

# Zig-Zag Sampler

A MCMC Game-Changer

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# Today's Menu

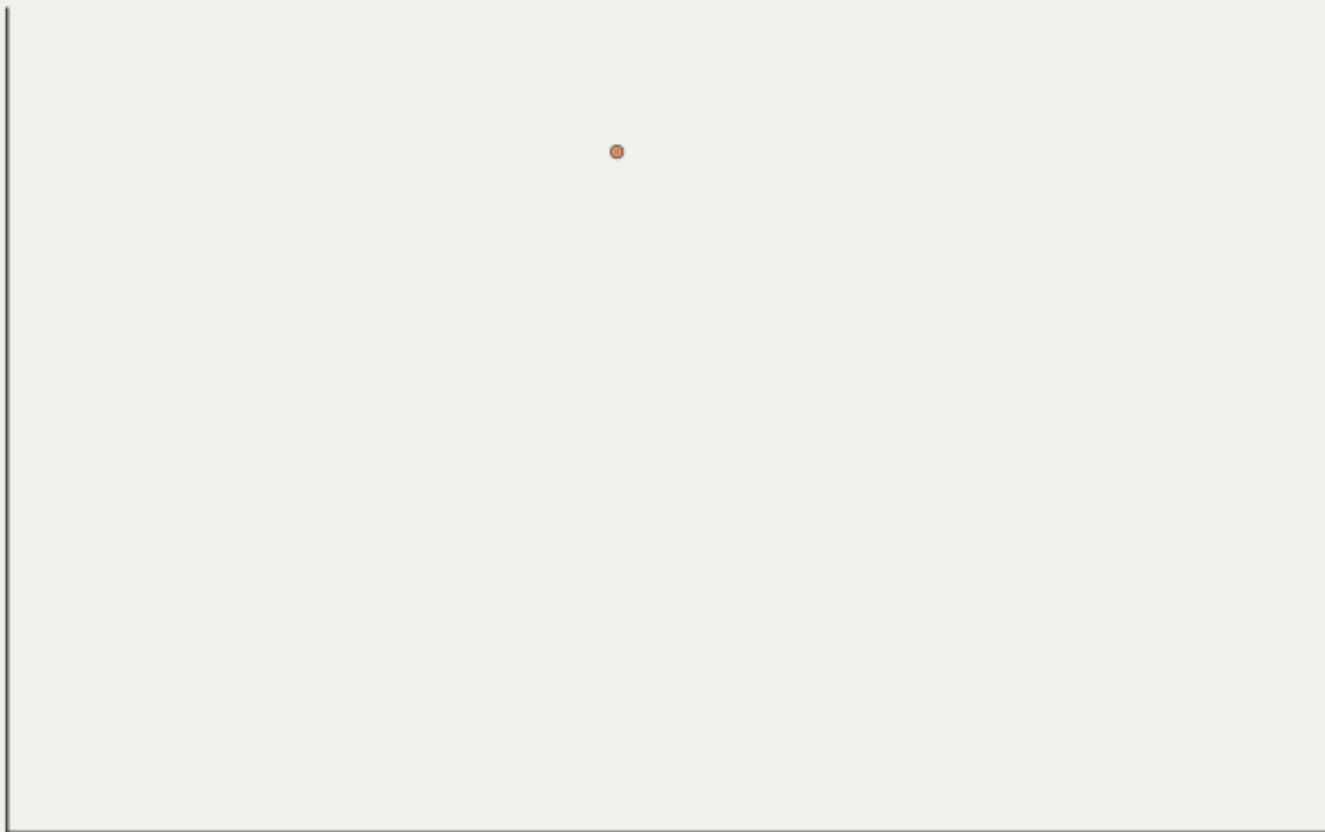
- 1 The Zig-Zag Sampler: What Is It?
- 2 The Algorithm: How to Use It?
- 3 Proof of Concept: How Good Is It?



# I The Zig-Zag Sampler: What Is It?

A continuous-time variant of MCMC algorithms

Zig-Zag



Trajectory for Zig-Zag Sampler. Please attribute Hirofumi Shiba. © ⓘ

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# 1.1 Keywords: PDMP (1/2)

PDMP (Piecewise Deterministic<sup>1</sup> Markov Process<sup>2</sup>) (Davis, 1984)

1. Mostly **deterministic** with the exception of random jumps happens at random times
  2. **Continuous-time**, instead of discrete-time processes
- Plays a **complementary role** to SDEs / Diffusions

Property	PDMP	SDE
Exactly simulatable?	✓	✗
Subject to discretization errors?	✗	✓
Driving noise	Poisson	Gauss



## History of PDMP Applications

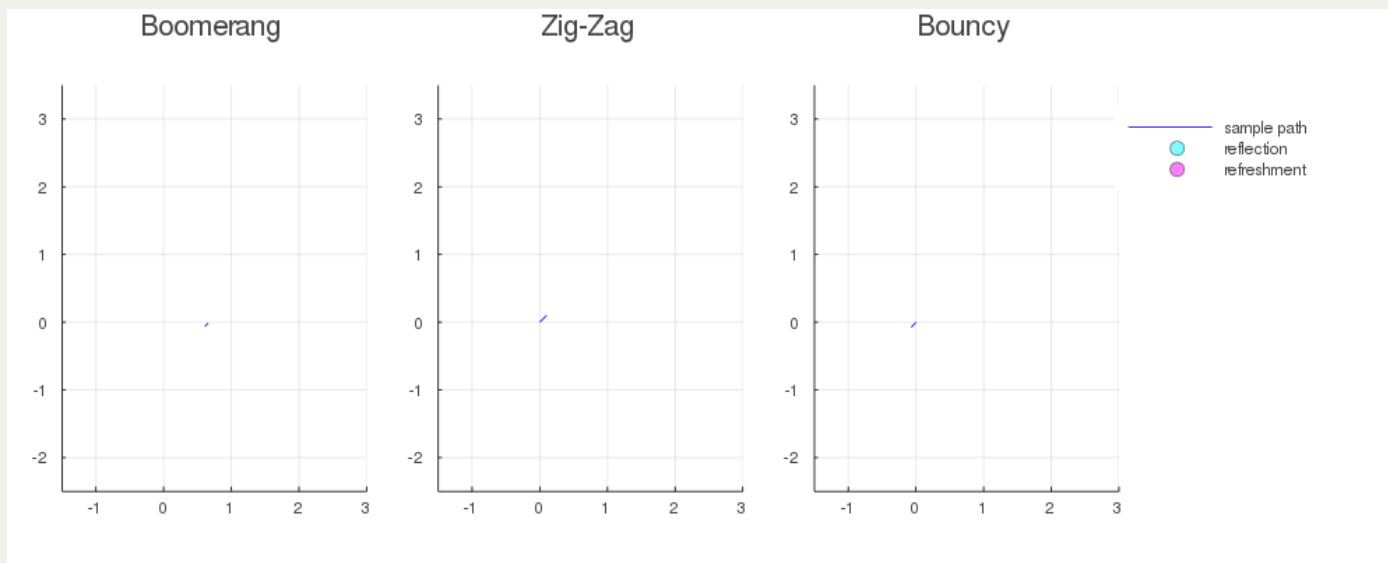
1. First applications: control theory, operations research, etc. (Davis, 1993)
2. Second applications: Monte Carlo simulation in material sciences (Peters and de With, 2012)
3. Third applications: Bayesian statistics (Bouchard-Côté et al., 2018)

1. Mostly **deterministic** with the exception of random jumps happens at random times
2. **Continuous-time**, instead of discrete-time processes



## I.2 Keywords: PDMP (2/2)

- We will concentrate on Zig-Zag sampler (Bierkens, Fearnhead, et al., 2019)
- Other PDMPs: Bouncy sampler (Bouchard-Côté et al., 2018), Boomerang sampler (Bierkens et al., 2020)



The most famous three PDMPs. Animated by (Grazzi, 2020)  
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# I.3 Menu

## What We've Learned

The new algorithm 'Zig-Zag Sampler' is based on continuous-time process called **PDMP**.

## What We'll Learn in the Rest of this Section I

We will review 3 instances of the standard (discrete-time) MCMC algorithm: **MH**, **Lifted MH**, and **MALA**.

1. Review: **MH** (Metropolis-Hastings) algorithm
2. Review: **Lifted MH**, A method bridging **MH** and Zig-Zag
3. Comparison: **MH** vs. **Lifted MH** vs. Zig-Zag
4. Review: **MALA** (Metropolis Adjusted Langevin Algorithm)
5. Comparison: Zig-Zag vs. **MALA**



# I.4 Review: Metropolis-Hastings (I/2)

(Metropolis et al., 1953)-(Hastings, 1970)

Input: Target distribution  $p$ , (symmetric) proposal distribution  $q$

1. Draw a  $X_t \sim q(\cdot | X_{t-1})$
2. Compute

$$\alpha(X_{t-1}, X_t) = \frac{p(X_t)}{p(X_{t-1})}$$

3. Draw a uniform random number  $U \sim U([0, 1])$ .
4. If  $\alpha(X_{t-1}, X_t) \leq U$ , then  $X_t \leftarrow X_t$ . Do nothing otherwise.
5. Return to Step 1.

