SDS 383C: Statistical Modeling I Fall 2022, Module VII

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"All models are wrong, but some are useful."- George E. P. Box

- We want to compute the integral $\int_{\mathcal{Y}} h(\mathbf{y}) d\mathbf{y}$, $\mathcal{Y} \subseteq \mathbb{R}^d$.
- Let h(y) = g(y)p(y) where p(y) is a density on \mathcal{Y} . Then

$$\mathbf{I} = \int_{\mathcal{Y}} h(\mathbf{y}) d\mathbf{y} = \int_{\mathcal{Y}} g(\mathbf{y}) p(\mathbf{y}) d\mathbf{y} = \mathbb{E}_{\mathbf{y} \sim p(\mathbf{y})} g(\mathbf{y}).$$

• Let y_1, \ldots, y_n be a random sample from p(y). Then

$$\mathbf{I} = \mathbb{E}_{p(\mathbf{y})} g(\mathbf{y}) \stackrel{\triangle}{=} \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{y}_i) = \widehat{\mathbf{I}}.$$

Monte Carlo standard error

$$SE^{2}(\widehat{\mathbf{I}}) \stackrel{\frown}{=} \frac{1}{n(n-1)} \sum_{i=1}^{n} \left\{ g(\mathbf{y}_{i}) - \widehat{\mathbf{I}} \right\}^{2}.$$

- The joint posterior may be complex or known only up to a normalizing constant but we may need to evaluate $\int a(\theta) v(\theta \mid \mathbf{v}_{1:n}) d\theta$.
- We may still be able to sample from the posterior and evaluate this as

$$\int g(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{y}_{1:n}) d\boldsymbol{\theta} \stackrel{\triangle}{=} \frac{1}{n} \sum_{i=1}^{n} g(\boldsymbol{\theta}_i)$$

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likelihood prior

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 $\int g(\mathbf{o})p(\mathbf{o} \mid \mathbf{y}_{1:n})d\mathbf{o} = \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{o}_i).$

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- The density p(y) is of interest but is difficult to sample from.
- The density q(y) roughly approximates p(y) and is easier to sample from.

• Then
$$\mathbf{I} = \int_{\mathcal{Y}} g(\mathbf{y}) p(\mathbf{y}) d\mathbf{y} = \int_{\mathcal{Y}} g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} q(\mathbf{y}) d\mathbf{y} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\}.$$

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An alternative formulation is

$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^{n} w_{i} g(\mathbf{y}_{i})}{\sum_{i=1}^{n} w_{i}} = \widehat{\mathbf{I}}_{2} \quad \text{where} \quad w_{i} = \frac{p(\mathbf{y}_{i})}{q(\mathbf{y}_{i})}.$$

- $\mathbb{E}(w_i) = \int \frac{p(\mathbf{y})}{q(\mathbf{y})} q(\mathbf{y}) d\mathbf{y} = \int p(\mathbf{y}) d\mathbf{y} = 1$ so that $\mathbb{E}\left(\sum_{i=1}^n w_i\right) = n$.
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$$SE^2(\widehat{\mathbf{I}}_2) \stackrel{\frown}{=} \frac{\sum_{i=1}^n w_i \left\{ g(\mathbf{y}_i) - \widehat{\mathbf{I}}_2 \right\}^2}{\sum_{i=1}^n w_i}$$

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- The density p(y) is of interest but is difficult to sample from.
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$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^{n} w_{i} g(\mathbf{y}_{i})}{\sum_{i=1}^{n} w_{i}} = \widehat{\mathbf{I}}_{2} \quad \text{where} \quad w_{i} = \frac{p(\mathbf{y}_{i})}{q(\mathbf{y}_{i})}.$$

- $\mathbb{E}(w_i) = \int \frac{p(\mathbf{y})}{q(\mathbf{y})} q(\mathbf{y}) d\mathbf{y} = \int p(\mathbf{y}) d\mathbf{y} = 1$ so that $\mathbb{E}\left(\sum_{i=1}^n w_i\right) = n$.
- Monte Carlo standard error

$$SE^2(\widehat{\mathbf{I}}_2) \stackrel{\frown}{=} \frac{\sum_{i=1}^n w_i \left\{ g(\mathbf{y}_i) - \widehat{\mathbf{I}}_2 \right\}^2}{\sum_{i=1}^n w_i}.$$

- $\widehat{\mathbf{I}}_1 \stackrel{P}{\to} \mathbf{I}$ and $\widehat{\mathbf{I}}_2 \stackrel{P}{\to} \mathbf{I}$ as $n \to \infty$.
- $\hat{\mathbf{I}}_2$ also works when the normalizing constant of $p(\mathbf{y})$ is NOT known

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- The density p(y) is of interest but is difficult to sample from.
- The density $q(\mathbf{y})$ roughly approximates $p(\mathbf{y})$ and is easier to sample from.
- Then $\mathbf{I} = \int_{\mathcal{Y}} g(\mathbf{y}) p(\mathbf{y}) d\mathbf{y} = \int_{\mathcal{Y}} g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} q(\mathbf{y}) d\mathbf{y} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\}.$
- Let y_1, \ldots, y_n be a random sample from q(y). Then

$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{y}_i) \frac{p(\mathbf{y}_i)}{q(\mathbf{y}_i)} = \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{y}_i) w_i = \widehat{\mathbf{I}}_1.$$

An alternative formulation is

$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^{n} w_{i} g(\mathbf{y}_{i})}{\sum_{i=1}^{n} w_{i}} = \widehat{\mathbf{I}}_{2} \quad \text{where} \quad w_{i} = \frac{p(\mathbf{y}_{i})}{q(\mathbf{y}_{i})}.$$

- $\mathbb{E}(w_i) = \int \frac{p(\mathbf{y})}{q(\mathbf{y})} q(\mathbf{y}) d\mathbf{y} = \int p(\mathbf{y}) d\mathbf{y} = 1$ so that $\mathbb{E}\left(\sum_{i=1}^n w_i\right) = n$.
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$$SE^2(\widehat{\mathbf{I}}_2) \stackrel{\triangle}{=} \frac{\sum_{i=1}^n w_i \left\{ g(\mathbf{y}_i) - \widehat{\mathbf{I}}_2 \right\}^2}{\sum_{i=1}^n w_i}.$$

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 \mathbf{I}_2 also works when the normalizing constant of $p(\mathbf{y})$ is NOT known.

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- Let y_1, \ldots, y_n be a random sample from q(y). Then

$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{y}_i) \frac{p(\mathbf{y}_i)}{q(\mathbf{y}_i)} = \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{y}_i) w_i = \widehat{\mathbf{I}}_1.$$

An alternative formulation is

$$\mathbf{I} = \mathbb{E}_{\mathbf{y} \sim q(\mathbf{y})} \left\{ g(\mathbf{y}) \frac{p(\mathbf{y})}{q(\mathbf{y})} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^{n} w_{i} g(\mathbf{y}_{i})}{\sum_{i=1}^{n} w_{i}} = \widehat{\mathbf{I}}_{2} \quad \text{where} \quad w_{i} = \frac{p(\mathbf{y}_{i})}{q(\mathbf{y}_{i})}.$$

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- $\hat{\mathbf{I}}_2$ also works when the normalizing constant of $p(\mathbf{y})$ is NOT known.

▶ Likelihood: $y_1, ..., y_n \stackrel{iid}{\sim} \text{Bernoulli}(\theta) \text{ with } p(y_i \mid \theta) = \theta^{y_i} (1 - \theta)^{1 - y_i}$

▶ Prior: $p(\theta) \propto \cos^2(4\pi\theta) = \widetilde{p}(\theta)$

▶ Posterior: $p(\theta \mid \mathbf{y}_{1:n}) \propto \cos^2(4\pi\theta) \ \theta^s (1-\theta)^{n-s} = \widetilde{p}(\theta \mid \mathbf{y}_{1:n})$

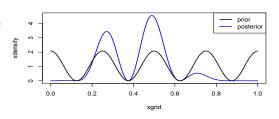
- ▶ Likelihood: $y_1, ..., y_n \stackrel{iid}{\sim} \text{Bernoulli}(\theta) \text{ with } p(y_i \mid \theta) = \theta^{y_i} (1 \theta)^{1 y_i}$
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$$\begin{split} p(\theta) &= \frac{\widetilde{p}(\theta)}{\mathbf{I}_{prior}}, \quad p(\theta \mid \mathbf{y}_{1:n}) = \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{\mathbf{I}_{post}}, \text{ where} \\ \mathbf{I}_{prior} &= \int_{\Theta} \widetilde{p}(\theta) d\theta = \int_{\Theta} \frac{\widetilde{p}(\theta)}{q(\theta)} q(\theta) d\theta = \mathbb{E}_{\theta \sim q(\theta)} \left\{ \frac{\widetilde{p}(\theta)}{q(\theta)} \right\}, \\ \mathbf{I}_{post} &= \int_{\Theta} \widetilde{p}(\theta \mid \mathbf{y}_{1:n}) d\theta = \int_{\Theta} \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{q(\theta)} q(\theta) d\theta = \mathbb{E}_{\theta \sim q(\theta)} \left\{ \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{q(\theta)} \right\}. \end{split}$$

