Topics in Retrospective simulation

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FoCSML, January 2025

Part 4: Principled subsampling and super-efficiency for Bayesian inference

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 (with discussion)" arXiv:1609.03436, JRSS B 2020

Both these ideas are examples of Continuous-time Monte Carlo algorithms, and they intrinsically rely on retrospective sampling.

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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 connsider (for example) the big (tall) data case:

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

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Does that mean that exact Bayesian inference is not realistically possible for huge data sets?

Maybe we can get away with just computing some of π 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

$$\frac{\mathrm{d}z_t}{\mathrm{d}t} = \Phi(z_t), \tag{1}$$

So

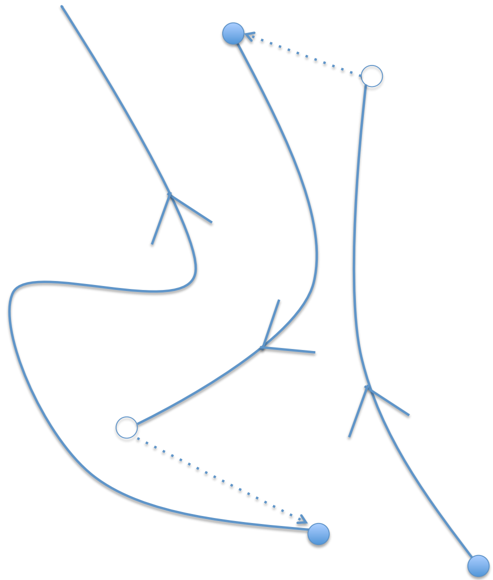
$$z_{s+t} = \Psi(z_t, s)$$

for some function Ψ.

(ii) The event rate. Events occur at rate, $\lambda(z_t)$,

(iii) The transition distribution at events. At each event time τ, 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)

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

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.... until recently

Non-reversibility for MCMC?

Reversible Markov chains are well-understood mathematically. They lead to flexible families of algorithms (Metropolsi-Hastings, etc) which can be implemented using only local computation (detailed balance equations leading to accept reject mechanisms).

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BUT it has long been known in probability that non-reversible chains can sometimes converge much more rapidly than reversible ones (see for instance Hwang, Hwang-Ma and Sheu (1993), Chen Lovasz and Pak (1999), Diaconis, Holmes and Neal (2000).

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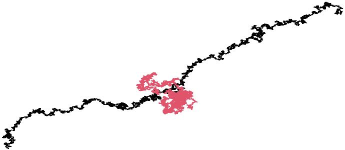
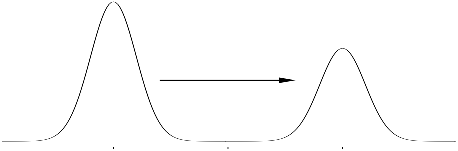
Hamiltonian MCMC (Hybrid Monte Carlo) tries to construct chains with non-reversible character, but ultimately it is also reversible because of the accept/reject step.

Why does non-reversibility help?

Breaking down random walk behaviour:



Or maybe helping to escape local modes

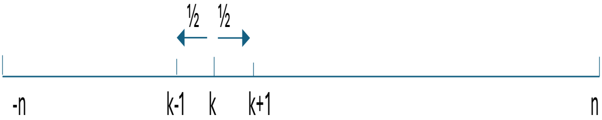


But if you had this momentum all the time, the chain would disproportionately visit the right hand mode.

How to choose the right direction for the momentum? Particularly in d dimensions.

Toy example

Consider one-dimensional random on the integers $-n, -(n-1), \ldots n-1, n$ started at $X_0 = 0$, ie

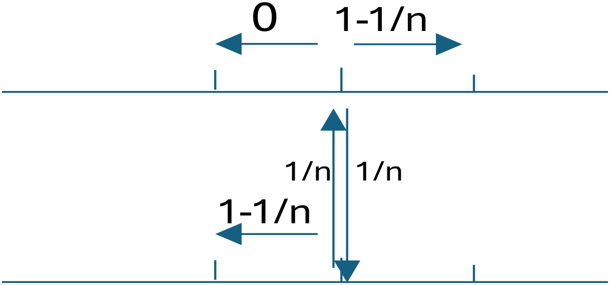


Imagine n is large. To have any chance of mixing, the chain needs to be able to reach $\pm n$.

