Exact simulation of diffusions with a finite boundary

Paul A. Jenkins

Departments of Statistics
University of Warwick

Statistics seminar, University of Bristol
26 Sep 2014

Joint work with Dario Spanò

Outline

Why are diffusions important?

Diffusion models crop up all over the place in scientific modelling:

- Molecular models of interacting particles
- Stock prices in perfect financial markets
- Communications systems with noise
- Neurophysiological activities with disturbances
- Ecological modelling
- Population genetics
- Fluid flows
- Queueing and network theory
- Learning theory

$\vdots$

Why are diffusions important?

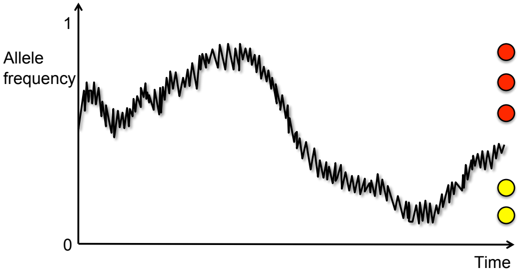
Diffusion models crop up all over the place in scientific modelling:

- Molecular models of interacting particles
- Stock prices in perfect financial markets
- Communications systems with noise
- Neurophysiological activities with disturbances
- Ecological modelling
- Population genetics
- Fluid flows
- Queueing and network theory
- Learning theory

  ⋮

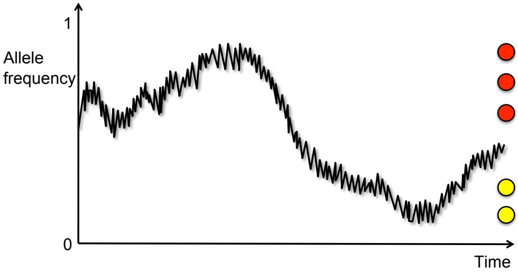
Diffusion model

The time-evolution of a genetic variant, or allele, is well approximated by a diffusion process on the interval [0, 1].



Diffusion model

The time-evolution of a genetic variant, or allele, is well approximated by a diffusion process on the interval [0, 1].



Wright-Fisher SDE

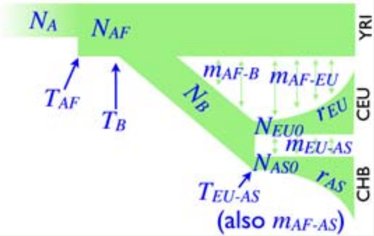
$$dX_t = \mu_\theta(X_t)dt + \sqrt{X_t(1 - X_t)}dW_t, \qquad X_0 = x, \quad t \geq 0.$$

The infinitesimal drift, $\mu_\theta(x)$, encapsulates directional forces such as natural selection, migration, mutation, ...

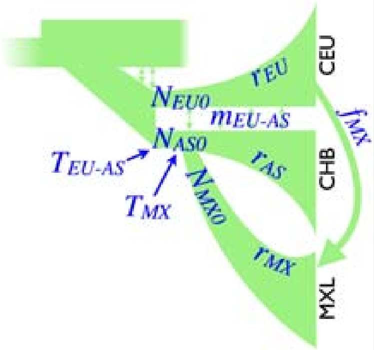
Population genetic Motivation I: Demographic inference

Given a sample of DNA sequences obtained in the present-day, what can we infer about the demographic history of the population?

Example (Gutenkunst *et al.*, 2009)



Expansion out-of-Africa

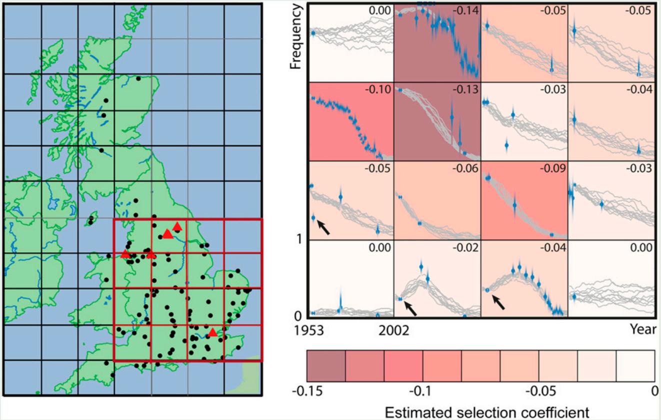


Settlement of the New World

Population genetic Motivation II: Time-series analysis of selection

Given a sample of genetic data obtained over several generations, what can we infer about the strength of natural selection?

Example (*Biston betulaeria*; Mathieson & McVean, 2013)



Inference from diffusion processes

- Like many interesting diffusions, the transition function of the Wright-Fisher diffusion is unknown.

Inference from diffusion processes

- Like many interesting diffusions, the transition function of the Wright-Fisher diffusion is unknown.
- Inference typically proceeds by
  1. Model-discretization such as an Euler approximation:

$$X_{t+dt} \mid (X_t = z) \sim \mathcal{N}(\mu_\theta(z)dt, \sigma^2(z)dt),$$

  2. ...followed by (sequential) Monte Carlo simulation (or numerical solution of Kolmogorov PDEs, or spectral expansions, ...)

Inference from diffusion processes

- Like many interesting diffusions, the transition function of the Wright-Fisher diffusion is unknown.
- Inference typically proceeds by
  1. Model-discretization such as an Euler approximation:
     $$X_{t+dt} \mid (X_t = z) \sim \mathcal{N}(\mu_\theta(z)dt, \sigma^2(z)dt),$$
  2. ...followed by (sequential) Monte Carlo simulation (or numerical solution of Kolmogorov PDEs, or spectral expansions, ...)
- But—discretization introduces a bias we would like to remove.

Inference from diffusion processes

- Like many interesting diffusions, the transition function of the Wright-Fisher diffusion is unknown.
- Inference typically proceeds by
  1. Model-discretization such as an Euler approximation:

$$X_{t+dt} \mid (X_t = z) \sim \mathcal{N}(\mu_\theta(z)dt, \sigma^2(z)dt),$$

  2. ...followed by (sequential) Monte Carlo simulation (or numerical solution of Kolmogorov PDEs, or spectral expansions, ...)
- But—discretization introduces a bias we would like to remove.

Inference from diffusion processes

- Like many interesting diffusions, the transition function of the Wright-Fisher diffusion is unknown.
- Inference typically proceeds by
  1. Model-discretization such as an Euler approximation:

$$X_{t+dt} \mid (X_t = z) \sim \mathcal{N}(\mu_\theta(z)dt, \sigma^2(z)dt),$$

  2. ...followed by (sequential) Monte Carlo simulation (or numerical solution of Kolmogorov PDEs, or spectral expansions, ...)
- But—discretization introduces a bias we would like to remove.

Three sentence summary

- There exist so-called exact algorithms for simulating diffusions without discretization error, even if the transition density is unknown.
- They can perform poorly when there are entrance boundaries.
- I will outline how to fix these problems.