MH algorithm works even without  $p$ 's normalizing constant. Hence, its ubiquity.





# I.5 Review: Metropolis-Hastings (2/2)

Alternative View: MH is a generic procedure to turn a **simple  $q$ -Markov chain** into a **Markov chain converging to  $p$** .

## The Choice of Proposal $q$

- Random Walk Metropolis (Metropolis et al., 1953): Uniform / Gaussian

$$q(y|x) = q(y - x) \in \left\{ \frac{dU([0, 1])}{d\lambda}(y - x), \frac{dN(0, \Sigma)}{d\lambda}(y - x) \right\}$$

- Hybrid / Hamiltonian Monte Carlo (Duane et al., 1987): Hamiltonian dynamics

$$q(y|x) = \delta_{x+\epsilon\rho}, \quad \epsilon > 0, \quad \rho : \text{momentum defined via Hamiltonian}$$

- Metropolis-adjusted Langevin algorithm (MALA) (Besag, 1994): Langevin diffusion

$$q(-|X_t) := \text{the transition probability of } X_t \text{ where } dX_t = \nabla \log p(X_t) dt + \sqrt{2\beta^{-1}} dB_t.$$





## I.6 Problem: Reversibility

Reversibility (a.k.a detailed balance):

$$p(x)q(x|y) = p(y)q(y|x).$$

In words:

$$\text{Probability}[\text{Going } x \rightarrow y] = \text{Probability}[\text{Going } y \rightarrow x].$$

→ Harder to explore the entire space

→ Slow mixing of MH

From the beginning of 21th century, many efforts have been made to make MH irreversible 

# 1.7 Lifting (1/3)

**Lifting**: A method to make MH's dynamics **irreversible**

How?: By adding an auxiliary variable  $\sigma \in \{\pm 1\}$ , called **momentum**

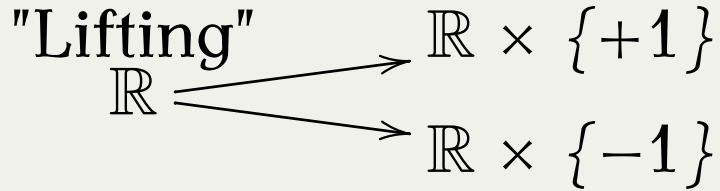
## Lifted MH (Turitsyn et al., 2011)

Input: Target  $p$ , **two** proposals  $q^{(+1)}, q^{(-1)}$ , and **momentum**  $\sigma \in \{\pm 1\}$

1. Draw  $X_t$  from  $q^{(\sigma)}$
2. Do a MH step
3. If accepted, go back to Step 1.
4. If rejected, **flip the momentum** and go back to Step 1.

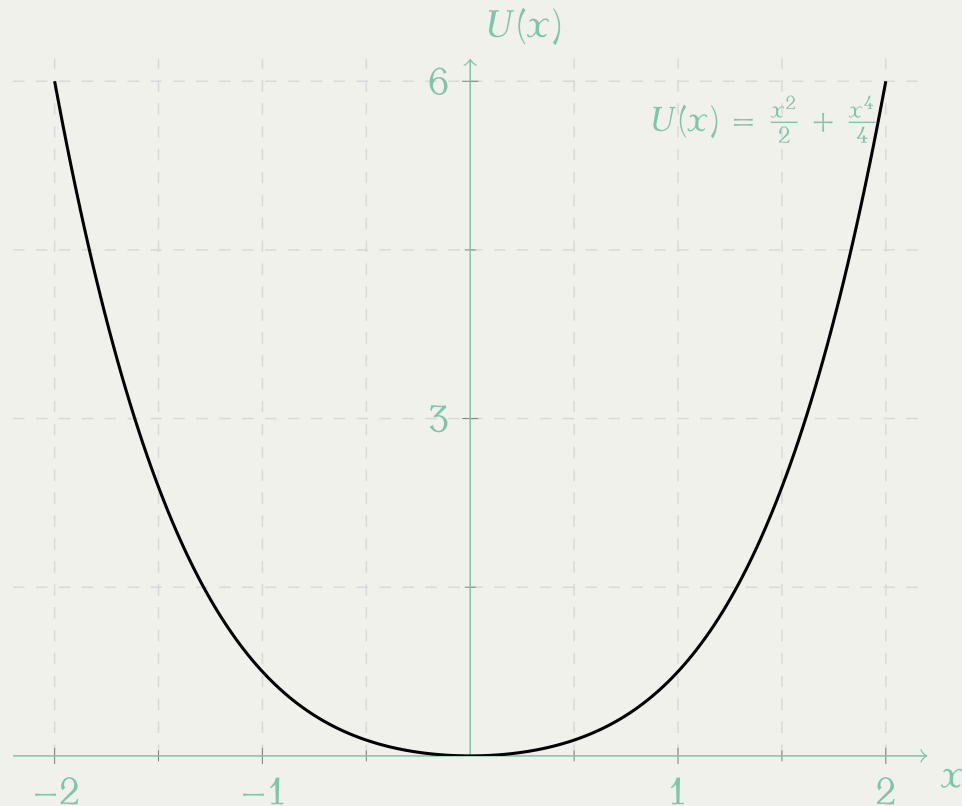


# I.8 Lifting (2/3)



$q^{(+1)}$ : Only propose  $\rightarrow$  moves

$q^{(-1)}$ : Only propose  $\leftarrow$  moves



$\rightarrow$  Once going uphill, it continues to go uphill.

$\rightarrow$  This is **irreversible**, since

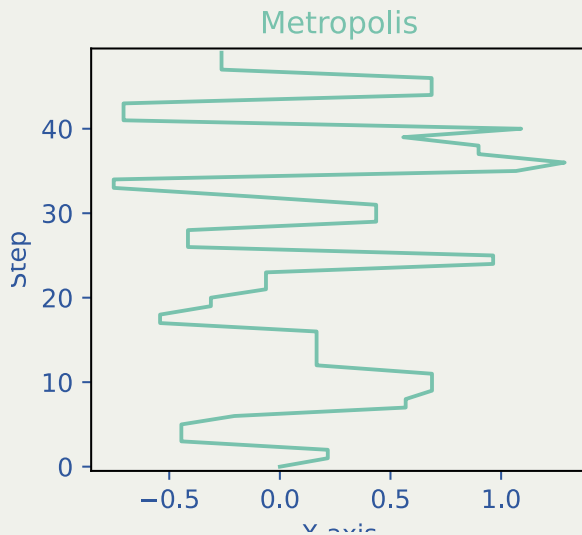
Probability $[x \rightarrow y]$

$\neq$  Probability $[y \rightarrow x]$ .

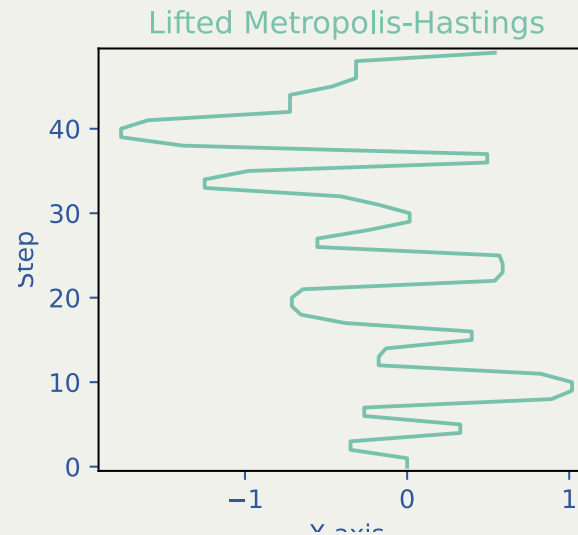


# 1.9 Lifting (3/3)

Reversible dynamic of MH has ‘irreversified’



MH



Lifted MH



**Caution**

**Scale is different**  
in the vertical axis!

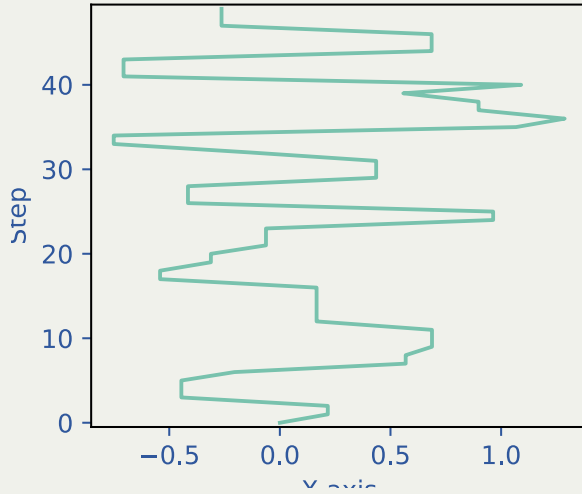
**Lifted MH** successfully explores the edges of the target distribution.

\*Irreversibility actually improves the efficiency of MCMC, as we observe in two slides later.