By the Central Limit Theorem, $X_t \approx N(0, t)$ ie standard deviation $\mathcal{O}(t^{1/2})$.

So we need $t^{1/2}$ to be at least $\mathcal{O}(n)$ to have non-negligible probability of reaching the edges, ie $t = \mathcal{O}(n^2)$ steps.

Now consider non-reversible (lifted) RW (Chen et al 1999)



We now have two copies of the state space, the upper one with momentum $+1$ and the lower one with momentum -1.

Now we have probability approximately e^{-1} of reaching $\pm n$ in time exactly n.

It can be shown in fact that the mixing time is $\mathcal{O}(n \log n)$ (Diaconis et al, 2000).

But can MCMC algorithms inherit this advantage?

Non-reversible MCMC algorithms

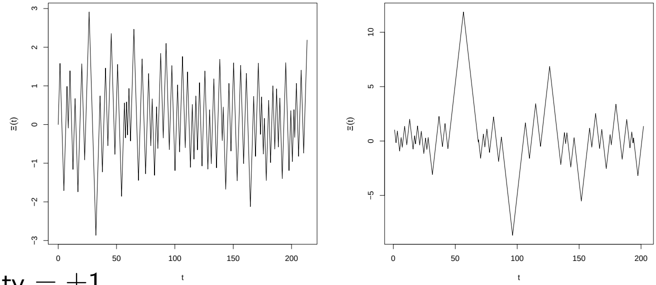
Much hype about non-reversibility in MCMC. There are still major challenges in implementation and software for these methods. However reasons for optimism:

1. High-dimensional scaling theory (methods scale well with dimension).
2. *Principled subsampling (major advantage over subsampled Langevin methods) - methods scale well with data size).*
3. Non-reversible algorithms can sometimes avoid **random walk behaviour**.

Here we are largely going to concentrate on the middle one of these .... although there are a lot of exciting recent developments in the other areas.

One-dimensional Zig-Zag

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

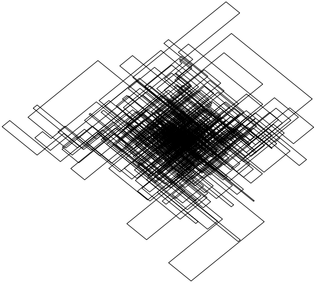


velocity $= \pm 1$.

Switching rate $= \max\{0, -v(\log \pi)'(x)\}$.

Canonical Zig-Zag (multiple dimensions)

State (X_t, V_t) in dimension d.
$V_{t,i} = \pm 1$ for each i.



$$dX_t = V_t \; dt$$

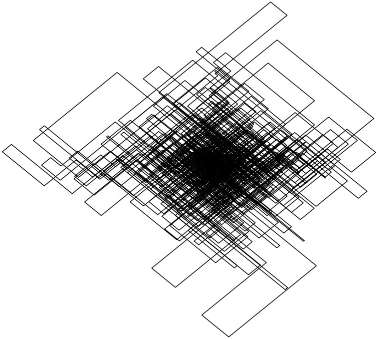
$V_{t-}^{(i)} \to 1 - V_{t-}^{(i)}$ at rate

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

Invariant distribution is

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

Ie in stationarity X and V are independent with V being uniform over all configerations: $(\pm 1, \pm 1, \ldots \pm 1)$



Marginal distribution in x is π.

Truly continuous time algorithm. Skeletons required (either equally spaced or random) to exptract ergodic estimates.

Markov chain from the jump times alone is biased.

Refreshment

But there is a lot more flexibility!

For instance, can take

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

for any function ν.

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Why might we do this?

