Gibbs sampling

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Announcements

- Homework 4 due tomorrow.

Outline

- Non-conjugate priors
- Full conditionals
- Gibbs sampling
- A simple example: bivariate normal
- In-class exercise

Bayesian inference (conjugacy recap)

- As we've seen so far, Bayesian inference is based on posterior distributions, that is,

$$p(\theta|y) = \frac{p(\theta)L(y;\theta)}{\int_\Theta p(\tilde{\theta})L(y;\tilde{\theta})\mathrm{d}\tilde{\theta}} = \frac{p(\theta)L(y;\theta)}{L(y)}$$

- Good news: we have the numerator in this expression.
- Bad news: the denominator is typically not available (may involve high dimensional integral)!
- How have we been getting by? Conjugacy! For conjugate priors, the posterior distribution of θ is available analytically.
- What if a conjugate prior does not represent our prior information well, or we have a more complex model, and our posterior is no longer in a convenient distributional form?

Some conjugate models

- We've already seen the following conjugate models.

Prior	Likelihood	Posterior
beta	binomial	beta
gamma	Poisson	gamma
gamma	exponential	gamma
normal-gamma	normal	normal-gamma

- Here are a few more we have not covered yet.

Prior	Likelihood	Posterior
beta	negative-binomial	beta
beta	geometric	beta
Dirichlet	multinomial	Dirichlet

- Clearly, we cannot restrict ourselves to conjugate models only.

Back to the normal model

- For conjugacy in the normal model, we had

$$\mu|\tau \sim \mathcal{N}\left(\mu_0, \frac{1}{\kappa_0 \tau}\right).$$
$$\tau \sim \mathrm{Gamma}\left(\frac{\nu_0}{2}, \frac{\nu_0\sigma_0^2}{2}\right)$$

- Suppose we wish to specify our uncertainty about μ as independent of τ, that is, we want $\pi(\mu, \tau) = \pi(\mu)\pi(\tau)$. For example,

$$\mu \sim \mathcal{N}\left(\mu_0, \sigma_0^2\right).$$
$$\tau \sim \mathrm{Gamma}\left(\frac{\nu_0}{2}, \frac{\nu_0}{2\tau_0}\right).$$

- When σ_0^2 is not proportional to $\dfrac{1}{\tau}$, the marginal density of τ is not a gamma density (or a density we can easily sample from).

- Side note: for conjugacy, the joint posterior should also be a product of two independent Normal and Gamma densities in μ and τ respectively.

Non-conjugate priors

- In general, conjugate priors are not available for generalized linear models (GLMs) other than the normal linear model.
- One can potentially rely on an asymptotic normal approximation.
- As $n \to \infty$, the posterior distribution is normal centered on MLE.
- However, even for moderate sample sizes, asymptotic approximations may be inaccurate.
- In logistic regression for example, for rare outcomes or rare binary exposures, posterior can be highly skewed.
- Appealing to avoid any reliance on large sample assumptions and base inferences on **exact posterior**.

NON-CONJUGATE PRIORS

- Even though we may not be able to sample from the marginal posterior of a particular parameter when using a non-conjugate prior, sometimes, we may still be able to sample from conditional distributions of those parameters given all other parameters and the data.

- These conditional distributions, known as full conditionals, will be very important for us.

- In our normal example with

$$\mu \sim \mathcal{N}\left(\mu_0, \sigma_0^2\right).$$
$$\tau \ \sim \text{Gamma}\left(\frac{\nu_0}{2}, \frac{\nu_0}{2\tau_0}\right),$$

  even though we cannot sample easily from $\tau|Y$, turns out we will be able to sample from $\tau|\mu, Y$. That is the full conditional for τ.

- By the way, note that we already know the full conditional for μ, i.e., $\mu|\tau, Y$ (last two classes).

Full conditional distributions

- Goal: try to take advantage of those full conditional distributions (without sampling directly from the marginal posteriors) to obtain samples from the said marginal posteriors.

