Markov Chain Monte Carlo

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1. Ergodicity of Markov chains

1.1 Markov Chains

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A sequence of random variables is called a **Markov chain** if there exists a function $P(x, \cdot)$ such that, for each $m = 0, 1, 2, \ldots$, the following holds:

$$\mathbb{P}(X_{m+1} \in A \mid X_m = x) = P(x, A)$$

Here, $P(x, \cdot)$ is called the **Markov kernel**.

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More generally, for any n,

$$P^n(x, A) = \mathbb{P}(X_{m+n} \in A \mid X_m = x)$$

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Let’s focus on initial value dependency.

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You do this N times, copying one stone each time.

Once the new jar is filled, the original jar is thrown away, and the process starts again.

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This gives the probability that the new jar will have exactly y **red** stones, where $\binom{N}{y}$ is the binomial coefficient, a way of counting how many ways you can choose y **red** stones out of N draws.

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This process, where the number of **red** stones in each new jar depends on the number from the previous jar, is called the **Wright-Fisher model**.

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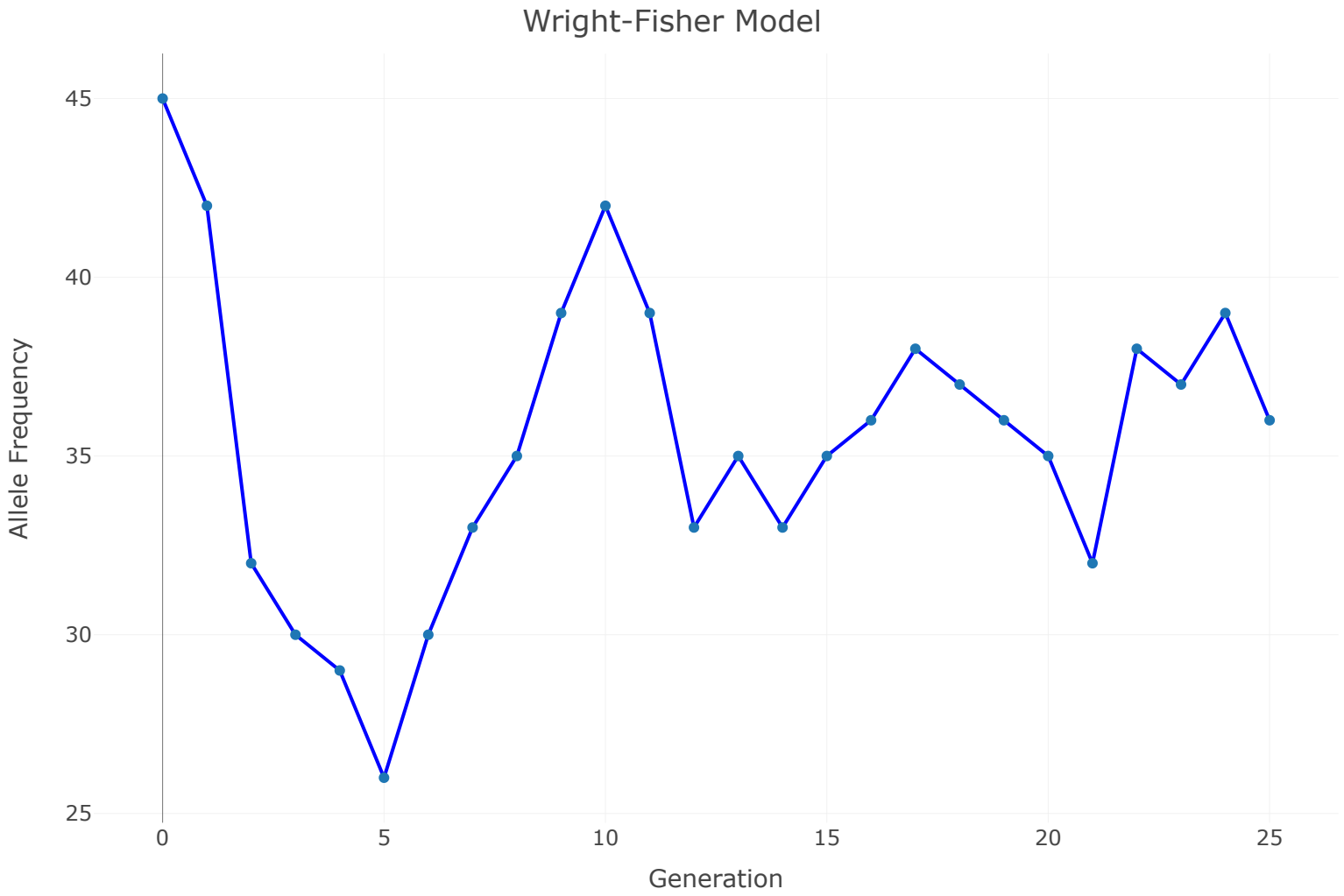
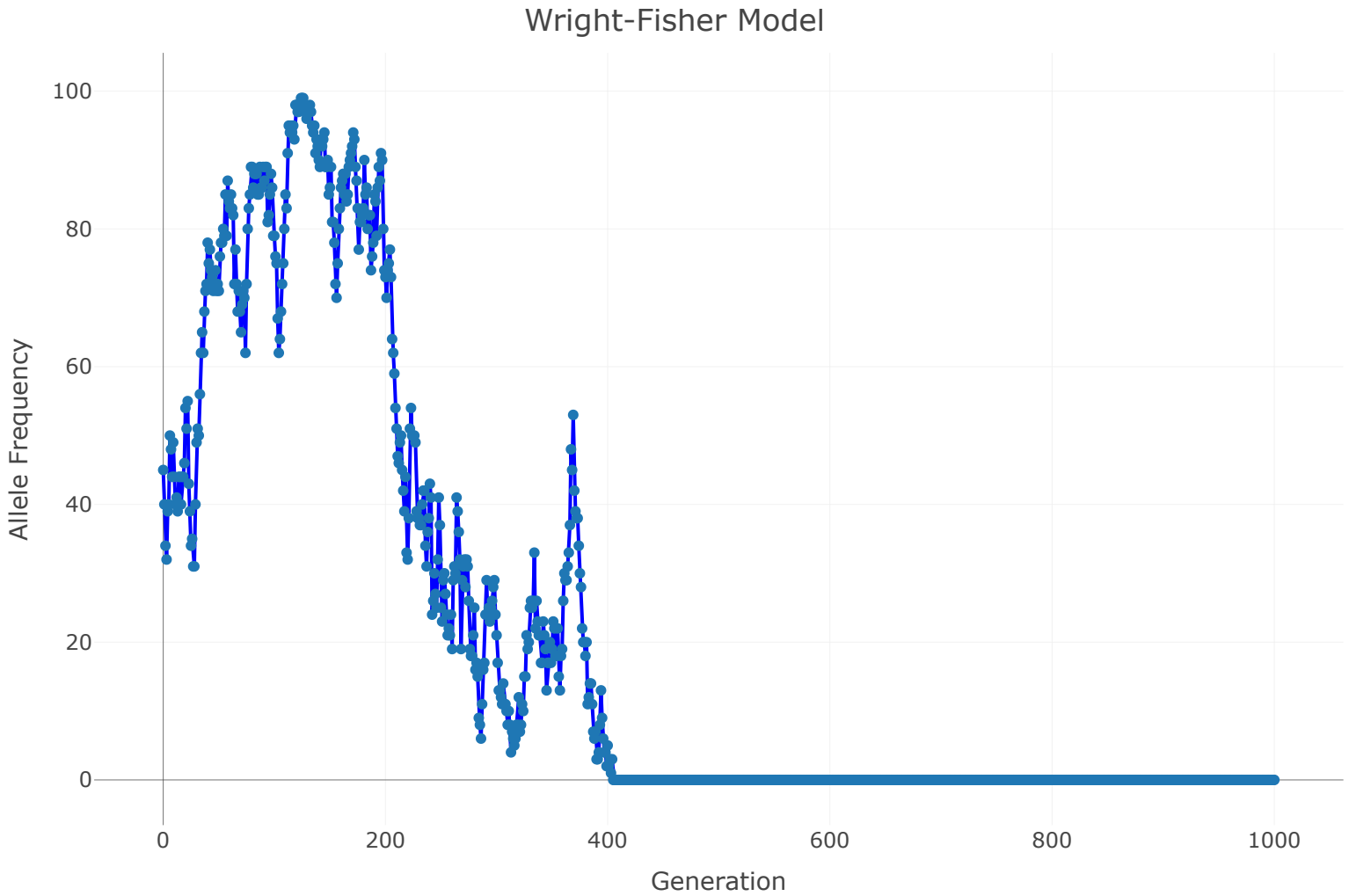
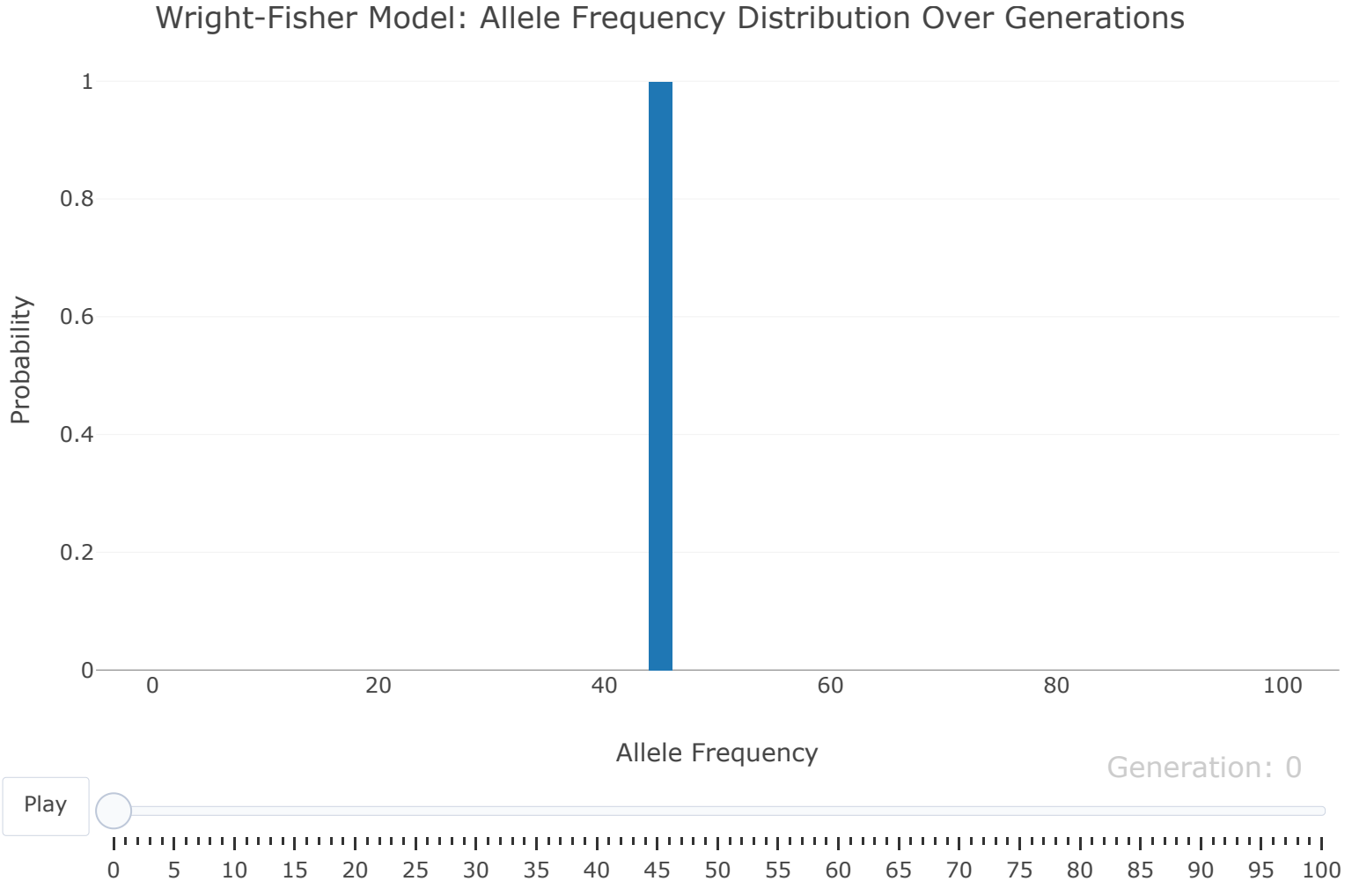
- The number of **red** stones in each new jar depends on how many **red** stones were in the previous jar.

