Markov Chain Monte Carlo

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Goal

We want to create Monte Carlo estimators of integrals:

$$I = \int f(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} \approx \frac{1}{S}\sum_{s=1}^{S} f(\mathbf{x}^{[s]}) = \hat{I} \qquad \text{with } \mathbf{x}^{[s]} \sim p(\mathbf{x})$$

Last lecture we saw

- rejection sampling — High rejection rate in high dim
- importance sampling — High variance in high dim

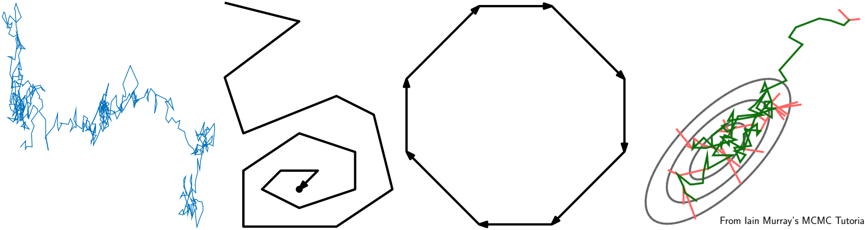
Today: Markov Chain methods for sampling from $p(\mathbf{x})$

Markov Chains

Instead of generating independent samples $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots$, use a proposal density q that depends on the previous sample (state) $\boldsymbol{x}^{(t)}$

- This generates a **sequence** with a joint $q(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(T)})$
- **Key idea**: For the marginal at T we want $q_{X^{(T)}}(\mathbf{x}) \approx p(\mathbf{x})$
- Simplify joint with **Markov property**: $q(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}) = q(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)}) = T(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)})$ only depends on the previous setting/state of the chain
- T is called a **transition operator**
- Example: $T(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)}) = \mathcal{N}\left(\boldsymbol{x}^{(t+1)} \,|\, \boldsymbol{x}^{(t)}, \sigma^2 \boldsymbol{I}\right)$
- Samples $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}$ form a **Markov chain**
- Samples $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}$ are no longer independent

Behaviour of Markov Chains

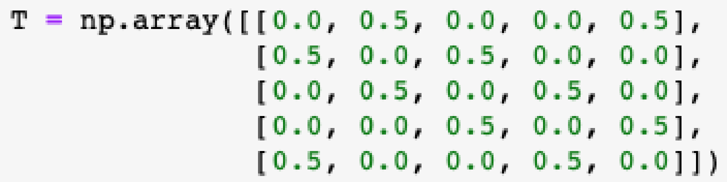


From Iain Murray's MCMC Tutorial

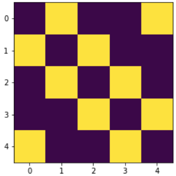
Four different behaviors of Markov chains:

- Diverge (e.g., random walk diffusion where $\boldsymbol{x}^{(t+1)} \sim \mathcal{N}\left(\boldsymbol{x}^{(t)}, \boldsymbol{I}\right)$)
- Converge to an absorbing state
- Converge to a (deterministic) limit cycle
- Converge to an equilibrium distribution p^*: Markov chain remains in a region, bouncing around in a random way

Example: Sampling from a uniform distribution



```
T = np.array([[0.0, 0.5, 0.0, 0.0, 0.5],
              [0.5, 0.0, 0.5, 0.0, 0.0],
              [0.0, 0.5, 0.0, 0.5, 0.0],
              [0.0, 0.0, 0.5, 0.0, 0.5],
              [0.5, 0.0, 0.0, 0.5, 0.0]])
```



Procedure:

1. Initialise state at $t = 1$ by sampling from initial distribution $p(\mathbf{x}^{(1)})$. Can be a delta function.
2. Repeat: Sample from $T(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)})$

What distribution are we sampling from?

We should ask:

At time t, what distribution are we sampling from?