- In our example, with $\pi(\mu) = \mathcal{N}\left(\mu_0, \sigma_0^2\right)$, we have

$$\mu | Y, \tau \sim \mathcal{N}(\mu_n, \tau_n^{-1}),$$

  where

  - $\mu_n = \dfrac{\frac{\mu_0}{\sigma_0^2} + n\tau\bar{y}}{\frac{1}{\sigma_0^2} + n\tau}$; and
  - $\tau_n = \frac{1}{\sigma_0^2} + n\tau$.

- Review results from previous two classes if you are not sure why this holds.

- Let's see if we can figure out the other full conditional $\tau | \mu, Y$.

Full conditional distributions

$$\pi(\tau|\mu, Y) = \frac{\Pr[\tau, \mu, Y]}{\Pr[\mu, Y]} = \frac{L(y; \mu, \tau)\pi(\mu, \tau)}{\Pr[\mu, Y]}$$

$$= \frac{L(y; \mu, \tau)\pi(\mu)\pi(\tau)}{\Pr[\mu, Y]}$$

$$\propto L(y; \mu, \tau)\pi(\tau)$$

$$\propto \underbrace{\tau^{\frac{n}{2}} \exp\left\{-\frac{1}{2}\tau \sum_{i=1}^{n}(y_i - \mu)^2\right\}}_{\propto L(Y;\mu,\tau)} \times \underbrace{\tau^{\frac{\nu_0}{2}-1} \exp\left\{-\frac{\tau\nu_0}{2\tau_0}\right\}}_{\propto \pi(\tau)}$$

$$= \underbrace{\tau^{\frac{\nu_0 + n}{2}-1} \exp\left\{-\frac{1}{2}\tau\left[\frac{\nu_0}{\tau_0} + \sum_{i=1}^{n}(y_i - \mu)^2\right]\right\}}_{\text{Gamma Kernel}}.$$

Full conditional distributions

$$\pi(\tau|\mu, Y) \propto \underbrace{\tau^{\frac{\nu_0+n}{2}-1} \exp\left\{-\frac{1}{2}\tau\left[\frac{\nu_0}{\tau_0} + \sum_{i=1}^{n}(y_i-\mu)^2\right]\right\}}_{\text{Gamma Kernel}}$$
$$= \text{Gamma}\left(\frac{\nu_n}{2}, \frac{\nu_n}{2\tau_n(\mu)}\right) \quad \text{OR} \quad \text{Gamma}\left(\frac{\nu_n}{2}, \frac{\nu_n\sigma_n^2(\mu)}{2}\right),$$

where

$$\nu_n = \nu_0 + n$$

$$\sigma_n^2(\mu) = \frac{1}{\nu_n}\left[\frac{\nu_0}{\tau_0} + \sum_{i=1}^{n}(y_i-\mu)^2\right] = \frac{1}{\nu_n}\left[\frac{\nu_0}{\tau_0} + ns_n^2(\mu)\right]$$

$$\text{OR} \quad \tau_n(\mu) = \frac{\nu_n}{\left[\frac{\nu_0}{\tau_0} + \sum_{i=1}^{n}(y_i-\mu)^2\right]} = \frac{\nu_n}{\left[\frac{\nu_0}{\tau_0} + ns_n^2(\mu)\right]};$$

$$\text{with} \quad s_n^2(\mu) = \frac{1}{n}\sum_{i=1}^{n}(y_i-\mu)^2.$$

Iterative scheme

- Now we have two full conditional distributions but what we really need is to sample from $\pi(\tau|Y)$.
- Actually, if we could sample from $\pi(\mu, \tau|Y)$, we already know that the draws for μ and τ will be from the two marginal posterior distributions. So, we just need a scheme to sample from $\pi(\mu, \tau|Y)$.
- Suppose we had a single sample, say $\tau^{(1)}$ from the marginal posterior distribution $\pi(\tau|Y)$. Then we could sample

$$\mu^{(1)} \sim p(\mu|\tau^{(1)}, Y).$$

- This is what we did in the last class, so that the pair $\{\mu^{(1)}, \tau^{(1)}\}$ is a sample from the joint posterior $\pi(\mu, \tau|Y)$.
- $\Rightarrow$ $\mu^{(1)}$ can be considered a sample from the marginal distribution of μ, which again means we can use it to sample

$$\tau^{(2)} \sim p(\tau|\mu^{(1)}, Y),$$

and so forth.

