

# Principled subsampling and super-efficiency for Bayesian inference

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Joint work with Paul Fearnhead, Joris Bierkens, Murray  
Pollock, Andi Wang, Adam Johansen, and others ...



**CoSInES**

## Talk outline

- The zig-zag as an alternative to MCMC. “The Zig-Zag Process and Super-Efficient Sampling for Bayesian Analysis of Big Data” arXiv:1607.03188, Ann Stat 2019
- Quasi-stationary Monte Carlo and the ScaLE algorithm “The scalable Langevin exact algorithm: Bayesian inference for big data” arXiv:1609.03436

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**Super-Efficiency:**

$$\frac{\text{computational cost of running algorithm}}{\text{cost of one single likelihood evaluation}} \longrightarrow 0$$

in the big data asymptotic.

## Likelihood intractability due to data size

MCMC is the workhorse of Bayesian inference. Since it requires large numbers of realisations of the posterior density  $\pi(x)$ , it relies on these evaluations to be quick. However consider (for example) the big (tall) data case:

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Maybe we can get away with just computing **some** of  $\pi$  at each step? This is known as a **subsampling** approach.

## Piecewise-deterministic Markov processes

Continuous time stochastic process, denote by  $Z_t$ .

The dynamics of the PDP involves random events, with deterministic dynamics between events and possibly random transitions at events.

(i) **The deterministic dynamics.** eg specified through an ODE

$$\frac{dz_t}{dt} = \Phi(z_t), \quad (1)$$

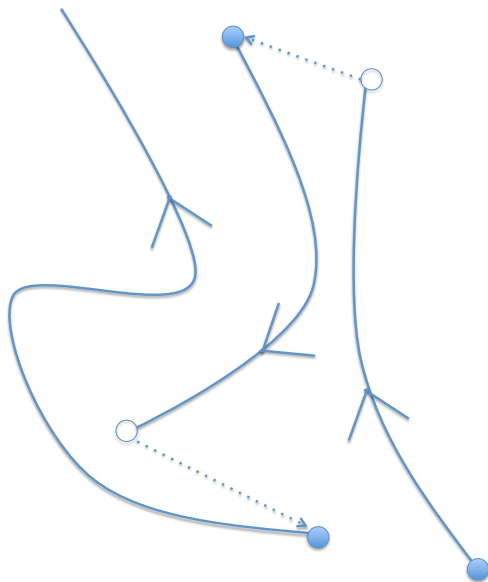
So

$$z_{s+t} = \Psi(z_t, s)$$

for some function  $\Psi$ .

- (ii) **The event rate.** Events occur at rate,  $\lambda(z_t)$ ,
- (iii) **The transition distribution at events.** At each event time  $\tau$ ,  $Z$  changes according to some transition kernel

## PDMP



# PDMP

Date back to 1951 paper by Mark Kac on the [telegraph process](#).

Mathematical foundations: Davis (1984, JRSS B)

**Non-reversible** Markov process.

Intrinsically continuous in time unlike (almost all) algorithms. Why would they ever be useful for simulation?

Unlike [diffusion processes](#) they are comparatively understudied, and underused (either for models or in stochastic simulation).

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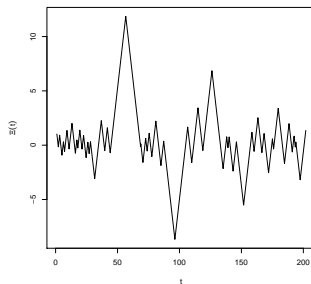
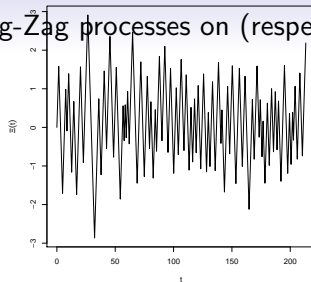
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.... **until recently**

One-dimensional Zig-Zag processes on (respectively) Gaussian and Cauchy targets.



