Stochastic Processes: Lecture 1

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UCLA Biostatistics 270

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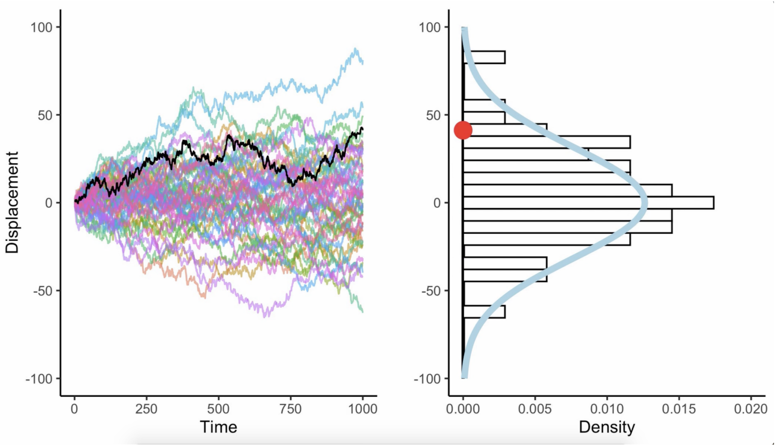
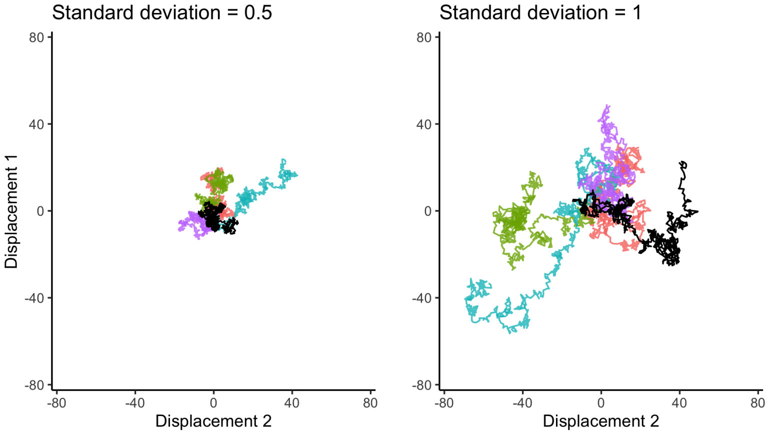
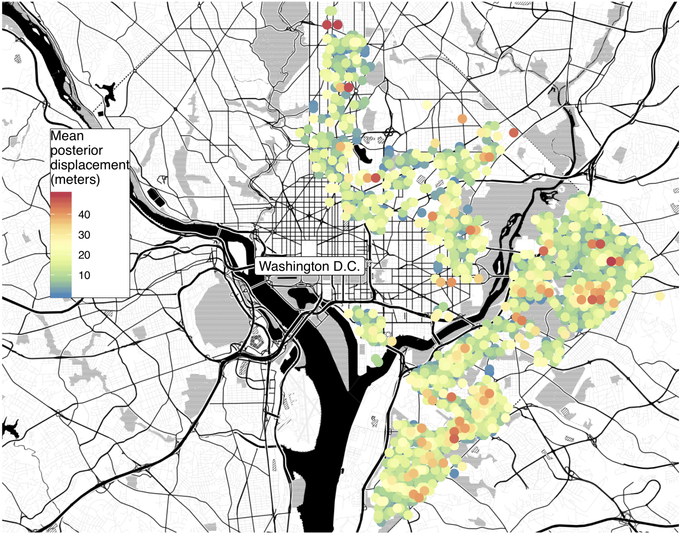
Brownian motion models diffusion



Brownian motion models diffusion

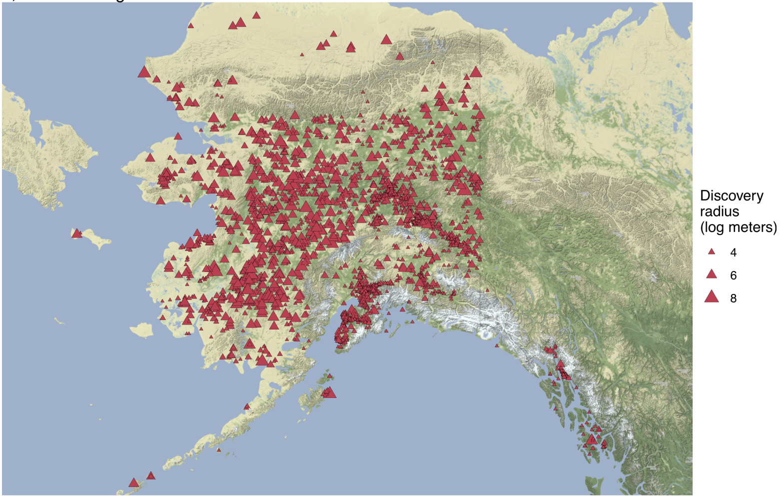


Hawkes processes model contagion



Hawkes processes model contagion

2,925 Wildfire ignition sites in Alaska: 2015–2019



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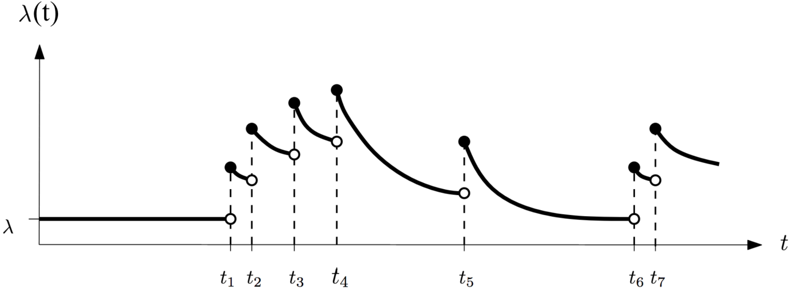
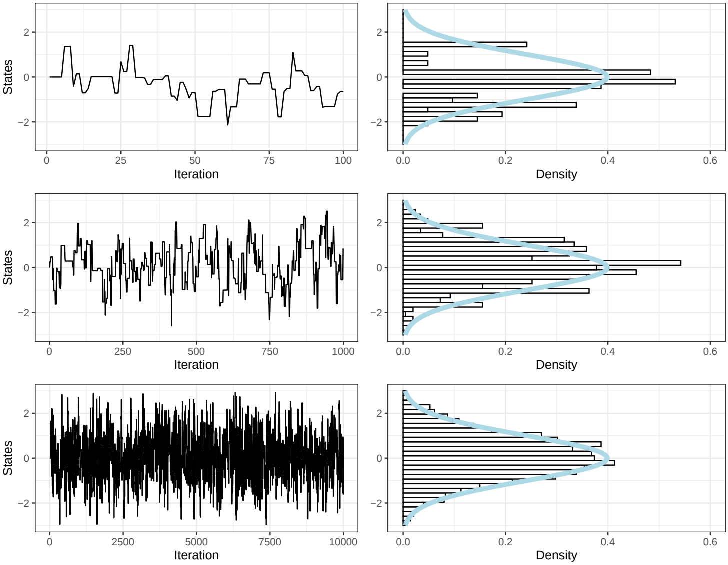


