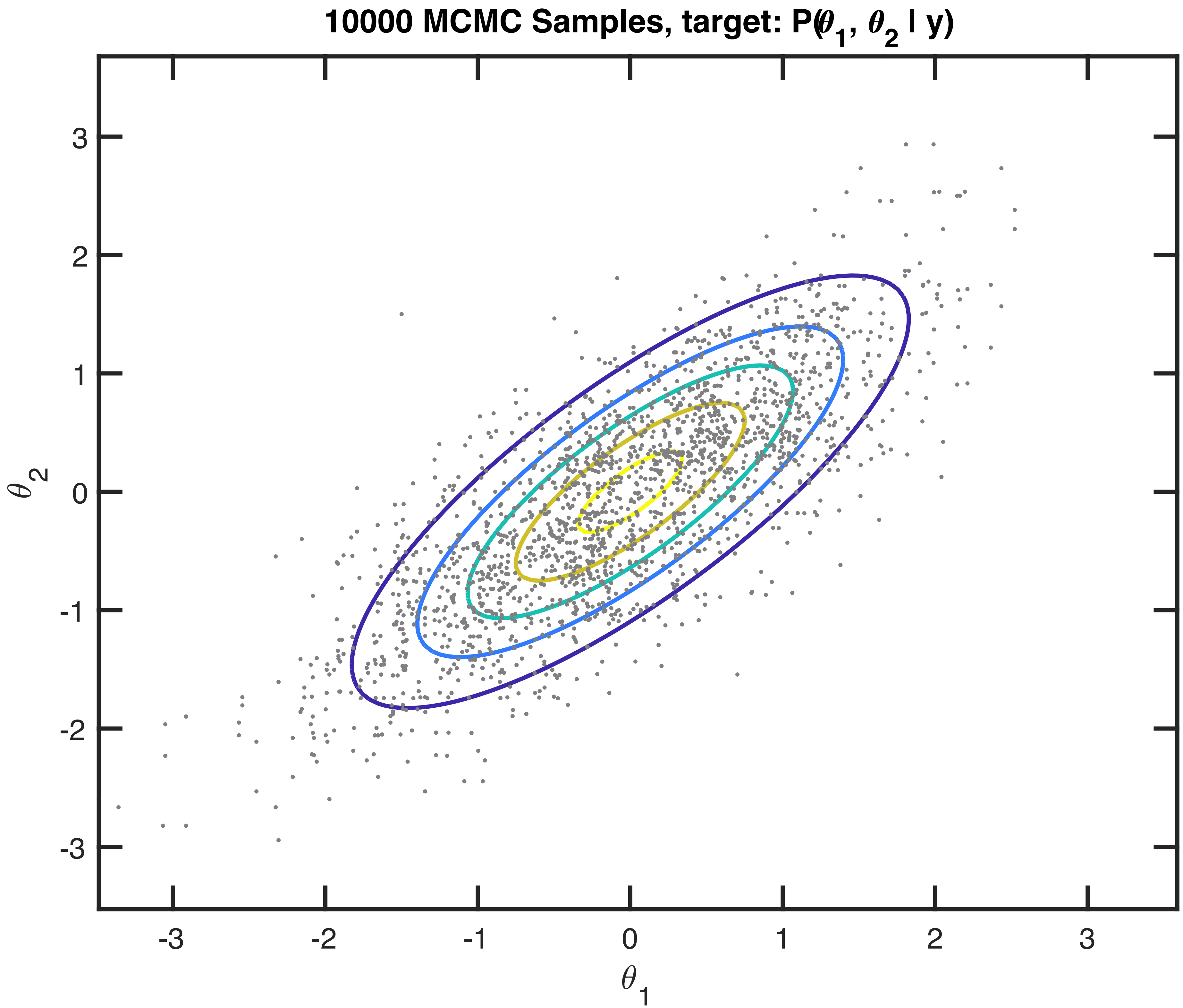
$$\theta_1|\theta_2, \boldsymbol{y} \sim N(y_1 + \rho(\theta_2 - y_2), 1 - \rho^2)$$

