Re-sampled Scalable Langevin Exact (ReScaLE) Method to Explore Bayesian Posterior using Quasi-stationarity regime

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OXWASP, University of Warwick

27 October 2015

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[7] Roberts, G. et al. (2015). Towards not being afraid of the big bad data set.

[8] Scott, S. L. et al. (2013). *Bayes and big data: The consensus Monte Carlo algorithm.*

Special Thanks

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Outline

Bayesian Inference for 'Big Data'

We are interested in Bayesian inference of parameter x in parameter space.

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

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- Break $\longrightarrow$ *Compute Posterior* $\longrightarrow$ *Recombine*[1]

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How do we simulate from π then?

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Gradient Method

Langevin Diffusion

$$dX_t = \frac{1}{2}\nabla \log \pi(X_t)\,dt + dB_t \quad X_0 = x,\, t \in [0, T]$$

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Gradient Method ...

Euler-Maruyama Scheme

$$X_{t+\delta} = X_t + \frac{1}{2}\nabla \log \pi(X_t)\delta + \epsilon$$
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- So, how do we perform rejection sampling on diffusion?

Exact simulation from diffusion

Rejection sampling on the diffusion path space!

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$$dX_t = \alpha(X_t)\,dt + dB_t \quad , X_0 = x_0, \quad 0 \le t \le T \tag{1}$$

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R-N Derivative using Girsanov's formula

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$$A(X_T) - A(x) - \frac{1}{2}\int_0^T \left(\alpha^2(X_s) + \alpha'(X_s)\right) ds = \int_0^T \alpha(X_s)dB_s - \frac{1}{2}\int_0^T \alpha^2(X_s)ds$$

Exact simulation from diffusion ...

$$\frac{d\mathbb{Q}}{d\mathbb{W}}(X) = \exp\left(A(X_T) - A(x) - \frac{1}{2}\int_0^T \left(\alpha^2(X_t) + \alpha'(X_t)\right) dt \right)$$

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Biased Brownian Motion

[1] Biased Brownian motion is a process $Z_t := (B_t | B_0 = x, B_T = y \sim h)$ with measure $\mathbb{Z}$ where $x, y \in \mathbb{R}$, $0 \leq t \leq T$ such that

$$h(y; x, T) \propto \exp\left(A(y) - \frac{(y-x)^2}{2T}\right)$$

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Theorem

[1] $\mathbb{Q}$ *is equivalent to* $\mathbb{Z}$

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$l \leq \frac{(\alpha(x)^2 + \alpha'(x))}{2} \leq u \quad x \in R$

$$\frac{d\mathbb{Q}}{d\mathbb{Z}}(X) \propto \exp\left\{-\int_0^T \underbrace{\left(\frac{1}{2}(\alpha^2(X_t) + \alpha'(X_t)) - l\right)}_{\phi(X_t)} dt\right\}$$

$$\frac{d\mathbb{Q}}{d\mathbb{Z}}(X) \propto \exp\left\{-\int_0^T \phi(X_t)\,dt\right\} \leq 1$$

How do we construct events of such probability?

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Poisson Thinning

Result [1]

Let $X = \{X_t : t \in [0, T]\}$ be a continuous path drawn from Biased Brownian Motion and $M(X)$ be the upper bound of the function $\phi(X)$. If Φ is a homogeneous Poisson process of unit intensity on the rectangle $[0, T] \times [0, M(X)]$ and
$N =$ Number of points found below the graph $\{t \to \phi(X_t)\}$, then

$$P(N = 0|X) = \exp\left\{-\int_0^T \phi(X_t)\,dt\right\} \tag{2}$$

Another interpretation of $\exp\left\{-\int_0^T \phi(X_t)\,dt\right\}$ is that events of hazard rate ϕ has not occurred by time T

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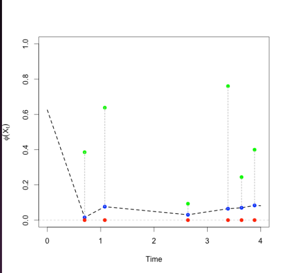
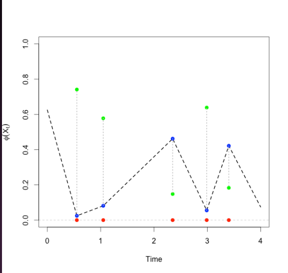