For irreducibility: to aid communication between different parts of the state space.

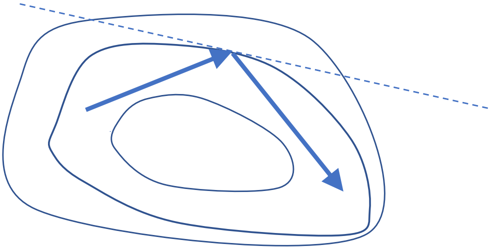
But the larger ν is, the *closer* to reversibility.

The canonical Zig-Zag is the *most non-reversible*. (Eg the limit as ν diverges is a reversible Langevin diffusion, suitably scaled, Bierkens+Duncan, 2017).

(See Andrieu+Livingstone 2019 for precise statement about the canonical algorithm minimising asymptotic Monte Carlo variances.)

Bouncy particle sampler

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



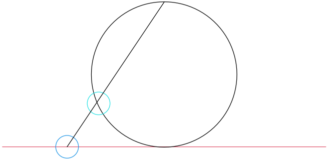
$$\lambda(x) = \max\{-\nabla \log \pi(x) \cdot v, 0\}$$

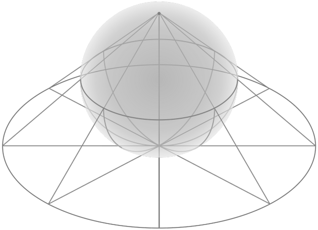
v constant until event occurs upon which it reflects.

Many alternatives/variants available (eg different inner products, refresh rate, excess switching rate, choice of velocity distribution...)

Stereographic Projection

Maps $\mathbb{R}^d$ to $\mathbb{S}^d$





Many attempts to curtail transient phases by transformations in the MCMC literature. Stereographic Projection is a very natural tool.

Inexpensive, and constant curvature gives great tractability and algorithmic advantages.

SBPS

Stereographic Bouncy Particle Sampler

Piecewise great circle trajectories on the hypersphere projected back onto $\mathbf{R}^d$:

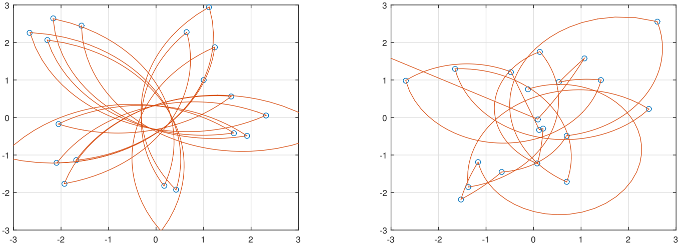


Figure: SBPS without (left) and with (right) refreshment for target distribution $\mathcal{N}(0, I_2)$.

Implementation

How do we simulate continuous time stochastic process like this?

Most general techniques using thinned poisson processes, but application specific to implement.

In its simplest form... 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.

Also automatic and numerical options, plus skew-Metropolised versions: eg Corbella et al (2021), Pagani et al (2020), Bertazzi et al (2022), and others, starting to make these methods accessible to non-specialist users.

Subsampling

Motivation: intractable likelihood problems where calculating π at any one fixed location is prohibitively expensive (given that very many evaluations will be required to run the algorithm. Here, concentrate on common context for (eg) 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. But this is not possible for a product without computing cost which is at least $O(N)$.

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) unbiased estimators of $\log \pi(x)$ and its derivatives.

For example take $I \sim \text{discrete}(\{1, \ldots, N\})$ and use

- Vanilla Subsampling $\widehat{\log \pi'(x)} = N \log \pi'_I(x)$
- Control Variate Subsampling $\widehat{\log \pi'(x)} = \log \pi'(x^*) + N(\log \pi'_I(x) - \log \pi'_I(x^*))$ where x^* is ideally taken to be at or near the mode of π.

Can we use this?

