Markov Chain Monte Carlo II

Probabilistic Decision Making VU

(Reinforcement Learning VO)

Thomas Wedenig

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Institute of Machine Learning and Neural Computation
Graz University of Technology, Austria

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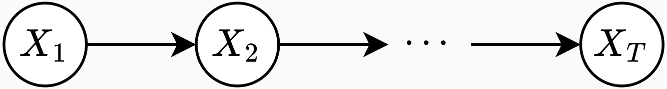
MCMC - Recap

Setup

- **Goal**: Draw **samples** from **distribution** $\pi(\mathsf{x})$
- Typically, only $\tilde{\pi}(\mathsf{x}) \propto \pi(\mathsf{x})$ is known
  - e.g., **Bayesian inference**: $\tilde{\pi}_{\mathsf{y}}(\mathsf{x}) := p(\mathsf{x}, \mathsf{y}) \propto p(\mathsf{x} \mid \mathsf{y})$
  - e.g., **Boltzmann distributions**: $\tilde{\pi}(\mathsf{x}) := \exp(-E(\mathsf{x}))$, $E : \mathcal{X} \to \mathbb{R}$
- We care about **samples** because...
  - they might be **the object of interest** (e.g., sample image from generative model), or
  - we may need samples to **approximate expectations** (Monte Carlo)

MCMC – Idea



- **Idea**: Construct **Markov Chain**

$$p(x_1, x_2, \ldots, x_T) = p(x_1)\, p(x_2 \mid x_1)\, p(x_3 \mid x_2) \ldots p(x_T \mid x_{T-1})$$

  - with **unique stationary distribution** π,
  - its **marginal distribution converges to** π when $T \to \infty$,
  - $p(x_1)$ and $p(x_t \mid x_{t-1})$ are **easy to sample from**

Sampling from the chain for “long enough” yields
samples with **marginal distribution close to** π !

MCMC

```
Initialize $x$
repeat:
    $x \leftarrow$ some (random) update to $x$
```

Running a

Markov Chain Monte Carlo

Algorithm

Metropolis-Hastings

Given: **Target** $\tilde{\pi}$ and **proposal distribution** $q(\mathsf{y} \mid \mathsf{x})$.

Initialize $X_1 \sim p(X_1)$ and repeat for $t = 1, \dots, T-1$:

1. Given current state $X_t = \mathsf{x}$, **propose:**

$$\mathsf{y} \sim q(\mathsf{y} \mid \mathsf{x})$$

2. **Compute acceptance probability:**

$$\alpha(\mathsf{x} \to \mathsf{y}) = \min\left(1, \frac{\tilde{\pi}(\mathsf{y})\, q(\mathsf{x} \mid \mathsf{y})}{\tilde{\pi}(\mathsf{x})\, q(\mathsf{y} \mid \mathsf{x})}\right)$$

3. **Accept or reject:**

$$\text{Sample } U \sim \mathsf{Uniform}(0,1), \qquad X_{t+1} = \begin{cases} \mathsf{y} & \text{if } U \leq \alpha(\mathsf{x} \to \mathsf{y}) \\ \mathsf{x} & \text{else} \end{cases}$$

Metropolis-Hastings (cont.)

Metropolis-Hastings Update

1️⃣ Propose $\mathbf{y} \sim q(\mathbf{y} \mid \mathbf{x})$ 2️⃣ Compute $\alpha = \min\left(1, \frac{\tilde{\pi}(\mathbf{y})\, q(\mathbf{x}|\mathbf{y})}{\tilde{\pi}(\mathbf{x})\, q(\mathbf{y}|\mathbf{x})}\right)$ 3️⃣ Accept $\mathbf{y}$ with probability α

- For continuous state spaces, we could choose a **Gaussian proposal**

$$q(\mathbf{y} \mid \mathbf{x}) := \mathcal{N}(\mathbf{y}; \mathbf{x}, \sigma^2 I)$$