Outline

Exact algorithm (EA)—one-dimensional bridge version

Goal: return exact bridge samples from the one-dimensional diffusion $X = (X_t : t \geq 0)$ on $\mathbb{R}$ satisfying

$$dX_t = \mu_\theta(X_t)dt + \sigma(X_t)dW_t, \qquad X_0 = x, \quad 0 \leq t \leq T.$$

Exact algorithm (EA)—one-dimensional bridge version

Goal: return exact bridge samples from the one-dimensional diffusion $X = (X_t : t \geq 0)$ on $\mathbb{R}$ satisfying

$$dX_t = \mu_\theta(X_t)dt + \sigma(X_t)dW_t, \qquad X_0 = x, \quad 0 \leq t \leq T.$$

1. Reduce the problem to unit diffusion coefficient via the Lamperti transform $X_t \mapsto Y_t$:

$$Y_t := \int^{X_t} \frac{1}{\sigma(u)} du,$$

so now we work with

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dW_t, \qquad Y_0 = y, \quad 0 \leq t \leq T.}$$

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dB_t, \qquad Y_0 = y, \quad 0 \leq t \leq T.}$$

Exact algorithm (EA)

2. Now we can consider a rejection algorithm using Brownian bridge paths as candidates.

   If $\mathbb{Q}_y$ is the target law (of Y) and $\mathbb{W}_y$ is the law of a Brownian motion then we need

$$\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y)$$

   to provide the rejection probability

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dB_t, \qquad Y_0 = y, \quad 0 \le t \le T.}$$

Exact algorithm (EA)

2. Now we can consider a rejection algorithm using Brownian bridge paths as candidates.

   If $\mathbb{Q}_y$ is the target law (of Y) and $\mathbb{W}_y$ is the law of a Brownian motion then we need

$$\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) = \exp\left\{\int_0^T \alpha_\theta(Y_t)dY_t - \frac{1}{2}\int_0^T \alpha_\theta^2(Y_t)dt\right\}$$

   to provide the rejection probability, by the Girsanov theorem.

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dB_t, \qquad Y_0 = y, \quad 0 \le t \le T.}$$

Exact algorithm (EA)

2. Now we can consider a rejection algorithm using Brownian bridge paths as candidates.

   If $\mathbb{Q}_y$ is the target law (of Y) and $\mathbb{W}_y$ is the law of a Brownian motion then we need

$$\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) = \exp\left\{\int_0^T \alpha_\theta(Y_t)dY_t - \frac{1}{2}\int_0^T \alpha_\theta^2(Y_t)dt\right\}$$

   to provide the rejection probability, by the Girsanov theorem.

- Such a rejection algorithm is impossible: it requires simulation of complete (infinite-dimensional) Brownian sample paths!

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dB_t, \qquad Y_0 = y, \quad 0 \le t \le T.}$$

Exact algorithm (EA)

3. Key observation: The Radon-Nikodým derivative can be put in the form

$$\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) \propto \exp\left\{-\int_0^T \phi(Y_s)ds\right\} \le 1,$$

where $\phi(\cdot) := \frac{1}{2}[\alpha_\theta^2(\cdot) + \alpha_\theta'(\cdot)] + C$.

$$\boxed{dY_t = \alpha_\theta(Y_t)dt + dB_t, \qquad Y_0 = y, \quad 0 \le t \le T.}$$

Exact algorithm (EA)

3. Key observation: The Radon-Nikodým derivative can be put in the form

$$\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) \propto \exp\left\{-\int_0^T \phi(Y_s)ds\right\} \le 1,$$

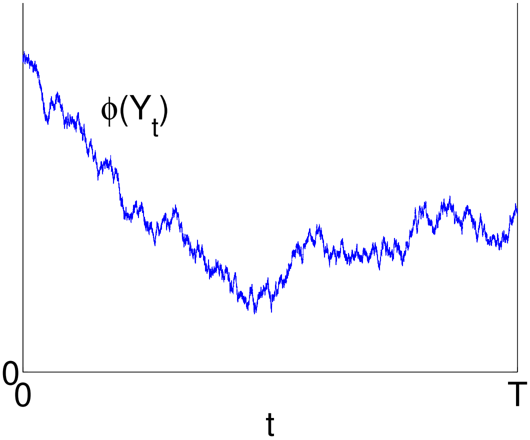
where $\phi(\cdot) := \frac{1}{2}[\alpha_\theta^2(\cdot) + \alpha_\theta'(\cdot)] + C$.

Assume we can arrange for $\phi \ge 0$. Then the right-hand side is the probability that a Poisson point process of unit rate on $[0, T] \times [0, \infty)$ has no points under the graph of $t \mapsto \phi(Y_s)$.

$$\boxed{\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) \propto \exp\left\{-\int_0^T \phi(Y_s)ds\right\} \leq 1.}$$

Exact algorithm (EA)

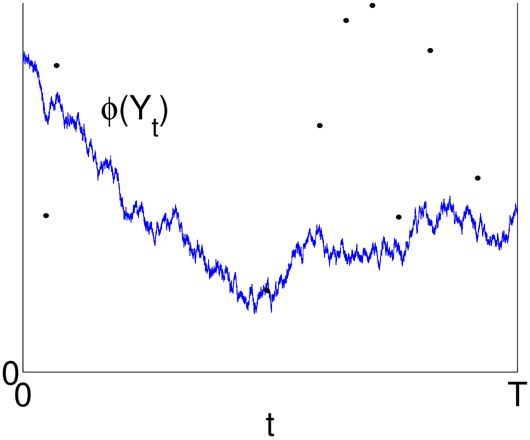
4. A proposed Brownian path should be rejected if a simulated Poisson point process has any points under its graph.



$$\boxed{\frac{d\mathbb{Q}_y}{d\mathbb{W}_y}(Y) \propto \exp\left\{-\int_0^T \phi(Y_s)ds\right\} \leq 1.}$$

Exact algorithm (EA)

4. A proposed Brownian path should be rejected if a simulated Poisson point process has any points under its graph.



Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0\leq t\leq T}$ from Y_0 to Y_T.

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0\leq t\leq T}$ from Y_0 to Y_T.
2. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0 \leq t \leq T}$ from Y_0 to Y_T.
2. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0 \le t \le T}$ from Y_0 to Y_T.
2. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

Problems

1. We still need an infinite-dimensional Brownian path.
2. The Poisson point process has unbounded intensity.

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0\leq t\leq T}$ from Y_0 to Y_T.
2. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

Problems

1. We still need an infinite-dimensional Brownian path.
2. The Poisson point process has unbounded intensity.

Solutions

1. Exploit retrospective sampling; switch the order of simulation!

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Brownian bridge $(Y_t)_{0\le t\le T}$ from Y_0 to Y_T.
2. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

Problems

1. We still need an infinite-dimensional Brownian path.
2. The Poisson point process has unbounded intensity.

Solutions

1. Exploit retrospective sampling; switch the order of simulation!

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
2. Simulate the Brownian bridge at the times of the Poisson points.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

Problems

1. We still need an infinite-dimensional Brownian path.
2. The Poisson point process has unbounded intensity.

Solutions

1. Exploit retrospective sampling; switch the order of simulation!

Retrospective sampling

Exact algorithm (EA) for simulating a bridge from Y_0 to Y_T

1. Simulate a Poisson point process of unit rate on $[0, T] \times [0, \infty)$.
2. Simulate the Brownian bridge at the times of the Poisson points.
3. Accept if all points are in the epigraph of $t \mapsto \phi(Y_t)$, otherwise return to 1.

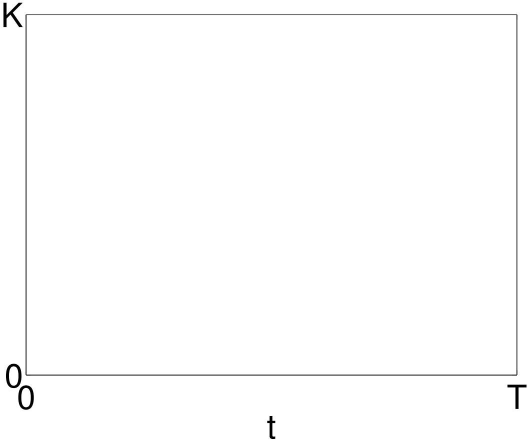
Problems

1. We still need an infinite-dimensional Brownian path.
2. The Poisson point process has unbounded intensity.

Solutions

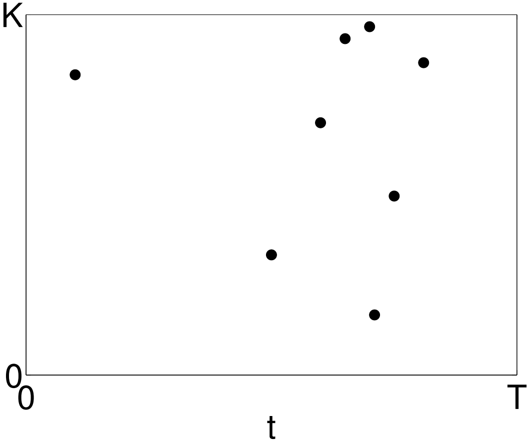
1. Exploit retrospective sampling; switch the order of simulation!
2. Assume ϕ is bounded, $\phi \leq K$ (for now), and use Poisson thinning (“EA1”).