## Canonical Zig-Zag

State  $(X_t, V_t)$  in dimension  $d$ .

$$dX_t = V_t dt$$

$V_{t-}^{(i)} \rightarrow 1 - V_{t-}^{(i)}$  at rate

$$\lambda_i(X_t, V_t) = \lambda_i^0(X_t, V_t) \equiv \max \left\{ 0, -V_{t-}^{(i)} \frac{\partial \log \pi(X_{t-})}{\partial X^{(i)}} \right\}$$

Invariant distribution is

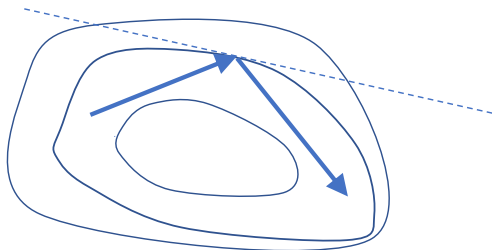
$$\pi_E(x, v) \propto \pi(x)$$

ie in stationarity  $X$  and  $V$  are independent with  $V$  being uniform over all configurations:  $(\pm 1, \pm 1, \dots, \pm 1)$



## Alternatives to Zig-Zag

Closely related to another PDMP scheme, the **bouncy particle sampler** (BPS), [Bouchard-Côté et al., 2015].



Many alternatives/variants available.

## Refreshment

Back to Zig-Zag

There is a lot more flexibility!

For instance, can take

$$\lambda_i(x, \nu) = \lambda_i^0(x, \nu) + \nu(x)$$

for **any** function  $\nu$ .

Why might we do this?

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Why might we do this?

To help visit different parts of the state space.

**But the larger  $\nu$  is, the *closer* to reversibility.**

The **canonical** Zig-Zag is the *most non-reversible*.

## Implementation

How do we simulate continuous time stochastic process like this?

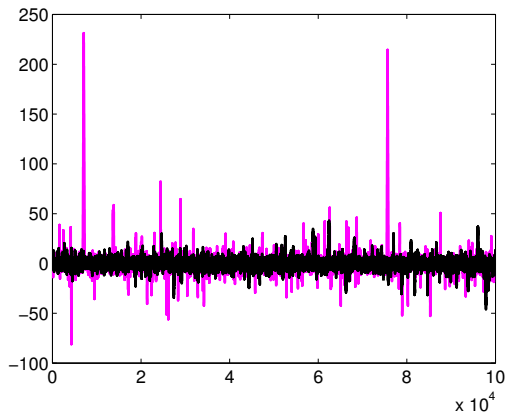
By using **thinned poisson processes**

For example, if  $|(\log \pi)'(x)| < c$ , simulate a Poisson process of rate  $c$  (by simulating the exponential inter-arrival times). Then at each poisson time, we accept as a direction change with probability  $\max(-(\log \pi)'(x), 0)/c$ .

This makes the algorithm **inexpensive** to implement as we only need to calculate  $(\log \pi)'(x)$  occasionally.

There are many other details .... though the method is not so complicated.

# Zig zag process for sampling the Cauchy distribution



$T = 10,000$

## Multi-dimensional zig zag process

Multi-dimensional zig zag process: here we have a multi-dimensional binary velocity, eg  $(1, -1, -1, 1, 1, -1, 1, 1)$ .

Efficient sampling (currently for potentials with locally Lipschitz gradients in multiple dimensions, but with obvious ways to extend).



## Subsampling

**Motivation:** intractable likelihood problems where calculating  $\pi$  at any one fixed location is prohibitively expensive (given that very many evaluations will be required to run the algorithm. For this talk, concentrate on the Bayesian setting:

$$\pi(x) = \prod_{i=1}^N \pi_i(x)$$

Eg we have  $N$  observations (but this method is not in any way restricted to the independent data case).

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For instance we might try **pseudo-marginal MCMC** (Beaumont, 2003, Andrieu and Roberts, 2009). But that would require an **unbiased non-negative estimate** of  $\pi(x)$  with variance which is stable as a function of  $N$ .

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## Subsampling within PDMP

PDMP for the exploration of high-dimensional distributions (such as zig-zag or the **ScaLE** algorithm, Fearnhead, Johansen, Pollock and Roberts, 2016) typically use  $\log \pi(x)$  rather than  $\pi(x)$  and

$$\log \pi(x) = \sum_{i=1}^N \log \pi_i(x)$$

for which there are well-behaved  $O(1)$  cost,  $O(1)$  variance (or sometime a little worse). **Can we use this?**

**Zig zag switching rate**  $\max \left( 0, -j \sum_{i=1}^N (\log \pi)'_i(x) \right) \rightsquigarrow O(N)$   
calculation at every switch

# Subsampling for zig-zag

## Sub-sampling

- Determine global upper bound  $M$  for switching rate
- Simulate  $\text{Exponential}(M)$  random variable  $T$
- Generate  $I \sim \text{discrete}(\{1, \dots, N\})$
- Accept the generated  $T$  as a “switching time” with probability  $N \max(0, -j(\log \pi_I)'(Y(T))) / M$