- Demo last week: Discrete state space with **proposal**

$$q(\mathbf{y} \mid \mathbf{x}) = \mathbf{Uniform}\left(\{\text{bitstrings that differ from } \mathbf{x} \text{ in exactly one bit}\}\right)$$

Analogy: Optimization

- Assume we want to find the **maximum** of $\tilde{\pi}$
- **Idea:** With current state $\mathbf{x}$, repeat
  1️⃣ Propose $\mathbf{y} \sim q(\mathbf{y} \mid \mathbf{x})$
  2️⃣ Set $\alpha = \tilde{\pi}(\mathbf{y})/\tilde{\pi}(\mathbf{x})$
  3️⃣ If $\alpha \geq 1$, accept $\mathbf{y}$, else stay at $\mathbf{x}$
- **"Greedy random search"**

Random-Walk Metropolis-Hastings Demo

`https://chi-feng.github.io/mcmc-demo/app.html`

Estimating Expectations with MCMC Samples

Dependency in MCMC Samples

Recall Goal: Draw i.i.d. samples from π.

Are samples from our Markov Chain **i.i.d.** samples from π? 🤔

No !

- If samples were i.i.d., X_t and X_{t+1} would be **independent**
- In the beginning, X_t is not even **marginally** distributed like π (not converged yet)
- Even when the chain has perfectly converged to π, and thus $X_t \sim \pi$, $X_{t+1} \sim \pi$ **marginally**, we still have **possibly large correlation** between X_t and X_{t+1}
- When the finite-state chain has converged, we have

$$p(X_t = j, X_{t+1} = i) = p(X_t = j)p(X_{t+1} = i \mid X_t = j) = \pi_j P_{ij} \neq \pi_j \pi_i = p(X_t = j)p(X_{t+1} = i)$$

Ergodic Theorem

Are we doomed? Monte Carlo estimators need **i.i.d.** samples 😰

Thankfully, no! 🥳

- There is an **MCMC counterpart** to classic i.i.d. Monte Carlo
- It assumes our Markov Chain has π as its **unique stationary distribution**
- And it assumes **certain properties**[1]

[1] Irreducible (when state space finite), irreducible and positive recurrent (state space countable), π-irreducible and Harris recurrent (state space uncountable.)

Ergodic Theorem

Ergodic Theorem

Assume $X_1, X_2, \ldots$ is a Markov Chain with above properties and stationary distribution π. Then,

$$\hat{\mathbb{E}}_T := \frac{1}{T}\sum_{t=1}^{T} f(X_t) \xrightarrow{\text{a.s.}} \mathbb{E}_{X\sim\pi}[f(X)]$$

as $T \to \infty$ for every initial state X_1.

- **Almost sure (a.s.) convergence** means

$$\mathbb{P}\left(\lim_{T\to\infty} \hat{\mathbb{E}}_T = \mathbb{E}_{X\sim\pi}[f(X)]\right) = 1$$

MCMC Estimate – Bias

Recap: Properties of MC Estimate

Given **i.i.d.** samples $Y_1, \ldots, Y_T \sim \pi$, the **Monte Carlo estimate** of $\mathbb{E}_{X\sim\pi}[f(X)]$ is

$$\hat{\mathbb{E}}_T^{(\mathrm{MC})} := \frac{1}{T}\sum_{t=1}^{T} f(Y_t).$$

- **Unbiased** for every T: $\mathbb{E}\left[\hat{\mathbb{E}}_T^{(\mathrm{MC})}\right] = \mathbb{E}_{X\sim\pi}[f(X)]$

Properties of MCMC Estimate

- MCMC estimate is generally[2] **biased** for any finite T
  - We can reduce bias by **discarding the first** B samples (**burn-in phase**)
- Bias goes to 0 as $T \to \infty$, i.e., **asymptotically unbiased**

[2] It would be unbiased if the initial distribution was already π, but we can't do that in practice.