Gibbs sampling

- So, we can use two **full conditional distributions** to generate samples from the **joint distribution**, once we have a starting value $\tau^{(1)}$.
- Formally, this sampling scheme is known as Gibbs sampling.
  - Purpose: Draw from a joint distribution, say $p(\mu, \tau|Y)$.
  - Method: Iterative conditional sampling
    - Draw $\tau^{(1)} \sim p(\tau|\mu^{(0)}, Y)$
    - Draw $\mu^{(1)} \sim p(\mu|\tau^{(1)}, Y)$
  - Purpose: Full conditional distributions have known forms, with sampling from the full conditional distributions fairly easy.
- More generally, we can use this method to generate samples of $\theta = (\theta_1, \ldots, \theta_p)$, the vector of p parameters of interest, from the joint density.

Gibbs sampling

- Procedure:
  - Start with initial value $\theta^{(0)} = (\theta_1^{(0)}, \ldots, \theta_p^{(0)})$.
  - For iterations $t = 1, \ldots, T$,
    1. Sample $\theta_1^{(t)}$ from the conditional posterior distribution

       $$\pi(\theta_1 | \theta_2 = \theta_2^{(t-1)}, \ldots, \theta_p = \theta_p^{(t-1)}, Y)$$

    2. Sample $\theta_2^{(t)}$ from the conditional posterior distribution

       $$\pi(\theta_2 | \theta_1 = \theta_1^{(t)}, \theta_3 = \theta_3^{(t-1)}, \ldots, \theta_p = \theta_p^{(t-1)}, Y)$$

    3. Similarly, sample $\theta_3^{(t)}, \ldots, \theta_p^{(t)}$ from the conditional posterior distributions given current values of other parameters.
  - This generates a **dependent** sequence of parameter values.

MCMC

- Gibbs sampling is one of several flavors of Markov chain Monte Carlo (MCMC).
  - Markov chain: a stochastic process in which future states are independent of past states conditional on the present state.
  - Monte Carlo: simulation.
- MCMC provides an approach for generating samples from posterior distributions.
- From these samples, we can obtain summaries (including summaries of functions) of the posterior distribution for θ, our parameter of interest.

How does MCMC work?

- Let $\theta^{(t)} = (\theta_1^{(t)}, \ldots, \theta_p^{(t)})$ denote the value of the $p \times 1$ vector of parameters at iteration t.
- Let $\theta^{(0)}$ be an initial value used to start the chain (*should not be sensitive*).
- MCMC generates $\theta^{(t)}$ from a distribution that depends on the data and potentially on $\theta^{(t-1)}$, but not on $\theta^{(1)}, \ldots, \theta^{(t-2)}$.
- This results in a Markov chain with **stationary distribution** $\pi(\theta|Y)$ under some conditions on the sampling distribution.
- The theory of Markov Chains (structure, convergence, reversibility, detailed balance, stationarity, etc) is well beyond the scope of this course so we will not dive into it.
- If you are interested, consider taking STA 531/831 or courses on stochastic process.

Properties

- **Note**: Our Markov chain is a collection of draws of θ that are (slightly we hope!) dependent on the previous draw.
- The chain will wander around our parameter space, only remembering where it had been in the last draw.
- We want to have our MCMC sample size, S, big enough so that we can
  - Move out of areas of low probability into regions of high probability (convergence)
  - Move between high probability regions (good mixing)
  - Know our Markov chain is stationary in time (the distribution of samples is the same for all samples, regardless of location in the chain)
- At the start of the sampling, the samples are **not** from the posterior distribution. It is necessary to discard the initial samples as a burn-in to allow convergence. We'll talk more about that in the next class.