- ▶ Likelihood: $y_1, ..., y_n \stackrel{iid}{\sim} \text{Bernoulli}(\theta) \text{ with } p(y_i \mid \theta) = \theta^{y_i} (1 \theta)^{1 y_i}$
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$$\begin{split} p(\theta) &= \frac{\widetilde{p}(\theta)}{\mathbf{I}_{prior}}, \quad p(\theta \mid \mathbf{y}_{1:n}) = \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{\mathbf{I}_{post}}, \text{ where} \\ \mathbf{I}_{prior} &= \int_{\Theta} \widetilde{p}(\theta) d\theta = \int_{\Theta} \frac{\widetilde{p}(\theta)}{q(\theta)} q(\theta) d\theta = \mathbb{E}_{\theta \sim q(\theta)} \left\{ \frac{\widetilde{p}(\theta)}{q(\theta)} \right\}, \\ \mathbf{I}_{post} &= \int_{\Theta} \widetilde{p}(\theta \mid \mathbf{y}_{1:n}) d\theta = \int_{\Theta} \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{q(\theta)} q(\theta) d\theta = \mathbb{E}_{\theta \sim q(\theta)} \left\{ \frac{\widetilde{p}(\theta \mid \mathbf{y}_{1:n})}{q(\theta)} \right\}. \end{split}$$

- Importance sampling density: $q(\theta) = \text{Beta}(2, 2)$
- lterations M = 500,000
- ightharpoonup I_{prior} pprox 0.4940351
- $n = 10, \ s = \sum_{i} y_i = 4$
- ▶ $I_{post} \approx 0.0002172$



- The density p(y) is of interest but is difficult to sample from.
- The density q(y) roughly approximates p(y) and is easier to sample from.
- Then

$$F_{p}(y) = \int_{-\infty}^{y} p(z)dz = \int_{-\infty}^{\infty} 1(z \le y)p(z)dz = \int_{-\infty}^{\infty} 1(z \le y)p(z)dz$$
$$= \int_{-\infty}^{\infty} 1(z \le y)\frac{p(z)}{q(z)}q(z)dz = \mathbb{E}_{z \sim q(z)}\left\{1(z \le y)\frac{p(z)}{q(z)}\right\}.$$

• Let z_1, \ldots, z_n be a random sample from q(z). Then

$$F_p(y) = \mathbb{E}_{z \sim q(z)} \left\{ 1(z \leq y) \frac{p(z)}{q(z)} \right\} \stackrel{\frown}{=} \frac{1}{n} \sum_{i=1}^n 1(z_i \leq y) \frac{p(z_i)}{q(z_i)} = \frac{1}{n} \sum_{i=1}^n 1(z_i \leq y) w_i = \widehat{F}_1(y) = 0$$

An alternative formulation is

$$F_p(y) = \mathbb{E}_{z \sim q(z)} \left\{ 1(z \le y) \frac{p(z)}{q(z)} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^n w_i 1(z_i \le y)}{\sum_{i=1}^n w_i} = \sum_{i=1}^n \widetilde{w}_i 1(z_i \le y) = \widehat{F}_2(y)$$

- $\widehat{F}_1(y) \stackrel{P}{\to} F_p(y)$ and $\widehat{F}_2(y) \stackrel{P}{\to} F_p(y)$ as $n \to \infty$.
- $\widehat{F}_2(y)$ also works when the normalizing constant of p(z) is NOT known
- $\widehat{F}_2(y)$ shows that sampling from p(y) can be approximated by resampling the z_i 's with weights \widetilde{w}_i 's.

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$$F_p(y) = \mathbb{E}_{z \sim q(z)} \left\{ 1(z \le y) \frac{p(z)}{q(z)} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^n w_i 1(z_i \le y)}{\sum_{i=1}^n w_i} = \sum_{i=1}^n \widetilde{w}_i 1(z_i \le y) = \widehat{F}_2(y).$$

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An alternative formulation is

$$F_p(y) = \mathbb{E}_{z \sim q(z)} \left\{ 1(z \le y) \frac{p(z)}{q(z)} \right\} \stackrel{\triangle}{=} \frac{\sum_{i=1}^n w_i 1(z_i \le y)}{\sum_{i=1}^n w_i} = \sum_{i=1}^n \widetilde{w}_i 1(z_i \le y) = \widehat{F}_2(y).$$

- $\widehat{F}_1(y) \stackrel{P}{\to} F_p(y)$ and $\widehat{F}_2(y) \stackrel{P}{\to} F_p(y)$ as $n \to \infty$.
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• $\bar{F}_2(y)$ shows that sampling from p(y) can be approximated by resampling the z_i 's with weights \widetilde{w}_i 's.

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_{t-1}) \longrightarrow (y_t) \longrightarrow (y_{t+1}) \longrightarrow \cdots$$

• Initial Distribution: probability that the chain starts with a state y:

$$p(y_0 = y) = \pi_0(y).$$

• Transition Probabilities: probability that the chain moves to a state y from a state x in a single step:

$$p(y_{t+1} = y \mid y_t = x) = p(y \mid x) = p(x \to y) = p(x, y).$$

- Transition Probability Matrix: $\mathbf{P} = \Big(\Big(p(x,y)\Big)\Big)$
- The probability that the chain is in state y at time t: $p(y_t = y) = \pi_t(y)$

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow \cdots$$

• **Initial Distribution:** probability that the chain starts with a state *y*:

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• **Initial Distribution:** probability that the chain starts with a state *y*:

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow \cdots$$

• **Initial Distribution:** probability that the chain starts with a state *y*:

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- The probability that the chain is in state y at time t: $p(y_t = y) = \pi_t(y)$.

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{\mathbf{y}_{t-2}} \quad y_{t-1} \xrightarrow{\mathbf{y}_{t}} \quad y_t \xrightarrow{\mathbf{y}_{t+1}} \quad \cdots$$

• **Initial Distribution:** probability that the chain starts with a state *y*:

$$p(y_0 = y) = \pi_0(y).$$

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$$p(y_{t+1} = y \mid y_t = x) = p(y \mid x) = p(x \to y) = p(x, y).$$

- Transition Probability Matrix: $\mathbf{P} = (p(x, y))$.
- The probability that the chain is in state y at time t: $p(y_t = y) = \pi_t(y)$.
- We have $\sum_{y \in \mathcal{Y}} p(x, y) = 1 \quad \forall \ x \in \mathcal{Y}, \qquad \sum_{y \in \mathcal{Y}} p(y_t = y) = 1.$

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{y_{t-2}} \quad y_{t-1} \xrightarrow{y_t} \quad y_t \xrightarrow{y_{t+1}} \quad \cdots$$

• **Initial Distribution:** probability that the chain starts with a state *y*:

$$p(y_0 = y) = \pi_0(y).$$

• **Transition Probabilities:** probability that the chain moves to a state *y* from a state *x* in a single step:

$$p(y_{t+1} = y \mid y_t = x) = p(y \mid x) = p(x \to y) = p(x, y).$$

- Transition Probability Matrix: $\mathbf{P} = (p(x, y))$.
- The probability that the chain is in state y at time t: $p(y_t = y) = \pi_t(y)$.
- We have P1 = 1, $\pi_t 1 = 1$.

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_{t-1}) \longrightarrow (y_t) \longrightarrow (y_{t+1}) \longrightarrow \cdots$$

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- We have P1 = 1, $\pi_t 1 = 1$.
- Chapman-Kolmogorov Equation: $\pi_{t+1}(y) = p(y_{t+1} = y)$ $= \sum_{x \in \mathcal{Y}} p(y_{t+1} = y \mid y_t = x) p(y_t = x)$ $= \sum_{x \in \mathcal{Y}} p(x, y) \pi_t(x).$

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow$$

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- We have $\pi_t = \pi_{t-1} \mathbf{P} = \pi_{t-2} \mathbf{P}^2 = \cdots = \pi_0 \mathbf{P}^t$.

Markov Chains - Stationarity

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{\mathbf{y}_{t-2}} \quad y_{t-1} \xrightarrow{\mathbf{y}_{t-1}} \quad y_t \xrightarrow{\mathbf{y}_{t+1}} \quad \cdots$$

• Irreducibility: A Markov chain is irreducible if the chain can move from any state to any other in finite steps - there exists some $n \in \mathbb{N}$ such that

$$p^n(x,y) > 0 \quad \forall \ x,y \in \mathcal{Y}.$$

 Aperiodicity: A Markov chain is aperiodic if the number of steps required to move between two states is not a multiple of some integer:

$$GCD\{n: p^n(x,y) > 0 \mid \forall x, y \in \mathcal{Y}\} = 1.$$

- Aperiodic Markov chains are NOT forced into cycles of fixed lengths between certain states.
- Stationarity: A Markov chain may reach stationarity when the probability of being in any particular state is independent of the initial state.
- The stationary distribution π satisfies

$$\pi = \pi \mathbf{P}$$
.

Irreducible and aperiodic Markov chains converge to stationarity

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Markov Chains - Stationarity

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{\mathbf{y}_{t-2}} \quad y_{t-1} \xrightarrow{\mathbf{y}_{t-1}} \quad y_t \xrightarrow{\mathbf{y}_{t+1}} \quad \cdots$$

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Irreducible and aperiodic Markov chains converge to stationarity

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Irreducible and aperiodic Markov chains converge to stationarity

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Irreducible and aperiodic Markov chains converge to stationarity

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Irreducible and aperiodic Markov chains converge to stationarity.

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{\mathbf{y}_{t-2}} \quad y_{t-1} \xrightarrow{\mathbf{y}_{t-1}} \quad y_t \xrightarrow{\mathbf{y}_{t+1}} \quad \cdots$$

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Irreducible and aperiodic Markov chains converge to stationarity.