Laub et al. 2015

Markov chains



In this course, we will learn to:

- simulate stochastic processes; and
- use stochastic process models to analyze data.

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Bayesian inference

We observe data $y_1, \dots, y_N \stackrel{iid}{\sim} p(y_n|\boldsymbol{\theta})$ and assume $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$. Here,

- $p(\mathrm{y}|\boldsymbol{\theta}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{\theta})$ is the *likelihood*,
- $p(\boldsymbol{\theta})$ is the *prior*,

and the goal of Bayesian inference is to obtain the *posterior*

$$p(\boldsymbol{\theta}|\mathrm{y}) = \frac{p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathrm{y})} = \frac{p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int_{\Theta} p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}}\,.$$

Bayesian inference

We're usually interested in computing another integral

$$\mathbb{E}_{\boldsymbol{\theta}|\mathrm{y}} f(\boldsymbol{\theta}) = \int_{\Theta} f(\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathrm{y}) \mathrm{d}\boldsymbol{\theta} \,,$$

so we do what statisticians have been doing forever. We collect samples and rely on the law of large numbers. Suppose $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_S \overset{iid}{\sim} p(\boldsymbol{\theta}|\mathrm{y})$ ($\mathbb{E}_{\boldsymbol{\theta}|\mathrm{y}} |\boldsymbol{\theta}| < \infty$) and $f(\cdot)$ *a.s.* continuous, then

- (WLLN) $\sum_{s=1}^{S} f(\boldsymbol{\theta}_s)/S \xrightarrow{P} \mathbb{E}_{\boldsymbol{\theta}|\mathrm{y}} f(\boldsymbol{\theta})$
- (SLLN) $\sum_{s=1}^{S} f(\boldsymbol{\theta}_s)/S \xrightarrow{a.s.} \mathbb{E}_{\boldsymbol{\theta}|\mathrm{y}} f(\boldsymbol{\theta})$

But where do we find our samples?

Generating (pseudo) random variables

We want to sample $Y \sim F(y)$, where $F(\cdot)$ is the (monotonically increasing) c.d.f.

Claim 1

Assume we can generate $U \sim U(0,1)$ and compute $F^{-1}(\cdot)$. Then

$$F^{-1}(U) \sim F(y)\,.$$

Proof.

$$\Pr(F^{-1}(U) < y) = \Pr(U < F(y)) = F(y).$$

□

Exponential random variables

Ingredients for $Y \sim \exp(\lambda)$:

1. $p(Y|\lambda) = \lambda \, exp(-\lambda Y)$
2. $F(y|\lambda) = \Pr(Y < y|\lambda) = \int_0^y \lambda \, exp(-\lambda Y) = 1 - \exp(-\lambda Y)$
3. $F^{-1}(u) = -\lambda^{-1} \log(1 - u)$

Easy but *extremely* limited!

Part 1. Monte Carlo

Rejection sampling

We want to sample from generic $p(\boldsymbol{\theta})$ but only know $p^*(\boldsymbol{\theta}) \propto p(\boldsymbol{\theta})$. We can easily sample from $q(\boldsymbol{\theta})$ and know a number $M > 0$ s.t. $p^*(\boldsymbol{\theta}) < Mq(\boldsymbol{\theta})$.

Algorithm for generating $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$:

1. Draw $\boldsymbol{\theta}^* \sim q(\boldsymbol{\theta})$ and $U \sim U(0,1)$
2. $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^*$ if $U < \frac{p*(\boldsymbol{\theta})}{Mq(\boldsymbol{\theta})}$

The tighter the envelope $Mq(\boldsymbol{\theta})$, the better. Suppose $p(\boldsymbol{\theta}) = c^* p^*(\boldsymbol{\theta})$. Then

$$\Pr(\text{Accept}) = \frac{1}{c^* M},$$

and expected number of iterations for one sample is $c^* M$.

Validity of rejection sampling

Importance sampling

We wish to know $\mathbb{E}f(\boldsymbol{\theta}) = \int f(\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$. We can evaluate $p^*(\boldsymbol{\theta}) \propto p(\boldsymbol{\theta})$ and can sample from $q(\boldsymbol{\theta})$ easily.

Algorithm for generating estimator $\widehat{\mathbb{E}f(\boldsymbol{\theta})}$:

1. Draw $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_S \sim q(\boldsymbol{\theta})$
2. Calculate $w_k = \frac{w(\boldsymbol{\theta}_k)}{\sum_{s=1}^{S} w(\boldsymbol{\theta}_s)}$, $w(\boldsymbol{\theta}_s) = \frac{p^*(\boldsymbol{\theta}_s)}{q(\boldsymbol{\theta}_s)}$ for $k = 1, \ldots, S$.
3. Return $\sum_{s=1}^{S} w_s f(\boldsymbol{\theta}_s)$

Validity of importance sampling

By the LLN,

$$\frac{1}{S}\sum_{s=1}^{S} w(\boldsymbol{\theta}_s)f(\boldsymbol{\theta}_s) \xrightarrow{a.s.} \int w(\boldsymbol{\theta})f(\boldsymbol{\theta})q(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} \quad \text{and}$$

$$\frac{1}{S}\sum_{s=1}^{S} w(\boldsymbol{\theta}_s) \xrightarrow{a.s.} \int w(\boldsymbol{\theta})q(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}\,.$$