Exact algorithm (EA1); Beskos & Roberts (2005)



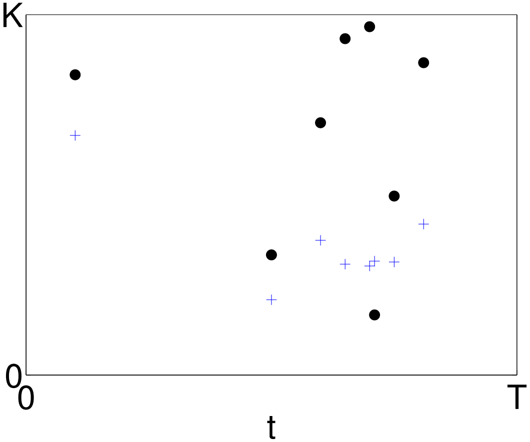
Exact algorithm (EA1); Beskos & Roberts (2005)

1. Simulate a Poisson point process on $[0, T] \times [0, K]$.



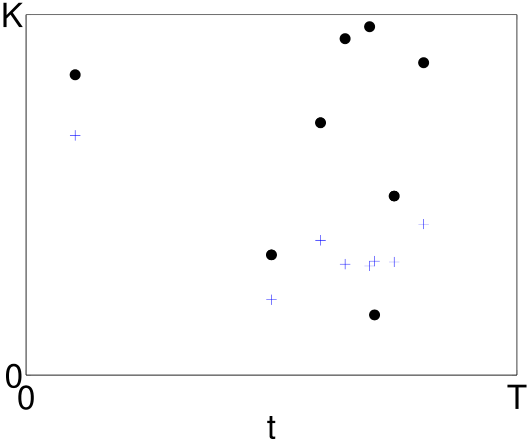
Exact algorithm (EA1); Beskos & Roberts (2005)

1. Simulate a Poisson point process on $[0, T] \times [0, K]$.
2. Simulate the Brownian bridge at the times of the Poisson points.



Exact algorithm (EA1); Beskos & Roberts (2005)

1. Simulate a Poisson point process on $[0, T] \times [0, K]$.
2. Simulate the Brownian bridge at the times of the Poisson points.
3. If any of the former are beneath any of the latter, return to 1.



Exact algorithm (EA)

- Output of the algorithm is a set of skeleton points of the bridge.
- Any further points can be filled in by further draws from the Brownian bridge—no further reference to the target law, $\mathbb{Q}_y$, is necessary!

Exact algorithm (EA)

- Output of the algorithm is a set of skeleton points of the bridge.
- Any further points can be filled in by further draws from the Brownian bridge—no further reference to the target law, $\mathbb{Q}_y$, is necessary!

$$\boxed{\phi(\cdot) = \frac{1}{2}[\alpha_\theta^2(\cdot) + \alpha'_\theta(\cdot)] + C.}$$

- There have been many further refinements to this algorithm (multidimensions, jumps, killing, reflection, . . .):
  Beskos *et al.* (2006, 2008, 2012), Casella & Roberts (2008, 2011), Chen & Huang (2013), Étoré & Martinez (2013), Giesecke & Smelov (2013), Gonçalves & Roberts (2013), Mousavi & Glynn (2013), Blanchet & Murthy (2014), Pollock *et al.* (2014).

Exact algorithm (EA)

- Output of the algorithm is a set of skeleton points of the bridge.
- Any further points can be filled in by further draws from the Brownian bridge—no further reference to the target law, $\mathbb{Q}_y$, is necessary!

$$\boxed{\phi(\cdot) = \frac{1}{2}[\alpha_\theta^2(\cdot) + \alpha_\theta'(\cdot)] + C.}$$

- There have been many further refinements to this algorithm (multidimensions, jumps, killing, reflection, ...):
  Beskos *et al.* (2006, 2008, 2012), Casella & Roberts (2008, 2011), Chen & Huang (2013), Étoré & Martinez (2013), Giesecke & Smelov (2013), Gonçalves & Roberts (2013), Mousavi & Glynn (2013), Blanchet & Murthy (2014), Pollock *et al.* (2014).
- In all cases the function ϕ is important.

Exact algorithm (EA)

- Output of the algorithm is a set of skeleton points of the bridge.
- Any further points can be filled in by further draws from the Brownian bridge—no further reference to the target law, $\mathbb{Q}_y$, is necessary!

$$\boxed{\phi(\cdot) = \frac{1}{2}[\alpha_\theta^2(\cdot) + \alpha_\theta'(\cdot)] + C.}$$

- There have been many further refinements to this algorithm (multidimensions, jumps, killing, reflection, ...):
  Beskos *et al.* (2006, 2008, 2012), Casella & Roberts (2008, 2011), Chen & Huang (2013), Étoré & Martinez (2013), Giesecke & Smelov (2013), Gonçalves & Roberts (2013), Mousavi & Glynn (2013), Blanchet & Murthy (2014), Pollock *et al.* (2014).
- In all cases the function ϕ is important.
- The assumption $\phi \leq K$ is restrictive, but it can in fact be relaxed ("EA2", Beskos *et al.*, 2006).

Exact algorithm 2 (EA2); Beskos *et al.* (2006)

- More realistic is that ϕ is well behaved in one direction:

$$\limsup_{u \to \infty} \phi(u) < \infty.$$

Exact algorithm 2 (EA2); Beskos *et al.* (2006)

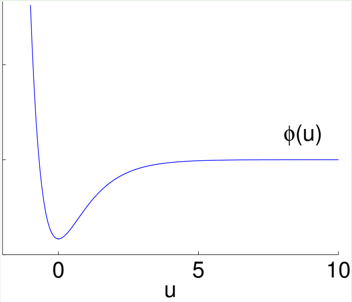
- More realistic is that ϕ is well behaved in one direction:

$$\limsup_{u\to\infty} \phi(u) < \infty.$$

Example: Logistic growth with noise (Beskos *et al.*, 2006)

$$dX_t = \theta X_t(1 - X_t)dt + X_t dB_t, \qquad X_0 = x > 0, \quad 0 \leq t \leq T.$$

- We find $\phi(u) = \theta^2 \left[\frac{1}{2}e^{-2u} - e^{-u}\right] + C$.



Exact algorithm 2 (EA2); Beskos *et al.* (2006)

- More realistic is that ϕ is well behaved in one direction:

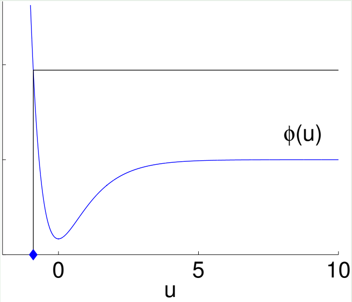
$$\limsup_{u\to\infty} \phi(u) < \infty.$$

Example: Logistic growth with noise (Beskos *et al.*, 2006)

$$dX_t = \theta X_t(1 - X_t)dt + X_t dB_t, \qquad X_0 = x > 0, \quad 0 \le t \le T.$$

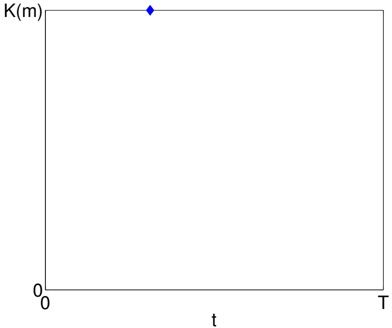
- We find $\phi(u) = \theta^2 \left[\frac{1}{2}e^{-2u} - e^{-u}\right] + C$.