Different flavors of MCMC

- The most commonly used MCMC algorithms are:
  - Metropolis sampling (Metropolis et al., 1953).
  - Metropolis-Hastings (MH) (Hastings, 1970).
  - Gibbs sampling (Geman & Geman, 1984; Gelfand & Smith, 1990).
- Overview of Gibbs - Casella & George (1992, The American Statistician, 46, 167-174). the first two
- Overview of MH - Chib & Greenberg (1995, The American Statistician).
- We will get to Metropolis and Metropolis-Hastings later in the course.

Example: bivariate normal

- Consider

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right]$$

  where ρ is known (and is the correlation between θ_1 and θ_2).

- We will review details of the multivariate normal distribution very soon but for now, let's use this example to explore Gibbs sampling.

- For this density, turns out that we have

$$\theta_1 | \theta_2 \sim \mathcal{N}\left(\rho\theta_2, 1 - \rho^2\right)$$

  and

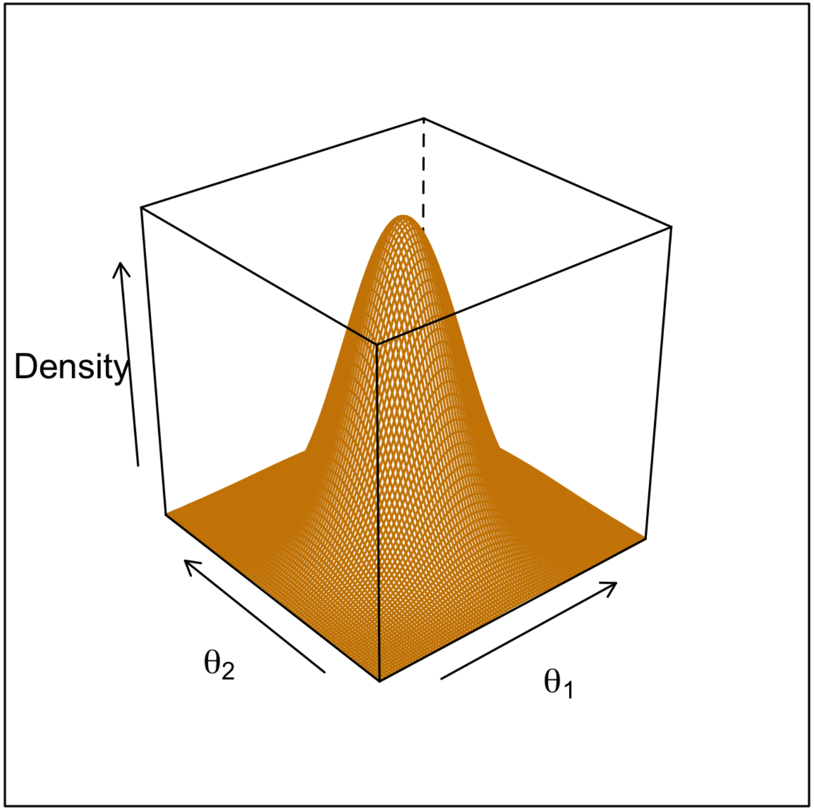
$$\theta_2 | \theta_1 \sim \mathcal{N}\left(\rho\theta_1, 1 - \rho^2\right)$$

- While we can easily sample directly from this distribution (using the `mvtnorm` or `MASS` packages in R), let's instead use the Gibbs sampler to draw samples from it.