: Accepted Path



: Rejected Path

Figure: Skeleton of ϕ function in two cases

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5. Output the skeleton $((0, X_0), (u_1, X_{u_1}), ..., (T, X_T))$

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An Example

$$dX_t = \frac{1}{1 + X_t^2} dt + dB_t \quad 0 \leq t \leq T, X_0 = 0$$

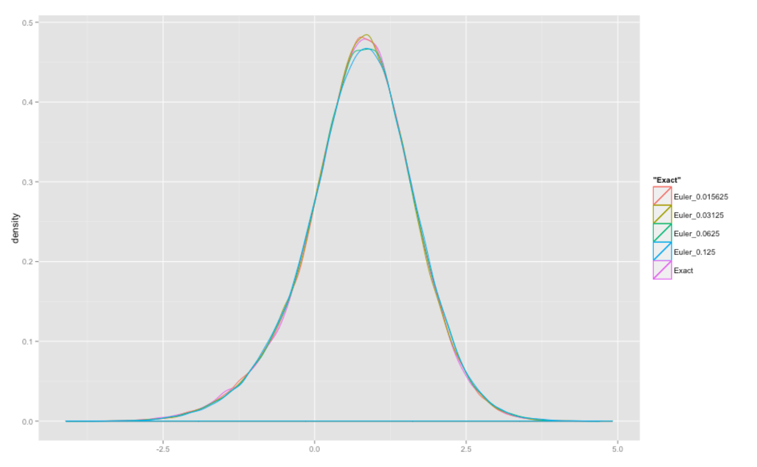

Figure: Exact vs Euler

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- Drawing from h is difficult.
- Can dropping $\{\pi(x)\}^{\frac{1}{2}}$ term help?

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Dacunha-Florens Lemma

Let P_t be the transition density of the diffusion defined by:

$$dX_t = \alpha(X_t) + \sigma dW_t$$

Denote $g = -\frac{1}{2}(\alpha^2 + \alpha')$ and suppose

- $|g(x)| = o(|x|^2) \quad \text{for} \quad |x| \to \infty$.
- $A(x) = \int_0^x \alpha(s) ds$.
- B_u be the standard Brownian Bridge
- $z_u(x, y) = (1-u)x + uy$ for $u \in [0, 1]$

then,

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then,

$$p_t(x, y) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp\left\{\frac{A(y) - A(x)}{\sigma^2} - \frac{(y-x)^2}{2\sigma^2 t}\right\} \times$$
$$\mathbb{E} \exp\left\{\sigma^2 t \int_0^1 g(z_u(x, y) + \sqrt{\sigma^2 t} B_u) du\right\}$$

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Transition Density [1]

Applying,

- $\sigma = 1$
- Transformation $\sqrt{\sigma^2 t}\, B_u = X_{tu} - x - u(X_t - x)$

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$$p_t(x|x_0) = \frac{1}{\sqrt{2\pi t}} \exp\left\{-\frac{(x-x_0)^2}{2t}\right\} \exp\left\{A(x) - A(x_0)\right\} \times$$
$$\mathbb{E}_{x_0,x}\left(\exp\left\{-\int_0^t \frac{(\alpha(X_s)^2 + \alpha'(X_s))}{2}\, ds\right\}\right)$$

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- Transformation $\sqrt{\sigma^2 t}\, B_u = X_{tu} - x - u(X_t - x)$

$$p_t(x|x_0) = \frac{1}{\sqrt{2\pi t}} \exp\left\{-\frac{(x-x_0)^2}{2t}\right\} \exp\left\{A(x) - A(x_0)\right\} \times \mathbb{E}_{x_0,x}\left(\exp\left\{-\int_0^t \frac{(\alpha(X_s)^2 + \alpha'(X_s))}{2} ds\right\}\right)$$

$$p_t(x|0) \propto \exp\left\{-\frac{(x)^2}{2t}\right\} \exp\left\{A(x)\right\} \mathbb{E}_{x_0,x}\left(\exp\left\{-\int_0^t \underbrace{\frac{((\alpha(X_s)^2 + \alpha'(X_s))}{2} - l}_{\phi(X_s)} ds\right\}\right)$$

$l := \inf_x \frac{\alpha^2+\alpha'}{2}(x)$

[1] Pollock, M. (2013). Some monte carlo methods for jump diffusions (phd thesis)