MCMC Estimate – Variance

Recap: Properties of MC Estimate

- **Variance** decreases **linearly** with T: $\mathrm{var}\left[\hat{\mathbb{E}}_T^{(\mathrm{MC})}\right] = \frac{\mathrm{var}[f(X)]}{T}$

Properties of MCMC Estimate

- As $T \to \infty$, the **variance** of the MCMC estimator is approximately

$$\mathrm{var}\left[\hat{\mathbb{E}}_T\right] \approx \frac{\sigma^2_{\mathrm{as}}}{T}$$

with

$$\sigma^2_{\mathrm{as}} = \mathrm{var}_\pi[f(X)] + 2\sum_{n=1}^{\infty} \mathrm{cov}_\pi(f(X_0), f(X_n)) \, .$$

where $X_0 \sim \pi, X_1 \sim \pi, \ldots$ (i.e., chain in **stationary** regime)

- **Note:** σ^2_{as} typically **larger** than $\mathrm{var}_\pi[f(X)]$, but still decreases **linearly** with T

Gibbs Sampling

Gibbs Sampling

- Target: $\pi(\mathbf{x})$ with $\mathbf{x} = (x_1, \ldots, x_d)^\top \in \mathcal{X}$
    - e.g., $\mathcal{X} = \mathbb{R}^d$ or $\mathcal{X} = \{-1, +1\}^d$
- Let $\mathbf{x}_{-i} := (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d)$
- Assume **conditionals** $\pi(x_i \mid \mathbf{x}_{-i})$ can be **sampled easily** for every i

Gibbs Sampling

Initialize $\mathbf{x}^{(1)} \sim p(\mathbf{x}^{(1)})$ and repeat for $t = 1, \ldots, T-1$:

- Given current state $\mathbf{x}^{(t)} := (x_1^{(t)}, \ldots, x_d^{(t)})$, sample

$$\begin{aligned}
x_1^{(t+1)} &\sim \pi\left(x_1 \mid x_2^{(t)}, x_3^{(t)}, \ldots, x_d^{(t)}\right) \\
x_2^{(t+1)} &\sim \pi\left(x_2 \mid x_1^{(t+1)}, x_3^{(t)}, \ldots, x_d^{(t)}\right) \\
x_3^{(t+1)} &\sim \pi\left(x_3 \mid x_1^{(t+1)}, x_2^{(t+1)}, x_4^{(t)}, \ldots, x_d^{(t)}\right) \\
&\vdots \\
x_d^{(t+1)} &\sim \pi\left(x_d \mid x_1^{(t+1)}, x_2^{(t+1)}, \ldots, x_{d-1}^{(t+1)}\right)
\end{aligned}$$

Gibbs Sampling Demo

`https://chi-feng.github.io/mcmc-demo/app.html`

Gibbs Sampling is a Metropolis-Hastings Algorithm

Metropolis-Hastings Update

1️⃣ Propose $\mathbf{y} \sim q(\mathbf{y} \mid \mathbf{x})$ 2️⃣ Compute $\alpha = \min\left(1, \frac{\tilde{\pi}(\mathbf{y})\, q(\mathbf{x}|\mathbf{y})}{\tilde{\pi}(\mathbf{x})\, q(\mathbf{y}|\mathbf{x})}\right)$ 3️⃣ Accept $\mathbf{y}$ with probability α

- Gibbs Sampling can be **viewed as an instance of Metropolis-Hastings (MH)**:

$$\mathbf{y} \sim q_i(\mathbf{y} \mid \mathbf{x}) \;:=\; \pi(y_i \mid \mathbf{x}_{-i})\, 1\{\mathbf{y}_{-i} = \mathbf{x}_{-i}\}.$$

- Hence, $\mathbf{y}_{-i} = \mathbf{x}_{-i}$, and thus

$$\pi(\mathbf{x}) = \pi(\mathbf{x}_{-i})\, \pi(x_i \mid \mathbf{x}_{-i}), \qquad \pi(\mathbf{y}) = \pi(\mathbf{x}_{-i})\, \pi(y_i \mid \mathbf{x}_{-i}),$$