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Markov Chains

$$\mathbf{P} = \begin{array}{ccc} 1 & 2 \\ 0.4 & 0.6 \\ 2 & \begin{bmatrix} 0.4 & 0.6 \\ 0.6 & 0.4 \end{bmatrix}, & \pi \mathbf{P} = \pi \quad \Rightarrow \quad \pi = (0.5, 0.5).$$

$$\mathbf{P} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 1 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 0 & 0 & 0 & 0 \end{bmatrix}$$

 $ightarrow \,$ irreducible, periodic Markov chain with period 4

Markov Chains

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \dots \quad \xrightarrow{y_{t-2}} \quad y_{t-1} \quad y_t \quad y_{t+1} \quad \dots$$

$$\begin{array}{c} 1 \quad 2 \quad 3 \quad 4 \quad 5 \\ 0.4 \quad 0.6 \quad 0 \quad 0 \quad 0 \\ 0.6 \quad 0.4 \quad 0 \quad 0 \quad 0 \\ 0 \quad 0 \quad 0.3 \quad 0.7 \quad 0 \\ 0 \quad 0 \quad 0.3 \quad 0.7 \quad 0 \\ 4 \quad 0 \quad 0 \quad 0.4 \quad 0.4 \quad 0.2 \\ 5 \quad 0 \quad 0 \quad 0 \quad 0.2 \quad 0.8 \end{array} \right], \qquad 1 \leftrightarrow 2,$$

$$3 \leftrightarrow 4 \leftrightarrow 5.$$

$$\mathbf{P} = \begin{array}{cc} 1 & 2 \\ 1 & \begin{bmatrix} 0.4 & 0.6 \\ 0.6 & 0.4 \end{bmatrix}, \end{array}$$

$$\boldsymbol{\pi}\mathbf{P} = \boldsymbol{\pi} \quad \Rightarrow \quad \boldsymbol{\pi} = (0.5, 0.5).$$

$$\mathbf{P} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 1 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 0 & 0 & 0 & 0 \end{bmatrix}$$

→ irreducible, periodic Markov chain with period 4.

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Markov Chains

$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{\mathbf{y}_{t-2}} \quad \underbrace{\mathbf{y}_{t-1}} \quad \underbrace{\mathbf{y}_{t}} \quad \underbrace{\mathbf{y}_{t+1}} \quad \cdots$$

$$\mathbf{P} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 0.4 & 0.6 & 0 & 0 & 0 \\ 2 & 0.6 & 0.4 & 0 & 0 & 0 \\ 0 & 0 & 0.3 & 0.7 & 0 \\ 4 & 0 & 0 & 0.4 & 0.4 & 0.2 \\ 5 & 0 & 0 & 0 & 0.2 & 0.8 \end{bmatrix}, \qquad 1 \leftrightarrow 2, \\ 3 \leftrightarrow 4 \leftrightarrow 5.$$

$$\mathbf{P} = \begin{array}{ccc} 1 & 2 \\ 0.4 & 0.6 \\ 0.6 & 0.4 \end{array} , \qquad \qquad \boldsymbol{\pi} \mathbf{P} = \boldsymbol{\pi} \quad \Rightarrow \quad \boldsymbol{\pi} = (0.5, 0.5).$$

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_{t-1}) \longrightarrow (y_t) \longrightarrow (y_{t+1}) \longrightarrow \cdots$$

- Detailed Balance Equation: $\pi^*(x)p(x,y) = \pi^*(y)p(y,x) \ \ \forall \ (x,y) \in \mathcal{Y}^2$.
- Reversibility: A Markov chain is reversible if the detailed balanced equation holds
- Detailed balance equation implies $\pi^* = \pi^* \mathbf{P}$.

$$(\pi^* \mathbf{P})_y = \sum_x \pi^*(x) p(x, y) = \sum_x \pi^*(y) p(y, x) = \pi^*(y) \sum_x p(y, x) = \pi^*(y)$$

• This implies $\pi^* = \pi$, the stationary distribution of **P**

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow$$

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$$(\boldsymbol{\pi}^{\star}\mathbf{P})_{y} = \sum_{x} \pi^{\star}(x) p(x,y) = \sum_{x} \pi^{\star}(y) p(y,x) = \pi^{\star}(y) \sum_{x} p(y,x) = \pi^{\star}(y)$$

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow$$

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow (y_t) \longrightarrow \cdots$$

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \xrightarrow{} (y_{t-2}) \xrightarrow{} (y_{t-1}) \xrightarrow{} (y_t) \xrightarrow{} \cdots$$

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow y_{t-2} \longrightarrow y_{t-1} \longrightarrow y_t \longrightarrow y_{t+1} \longrightarrow \cdots$$

- Transition Probability Kernel: $\int p(x,y)dy = 1$.
- Chapman-Kolmogorov Equation: $\pi_t(y) = \int \pi_{t-1}(x) p(x,y) dx$
- Detailed Balance Equation: $\pi(x)p(x,y) = \pi(y)p(y,x) \ \forall \ (x,y) \in \mathcal{Y}^2$
- Stationary Distribution: $\pi(y) = \int \pi(x)p(x,y)dx$.

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$$p(y_{t+1} \mid y_0, y_1, \dots, y_t) = p(y_{t+1} \mid y_t) \quad \cdots \quad \longrightarrow (y_{t-2}) \longrightarrow (y_{t-1}) \longrightarrow (y_t) \longrightarrow (y_{t+1}) \longrightarrow \cdots$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

- Goal is to draw random samples from a (generic) distribution $p(\theta)$ possibly known only up to its normalizing constant, e.g., a complex joint posterior $p(\theta \mid \mathbf{y}_{1:n})$.
- Iterative Algorithm (Metropolis Sampler): Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.
 - (a) Generate a candidate θ^* using a 'proposal distribution' $q(\theta^{(t-1)} \to \theta^*)$ satisfying $q(\theta^{(t-1)} \to \theta^*) = q(\theta^* \to \theta^{(t-1)})$.
 - (b) Compute $\alpha = \min \left\{ 1, \frac{p(\theta^*)}{p(\theta^{(t-1)})} \right\}$
 - (c) With probability α , set $\theta^{(t)} = \theta^*$. With probability (1α) , set $\theta^{(t)} = \theta^{(t-1)}$
- Iterative Algorithm (Metropolis-Hastings Sampler): Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.
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• Step (c): Draw $r \sim \text{Unif}(0,1)$. If $r \leq \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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- Iterative Algorithm (Metropolis-Hastings Sampler): Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.
 - (a) Generate a candidate θ^* using a 'proposal distribution' $q(\theta^{(t-1)} \to \theta^*)$.
 - (b) Compute $\alpha = \min \left\{ 1, \frac{p(\boldsymbol{\theta}^*)q(\boldsymbol{\theta}^* \to \boldsymbol{\theta}^{(t-1)})}{p(\boldsymbol{\theta}^{(t-1)})q(\boldsymbol{\theta}^{(t-1)} \to \boldsymbol{\theta}^*)} \right\}$.
 - (c) With probability α , set $\theta^{(t)} = \theta^*$. With probability (1α) , set $\theta^{(t)} = \theta^{(t-1)}$.

• Step (c): Draw $r \sim \text{Unif}(0,1)$. If $r \leq \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

- Goal is to draw random samples from a (generic) distribution $p(\theta)$ possibly known only up to its normalizing constant, e.g., a complex joint posterior $p(\theta \mid \mathbf{y}_{1:n})$.
- Iterative Algorithm (Metropolis Sampler):

Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.

- (a) Generate a candidate θ^* using a 'proposal distribution' $q(\theta^{(t-1)} \to \theta^*)$ satisfying $q(\theta^{(t-1)} \to \theta^*) = q(\theta^* \to \theta^{(t-1)})$.
- (b) Compute $\alpha = \min \left\{ 1, \frac{p(\boldsymbol{\theta}^*)}{p(\boldsymbol{\theta}^{(t-1)})} \right\}$.
- (c) With probability α , set $\theta^{(t)} = \theta^*$. With probability (1α) , set $\theta^{(t)} = \theta^{(t-1)}$.
- Iterative Algorithm (Metropolis-Hastings Sampler):

Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.

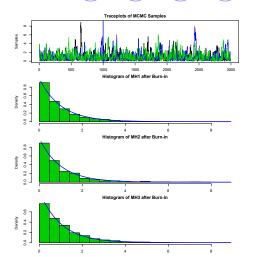
- (a) Generate a candidate θ^* using a 'proposal distribution' $q(\theta^{(t-1)} \to \theta^*)$.
- (b) Compute $\alpha = \min \left\{ 1, \frac{p(\boldsymbol{\theta}^*)q(\boldsymbol{\theta}^* \to \boldsymbol{\theta}^{(t-1)})}{p(\boldsymbol{\theta}^{(t-1)})q(\boldsymbol{\theta}^{(t-1)} \to \boldsymbol{\theta}^*)} \right\}$.
- (c) With probability α , set $\theta^{(t)} = \theta^*$. With probability (1α) , set $\theta^{(t)} = \theta^{(t-1)}$.
- Step (c): Draw $r \sim \text{Unif}(0,1)$. If $r \leq \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

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Metropolis-Hastings Sampler - Sampling from an Exponential

$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \theta_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t+1} \end{pmatrix} \longrightarrow$$

- ▶ Target: $p(\theta) = \exp(-\theta)$
- ► Proposal: $q(\theta^* | \theta^{(t-1)}) =$ Normal $(\theta^* | \theta^{(t-1)}, \sigma_{\theta}^2)$
- ▶ Start with some $\theta^{(0)}$.
- Propose θ^* according to $q(\theta^*|\theta^{(t-1)})$.
- Compute $\alpha = \min \left\{ 1, \frac{p(\theta^*)}{p(\theta^{(t-1)})} \right\}.$
- ightharpoonup Draw r = Unif(0, 1).
- ▶ If $r \le \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$



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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• The transition probability kernel of the MH sampler is

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

• For all $(x,y) \in \mathcal{Y}^2$, either $\alpha(x,y) = 1$ or $\alpha(y,x) = 1$. If $\alpha(x,y) = 1$, then

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

$$\Leftrightarrow \alpha(y,x)p(y)q(y,x) = p(x)q(x,y)\alpha(x,y)$$

$$\Leftrightarrow p(y)p(y,x) = p(x)p(x,y).$$

- ructs a Markov chain with stationary distribution n(u)
- Irrespective of initial values, when run long enough, MH sampler eventually draws samples from the stationary distribution p(u).