Let's experiment with this model for $N = 100$, starting with 45 red stones, over 25 trials:



Now, let's extend the experiment to 1000 trials. Note that the number of red stones becomes 0 at some point, and once this happens, the number does not change:




Wright-Fisher Model: Allele Frequency Distribution Over Generations
Probability
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
Allele Frequency
Generation: 0
Play
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100

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In the Wright-Fisher model, the final state will end up in an absorbing set, either 0 or N, and the proportion of each is determined probabilistically based on the initial number of red stones.

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$$\mathbb{E}[X_{m+1}(N - X_{m+1}) \mid X_m = x] = \left(1 - \frac{1}{N}\right) x(N - x).$$

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1.3 From the above equation, conclude that X_m converges in probability to 0 or N when $m \to \infty$.

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A Markov chain defined by

$$X_{m+1} = \alpha X_m + W_{m+1}, \quad W_{m+1} \sim \mathcal{N}(0, \sigma^2),$$

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From this equation, we can derive:

$$X_m = \alpha^m X_0 + \sum_{n=0}^{m-1} \alpha^n W_{m-n}.$$

Due to the reproductive property of normal distributions, we find that X_m follows a normal distribution:

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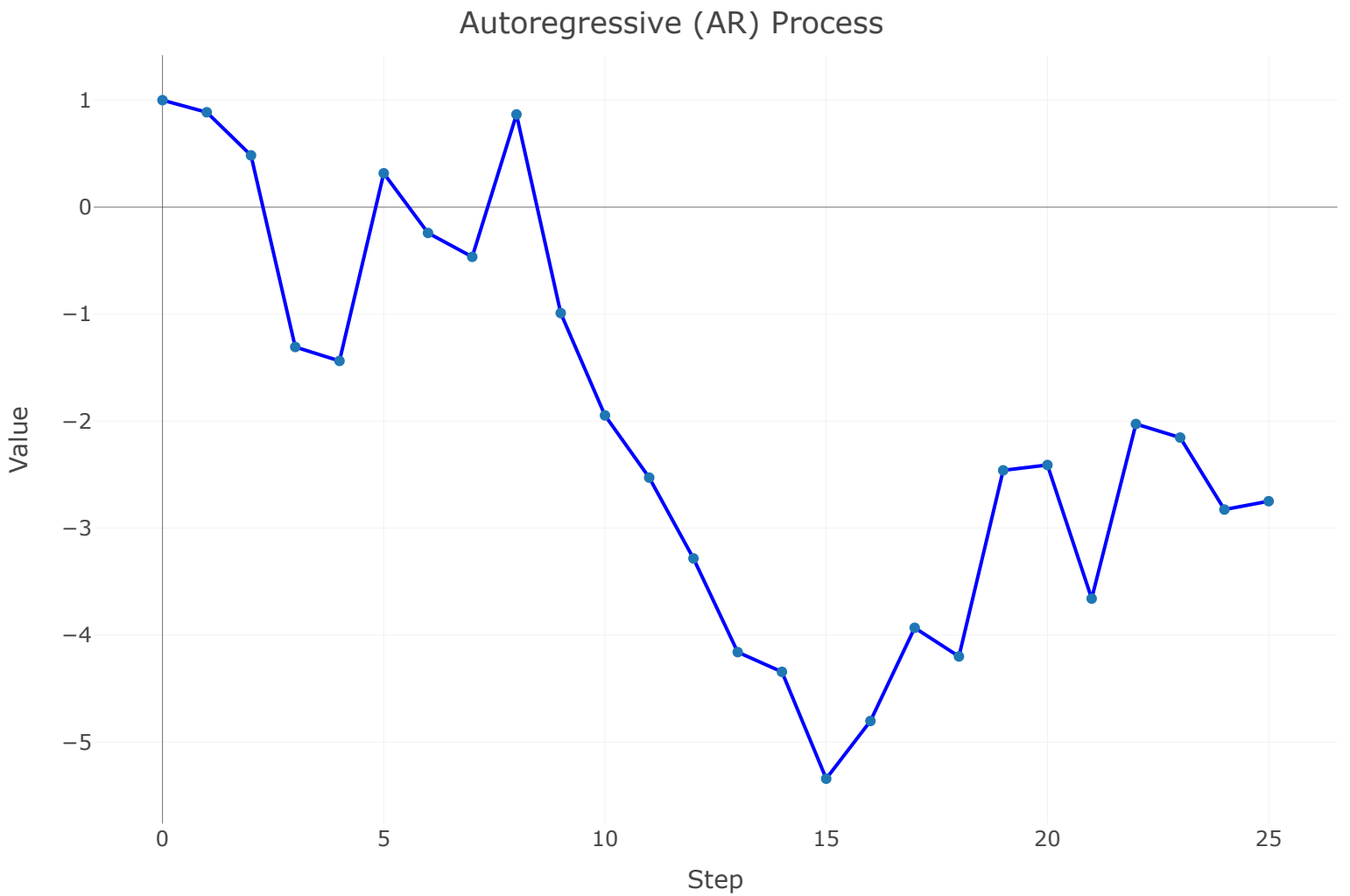
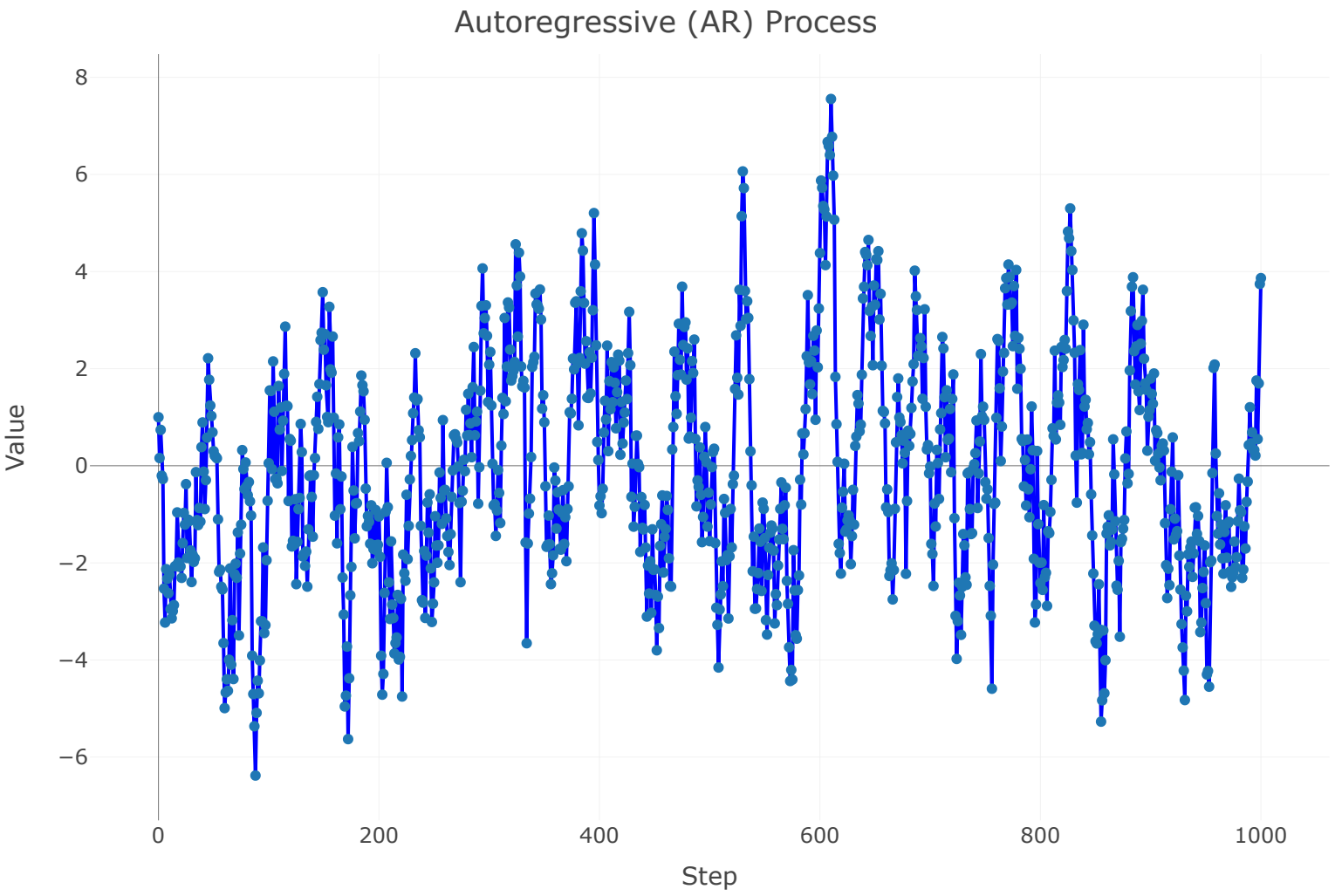
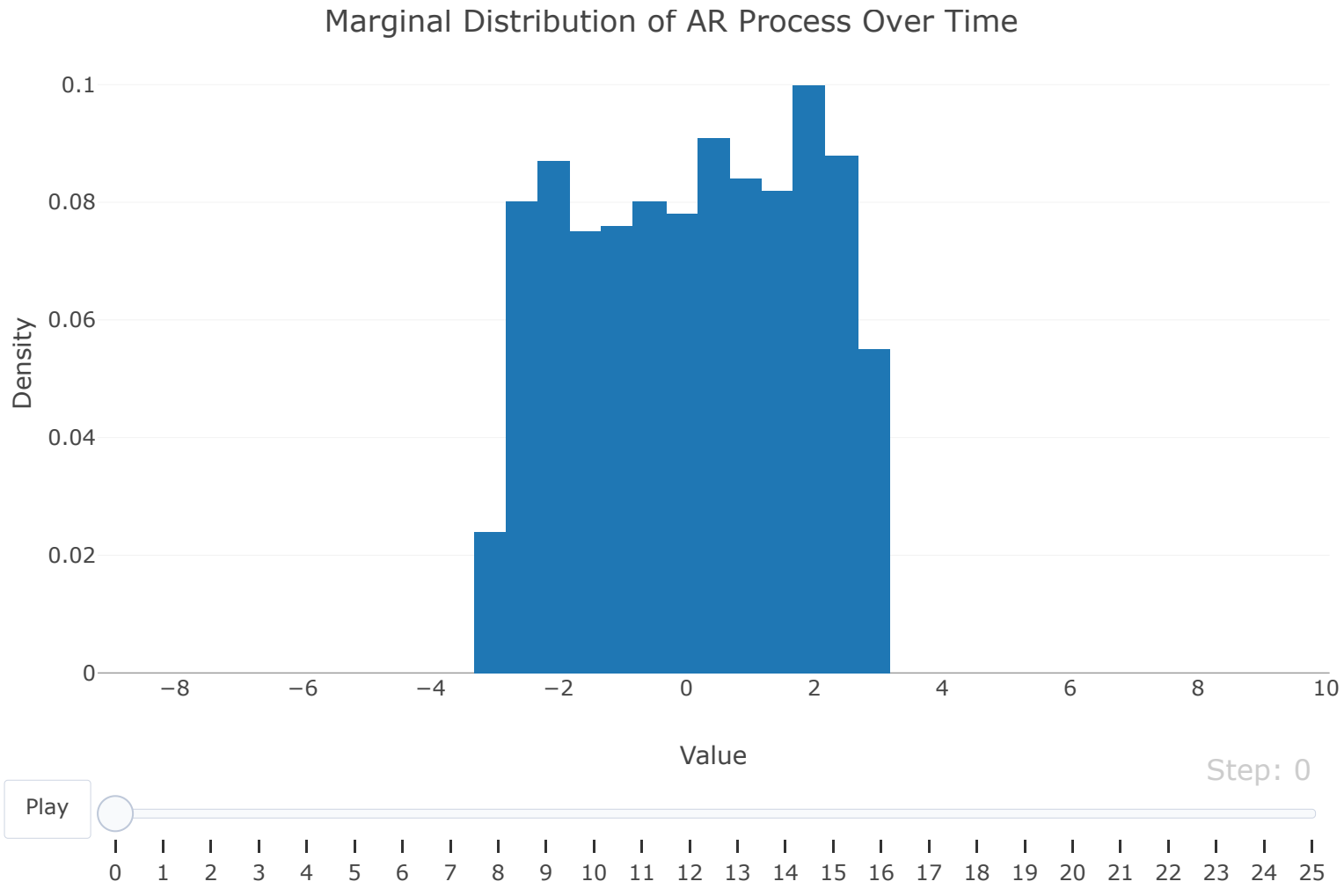
The autoregressive model differs from the Wright-Fisher model in that the limiting distribution does not depend on the initial value.

Example: Autoregressive Process




Autoregressive (AR) Process
Value
Step
8
6
4
2
0
−2
−4
−6
0
200
400
600
800
1000


Marginal Distribution of AR Process Over Time
Density
0.1
0.08
0.06
0.04
0.02
0
−8
−6
−4
−2
0
2
4
6
8
10
Value
Play
Step: 0
0
1
2
3
4
5
6
7
8
9
10
11
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Let’s continue with a more detailed explanation of ergodicity and the concepts involved in the behavior of Markov chains.

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2. **Singularity**
3. **Total Variation**

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If $X_0 \sim \Pi$, then $X_1 \sim \Pi$ must also hold. A probability distribution Π that satisfies this property is called an **invariant probability measure**.

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In this case, we write $P \perp Q$. If P and Q are not mutually singular, we write $P \not\perp Q$.

