Sampling from Unknown Transition Densities of Diffusion processes

Yasin Kikabi, Juma Kasozi
Department of Mathematics, College of Natural Sciences, Makerere University.
P.O. Box: 7062 Kampala, Uganda.

Abstract
In this paper, we introduce a new method of sampling from transition densities of diffusion processes including those unknown in closed forms by solving a partial differential equation satisfied by the quotient of transition densities. We demonstrate the performance of the developed method on processes with known densities and the obtained results are consistent with theoretical values. The method is applied to Wright-Fisher diffusions owing to their importance in population genetics in studying interaction networks inherent in genetic data. Diffusion processes with bounded drift and non degenerate diffusion are considered as reference processes.

Keywords: Stochastic differential equation (SDE), Transition density, Fokker-Planck partial differential equation, Aronson’s bound, Rejection sampling, Wright-Fisher diffusion.

1 Introduction

There are several ways of representing stochastic systems mathematically for instance using stochastic differential equations. A stochastic differential equation (SDE) is an equation of the form

$$dX_t = a(X_t,t)dt + b(X_t,t)dW_t,$$

where $a(X_t,t)$ is the drift term, $b(X_t,t)$ is diffusion coefficient and $W_t$ is the Wiener process. Due to the interplay between stochastic differential equations and the Fokker-Planck equation see (Gardiner 1985, chapter 5)\textsuperscript{[11]}, the transition density of the process described by (1.1) is obtained by solving the Fokker-Planck equation associated with the SDE. The Fokker-Planck equation is a partial differential equation that describes the evolution of the conditional probability distribution say $P(x,t/x_0,t_0)$ of a stochastic system through time in terms of state-space variables $x$. For instance, following Grigoris (2014)\textsuperscript{[17]}, the one dimensional, the Fokker-Planck equation associated with (1.1) is given by

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}[a(x,t)P(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b(x,t)P(x,t)]$$

with initial condition $P(x,t_0/x_0,t_0) = \delta(x - x_0)$. 

1
In equation (1.2), \( P(x,t) \) denotes the conditional density \( P(x,t|x_0,t_0) \).

Unfortunately, obtaining closed form solutions to Fokker-Planck equations associated with many diffusion processes of practical interest such as the Wright-Fisher diffusion remains a challenging problem Yun & Steinrücken (2012)\(^{[18]} \). This has always hampered the likelihood based inference for diffusion models with discretely observed data due to the fact it requires the transition density to be known explicitly which is hardly the case. However, several methods have been proposed in literature to circumvent the intractable likelihoods in statistical inference of diffusion models described by SDEs. These include approximating the transition density \( P \) by a Gaussian density (Florens-Zmirou 1989; Yoshida 1992; Sorensen & Uchida 2003)\(^{[10, 21, 19]} \), approximating \( P \) by orthogonal polynomials, Ait-Sahalia (2002, 2008)\(^{[1, 2]} \) and approximating \( P \) by solving the Fokker-Planck Equation numerically Bollback et al. (2008)\(^{[8]} \).

On the other hand, alternative inference methods such as the so-called Approximately Bayesian Computation (ABC) for diffusion models found for instance in Tina at el. (2009)\(^{[20]} \), require obtaining exact sample paths from the diffusion models. That is, sampling exactly from the transition densities associated with the SDEs describing the process. However, these transition densities are mostly known by eigen-fuction expansion or by their Fokker-Planck equations which itself is a challenge to solve to obtain closed forms of transition densities.

Recently, exact simulation methods for diffusion process have been proposed by Beskos et al. (2005, 2006, 2008)\(^{[7, 6, 5]} \). These are based on equivalence of measures induced by SDEs that comprise the same diffusion coefficient where rejection sampling is obtained via the Radon-Nikodym derivative. These methods require obtaining exact sample paths from one of the diffusions which are used as proposal paths in the rejection sampling. Generally, Beskos’s utilizes the absolute continuity of measures induced by diffusions with the same diffusion coefficient via Girsanov’s theorem to carry out rejection sampling of diffusion paths.

In this work, we explore the possibility of obtaining sample paths for diffusions by rejection sampling via Fokker-Planck equations. We consider diffusions that have the same diffusion coefficient. Our method is based on the assumption that the transition density of one of the diffusions (proposal diffusion) is known so that we can obtain samples from it at any discrete time points. This method involves solving a partial differential equation that involves quotients of transition densities of the target diffusion and proposal diffusion. Each of the two diffusion processes is defined by a system of stochastic differential equations.