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• The transition probability kernel of the MH sampler is

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

- For all $(x,y) \in \mathcal{Y}^2$, either $\alpha(x,y) = 1$ or $\alpha(y,x) = 1$. If $\alpha(x,y) = 1$, then $\alpha(y,x) = \frac{p(x)q(x,y)}{p(y)q(y,x)} = \frac{p(x)q(x,y)\alpha(x,y)}{p(y)q(y,x)}$ $\Leftrightarrow \alpha(y,x)p(y)q(y,x) = p(x)q(x,y)\alpha(x,y)$ $\Leftrightarrow p(y)p(y,x) = p(x)p(x,y).$
- MH sampler constructs a Markov chain with stationary distribution p(y)
- Irrespective of initial values, when run long enough, MH sampler eventually draws samples from the stationary distribution p(y).

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• The transition probability kernel of the MH sampler is

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

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- MH sampler constructs a Markov chain with stationary distribution p(y).
- Irrespective of initial values, when run long enough, MH sampler eventually draws samples from the stationary distribution p(y).

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• The transition probability kernel of the MH sampler is

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

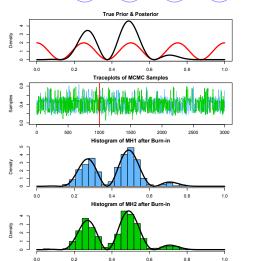
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- MH sampler constructs a Markov chain with stationary distribution p(y).
- Irrespective of initial values, when run long enough, MH sampler eventually draws samples from the stationary distribution p(y).

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Metropolis-Hastings Sampler - Sampling from a Complex Posterior

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \left(\boldsymbol{\theta}_{t-2}\right) \rightarrow \left(\boldsymbol{\theta}_{t-1}\right) \rightarrow \left(\boldsymbol{\theta}_t\right) \rightarrow \left(\boldsymbol{\theta}_{t+1}\right) \rightarrow \cdots$$

- Likelihood: $p(y_i \mid \theta) = \theta^{y_i} (1 \theta)^{1 y_i}$
- ▶ Prior: $p(\theta) \propto \cos^2(4\pi\theta)$
- Target: $p(\theta \mid \mathbf{y}_{1:n}) \propto \cos^2(4\pi\theta) \, \theta^s (1-\theta)^{n-s}$
- ▶ Proposal: $q(\theta^{\star}|\theta^{(t-1)}) = \text{Normal}(\theta^{\star}|\theta^{(t-1)}, \sigma_{\theta}^2)$
- ▶ Start with some $\theta^{(0)}$.
- Propose θ^* according to $q(\theta^*|\theta^{(t-1)})$.
- ightharpoonup Draw r = Unif(0, 1).
- If $r \le \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

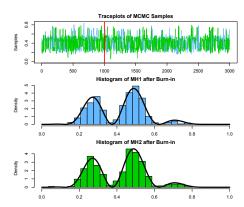


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Metropolis-Hastings Sampler - Mixing

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

- Good Mixing: The chain explores the whole parameter space well.
- Poor Mixing 1: The chain stays in small regions of the parameter space
- Poor Mixing 2: The chain makes big jumps with little acceptance
 - Likelihood: $p(y_i \mid \theta) = \theta^{y_i} (1 - \theta)^{1 - y_i}$
 - Prior: $p(\theta) \propto \cos^2(4\pi\theta)$
- Target: $p(\theta \mid \mathbf{y}_{1:n}) \propto \cos^2(4\pi\theta) \, \theta^s (1-\theta)^{n-s}$
- ► Proposal: $q(\theta^*|\theta^{(t-1)}) =$ Normal $(\theta^*|\theta^{(t-1)}, \frac{\textbf{0.25}^2}{\textbf{0.25}^2})$
- ► Starting points: MH1: $\theta^{(0)} = 0.50$, MH2: $\theta^{(0)} = 0.25$



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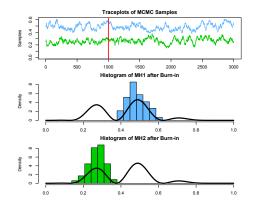
Metropolis-Hastings Sampler - Mixing

$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \rightarrow \left(\theta_{t-2}\right) \rightarrow \left(\theta_{t-1}\right) \rightarrow \left(\theta_t\right) \rightarrow \left(\theta_{t+1}\right) \rightarrow \cdots$$

- Good Mixing: The chain explores the whole parameter space well.
- **Poor Mixing 1:** The chain stays in small regions of the parameter space.
- Poor Mixing 2: The chain makes big jumps with little acceptance.
 - Likelihood:

$$p(y_i \mid \theta) = \theta^{y_i} (1 - \theta)^{1 - y_i}$$

- Prior: $p(\theta) \propto \cos^2(4\pi\theta)$
- ► Target: $p(\theta \mid \mathbf{y}_{1:n}) \propto \cos^2(4\pi\theta) \, \theta^s (1-\theta)^{n-s}$
- ► Proposal: $q(\theta^*|\theta^{(t-1)}) = \text{Normal}(\theta^*|\theta^{(t-1)}, \frac{\textbf{0.01}^2}{\textbf{0.01}^2})$
- Starting points: MH1: $\theta^{(0)} = 0.50$, MH2: $\theta^{(0)} = 0.25$

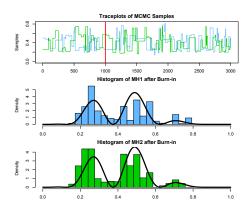


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Metropolis-Hastings Sampler - Mixing

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

- Good Mixing: The chain explores the whole parameter space well.
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 - Likelihood: $p(y_i \mid \theta) = \theta^{y_i} (1 - \theta)^{1 - y_i}$
 - Prior: $p(\theta) \propto \cos^2(4\pi\theta)$
- Target: $p(\theta \mid \mathbf{y}_{1:n}) \propto \cos^2(4\pi\theta) \, \theta^s (1-\theta)^{n-s}$
- Proposal: $q(\theta^*|\theta^{(t-1)}) = \text{Normal}(\theta^*|\theta^{(t-1)}, \mathbf{4^2})$
- ► Starting points: MH1: $\theta^{(0)} = 0.50$, MH2: $\theta^{(0)} = 0.25$



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Metropolis-Hastings Sampler - Simulated Annealing

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

Metropolis-Hastings Sampler:

- Start with some $\theta^{(0)}$.
- Propose θ^* according to $q(\theta^*|\theta^{(t-1)})$.
- $\bullet \ \ \mathsf{Compute} \ \alpha = \min \left\{ 1, \frac{p(\pmb{\theta}^\star)q(\pmb{\theta}^\star \to \pmb{\theta}^{(t-1)})}{p(\pmb{\theta}^{(t-1)})q(\pmb{\theta}^{(t-1)} \to \pmb{\theta}^\star)} \right\}$
- Draw r = Unif(0, 1).
- If $r \leq \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

Metropolis-Hastings Sampler with Simulated Annealing:

- Modify the acceptance probability as $\alpha = \min \left\{ 1, \left\{ \frac{p(\boldsymbol{\theta}^{\star})q(\boldsymbol{\theta}^{\star} \to \boldsymbol{\theta}^{(t-1)})}{p(\boldsymbol{\theta}^{(t-1)})q(\boldsymbol{\theta}^{(t-1)} \to \boldsymbol{\theta}^{\star})} \right\}^{1/T(t)} \right\}$
 - ullet Start with temperature T_0 and cool down to a final temperature T_f over n iterations:

$$T(t) = \max \left\{ T_0 \left(\frac{T_f}{T_0} \right)^{t/n}, T_f \right\}.$$

• Start with temperature T_0 and cool down to original MH over n iterations $T(t) = \max \left\{ T^{1-t/n} \right\}$

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Metropolis-Hastings Sampler - Simulated Annealing

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

Metropolis-Hastings Sampler:

- Start with some $\theta^{(0)}$.
- Propose θ^* according to $q(\theta^*|\theta^{(t-1)})$.
- $\bullet \ \ \mathsf{Compute} \ \alpha = \min \left\{ 1, \frac{p(\pmb{\theta}^\star)q(\pmb{\theta}^\star \to \pmb{\theta}^{(t-1)})}{p(\pmb{\theta}^{(t-1)})q(\pmb{\theta}^{(t-1)} \to \pmb{\theta}^\star)} \right\}$
- Draw r = Unif(0, 1).
- If $r \leq \alpha$, set $\theta^{(t)} = \theta^*$, otherwise, set $\theta^{(t)} = \theta^{(t-1)}$.

Metropolis-Hastings Sampler with Simulated Annealing:

- Modify the acceptance probability as $\alpha = \min \left\{ 1, \left\{ \frac{p(\boldsymbol{\theta}^{\star})q(\boldsymbol{\theta}^{\star} \to \boldsymbol{\theta}^{(t-1)})}{p(\boldsymbol{\theta}^{(t-1)})q(\boldsymbol{\theta}^{(t-1)} \to \boldsymbol{\theta}^{\star})} \right\}^{1/T(t)} \right\}$
 - Start with temperature T_0 and cool down to a final temperature T_f over n iterations: $T(t) = \max \left\{ T_0 \left(\frac{T_f}{T_0} \right)^{t/n}, T_f \right\}.$
 - Start with temperature T_0 and cool down to original MH over n iterations: $T(t) = \max \left\{ T_0^{1-t/n}, 1 \right\}$.