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Quasi-Stationary π

$$p_t(x|x_0=0) \propto \overbrace{\exp\left\{-\frac{x^2}{2t}\right\}\exp\{A(x)\}}^{\propto h}\,\overbrace{\mathbb{E}_{x_0,x}\left(\exp\left\{-\int_0^t \phi(X_s)\,ds\right\}\right)}^{(II)}$$

$$\propto \exp\left\{-\frac{x^2}{2t}\right\}\{\pi(x)\}^{\frac{1}{2}}\,\mathbb{E}_{x_0,x}\left(\exp\left\{-\int_0^t \phi(X_s)\,ds\right\}\right) \longrightarrow \pi(x)$$

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- $\exp\left\{-\frac{x^2}{2t}\right\}$ suggests to start simulating according to Brownian motion.
- Need to construct the events of probability $\exp\left\{-\int_0^t \phi(X_t)\,dt\right\}$

[1] Roberts, G. et al. (2015). Towards not being afraid of the big bad data set

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Poisson Thinning revisited

Coloring Scheme [1]

Let $\tau_1, \ldots, \tau_k$ be the Poisson Process with rate M where M is such that $\sup_x \phi(x) \leq M$. Let $X_{\tau_1}, \ldots, X_{\tau_k}$ be the realised skeleton of process $\{X_t : t \geq 0\}$ at times $\tau_1, \ldots, \tau_k$. If process is killed at τ_j with probability $\frac{\phi(X_{\tau_j})}{M}$. Then,

$$\mathbb{P}(\text{Process survived until time } t) = \exp\left\{ -\int_0^t \phi(X_t)\, dt \right\}$$

- Suggests to simulate $\tau_1, \ldots, \tau_k$ from homogeneous Poisson Process of rate M and decide to kill the process at time of event τ_j with probability $\frac{\phi(X_{\tau_j})}{M}$.

[1] Kingman, J. F. (1993). *Poisson Processes.* Clarendon Press, Oxford

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Quasi Stationary distribution

How do we sample from QSD?

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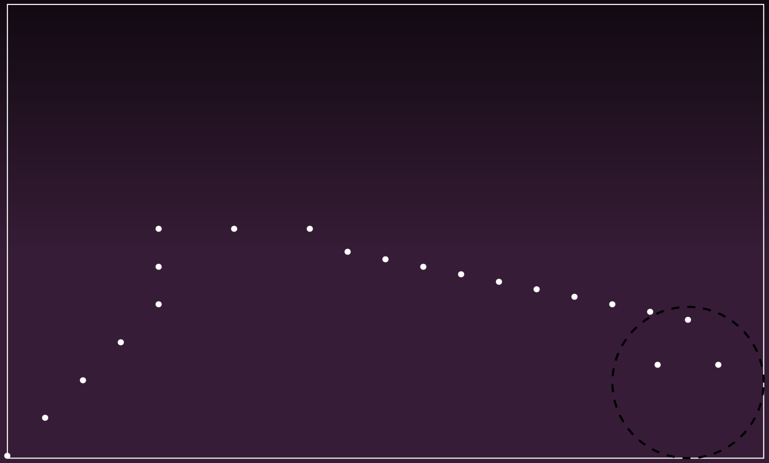
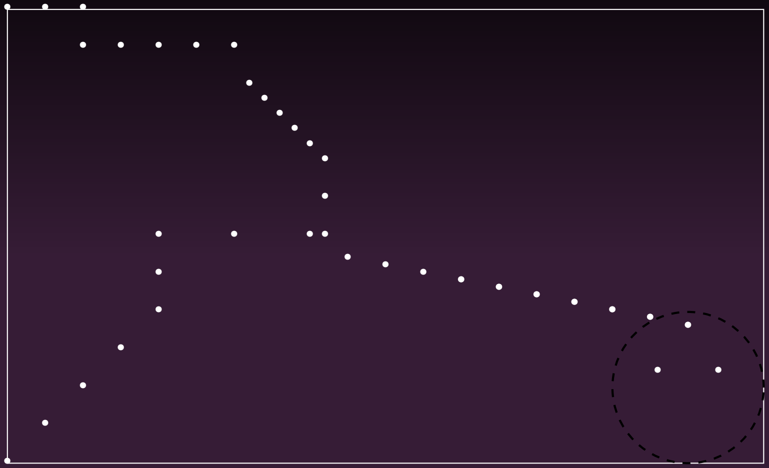
Quasi Stationary distribution



How do we sample from QSD?