- The MH ratio becomes

$$\frac{\pi(\mathbf{y})\, q_i(\mathbf{x} \mid \mathbf{y})}{\pi(\mathbf{x})\, q_i(\mathbf{y} \mid \mathbf{x})} = \frac{\left[\pi(\mathbf{x}_{-i})\, \pi(y_i \mid \mathbf{x}_{-i})\right]\, \pi(x_i \mid \mathbf{x}_{-i})}{\left[\pi(\mathbf{x}_{-i})\, \pi(x_i \mid \mathbf{x}_{-i})\right]\, \pi(y_i \mid \mathbf{x}_{-i})} = 1$$

and we accept with **probability $\alpha = 1$**.

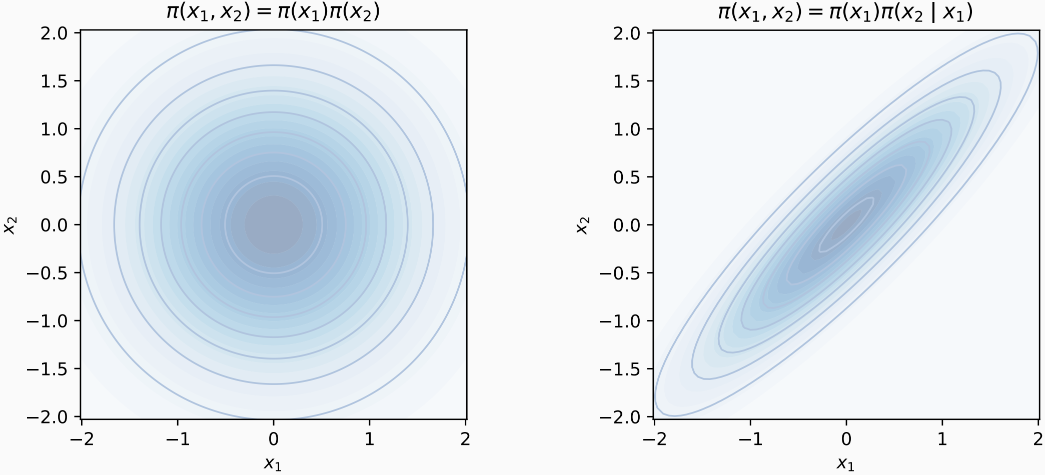
Gibbs Sampling is a Metropolis-Hastings Algorithm

- **Every coordinate update can be seen as a MH step that always accepts** 😍

- Gibbs Sampling typically only stores **every d^{th} MH sample**
  - Technically, this is not necessary if we e.g. apply the **ergodic theorem**
  - But it **reduces autocorrelation**
  - ...at the expense of “throwing away” samples

- Theoretical caveat: In this view, q_i is **time-dependent**
  - Issue: the ergodic theorem assumes a **time-homogeneous** chain
  - Luckily, we can make it time-homogeneous by augmenting the state space $\mathbf{z} := (\mathbf{x}, i)$
  - We then consider $q(\mathbf{y} \mid \mathbf{z})$ in this augmented space, which also updates i accordingly

Gibbs Sampling from a Gaussian



$\pi(x_1, x_2) = \pi(x_1)\pi(x_2)$

$\pi(x_1, x_2) = \pi(x_1)\pi(x_2 \mid x_1)$

Gibbs Sampling Highly Correlated Variables

- Per-coordinate updates may yield **large autocorrelation**
  - Especially for **highly correlated variables**
  - We cannot **“move diagonally”** in the state space
- In the above example, we of course could sample both coordinates at once ❗
  - In general, we can’t sample **all coordinates at once**
  - ...otherwise we would not need MCMC 😂
- Is there something in the middle? 🤔
- **Blocked Gibbs Sampling**: Sample **multiple coordinates** at once