**Theorem:** This works! (invariant distribution  $\pi$ )

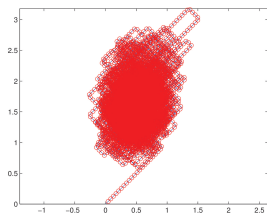
## Subsampling + control variates

Crudely, for an  $O(1)$  update in state space:

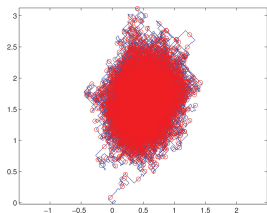
- Without subsampling,  $O(N)$  computations required
- Using **subsampling**, gain **factor  $N^{1/2}$**   $\rightsquigarrow$  complexity  $O(N^{1/2})$  per step
- Using **control variates**, gain **additional factor  $N^{1/2}$**   $\rightsquigarrow$  complexity  $O(1)$  per step

**Superefficiency** We call an **epoch** the time taken to make one function evaluation of the target density  $\pi$ . The control variate subsampled zig-zag is **superefficient** in the sense that the **effective sample size** from running the algorithm per epoch diverges.

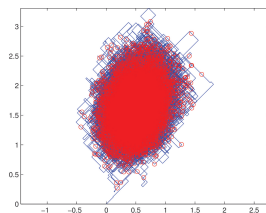
# Subsampling + control variates – Logistic growth



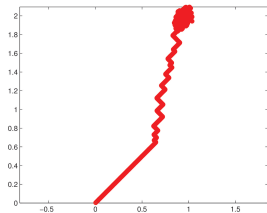
(a)  $N = 100$



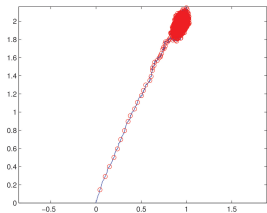
(b)  $N = 100$



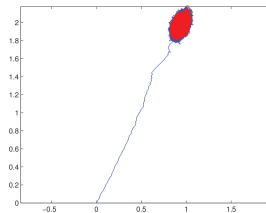
(c)  $N = 100$



(d)  $N = 10,000$



(e)  $N = 10,000$

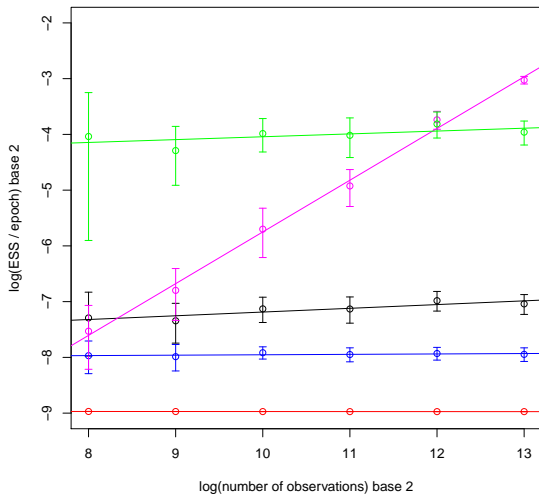


(f)  $N = 10,000$

[Bierkens, Roberts, 2015, <http://arxiv.org/abs/1509.00302>]

[Bierkens, Fearnhead, Roberts, Ann Stat to appear]

# Effective Sample Size per epoch



## Summary of Zig-Zag

- PDMPs have many uses for simulation of stochastic processes (even those very different from PDMPs) as well as **steady state** simulation.



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- Zigzag is a flexible and usually easy-to-implement method for simulating from a target distribution.
- Can zigzag be a competitor to Hamiltonian MCMC?

# Quasi-stationary Monte Carlo

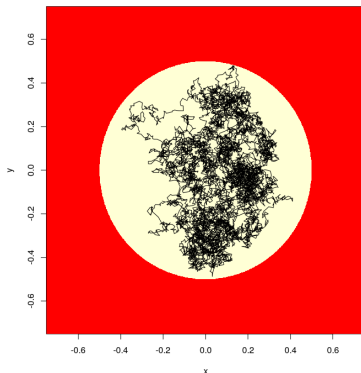
Traditional Markov chain Monte Carlo rests on the construction of an **ergodic Markov chain** designed to have a prescribed stationary distribution  $\pi$ .

**Quasi-stationary Monte Carlo** instead makes use of the **conditional** distribution of an killed stochastic process conditioned on not being killed.

This turns out to be a natural framework for subsampling without approximation.

## Quasi-stationarity: boundary killing

Ant on a volcanic island undergoing Brownian motion, killed at  $\tau_{\partial}$  when it touches lava.



What can be said about  $\mathbb{P}(X_t \in \cdot \mid \tau_{\partial} > t)$  for large  $t$ ?