- Idea: Simulate the minimum of $(Y_t)_{0\le t\le T}$ to get a path-specific bound on ϕ.



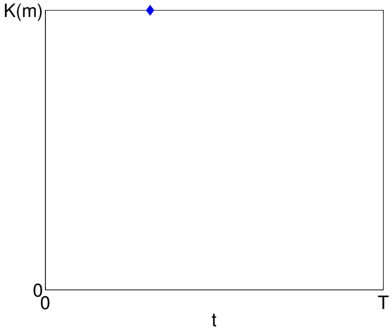
Exact algorithm 2 (EA2); Beskos *et al.* (2006)

1. Simulate the minimum m_T (and the time, t_m, it is attained) of a Brownian bridge from Y_0 to Y_T.



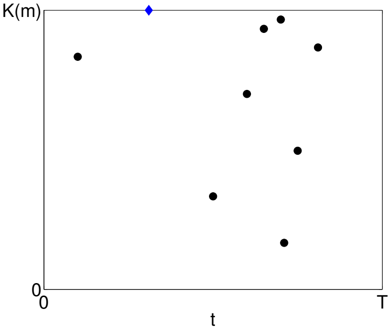
Exact algorithm 2 (EA2); Beskos *et al.* (2006)

1. Simulate the minimum m_T (and the time, t_m, it is attained) of a Brownian bridge from Y_0 to Y_T.
2. Find a bound $K(m_T)$ on $\phi(u)$ over the interval $[m_T, \infty)$.



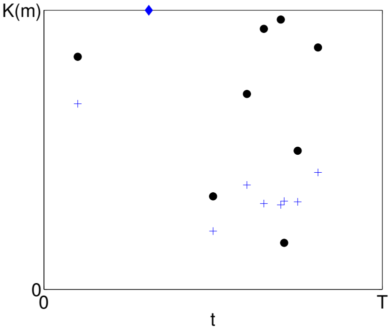
Exact algorithm 2 (EA2); Beskos *et al.* (2006)

1. Simulate the minimum m_T (and the time, t_m, it is attained) of a Brownian bridge from Y_0 to Y_T.
2. Find a bound $K(m_T)$ on $\phi(u)$ over the interval $[m_T, \infty)$.
3. Simulate a Poisson point process on $[0, T] \times [0, K(m_T)]$.



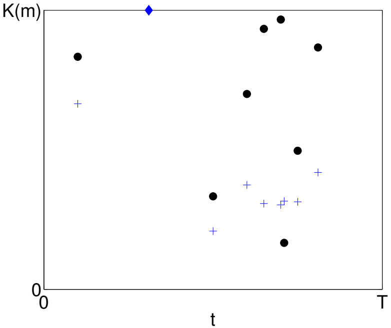
Exact algorithm 2 (EA2); Beskos *et al.* (2006)

1. Simulate the minimum m_T (and the time, t_m, it is attained) of a Brownian bridge from Y_0 to Y_T.
2. Find a bound $K(m_T)$ on $\phi(u)$ over the interval $[m_T, \infty)$.
3. Simulate a Poisson point process on $[0, T] \times [0, K(m_T)]$.
4. Simulate the Brownian bridge at the times of the Poisson points, conditioned on m_T and t_m.



Exact algorithm 2 (EA2); Beskos *et al.* (2006)

1. Simulate the minimum m_T (and the time, t_m, it is attained) of a Brownian bridge from Y_0 to Y_T.
2. Find a bound $K(m_T)$ on $\phi(u)$ over the interval $[m_T, \infty)$.
3. Simulate a Poisson point process on $[0, T] \times [0, K(m_T)]$.
4. Simulate the Brownian bridge at the times of the Poisson points, conditioned on m_T and t_m.
5. If any of the former are beneath any of the latter, return to 1.



Efficiency

- It is possible to relax assumptions on the size of ϕ entirely ("EA3"; Beskos *et al.*, 2008).
- The exact algorithms will be less efficient wherever $\phi(X_t)$ is very large—unavoidable when the diffusion travels through a region where the drift (or its derivative) is very large.

Efficiency

- It is possible to relax assumptions on the size of ϕ entirely ("EA3"; Beskos *et al.*, 2008).
- The exact algorithms will be less efficient wherever $\phi(X_t)$ is very large—unavoidable when the diffusion travels through a region where the drift (or its derivative) is very large.

Example: Entrance boundary at 0

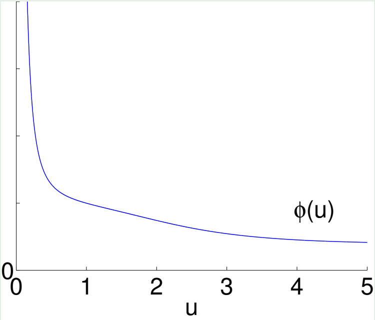
- "A diffusion at x will almost surely not hit 0 before hitting any $b > x$.
  A diffusion started at 0 will enter $(0, \infty)$ in finite time."
- If $\sigma^2(x) = 1$, then ϕ explodes at the boundary.

Efficiency

- It is possible to relax assumptions on the size of ϕ entirely ("EA3"; Beskos *et al.*, 2008).
- The exact algorithms will be less efficient wherever $\phi(X_t)$ is very large—unavoidable when the diffusion travels through a region where the drift (or its derivative) is very large.

Example: Entrance boundary at 0

- "A diffusion at x will almost surely not hit 0 before hitting any $b > x$. A diffusion started at 0 will enter $(0, \infty)$ in finite time."
- If $\sigma^2(x) = 1$, then ϕ explodes at the boundary.

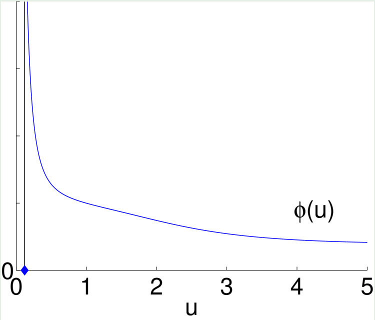


Efficiency

- It is possible to relax assumptions on the size of ϕ entirely ("EA3"; Beskos *et al.*, 2008).
- The exact algorithms will be less efficient wherever $\phi(X_t)$ is very large—unavoidable when the diffusion travels through a region where the drift (or its derivative) is very large.

Example: Entrance boundary at 0

- "A diffusion at x will almost surely not hit 0 before hitting any $b > x$.
  A diffusion started at 0 will enter $(0, \infty)$ in finite time."
- If $\sigma^2(x) = 1$, then ϕ explodes at the boundary.



- Large ϕ is a symptom of a poor likelihood ratio, i.e. Brownian motion is a poor mimic of the target diffusion.

- Large ϕ is a symptom of a poor likelihood ratio, i.e. Brownian motion is a poor mimic of the target diffusion.
- Idea: Replace Brownian motion with a different candidate process—one with an entrance boundary.

- Large ϕ is a symptom of a poor likelihood ratio, i.e. Brownian motion is a poor mimic of the target diffusion.
- Idea: Replace Brownian motion with a different candidate process—one with an entrance boundary.
- But: the exact algorithms rely heavily on our knowledge about Brownian bridges:
    - The distribution of bridge coordinates.
    - The distribution of the minimum, m_T, and its time, t_m.
    - The distribution of bridge coordinates conditioned on (m_T, t_m).
    - The ability to sample from these distributions *exactly*.

- Large ϕ is a symptom of a poor likelihood ratio, i.e. Brownian motion is a poor mimic of the target diffusion.
- Idea: Replace Brownian motion with a different candidate process—one with an entrance boundary.
- But: the exact algorithms rely heavily on our knowledge about Brownian bridges:
  - The distribution of bridge coordinates.
  - The distribution of the minimum, m_T, and its time, t_m.
  - The distribution of bridge coordinates conditioned on (m_T, t_m).
  - The ability to sample from these distributions *exactly*.