Apply sum rule:

$$\begin{aligned} q(x^{(t)}) &= \sum_{x=1}^{5} T(x^{(t)}|x^{(t-1)} = x)q(x^{(t-1)} = x) \\ &= \mathbf{T}\mathbf{q}^{(t-1)} \end{aligned}$$

Why does it converge?

$$\mathbf{q}^{(t)} = \mathbf{T}\mathbf{q}^{(t-1)} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}\mathbf{q}^{(t-1)}$$

For this simple-to-analyse case:

- Only one eigenvector with $\lambda = 1$, which is $\mathbf{p}$.
- All other eigenvectors have $\lambda < 1$.

Using Markov Chain samples: Independent chains

If after T steps, we converge to $q_{\mathbf{x}^{(T)}}(\mathbf{x}) \approx p(\mathbf{x})$.

$$\hat{I} \approx \frac{1}{S}\sum_{s=1}^{S} g(\mathbf{x}_s)\,, \qquad \mathbf{x}_s \sim q(\mathbf{x}^{(T)})\,. \tag{1}$$

Where $q(\mathbf{x}_T)$ is generated from the Tth step of a Markov Chain. Time for a sample to be "good enough" is called **burn-in time**.

- We run S separate Markov Chains for T steps. Samples are **independent**, because the Markov Chains are independent.
- Samples are approximate. May contain bias from T not being large enough for the distribution to converge.

Using Markov Chain samples: Single long chain

Alternative: After T steps, average all samples

$$\hat{I} \approx \frac{1}{S} \sum_{s=1}^{S} g(\mathbf{x}^{(T+s)}) , \qquad \mathbf{x}^{(T+1)}, \dots, \mathbf{x}^{(T+S)} \sim q(\mathbf{x}_{T+1}, \dots, \mathbf{x}_{T+S}) . \tag{2}$$

$$q(\mathbf{x}^{(T+1)}, \dots, \mathbf{x}^{(T+S)}) = q(\mathbf{x}^{(T)}) \prod_{s=1}^{S-1} q(\mathbf{x}^{(T+s)} \mid \mathbf{x}^{(T+s-1)}) \tag{3}$$

- Remember, we choose T such that $q_{\mathbf{x}^{(T)}}(\mathbf{x}) \approx p(\mathbf{x})$.
- Only requires T steps for burn-in time **once**.
- Then can get a single sample per step. However, samples are **correlated**.

Usually more efficient to generate **many correlated samples**, than few independent ones.

Markov Chain Monte Carlo

Markov Chain Monte Carlo estimates an integral using correlated samples from a Markov Chain. If the chain has converged, the estimate is **unbiased**.

$$\hat{I} \approx \frac{1}{S}\sum_{s=1}^{S} g(\mathbf{x}^{(s)}) \tag{4}$$

with $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots\}$ from Markov Chain.

$$\mathbb{E}_{q\left(\mathbf{x}^{(1)},\mathbf{x}^{(2)},\dots\right)}\left[\hat{I}\right] = \frac{1}{S}\sum_{s=1}^{S} \mathbb{E}_{q(\mathbf{x}^{(s)})}\left[g(\mathbf{x}^{(s)})\right] = I \tag{5}$$

Variance decreases depending on **covariance**

$$\mathbb{V}_{q(\{\mathbf{x}^{(s)}\})}\left[\hat{I}\right] = \frac{1}{S^2}\left[\sum_{s=1}^{S} \mathbb{V}_{q(\mathbf{x}^{(s)})}\left[g(\mathbf{x}^{(s)})\right] + \sum_{t}\sum_{t' \neq t} \mathbb{C}_{q(\mathbf{x}^{(t)},\mathbf{x}^{(t')})}\left[g(\mathbf{x}^{(t)}), g(\mathbf{x}^{(t')})\right]\right]$$

$$= \frac{1}{S}\mathbb{V}_{p(\mathbf{x})}[g(\mathbf{x})] + \left[\sum_{t}\sum_{t' \neq t} \mathbb{C}_{q(\mathbf{x}^{(t)},\mathbf{x}^{(t')})}\left[g(\mathbf{x}^{(t)}), g(\mathbf{x}^{(t')})\right]\right]$$

Correlation vs steps trade-off

Independent chains:

- Require $T \cdot S$ transitions for S samples
- Generate independent samples, so don't need too many S.