## Quasi-stationarity: interior killing

Take a continuous-time Markov process on  $\mathbb{R}^d$

$$(X_t, \quad t \geq 0).$$

We then augment this process with an inhomogeneous Poisson process:

$$\tau_{\partial} := \inf \left\{ t \geq 0 : \int_0^t \kappa(X_s) ds \geq \xi \right\},$$

where  $\xi \sim \text{Exp}(1)$ , independent of  $X$ .

Here  $\kappa : \mathbb{R}^2 \rightarrow [0, \infty)$  is a locally bounded function, the **killing rate**.

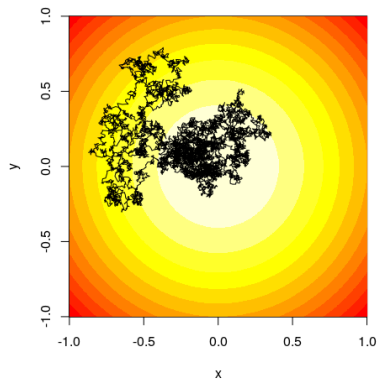
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Take  $X$  to be a standard **Brownian motion** on  $\mathbb{R}^2$ ,  $\kappa(y) = \|y\|^2$ .



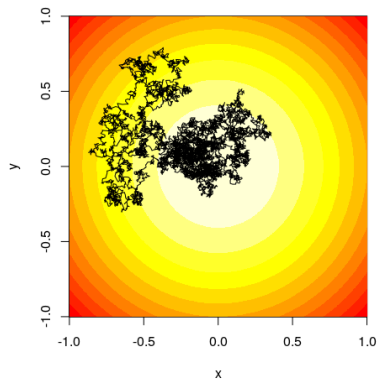
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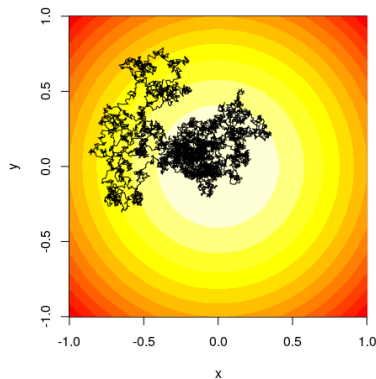
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What can be said about  $\mathbb{P}(X_t \in \cdot \mid \tau_\partial > t)$  for large  $t$ ? Gaussian.

## Quasi-stationarity

Say a probability measure  $\mu$  is **quasi-stationary** if for any  $t \geq 0$ ,

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Rich literature in probability theory; e.g. population dynamics, and textbook of Collet et al (2013).

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This actually arises quite naturally in computing:

$$\tau_\partial = \{\text{algorithm behaves very badly}\},$$

e.g. stack overflow, very slow runs, *cf. user-impatience bias*.

# Characterisation of quasi-stationarity distributions

## Discrete time

- Transition matrix  $P$ .
- $\pi$  is **stationary** if

$$\pi P = \pi.$$

- $\pi$  **quasi-stationary** if

$$\pi P = \lambda \pi,$$

some  $0 < \lambda < 1$ .

- Semigroup

$$\pi P^n = \lambda^n \pi.$$

## Continuous time

- Rate matrix  $Q$ .
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Theory of quasi-stationarity more delicate, so why bother ....

## Quasi-stationary Monte Carlo

Start with a diffusion, for simplicity assume  $X$  is Brownian motion.

At time  $t$ , kill  $X$  at rate  $\kappa(X_t)$ .

Idea of quasi-stationary Monte Carlo: choose  $\kappa$  in such a way that the quasi-limiting distribution coincides with the target distribution  $\pi$ .

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Need to take

$$\kappa(x) = \frac{1}{2} \frac{\Delta \pi(x)}{\pi(x)} + C$$

where  $\Delta$  denotes the Laplacian and  $C$  is an arbitrary constant (which needs to be chosen so that  $\kappa$  is always non-negative).

## How to extract samples from $\pi$ ?

For MCMC it is obvious to just take values of the chain after a while which should be close to samples from  $\pi$ .

It is clearly inefficient to take long runs of Brownian motion and just keep the ones which have not been killed.

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Instead we have two approaches

- The **Scalable Langevin Exact Algorithm: ScaLE** which propagates a population of particles. Once one dies, it is resurrected from the location of one of the other particles.
- **ReScaLE** which uses a single trajectory which on death regenerates from a point along the trajectory to date.

## Some implementational comments about ScaLE

The algorithm is implemented via an **SMC** framework.

In practice, we don't automatically kill particles and carry weighted particles instead in a more traditional SMC way. This is more efficient.