Differently from Beskos’s method, where the entire path is either accepted or rejected, a path is developed by sampling from transition densities at discrete time points using the classical rejection sampling from probability density functions. This method is based on the assumption that we can solve the PDE that involves quotients of conditional transition densities.

The remainder of this paper is organised as follows. In Section 2 we present the classical rejection sampling method for purposes of development of our method. In Section 3, we present our rejection method, and its implementation. In Section 4 we apply our method to diffusion processes with bounded drift and non degenerate diffusion coefficients that satisfy Aronson’s bound with specific application to the Wright-Fisher diffusion. Later, we consider processes with unbounded drift . We discuss conclusions and possible directions for future research in the last section.
2 General rejection sampling

Rejection sampling is a widely applied technique of sampling from one probability density using samples from another density. Following Beskos (2005) [7], the classical rejection method is presented as follows.

Assume that $P_1$ and $P_2$ are probability densities with respect to some measure on $\mathbb{R}^d$ $d > 0$ and that there exists $\epsilon > 0$ such that $\frac{P_2}{\epsilon P_1} \leq 1$. Then, the following algorithm returns samples distributed according to $P_2$. Observe that, the rejection condition requires obtaining values of the quotient of probability densities at the sample points $Y$. Obtaining such values is challenging specifically in cases where the closed form of $P_2$ is unknown. In our method presented in the next section, obtaining such values involves solving a partial differential equation of quotients of probability densities so that (Algorithm 1) is then applicable.

Algorithm 1 Rejection algorithm

1: SAMPLE $Y \sim P_1$.
2: SAMPLE $U \sim \text{Unif}(0,1)$.
3: IF $U < \frac{P_2}{\epsilon P_1}(Y)$
4: return $Y$
5: ELSE go to 1

of probability densities at the sample points $Y$. Obtaining such values is challenging specifically in cases where the closed form of $P_2$ is unknown. In our method presented in the next section, obtaining such values involves solving a partial differential equation of quotients of probability densities so that (Algorithm 1) is then applicable.

3 Rejection sampling via the Fokker-Planck equation

Consider the following multidimensional stochastic differential equations

$$dX_t = S_i(X_t)dt + \sqrt{\sigma(X_t)}dW_t, \; X_0, \; 0 \leq t \leq T, \; i = 1, 2,$$

(3.1)

where $S_i, X_t \in \mathbb{R}^d$, $d \in \mathbb{N}$ and $\sigma(X_t)$ is a $d$–square matrix.

Let $P_1$ and $P_2$ be the corresponding conditional probability densities with $P_1$ known explicitly in its closed form. Then the corresponding Fokker-Planck equations are given by

$$\frac{\partial}{\partial t} P_i(x,t) = -\nabla^T_x(S_i(x)P_i) + \frac{1}{2} \nabla^T_x(\sigma(x)P_i) \nabla_x,$$

(3.2)

subject to initial condition $P_i(x, t_0) = \delta(x - x_0)$ $i = 1, 2$. $\nabla^T_x$ denotes the multivariate differential operator, $\nabla_x = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n})$.

Assumptions: Let us introduce the following set of assumptions,

A1. the Fokker-Planck equation for $P_2$ yields a solution on time interval $[0, T]$ such there exists $c \in \mathbb{R}$, $c > 0$ for which $\frac{P_2(x,t)}{P_1(x,t)} \leq c$ for any $x \in \mathbb{R}^d$ and $t \in [0, T]$. 


A2. $S_1(x)$, $S_2(x)$ and $\sigma_{k,j}(x)$, $j,k = 1,2,...,d.$ are differentiable functions.

Then, the quotient of transition densities $\frac{P_2}{P_1}(x,t)$ satisfies a partial differential equation given in the following theorem.