Eg: subsampling for one-dimensional zig-zag

Eg one-dimensional Zig zag switching rate

$\max\left(0, -v\sum_{i=1}^{N}(\log\pi_i)'(x)\right) \rightsquigarrow O(N)$ calculation at every switch (or attempted switch).

Sub-sampling version

- Determine global upper bound M for switching rate
- Simulate Exponential(M) random variable T
- Generate $I \sim \text{discrete}(\{1,\ldots,N\})$
- Accept the generated T as a "switching time" wp $\frac{\max\left(0, -V_{T-}\log\widehat{\pi'(X_T)}\right)}{M}$.

Theorem: This works! (invariant distribution π)

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Why? Subsampling is statistically equivalent to adding a (state-dependent) refresh rate.

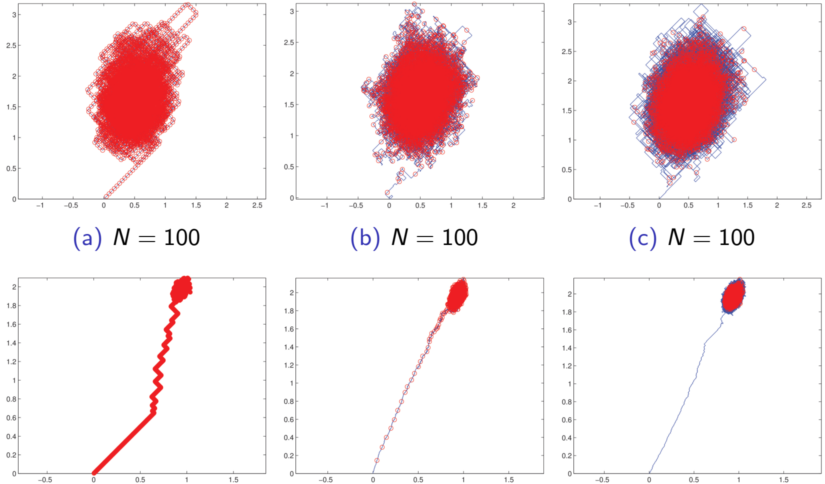
Subsampling: implementational complexity - the transient phase

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

- Canonical Zig-Zag, $O(N)$ 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 π. 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) $N = 100$

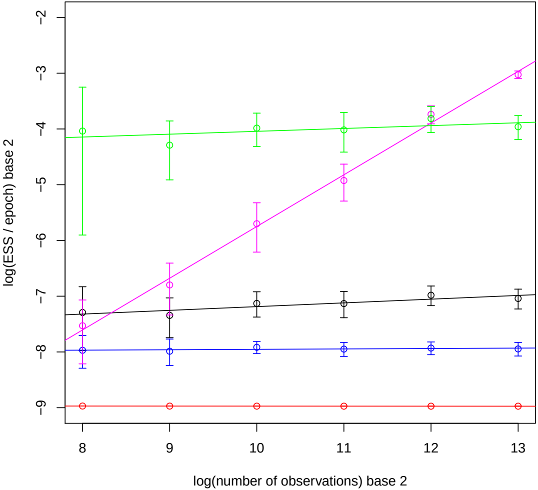
(d) $N = 10,000$

(e) $N = 10,000$

(f) $N = 10,000$

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

Effective Sample Size per epoch



Is the zig-zag ergodic?

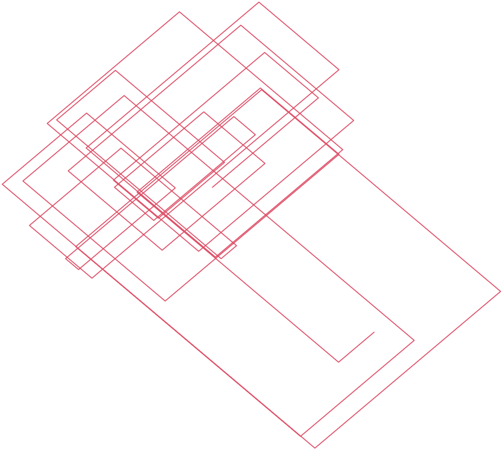
An invariant distribution for (x, v) for the zig-zag is just