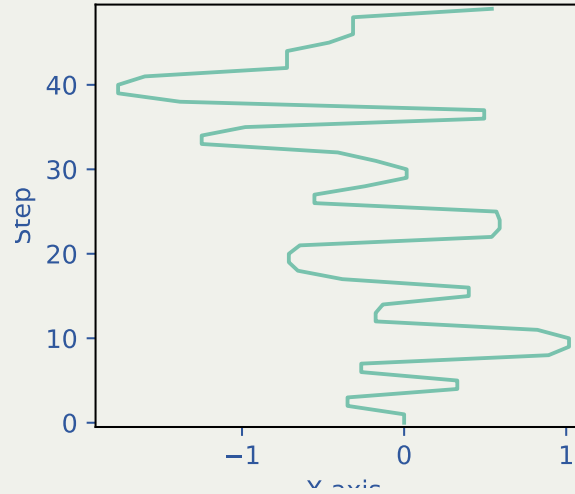
# I.10 Comparison: MH vs. LMH vs. Zig-Zag (1/2)

Metropolis



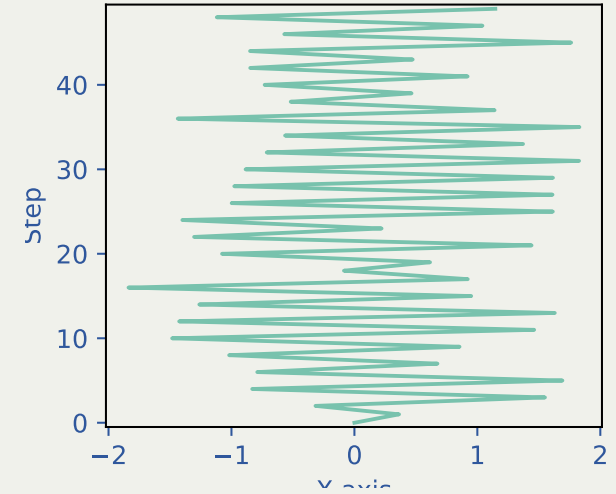
MH

Lifted Metropolis-Hastings



Lifted MH

Zig-Zag sampler



Zig-Zag

Zig-Zag corresponds to the **limiting case of lifted MH** as the step size of proposal  $q$  goes to zero, as we'll learn later.

→ Zig-Zag has a maximum **irreversibility**.

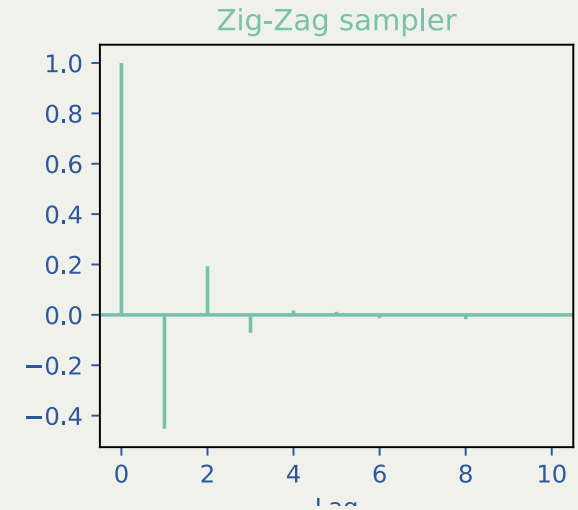
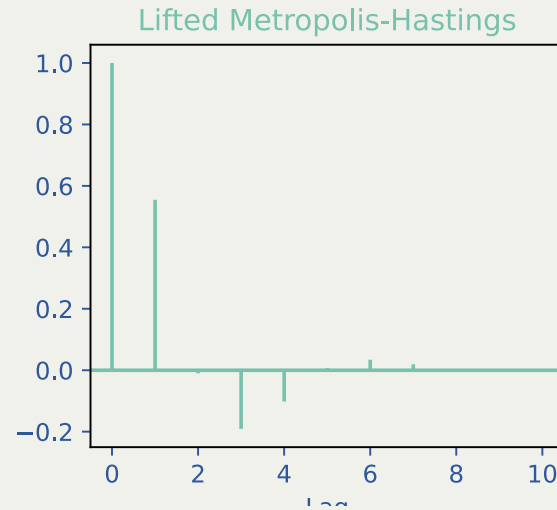
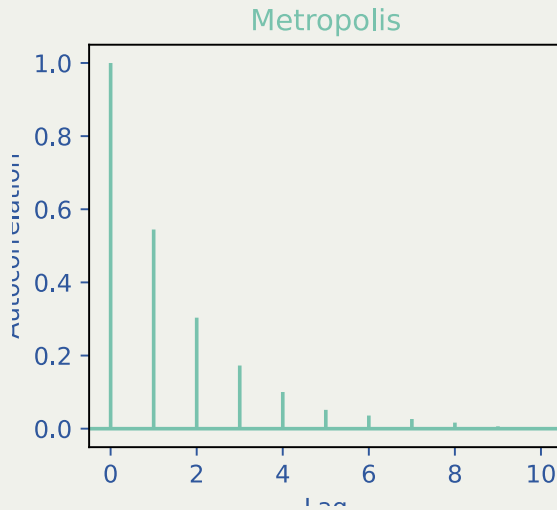


# 1.1 Comparison: MH vs. LMH vs. Zig-Zag (2/2)

**Irreversibility** actually improves the efficiency of MCMC.

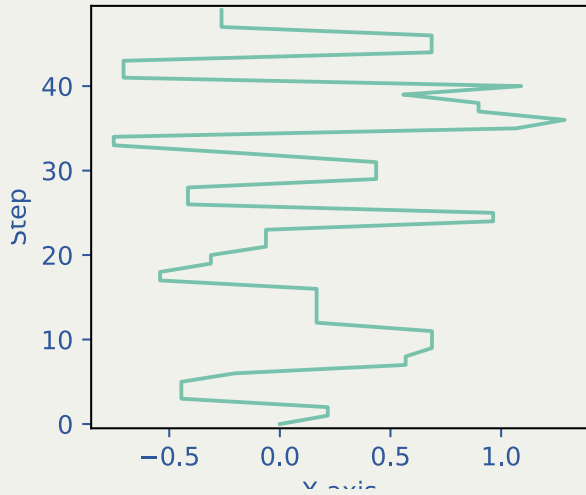
Faster decay of **autocorrelation**  $\rho_t \approx \text{Corr}[X_0, X_t]$  implies

1. faster mixing of MCMC
2. lower variance of Monte Carlo estimates



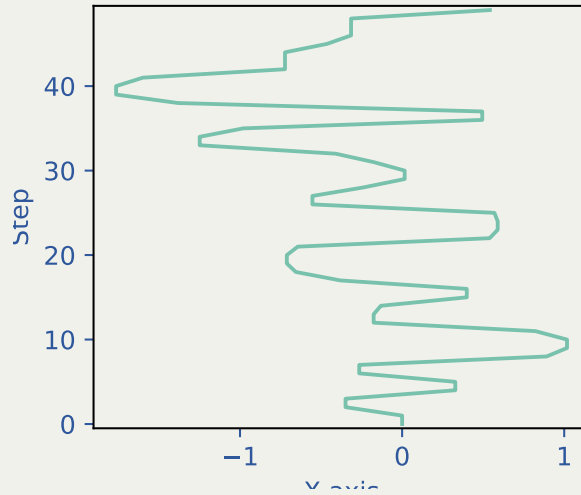


Metropolis



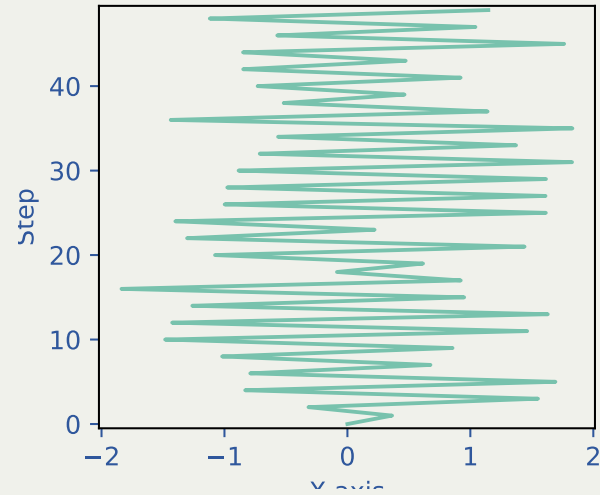
MH

Lifted Metropolis-Hastings



Lifted MH

Zig-Zag sampler



Zig-Zag



# 1.12 Review: MALA

**Langevin diffusion:** A diffusion process defined by the following SDE:

$$dX_t = \nabla \log p(X_t) dt + \sqrt{2\beta^{-1}} dB_t.$$

**Langevin diffusion** itself converges to the target distribution  $p$  in the sense that <sup>1</sup>

$$\|p_t - p\|_{L^1} \rightarrow 0, \quad t \rightarrow \infty.$$

Two MCMC algorithms derived from **Langevin diffusion**:

ULA (Unadjusted Langevin Algorithm)

Use the discretization of  $(X_t)$ . **Discretization errors accumulate.**

MALA (Metropolis Adjusted Langevin Algorithm)

Use ULA as a proposal in MH, erasing the errors by MH steps.