Therefore,

$$\begin{aligned}\sum_{s=1}^{S} w_s f(\boldsymbol{\theta}_s) &= \frac{\frac{1}{S}\sum_{s=1}^{S} w(\boldsymbol{\theta}_s)f(\boldsymbol{\theta}_s)}{\frac{1}{S}\sum_{s=1}^{S} w(\boldsymbol{\theta}_s)} \xrightarrow{a.s.} \frac{\int w(\boldsymbol{\theta})f(\boldsymbol{\theta})q(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}}{\int w(\boldsymbol{\theta})q(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}} \\ &= \frac{\int f(\boldsymbol{\theta})p^*(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}}{\int p^*(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}} = \int f(\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} = \mathbb{E}f(\boldsymbol{\theta})\,.\end{aligned}$$

Variance of IS estimator

An estimator for the variance of $\widehat{\mathbb{E}f(\boldsymbol{\theta})} = \sum_{s=1}^{S} w_s f(\boldsymbol{\theta}_s)$ is

$$\widehat{\mathrm{Var}}\left(\widehat{\mathbb{E}f(\boldsymbol{\theta})}\right) \approx \sum_{s=1}^{S} w_s^2 (f(\boldsymbol{\theta}_s) - \widehat{\mathbb{E}f(\boldsymbol{\theta})})^2 \, .$$

The variance can be large if even a single w_s is large.

Question: is it better to use a t-distribution to sample a normal or vice-versa?

Part 2. Discrete time, discrete space, time-homogeneous Markov chains

The setup

Our Markov chain is a discrete time stochastic process $\{\boldsymbol{\theta}^{(s)}, s \in \mathbb{N}\}$ satisfying

$$\Pr(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)}, \boldsymbol{\theta}^{(s-2)}, \ldots, \boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(0)}) = \Pr(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)}) \, .$$

Ingredients:

1. The state space $\mathcal{S}$ is a finite or countable set.
2. Initial distribution $\{p_i^{(0)}\}_{i \in \mathcal{S}}$, satisfying
   2.1 $p_i^{(0)} = \Pr(\boldsymbol{\theta}^{(0)} = i)$
   2.2 $p_i^{(0)} \geq 0$
   2.3 $\sum_{i \in \mathcal{S}} p_i^{(0)} = 1$
3. Transition probabilities $\{q_{ij}\}_{i,j \in \mathcal{S}}$
   3.1 $q_{ij} = \Pr(\boldsymbol{\theta}^{(s)} = j|\boldsymbol{\theta}^{(s-1)} = i)$
   3.2 $q_{ij} \geq 0$
   3.3 $\sum_{j \in \mathcal{S}} q_{ij} = 1$

Finite state space

When $\mathcal{S} = \{1, \ldots, M\}$, then we can write state probabilities as row-vectors:

$$\mathrm{p}^{(s)} = \Big(\Pr(\boldsymbol{\theta}^{(s)} = 1), \Pr(\boldsymbol{\theta}^{(s)} = 2), \ldots, \Pr(\boldsymbol{\theta}^{(s)} = M)\Big)$$

Similarly, the transition probabilities q_{ij} form the matrix

$$\mathrm{Q} = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1M} \\ q_{21} & q_{22} & \cdots & q_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ q_{M1} & q_{M2} & \cdots & q_{MM} \end{bmatrix}$$

and

$$\mathrm{p}^{(s)} = \mathrm{p}^{(s-1)}\mathrm{Q} = \mathrm{p}^{(s-2)}\mathrm{Q}^2 = \cdots = \mathrm{p}^{(0)}\mathrm{Q}^s \,.$$

Perron-Frobenius theorem

Let A be a square matrix, satisfying $A \geq 0$ and $A^k > 0$ for some k.

1. There exists a real eigenvalue $\lambda_{PF} > 0$ with associated *positive* left/right eigenvectors.

2. For any other eigenvalue λ of A, $|\lambda| < |\lambda_{PF}|$

3. λ_{PF} has multiplicity 1 and corresponds to 1×1 Jordan block.

Transition matrix

Assume that our transition matrix satisfies $Q^k > 0$ for some k. We know:

- $Q \geq 0$
- If $\mathbb{1} = (1, \ldots, 1)$, then $Q\mathbb{1}^T = \mathbb{1}^T$, so 1 is an eigenvalue with right eigenvector $\mathbb{1}^T$.
- But the eigenvalues of Q satisfy $|\lambda| \leq 1$ (Gershgorin circle theorem) .

Therefore $\lambda_{PF} = 1$ and there exists a positive left eigenvector $\boldsymbol{\pi}$ for which

$$\boldsymbol{\pi} Q = \boldsymbol{\pi} \quad \text{and} \quad \boldsymbol{\pi}\mathbb{1}^T = 1 \quad \text{(Why?)}$$

We call such a $\boldsymbol{\pi}$ *the* stationary distribution.

Stationary distributions

Because all other eigenvalues are bounded below 1, they die away, and (remembering that Q is a sum of outer products)

$$\lim_{s \longrightarrow \infty} \mathrm{Q}^s = \mathbb{1}^T \boldsymbol{\pi} = \begin{pmatrix} -\boldsymbol{\pi}- \\ \vdots \\ -\boldsymbol{\pi}- \end{pmatrix}$$

On the other hand, even without the regularity assumption ($\mathrm{Q}^k > 0$), any limiting distribution is a stationary distribution. Take p an arbitrary limiting distribution, i.e.,

$$\lim_{s \longrightarrow \infty} \mathrm{Q}^s = \mathbb{1}^T \mathrm{p} \quad \text{or} \quad \lim_{s \to \infty} \mathrm{Q}^s_{ik} = \mathrm{p}_k$$

for any i. Then,

$$\mathrm{p}_j = \lim_{s \to \infty} \mathrm{Q}^{s+1}_{ij} = \lim_{s \to \infty} \sum_k \mathrm{Q}^s_{ik} \mathrm{Q}_{kj} = \sum_k \lim_{s \to \infty} \mathrm{Q}^s_{ik} \mathrm{Q}_{kj} = \sum_k \mathrm{p}_k \mathrm{Q}_{kj} \,.$$

Law of large numbers

Consider a Markov chain with finite state space and regular transition matrix. If a function $f(\cdot)$ is bounded on $\mathcal{S}$, then

$$\frac{1}{S}\sum_{s=0}^{S} f(\boldsymbol{\theta}^{(s)}) \xrightarrow{a.s.} \mathbb{E}_{\boldsymbol{\pi}} f(\boldsymbol{\theta}) = \sum_{i\in\mathcal{S}} f(i)\boldsymbol{\pi}_i\,.$$

This result holds irrespective of initial state $\mathrm{p}^{(0)}$.