Blocked Gibbs Sampling

Let

$$\mathbf{x} = (\mathbf{x}_{B_1}, \mathbf{x}_{B_2}, \ldots, \mathbf{x}_{B_K}), \qquad B_1 \cup \cdots \cup B_K = \{1, \ldots, d\}.$$

Initialize $\mathbf{x}^{(1)} \sim p(\mathbf{x}^{(1)})$ and repeat for $t = 1, \ldots, T-1$:

- Given current state $\mathbf{x}^{(t)} := (\mathbf{x}_{B_1}^{(t)}, \ldots, \mathbf{x}_{B_K}^{(t)})$, sample

$$\mathbf{x}_{B_1}^{(t+1)} \sim \pi\left(\mathbf{x}_{B_1} \,\middle|\, \mathbf{x}_{B_2}^{(t)}, \mathbf{x}_{B_3}^{(t)}, \ldots, \mathbf{x}_{B_K}^{(t)}\right)$$

$$\mathbf{x}_{B_2}^{(t+1)} \sim \pi\left(\mathbf{x}_{B_2} \,\middle|\, \mathbf{x}_{B_1}^{(t+1)}, \mathbf{x}_{B_3}^{(t)}, \ldots, \mathbf{x}_{B_K}^{(t)}\right)$$

$$\mathbf{x}_{B_3}^{(t+1)} \sim \pi\left(\mathbf{x}_{B_3} \,\middle|\, \mathbf{x}_{B_1}^{(t+1)}, \mathbf{x}_{B_2}^{(t+1)}, \mathbf{x}_{B_4}^{(t)}, \ldots, \mathbf{x}_{B_K}^{(t)}\right)$$

$$\vdots$$

$$\mathbf{x}_{B_K}^{(t+1)} \sim \pi\left(\mathbf{x}_{B_K} \,\middle|\, \mathbf{x}_{B_1}^{(t+1)}, \mathbf{x}_{B_2}^{(t+1)}, \ldots, \mathbf{x}_{B_{K-1}}^{(t+1)}\right)$$

Metropolis-within-Gibbs

What if we cannot directly sample from some **conditional distribution** ?

$$\mathbf{x}_{B_i}^{(t+1)} \sim \pi\left(\mathbf{x}_{B_i} \,\middle|\, \mathbf{x}_{B_1}^{(t+1)}, \ldots, \mathbf{x}_{B_{i-1}}^{(t+1)}, \mathbf{x}_{B_{i+1}}^{(t)}, \ldots, \mathbf{x}_{B_K}^{(t)}\right)$$

- We could use MCMC again **just for this block** !
    - e.g., random walk MH (or something smarter)
- This is called **Metropolis-within-Gibbs**

Langevin MCMC

Langevin MCMC – Motivation

Maximizing $\tilde{\pi}$ via greedy random search

With current state $\mathbf{x}$, repeat:

1️⃣ Propose $\mathbf{y} \sim q(\mathbf{y} \mid \mathbf{x})$ 2️⃣ Set $\alpha = \tilde{\pi}(\mathbf{y})/\tilde{\pi}(\mathbf{x})$ 3️⃣ If $\alpha \geq 1$, accept $\mathbf{y}$, else stay at $\mathbf{x}$

This is clearly **ridiculous** in most cases 😂

- If $\tilde{\pi}$ is a **differentiable** PDF, we can use **gradient information** to find a maximum
  - e.g., **gradient ascent**
- In MCMC **sampling**, we want to **explore regions of high probability**
  - Gradients can guide us towards regions of **high density**

Metropolis-Adjusted Langevin Algorithm (MALA)

- Metropolis-Adjusted Langevin Algorithm (MALA)

- MALA is an instance of Metropolis-Hastings with
$$q(\mathrm{y} \mid \mathrm{x}) = \mathcal{N}\left(\mathrm{y};\ \mathrm{x} + \frac{\eta}{2}\nabla_{\mathrm{x}} \log \pi(\mathrm{x}),\ \eta I\right)$$
  with step size $\eta > 0$.