Quasi Stationary distribution



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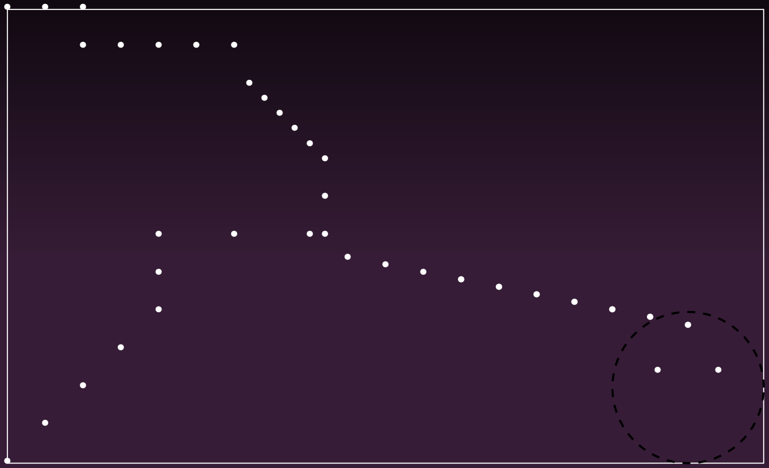

How do we sample from QSD?

An Example [1]

- Suppose we have **K BINS** (One for each non-absorbing state) and **1 TRAP**!

[1] Glynn, P. et al. (2014). Analysis of a stochastic aproximation algorithm for computing quasi-stationary distributions

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- If K=2 and there are 5 balls in Bin-1 and 4 in Bin-2 then

$$P(State - 1) = \frac{5}{9} \quad P(State - 2) = \frac{4}{9}$$

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- Run first tour of the chain until absorption.
- During the tour State-1 is visited 3 times and state-2 is visited 2 times.

$$P(State-1) = \frac{8}{14} \quad P(State-2) = \frac{6}{14}$$

[1] Glynn, P. et al. (2014). Analysis of a stochastic aproximation algorithm for computing quasi-stationary distributions

Physicist's Heuristic [1]

- R— transition rate matrix.

[1]Oliveira, M. d. and Dickamn, R. (2008). How to simulate the quasi-stationary state

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$$\pi_j := \lim_{t \to \infty} \frac{p_{0,t}(i,j)}{p_{0,t}(i,k)} \tag{5}$$

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$$\frac{d}{dt}(p_{0,t}(i,j)) = \sum_{l} p_{0,t}(i,l) R(l,j)$$

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Approximating Quasi-Stationary distribution

- $\pi_j p_{0,t}(i, k) \approx p_{0,t}(i, j)$ for large enough t.

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$$= -\sum_l \pi_l\, p_{0,t}(i,k) R(l,d) \tag{10}$$

- Multiply (10) by π_j and subtract from (8) to get,

$$\sum_l \pi_l\, R(l,j) + \pi_j \left(\sum_l \pi_l\, R(l,d) \right) = \frac{d}{dt}(\pi_j) \tag{11}$$

Algorithm for Quasi-Stationary distribution

$$\frac{d}{dt}(\pi_j) = \underbrace{\sum_l \pi_l R(l,j)}_{\text{Forward part}} + \underbrace{\pi_j \left(\sum_l \pi_l R(l,d) \right)}_{\text{Redeposited Probability}}$$

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Algorithm 5.3: *a* Estimating Quasi-Stationary distribution (π)

1. Begin the chain in transient state.
2. Simulate the chain normally.
3. If the chain hits the absorbing state, re-sample the starting position using the empirical estimate of the quasi-stationary distribution up until that point and then **GOTO** 2.

---

*a*Glynn, P. et al. (2006). Empirical analysis of a stochastic aproximation algorithm for computing quasi-stationary distributions

The idea of proof [1]

- π^n: sequence of probability vectors over the transient states. Stores cumulative empirical distribution until n-th iteration.

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- π^n: sequence of probability vectors over the transient states. Stores cumulative empirical distribution until n-th iteration.
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- $\tau^{(n)} = \min\{k \geq 0 : X_k^{(n)}$ is not in transient state$\}$. Time to absorption in n-th iteration.