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

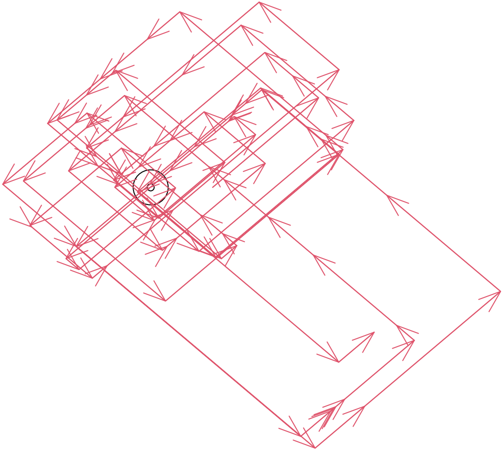
ie $X \sim \pi$ and independently the velocity v is uniformly distributed within $\{-1, 1\}^d$.

Ergodicity requires that we can reach all locations in (x, v) space.
But can we ensure this?

Perfectly well-mixing Zig Zag?

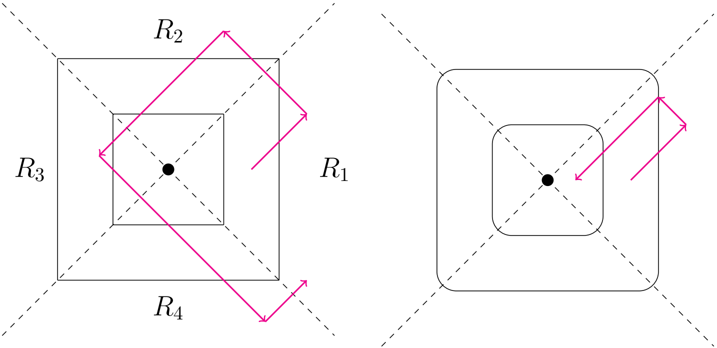


Turns out to be reducible!



A counter example

$\pi(x, y) \propto \exp\{-\max(|x|, |y|)\}$



(a) Contour lines, the regions R_1, R_2, R_3 and R_4, and a typical trajectory for the potential function $U(x) = \max(|x_1|, |x_2|)$. From the displayed starting position it is impossible to reach a point in R_1 with direction $(-1, -1)$.

(b) Once we smooth the density function slightly, it becomes possible to switch the second coordinate of the direction vector, making the process irreducible.

Possible solution

Include a refresh jump rate γ_i which is uniformly positive, eg $\gamma_i(x) = \tilde{\gamma} > 0$.

This makes proving ergodicity easy under minimal assumptions on π

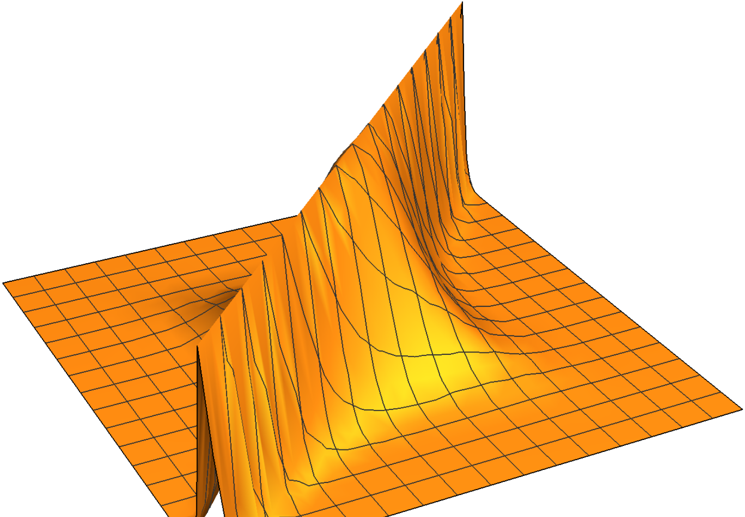
But for large $\tilde{\gamma}$, the zig-zag then looks more and more like a Langevin diffusion which is reversible. Many of the advantages of non-reversibility are therefore lost.