Single chain:

- Require $T + S$ transitions for S samples
- Generates dependent samples so may need more S.

Converging to an Equilibrium Distribution

To get a Markov Chain that converges to a desired distribution $p(\mathbf{x})$, we need two properties:

1. Transition leaves $p(\mathbf{x})$ **invariant**:

$$p(\mathbf{x}) = \int T(\mathbf{x}|\mathbf{x}')p(\mathbf{x}')\mathrm{d}\mathbf{x}' \tag{6}$$

   i.e. if we start with a sample from $p(\mathbf{x})$, the marginal distribution after the transition is unchanged.

2. Transition is **ergodic**. Definition is technical, but it is needed to ensure that $\pi(\mathbf{x}^{(t)}) \to p(\mathbf{x})$ as $t \to \infty$.
   Ergodic chains only have one equilibrium distribution.

Invariance and Detailed Balance

- Invariance: Each step leaves the distribution p invariant (we stay in p):

  $$p(\boldsymbol{x}') = \sum_{\boldsymbol{x}} T(\boldsymbol{x}'|\boldsymbol{x})p(\boldsymbol{x}) \qquad p(\boldsymbol{x}') = \int T(\boldsymbol{x}'|\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x}$$

  Once we sample from p, the transition operator will not change this, i.e., we do not fall back to some funny distribution $\pi \neq p$

- Sufficient condition for p being invariant:

  Detailed balance:

  $$p(\boldsymbol{x})T(\boldsymbol{x}'|\boldsymbol{x}) = p(\boldsymbol{x}')T(\boldsymbol{x}|\boldsymbol{x}')$$

Why is invariance not enough?

- Invariance only says something about the transitions once we have **reached** the stationary distribution.
- Invariance doesn't say anything about how the chain converges.

Trivial solutions leave $p(\mathbf{x})$ invariant, e.g. $T(\mathbf{x}_{t+1} \,|\, \mathbf{x}_t) = \delta(\mathbf{x}_{t+1} - \mathbf{x}_t)$:

$$\int T(\mathbf{x}_{t+1} = \mathbf{x} \,|\, \mathbf{x}_t = \mathbf{x}') p(\mathbf{x}') \mathrm{d}\mathbf{x}' = p(\mathbf{x}) \tag{7}$$

Ergodicity has a rather technical definition, but thankfully it is easy to guarantee!

Ergodicity and communication

A Markov Chain is ergodic if there is some probability for any state to reach any state in bounded steps. If this is true, all states are said to **communicate**.

When designing Markov Chains, the easiest way to guarantee this is to have transitions that satisfy:

$$T(\mathbf{x}^{(t+1)} \mid \mathbf{x}^{(t)}) > 0 \qquad\qquad \forall \mathbf{x}^{(t+1)}, \mathbf{x}^{(t)} \tag{8}$$

Then, all states will communicate in 1 step.

Metropolis-Hastings

- Assume that $\tilde{p} = Zp$ can be evaluated easily
- Proposal density $\hat{T}(\boldsymbol{x}'|\boldsymbol{x}^{(t)})$ depends on last sample $\boldsymbol{x}^{(t)}$.
  Example: Gaussian with mean $\boldsymbol{x}^{(t)}$: $\hat{T}(\boldsymbol{x}'|\boldsymbol{x}^{(t)}) = \mathcal{N}\big(\boldsymbol{x}^{(t)}, \boldsymbol{\Sigma}\big)$