- As usual, we accept $\mathbf{y}$ with probability
$$\alpha(\mathrm{x} \to \mathrm{y}) = \min\left(1, \frac{\tilde{\pi}(\mathrm{y})\, q(\mathrm{x} \mid \mathrm{y})}{\tilde{\pi}(\mathrm{x})\, q(\mathrm{y} \mid \mathrm{x})}\right)$$

- **Note:** We have to be able to compute $\nabla_{\mathrm{x}} \log \tilde{\pi}(\mathrm{x}) = \nabla_{\mathrm{x}} \log \pi(\mathrm{x})$
  - And evaluate $\tilde{\pi}$ in the **acceptance step**

MALA Demo

`https://chi-feng.github.io/mcmc-demo/app.html`

MALA – Background and Motivation

- This **choice of** q is motivated by the **Langevin Stochastic Differential Equation (SDE)**:

$$dX_t = \frac{1}{2}\nabla \log \pi(X_t)\, dt + dW_t$$

where W_t is a **Wiener process** (Brownian motion)

- Discretizing this SDE using **Euler-Maruyama** gives:

$$X_{t+1} = X_t + \frac{\eta}{2}\nabla \log \pi(X_t) + \sqrt{\eta}\mathbf{z}, \quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, I)$$

which is **exactly a sample from this** $q(\mathbf{y} \mid \mathbf{x})$

Unadjusted Langevin Algorithm

- For MALA, we need to know $\nabla_x \log \tilde{\pi}(x)$ and $\tilde{\pi}(x)$
- Sometimes, we **do not have access to** $\tilde{\pi}$, but **only to** $\nabla_x \log \tilde{\pi}(x)$
  - e.g., **Score-based Generative Models** (**Diffusion Models**)
- Idea: Let's just **always accept** 😂
- This is called the **Unadjusted Langevin Algorithm (ULA)**
- **Not a MH algorithm anymore**, and the stationary distribution is $\pi_\eta \neq \pi$ ❗
  - It has **stationary bias** $\mathbb{E}_{\pi_\eta}[f] - \mathbb{E}_\pi[f]$ of order $O(\eta)$ in general (even as $T \to \infty$)

Hamiltonian Monte Carlo

Hamiltonian Monte Carlo – Motivation

- To explore π, we want to make “large steps”
    - while still staying in **high probability regions**
- Also, we wish to incorporate **momentum**
    - Don’t forget direction immediately
    - Physical analog: ball with **mass**

Hamiltonian Monte Carlo

- If $\mathbf{x} \in \mathbb{R}^d$, augment the state space by a **new momentum variable $\mathbf{p} \in \mathbb{R}^d$**
- Define the **Hamiltonian**

$$H(\mathbf{x}, \mathbf{p}) = \overbrace{-\log \tilde{\pi}(\mathbf{x})}^{E(\mathbf{x})} + \overbrace{\tfrac{1}{2}\mathbf{p}^\top M^{-1}\mathbf{p}}^{K(\mathbf{p})}.$$

  where M is the **mass matrix**.

- This defines a **new joint distribution**

$$\pi_{\text{aug}}(\mathbf{x}, \mathbf{p}) = Z_H^{-1} \exp(-H(\mathbf{x}, \mathbf{p})) = Z_H^{-1} \tilde{\pi}(\mathbf{x}) \exp(-\tfrac{1}{2}\mathbf{p}^\top M^{-1}\mathbf{p}).$$

  with **marginal** $\pi_{\text{aug}}(\mathbf{x}) = \int \pi_{\text{aug}}(\mathbf{x}, \mathbf{p})\, d\mathbf{p} = \pi(\mathbf{x})$

- HMC is again an instance of **Metropolis-Hastings**, but **sampling from** $\pi_{\text{aug}}(\mathbf{x}, \mathbf{p})$
  - Since we want to **sample from** π (the marginal), we **throw away the sampled $\mathbf{p}$**

Hamiltonian Monte Carlo (cont.)