See Peskun Tierney ordering result of Andrieu-Livingstone 2019) which shows that adding refresh increases asymptotic Monte Carlo variance.

Can we establish an ergodicity result for the canonical zig-zag, ie $\tilde{\gamma} = 0$?

What else could go wrong?

We also need to preclude evanesence



Theorem

Assume that

1. π *is positive and* $\mathcal{C}^3$
2. $\lim_{|x|\to\infty} \pi(x) = 0$, *and*
3. *has a non-degenerate local maximum, ie the Hessian at the local maximum is strictly negative definite.*

Then the chain is irreducible and converges to π *from any starting distribution.*

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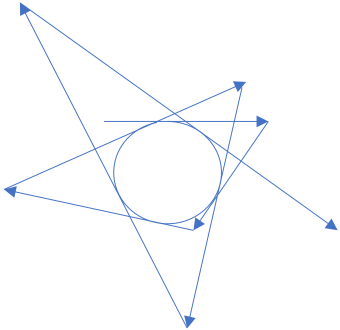
Method of proof relies heavily upon smoothness and the ability to approximate by a Gaussian around the local mode. (3) can no doubt be weakened.

Irreducibility of BPS?

Without refreshment, canonical BPS can easily be irreducible. Eg for 2-dimensional isotropic Normal Distribution:



Uncountably infinite number of reducibility classes!

More generally ..

For distributions which are close to spherical symmetry, mixing will be extremely slow.

For higher-dimensional Gaussians we just need any two eigenvalues of Σ to be equal to replicate this extreme reducibility.

So, strangely, the eigenvalues of Σ need to be well-separated to even hope for mixing, leading itself to heterogeneity of scale and again very slow mixing.

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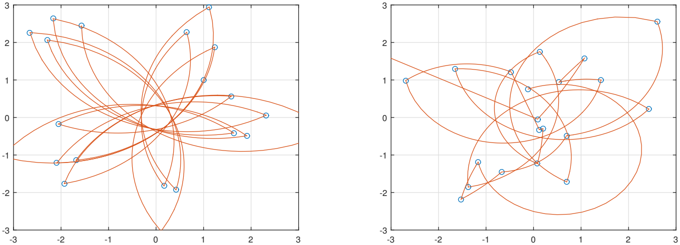
But how much refreshment?

SBPS irreducibility

SBPS chain is also potentially not irreducible without refreshment.

Piecewise great circle trajectories on the hypersphere projected back onto $\mathbf{R}^d$:



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- More work is needed on studying the theoretical and empirical properties of these algorithms, and exploiting their flexibility. (Though lots more I have not told you ...)
- 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

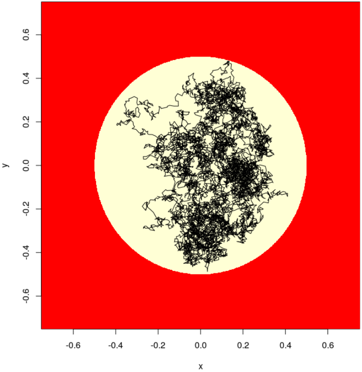
Traditional Markov chain Monte Carlo rests on the construction of an ergodic Markov chain designed to have a prescribed stationary distribution π.

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 τ_∂ when it touches lava.