The punchline

- We construct Markov chains so that they have a specific stationary distribution $\boldsymbol{\pi}$ (e.g., the posterior).

- By simulating the Markovian dynamics, we may obtain an *empirical* estimate of $\mathbb{E}_{\boldsymbol{\pi}} f(\boldsymbol{\theta})$.

Detailed balance

Satisfying the *detailed balance* equations

$$\boldsymbol{\pi}_i \mathsf{Q}_{ij} = \boldsymbol{\pi}_j \mathsf{Q}_{ji}$$

is sufficient (assuming regularity, of course) for guaranteeing that $\boldsymbol{\pi}$ is the invariant distribution of the Markov chain:

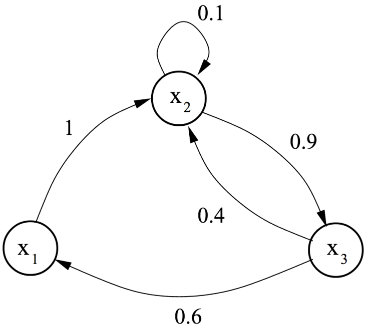
$$\sum_i \boldsymbol{\pi}_i \mathsf{Q}_{ij} = \sum_i \boldsymbol{\pi}_j \mathsf{Q}_{ji} = \boldsymbol{\pi}_j \sum_i \mathsf{Q}_{ji} = \boldsymbol{\pi}_j$$

We say:

- The Markov chain is reversible with respect to $\boldsymbol{\pi}$ *or*
- the Markov chain satisfies detailed balance with respect to $\boldsymbol{\pi}$.

Two concepts

A chain is *irreducible* if for any two states i and j, there exists a k such that $(Q^k)_{ij} > 0$. Intuitively, this means the transition graph is connected.



Andrieu et al. 2003

The *period* of a state i is the *gcd* of the times at which it is possible to move from i to i. A Markov chain is *aperiodic* if the period of all states is 1.

Existence and uniqueness of stationary distribution

Finite state space:

$$\text{Irreducibility} + \text{Aperiodicity} \iff \text{Regular} \iff \text{Ergodic}$$

Countable state space:

$$\text{Irreducibility} + \text{Aperiodicity} + \text{Positive recurrence} \iff \text{Ergodic}$$

A state is *positive recurrent* if the expected time to return is finite.
A chain is positive recurrent if all states are positive recurrent.

Part 3. Discrete time, continuous space, time-homogeneous Markov chains

Analogies: the Markov property

The Markov property

$$\Pr(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)},\ldots,\boldsymbol{\theta}^{(1)},\boldsymbol{\theta}^{(0)}) = \Pr(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)})$$

now becomes

$$\Pr(\boldsymbol{\theta}^{(s)} \in A|\boldsymbol{\theta}^{(s-1)},\ldots,\boldsymbol{\theta}^{(1)},\boldsymbol{\theta}^{(0)}) = \Pr(\boldsymbol{\theta}^{(s)} \in A|\boldsymbol{\theta}^{(s-1)}) \,.$$

Analogies: transition kernel

The previous fact that

$$(\mathrm{p}^{(s)})_j = (\mathrm{p}^{(0)}\mathrm{Q}^s)_j = \sum_{i_0, i_1, \ldots, i_{s-2}, i_{s-1}} \mathrm{p}^{(0)}_{i_0} \mathrm{Q}_{i_0 i_1} \ldots \mathrm{Q}_{i_{s-2} i_{s-1}} \mathrm{Q}_{i_{s-1} j}$$

becomes

$$\Pr(\boldsymbol{\theta}^{(s)} \in A) = \int_A p_s(\boldsymbol{\theta}^{(s)}) \mathrm{d}\boldsymbol{\theta}^{(s)} =$$
$$\int_A \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} q(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)}) \ldots q(\boldsymbol{\theta}^{(1)}|\boldsymbol{\theta}^{(0)}) p_0(\boldsymbol{\theta}^{(0)})\, \mathrm{d}\boldsymbol{\theta}^{(0)} \ldots \mathrm{d}\boldsymbol{\theta}^{(s-1)} \mathrm{d}\boldsymbol{\theta}^{(s)}\,,$$

i.e., we replace the transition matrix with the integral kernel

$$\int p_{s-1}(\boldsymbol{\theta}^{(s-1)}) q(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)}) \mathrm{d}\boldsymbol{\theta}^{(s-1)} = p_s(\boldsymbol{\theta}^{(s)})\,.$$

Analogies: stationary distributions

The definition of a stationary distribution

$$\boldsymbol{\pi}\mathsf{Q} = \boldsymbol{\pi}$$

becomes

$$\pi(\boldsymbol{\theta}^{(s)}) = \int q(\boldsymbol{\theta}^{(s)}|\boldsymbol{\theta}^{(s-1)})\pi(\boldsymbol{\theta}^{(s-1)})\mathrm{d}\boldsymbol{\theta}^{(s-1)}\,,$$

i.e., $\pi(\cdot)$ is an eigenfunction of the transition kernel with eigenvalue 1.

Analogies: detailed balance

Detailed balance equations

$$\boldsymbol{\pi}_i \mathsf{Q}_{ij} = \boldsymbol{\pi}_j \mathsf{Q}_{ji}$$

becomes (a.s.)

$$\pi(\boldsymbol{\theta})q(\boldsymbol{\theta}^*|\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}^*)q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)\,.$$

If the chain satisfies detailed balance with respect to $\pi(\cdot)$, then

$$\int \pi(\boldsymbol{\theta}^*)q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)\mathrm{d}\boldsymbol{\theta}^* = \int \pi(\boldsymbol{\theta})q(\boldsymbol{\theta}^*|\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}^* = \pi(\boldsymbol{\theta})\,,$$

i.e., $\pi(\cdot)$ is a stationary distribution of the Markov chain.

Useful concepts

- An MC is p-*irreducible* if there is a positive probability of reaching any set A for which $\int_A \mathrm{p}(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} > 0$, regardless of initial state.
- A chain is *periodic* if it returns to any set A at regular intervals (*gcd* of return times > 1). Otherwise it is *aperiodic*.