- In a single MH proposal step, we will consider $\mathbf{x}, \mathbf{p}$ to change over "time" t
    - This is **not** time t in the Markov chain
- We want that the **Hamiltonian is conserved over time**:

$$\frac{dH(\mathbf{x}, \mathbf{p})}{dt} = \frac{\partial H}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial t} + \frac{\partial H}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial t} \overset{!}{=} 0$$

- Which we enforce by letting $\mathbf{x}, \mathbf{p}$ evolve via **Hamiltonian dynamics:**

$$\frac{\partial \mathbf{x}}{\partial t} := \frac{\partial H}{\partial \mathbf{p}} \qquad \frac{\partial \mathbf{p}}{\partial t} := -\frac{\partial H}{\partial \mathbf{x}}$$

- Let $(\mathbf{y}, \mathbf{p}') = \Phi_\tau(\mathbf{x}, \mathbf{p})$ be a **ODE solver** that **integrates this ODE** over some time τ
    - If we made no numerical error, then $H(\mathbf{x}, \mathbf{p}) = H(\Phi_\tau(\mathbf{x}, \mathbf{p}))$ for any τ and $(\mathbf{x}, \mathbf{p})$
    - In practice, we set step size ε and number of steps L, where then $\tau = L\varepsilon$

HMC – Algorithm

Hamiltonian Monte Carlo

Initialize $X_1 \sim p(X_1)$ and repeat for $t = 1, \ldots, T-1$:

1. Given current state $X_t = \mathbf{x}$, sample $\mathbf{p} \sim \mathcal{N}(\mathbf{p}; \mathbf{0}, M)$ and **propose** (deterministically)

$$(\mathbf{y}, \mathbf{p}') = \Phi_\tau(\mathbf{x}, \mathbf{p}) \qquad \text{i.e., } q\big((\mathbf{y}, \mathbf{p}') \mid (\mathbf{x}, \mathbf{p})\big) = \delta_{\Phi_\tau(\mathbf{x},\mathbf{p})}(\mathbf{y}, \mathbf{p}')$$

2. **Compute acceptance probability:**

$$\begin{aligned}\alpha((\mathbf{x}, \mathbf{p}) \to (\mathbf{y}, \mathbf{p}')) &= \min\big(1,\ \exp\big(-H(\mathbf{y}, \mathbf{p}') + H(\mathbf{x}, \mathbf{p})\big)\big) \\ &= 1 \qquad \text{if ODE solver has no numerical error}\end{aligned}$$

3. **Accept or reject:**

$$\text{Sample } U \sim \mathrm{Uniform}(0,1), \qquad X_{t+1} = \begin{cases} \mathbf{y} & \text{if } U \leq \alpha \\ \mathbf{x} & \text{else} \end{cases}$$

Extensions to HMC

- **Issue:** L and ε are sometimes **hard to tune**
  - Problem specific, brittle hyperparameters

- **NUTS (No U-Turn Sampler)**: Variant of HMC which
  - **Auto-tunes** ε in a **warm-up phase**
  - Picks L **adaptively** per MH step (integration stops when trajectory want to “turn around”)

HMC Demo

`https://chi-feng.github.io/mcmc-demo/app.html`

Diagnosing MCMC

MCMC – What can go wrong?