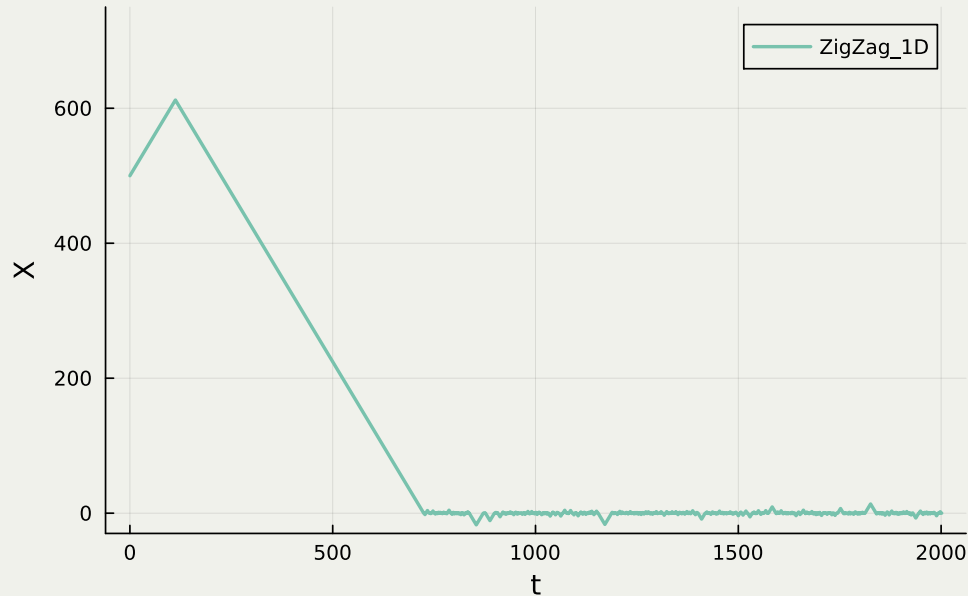
1. under fairly general conditions on  $p$ .



# 1.13 Comparison: Zig-Zag vs. MALA (1/3)

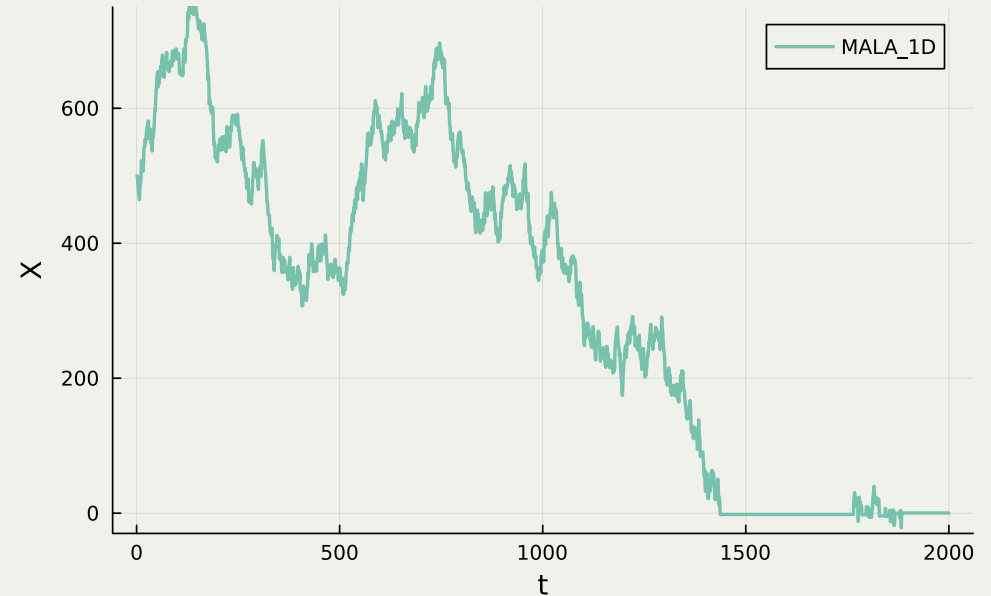
How fast do they go back to high-probability regions? <sup>1</sup>

1D ZigZag Sampler (Cauchy Distribution)



Zig-Zag

1D MALA Sampler (Cauchy Distribution)



MALA

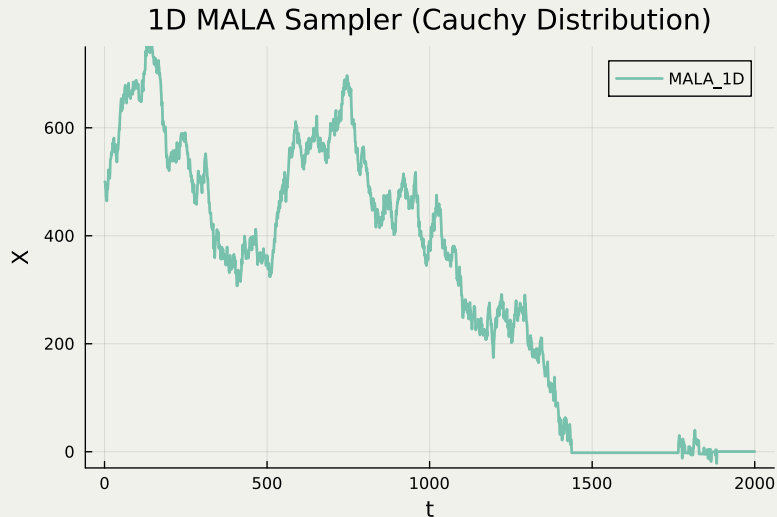
**Irreversibility** of Zig-Zag accelerates its convergence.



I. The target here is the standard Cauchy distribution  $C(0, 1)$ , equivalent to  $t(1)$  distribution. Its heavy tails hinder the convergence of MCMC.



# I.14 Comparison: Zig-Zag vs. MALA (2/3)



## Caution: Fake Continuity

The left plot looks continuous, but **it actually is not.**

MALA trajectory

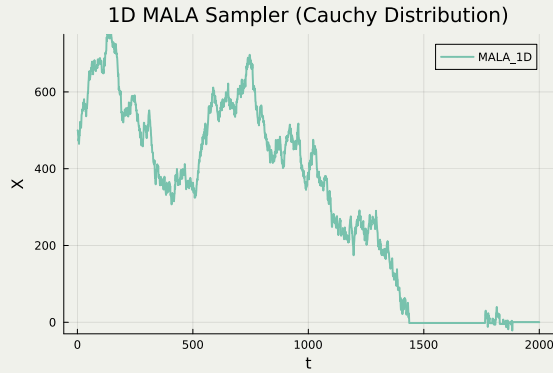
MH, including MALA, is actually a discrete-time process.

The plot is obtained by connecting the points by line segments.



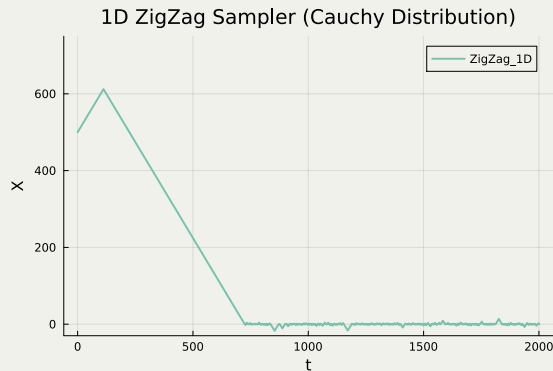
# I.15 Comparison: Zig-Zag vs. MALA (3/3)

Monte Carlo estimation is also done differently:



MALA outputs  $(X_n)_{n \in [N]}$  defines

$$\frac{1}{N} \sum_{n=1}^N f(X_n) \xrightarrow{N \rightarrow \infty} \int_{\mathbb{R}^d} f(x) p(x) dx.$$