A sufficient condition for aperiodicity and p-irreducibility is that

$$\int_A q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(0)})\mathrm{d}\boldsymbol{\theta} > 0\,,\ \forall \boldsymbol{\theta}^{(0)} \quad \text{if} \quad \int_A p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} > 0\,.$$

Limiting distribution

If a chain has a stationary distribution $\pi(\cdot)$ and is π-irreducible and aperiodic, then

1. $\pi(\cdot)$ is the unique stationary distribution, and
2. $\lim_{s\to\infty} \Pr(\boldsymbol{\theta}^{(s)} \in A | \boldsymbol{\theta}^{(0)} = \boldsymbol{\theta}^*) = \int_A \pi(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta}$,

where we have asserted that the initial state has some value with probability 1.

Existence and uniqueness of stationary distribution

Finite state space:

$$\text{Irreducibility} + \text{Aperiodicity} \iff \text{Regular} \iff \text{Ergodic}$$

Countable state space:

$$\text{Irreducibility} + \text{Aperiodicity} + \text{Positive recurrence} \iff \text{Ergodic}$$

Continuous state space:

$$\pi\text{-Irreducibility} + \text{Aperiodicity} + \text{Harris recurrence} \iff \text{Ergodic}$$

A state is *Harris recurrent* if for any starting value and any set A with $\int_A \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} > 0$, the probability A is returned to infinitely often is 1.

Consequences of ergodicity

For an ergodic chain with stationary distribution $\pi(\cdot)$,

1. $\lim_{s\to\infty} \Pr(\boldsymbol{\theta}^{(s)} \in A) = \int_A \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$, and
2. $\frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{\theta}^{(s)}) \xrightarrow{a.s.} \mathbb{E}_\pi f(\boldsymbol{\theta})$,,

provided the expectation is finite.

In practice

Three things we can actually check:

1. Sufficient condition for $\pi(\cdot)$ being a stationary distribution is reversibility / detailed balance:

$$\pi(\boldsymbol{\theta})q(\boldsymbol{\theta}^*|\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}^*)q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)\,.$$

2. Sufficient condition for aperiodicity and π-irreducibility is that

$$\int_A q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(0)})\mathrm{d}\boldsymbol{\theta} > 0\,,\ \forall\boldsymbol{\theta}^{(0)} \quad \text{if} \quad \int_A \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} > 0\,.$$

3. Sufficient condition for Harris recurrence is π-irreducibility and *absolute continuity* of $q(\cdot|\boldsymbol{\theta}^*)$ wrt $\pi(\cdot)$:

$$\int_A \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} = 0 \quad \Longrightarrow \quad \int_A q(\boldsymbol{\theta}|\boldsymbol{\theta}^*)\mathrm{d}\boldsymbol{\theta}\,.$$

Part 4. Classical MCMC

Time for a 180°

So far: $\mathcal{S} + q(\cdot,\cdot) \Longrightarrow \pi(\cdot)$

Markov chain Monte Carlo: $\mathcal{S} + \pi(\cdot) \Longrightarrow q(\cdot,\cdot)$

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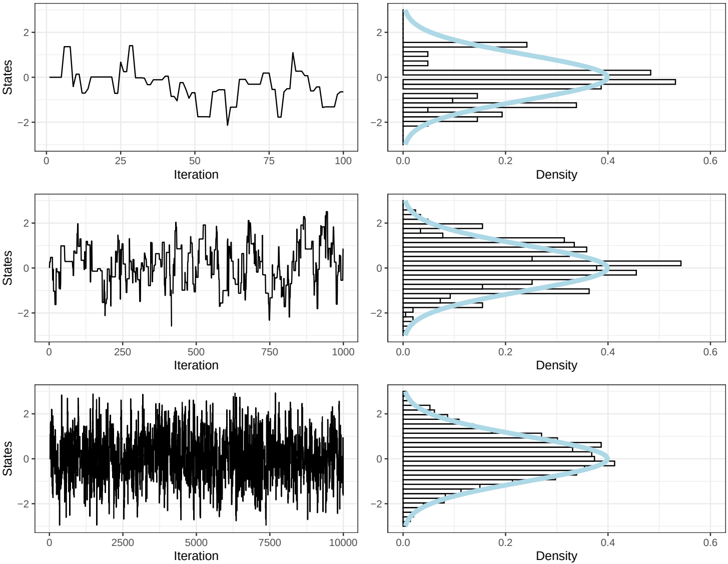
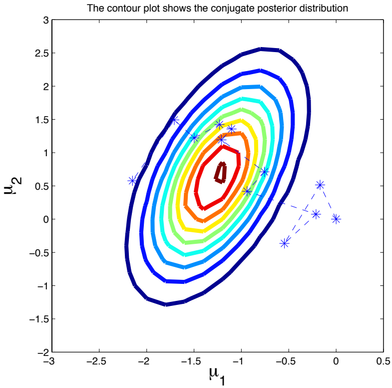
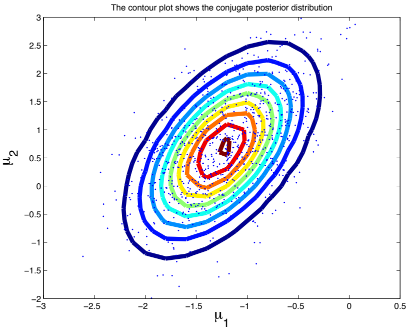
Markov chain Monte Carlo



Markov chain Monte Carlo





The Metropolis algorithm

Our target stationary distribution is $\pi(\boldsymbol{\theta}) = p(\boldsymbol{\theta}|\mathrm{y}) \propto p^*(\boldsymbol{\theta}|\mathrm{y})$.