- Large ϕ is a symptom of a poor likelihood ratio, i.e. Brownian motion is a poor mimic of the target diffusion.
- Idea: Replace Brownian motion with a different candidate process—one with an entrance boundary.
- But: the exact algorithms rely heavily on our knowledge about Brownian bridges:
  - The distribution of bridge coordinates.
  - The distribution of the minimum, m_T, and its time, t_m.
  - The distribution of bridge coordinates conditioned on (m_T, t_m).
  - The ability to sample from these distributions *exactly*.

Question. Does there exist a diffusion:

- with infinitesimal variance equal to 1,
- with an entrance boundary, and such that
- the finite-dimensional distributions of its bridges are known, and
- which can be simulated exactly, and
- (bonus) whose extrema are well characterized?

Outline

Bessel process

- Infinitesimal variance 1?
- Entrance boundary?
- Finite-dimensional distributions?
- Exact simulation?
- Distributions of extrema?

✓ Drift $\beta(y) = (\delta - 1)/(2y)$, variance $\sigma^2(y) = 1$.

Bessel process

- Infinitesimal variance 1?
- Entrance boundary?
- Finite-dimensional distributions?
- Exact simulation?
- Distributions of extrema?

✓ Drift $\beta(y) = (\delta - 1)/(2y)$, variance $\sigma^2(y) = 1$.

✓ Zero is an entrance boundary when $\delta \geq 2$.

Bessel process

- Infinitesimal variance 1?
  ✓ Drift $\beta(y) = (\delta - 1)/(2y)$, variance $\sigma^2(y) = 1$.
- Entrance boundary?
  ✓ Zero is an entrance boundary when $\delta \geq 2$.
- Finite-dimensional distributions?
  ✓ $p_{(y,0)\to(z,T)}(x;t) =$
  $$\frac{T}{2t(T-t)} e^{-\left(\frac{z(T-t)}{2tT} + \frac{xT}{2t(T-t)} + \frac{yt}{2T(T-t)}\right)} \frac{I_\nu\left(\frac{\sqrt{xz}}{t}\right) I_\nu\left(\frac{\sqrt{xy}}{(T-t)^2}\right)}{I_\nu\left(\frac{\sqrt{yz}}{T^2}\right)},$$
  where $\nu = 2(\delta + 1)$, is the transition density of the (squared) Bessel bridge.
- Exact simulation?
- Distributions of extrema?

Bessel process

- Infinitesimal variance 1?
- Entrance boundary?
- Finite-dimensional distributions?
- Exact simulation?
- Distributions of extrema?

✓ Drift $\beta(y) = (\delta - 1)/(2y)$, variance $\sigma^2(y) = 1$.

✓ Zero is an entrance boundary when $\delta \geq 2$.

✓ $p_{(y,0)\to(z,T)}(x;t) =$

$$\frac{T}{2t(T-t)} e^{-\left(\frac{z(T-t)}{2tT} + \frac{xT}{2t(T-t)} + \frac{yt}{2T(T-t)}\right)} \frac{I_\nu(\frac{\sqrt{xz}}{t}) I_\nu(\frac{\sqrt{xy}}{(T-t)^2})}{I_\nu(\frac{\sqrt{yz}}{T^2})},$$

where $\nu = 2(\delta + 1)$, is the transition density of the (squared) Bessel bridge.

✓ $\delta \in \mathbb{Z}_{\geq 0}$: radial part of a δ-dimensional Brownian motion.
$\delta \in \mathbb{R}_{\geq 0}$: See Makarov & Glew (2010).

Bessel process

- Infinitesimal variance 1? ✓ Drift $\beta(y) = (\delta - 1)/(2y)$, variance $\sigma^2(y) = 1$.
- Entrance boundary? ✓ Zero is an entrance boundary when $\delta \geq 2$.
- Finite-dimensional distributions? ✓ $p_{(y,0)\to(z,T)}(x;t) =$

$$\frac{T}{2t(T-t)} e^{-\left(\frac{z(T-t)}{2tT} + \frac{xT}{2t(T-t)} + \frac{yt}{2T(T-t)}\right)} \frac{I_\nu(\frac{\sqrt{xz}}{t}) I_\nu(\frac{\sqrt{xy}}{(T-t)^2})}{I_\nu(\frac{\sqrt{yz}}{T^2})},$$

  where $\nu = 2(\delta + 1)$, is the transition density of the (squared) Bessel bridge.
- Exact simulation? ✓ $\delta \in \mathbb{Z}_{\geq 0}$: radial part of a δ-dimensional Brownian motion. $\delta \in \mathbb{R}_{\geq 0}$: See Makarov & Glew (2010).
- Distributions of extrema? (✓) Partly.

Bessel-EA

- Exact simulation from a diffusion with law $\mathbb{Q}_y$ using the Bessel process (law $\mathbb{B}_y^\delta \gg \mathbb{Q}_y$) is possible by the following:

Theorem.

Under regularity conditions (similar to EA), $\mathbb{Q}_y$ is the marginal distribution of Y when

$$(Y, \Phi) \sim (\mathbb{B}_y^\delta \otimes \mathbb{PPP}) \Big| \left\{ \Phi \subseteq \text{epigraph} \left[\widetilde{\phi}(Y) \right] \right\},$$

where $\mathbb{PPP}$ is the law of a Poisson point process Φ of unit rate on $[0, T] \times [0, \infty)$,and

$$\widetilde{\phi}(u) := \frac{1}{2}[\alpha_\theta^2(u) - \beta^2(u) + \alpha'_\theta(u) - \beta'(u)] + C.$$

Outline of proof.

Similar to the Brownian case: regularity conditions permit a Girsanov transformation and rearrangement so that

$$\frac{d\mathbb{Q}_y}{d\mathbb{B}_y^\delta}(Y) \propto \exp\left\{-\int_0^T \widetilde{\phi}(Y_t)dt\right\} \leq 1,$$

provides the rejection probability for sampling from the conditional law

$$(\mathbb{B}_y^\delta \otimes \mathbb{L})\Big| \left\{\Phi \subseteq \text{epigraph}\left[\widetilde{\phi}(Y)\right]\right\}. \quad \square$$

Outline of proof.

Similar to the Brownian case: regularity conditions permit a Girsanov transformation and rearrangement so that

$$\frac{d\mathbb{Q}_y}{d\mathbb{B}^\delta_y}(Y) \propto \exp\left\{-\int_0^T \widetilde{\phi}(Y_t)dt\right\} \leq 1,$$

provides the rejection probability for sampling from the conditional law

$$(\mathbb{B}^\delta_y \otimes \mathbb{L})\Big| \left\{\Phi \subseteq \text{epigraph}\left[\widetilde{\phi}(Y)\right]\right\}. \quad \square$$

So what?

- We have just replaced one candidate process for another, the only substantial difference the appearance of

$$\widetilde{\phi}(u) := \frac{1}{2}[\alpha^2_\theta(u) - \beta^2(u) + \alpha'_\theta(u) - \beta'(u)] + C.$$

instead of

$$\phi(u) := \frac{1}{2}[\alpha^2_\theta(u) + \alpha'_\theta(u)] + C.$$

Example: A population growth model.

- A diffusion $(X_t)_{0\leq t\leq T}$ with drift and diffusion coefficients

$$\mu(x) = \kappa x, \qquad \sigma^2(x) = x + \omega x^2,$$

commenced from $X_0 = x_0$ and grown to $X_T = x_T$.

Example: A population growth model.

- A diffusion $(X_t)_{0 \leq t \leq T}$ with drift and diffusion coefficients

$$\mu(x) = \kappa x, \qquad \sigma^2(x) = x + \omega x^2,$$

  commenced from $X_0 = x_0$ and grown to $X_T = x_T$.
- The population has not died out, so we can condition the process on non-absorption at 0.

Example: A population growth model.

- A diffusion $(X_t)_{0\leq t\leq T}$ with drift and diffusion coefficients

$$\mu(x) = \kappa x, \qquad \sigma^2(x) = x + \omega x^2,$$

commenced from $X_0 = x_0$ and grown to $X_T = x_T$.