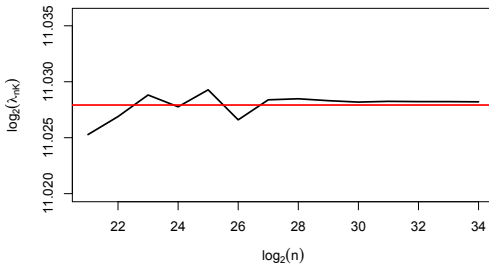
Crucial to efficiency is subsampling. Need tractability of  $f$  as well as a thinned Poisson process approach. All of this is analogous to the Zig-Zag set-up.

The underlying stochastic process is just Brownian motion. Simulation of Brownian motion is complicated by the need to simulate random variable such as BM's first exit time of a suitable hypercube. (Needed to ensure we can exactly implement the thinned PP method.)

# ScaLE

The key is that deciding on whether to kill a particle or not can be done using subsamples of the data set of size 2, with no loss of algorithmic efficiency.

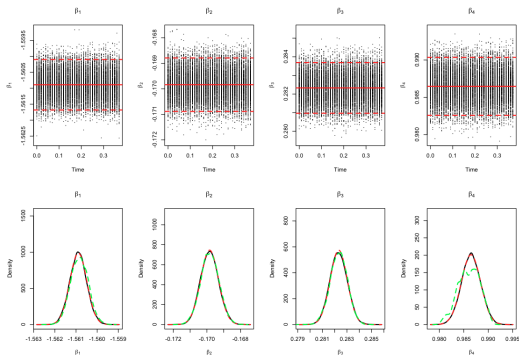
For example a logistic regression example using control variates:



## Logistic regression example

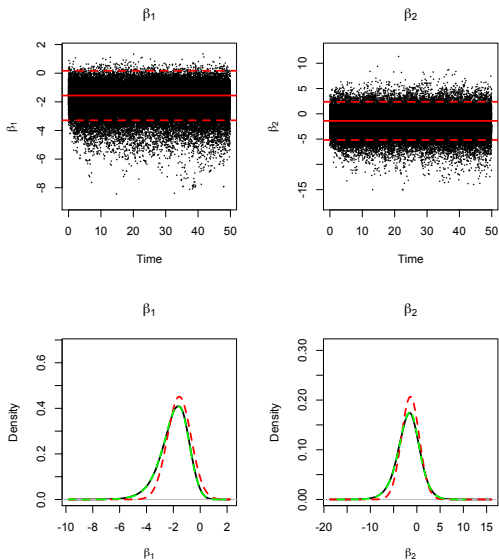
Airline data set (all flights in US over an extended period). Binary output of whether the flight was late.

49,665,450 individual records of the data set were accessed (equivalent to roughly 0.0029 full data evaluations) for the following output.





# Skewed distribution



## Summary of ScaLE properties

ScaLE has remarkable scaling properties for large data. **BUT** it does require

1. smoothness of the likelihood;
2. posterior contraction
3. to get the best scaling with dimension, require to find at least one point "close" to a mode of  $\pi$ .

Current implementation (in R!) is fairly slow and only suitable for fairly low dimensional parameter sets. But the scaling properties can be clearly seen.

## Final comments

We have introduced two *principled subsampling* methods which exhibit **iterative** super-efficiency.

Note that with highly heterogenous data (eg all the information comes from a tiny fraction of the data) no method can be super-efficient.

ScaLE is statistically identical to the algorithm which would carry out no subsampling and fully evaluate the target at each step. Zig-Zag is not statistically identical and can converge slower with subsampling.

Zig-Zag (and other PDMPS) are currently the more promising method for higher-dimensional problems.

Continuous-time algorithms involve many new implementational details and challenges. But these methods can often be **more robust** than their continuous-time competitors.

## Final comment (continued)

### Software:

<https://github.com/mpoll/scale>

RZigZag, see

<https://diamweb.ewi.tudelft.nl/joris/pdmps.html>

### Current/future directions:

1. **ReScaLE**. While ScaLE uses a population approach (SMC) to realise the quasi-stationary distribution, ReScaLE is a single trajectory algorithm: rebirths come from the past trajectory rather than the remaining population of particles. Compared to ScaLE, ReScaLE is very fast, but has less robust convergence.
2. **Restore**. This is a pure non-reversible MCM algorithm involving rebirths together with local dynamics.  
<http://arxiv.org/abs/1910.05037>
3. Theoretical underpinning for all these methods!
4. Generic software using automatic differentiation.
5. Applications in infectious disease epidemiology