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$$\pi_j^{n+1} = \frac{\left(\sum_{k=0}^{n} \tau^{(k)}\right) \pi_j^n + \sum_{k=0}^{\tau^{(n+1)}-1} \mathbb{I}(X_k^{(n+1)} = j | X_0^{(n+1)} \sim \pi^n)}{\sum_{k=0}^{n+1} \tau^{(k)}}$$

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ReScaLE Algorithm

Algorithm 5.4: ReScaLE Algorithm(α, x_0)

1. $l \leftarrow \inf_{x \in \mathbb{R}} \frac{\alpha^2 + \alpha'}{2}, \phi \leftarrow \frac{\alpha^2 + \alpha'}{2} - l, M \leftarrow \sup_{x \in \mathbb{R}} \phi(x)$
2. $t_0 \leftarrow 0; X_{t_0} \leftarrow x_0$
3. **do** $\begin{cases} (t_1, t_2, \ldots) \sim \text{Poisson Process of rate } M \text{ starting at } t_0 \\ (X_{t_1}, X_{t_2}, \ldots) \sim \text{Brownian Motion started at position } X_{t_0} \\ \text{Kill the process at } X_{t_i} \text{ with probability } \phi(X_{t_i})/M \\ \textbf{exit} \text{ once it kills} \end{cases}$
4. starting time $\sim U[0, \text{Time of Kill}]$
5. starting value $\sim$ Brownian Bridge
6. **GOTO** 2. with $t_0 \leftarrow$ starting time ; $X_{t_0} \leftarrow$ starting value

return $((X_{t_1}, X_{t_2}, \ldots))$

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Illustration of ReScaLE

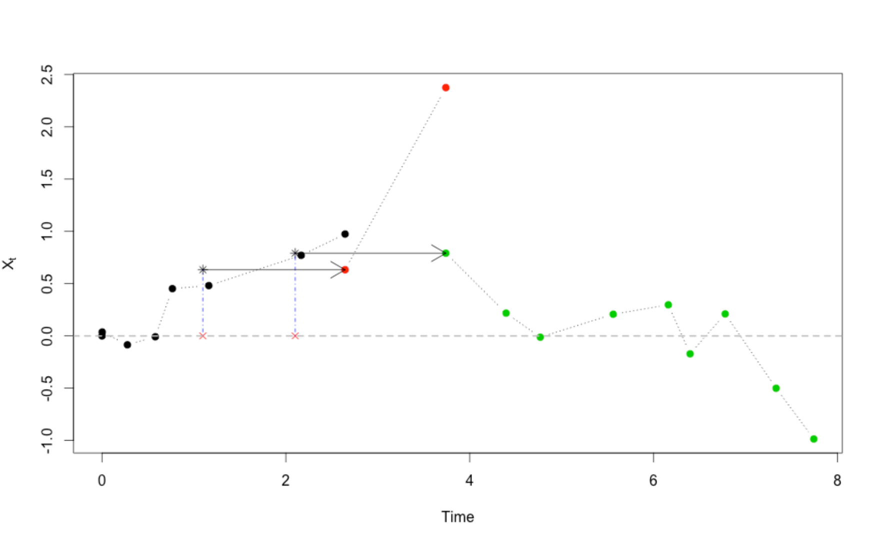
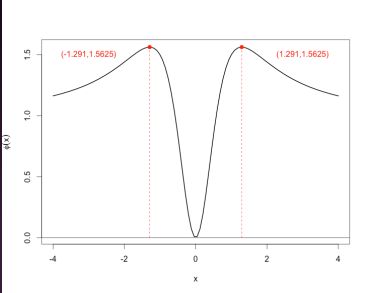
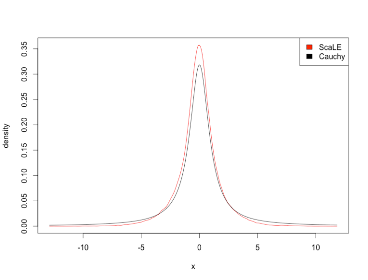


Figure: A run of ReScaLE

An Example



: $\phi-$ function



: Density Comparison

Figure: Implementation of ReScaLE algorithm to Cauchy density

Summary

- Exact method to simulate from diffusion.

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Further Work:

- Adaptive version of ReScaLE!
- Parallel Execution and its theory.
- Optimal version and its rate of convergence.

Thanks!