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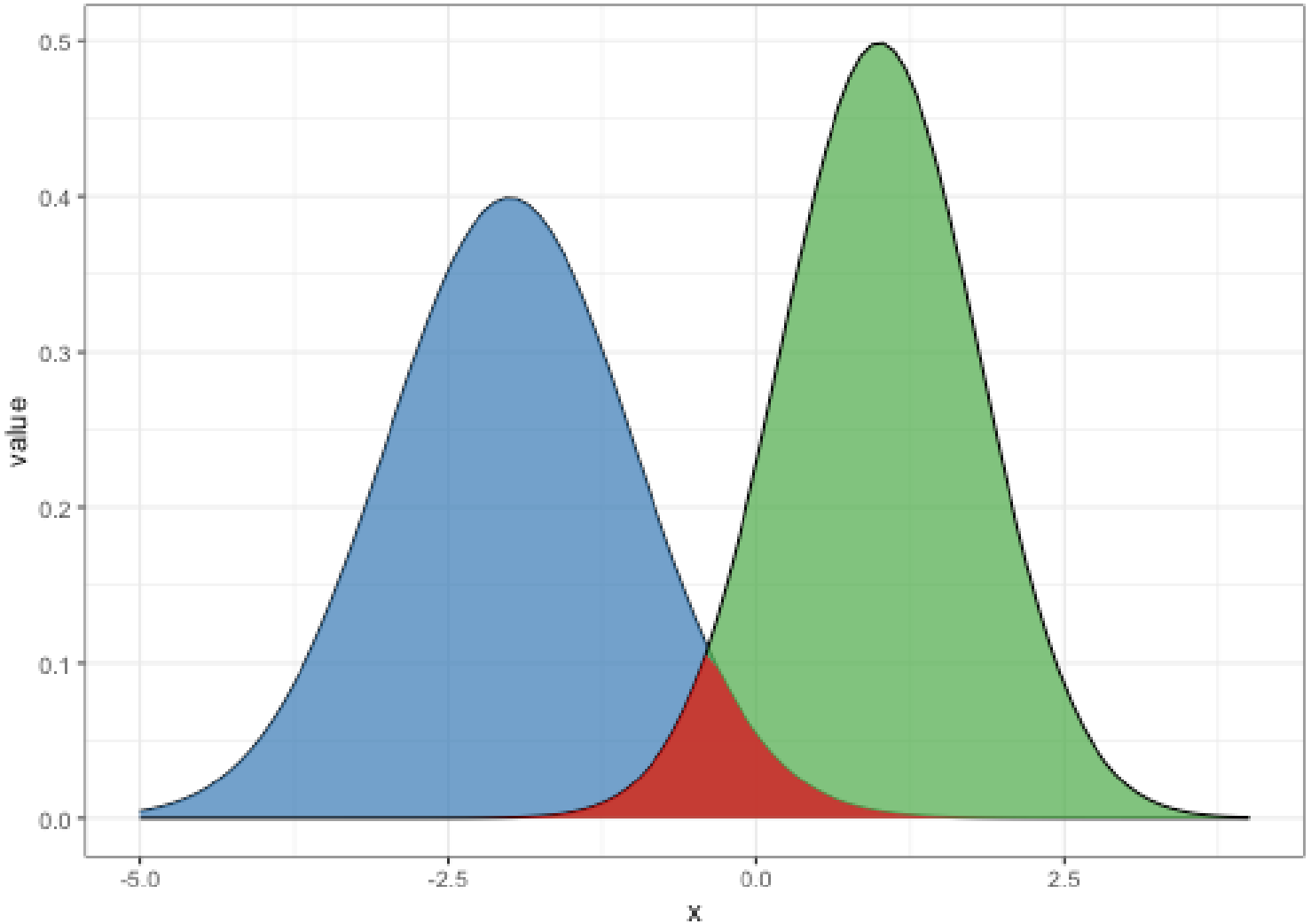
If there is a shared **red region** under both probability density functions, then $P \not\perp Q$. If no such region exists, then $P \perp Q$.


0.5
0.4
0.3
0.2
0.1
0.0
value
-5.0
-2.5
0.0
2.5
x

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This measures the difference between the probability density functions $p(x)$ and $q(x)$.

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Hence, the area of the red region is:

$$\text{Red Region} = 1 - \frac{1}{2}\|P - Q\|_{\mathrm{TV}}.$$

If $P \perp Q$, the area of the red region is 0, meaning that $\|P - Q\|_{\mathrm{TV}} = 2$, and conversely, if $P \not\perp Q$, then $\|P - Q\|_{\mathrm{TV}} < 2$.

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- If the red region of the graph is zero, we say that the two probability measures are **mutually singular**.
- This red region can be expressed as $1 - \|P - Q\|_{\mathrm{TV}}/2$, where $\|P - Q\|_{\mathrm{TV}}$ is the total variation distance between the measures P and Q.

Exercise 2.

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2.3 Prove that no invariant probability measure exists for the Autoregressive model when $\alpha = 1$. (Hint: Evaluate the characteristic function. Recall that every characteristic function $\psi(u)$ satisfies $\psi(0) = 1$ and is continuous at $u = 0$.)

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Moreover, if $X_0 = x$, the law of large numbers holds:

$$\frac{1}{M} \sum_{m=0}^{M-1} f(X_m) \longrightarrow_{M \to \infty} \int f(x) \Pi(\mathrm{d}x),$$

as long as the right-hand side exists.

Proof Outline:

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For more details, see "Kulik (2017)" Theorem 2.5.1.

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even if P and Q are very close or even identical.

However, with **coupling**, we can construct the pair (X, Y) in such a way that we increase the probability $\mathbb{P}(X = Y)$ or reduce the difference $|X - Y|$.

Coupling (continued)

Coupling is a method for constructing a pair (X, Y), where $X \sim P$ and $Y \sim Q$, in such a way that we increase the probability $\mathbb{P}(X = Y)$ or make $|X - Y|$ smaller.

In Markov chain convergence theory, **optimal coupling** plays an important role. Optimal coupling maximizes $\mathbb{P}(X = Y)$, which is beneficial for proving convergence.

Imagine we have 100 **German** and 100 Japanese male Judo players (Judoka). Our goal is to pair them by matching those in the same weight class. Ideally, we want to create as many matches where the weight classes of the players, X and Y, are identical, meaning $X = Y$.

The beautiful image was shared by Joshua Jamias on Unsplash

However, even with careful pairing, there’s a limit to the number of same-class matches we can create.

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For example:

- If there are 3 **German** and 5 **Japanese** players in the under-66 kg weight class, the maximum number of same-class matches is 3.
- If there are 6 **German** and 2 **Japanese** players in the 81 kg weight class, the maximum number of same-class matches is 2.

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Therefore, the total number of same-class matches is determined by the smaller number of players from each group in every weight class. Any remaining players will participate in mixed-class matches, where $X \neq Y$.

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Mathematically, when two distributions P and Q are coupled, the maximum probability of forming a match $X = Y$ is:

$$\mathbb{P}(X = Y) = 1 - \frac{1}{2}\|P - Q\|_{\mathrm{TV}}.$$

This coupling, which achieves this maximum probability, is called **optimal coupling**.

Sequential Coupling in Markov Chains

Now, let's apply coupling sequentially to Markov chains. Consider two Markov chains starting from different initial values x_0 and y_0.

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This process is repeated indefinitely.

Once $X_m = Y_m$, they remain coupled for all future steps.

The inequality

$$\mathbb{P}(X_m = Y_m) \leq 1 - \frac{1}{2}\|P^m(x, \cdot) - P^m(y, \cdot)\|_{\mathrm{TV}}.$$

is always true.

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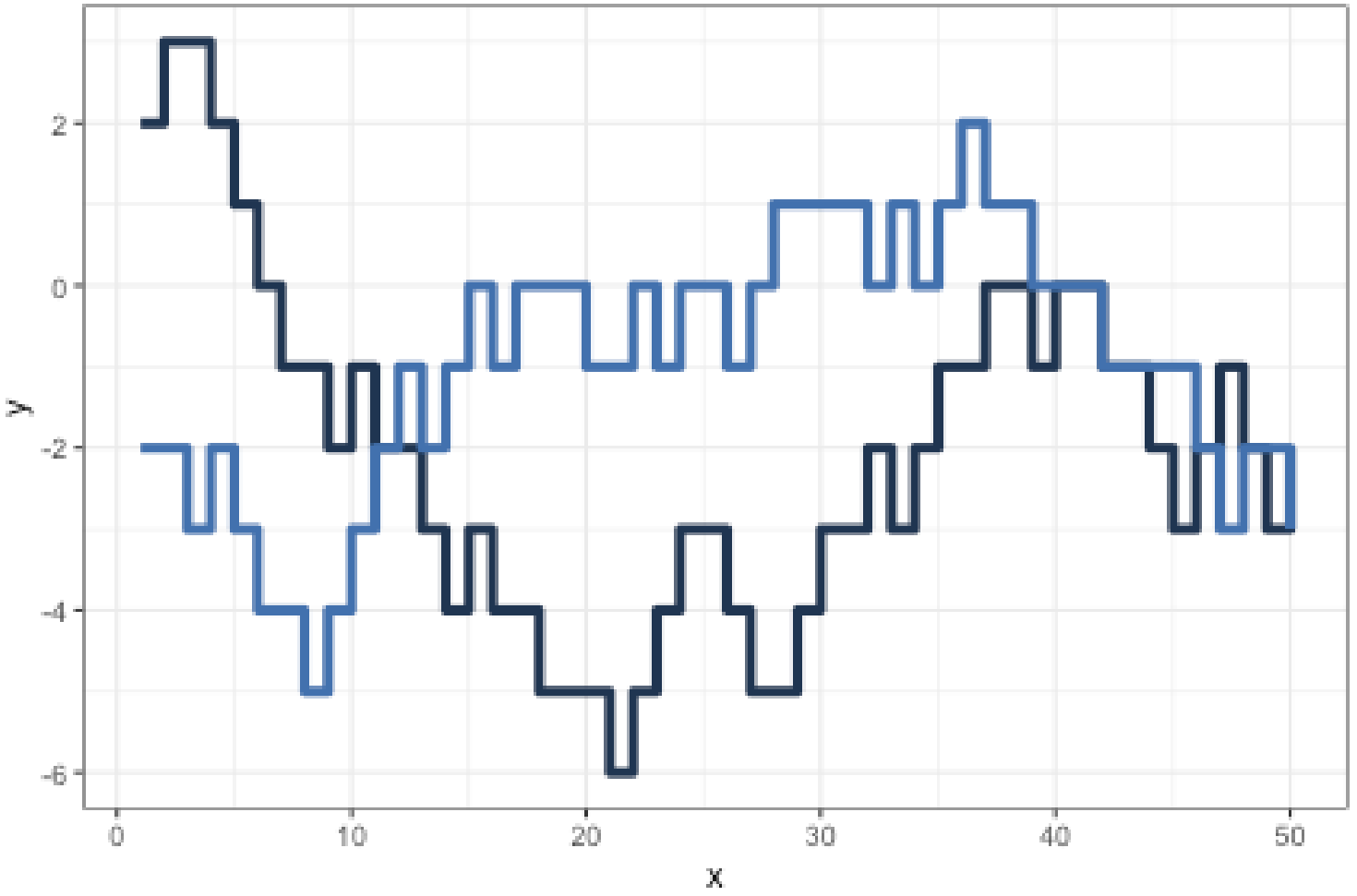
is always true.