**Theorem 3.1.** Let

$$dX_t = S_i(X_t)dt + \sqrt{\sigma(X_t)}dW_t, \ X_0, \ 0 \leq t \leq T, \ i = 1,2.$$ be SDEs satisfying assumptions (A1) and (A2) above. Then the quotient of transition densities $\frac{P_2}{P_1}(x,t)$ satisfies the partial differential equation

$$\frac{\partial}{\partial t} \left[ \frac{P_2}{P_1}(x,t) \right] = \left\{ \nabla_x^T(S_1 - S_2) + \nabla_x^T \log(P_1)(S_1 - S_2) \right\} \left[ \frac{P_2}{P_1} \right] +$$

$$\left\{ (\nabla_x^T \log(P_1))\sigma(x) + \nabla_x^T \sigma(x) - S_2 \right\}^T \nabla_x \left[ \frac{P_2}{P_1} \right] + \frac{1}{2} \text{trace} \left\{ \sigma(x) \nabla_x (\nabla_x \left[ \frac{P_2}{P_1} \right]) \right\}. \quad (3.3)$$

$A^T$ denotes the transpose of the matrix $A$.

**Proof.** We sketch the proof for $d = 1$, the general case being straightforward. Let $d=1$ and denote the second partial derivative of $P$ with respect to $x$ by $\partial^2_{xx}P$.

Consider

$$\frac{\partial}{\partial t} \left[ \frac{P_2}{P_1}(x,t) \right] = \frac{P_1 \partial_t P_2 - P_2 \partial_t P_1}{P_1^2}. \quad (3.4)$$

Using the Fokker-Planck equations associated with the constituent SDEs equation (3.2), yields

$$\frac{\partial}{\partial t} \left[ \frac{P_2}{P_1}(x,t) \right] = \frac{-P_1 \partial_x(S_2(x)P_2) + P_2 \partial_x(S_1(x)P_1)}{P_1^2} + \frac{P_1 \partial_{xx}^2(\sigma(x)P_2) - P_2 \partial_{xx}^2(\sigma(x)P_1)}{2P_1^2}. \quad (3.5)$$

Note that the second order partial derivatives in equation (3.5) can be expressed as

$$\partial_{xx}^2(\sigma(x)P_2) = \sigma(x)\partial_{xx}^2 P_2 + 2\partial_x \sigma(x) \partial_x P_2 + \partial_{xx}^2 \sigma(x) P_2, \quad (3.6)$$

and similarly,

$$\partial_{xx}^2(\sigma(x)P_1) = \sigma(x)\partial_{xx}^2 P_1 + 2\partial_x \sigma(x) \partial_x P_1 + \partial_{xx}^2 \sigma(x) P_1. \quad (3.7)$$
By equation (3.6) and (3.7),
\[ P_1 \partial_{xx}^2 \sigma(x)P_2 - P_2 \partial_{xx}^2 \sigma(x)P_1 = \sigma(x)(P_1 \partial_{xx}^2 P_2 - P_2 \partial_{xx}^2 P_1) + 2 \partial_x \sigma(x)(P_1 \partial_x P_2 - P_2 \partial_x P_1). \]  
(3.8)

Thus, the last term in equation (3.5) simplifies to
\[ \frac{\sigma(x)}{2P_1^2} \partial_x \left(P_2^2 \partial_x \frac{P_2}{P_1}\right) + \partial_x \sigma(x) \partial_x \left(\frac{P_2}{P_1}\right), \]  
(3.9)

which further reduces to
\[ \frac{1}{2} \sigma(x) \partial_{xx} \left[ \frac{P_2}{P_1} \right] + (\sigma(x) \frac{\partial_x P_1}{P_1} + \partial_x \sigma(x)) \partial_x \left[ \frac{P_2}{P_1} \right]. \]  
(3.10)

On the other hand, the remaining term on the right side of equation (3.5) reduces to
\[ -S_2(x) \{ \partial_x \left[ \frac{P_2}{P_1} \right] + \frac{P_2}{P_1} \partial_x P_1 \} + S_1(x) \frac{P_2}{P_1} \partial_x P_1 - (\partial_x S_2(x) - \partial_x S_1(x)) \frac{P_2}{P_1}. \]  
(3.11)

Using (3.10) and (3.11) yields the partial differential equation (3.12) which is satisfied by the ratio of transition densities,
\[ \frac{\partial}{\partial t} V(x,t) = \left\{ \partial_x[S_1(x) - S_2(x)] + [S_1(x) - S_2(x)] \partial_x \log P_1 \right\} V(x,t) + \left\{ \sigma(x) \partial_x \log P_1 + \sigma(x) \partial_x S_2(x) \right\} \frac{\partial}{\partial x} V(x,t) + \frac{1}{2} \sigma(x) \frac{\partial^2}{\partial x^2} V(x,t), \]  
(3.12)

with initial condition \( V(x, t_0/x_0, t_0) = 1 \), where \( V(x, t) = \frac{P_2}{P_1}(x, t) \).