Inputs:

- $p^*(\boldsymbol{\theta}|\mathrm{y})$
- a *proposal distribution* $h(\boldsymbol{\theta}^*|\boldsymbol{\theta})$ such that $h(\boldsymbol{\theta}|\boldsymbol{\theta}^*) = h(\boldsymbol{\theta}^*|\boldsymbol{\theta})$
- $\boldsymbol{\theta}^{(0)}$ (chosen or randomly generated however you want)

For $s = 1, \ldots, S$,

1. Generate $\boldsymbol{\theta}^* \sim h(\boldsymbol{\theta}|\boldsymbol{\theta}^{(s-1)})$ and $U \sim Uni(0, 1)$
2. Compute

$$a \leftarrow 1 \wedge \frac{p^*(\boldsymbol{\theta}^*|\mathrm{y})}{p^*(\boldsymbol{\theta}^{(s-1)}|\mathrm{y})} = 1 \wedge \frac{\pi(\boldsymbol{\theta}^*)}{\pi(\boldsymbol{\theta}^{(s-1)})}$$

3. IF $U < a$: $\quad \boldsymbol{\theta}^{(s)} \leftarrow \boldsymbol{\theta}^*$;
   ELSE: $\quad \boldsymbol{\theta}^{(s)} \leftarrow \boldsymbol{\theta}^{(s-1)}$

The Metropolis algorithm

The Metropolis algorithm generates Markov chains that are reversible wrt the target distribution $\pi(\boldsymbol{\theta})$:

$$\begin{aligned}
\pi(\boldsymbol{\theta})q(\boldsymbol{\theta}'|\boldsymbol{\theta}) &= \pi(\boldsymbol{\theta})h(\boldsymbol{\theta}'|\boldsymbol{\theta})a(\boldsymbol{\theta}',\boldsymbol{\theta}) \\
&= \pi(\boldsymbol{\theta})h(\boldsymbol{\theta}'|\boldsymbol{\theta})\left(1 \wedge \frac{\pi(\boldsymbol{\theta}')}{\pi(\boldsymbol{\theta})}\right) \\
&= h(\boldsymbol{\theta}'|\boldsymbol{\theta})\left(\pi(\boldsymbol{\theta}) \wedge \pi(\boldsymbol{\theta}')\right) \\
&= h(\boldsymbol{\theta}|\boldsymbol{\theta}')\left(\pi(\boldsymbol{\theta}') \wedge \pi(\boldsymbol{\theta})\right) \\
&= \pi(\boldsymbol{\theta}')h(\boldsymbol{\theta}|\boldsymbol{\theta}')\left(1 \wedge \frac{\pi(\boldsymbol{\theta})}{\pi(\boldsymbol{\theta}')}\right) \\
&= \pi(\boldsymbol{\theta}')h(\boldsymbol{\theta}|\boldsymbol{\theta}')a(\boldsymbol{\theta},\boldsymbol{\theta}') \\
&= \pi(\boldsymbol{\theta}')q(\boldsymbol{\theta}|\boldsymbol{\theta}')\,.
\end{aligned}$$

The Metropolis algorithm

For unbounded targets (why?), the classic symmetric proposal is a Gaussian centered at the current state:

$$\boldsymbol{\theta}^* \sim h(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(s-1)}) \equiv N_D(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(s-1)}, \Sigma) \,.$$

The Metropolis algorithm

For unbounded targets (why?), the classic symmetric proposal is a Gaussian centered at the current state:

$$\boldsymbol{\theta}^* \sim h(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(s-1)}) \equiv N_D(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(s-1)}, \Sigma)\,.$$

Metropolis-Hastings

Our target stationary distribution is $\pi(\boldsymbol{\theta}) = p(\boldsymbol{\theta}|\mathrm{y}) \propto p^*(\boldsymbol{\theta}|\mathrm{y})$.

Inputs:

- $p^*(\boldsymbol{\theta}|\mathrm{y})$
- a not-necessarily-symmetric proposal distribution $h(\boldsymbol{\theta}^*|\boldsymbol{\theta})$
- $\boldsymbol{\theta}^{(0)}$ (chosen or randomly generated however you want)

For $s = 1, \ldots, S$,

1. Generate $\boldsymbol{\theta}^* \sim h(\boldsymbol{\theta}|\boldsymbol{\theta}^{(s-1)})$ and $U \sim Uni(0,1)$
2. Compute

$$a \leftarrow 1 \wedge \frac{p^*(\boldsymbol{\theta}^*|\mathrm{y})\, h(\boldsymbol{\theta}|\boldsymbol{\theta}^*)}{p^*(\boldsymbol{\theta}^{(s-1)}|\mathrm{y})h(\boldsymbol{\theta}^*|\boldsymbol{\theta})} = 1 \wedge \frac{\pi(\boldsymbol{\theta}^*)h(\boldsymbol{\theta}|\boldsymbol{\theta}^*)}{\pi(\boldsymbol{\theta}^{(s-1)})h(\boldsymbol{\theta}^*|\boldsymbol{\theta})}$$

3. IF $U < a$: $\quad \boldsymbol{\theta}^{(s)} \leftarrow \boldsymbol{\theta}^*$;
   ELSE: $\quad \boldsymbol{\theta}^{(s)} \leftarrow \boldsymbol{\theta}^{(s-1)}$

Decomposing the parameter space

- Sometimes it is useful/easier to decompose the parameter space into several components.
- We want to use MH to sample from $\pi(\boldsymbol{\theta}) = \pi(\theta_1, \ldots, \theta_D)$.
- Keep all but one component θ_d fixed and use a univariate proposal to update θ_d.

Decomposing the parameter space

To update the dth component within global MCMC iteration s with state $(\theta_1^{(s)}, \ldots, \theta_{d-1}^{(s)}, \theta_d^{(s-1)}, \ldots, \theta_D^{(s-1)})$.

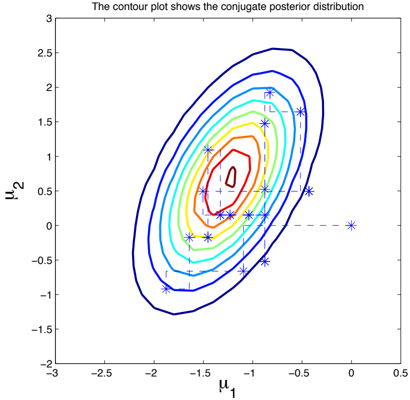
1. Propose $\theta_d^* \sim h_d(\theta_d^* | \theta_1^{(s)}, \ldots, \theta_{d-1}^{(s)}, \theta_d^{(s-1)}, \ldots, \theta_D^{(s-1)})$
   $\equiv h_d(\boldsymbol{\theta}^* | \boldsymbol{\theta})$

2. Accept with probability

$$1 \wedge \frac{\pi(\theta_1^{(s)}, \ldots, \theta_{d-1}^{(s)}, \theta_d^*, \ldots, \theta_D^{(s-1)}) h_d(\boldsymbol{\theta} | \boldsymbol{\theta}^*)}{\pi(\theta_1^{(s)}, \ldots, \theta_{d-1}^{(s)}, \theta_d^{(s-1)}, \ldots, \theta_D^{(s-1)}) h_d(\boldsymbol{\theta}^* | \boldsymbol{\theta})}$$

Decomposing the parameter space

- We can decompose into blocks of components.
- We can use a random scan instead of sequential updates.
- If $\pi(\boldsymbol{\theta})$ invariant to h_1, h_2, then $\pi(\boldsymbol{\theta})$ invariant to $h_1 \circ h_2$.