- Recall that for a **stationary** Markov Chain, the **MCMC estimator**

$$\hat{\mathbb{E}}_T = \frac{1}{T}\sum_{t=1}^{T} f(X_t), \qquad X_t \sim \pi$$

has variance

$$\mathrm{var}\left[\hat{\mathbb{E}}_T\right] \approx \frac{\sigma^2_{\mathrm{as}}}{T}, \qquad \sigma^2_{\mathrm{as}} = \mathrm{var}_\pi[f(X)] + 2\sum_{k=1}^{\infty} \mathrm{cov}_\pi(f(X_0), f(X_k)).$$

- **Note:** This formula is only valid **after burn-in**

Diagnostics

When running MCMC at time t, we want to answer **two questions**:

1. Are we **in stationarity**, i.e., is $p_t \approx \pi$ **?**
2. How **large** is σ^2_{as}, i.e., how **inefficient is the chain** **?**

Burn-in Phase

- We suffer from **initialization bias** since $p_1 \neq \pi$
- Thus, discard the first B samples (**burn-in phase**)
- **Unfortunately, there is no good data-driven way to pick** B 😩
- **Note:** B only affects **bias** and is **not related** to σ_{as} ⚠️

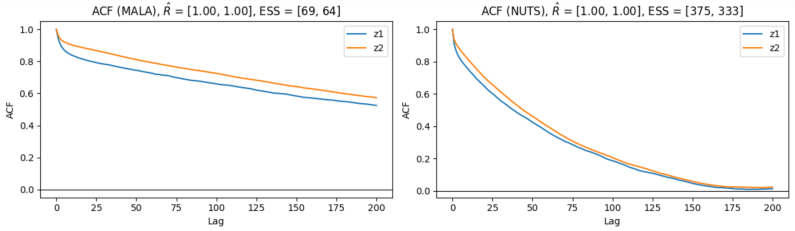
Autocorrelation Function (ACF)

- For a **stationary** chain, we can write

$$\rho_k = \frac{\text{cov}_\pi(f(X_0), f(X_k))}{\text{var}_\pi(f(X))}, \qquad \sigma^2_{\text{as}} = \text{var}_\pi[f(X)] \left(1 + 2\sum_{k=1}^{\infty} \rho_k\right)$$

  where ρ_k is the **autocorrelation** at lag k.

- We can plot an **estimate** $\hat{\rho}_k$ over k **after burn-in**:



- ACF diagnoses **within-chain dependence, not convergence to** π ⚠

Effective Sample Size (ESS)

- We would like to define **Effective Sample Size (ESS)** such that

$$\text{var}\left[\hat{\mathbb{E}}_T\right] = \frac{\text{var}_\pi[f(X)]}{\text{ESS}}$$

- ESS tells us **how many i.i.d. samples would give the same variance** !

- For a **stationary** chain, we thus have

$$\text{ESS} = \frac{\text{var}_\pi[f(X)]}{\sigma^2_{\text{as}}/T} = \frac{T}{1 + 2\sum_{k=1}^{\infty} \rho_k}$$

  which we can estimate from **samples post burn-in**

Gelman-Rubin $\hat{R}$

- We want to check if MCMC has **converged to “stationary” distribution**
  - By construction, we will **converge** to the **unique stationary distribution** π as $T \to \infty$
  - However, for finite T, we can get **stuck** in quasi-stationary distributions $\neq \pi$ **!**

- Run $M \geq 2$ **independent chains** and discard **burn-in**

- **Idea:** Compare **within-chain variance** W with **between-chain variance** B:

$$\hat{R} := \sqrt{\frac{(1 - \frac{1}{T})W + \frac{1}{T}B}{W}}$$

- If all chains converged to the same distribution, we should have $\hat{R} \approx 1$
  - Often, one checks if $\hat{R} \leq 1.01$

MCMC – Summary

- **Goal**: Sample from **complicated, high-dimensional distribution** π
  - Where typically only $\tilde{\pi}$ is known
- Almost all MCMC algorithms presented are **instances of Metropolis-Hastings**
  - Random-walk MH, Gibbs Sampling, MALA, HMC, NUTS
- In **high dimensions**, HMC/NUTS is the **go-to choice**
  - If you have **tractable conditionals**, Gibbs sampling may be a **good option**
- However, even well-tuned MCMC methods **can take a long time to converge**
  - This is called **mixing time**
- **Diagnosis** of MCMC is **hard in general**
  - Common tools: ACF, ESS, $\hat{R}$