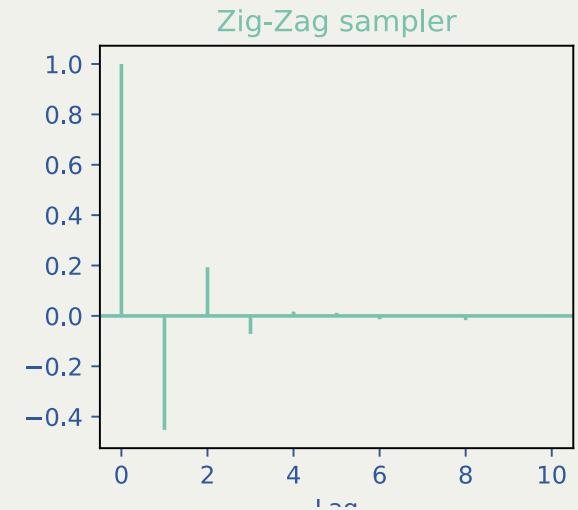
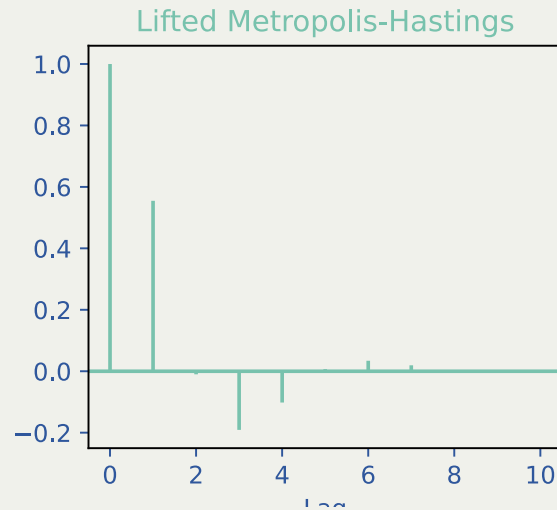
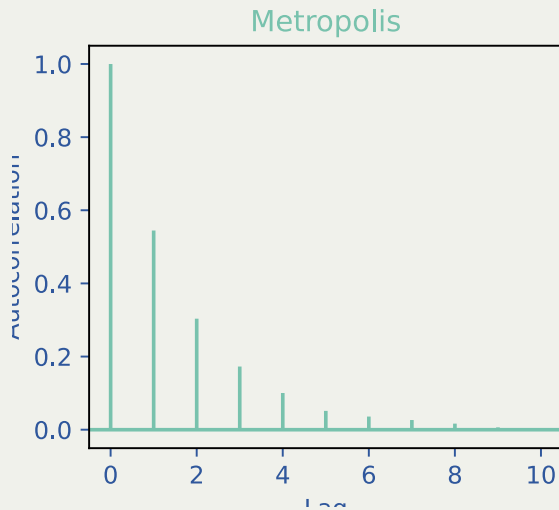
Zig-Zag outputs  $(X_t)_{t \in [0, T]}$  defines

$$\int_0^T f(X_t) dt \xrightarrow{T \rightarrow \infty} \int_{\mathbb{R}^d} f(x) p(x) dx.$$

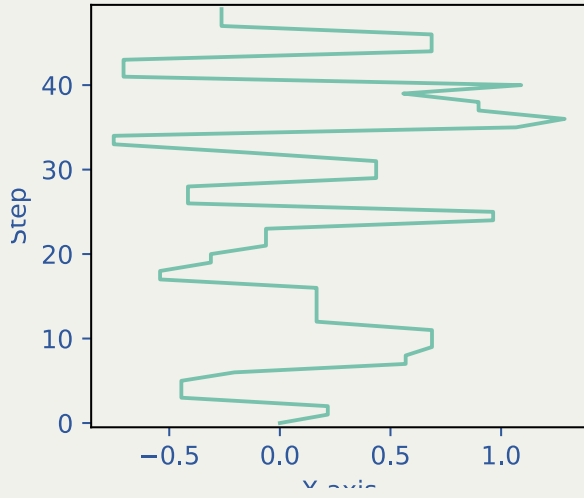


## I.16 Recap of Section I

- Zig-Zag Sampler's trajectory is a PDMP.
- PDMP, by design, has maximum **irreversibility**.
- **Irreversibility** leads to faster convergence of Zig-Zag in comparisons against **MH**, **Lifted MH**, and especially **MALA**.

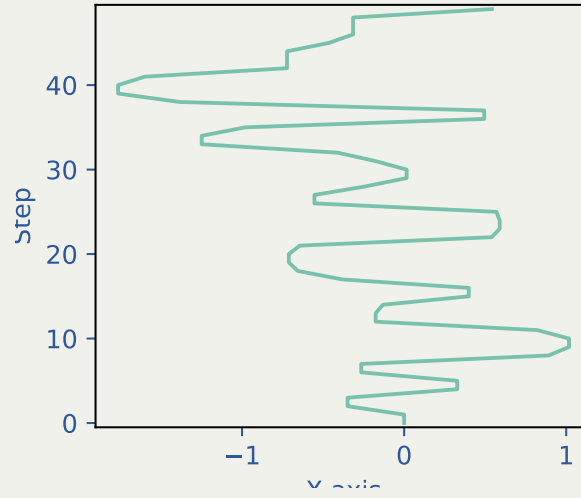


Metropolis



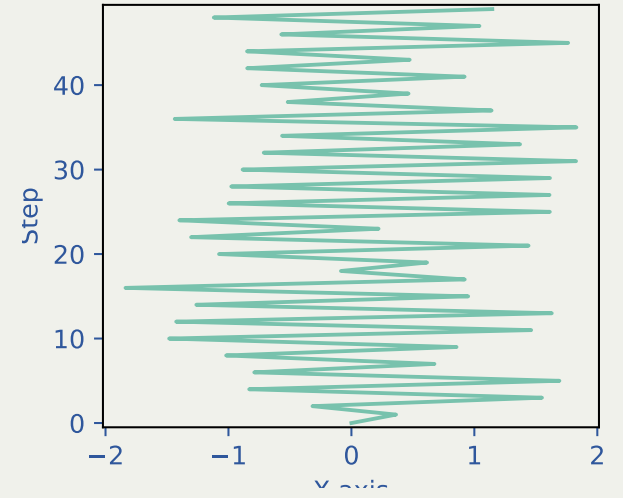
MH

Lifted Metropolis-Hastings



Lifted MH

Zig-Zag sampler



Zig-Zag





# 2 The Algorithm: How to Use It?

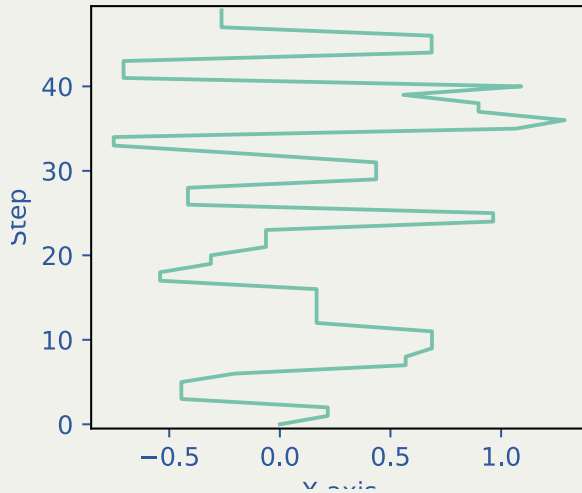
Fast and exact simulation of continuous trajectory.



## 2.1 Review: MH vs. LMH vs. Zig-Zag (1/2)

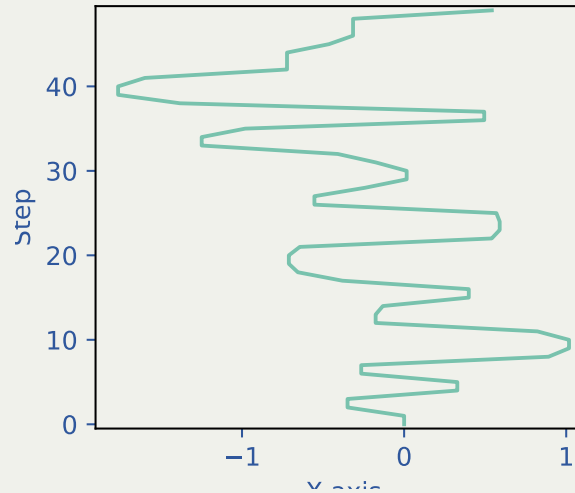
As we've learned before, Zig-Zag corresponds to the **limiting case of lifted MH** as the step size of proposal  $q$  goes to zero.