What can be said about $\mathbb{P}(X_t \in \cdot \,|\tau_\partial > t)$ 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:

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

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

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

Quasi-stationarity: interior killing example

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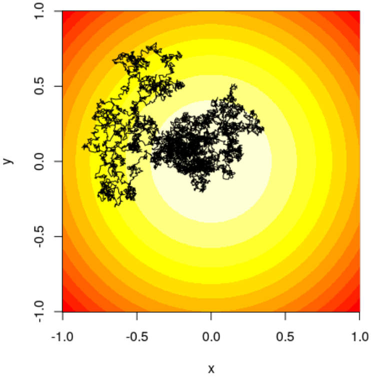

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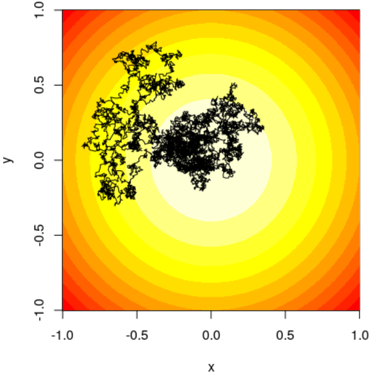

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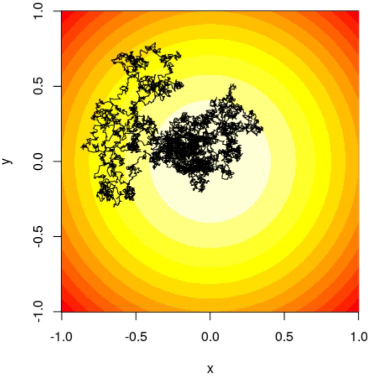

What can be said about $\mathbb{P}(X_t \in \cdot \,|\tau_\partial > t)$ for large t? Gaussian.

Quasi-stationarity

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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.
- π is stationary if

$$\pi P = \pi.$$

- π quasi-stationary if

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

some $0 < \lambda < 1$.

- Semigroup

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

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- 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 $\kappa(X_t)$.

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Need to take

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

where Δ denotes the Laplacian and C is an arbitrary constant (which needs to be chosen so that κ is always non-negative.

How to extract samples from π?

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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.

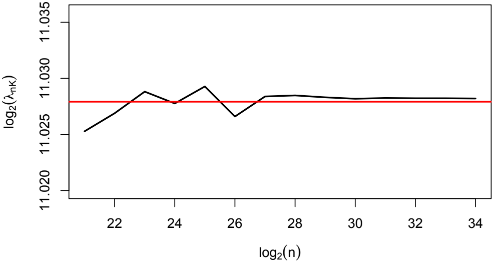
Crucial to efficiency is subsampling. Need tractability of f as well as a thinned Poisson process approach. All of this is analogous to the Zig-Zag set-up.

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.

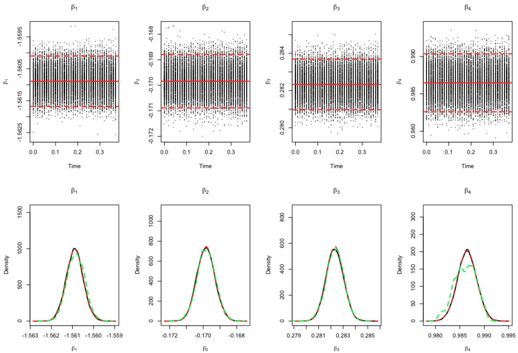
For example a logistic regression example using control variates:



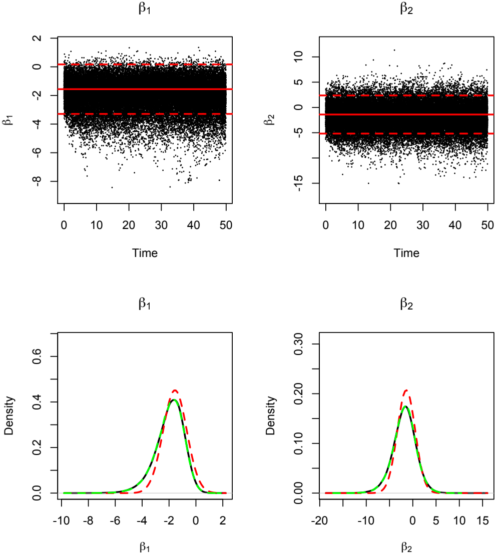
Logistic regression example

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 properies 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 π.

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 the 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