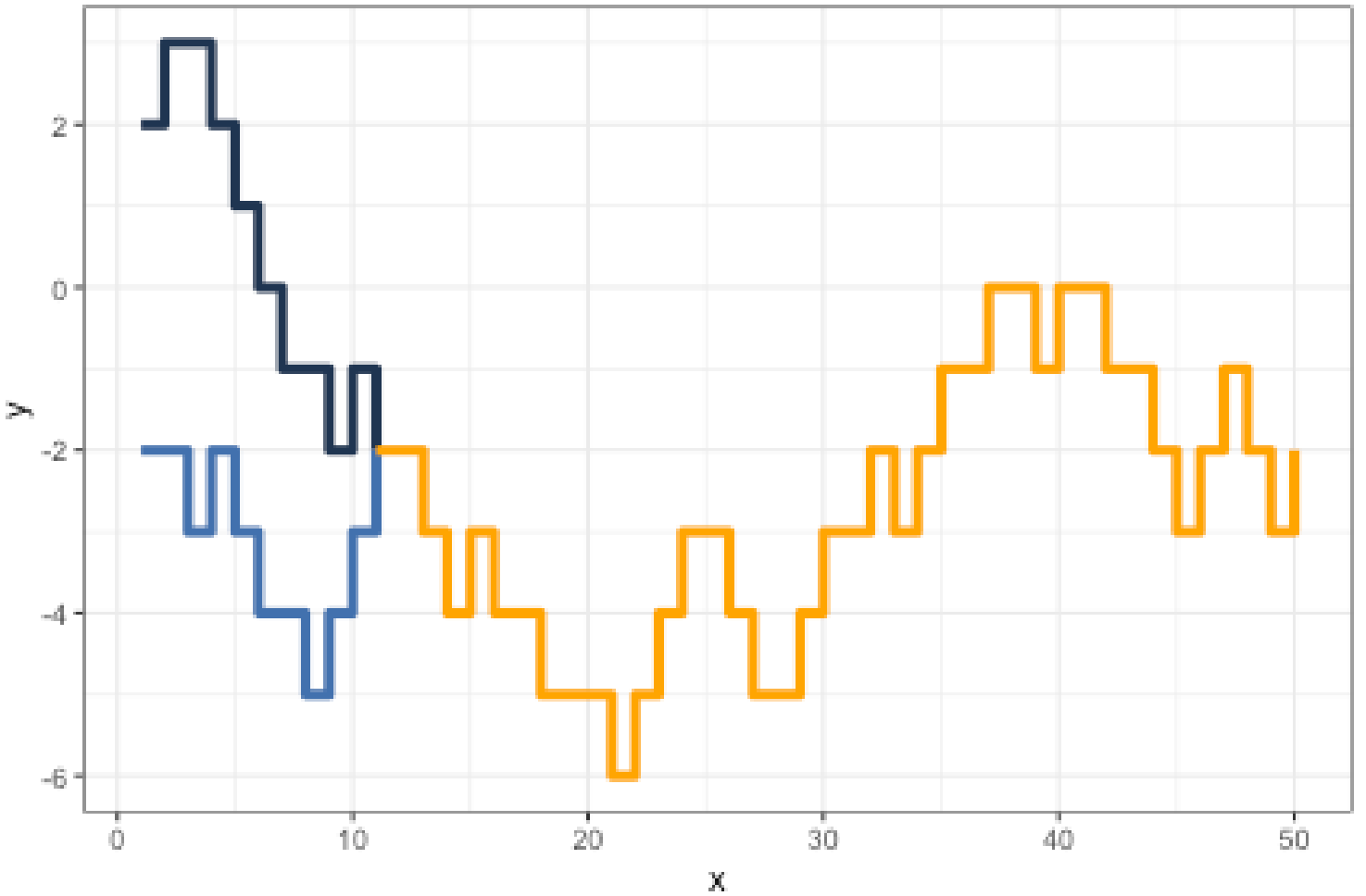
Through coupling, the left-hand side provides a good bound of the right-hand side, and is **easier** to estimate.

Coupling Before and After

Before coupling (left side of the plot):



After coupling (right side of the plot):



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- A sufficient condition for this is that $P(x, \cdot)$ and $P(y, \cdot)$ are not mutually singular, and that an invariant probability measure exists.
- **Coupling** is a powerful technique used to establish the law of large numbers in Markov chains.

From here ...

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- We introduced the law of large numbers for Markov chains.
- From here, we will introduce a Monte Carlo method using the theorem.

2. Markov chain Monte Carlo

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> The **Markov Chain Monte Carlo (MCMC)** method is a powerful numerical technique used to approximate expectations by leveraging the law of large numbers of Markov chains. It generates samples from a target distribution by constructing a Markov chain that converges to this distribution, allowing for the estimation of complex integrals or probabilistic quantities that are otherwise intractable

2.1 Metropolis Algorithm

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Now, assume stationarity has been reached, meaning that the random variable X satisfies $\mathbb{P}(X = x) = \pi(x)$.

The **outflow** from x to y in one step is the original probability $\pi(x)$ multiplied by the transition probability $q(x, y)$:

$$\pi(x)q(x, y).$$

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Conversely, the **inflow** from y to x is:

$$\pi(y)q(y, x).$$

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If the transition is not allowed, the process stays at x.

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This acceptance function $\alpha(x,y)$ is the core idea behind the **Metropolis algorithm**.

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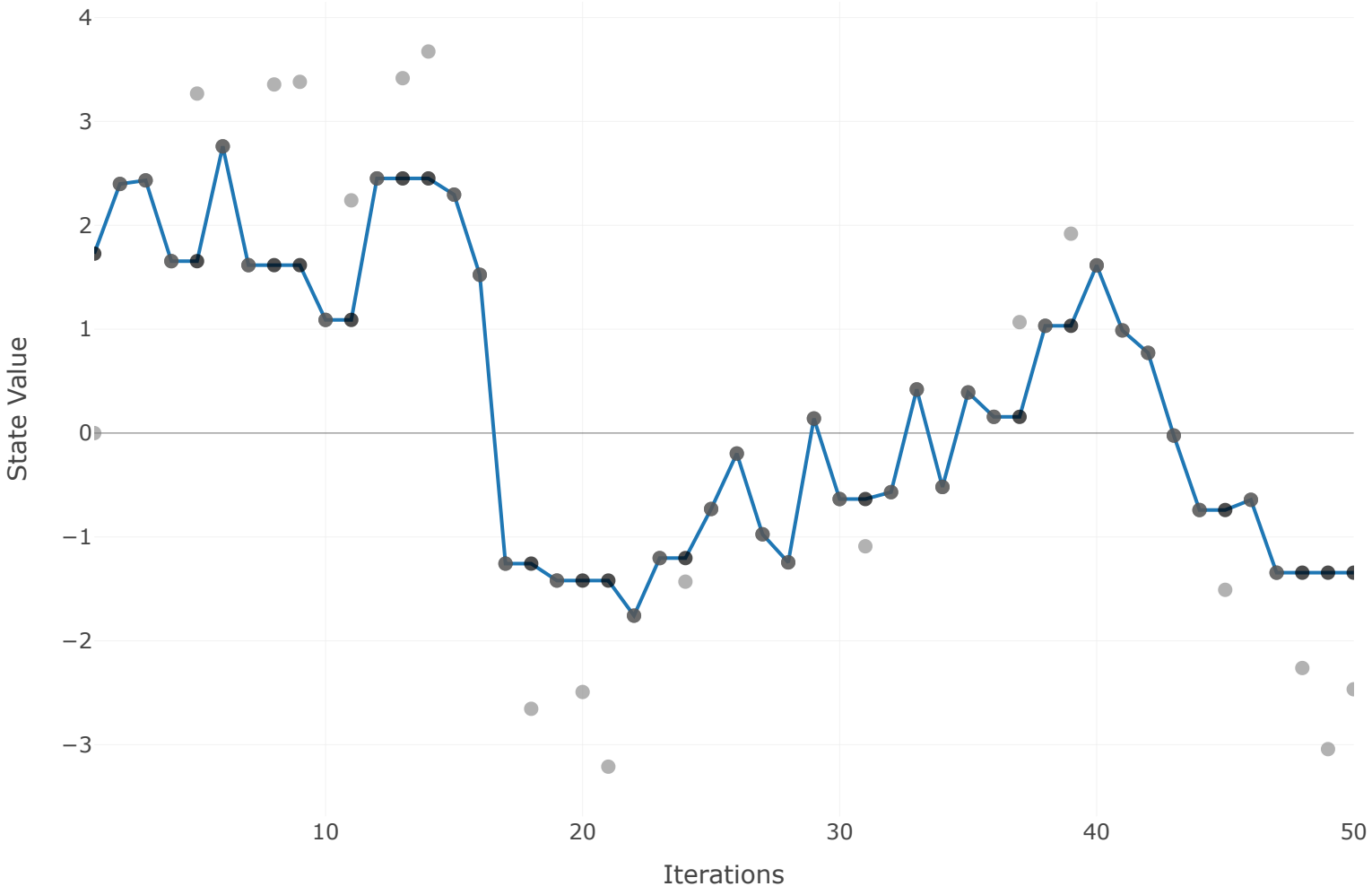
2. Propose a new state y by generating $y \sim Q(x, \cdot)$.
3. Draw $u \sim \mathcal{U}[0, 1]$.
4. If $u \leq \alpha(x, y)$, move to y, otherwise stay at x.