Our rejection sampling method is based on Theorem 3.1. To enhance our method, it requires establishing existence of solution to the partial differential (3.12) which we briefly consider in Subsection 3.1. In application of theorem 3.1, we restrict our consideration to a class of multidimensional diffusion processes that satisfy Aronson’s bound and later to diffusions with unbounded drift term in the one dimensional case. Before that, we state the following theorem due to Aronson (1967) [3]. This theorem will be vital in ensuring that assumption A_1 to Theorem 3.1 holds in our application.
Theorem 3.2. Aronson's bound
Consider the stochastic differential equation
\[ dX_t = S(X_t)dt + \sigma(X_t)dW_t, \quad X_0, \ 0 \leq t \leq T, \] (3.13)
with state space \( S \). Assume there exists a constant \( \lambda > 0 \) such that
\[ \lambda^{-1}I \leq \sigma(x)\sigma(x)^T \leq \lambda I \]
for all \( x \in S \) and that \( S(x) \) is bounded over \( S \). Then the bound to the transition density \( p(x,s;y,t) \)
associated with the SDE is given by
\[ K_1 g(x,s;y,t) \leq p(x,s;y,t) \leq K_2 g(x,s;y,t), \]
where \( K_1, K_2 \) are constants and \( g \) is the transition density of Brownian motion.

3.1 Numerical solution to the partial differential equation satisfied by ratio of transition densities

By Theorem 3.1, the partial differential equation (3.12) satisfied by ratio of transition densities is
is of a general form
\[ \frac{\partial}{\partial t} V(x,t) = c(x,t)V(x,t) + b(x,t)\frac{\partial}{\partial x} V(x,t) + a(x,t)\frac{\partial^2}{\partial x^2} V(x,t), \] (3.14)
with initial condition \( V(x,t_0) = 1 \). This is a second order, variable coefficient, linear parabolic
partial differential equation whose approximate solutions are obtained by numerical methods such
as finite difference methods. Obtaining numerical solutions to (3.14) over the time interval \([0,T]\)
and spatial interval \([x_{min}, x_{max}]\) leads to solving an initial value boundary value PDE numerically.
\( x_{min} \) and \( x_{max} \) denote the minimum and maximum sample values along the path obtained from
\( P_1 \) respectively.

In this work, we apply the Cranck-Nicolson finite difference scheme to solve the developed PDE
of quotients of densities. This is largely attributed to its unconditional stability and consistency
properties Marques (2017)\(^{15}\). In the multidimensional case (Section 4.2), the Alternating Direction
Implicit (ADI) method is used.

Following Marques (2017)\(^{15}\), for a general PDE of the form (3.14), consider mesh points \((x_j, t_i)\)
with spatial and time spacing \( h \) and \( k \) respectively. That is, \( x_j = jh, \ t_i = ik \) \( i = 1,2,...,N, \)
\( j = 1,2,...,M; M, N \in \mathbb{N} \). Let \( u^i_j = u(x_j, t_i), \ a^i_j = a(x_j, t_i), \ b^i_j = b(x_j, t_i), \ c^i_j = c(x_j, t_i) \). The
Cranck-Nicolson scheme is given by
\[ A_i u^{i+1}_{j+1} + B_i u^{i+1}_j + C_i u^{i+1}_{j-1} = D_i, \] (3.15)
where \( A_i = 2ka^i_{j+1} + hkb^{i+1}_j, \ B_i = -4h^2 - 4ka^i_{j+1} + 2h^2kc^{i+1}_j, \ C_i = 2ka^i_{j+1} - hkb^{i+1}_j, \)
\( D_i = - [u^i_{j+1} - (2ka_j + hkb^i_j) + u^i_j(4h^2 - 4ka^i_j + 2h^2c^i_j) + u^i_{j-1}(2ka^i_j - hkb^i_j)], \ i = 1,2,...,N, \)
$j = 1, 2, ..., M$.

$N$ and $M$ are the number of subintervals time in time and space respectively.