$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \theta_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t+1} \end{pmatrix} \longrightarrow$$

• Autocorrelation: The k^{th} order autocorrelation based on n samples after burn-in:

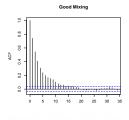
$$\rho_k = \frac{\operatorname{cov}(\theta^{(t)}, \theta^{(t+k)})}{\operatorname{var}(\theta^{(t)})} \stackrel{\triangle}{=} \frac{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta})(\theta^{(t+k)} - \overline{\theta})}{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta})^2} = \widehat{\rho}_k, \quad \overline{\theta} = \frac{1}{n} \sum_{t=1}^n \theta^{(t)}.$$

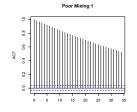
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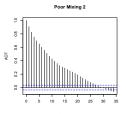
$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• Autocorrelation: The k^{th} order autocorrelation based on n samples after burn-in:

$$\rho_k = \frac{\operatorname{cov}(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t+k)})}{\operatorname{var}(\boldsymbol{\theta}^{(t)})} \stackrel{\triangle}{=} \frac{\sum_{t=1}^{n-k} (\boldsymbol{\theta}^{(t)} - \overline{\boldsymbol{\theta}}) (\boldsymbol{\theta}^{(t+k)} - \overline{\boldsymbol{\theta}})}{\sum_{t=1}^{n-k} (\boldsymbol{\theta}^{(t)} - \overline{\boldsymbol{\theta}})^2} = \widehat{\rho}_k, \quad \overline{\boldsymbol{\theta}} = \frac{1}{n} \sum_{t=1}^n \boldsymbol{\theta}^{(t)}.$$







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$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \theta_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t+1} \end{pmatrix} \longrightarrow$$

• Autocorrelation: The k^{th} order autocorrelation based on n samples after burn-in:

$$\begin{split} \rho_k &= \frac{\text{cov}(\theta^{(t)}, \theta^{(t+k)})}{\text{var}(\theta^{(t)})} \triangleq \frac{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta}) (\theta^{(t+k)} - \overline{\theta})}{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta})^2} = \widehat{\rho}_k, \quad \overline{\theta} = \frac{1}{n} \sum_{t=1}^n \theta^{(t)}. \end{split}$$
• Sample Size Inflation: For an AR(1) process $\theta^{(t)} = \mu + \alpha(\theta^{(t-1)} - \mu) + \epsilon_t$ with

• Sample Size Inflation: For an AR(1) process $\theta^{(t)} = \mu + \alpha(\theta^{(t-1)} - \mu) + \epsilon_t$ with $\epsilon_t \stackrel{iid}{\sim} \text{Normal}(0, \sigma^2)$, we have $\rho_k = \alpha^k, \quad \mathbb{E}(\overline{\theta}_T) = \mu, \quad SE(\overline{\theta}_T) \approx \frac{\sigma}{\sqrt{T}} \frac{1}{(1 - \rho)}.$

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• Autocorrelation: The k^{th} order autocorrelation based on n samples after burn-in:

$$\begin{split} \rho_k &= \frac{\text{cov}(\theta^{(t)}, \theta^{(t+k)})}{\text{var}(\theta^{(t)})} \stackrel{\triangle}{=} \frac{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta}) (\theta^{(t+k)} - \overline{\theta})}{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta})^2} = \widehat{\rho}_k, \quad \overline{\theta} = \frac{1}{n} \sum_{t=1}^n \theta^{(t)}. \end{split}$$
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• Sample Size Inflation: For an AR(1) process $\theta^{(t)} = \mu + \alpha(\theta^{(t-1)} - \mu) + \epsilon_t$ with $\epsilon_t \stackrel{iid}{\sim} \text{Normal}(0, \sigma^2)$, we have $\rho_k = \alpha^k$, $\mathbb{E}(\overline{\theta}_T) = \mu$, $SE(\overline{\theta}_T) \approx \frac{\sigma}{\sqrt{T}} \frac{1}{(1 - \rho)}$.

Therefore, $\bar{\theta}$ is unbiased for μ but with inflated variance.

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• Autocorrelation: The k^{th} order autocorrelation based on n samples after burn-in:

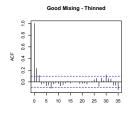
$$\begin{split} & \rho_k = \frac{\text{cov}(\theta^{(t)}, \theta^{(t+k)})}{\text{var}(\theta^{(t)})} \cong \frac{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta}) (\theta^{(t+k)} - \overline{\theta})}{\sum_{t=1}^{n-k} (\theta^{(t)} - \overline{\theta})^2} = \widehat{\rho}_k, \quad \overline{\theta} = \frac{1}{n} \sum_{t=1}^n \theta^{(t)}. \end{split}$$

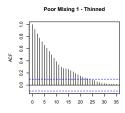
$$\bullet \text{ Sample Size Inflation: For an AR(1) process } \theta^{(t)} = \mu + \alpha(\theta^{(t-1)} - \mu) + \epsilon_t \text{ with } \theta^{(t)}.$$

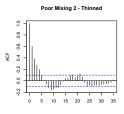
• **Sample Size Inflation:** For an AR(1) process $\theta^{(t)} = \mu + \alpha(\theta^{(t-1)} - \mu) + \epsilon_t$ with $\epsilon_t \stackrel{iid}{\sim} \text{Normal}(0, \sigma^2)$, we have

$$\rho_k = \alpha^k, \quad \mathbb{E}(\overline{\theta}_T) = \mu, \quad SE(\overline{\theta}_T) \approx \frac{\sigma}{\sqrt{T}} \frac{1}{(1-\rho)}.$$

• Thinning: Thin the samples after burn-in, e.g. take every 5th value etc.







$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

- Let $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)^T$ and $\boldsymbol{\theta}_{-j} = (\theta_1, \dots, \theta_{j-1}, \theta_{j+1}, \dots, \theta_p)^T$ for each j.
- Sampling from the *p*-dimensional joint (posterior) distribution is often difficult
- Computing smaller dimensional marginal (posterior) distributions is often difficult

$$p(\theta_j) = \int p(\theta_j, \boldsymbol{\theta}_{-j}) d\boldsymbol{\theta}_{-j}$$

Computing smaller dimensional conditional (posterior) distributions is often easy.

$$p(heta_j \mid m{ heta}_{-j}) \propto p(heta_j, m{ heta}_{-j})$$
 with $m{ heta}_{-j}$ held constant

- Special type of MH sampler when the proposal is never rejected ($\alpha = 1$)
- Samples only from smaller dimensional conditional (posterior) distributions.
- Iterative Algorithm: Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.

$$p(\theta_j^{(t)} \mid \theta_1 = \theta_1^{(t)}, \dots, \theta_{j-1} = \theta_{j-1}^{(t)}, \theta_{j+1} = \theta_{j+1}^{(t-1)}, \dots, \theta_p = \theta_p^{(t-1)})$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(heta_j) = \int p(heta_j, oldsymbol{ heta}_{-j}) doldsymbol{ heta}_{-j}$$

• Computing smaller dimensional conditional (posterior) distributions is often easy. $n(\theta_1 \mid \theta_2) \propto n(\theta_1 \mid \theta_2)$ with θ_2 held constant

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix} \rightarrow \cdots$$

- Let $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)^{\mathrm{T}}$ and $\boldsymbol{\theta}_{-j} = (\theta_1, \dots, \theta_{j-1}, \theta_{j+1}, \dots, \theta_p)^{\mathrm{T}}$ for each j.
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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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 with $\boldsymbol{\theta}_{-i}$ held constant

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 with $\boldsymbol{\theta}_{-j}$ held constant

Gibbs Sampler:

- Special type of MH sampler when the proposal is never rejected ($\alpha = 1$).
- Samples only from smaller dimensional conditional (posterior) distributions.
- Iterative Algorithm:
 Starting with some $\theta^{(0)}$, iteratively sample $\theta^{(t)}$ until convergence.
 At each iteration t, for each $j=1,\ldots,p$, sample $\theta_j^{(t)}$ from $\pi(\rho^{(t)} \mid \rho = \rho^{(t)}) \qquad \pi(\rho^{(t)} \mid \rho$

$$p(\theta_j^{(t)} \mid \theta_1 = \theta_1^{(t)}, \dots, \theta_{j-1} = \theta_{j-1}^{(t)}, \theta_{j+1} = \theta_{j+1}^{(t-1)}, \dots, \theta_p = \theta_p^{(t-1)}).$$

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(x,y) = \frac{1}{\text{Beta}(\alpha,\beta)} \binom{n}{x} y^{x+\alpha-1} (1-y)^{n-x+\beta-1}, \quad x = 0,1,\ldots,n, \ y \in (0,1).$$

- $p(x \mid y) = Bin(n, y).$
- $\triangleright p(y \mid x) = \text{Beta}(x + \alpha, n x + \beta)$
- $ightharpoonup n = 10, \quad \alpha = 3, \quad \beta = 3.$

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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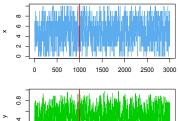
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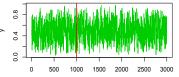
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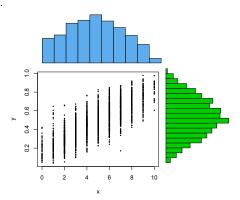
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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

• For each $j = 1, \ldots, p$, define

$$\begin{split} P_{j,t}^G &= p(\theta_j^{\star} \mid \boldsymbol{\theta}_{-j}^{(t)}, \mathbf{y}_{1:n}), \\ \text{where} \quad \boldsymbol{\theta}_{-j}^{(t)} &= (\theta_1^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_{j+1}^{(t-1)}, \dots, \theta_p^{(t-1)}). \end{split}$$

• $P_{j,t}^G = q(\theta_j^{(t)} \to \theta_j^*)$ is the proposal to move from $\theta_j^{(t)}$ to θ_j^* where

$$\theta_j^{(t)} = (\theta_1^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_j^{(t-1)}, \theta_{j+1}^{(t-1)}, \dots, \theta_p^{(t-1)})$$

$$\theta_j^* = (\theta_1^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_j^*, \theta_{j+1}^{(t-1)}, \dots, \theta_p^{(t-1)}).$$

• Also, $\theta_{-i}^{\star} = \theta_{-i}^{(t)}$ since other components do not change.