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

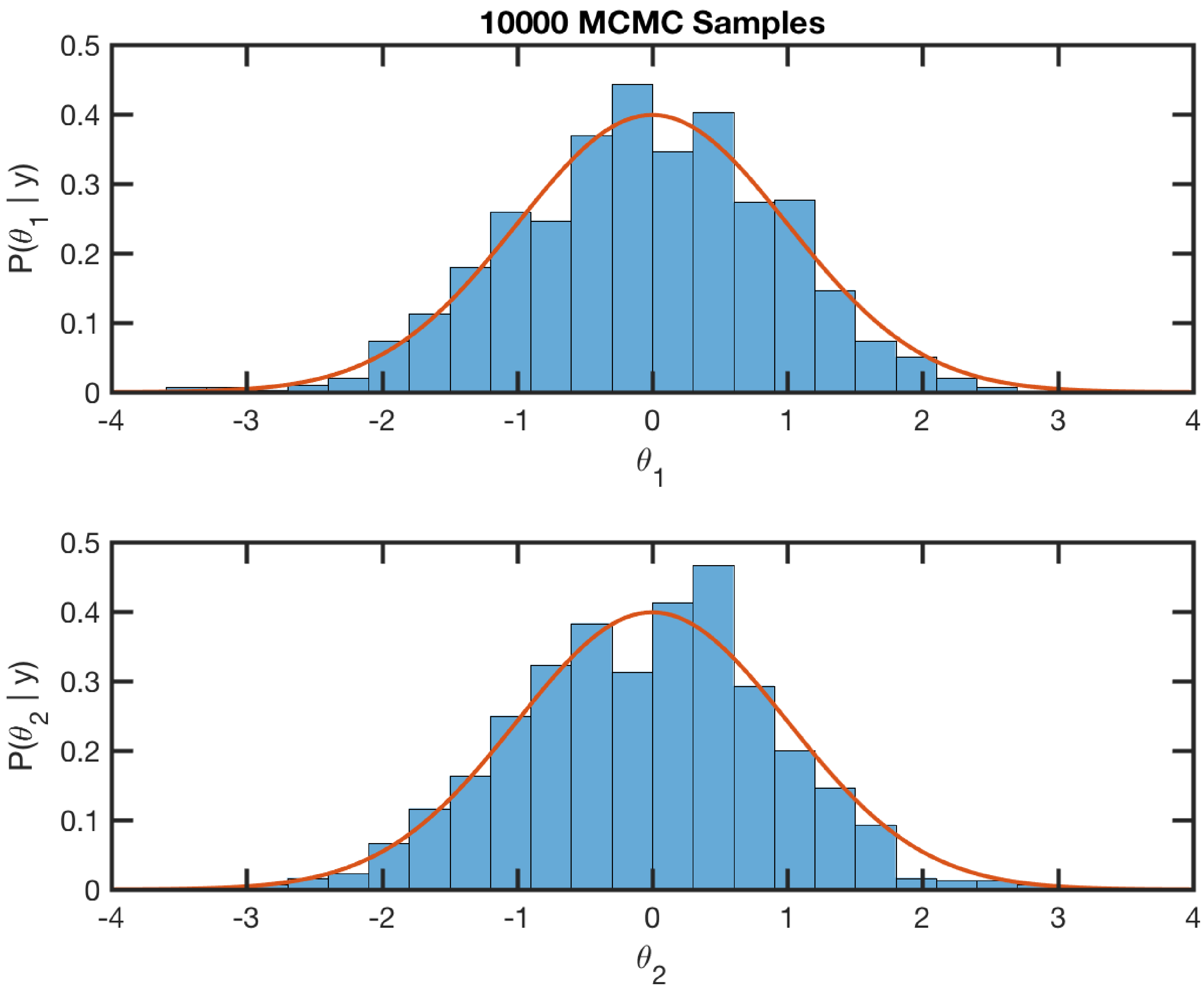
Gibbs Sampling: demo
gibbs_example.m
2D Trace Paths for 50 iterations



Gibbs Sampling: demo
gibbs_example.m
Joint Posterior Densities



Gibbs Sampling: demo
gibbs_example.m
Marginal Posterior Densities



Metropolis-within-Gibbs

$$\boldsymbol{\theta} = (\theta_1 \ldots \theta_d) \qquad \boldsymbol{\theta}_{-j} \equiv (\theta_1, \ldots \theta_{j-1}, \theta_{j+1} \ldots \theta_d)$$

- When you can't solve for tractable conditional distributions for all θ_j: $P(\theta_j | \boldsymbol{\theta}_{-j}, \boldsymbol{D})$
- Replace each substep for updating each jth parameter θ_j with a separate Metropolis rule, compute Metropolis ratio, and accept/reject
- Cycle through all parameters, and repeat all for N MCMC steps

d-dim Metropolis-within-Gibbs Sampler

$$\boldsymbol{\theta} = (\theta_1 \ldots \theta_d) \qquad \boldsymbol{\theta}_{-j} \equiv (\theta_1, \ldots \theta_{j-1}, \theta_{j+1} \ldots \theta_d)$$

1. Choose a random starting point θ_0
2. At step i = 1…N, cycle through the d-parameters:
   1. For each j = 1… d, propose a new jth parameter from a 1-Dimensional Gaussian: $\theta_j^* \sim N(\theta_j^{i-1}, \tau^2)$
   2. Evaluate ratio of posteriors at proposed vs current values:

$$r = P(\theta_j^*, \boldsymbol{\theta}_{-j}^{i-1} | \boldsymbol{y}) / P(\boldsymbol{\theta}^{i-1} | \boldsymbol{y}) = P(\theta_j^* | \boldsymbol{\theta}_{-j}^{i-1}, \boldsymbol{y}) / P(\theta_j^{i-1} | \boldsymbol{\theta}_{-j}^{i-1}, \boldsymbol{y})$$

   3. Accept $\theta_j^i = \theta_j^*$ with probability min(r,1), otherwise $\theta_j^i = \theta_j^{i-1}$
3. Repeat steps 2 for all parameters until reach some measure of convergence (G-R) and gather enough independent samples to compute your inference (reduce Monte Carlo error)

Metropolis-within-Gibbs Sampling: Example: Gelman BDA Section 11.1)

Likelihood: $$\boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \sim N\left(\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right) \qquad \rho \text{ known}$$

Priors: $$P(\theta_1) = P(\theta_2) \propto 1$$

Posterior: $$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \Big| \boldsymbol{y} \sim N\left(\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

Suppose we can't solve for the Conditional Posteriors.

Metropolis-within-Gibbs Sampling: Code Demo metropolisgibbs_example.m

A sketch of Markov Chain Theory

- See Robert & Casella “Monte Carlo Statistical Methods” Chapter 6 “Markov Chains” for the technical details

- Existence of a stationary limiting distribution (irreducible, aperiodic).

- The target distribution (posterior) is the invariant, stationary distribution under your chosen transition probabilities