State Value
4
3
2
1
0
−1
−2
−3
10
20
30
40
50
Iterations

Reversiblity

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A Markov kernel $P(x, \cdot)$ is called Π-**reversible** for a measure Π if

$$\int_A \Pi(\mathrm{d}x) P(x, B) = \int_B \Pi(\mathrm{d}x) P(x, A)$$

are the same for any A and B.

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If Π is a probability measure, then Π is an invariant probability measure.

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- The **Metropolis algorithm**, a core MCMC technique, relies on the principle of reversibility.
- The Metropolis algorithm operates by repeating a two-step process: **Propose** a new state and then either **Accept** or **Reject** it.

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Here's an example of a random walk Metropolis algorithm in R:

```r
sd <- 0.25
target <- function(x) 1/(1 + x^2)

v <- numeric(1e2)
x <- runif(1)
for(i in 1:length(v)) {
  y <- x + sd * rnorm(1)
  if(runif(1) < target(y)/target(x)) x <- y #<< Acceptance step
  v[i] <- x
}
```

In this algorithm:

$$y = x + \sigma w, \quad w \sim \mathcal{N}(0, I_d),$$

where σ is a step size, and w is a random sample from the normal distribution.

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If the new state y is accepted, it becomes the next state of the Markov chain; otherwise, the chain remains at x.

Choice of σ and dimensionality

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- The **Metropolis-Hastings algorithm** is affected by the **curse of dimensionality**, directly tied to the choice of the step size, σ.
- Balancing **outflow** and **inflow** (reversibility), can introduce challenges for the algorithm's efficiency.

Average acceptance probability

For a Markov chain generated by the random-walk Metropolis algorithm $(X_m)_m$, if $\|X_0\| \neq \|X_1\|$, it means the move at time $t = 1$ has been **accepted**.

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$$\mathbb{P}(\|X_0\|^2 < \|X_1\|^2) = \mathbb{P}(\|X_0\|^2 > \|X_1\|^2).$$

Thus, the acceptance probability equals:

$$\mathbf{2} \cdot \mathbb{P}(\|X_0\|^2 > \|X_1\|^2).$$

Average acceptance probability

For a Markov chain generated by the random-walk Metropolis algorithm $(X_m)_m$, if $\|X_0\| \neq \|X_1\|$, it means the move at time $t = 1$ has been **accepted**.

Therefore, the probability of accepting a move is:

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Denote the proposed state as Y_1, then the acceptance probability is **less than**:

$$2 \cdot \mathbb{P}(\|X_0\|^2 > \|Y_1\|^2).$$

The proposed state is generated as follows:

$$Y_1 = X_0 + \sigma W, \quad W \sim \mathcal{N}_d(0, \sigma I_d).$$

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where $e = W/\|W\|$ follows a uniform distribution on the unit sphere.

Dimensionality Effects

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- Conversely, if $\sigma = O(d^{-1/2})$, the algorithm cannot **make large moves**, revealing the curse of dimensionality.

Taking it Further

If X_0 follows a d-dimensional standard normal distribution, the right-hand side becomes:

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A useful performance measure for the random-walk Metropolis algorithm is the **expected squared jump distance (ESJD)**:

$$\mathbb{E}\left[\|X_1 - X_0\|^2\right].$$

> There are few reliable measures for assessing the performance of MCMC methods. ESJD is sometimes used because it is relatively straightforward to analyze theoretically. However, like many performance metrics, the direct link between ESJD and actual algorithm efficiency remains unclear.

ESJD can be simplified as:

$$2\mathbb{E}\left[\|X_1 - X_0\|^2, \|X_0\|^2 > \|X_1\|^2\right] = \mathbb{E}\left[\sigma^2\|W\|^2, -2X_0^\top e > \sigma\|W\|\right].$$

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So we may use **23.4%** ratio as a criterion of the choice of the tuning parameter σ.

We initially assumed $X_0 \sim \mathcal{N}(0, I_d)$, meaning $\Pi = \mathcal{N}(0, I_d)$. However, this assumption can be relaxed. Empirically, it is believed that this criterion is relatively robust across different settings.

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- This impact can be quantified using the **expected squared jump distance (ESJD)**, a measure of how far the chain moves.
- There is an optimal value of σ that maximizes the ESJD. When this is achieved, the average acceptance rate is approximately **23.4%**.

Exercise 3.

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3.1 Verify that

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

also satisfies the balance between **inflow** and **outflow**.

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3.3 Discuss the use of a heavy-tailed distribution as the law of W in terms of the Expected Squared Jump Distance when the target distribution is standard normal.

2.3 Preconditioned Crank-Nicolson (pCN) and Gaussian perturbation

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A variant of the Metropolis algorithm is the **preconditioned Crank-Nicolson (pCN)** method, often used in Bayesian computation. This method is well-suited for high-dimensional problems.

The proposed state in the pCN algorithm is given by:

$$y = \rho x + \sigma\sqrt{1-\rho^2}w, \quad w \sim \mathcal{N}(0, I_d),$$

where $\rho \in (-1, 1)$ is a tuning parameter.

Bayesian Inverse Problem

In Bayesian statistics, we are concerned with the posterior distribution, which is defined as:

$$\Pi(\mathrm{d}\theta) = \frac{\exp(l(\theta))P(\mathrm{d}\theta)}{\int_\Theta \exp(l(\theta))P(\mathrm{d}\theta)},$$

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In this setting, the random-walk Metropolis algorithm tends to perform poorly. But how does the pCN algorithm fare?

Assume $P = \mathcal{N}(0, 1)$ and let $\sigma = 1$.

Thanks to the autoregressive nature of the pCN model, the transition:

$$y = \rho x + \sqrt{1-\rho^2} w, \quad w \sim \mathcal{N}(0, I_d),$$

is **reversible** with respect to $\mathcal{N}(0, I_d)$.

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Even in high dimensions, sometimes this ratio tends to be stable, unlike the behavior seen with the random-walk Metropolis algorithm.

Summary

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- In high-dimensional settings, it often maintains a high acceptance probability.
- However, it's important to note that its performance deteriorates significantly when the target distribution deviates far from Gaussian. This method is sometimes not robust.

Exercise 4.

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4.1 Verify that the acceptance ratio for the preconditioned Crank-Nicolson algorithm, with the target distribution

$$\Pi(\mathrm{d}x) \propto \exp(-U(x) - x^2/2)\mathrm{d}x$$

is given by

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4.2 Write code (in R, Python, etc.) for the preconditioned Crank-Nicolson algorithm targeting the distribution $\pi(x) \propto \frac{1}{1+x^2}$. Conclude that the performance, although not mathematically defined, is worse compared to the random walk Metropolis algorithm.

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4.3 Discuss the reason behind this observation.

3. (Advanced) Non-reversiblility

3.1 Non-Reversibility in descrete time

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Reversibility simplifies algorithm design but can sometimes lead to inefficiency.

In certain cases, the Markov chain spends too much time exploring the same areas, leading to longer travel distances before covering the state space adequately.