- The population has not died out, so we can condition the process on non-absorption at 0.
- Conditioning and Lamperti transforming leads to new drift

$$\alpha(y) = \frac{\kappa}{\sqrt{\omega}} \tanh\left[\frac{\sqrt{\omega}y}{2}\right] - \frac{\sqrt{\omega}}{2} \coth\left[\sqrt{\omega}y\right] + \frac{\omega - 2\kappa}{\sqrt{w}} \frac{\tanh\left[\frac{\sqrt{\omega}y}{2}\right]}{1 - \cosh^{\frac{4\kappa}{\omega}-2}\left[\frac{\sqrt{\omega}y}{2}\right]},$$

with an entrance boundary at 0.

Example: A population growth model.

- What does the drift look like at the boundary?

$$\alpha(y) = \frac{3}{2y} + O(y) \qquad \text{as } y \to 0.$$

Example: A population growth model.

- What does the drift look like at the boundary?

$$\alpha(y) = \frac{3}{2y} + O(y) \qquad \text{as } y \to 0.$$

- Compare with the Bessel process: $$\beta(y) = \frac{\delta - 1}{2y}.$$

  So we should choose $\delta = 4$ for our candidate process.

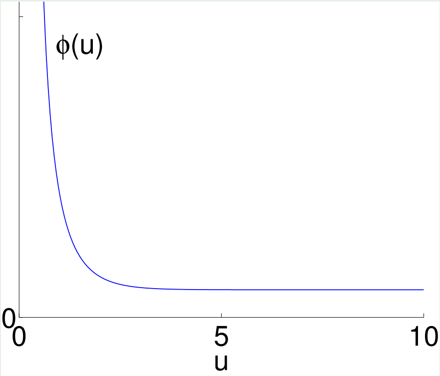
Example: A population growth model.

- What does the drift look like at the boundary?

$$\alpha(y) = \frac{3}{2y} + O(y) \qquad \text{as } y \to 0.$$

- Compare with the Bessel process: $\beta(y) = \dfrac{\delta - 1}{2y}$.

  So we should choose $\delta = 4$ for our candidate process.



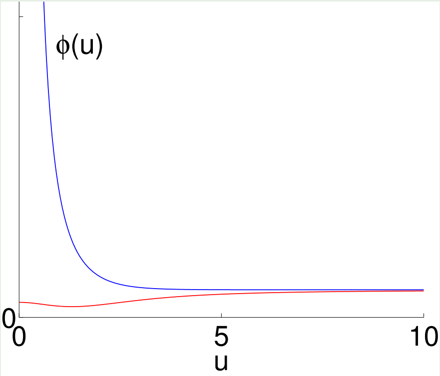
Example: A population growth model.

- What does the drift look like at the boundary?

$$\alpha(y) = \frac{3}{2y} + O(y) \qquad \text{as } y \to 0.$$

- Compare with the Bessel process: $\beta(y) = \frac{\delta - 1}{2y}$.

  So we should choose $\delta = 4$ for our candidate process.



Example: A population growth model.

- $\widetilde{\phi}$ is (tightly) bounded (by K say), while ϕ is unbounded as $y \to 0$.

Example: A population growth model.

- $\widetilde{\phi}$ is (tightly) bounded (by K say), while ϕ is unbounded as $y \to 0$.
- Hence we can use the following Bessel-EA to return skeleton bridges:
  1. Simulate a Poisson point process on $[0, T] \times [0, K]$.
  2. Simulate a Bessel bridge of dimension $\delta = 4$ at the times of the Poisson points.
  3. If any of the former are beneath any of the latter, return to 1.

Results

Bessel-EA1 $Y_0 = y$ to $Y_{0.15} = 1$, $\omega = 3$.

κ	y	Attempts	Poisson points	Skeleton points	Random variables	Total Time (s)
1.0	10.0	1.1	0.2	0.2	1.9	0
1.0	1.0	1.0	0.2	0.2	1.9	0
1.0	0.25	1.0	0.2	0.2	2.0	0
1.0	0.15	1.0	0.2	0.2	2.0	1
1.0	0.1	1.1	0.2	0.2	2.0	1
1.0	0.025	1.0	0.2	0.2	2.0	0

Brownian-EA (“EA2”)

κ	y	Attempts	Poisson points	Skeleton points	Random variables	Total Time (s)
1.0	10.0	1.0	0.1	0.1	7.3	0
1.0	1.0	1.1	0.1	0.1	7.4	0
1.0	0.25	1.2	1288.6	420.6	3846.1	6
1.0	0.15	1.4	7531.1	617.4	16921.4	16
1.0	0.1	DNF	DNF	DNF	DNF	DNF
1.0	0.025	DNF	DNF	DNF	DNF	DNF

Results

Bessel-EA1 $Y_0 = y$ to $Y_{0.15} = 1$, $\omega = 3$.

κ	y	Attempts	Poisson points	Skeleton points	Random variables	Total Time (s)
10.0	10.0	5.2	14.1	6.8	56.4	1
10.0	1.0	3.0	7.9	4.9	36.4	1
10.0	0.25	2.3	6.1	4.4	30.8	1
10.0	0.15	2.2	6.0	4.3	30.3	0
10.0	0.1	2.2	5.9	4.4	30.4	0
10.0	0.025	2.1	5.8	4.3	29.6	1

Brownian-EA (“EA2”)

κ	y	Attempts	Poisson points	Skeleton points	Random variables	Total Time (s)
10.0	10.0	5.0	9.8	4.8	40.9	0
10.0	1.0	2.9	5.9	3.6	29.8	0
10.0	0.25	2.6	81.4	10.7	201.9	0
10.0	0.15	2.9	23052.1	1981.9	52056.9	52
10.0	0.1	DNF	DNF	DNF	DNF	DNF
10.0	0.025	DNF	DNF	DNF	DNF	DNF

When is the singularity in the drift at an entrance boundary matched by a Bessel process?

When is the singularity in the drift at an entrance boundary matched by a Bessel process?
Here's a partial answer.

Theorem.

Suppose we have a diffusion Y satisfying the requirements of EA1. Then the diffusion Y^* obtained by conditioning this process on $\{T_b < T_0\}$, can be simulated via Bessel-EA1 with $\delta = 3$.

When is the singularity in the drift at an entrance boundary matched by a Bessel process?
Here's a partial answer.

Theorem.

Suppose we have a diffusion Y satisfying the requirements of EA1. Then the diffusion Y^* obtained by conditioning this process on $\{T_b < T_0\}$, can be simulated via Bessel-EA1 with $\delta = 3$.

Outline of proof.

- Deduce regularity requirements for Bessel-EA1 from the assumptions of EA1.
- Compute the conditioned drift $\alpha^*(y)$ by bare hands, using a Doob h-transform.
- We find $\widetilde{\phi}^*(u)$ is bounded iff $\delta = 3$ (among all possible $\delta \geq 2$). □

Remarks

1. The previous result is perhaps not surprising given the well known observation:

A Brownian bridge conditioned to remain positive is a Bessel bridge of dimension $\delta = 3$.

Remarks

1. The previous result is perhaps not surprising given the well known observation:

A Brownian bridge conditioned to remain positive is a Bessel bridge of dimension $\delta = 3$.

2. The close relationship between Brownian bridges and Bessel(3) bridges is exploited in EA2—to simulate a Brownian bridge conditioned on its minimum (Beskos *et al.*, 2006).

Remarks

1. The previous result is perhaps not surprising given the well known observation:

> A Brownian bridge conditioned to remain positive is a Bessel bridge of dimension $\delta = 3$.

2. The close relationship between Brownian bridges and Bessel(3) bridges is exploited in EA2—to simulate a Brownian bridge conditioned on its minimum (Beskos *et al.*, 2006).
3. Hence, Bessel-EA1 and (Brownian)-EA2 are similar when applied to conditioned diffusions.