Bivariate normal

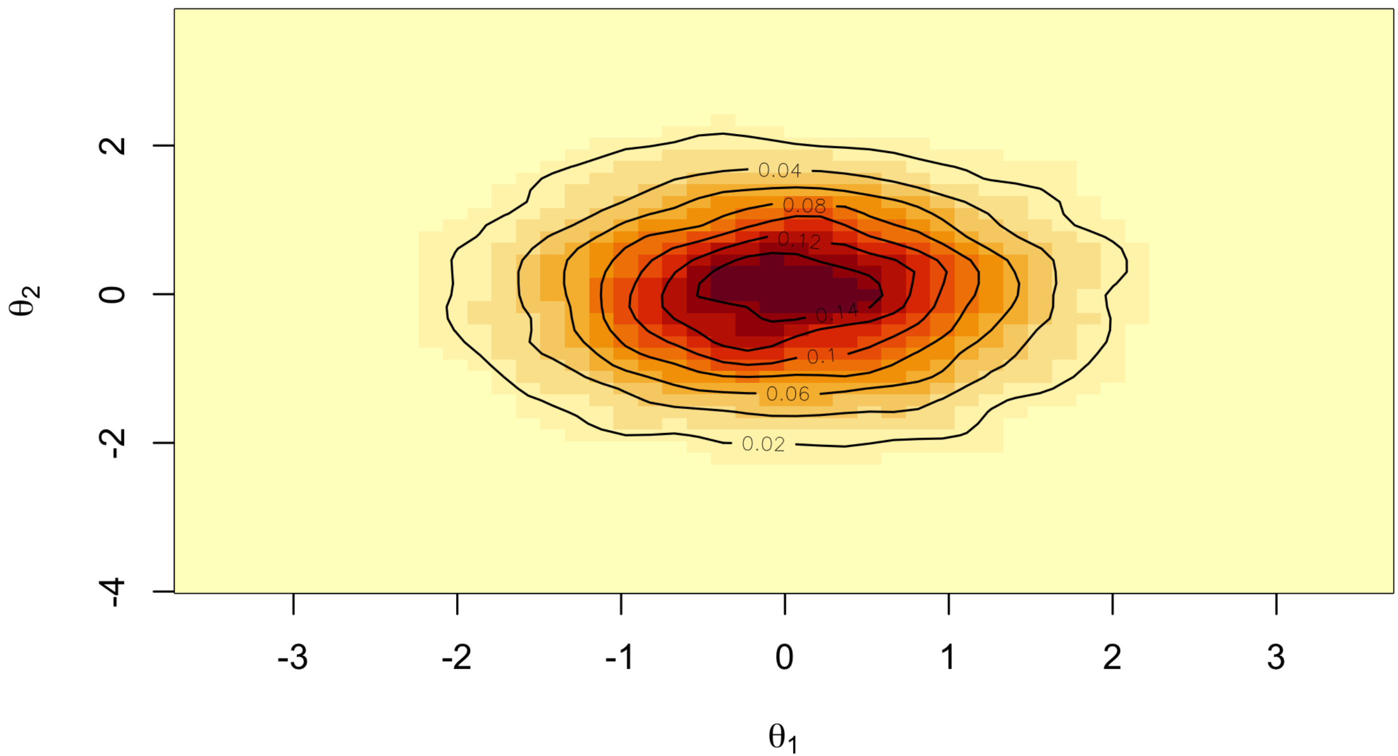
First, a few examples of the bivariate normal distribution.