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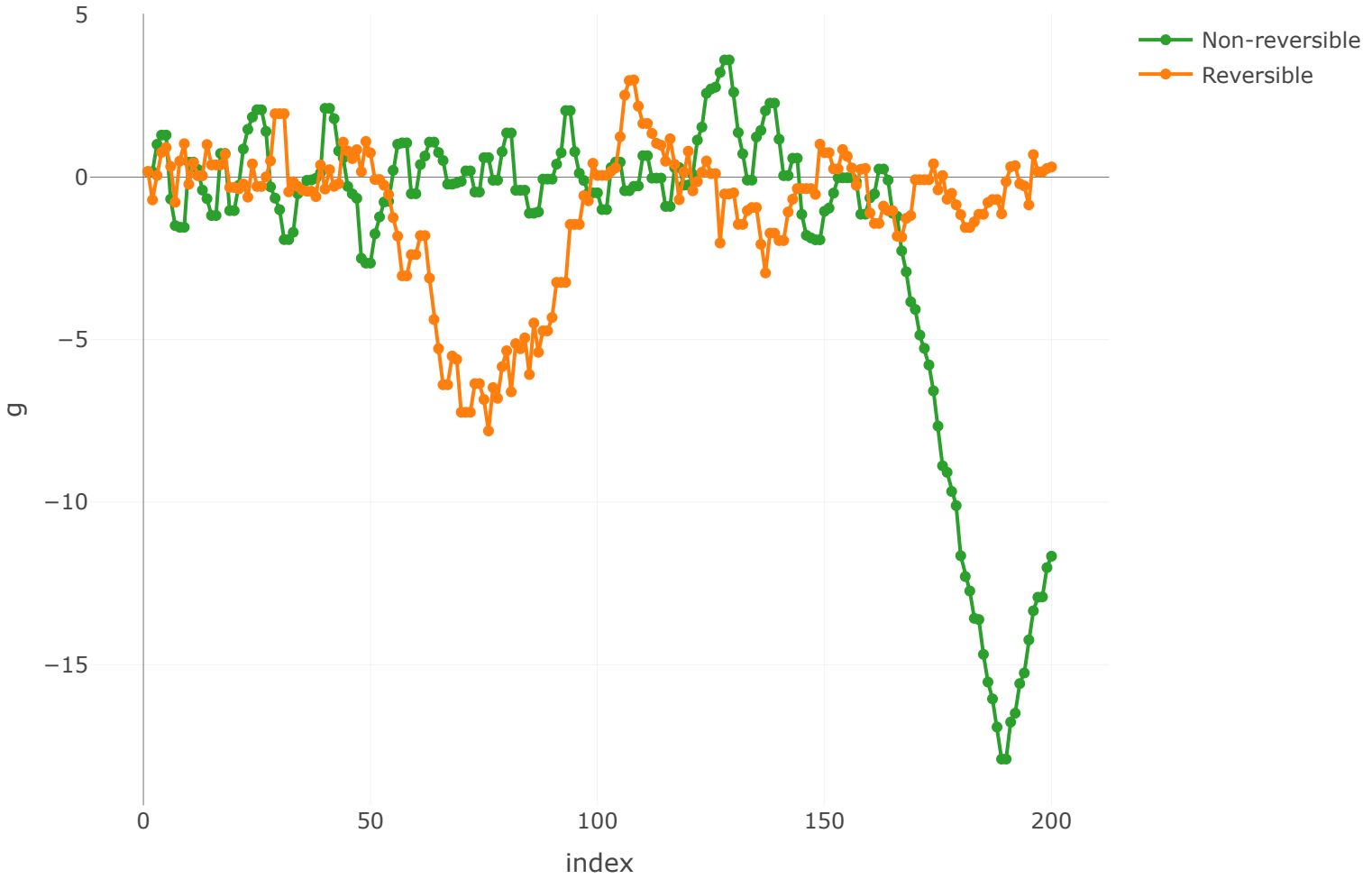
In lifting, we introduce a velocity variable $v \in \{-1, +1\}$ and allow the chain to switch directions at certain points.

For example, starting from $(x, +1)$, the algorithm can move to $(x + |w|, -1)$ if the proposal is accepted. If rejected, it stays at $(x, +1)$.

Lifting Visualization: Example by Gustafson 1996

Here’s an example of how lifting works in practice:



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This method works well in one dimension. However, extending it to multiple dimensions requires special care.

Some recent progress in puctures (K., Song 2023)

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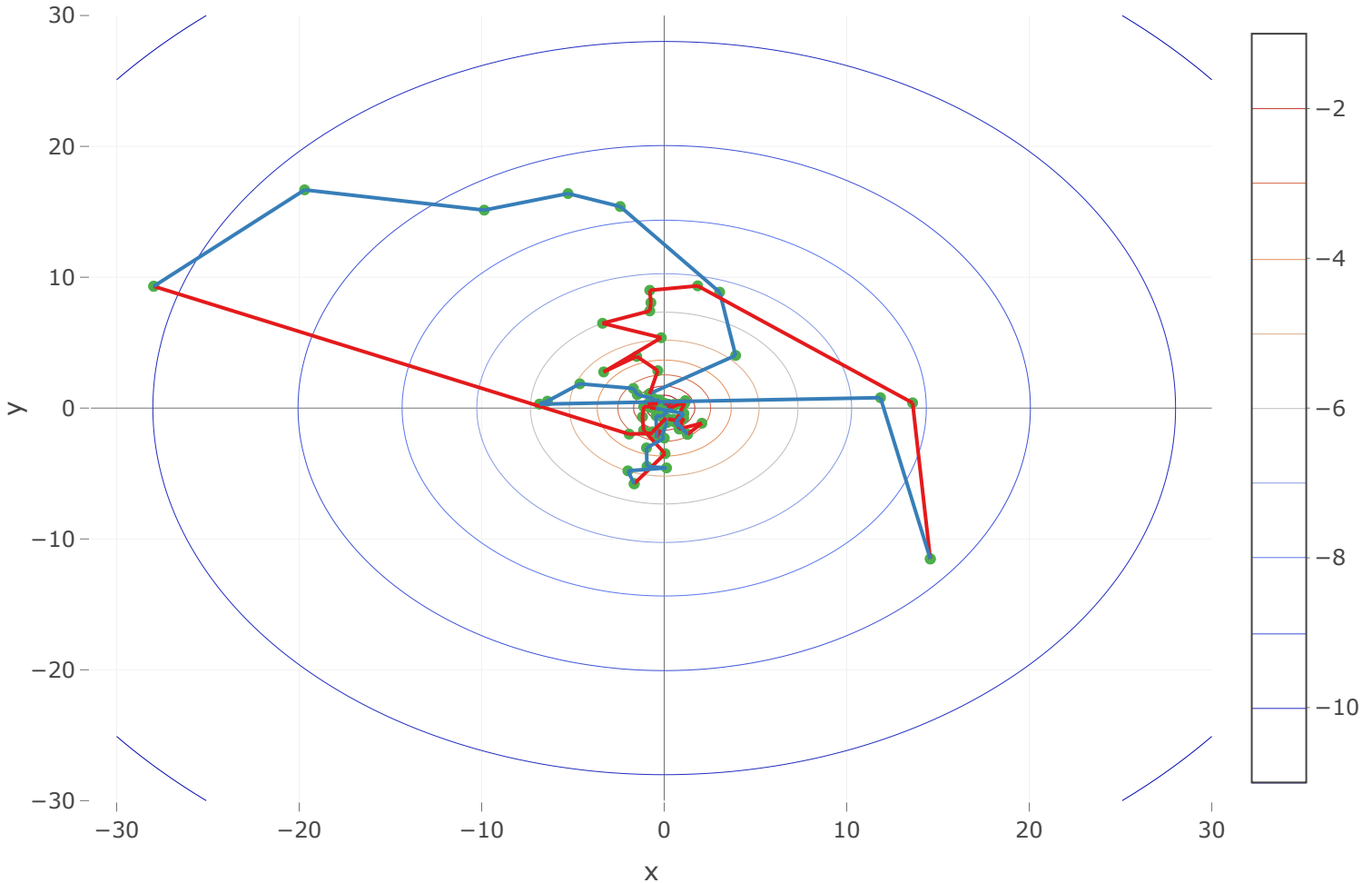
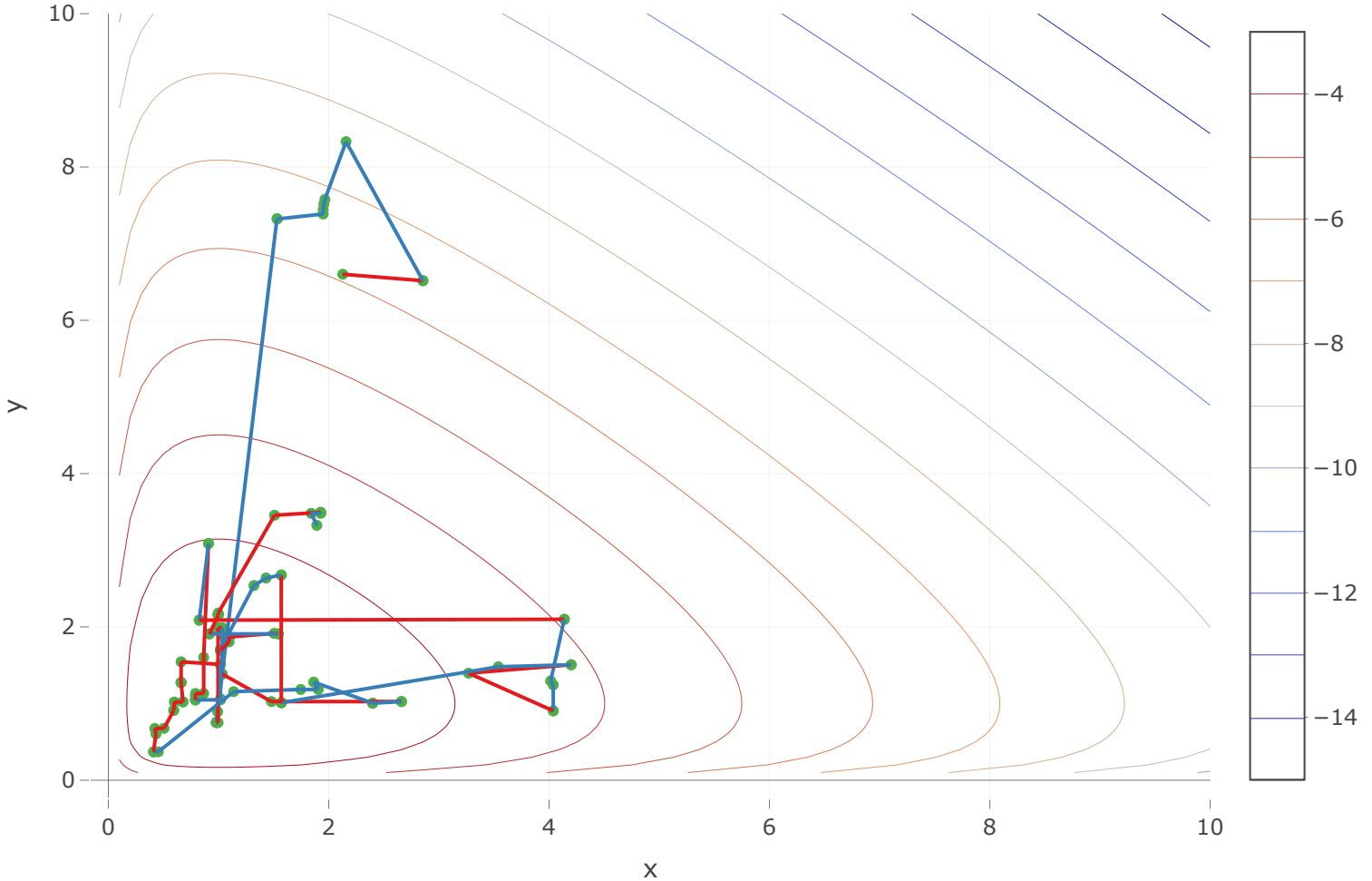
> Extending the previous method to the multidimensional case in a more useful direction was challenging. Due to time constraints, we present the recent results in pictures only.