Neat trick!

Suppose we divide $\boldsymbol{\theta}$ into two components: $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and that

$$h_1(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta})/\pi(\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta}) \,/ \int \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}_1$$

and analogous for $h_2(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)$. Then the MH acceptance criterion is $\boldsymbol{\theta}_1^{(s)}$

$$\begin{aligned} a &= 1 \wedge \frac{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_1^{(s-1)}|\boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^*|\boldsymbol{\theta}_2^{(s-1)})} \\ &= 1 \wedge \frac{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_2^{(s-1)})} \quad = 1 \end{aligned}$$

and similar for $\boldsymbol{\theta}_2^{(s)}$. Thus, we can avoid wasted compute time on rejected proposals.

Neat trick!

But when can we use it?

Part 5. Introduction (?) to Bayesian inference

Bayesian inference

We observe data $y_1, \ldots, y_N \overset{iid}{\sim} p(y_n|\boldsymbol{\theta})$ and assume $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$.
Here,

- $p(\mathrm{y}|\boldsymbol{\theta}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{\theta})$ is the *likelihood*,
- $p(\boldsymbol{\theta})$ is the *prior*,

and the goal of Bayesian inference is to obtain the *posterior*

$$p(\boldsymbol{\theta}|\mathrm{y}) = \frac{p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathrm{y})} = \frac{p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int_{\Theta} p(\mathrm{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}}\,.$$

Conjugate priors

- *Conjugacy* refers to the situation when the prior $p(\boldsymbol{\theta})$ and posterior $p(\boldsymbol{\theta}|\mathrm{y})$ belong to the same distribution (albeit with "updated" parameters).
- When one combines a *conjugate* prior with a specific likelihood, one may obtain the posterior in closed form, no computations necessary!
- Unfortunately, conjugacy only works for a limited class of simple models.

Exponential family distributions

- Exponential family distributions include the normal, beta, Bernoulli, gamma and Poisson distributions.
- If y follows an exponential family distribution, then

$$p(y|\theta) = h(y)g(\boldsymbol{\theta}) \exp\left(\phi(\boldsymbol{\theta})^T s(y)\right) .$$

- The joint distribution for independent $\mathrm{y} = (y_1, \ldots, y_N)$ is

$$p(\mathrm{y}|\boldsymbol{\theta}) = \left(\prod_{n=1}^{N} h(y_n)\right) g^N(\boldsymbol{\theta}) \exp\left(\phi(\boldsymbol{\theta})^T \sum_{n=1}^{N} s(y_n)\right) .$$

- $\phi(\boldsymbol{\theta})$ is the *natural parameter* and $t(\mathrm{y}) = \sum_n s(y_n)$ is the *sufficient statistic*.

Conjugate priors

Again, our likelihood is

$$p(\mathrm{y}|\boldsymbol{\theta}) \propto g^N(\boldsymbol{\theta}) \exp\left(\phi(\boldsymbol{\theta})^T t(\mathrm{y})\right) \ ,$$

and we specify $\boldsymbol{\theta}$ follows an exponential family distribution with prior

$$p(\boldsymbol{\theta}) \propto g(\boldsymbol{\theta})^\eta \exp\left(\phi(\boldsymbol{\theta})^T \nu\right) \ .$$

It follows that

$$p(\boldsymbol{\theta}|\mathrm{y}) \propto g^{N+\eta}(\boldsymbol{\theta}) \exp\left(\phi(\boldsymbol{\theta})^T (t(\mathrm{y}) + \nu)\right) \ .$$

Beta-binomial model

$$p(y|\theta, N) \propto \theta^y (1-\theta)^{N-y} \propto (1-\theta)^N \exp\left(y \log\left(\frac{\theta}{1-\theta}\right)\right)$$

$$\implies \quad g(\theta) = 1-\theta \quad \text{and} \quad \phi(\theta) = \log\left(\frac{\theta}{1-\theta}\right)$$

$$\implies \quad p(\theta) \propto (1-\theta)^\eta \exp\left(\nu \log\left(\frac{\theta}{1-\theta}\right)\right) \propto (1-\theta)^{\eta-\nu}\theta^\nu$$

$$\implies \quad p(\theta) \equiv \text{beta}(\alpha = \nu + 1,\, \beta = \eta - \nu + 1)$$

$$\implies \quad p(\theta|y) \propto (1-\theta)^{(\eta-\nu+N-y)}\theta^{\nu+y}$$

$$\implies \quad p(\theta|y) \equiv \text{beta}(\alpha + y,\, \beta + N - y)$$

$$\implies \quad \mathbb{E}(\theta|y) = (\alpha + y)/(\alpha + \beta + N)$$

Univariate normal, known variance

$$p(\mathrm{y}|\theta,\sigma^2) \propto \exp\left(-\frac{1}{2\sigma^2}\sum_n (y_n-\theta)^2\right) \propto \exp\left(-\frac{N\theta^2}{2\sigma^2}+\frac{\theta}{\sigma^2}\sum_n y_n\right)$$

$$\implies \quad p(\theta) \propto \exp\left(-\frac{\theta^2}{2\tau_0^2}+\frac{\mu_0\theta}{\tau_0^2}\right) \propto \exp\left(-\frac{1}{2\tau_0^2}(\theta-\mu_0)^2\right)$$

$$\begin{aligned}\implies \quad p(\theta|\mathrm{y},\sigma^2) &\propto \exp\left(-\frac{\theta^2}{2\tau_0^2}+\frac{\mu_0\theta}{\tau_0^2}\right)\exp\left(-\frac{N\theta^2}{2\sigma^2}+\frac{\theta}{\sigma^2}\sum_n y_n\right)\\ &\propto \exp\left(-\frac{1}{2}\left(\frac{1}{\tau_0^2}+\frac{N}{\sigma^2}\right)\theta^2+\left(\frac{\mu_0}{\tau_0^2}+\frac{\sum_n y_n}{\sigma^2}\right)\theta\right)\\ &\equiv \mathrm{N}\left(\left(\frac{\mu_0}{\tau_0^2}+\frac{\sum_n y_n}{\sigma^2}\right)\left(\frac{1}{\tau_0^2}+\frac{N}{\sigma^2}\right)^{-1}, \left(\frac{1}{\tau_0^2}+\frac{N}{\sigma^2}\right)^{-1}\right)\end{aligned}$$