Metropolis



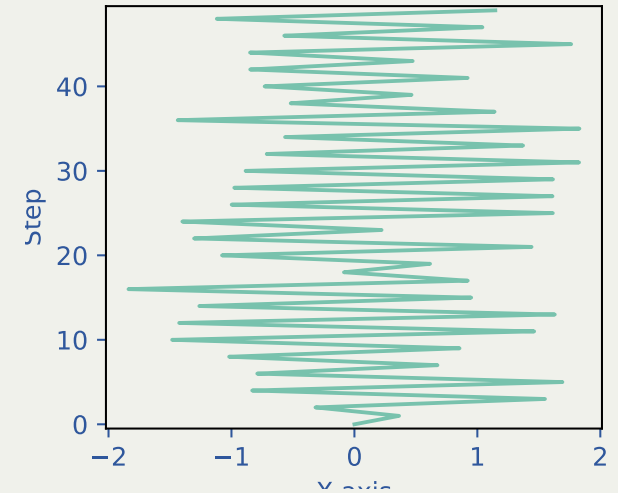
MH

Lifted Metropolis-Hastings



Lifted MH

Zig-Zag sampler

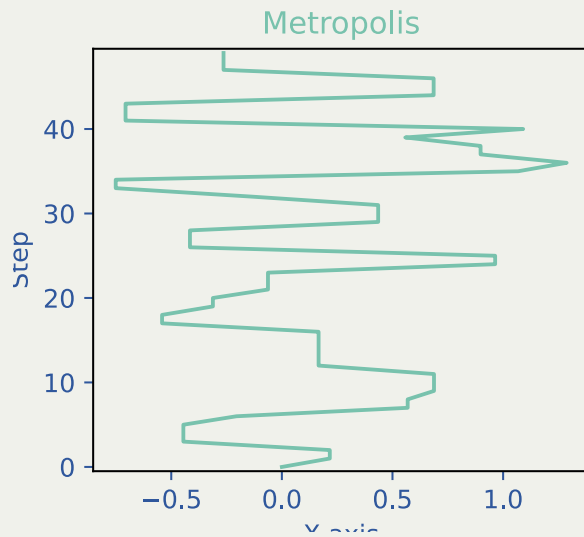


Zig-Zag

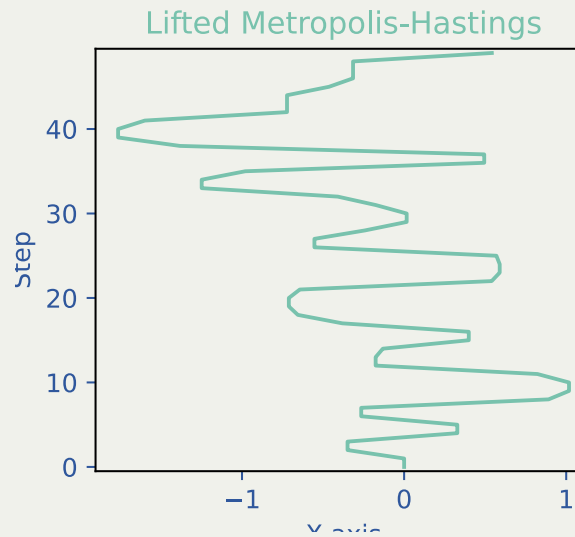


## 2.2 Review: MH vs. LMH vs. Zig-Zag (2/2)

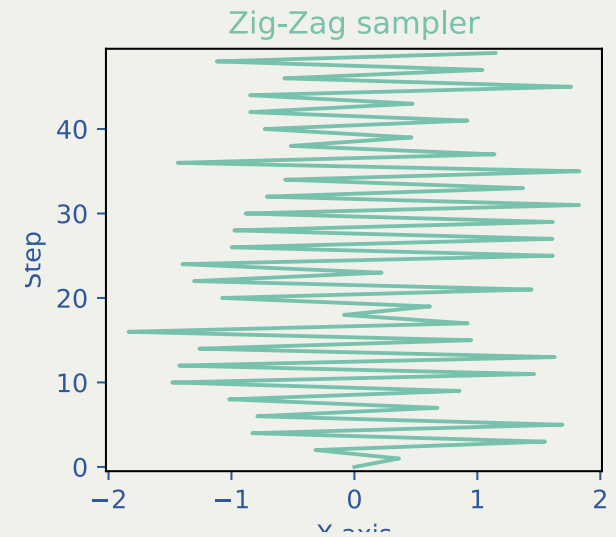
‘Limiting case of lifted MH’ means that we only simulate where we should flip the momentum  $\sigma \in \{\pm 1\}$  in Lifted MH.



MH



Lifted MH



Zig-Zag



## 2.3 Algorithm (1/2)

‘**Limiting case of lifted MH**’ means that we only simulate where we should flip the momentum  $\sigma \in \{\pm 1\}$  in Lifted MH.

(Id | Zig Zag sampler Bierkens, Fearnhead, et al., 2019)

**Input:** Gradient  $\nabla \log p$  of log target density  $p$

For  $n \in \{1, 2, \dots, N\}$ :

1. Simulate an first arrival time  $T_n$  of a **Poisson point process** (described in the next slide)
2. Linearly interpolate until time  $T_n$ :

$$X_t = X_{T_{n-1}} + \sigma(t - T_{n-1}), \quad t \in [T_{n-1}, T_n].$$

3. Go back to Step 1 with the momentum  $\sigma \in \{\pm 1\}$  flipped

1. Multidimensional extension is straightforward, but we won't cover it today.



## 2.4 Algorithm (2/2)

**(Fundamental Property of Zig-Zag Sampler (I d) Bierkens, Fearnhead, et al., 2019)**

Let  $U(x) := -\log p(x)$ . Simulating a **Poisson point process** with a rate function

$$\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x)$$

ensures the Zig-Zag sampler converges to the target  $p$ , where  $\gamma$  is an arbitrary non-negative function.

Its ergodicity is ensured as long as there exists  $c, C > 0$  such that<sup>1</sup>

$$p(x) \leq C|x|^{-c}.$$

1. With some regularity conditions on  $U$ . (See [Bierkens, Roberts, et al., 2019](#)).



## 2.5 Core of the Algorithm

Given a rate function

$$\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x)$$

how to simulate a corresponding **Poisson point process**?

### What We'll Learn in the Rest of this Section 2

1. What is **Poisson Point Process**?
2. How to Simulate It?
3. Core Technique: **Poisson Thinning**

**Take Away: Zig-Zag sampling reduces to **Poisson Thinning**.**



## 2.6 Simulating Poisson Point Process (1/2)

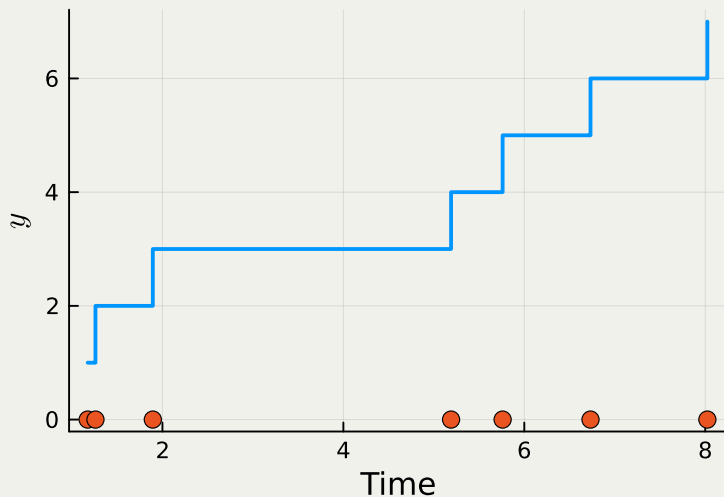
### What is a Poisson Point Process with rate $\lambda$ ?

The number of points in  $[0, t]$  follows a Poisson distribution with mean  $\int_0^t \lambda(x_s, \sigma_s) ds$ :

$$N([0, t]) \sim \text{Pois}(M(t)), \quad M(t) := \int_0^t \lambda(x_s, \sigma_s) ds.$$

We want to know when the first point  $T_1$  falls on  $[0, \infty)$ .

Poisson Point Process with  $\lambda \equiv 1$



When  $\lambda(x, \sigma) \equiv c$  (constant),

- blue line: Poisson Process
- red dots: Poisson Point Process

satisfying  $N_t = N([0, t]) \sim \text{Pois}(ct)$ .



## 2.7 Simulating Poisson Point Process (2/2)

### Proposition (Simulation of Poisson Point Process)

The first arrival time  $T_1$  of a **Poisson Point Process** with rate  $\lambda$  can be simulated by

$$T_1 \stackrel{d}{=} M^{-1}(E), \quad E \sim \text{Exp}(1), \quad M(t) := \int_0^t \lambda(x_s, \sigma_s) ds,$$

where  $\text{Exp}(1)$  denotes the exponential distribution with parameter 1.

Since  $\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x)$ ,  $M$  can be quite complicated.

→ Inverting  $M$  can be impossible.

→ We need more general techniques: **Poisson Thinning**.





## 2.8 Poisson Thinning (1/2)

(Lewis and Shedler, 1979)

To obtain the first arrival time  $T_1$  of a **Poisson Point Process** with rate  $\lambda$ ,

1. Find a bound  $M$  that satisfies

$$m(t) := \int_0^t \lambda(x_s, \sigma_s) ds \leq M(t).$$

2. Simulate a point  $T$  from the **Poisson Point Process** with intensity  $M$ .

3. Accept  $T$  with probability  $\frac{m(T)}{M(T)}$ .

- $m(t)$ : Defined via  $\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x)$ .
- $M(t)$ : Simple upper bound  $m \leq M$ , such that  $M^{-1}$  is analytically tractable.



## 2.9 Poisson Thinning (2/2)

In order to simulate a **Poisson Point Process** with rate

$$\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x),$$

we find a **invertible upper bound  $M$**  that satisfies

$$\int_0^t \lambda(x_s, \sigma_s) ds = m(t) \leq M(t).$$

for all possible Zig-Zag trajectories  $\{(x_s, \sigma_s)\}_{s \in [0, T]}$ .



## 2.10 Recap of Section 2

1. Continuous-time MCMC, based on PDMP, has an entirely different algorithm and strategy.
2. To simulate PDMP is to simulate **Poisson Point Process**.
3. The core technology to simulate **Poisson Point Process** is **Poisson Thinning**.
4. **Poisson Thinning** is about finding an **upper bound  $M$** , with tractable inverse  $M^{-1}$ ; Typically a polynomial function.
5. The **upper bound  $M$**  has to be given on a case-by-case basis.