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]$$



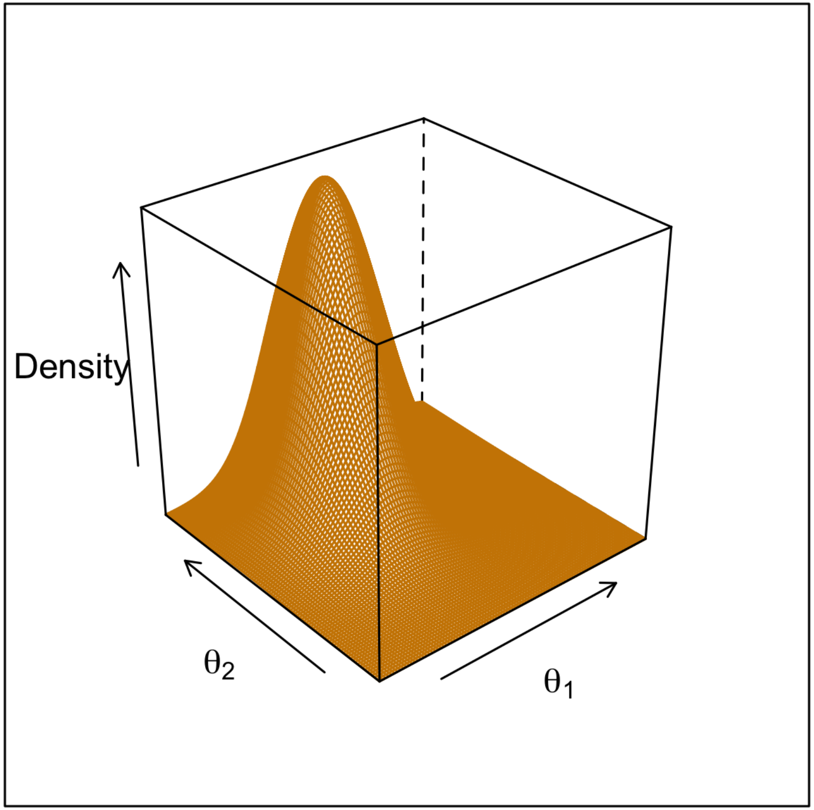
Bivariate normal

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]$$



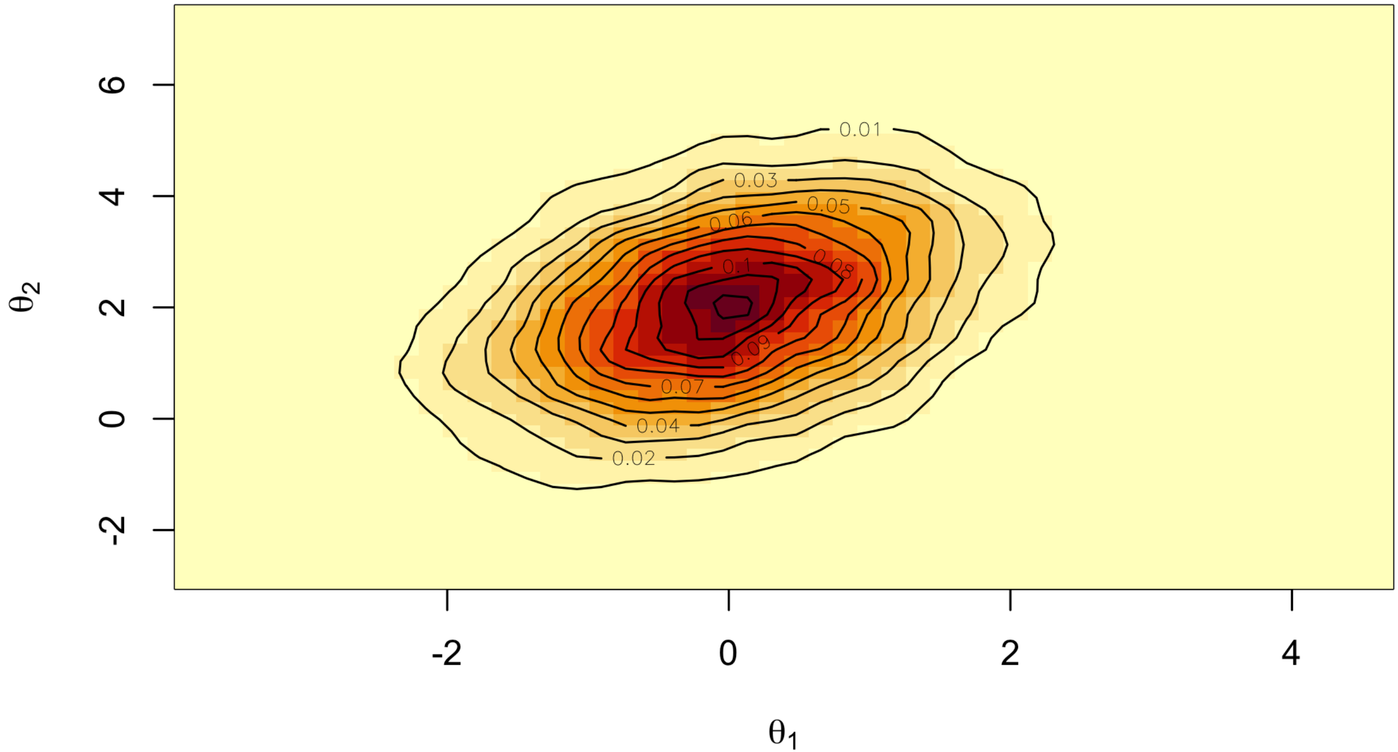
Bivariate normal