Remarks

1. The previous result is perhaps not surprising given the well known observation:

A Brownian bridge conditioned to remain positive is a Bessel bridge of dimension $\delta = 3$.

2. The close relationship between Brownian bridges and Bessel(3) bridges is exploited in EA2—to simulate a Brownian bridge conditioned on its minimum (Beskos *et al.*, 2006).
3. Hence, Bessel-EA1 and (Brownian)-EA2 are similar when applied to conditioned diffusions.
4. The theorem does not apply to the population growth example; an ‘extra’ $1/(2y)$ comes from the Lamperti transform.

Outline

The Wright-Fisher diffusion with mutation but no selection

$$dX_t = [\theta_1(1 - X_t) - \theta_2 X_t]dt + \sqrt{X_t(1 - X_t)}dW_t, \qquad X_0 = x, \quad t \geq 0.$$

The transition density has eigenfunction expansion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

where $q_m(t)$ is the transition function of a certain pure death process on $\mathbb{N}$ (related to Kingman's coalescent):

$$m \mapsto m - 1 \quad \text{at rate} \quad \frac{m(m + \theta_1 + \theta_2 - 1)}{2}.$$

The Wright-Fisher diffusion with mutation but no selection

$$dX_t = [\theta_1(1 - X_t) - \theta_2 X_t]dt + \sqrt{X_t(1 - X_t)}dW_t, \qquad X_0 = x, \quad t \geq 0.$$

The transition density has eigenfunction expansion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

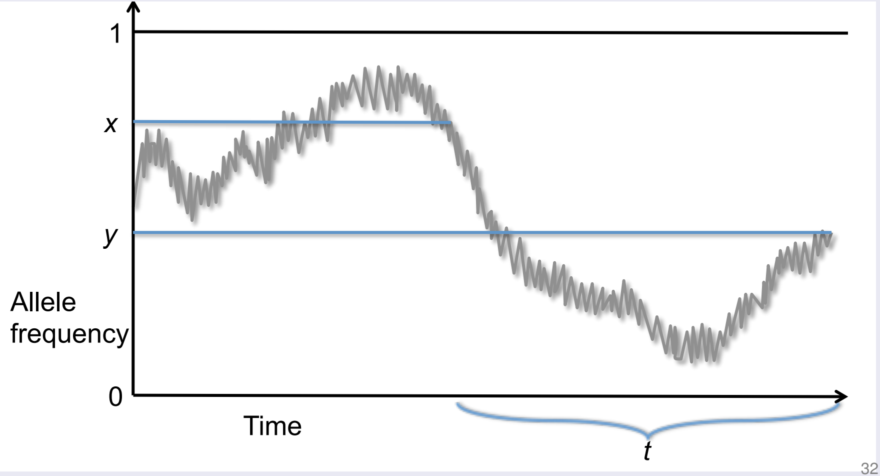
where $q_m(t)$ is the transition function of a certain pure death process on $\mathbb{N}$ (related to Kingman's coalescent):

$$m \mapsto m - 1 \quad \text{at rate} \quad \frac{m(m + \theta_1 + \theta_2 - 1)}{2}.$$

- So $f(x, y; t)$ is a known infinite mixture of beta random variables.

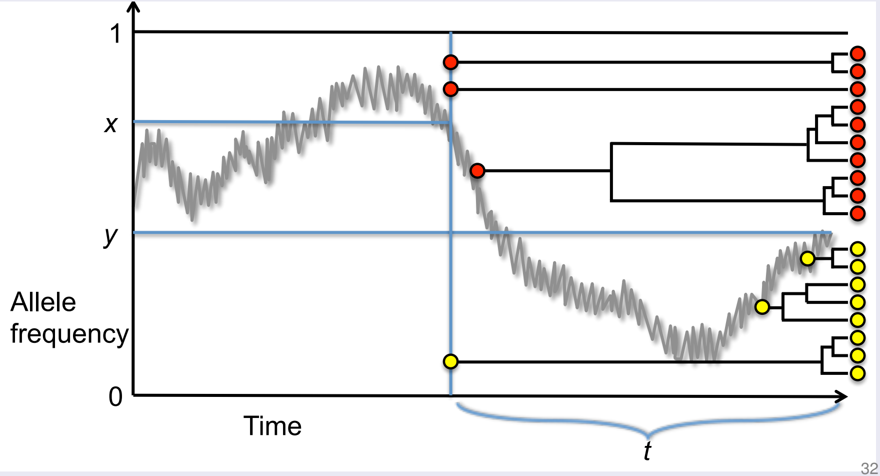
Duality and the transition density of the Wright-Fisher diffusion

$$f(x,y;t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$



Duality and the transition density of the Wright-Fisher diffusion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$



Duality and the transition density of the Wright-Fisher diffusion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

Convenient for simulation! (Griffiths & Li, 1983)

1. Simulate $M \sim \{q_m(t) : m = 0, 1, \ldots\}$.

   (a realization of Kingman's coalescent with mutation, time t).

Duality and the transition density of the Wright-Fisher diffusion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

Convenient for simulation! (Griffiths & Li, 1983)

1. Simulate $M \sim \{q_m(t) : m = 0, 1, \ldots\}$.
   (a realization of Kingman's coalescent with mutation, time t).
2. Simulate $L \sim \text{Binomial}(M, x)$.

Duality and the transition density of the Wright-Fisher diffusion

$$f(x, y; t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

Convenient for simulation! (Griffiths & Li, 1983)

1. Simulate $M \sim \{q_m(t) : m = 0, 1, \ldots\}$.
   (a realization of Kingman's coalescent with mutation, time t).
2. Simulate $L \sim \text{Binomial}(M, x)$.
3. Return $Y \sim \text{Beta}(\theta_1 + L, \theta_2 + M - L)$.

Exact simulation with the Wright-Fisher diffusion

- We can simulate from this Wright-Fisher diffusion directly.
- Key idea: Use it as the candidate in an exact algorithm for more complicated drifts.

With proposal drift $\alpha(x)$ and target drift $\beta(x)$, the Radon-Nikodým derivative is:

$$\frac{d\mathbb{WF}_\beta}{d\mathbb{WF}_\alpha}(X) \propto \exp\left\{\int_0^T \widehat{\phi}(X_t)dt\right\},$$

where

$$\widehat{\phi}(x) := \frac{1}{2}\left[\frac{\beta^2(x)-\alpha^2(x)}{x(1-x)} + \beta'(x) - \alpha'(x) - [\beta(x)-\alpha(x)]\frac{1-2x}{x(1-x)}\right].$$

This provides the required rejection probability.

Example (Natural selection)

$$\text{Proposal drift: } \alpha(x) = \theta_1(1-x) - \theta_2 x.$$
$$\text{Target drift: } \beta(x) = \alpha(x) + \gamma x(1-x).$$

Radon-Nikodým derivative:

$$\frac{d\mathbb{WF}_\beta}{d\mathbb{WF}_\alpha}(X) \propto \exp\left\{ \int_0^T \underbrace{\left[\frac{1}{2}\gamma^2 x(1-x) + \gamma\theta_1(1-x) - \gamma\theta_2 x\right]}_{\widehat{\phi}(x)} dt \right\}.$$

$\widehat{\phi}(x)$ is just a quadratic polynomial on a compact interval, so bounded!

Issues

$$f(x,y;t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

Simulating from $\mathbb{WF}_{\alpha}$.

1. Simulate $M \sim \{q_m(t) : m = 0, 1, \ldots\}$.
   (a realization of Kingman's coalescent with mutation, time t).
2. Simulate $L \sim \text{Binomial}(M, x)$.
3. Return $Y \sim \text{Beta}(\theta_1 + L, \theta_2 + M - L)$.

Issues

$$f(x,y;t) = \sum_{m=0}^{\infty} q_m(t) \sum_{l=0}^{m} \underbrace{\mathcal{B}_{m,x}(l)}_{\text{Binomial PMF}} \cdot \underbrace{\mathcal{D}_{\theta_1+l,\theta_2+m-l}(y)}_{\text{Beta density}},$$

Simulating from $\mathbb{WF}_\alpha$.