Then
$$\alpha = \frac{p(\theta_{j}^{\star} \mid \mathbf{y}_{1:n})}{p(\theta_{j}^{(t)} \mid \mathbf{y}_{1:n})} \times \frac{P_{j,t}^{G}(\theta_{j}^{(t)} \mid \theta_{j}^{\star})}{P_{j,t}^{G}(\theta_{j}^{\star} \mid \theta_{j}^{(t)})} = \frac{p(\theta_{j}^{\star} \mid \mathbf{y}_{1:n})}{p(\theta_{j}^{(t)} \mid \mathbf{y}_{1:n})} \times \frac{p(\theta_{j}^{(t-1)} \mid \theta_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\theta_{j}^{\star} \mid \theta_{-j}^{\star}, \mathbf{y}_{1:n})} = \frac{p(\theta_{j}^{\star} \mid \theta_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\theta_{j}^{(t-1)} \mid \theta_{-j}^{(t)}, \mathbf{y}_{1:n})} \times \frac{p(\theta_{j}^{(t-1)} \mid \theta_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\theta_{j}^{(t-1)} \mid \theta_{-j}^{\star}, \mathbf{y}_{1:n})} = 1.$$

$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \rightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \rightarrow \left(\boldsymbol{\theta}_{t-2}\right) \rightarrow \left(\boldsymbol{\theta}_{t-1}\right) \rightarrow \left(\boldsymbol{\theta}_t\right) \rightarrow \left(\boldsymbol{\theta}_{t+1}\right) \rightarrow \cdots$$

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 where $\boldsymbol{\theta}_{-j}^{(t)} = (\theta_1^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_{j+1}^{(t-1)}, \dots, \theta_p^{(t-1)}).$

• $P_{j,t}^G = q(\boldsymbol{\theta}_j^{(t)} \to \boldsymbol{\theta}_j^{\star})$ is the proposal to move from $\boldsymbol{\theta}_j^{(t)}$ to $\boldsymbol{\theta}_j^{\star}$ where

$$\begin{aligned} \boldsymbol{\theta}_{j}^{(t)} &= (\theta_{1}^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_{j}^{(t-1)}, \theta_{j+1}^{(t-1)}, \dots, \theta_{p}^{(t-1)}), \\ \boldsymbol{\theta}_{j}^{\star} &= (\theta_{1}^{(t)}, \dots, \theta_{j-1}^{(t)}, \theta_{j}^{\star}, \theta_{j+1}^{(t-1)}, \dots, \theta_{p}^{(t-1)}). \end{aligned}$$

- Also, $\theta_{-j}^{\star} = \theta_{-j}^{(t)}$ since other components do not change.
- $$\begin{split} & \text{Then} \\ & \alpha = \frac{p(\boldsymbol{\theta}_{j}^{\star} \mid \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{j}^{(t)} \mid \mathbf{y}_{1:n})} \times \frac{P_{j,t}^{G}(\boldsymbol{\theta}_{j}^{(t)} \mid \boldsymbol{\theta}_{j}^{\star})}{P_{j,t}^{G}(\boldsymbol{\theta}_{j}^{\star} \mid \boldsymbol{\theta}_{j}^{(t)})} = \frac{p(\boldsymbol{\theta}_{j}^{\star} \mid \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{j}^{(t)} \mid \mathbf{y}_{1:n})} \times \frac{p(\boldsymbol{\theta}_{j}^{(t-1)} \mid \boldsymbol{\theta}_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{j}^{\star} \mid \boldsymbol{\theta}_{-j}^{(t)}, \mathbf{y}_{1:n})} \\ & = \frac{p(\boldsymbol{\theta}_{j}^{\star} \mid \boldsymbol{\theta}_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{j}^{(t-1)} \mid \boldsymbol{\theta}_{-j}^{(t)}, \mathbf{y}_{1:n})} \times \frac{p(\boldsymbol{\theta}_{-j}^{\star} \mid \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{-j}^{(t)} \mid \mathbf{y}_{1:n})} \times \frac{p(\boldsymbol{\theta}_{j}^{(t-1)} \mid \boldsymbol{\theta}_{-j}^{\star}, \mathbf{y}_{1:n})}{p(\boldsymbol{\theta}_{j}^{\star} \mid \boldsymbol{\theta}_{-j}^{(t)}, \mathbf{y}_{1:n})} = 1. \end{split}$$

Normal Model Under Conjugate Prior (From Module V)

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- Normal-Inverse-Gamma Prior: $(\mu, \sigma^2) \sim \text{NIG}\left(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2\right)$ $p(\mu, \sigma^2) = p(\sigma^2)p(\mu \mid \sigma^2) = \text{Inv-Ga}\left(\sigma^2 \mid \nu_0/2, \nu_0 \sigma_0^2/2\right) \cdot \text{Normal}(\mu \mid \mu_0, \sigma^2/\kappa_0)$
- **▶** Normal-Inverse-Gamma Posterior:

$$\begin{split} & p(\mu, \sigma^2 \mid \mathbf{y}_{1:n}) \\ & \propto \left(\sigma^2\right)^{-\left\{\frac{(\nu_0 + n)}{2} + 1 + \frac{1}{2}\right\}} \exp\left[-\frac{1}{2\sigma^2} \left\{\nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} - \mu_0)^2 + (\kappa_0 + n)(\mu - \mu_n)^2\right\}\right] \\ & \equiv \text{NIG}\left(\mu_n, \sigma_n^2 / \kappa_n, \nu_n, \sigma_n^2\right), \quad \nu_n = (\nu_0 + n), \quad \kappa_n = (\kappa_0 + n), \quad \mu_n = (\kappa_0 \mu_0 + n\overline{y})/(\kappa_0 + n), \\ & \sigma_n^2 = \frac{1}{\nu_n} \left\{\nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} - \mu_0)^2\right\} \end{split}$$

- \blacktriangleright Gibbs: Iteratively Sample $\{(\mu^{(m)},\sigma^{2(m)})\}_{m=1}^M$ from the Conditional Posteriors:
 - $\triangleright p(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \text{Normal}(\mu_n, \sigma^2/\kappa_n)$
 - ▶ $p(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \text{Inv-Ga}[(\nu_n + 1)/2, {\kappa_n(\mu \mu_n)^2 + \nu_n \sigma_n^2}/2]$
- ► Collapsed: Collectively Sample $\{(\mu^{(m)}, \sigma^{2(m)})\}_{m=1}^{M}$ from the Marginal Posteriors: ► $p(\mu \mid \mathbf{y}_{1:n}) = t_{\nu_n}(\mu_n, \sigma_n^2/\kappa_n)$ ► $p(\sigma^2 \mid \mathbf{y}_{1:n}) = \text{Inv-Ga}(\nu_n/2, \nu_n \sigma_n^2/2)$

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Normal Model Under Conjugate Prior (From Module V)

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

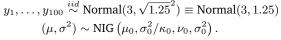
- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- Normal-Inverse-Gamma Prior: $(\mu, \sigma^2) \sim \text{NIG}\left(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2\right)$ $p(\mu, \sigma^2) = p(\sigma^2)p(\mu \mid \sigma^2) = \text{Inv-Ga}\left(\sigma^2 \mid \nu_0/2, \nu_0 \sigma_0^2/2\right) \cdot \text{Normal}(\mu \mid \mu_0, \sigma^2/\kappa_0)$
- **▶** Normal-Inverse-Gamma Posterior:

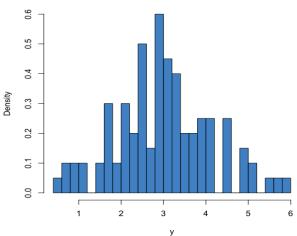
$$\begin{split} & p(\mu, \sigma^2 \mid \mathbf{y}_{1:n}) \\ & \propto \left(\sigma^2\right)^{-\left\{\frac{(\nu_0 + n)}{2} + 1 + \frac{1}{2}\right\}} \exp\left[-\frac{1}{2\sigma^2} \left\{\nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} - \mu_0)^2 + (\kappa_0 + n)(\mu - \mu_n)^2\right\}\right] \\ & \equiv \text{NIG}\left(\mu_n, \sigma_n^2 / \kappa_n, \nu_n, \sigma_n^2\right), \quad \nu_n = (\nu_0 + n), \quad \kappa_n = (\kappa_0 + n), \quad \mu_n = (\kappa_0 \mu_0 + n\overline{y})/(\kappa_0 + n), \\ & \sigma_n^2 = \frac{1}{\nu_n} \left\{\nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} - \mu_0)^2\right\} \end{split}$$

- \blacktriangleright Gibbs: Iteratively Sample $\{(\mu^{(m)},\sigma^{2(m)})\}_{m=1}^M$ from the Conditional Posteriors:
 - $\triangleright p(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \text{Normal}(\mu_n, \sigma^2/\kappa_n)$
 - ▶ $p(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \text{Inv-Ga}[(\nu_n + 1)/2, {\kappa_n(\mu \mu_n)^2 + \nu_n \sigma_n^2}/2]$
- lacktriangle Collapsed: Collectively Sample $\{(\mu^{(m)},\sigma^{2(m)})\}_{m=1}^M$ from the Marginal Posteriors:

$$\blacktriangleright p(\mu \mid \mathbf{y}_{1:n}) = t_{\nu_n}(\mu_n, \sigma_n^2/\kappa_n) \quad \blacktriangleright p(\sigma^2 \mid \mathbf{y}_{1:n}) = \text{Inv-Ga}(\nu_n/2, \nu_n \sigma_n^2/2)$$

Gibbs Sampler for Normal Model Under NIG Prior - Data

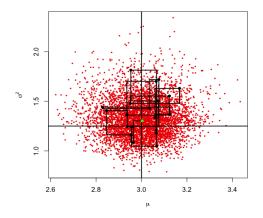




Gibbs Sampler for Normal Model Under NIG Prior - Sample Path

$$y_1, \dots, y_{100} \stackrel{iid}{\sim} \text{Normal}(3, \sqrt{1.25}^2) \equiv \text{Normal}(3, 1.25)$$