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 & 0.5 \\ 0.5 & 2 \end{pmatrix}\right]$$



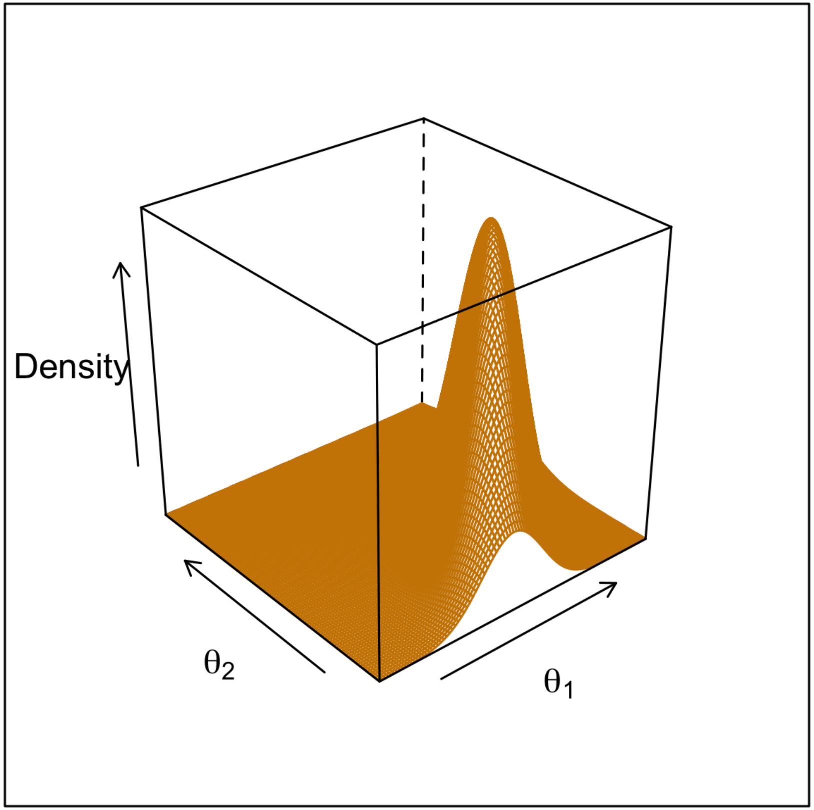
Bivariate normal

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 & 0.5 \\ 0.5 & 2 \end{pmatrix}\right]$$