# 3 Proof of Concept: How Good Is It?

Quick demonstration of the state-of-the-art performance on a toy example.



## 3.1 Review: The 3 Steps of Zig-Zag Sampling

Given a target  $p$ ,

1. Calculate the negative log-likelihood  $U(x) := -\log p(x)$
2. Fix a refresh rate  $\gamma(x)$  and compute the rate function

$$\lambda(x, \sigma) := \left( \sigma U'(x) \right)_+ + \gamma(x).$$

3. Find an **invertible upper bound**  $M$  that satisfies

$$\int_0^t \lambda(x_s, \sigma_s) ds =: m(t) \leq M(t).$$



## 3.2 Model: 1d Gaussian Mean Reconstruction

### Setting

- Data:  $y_1, \dots, y_n \in \mathbb{R}$  acquired by

$$y_i \stackrel{\text{iid}}{\sim} \mathbf{N}(x_0, \sigma^2), \quad i \in [n],$$

with  $\sigma > 0$  known,  $x_0 \in \mathbb{R}$  unknown.

- Prior:  $\mathbf{N}(0, \rho^2)$  with known  $\rho > 0$ .
- Goal: Sampling from the posterior

$$p(x) \propto \left( \prod_{i=1}^n \phi(x|y_i, \sigma^2) \right) \phi(x|0, \rho^2),$$

where  $\phi(x|y, \sigma^2)$  is the  $\mathbf{N}(y, \sigma^2)$  density.

The negative log-likelihood:

$$U(x) = -\log p(x)$$

$$= \frac{x^2}{2\rho^2} + \frac{1}{2\sigma^2} \sum_{i=1}^n (x - y_i)^2$$

$$U'(x) = \frac{x}{\rho^2} + \frac{1}{\sigma^2} \sum_{i=1}^n (x - y_i),$$

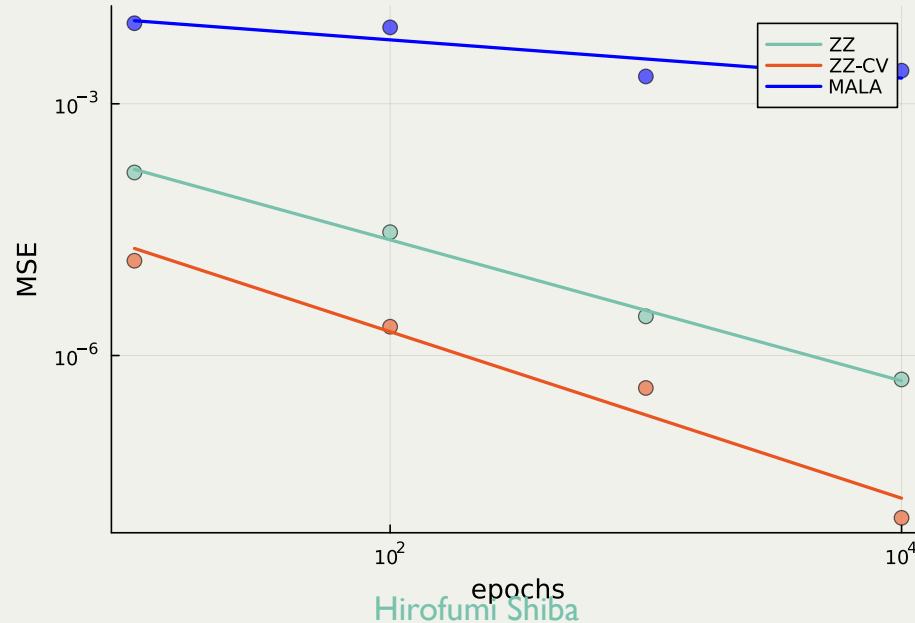
$$U''(x) = \frac{1}{\rho^2} + \frac{n}{\sigma^2}.$$



## 3.3 Menu

In the rest of this Section 3, we'll learn:

1. Even a simple Zig-Zag Sampler with  $\gamma \equiv 0$  surpasses MALA.
2. Incorporating sub-sampling, Zig-Zag with Control Variates further improves the efficiency.



### 3.4 Simple Zig-Zag Sampler with $\gamma \equiv 0$ (1/2)

Fixing  $\gamma \equiv 0$ , we obtain the upper bound  $M$

$$\begin{aligned}
 m(t) &= \int_0^t \lambda(x_s, \sigma_s) ds = \int_0^t \left( \sigma U'(x_s) \right)_+ ds \\
 &\leq \left( \frac{\sigma x}{\rho^2} + \frac{\sigma}{\sigma^2} \sum_{i=1}^n (x - y_i) + t \left( \frac{1}{\rho^2} + \frac{n}{\sigma^2} \right) \right)_+ \\
 &=: (a + bt)_+ = M(t),
 \end{aligned}$$

where



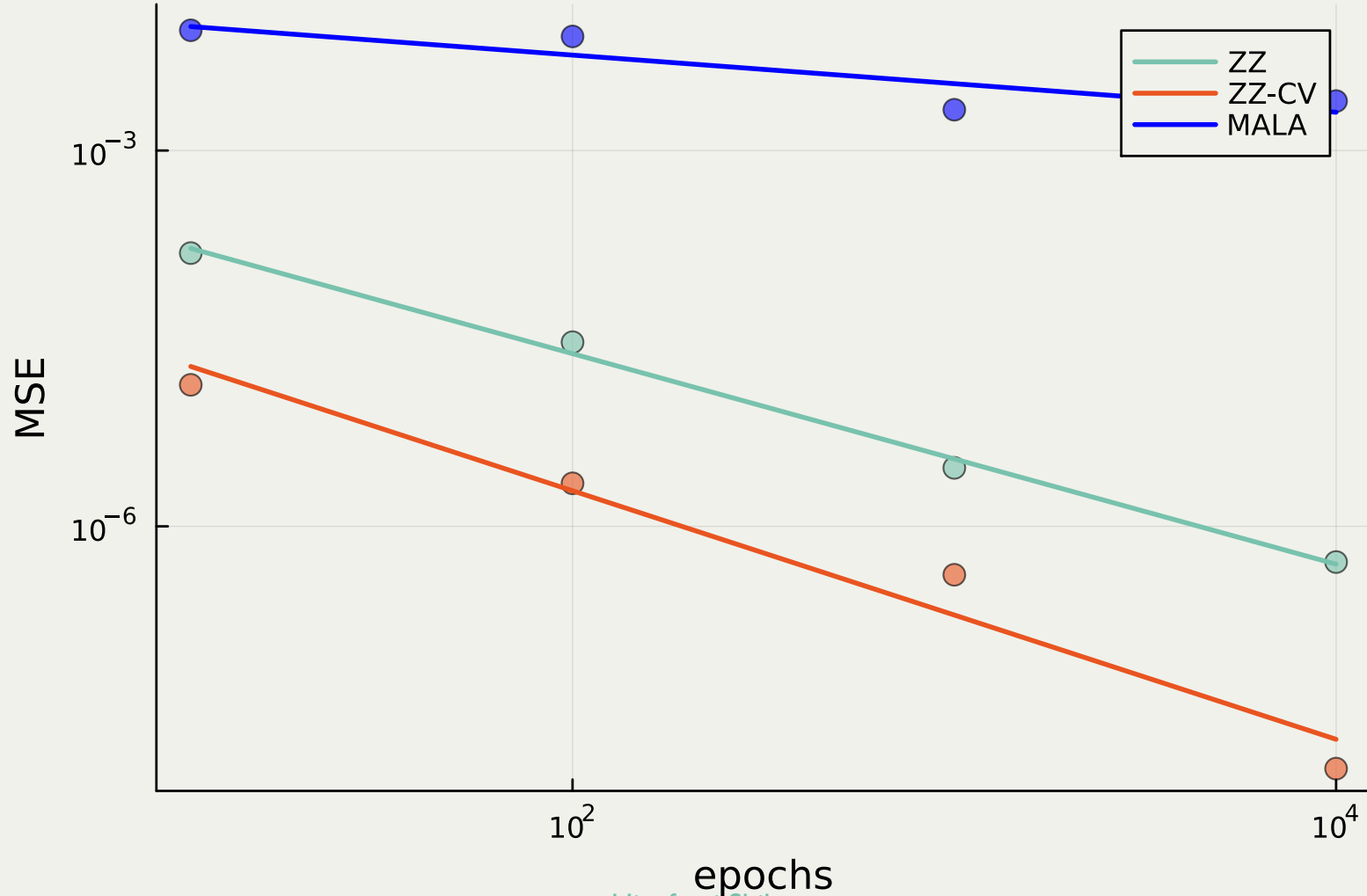


$$a = \frac{\sigma x}{\rho^2} + \frac{\sigma}{\sigma^2} \sum_{i=1}^n (x - y_i), \quad b = \frac{1}{\rho^2} + \frac{n}{\sigma^2}.$$



## 3.5 Result: 1d Gaussian Mean Reconstruction

We generated 100 samples from  $\mathcal{N}(x_0, \sigma^2)$  with  $x_0 = 1$ .