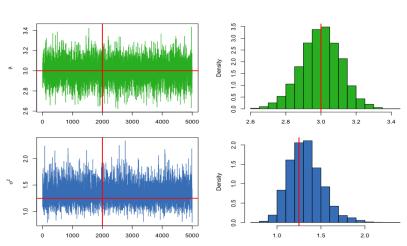
 $(\mu, \sigma^2) \sim \text{NIG}(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2).$



Gibbs Sampler for Normal Model Under NIG Prior - Trace Plots

$$y_1, \dots, y_{100} \stackrel{iid}{\sim} \text{Normal}(3, \sqrt{1.25}^2) \equiv \text{Normal}(3, 1.25)$$

 $(\mu, \sigma^2) \sim \text{NIG}(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2).$



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$$p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t) = p(\boldsymbol{\theta}_{t+1} \mid \boldsymbol{\theta}_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \boldsymbol{\theta}_{t+1} \end{pmatrix}$$

$$\mathbb{E}_x(x) = \mathbb{E}_y(\mathbb{E}_{x\mid y}(x\mid y)), \quad \operatorname{var}_x(x) = \operatorname{var}_y(\mathbb{E}_{x\mid y}(x\mid y)) + \mathbb{E}_y(\operatorname{var}_{x\mid y}(x\mid y))$$

Moments:

ullet Moments of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$ as

$$\mathbb{E}(x) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} x^{(t)}.$$

• An alternative estimate constructed using Gibbs samples $y^{(t)}$ is

$$\mathbb{EE}(x \mid y) = \mathbb{E}\{g(y)\} \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} g\left(y^{(t)}\right)$$

- Marginal of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$.
- ullet An alternative estimate that often better estimates the uses Gibbs samples $y^{(t)}$ as

$$p(x) = \int p(x \mid y)p(y)dy = \mathbb{E}_{y \sim p(y)}p(x \mid y) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} p(x \mid y^{(t)})$$

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$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \longrightarrow \begin{pmatrix} \theta_{t-2} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t-1} \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_t \end{pmatrix} \longrightarrow \begin{pmatrix} \theta_{t+1} \end{pmatrix} \longrightarrow \cdots$$

$$\mathbb{E}_x(x) = \mathbb{E}_y(\mathbb{E}_{x|y}(x \mid y)), \quad \text{var}_x(x) = \text{var}_y(\mathbb{E}_{x|y}(x \mid y)) + \mathbb{E}_y(\text{var}_{x|y}(x \mid y))$$

Moments:

• Moments of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$ as

$$\mathbb{E}(x) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} x^{(t)}$$
.

ullet An alternative estimate constructed using Gibbs samples $y^{(t)}$ is

$$\mathbb{EE}(x \mid y) = \mathbb{E}\{g(y)\} \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} g\left(y^{(t)}\right).$$

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- ullet An alternative estimate that often better estimates the uses Gibbs samples $y^{(t)}$ as

$$p(x) = \int p(x \mid y)p(y)dy = \mathbb{E}_{y \sim p(y)}p(x \mid y) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} p(x \mid y^{(t)})$$

$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \longrightarrow \underbrace{\theta_{t-2}} \longrightarrow \underbrace{\theta_{t-1}} \longrightarrow \underbrace{\theta_t} \longrightarrow \underbrace{\theta_{t+1}} \longrightarrow \cdots$$

$$\mathbb{E}_x(x) = \mathbb{E}_y(\mathbb{E}_{x\mid y}(x\mid y)), \quad \text{ } \operatorname{var}_x(x) = \operatorname{var}_y(\mathbb{E}_{x\mid y}(x\mid y)) + \mathbb{E}_y(\operatorname{var}_{x\mid y}(x\mid y))$$

Moments:

• Moments of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$ as

$$\mathbb{E}(x) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} x^{(t)}.$$

ullet An alternative estimate constructed using Gibbs samples $y^{(t)}$ is

$$\mathbb{EE}(x \mid y) = \mathbb{E}\{g(y)\} \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} g\left(y^{(t)}\right).$$

Marginal Distributions:

- Marginal of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$.
- ${\color{blue}\bullet}$ An alternative estimate that often better estimates the uses Gibbs samples $y^{(t)}$ as

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$$p(\theta_{t+1} \mid \theta_0, \theta_1, \dots, \theta_t) = p(\theta_{t+1} \mid \theta_t) \quad \cdots \quad \bullet \underbrace{\theta_{t-2}} \quad \bullet \underbrace{\theta_{t-1}} \quad \bullet \underbrace{\theta_{t}} \quad \bullet \underbrace{\theta_{t+1}} \quad \bullet$$

$$\mathbb{E}_x(x) = \mathbb{E}_y(\mathbb{E}_{x\mid y}(x\mid y)), \quad \text{var}_x(x) = \text{var}_y(\mathbb{E}_{x\mid y}(x\mid y)) + \mathbb{E}_y(\text{var}_{x\mid y}(x\mid y))$$

Moments:

• Moments of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$ as

$$\mathbb{E}(x) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} x^{(t)}.$$

ullet An alternative estimate constructed using Gibbs samples $y^{(t)}$ is

$$\mathbb{EE}(x \mid y) = \mathbb{E}\{g(y)\} \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} g\left(y^{(t)}\right).$$

Marginal Distributions:

- Marginal of x can be estimated straightforwardly using Gibbs samples $x^{(t)}$.
- ullet An alternative estimate that often better estimates the uses Gibbs samples $y^{(t)}$ as

$$p(x) = \int p(x \mid y) p(y) dy = \mathbb{E}_{y \sim p(y)} p(x \mid y) \stackrel{\triangle}{=} \frac{1}{T} \sum_{t=1}^{T} p(x \mid y^{(t)}).$$

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- ▶ Normal-Inverse-Gamma Prior: $(\mu, \sigma^2) \sim \text{NIG}\left(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2\right)$

$$p(\mu,\sigma^2) = p(\sigma^2)p(\mu \mid \sigma^2) = \text{Inv-Ga}\left(\sigma^2 \mid \nu_0/2,\nu_0\sigma_0^2/2\right) \cdot \text{Normal}(\mu \mid \mu_0,\sigma^2/\kappa_0)$$

► Normal-Inverse-Gamma Posterior:

$$\begin{split} & p(\mu, \sigma^2 \mid \mathbf{y}_{1:n}) = \mathrm{NIG}\left(\mu_n, \sigma_n^2/\kappa_n, \nu_n, \sigma_n^2\right), \quad \nu_n = (\nu_0 + n), \quad \kappa_n = (\kappa_0 + n), \quad \mu_n = (\kappa_0 \mu_0 + n\overline{y})/(\kappa_0 + n), \\ & \sigma_n^2 = \frac{1}{1-\epsilon} \left\{\nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n-1)s^2} (\overline{y} - \mu_0)^2\right\} \end{split}$$

► Gibbs: Iteratively Sample $\{(\mu^{(m)}, \sigma^{2(m)})\}_{m=1}^{M}$ from the Conditional Posteriors:

Collapsed: Collectively Sample from the Marginal Poster

Rao-Blackwellized: Iteratively Sample from the Conditional Posteriors

 $\blacktriangleright \mathbb{E}(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \mu_{n \mid \sigma^2} = \mu_n = (\kappa_0 \mu_0 + n \overline{y}) / (\kappa_0 + n)$

 $\mathbb{E}(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \sigma_{n|\mu}^2 = \{\kappa_n(\mu - \mu_n)^2 + \nu_n \sigma_n^2\} / (\nu_n - 1)$

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- \blacktriangleright Normal-Inverse-Gamma Prior: $(\mu,\sigma^2) \sim {\rm NIG}\left(\mu_0,\sigma_0^2/\kappa_0,\nu_0,\sigma_0^2\right)$

$$p(\mu,\sigma^2) = p(\sigma^2)p(\mu \mid \sigma^2) = \text{Inv-Ga}\left(\sigma^2 \mid \nu_0/2,\nu_0\sigma_0^2/2\right) \cdot \text{Normal}(\mu \mid \mu_0,\sigma^2/\kappa_0)$$

► Normal-Inverse-Gamma Posterior:

$$\begin{split} p(\mu,\sigma^2\mid\mathbf{y}_{1:n}) &= \mathrm{NIG}\left(\mu_n,\sigma_n^2/\kappa_n,\nu_n,\sigma_n^2\right), \quad \nu_n = (\nu_0+n), \quad \kappa_n = (\kappa_0+n), \quad \mu_n = (\kappa_0\mu_0+n\overline{y})/(\kappa_0+n), \\ \sigma_n^2 &= \frac{1}{1-}\left\{\nu_0\sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n-1)s^2}(\overline{y}-\mu_0)^2\right\} \end{split}$$

▶ Gibbs: Iteratively Sample $\{(\mu^{(m)}, \sigma^{2(m)})\}_{m=1}^{M}$ from the Conditional Posteriors:

$$\blacktriangleright \ p(\boldsymbol{\sigma}^2 \mid \boldsymbol{\mu}, \mathbf{y}_{1:n}) = \text{Inv-Ga}[(\nu_n + 1)/2, \{\kappa_n(\boldsymbol{\mu} - \boldsymbol{\mu}_n)^2 + \nu_n \sigma_n^2\}/2] \\ \Rightarrow \mathbb{E}(\boldsymbol{\sigma}^2 \mid \mathbf{y}_{1:n}) = \frac{1}{M} \sum_{m=1}^{M} \sigma^{2(m)} + \nu_n \sigma_n^2 + \nu$$

► Collapsed: Collectively Sample from the Marginal Posteriors:

Rao-Blackwellized: Iteratively Sample from the Conditional Posteriors:

 $\blacktriangleright \mathbb{E}(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \mu_{n \mid \sigma^2} = \mu_n = (\kappa_0 \mu_0 + n \overline{y}) / (\kappa_0 + n)$

 $\mathbb{E}(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \sigma_{n|\mu}^2 = \{ \kappa_n (\mu - \mu_n)^2 + \nu_n \sigma_n^2 \} / (\nu_n - 1)$

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp \left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- Normal-Inverse-Gamma Prior: $(\mu, \sigma^2) \sim \text{NIG}(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2)$

$$p(\mu,\sigma^2) = p(\sigma^2)p(\mu\mid\sigma^2) = \text{Inv-Ga}\left(\sigma^2\mid\nu_0/2,\nu_0\sigma_0^2/2\right)\cdot \text{Normal}(\mu\mid\mu_0,\sigma^2/\kappa_0)$$

Normal-Inverse-Gamma Posterior:

$$p(\mu, \sigma^2 \mid \mathbf{y}_{1:n}) = \mathrm{NIG}\left(\mu_n, \sigma_n^2/\kappa_n, \nu_n, \sigma_n^2\right), \quad \nu_n = (\nu_0 + n), \quad \kappa_n = (\kappa_0 + n), \quad \mu_n = (\kappa_0 \mu_0 + n\overline{y})/(\kappa_0 + n),$$

- $$\begin{split} &\sigma_n^2 = \frac{1}{\nu_n} \left\{ \nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} \mu_0)^2 \right\} \\ &\blacktriangleright \text{ Gibbs: Iteratively Sample } \{ (\mu^{(m)}, \sigma^{2(m)}) \}_{m=1}^M \text{ from the Conditional Posteriors:} \end{split}$$
- $\triangleright p(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \text{Normal}(\mu_n, \sigma^2/\kappa_n)$
- $\Rightarrow \mathbb{E}(\mu \mid \mathbf{y}_{1:n}) = \frac{1}{M} \sum_{m=1}^{M} \mu^{(m)}$
- Collapsed: Collectively Sample from the Marginal Posteriors:
- $\triangleright p(\mu \mid \mathbf{y}_{1:n}) = t_{\nu_n}(\mu_n, \sigma_n^2/\kappa_n)$ $\Rightarrow \mathbb{E}(\mu \mid \mathbf{y}_{1:n}) = \frac{1}{M} \sum_{m=1}^{M} \mu^{(m)}$
- $\Rightarrow \mathbb{E}(\sigma^2 \mid \mathbf{y}_{1:n}) = \frac{1}{M} \sum_{m=1}^{M} \sigma^{2(m)}$ $\triangleright p(\sigma^2 \mid \mathbf{y}_{1:n}) = \text{Inv-Ga}(\nu_n/2, \nu_n \sigma_n^2/2)$
 - ► Rao-Blackwellized: Iteratively Sample from the Conditional Posteriors:

$$\mathbf{E}(\mu \mid \sigma^{2}, \mathbf{y}_{1:n}) = \mu_{n \mid \sigma^{2}} = \mu_{n} = (\kappa_{0}\mu_{0} + n\overline{y})/(\kappa_{0} + n) \qquad \Rightarrow \mathbb{E}(\mu \mid \mathbf{y}_{1:n}) \widehat{=} \mu_{n}$$

$$\mathbf{E}(\sigma^{2} \mid \mu, \mathbf{y}_{1:n}) = \sigma_{n \mid \mu}^{2} = {\kappa_{n}(\mu - \mu_{n})^{2} + \nu_{n}\sigma_{n}^{2}}/(\nu_{n} - 1) \qquad \Rightarrow \mathbb{E}(\sigma^{2} \mid \mathbf{y}_{1:n}) \widehat{=} \frac{1}{M} \sum_{m=1}^{M} \sigma_{n \mid \mu}^{2(m)}$$

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 $\Rightarrow \mathbb{E}(\mu \mid \mathbf{y}_{1:n}) \widehat{=} \mu_n$

$$y_1, \ldots, y_n \stackrel{iid}{\sim} \text{Normal}(\mu, \sigma^2)$$
 with μ, σ^2 both unknown

- Normal Likelihood: $p(\mathbf{y}_{1:n} \mid \mu, \sigma^2) \propto \left(\sigma^2\right)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left\{(n-1)s^2 + n(\overline{y} \mu)^2\right\}\right]$
- \blacktriangleright Normal-Inverse-Gamma Prior: $(\mu,\sigma^2) \sim {\rm NIG}\left(\mu_0,\sigma_0^2/\kappa_0,\nu_0,\sigma_0^2\right)$

$$p(\mu,\sigma^2) = p(\sigma^2)p(\mu \mid \sigma^2) = \text{Inv-Ga}\left(\sigma^2 \mid \nu_0/2,\nu_0\sigma_0^2/2\right) \cdot \text{Normal}(\mu \mid \mu_0,\sigma^2/\kappa_0)$$

► Normal-Inverse-Gamma Posterior:

$$p(\mu,\sigma^2\mid \mathbf{y_{1:n}}) = \mathrm{NIG}\left(\mu_n,\sigma_n^2/\kappa_n,\nu_n,\sigma_n^2\right), \quad \nu_n = (\nu_0+n), \quad \kappa_n = (\kappa_0+n), \quad \mu_n = (\kappa_0\mu_0+n\overline{y})/(\kappa_0+n), \quad \kappa_n = (\kappa_0+n), \quad \mu_n = (\kappa_0\mu_0+n\overline{y})/(\kappa_0+n), \quad \kappa_n = (\kappa_0+n), \quad$$

$$\sigma_n^2 = \frac{1}{\nu_n} \left\{ \nu_0 \sigma_0^2 + (n-1)s^2 + \frac{n\kappa_0}{(n+\kappa_0)} (\overline{y} - \mu_0)^2 \right\}$$

▶ Gibbs: Iteratively Sample $\{(\mu^{(m)}, \sigma^{2(m)})\}_{m=1}^M$ from the Conditional Posteriors:

$$\blacktriangleright p(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \text{Normal}(\mu_n, \sigma^2 / \kappa_n)$$

$$\Rightarrow \mathbb{E}(\mu \mid \mathbf{y}_{1:n}) = \frac{1}{M} \sum_{m=1}^{M} \mu^{(m)}$$

▶
$$p(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \text{Inv-Ga}[(\nu_n + 1)/2, {\kappa_n(\mu - \mu_n)}^2 + \nu_n \sigma_n^2 }/2]$$
 $\Rightarrow \mathbb{E}(\sigma^2 \mid \mathbf{y}_{1:n}) \stackrel{\triangle}{=} \frac{1}{M} \sum_{m=1}^{M} \sigma^{2(m)}$

▶ Collapsed: Collectively Sample from the Marginal Posteriors:

▶ Rao-Blackwellized: Iteratively Sample from the Conditional Posteriors:

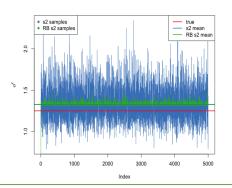
$$\blacktriangleright \mathbb{E}(\mu \mid \sigma^2, \mathbf{y}_{1:n}) = \mu_{n \mid \sigma^2} = \mu_n = (\kappa_0 \mu_0 + n\overline{y})/(\kappa_0 + n) \qquad \rightarrow \text{Does not depend on the samples at all!}$$

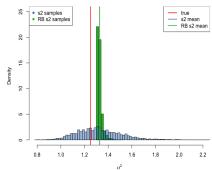
$$\blacktriangleright \ \mathbb{E}(\sigma^2 \mid \mu, \mathbf{y}_{1:n}) = \sigma^2_{n \mid \mu} = \{\kappa_n(\mu - \mu_n)^2 + \nu_n \sigma^2_n\} / (\nu_n - 1) \ \to \ \text{Depends only on the samples of } \mu!$$

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Gibbs Sampler for Normal Model Under NIG Prior - Rao-Blackwellization

$$\begin{split} y_1, \dots, y_{100} &\stackrel{iid}{\sim} \text{Normal}(3, \sqrt{1.25}^2) \equiv \text{Normal}(3, 1.25) \\ &(\mu, \sigma^2) \sim \text{NIG}\left(\mu_0, \sigma_0^2/\kappa_0, \nu_0, \sigma_0^2\right). \\ &\widehat{\sigma}_{post-mean}^2 = \frac{1}{M} \sum_{m=1}^M \sigma^{2(m)} \\ &\widehat{\sigma}_{RB-post-mean}^2 = \frac{1}{M} \sum_{m=1}^M \frac{\kappa_n(\mu^{(m)} - \mu_n)^2 + \nu_n \sigma_n^2}{\nu_n - 1} \end{split}$$





• Monte Carlo integration

- Approximates integrals writing it as an expectation then sampling from the corresponding density
- Importance sampling

- Sampling from a target density when direct sampling is difficult

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- Monte Carlo integration
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- Sampling from a target density when direct sampling is difficult
- Markov chain Monte Carlo

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 - Allows Monte Carlo integration when sampling from the target density is difficul-
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 - Applicable even when the target density is known only up to a normalizing constan
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Markov chain Monte Carlo

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Sampling from a target density when direct sampling is difficult

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 - Markov chain Monte Carlo
 - Samples from a stationary Markov chain with the target density as the stationary distribution

- Markov chains
 - The two components that define an MC are
 - Initial distribution $p(z_1)$
 - Transition distributions $p(z_t \mid z_{t-1})$
 - Important properties

Metropolis-Hastings sampler

Gibbs sample

Convergence diagnostic

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29/29 115/133

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Convergence diagnostics

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Convergence diagnostics

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Convergence diagnostics

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Convergence diagnostics

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Convergence diagnostics

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 - Burn-in and thinning

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 - Trace plots and autocorrelation plots

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