Metropolis-Hastings Algorithm

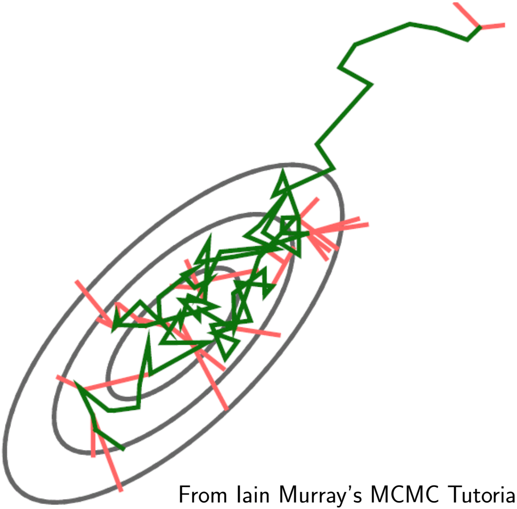
1. Generate proposal $\boldsymbol{x}' \sim \hat{T}(\boldsymbol{x}'|\boldsymbol{x}^{(t)})$
2. If

$$\frac{\hat{T}(\boldsymbol{x}^{(t)}|\boldsymbol{x}')\tilde{p}(\boldsymbol{x}')}{\hat{T}(\boldsymbol{x}'|\boldsymbol{x}^{(t)})\tilde{p}(\boldsymbol{x}^{(t)})} \geqslant u\,, \qquad u \sim U[0,1]$$

accept the sample $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}'$. Otherwise set $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)}$.

- $q(\boldsymbol{x}^{(t)}) \xrightarrow{t\to\infty} p(\boldsymbol{x})$ ⏩ Converge to equilibrium distribution
- If proposal distribution is symmetric: Metropolis Algorithm (Metropolis et al., 1953); Otherwise Metropolis-Hastings

Example



From Iain Murray's MCMC Tutorial

Step-Size Demo

- Explore $p(x) = \mathcal{N}\left(x \,|\, 0,\, 1\right)$ for different step sizes σ.
- We can only evaluate $\log \tilde{p}(x) = -x^2/2$
- Proposal distribution q: Gaussian $\mathcal{N}\left(x^{(t+1)} \,|\, x^{(t)},\, \sigma^2\right)$ centered at the current state for various step sizes σ
- Expect to explore the space between $-2, 2$ with high probability

Step-Size Demo: Discussion

- Acceptance rate depends on the step size of the proposal distribution
  - ▶▶ Exploration parameter
- If we do not reject enough, the method does not work.
- In rejection sampling we do not like rejections, but in MH rejections tell you where the target distribution is.
- Theoretical results: in 1D 44%, in higher dimensions about 25% acceptance rate for good mixing properties
- Tune the step size

Properties

- Samples are correlated
- If $\hat{T} > 0$ everywhere, we will end up in the equilibrium distribution: $\pi(\boldsymbol{x}^{(t)}) \xrightarrow{t\to\infty} p^*(\boldsymbol{x})$
- Explore the state space by random walk

  ⏩ May take many steps, if the steps are short compared to the distribution
- No further catastrophic problems in high dimensions

MCMC Diagnostics: Trace Plots

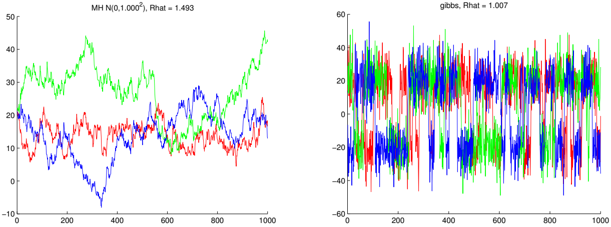


Figure from Murphy (2012)

- Mixing time: Amount of time it takes the Markov chain to converge to the stationary distribution and forget its initial state.
- Trace plots: Run multiple chains from very different starting points, plot the samples of the variables of interest. If the chain has mixed, the trace plots should converge to the same distribution.

Summary

- MCMC generates a Markov chain of dependent samples that allow us to generate samples from the target distribution
- Metropolis Hastings algorithm

Further Reading

- MacKay, ch 29
- Murphy, ch 24

References I