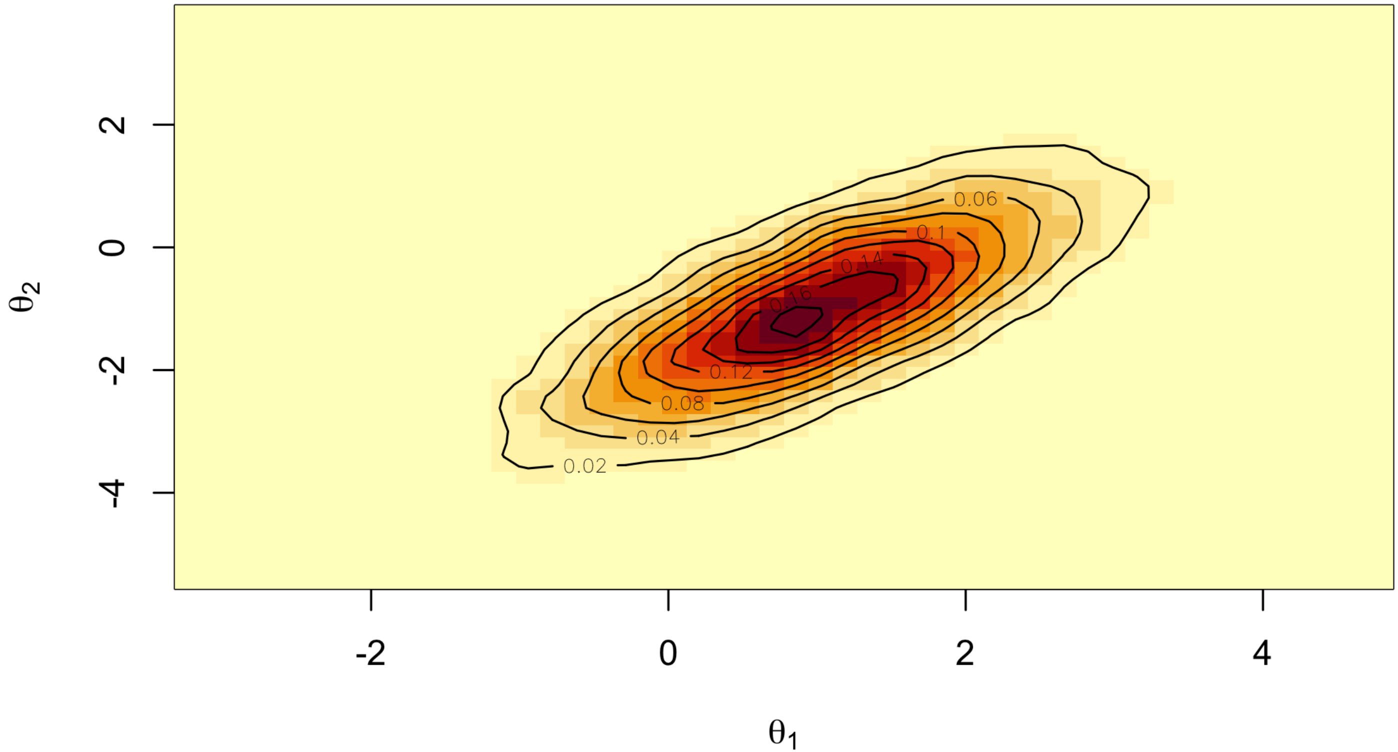
BIVARIATE NORMAL

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 & 0.9 \\ 0.9 & 0.5 \end{pmatrix}\right]$$



Bivariate normal

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 & 0.9 \\ 0.9 & 0.5 \end{pmatrix}\right]$$



Back to the example

- Again, we have

$$\theta_1|\theta_2 \sim \mathcal{N}\left(\rho\theta_2, 1-\rho^2\right); \quad \theta_2|\theta_1 \sim \mathcal{N}\left(\rho\theta_1, 1-\rho^2\right)$$

- Here's a code to do Gibbs sampling using those full conditionals:

```
rho <- #set correlation
S <- #set number of MCMC sample
thetamat <- matrix(0,nrow=S,ncol=2)
theta <- c(10,10) #initialize values of theta
for (s in 1:S) {
theta[1] <- rnorm(1,rho*theta[2],sqrt(1-rho^2)) #sample theta1
theta[2] <- rnorm(1,rho*theta[1],sqrt(1-rho^2)) #sample theta2
thetamat[s,] <- theta
}
```

- Here's a code to do sample directly instead:

```
library(mvtnorm)
rho <- #set correlation; no need to set again once you've used previous code
S <- #set number of MCMC sample; no need to set again once you've used previous code
Mu <- c(0,0)
Sigma <- matrix(c(1,rho,rho,1),ncol=2)
thetamat_direct <- rmvnorm(S, mean = Mu,sigma = Sigma)
```