Univariate normal, known mean

$$p(\mathrm{y}|\theta, \sigma^2) \propto (\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2}\sum_n (y_n - \theta)^2\right)$$

$$\implies \quad p(\sigma^2) \propto (\sigma^2)^{-\alpha-1} \exp\left(-\frac{\beta}{\sigma^2}\right) \equiv \Gamma^{-1}(\alpha, \beta)$$

$$\implies \quad p(\sigma^2|\mathrm{y}, \theta) \propto (\sigma^2)^{-\alpha-N/2-1} \exp\left(-\frac{\beta}{\sigma^2} + \frac{\sum_n (y_n - \theta)^2}{2\sigma^2}\right)$$
$$\equiv \Gamma^{-1}\left(\alpha + \frac{N}{2}, \beta + \frac{\sum_n (y_n - \theta)^2}{2}\right)$$

Limitations to conjugacy

- We rarely know the variance but not the mean (and vice-versa).
- We don't have the joint posterior for both mean and variance in closed form.
- All we know is the conditional posteriors for either parameter.
- It turns out, this kind of situation is rather common for Bayesian hierarchical models that arise out of pieced together exponential family distributions.

Part 6. Classical MCMC (again)

Neat trick!

Suppose we divide $\boldsymbol{\theta}$ into two components: $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and that

$$h_1(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta})/\pi(\boldsymbol{\theta}_2) = \pi(\boldsymbol{\theta}) \Big/ \int \pi(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}_1$$

and analogous for $h_2(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)$. Then the MH acceptance criterion is $\boldsymbol{\theta}_1^{(s)}$

$$\begin{aligned} a &= 1 \wedge \frac{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_1^{(s-1)}|\boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^*|\boldsymbol{\theta}_2^{(s-1)})} \\ &= 1 \wedge \frac{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_1^{(s-1)}, \boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^{(s-1)})} \times \frac{\pi(\boldsymbol{\theta}_2^{(s-1)})}{\pi(\boldsymbol{\theta}_2^{(s-1)})} \quad = 1 \end{aligned}$$

and similar for $\boldsymbol{\theta}_2^{(s)}$. Thus, we can avoid wasted compute time on rejected proposals.

Neat trick!

But when can we use it?

A Gibbs sampler

We assume our data $\mathrm{y} = (y_1, \ldots, y_N) \stackrel{iid}{\sim} N(\theta, \sigma^2)$ and priors

$$\theta \sim \mathrm{N}(\mu_0, \tau_0^2) \quad \text{and} \quad \sigma^2 \sim \Gamma^{-1}(\alpha, \beta)\,.$$

We wish to generate samples from $p(\theta, \sigma^2 | \mathrm{y})$. Initialize $\theta^{(0)}$ and $\sigma^{(0)}$. For $s = 1, \ldots, S$,

1. Draw from $p(\theta | \mathrm{y}, \sigma^2)$ with $\sigma^2 = \sigma^{2(s-1)}$:

$$\theta^{(s)} \sim \mathrm{N}\left(\left(\frac{\mu_0}{\tau_0^2} + \frac{\sum_n y_n}{\sigma^2}\right)\left(\frac{1}{\tau_0^2} + \frac{N}{\sigma^2}\right)^{-1}, \left(\frac{1}{\tau_0^2} + \frac{N}{\sigma^2}\right)^{-1}\right).$$

2. Draw from $p(\sigma^2 | \mathrm{y}, \theta)$ with $\theta = \theta^{(s)}$:

$$\sigma^{2(s)} \sim \Gamma^{-1}\left(\alpha + \frac{N}{2}, \beta + \frac{\sum_n (y_n - \theta)^2}{2}\right)$$

No need for the accept/reject step!

Another Gibbs sampler

We assume our data $y_n \overset{ind}{\sim} N(\theta_n, \sigma^2)$, $n = 1, \ldots, N$,

$$\theta_n \overset{iid}{\sim} N(\theta_0, \tau_0^2) \quad \text{and} \quad \theta_0 \sim N(0, 10)\,.$$

We wish to sample from $p(\theta_0, \theta_1, \ldots, \theta_N | \mathrm{y}, \sigma^2, \tau^2)$. After initialization, for $s = 1, \ldots, S$:

1. Draw from $p(\theta_0 | \mathrm{y}, \tau^2, \theta_1^{(s-1)}, \ldots, \theta_N^{(s-1)})$:

$$\theta_0^{(s)} \sim \mathrm{N}\left(\left(\frac{\sum_n \theta_n^{(s-1)}}{\tau_0^2}\right)\left(\frac{N}{\tau_0^2} + \frac{1}{10}\right)^{-1}, \left(\frac{N}{\tau_0^2} + \frac{1}{10}\right)^{-1}\right)$$

2. For $n = 1, \ldots, N$, draw from $p(\theta_n | \mathrm{y}, \sigma^2, \tau^2, \theta_0^{(s)})$:

$$\theta_1^{(s)} \sim \mathrm{N}\left(\left(\frac{\theta_0^{(s)}}{\tau_0^2} + \frac{y_n}{\sigma^2}\right)\left(\frac{1}{\tau_0^2} + \frac{1}{\sigma^2}\right)^{-1}, \left(\frac{1}{\tau_0^2} + \frac{1}{\sigma^2}\right)^{-1}\right).$$

Pros and cons of Gibbs sampling

Pros:

- No wasted compute time on rejected proposals.
- For big data, factorization helps
    1. data storage
    2. parallel computing.

Cons:

- You're only as strong as your weakest link. (But isn't this always true?)
- Coding by hand can be time intensive. (But isn't there software for that?)
- Conditional posteriors aren't always known. (But isn't there Metropolis-within-Gibbs for that?)