1. Simulate $M \sim \{q_m(t) : m = 0, 1, \ldots\}$.
   (a realization of Kingman's coalescent with mutation, time t).
2. Simulate $L \sim \text{Binomial}(M, x)$.
3. Return $Y \sim \text{Beta}(\theta_1 + L, \theta_2 + M - L)$.

Problem.

Mixture weights are known only as an infinite series:

$$q_m(t) = \sum_{k=m}^{\infty} (-1)^{k-m} \frac{(\theta + 2k - 1)\Gamma(\theta + m + k - 1)}{m!(k-m)!\Gamma(\theta + m)} e^{-k(k+\theta-1)t/2}.$$

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty} (-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty} (-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Then for each M, K,

$$\sum_{m=0}^{M} \sum_{k=0}^{2K+1} (-1)^k b_k(m) \leq \sum_{m=0}^{M} p_m \leq \sum_{m=0}^{M} \sum_{k=0}^{2K} (-1)^k b_k(m),$$

and these lower and upper bounds converge monotonically to the required CDF.

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty}(-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Then for each M, K,

$$\sum_{m=0}^{M}\sum_{k=0}^{2K+1}(-1)^k b_k(m) \leq \sum_{m=0}^{M} p_m \leq \sum_{m=0}^{M}\sum_{k=0}^{2K}(-1)^k b_k(m),$$

and these lower and upper bounds converge monotonically to the required CDF.

Hence, we can employ standard inversion sampling:

- Sample $U \sim \text{Uniform}[0, 1]$; then

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty}(-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Then for each M, K,

$$\sum_{m=0}^{M}\sum_{k=0}^{2K+1}(-1)^k b_k(m) \le \sum_{m=0}^{M} p_m \le \sum_{m=0}^{M}\sum_{k=0}^{2K}(-1)^k b_k(m),$$

and these lower and upper bounds converge monotonically to the required CDF.

Hence, we can employ standard inversion sampling:

- Sample $U \sim \text{Uniform}[0, 1]$; then
- $\inf\left\{M \in \mathbb{N} : \sum_{m=0}^{M} p_m > U\right\} \overset{d}{=} X$,

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty} (-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Then for each M, K,

$$\sum_{m=0}^{M} \sum_{k=0}^{2K+1} (-1)^k b_k(m) \leq \sum_{m=0}^{M} p_m \leq \sum_{m=0}^{M} \sum_{k=0}^{2K} (-1)^k b_k(m),$$

and these lower and upper bounds converge monotonically to the required CDF.

Hence, we can employ standard inversion sampling:

- Sample $U \sim \text{Uniform}[0, 1]$; then
- $\inf \left\{ M \in \mathbb{N} : \sum_{m=0}^{M} p_m > U \right\} \stackrel{d}{=} X,$

Solution: A variant of the alternating series method (Devroye, 1986).

Suppose X has PMF $\{p_m : m = 0, 1, \ldots\}$ of the form

$$p_m = \sum_{k=0}^{\infty} (-1)^k b_k(m), \text{ where } b_k(m) \downarrow 0 \text{ as } k \to \infty.$$

Then for each M, K,

$$\sum_{m=0}^{M} \sum_{k=0}^{2K+1} (-1)^k b_k(m) \leq \sum_{m=0}^{M} p_m \leq \sum_{m=0}^{M} \sum_{k=0}^{2K} (-1)^k b_k(m),$$

and these lower and upper bounds converge monotonically to the required CDF.

Hence, we can employ standard inversion sampling:

- Sample $U \sim \text{Uniform}[0, 1]$; then
- $\inf \left\{ M \in \mathbb{N} : \sum_{m=0}^{M} p_m > U \right\} \stackrel{d}{=} X$,

—except computing only as many terms in the series as needed in order to determine whether or not the inequality holds (testing each M in turn).

Proposition (Jenkins & Spanò, in preparation).

The coefficients of the ancestral process of Kingman's coalescent,

$$\{q_m(t) : m = 0, 1, \ldots\},$$

can be rearranged so that the alternating series method applies.

Outline

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.
- Candidate diffusions other than Brownian motion:
  - Bessel process
  - Wright-Fisher diffusion

  suggest the potential for further generalizing the exact algorithms.

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.
- Candidate diffusions other than Brownian motion:
  - Bessel process
  - Wright-Fisher diffusion

  suggest the potential for further generalizing the exact algorithms.

Further work

- Extend to an inference algorithm; applications to population genetic data.

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.
- Candidate diffusions other than Brownian motion:
    - Bessel process
    - Wright-Fisher diffusion

  suggest the potential for further generalizing the exact algorithms.

Further work

- Extend to an inference algorithm; applications to population genetic data.
- Other types of boundary (sticky, absorbing, . . .)

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.
- Candidate diffusions other than Brownian motion:
  - Bessel process
  - Wright-Fisher diffusion

  suggest the potential for further generalizing the exact algorithms.

Further work

- Extend to an inference algorithm; applications to population genetic data.
- Other types of boundary (sticky, absorbing, . . .)
- What other candidate processes are both easy to simulate and useful?

Summary

- It is possible to simulate efficiently from several diffusions with a finite entrance boundary, without discretization error.
- Candidate diffusions other than Brownian motion:
  - Bessel process
  - Wright-Fisher diffusion

  suggest the potential for further generalizing the exact algorithms.

Further work

- Extend to an inference algorithm; applications to population genetic data.
- Other types of boundary (sticky, absorbing, ...)
- What other candidate processes are both easy to simulate and useful?
- Extensions to infinite-dimensions (cf. Fleming-Viot process)?

Plug

Jenkins, P. A. “Exact simulation of the sample paths of a diffusion with a finite entrance boundary.” arXiv:1311.5777.

Acknowledgements

Many helpful conversations:

- Steve Evans
- Murray Pollock
- Gareth Roberts
- Joshua Schraiber

Plug

Jenkins, P. A. "Exact simulation of the sample paths of a diffusion with a finite entrance boundary." arXiv:1311.5777.

Acknowledgements

Many helpful conversations:

- Steve Evans
- Murray Pollock
- Gareth Roberts
- Joshua Schraiber

Thank you for listening!

Outline

Conditioned diffusion:

$$\widetilde{\phi}^*(u) = \frac{1}{2}\left[\alpha^2(u) + \alpha'(u) + \frac{(\delta-3)(\delta-1)}{4u^2}\right] + C. \quad \square$$

Convergent series method

$f(m) = \sum_{k=1}^{\infty} a_k(m)$.
REPEAT

- Generate $X \sim h$.
- Generate $U \sim U[0,1]$.
- Set $W := Uch(X)$, $S = 0$, $k = 0$.
- REPEAT
  - $k \mapsto k+1$,
  - $S \mapsto S + a_k(X)$,
- UNTIL $|S - W| > R_{k+1}(X)$

UNTIL $S \leq W$. RETURN X.

Alternating series method

$f(m) = ch(m) \sum_{n=0}^{\infty} (-1)^n b_n(m)$ and $b_n(m) \downarrow 0$.
REPEAT

- Generate $X \sim h$.
- Generate $U \sim U[0, c]$.
- Set $W := 0$, $n = 0$.
- REPEAT
  - $n \mapsto n + 1$,
  - $W \mapsto W + b_n(X)$,
  - IF $U \geq W$ THEN RETURN X.
  - $n \mapsto n + 1$,
  - $W \mapsto W - b_n(X)$.
- UNTIL $U < W$

UNTIL FALSE.
This works because

$$1 + \sum_{n=1}^{k} (-1)^n b_n(x) \leq \frac{f(x)}{ch(x)} \leq 1 + \sum_{n=1}^{k+1} (-1)^n b_n(x), \qquad k \text{ odd}.$$