Multi-dim case: $\mathbb{R}^d$ (Autoregressive)



Multi-dim case: $\mathbb{R}_+^d$ (Beta-Gamma)



Exercise 5.

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5.1 Write code (in R, Python, etc.) for the random walk Metropolis algorithm with lifting with targeting the distribution $\pi(x) \propto \frac{1}{1+x^2}$. Plot a path and compare it to that of the random walk Metropolis algorithm.

3.2 Non-reversibility in continous time

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These algorithms define **piecewise determinsitic Markov processes**.

These methods remove the need to define discrete-time steps and allow the chain to move continuously through the state space.

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Also PDMPs seem to be suitable for a sub-sampling implementation.

PDMP triplet Davis1984

Let E be the state space. The triplet (φ, λ, Q) consists of:

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- **Conditional intensity**: $\lambda(x) \geq 0$.
- **Jump size**: $Q(x, A)$, which is a Markov kernel.

$$E_1 \sim \mathcal{E}(1) \quad \rightsquigarrow \quad T_1 = \inf\left\{t > 0 : E_1 \leq \int_0^t \lambda(\varphi_s(x))\mathrm{d}s\right\}$$

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This determines $x(t)$ up to time T_1.

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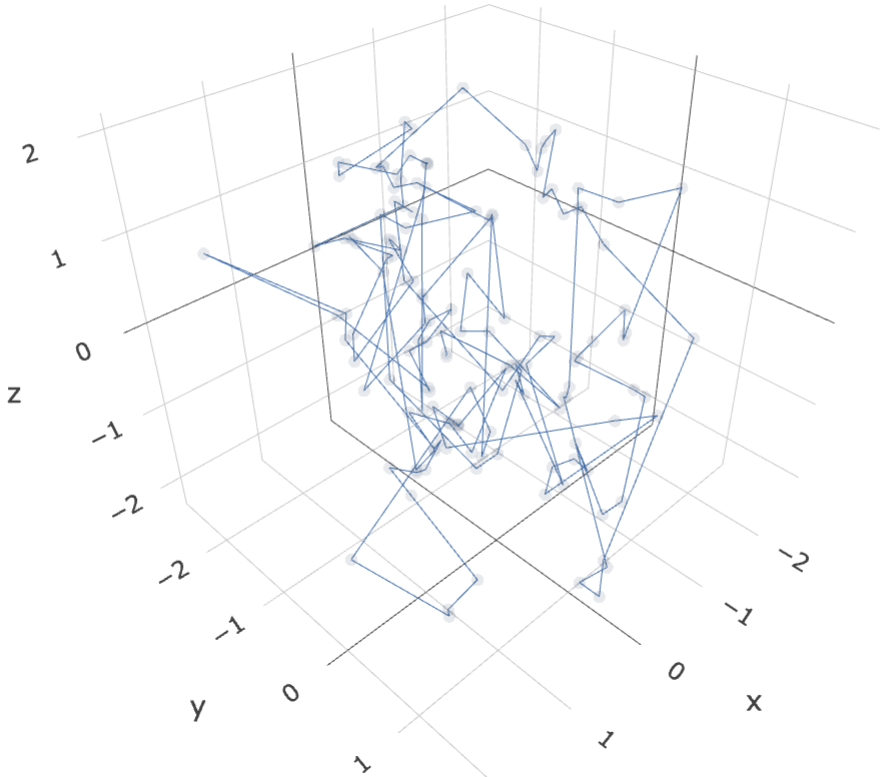
Here’s an example in three dimensions:



Extended generator

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$$\mathcal{L}f(x, v) = v^\top \partial_x f(x, v) + (v^\top \nabla U(x))^+ \, (\mathcal{B} - \mathrm{id}) f(x, v) + \rho \, (\mathcal{R} - \mathrm{id}) f(x, v)$$

where $\mathcal{B}f(x, v) = f(x, B(x)v)$ and $B(x)v = (I - 2n(x)n(x)^\top)v$, and $\mathcal{R}$ is the **refresh** operator which changes the direction v randomly.

Example Zig-Zag sampler Bierkens, Fearnhead, and Roberts (2019)

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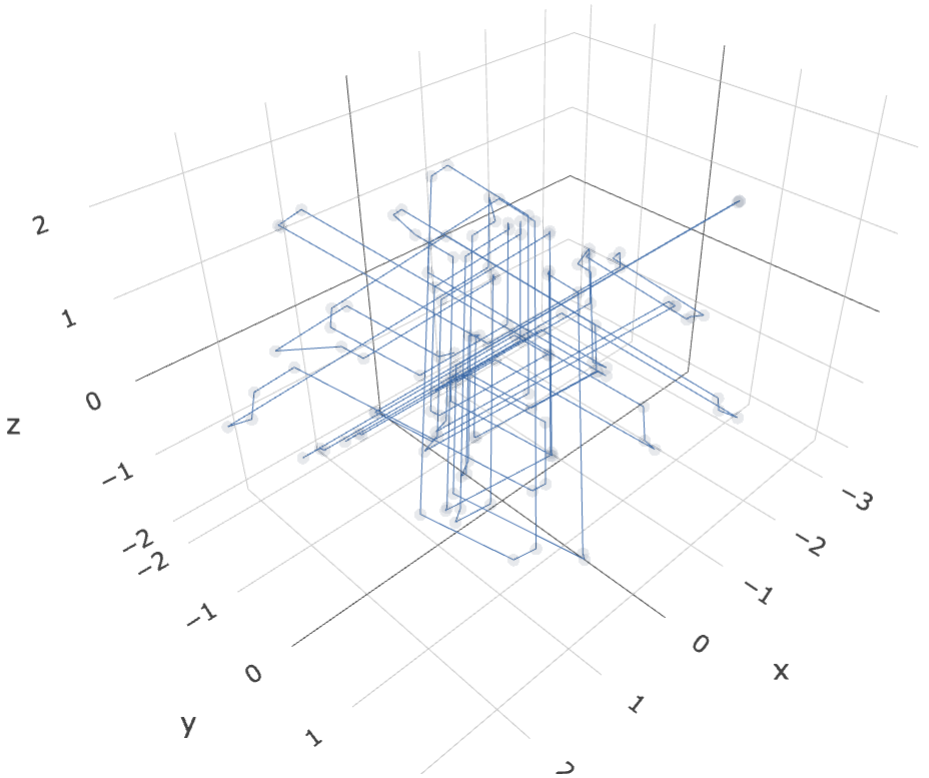
Here’s an example of the Zig-Zag Sampler in three dimensions:



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where $\mathcal{F}_i f(x, v) = f(x, F_i v)$ and F_i switches the i-th coordinate of v.

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- Non-reversible $\rightsquigarrow$ Avoid diffusive behaviour (?)
- Scalable (I do not have enough time to explain this.)
- (Anyway,) Different from MCMC

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- Additionally, check out the brand new **pdmp-jax** by Charly Andral!

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- **Markov Chain Monte Carlo (MCMC)** methods can approximate integrals, and we understand both how to design them and why they converge.
- As an advanced topic, we treat Continuous-time methods, such as the **Zig-Zag Sampler** and **Bouncy Particle Sampler**.