## 3.6 MSE per Epoch: The Vertical Axis

MSE (Mean Squared Error) of  $\{X_i\}_{i=1}^n$  is defined as

$$\frac{1}{n} \sum_{i=1}^n (X_i - x_0)^2.$$

Epoch: Unit computational cost.

**The following is considered as one epoch:**

- One evaluation of a likelihood ratio

$$\frac{p(X_{n+1})}{p(X_n)}.$$

- One evaluation of a **Poisson Point Process**.



## 3.7 Good News!

Case-by-case construction of an **upper bound  $M$**  is too complicated / demanding.

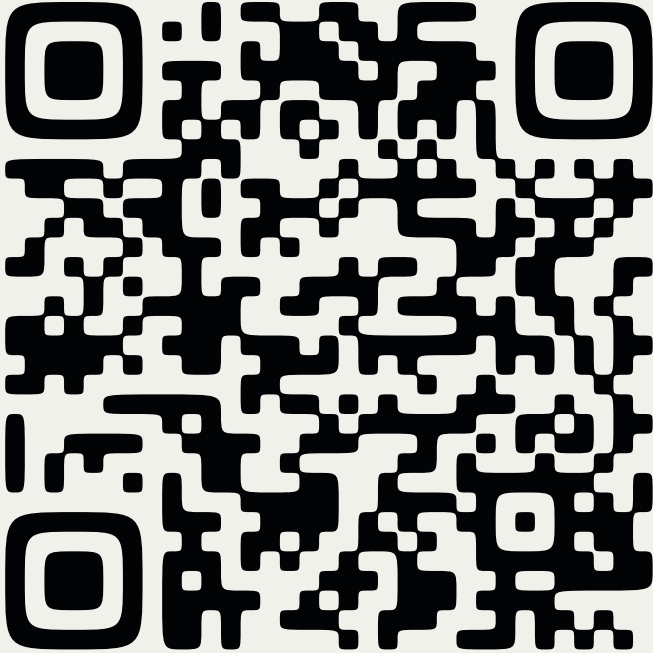
Therefore, we are trying to **automate** the whole procedure.

### **Automatic Zig-Zag**

1. Automatic Zig-Zag ([Corbella et al., 2022](#))
2. Concave-Convex PDMP ([Sutton and Fearnhead, 2023](#))
3. NuZZ (numerical Zig-Zag) ([Pagani et al., 2024](#))



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Slides and codes are available here

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# Appendix: Scalability by Subsampling

Construction of **ZZ-CV** (Zig-Zag with Control Variates).



## 3.8 Review: 1d Gaussian Mean Reconstruction

$U'$  has an alternative form:

$$U'(x) = \frac{x}{\rho^2} + \frac{1}{\sigma^2} \sum_{i=1}^n (x - y_i) =: \frac{1}{n} \sum_{i=1}^n U'_i(x),$$

where

$$U'_i(x) = \frac{x}{\rho^2} + \frac{n}{\sigma^2} (x - y_i).$$

→ We only need one sample  $y_i$  to evaluate  $U'_i$ .



## 3.9 Randomized Rate Function

Instead of

$$\lambda_{\mathbf{ZZ}}(x, \sigma) = \left( \sigma U'(x) \right)_+$$

we use

$$\lambda_{\mathbf{ZZ-CV}}(x, \sigma) = \left( \sigma U'_I(x) \right)_+, \quad I \sim \mathbf{U}([n]).$$

Then, the latter is an unbiased estimator of the former:

$$\mathbf{E}_{I \sim \mathbf{U}([n])} \left[ \lambda_{\mathbf{ZZ-CV}}(x, \sigma) \right] = \lambda_{\mathbf{ZZ}}(x, \sigma).$$



### 3.10 Last Step: Poisson Thinning

Find an invertible upper bound  $M$  that satisfies

$$\int_0^t \lambda_{\text{ZZ-CV}}(x_s, \sigma_s) ds =: m_I(t) \leq M(t), \quad I \sim \text{U}([n]).$$

It is harder to bound  $\lambda_{\text{ZZ-CV}}$ , since it is now an estimator (random function).



## 3.1 | Upper Bound $M$ with Control Variates

### Preprocessing (once and for all)

1. Find

$$x_* := \operatorname{argmin}_{x \in \mathbb{R}} U(x)$$

2. Compute

$$U'(x_*) = \frac{x_*}{\rho^2} + \frac{1}{\sigma^2} \sum_{i=1}^n (x_* - y_i).$$

Then, with a re-parameterization of  $m_i$ ,

$$m_i(t) \leq M(t) := a + bt,$$



where

$$a = (\sigma U'(x_*))_+ + \|U'\|_{\text{Lip}} \|\mathbf{x} - \mathbf{x}_*\|_p, \quad b := \|U'\|_{\text{Lip}}.$$

And  $m_i$  is redefined as

$$m_i(t) = U'(x_*) + U'_i(x) - U'_i(x_*).$$



## 3.12 Subsampling with Control Variates

Zig-Zag sampler with the random rate function

$$\lambda_{\text{ZZ-CV}}(x, \sigma) = \left( \sigma U'_I(x) \right)_+, \quad I \sim \text{U}([n]).$$

and the upper bound

$$M(t) = a + bt$$

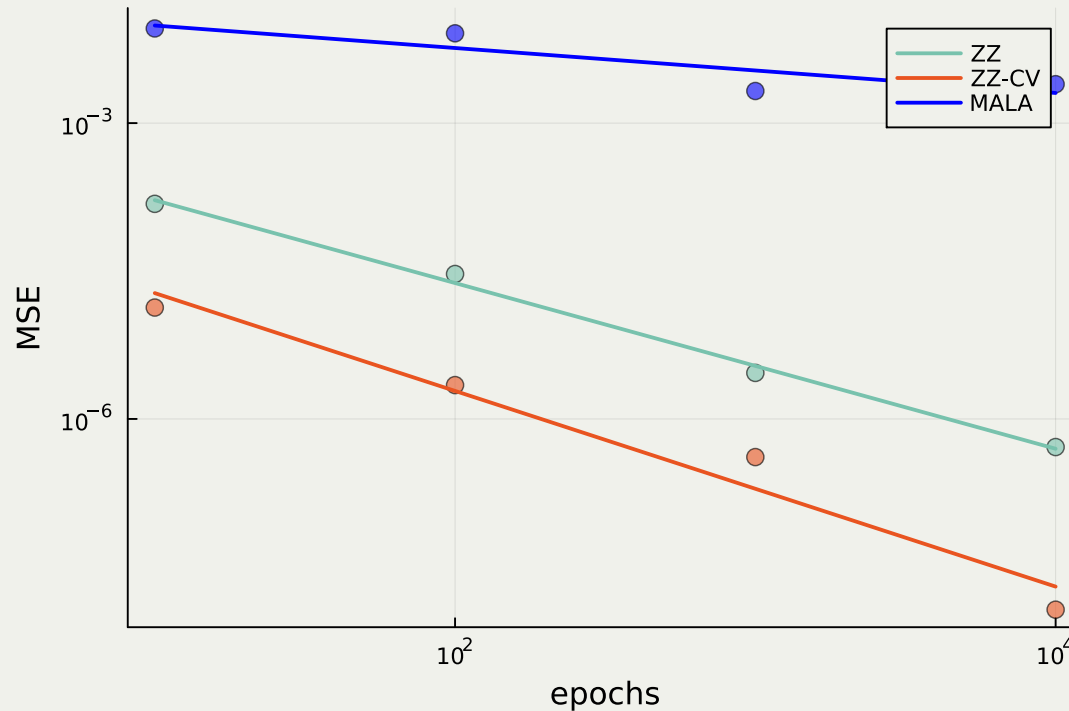
is called **Zig-Zag with Control Variates** (Bierkens, Fearnhead, et al., 2019).





## 3.13 Zig-Zag with Control Variates

1. has  $O(1)$  efficiency as the sample size  $n$  grows.<sup>1</sup>
2. is exact (no bias).



I. As long as the preprocessing step is properly done.



## 3.14 Scalability (1/3)

There are currently two main approaches to scaling up MCMC for large data.

### 1. Devide-and-conquer

Devide the data into smaller **chunks** and run MCMC on each **chunk**.

### 2. Subsampling

Use a subsampling estimate of the likelihood, which does not require the entire data.



### 3.15 Scalability (2/3) by Devide-and-conquer

Devide the data into smaller chunks and run MCMC on each chunk.

<b>Unbiased?</b>	<b>Method</b>	<b>Reference</b>
✗	WASP	(Srivastava et al., 2015)
✗	Consensus Monte Carlo	(Scott et al., 2016)
✓	Monte Carlo Fusion	(Dai et al., 2019)



## 3.16 Scalability (3/3) by Subsampling

Use a subsampling estimate of the likelihood, which does not require the entire data.

Unbiased?	Method	Reference
✗	Stochastic Gradient MCMC	(Welling and Teh, 2011)
✓	Zig-Zag with Subsampling	(Bierkens, Fearnhead, et al., 2019)
✗	Stochastic Gradient PDMP	(Fearnhead et al., 2024)



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