To obtain the solution at the next time line, we solve linear system given by (3.15).

Having described how to obtain values of $\frac{P_2}{P_1}(x_i, t_i)$ via the developed PDE, we now describe how to obtain sample path points from $P_2$ using exact sample paths from $P_1$. The idea of obtaining such samples from $P_2$ is as follows:

Obtain sample path points from $P_1$ at time instances $(t_1, t_2, ..., t_T)$. Denote the minimum observation by $x_{\text{min}}$ and similarly the maximum observation by $x_{\text{max}}$.

Solve the PDE (3.12) numerically at time instances $(t_1, t_2, ..., t_T)$ subject to boundary conditions $V(x_{\text{min}}, t) = 1 = V(x_{\text{max}}, t)$. The $x$-mesh is strategically chosen such that it contains both $x_{\text{min}}$ and $x_{\text{max}}$ and all the sample points. This solution gives the approximate value of $\frac{P_2}{P_1}$ at sample points and thus the usual rejection sampling procedure of using uniformly generated random numbers on unit interval. That is, a sample point is rejected, if random number generated uniformly on the unit interval falls above $\frac{P_2}{P_1}(x_i, t_i)$, otherwise it is accepted as a sample point from $P_2$. This rejection step can be carried out simultaneously for all sample path points by generating $T$ uniform random numbers. The values at any of the rejected points can be obtained by interpolation between any two accepted points using a diffusion bridge. The sampling procedure is summarised in the following algorithm.

**Algorithm 2** Rejection sampling algorithm

1: Sample paths points $x_i$ from $P_1$ at time times $t_i$ $i = 1, 2, ..., T \in \mathbb{N}$

2: Approximate the solution to the PDE (3.12) at time instances $\{t_1, t_2, ..., t_T\}$ with $x$-grid that includes all the sample points with boundaries at $x_{\text{min}}$ and $x_{\text{max}}$

3: return $\frac{P_2}{P_1}(x_i, t_i)$ $i = 1, 2, ..., T$

4: Generate $T$ uniformly distributed numbers on $[0, 1]$

5: For $i = 1, 2, ..., T$, if $u_i \leq \frac{P_2}{P_1}(x_i, t_i)$, accept $(x_i, t_i)$ else reject $(x_i, t_i)$

6: return Accepted sample path points $(x_i, t_i)$.

4 Numerical Results

4.1 Diffusions with bounded Drift:

4.1.1 The 1-dimensional Wright-Fisher diffusion with selection.

The Wright-Fisher diffusion is a continuous time Markov process with a continuous state space that is used to model fluctuations in size of finite populations under the influence of evolutionary forces such as selection and mutations. In population genetics, the Wright-Fisher diffusion in form of a stochastic differential equation is used to model the changes in allele frequencies in finite populations. For instance, considering a population under selection evolutionary force, the
Wright-Fisher diffusion in the univariate case is given by

\[ dx_t = \gamma x_t (1 - x_t) dt + \sqrt{x_t(1 - x_t)} dW_t \quad (4.1) \]

where \( x_t \) is allele frequency at time \( t \) and \( \gamma \) is the selection parameter. Observe that the drift function is bounded on the state space \([0, 1]\). Data on such diffusion processes is increasing becoming available due to advancement in biotechnology as earlier mentioned in the introduction of chapter 1 with a challenge being the development reliable statistical methods that can accurately determine the parameters underlying such processes such as selection and mutation parameters in the univariate cases and interaction parameters in the multivariate cases.

Such statistical methods in cases of (4.1) has always been hampered by lack of closed form transition densities associated with the diffusion to explicitly express the likelihood function. However, lack of a likelihood function can be circumvented by using likelihood free inferential methods such the Approximately Bayesian methods. These rely on the possibility of simulating exactly from models which in this cases implies the need for simulating sample paths of the diffusion (4.1). In this section, we show how to sample from the transition density of (4.1) using the transition density of a derived process from a Brownian bridge using our method.

Consider Brownian motion \( x_t \) on the time interval \([0, T]\) started at \( x_0 \). This is described by the stochastic differential equation,

\[ dx_t = dW_t, \quad x(0) = x_0. \quad (4.2) \]

Take the transformation of \( x_t \) under the map

\[ g(x) = \frac{1}{1 + e^{-x}}, \quad (4.3) \]

and denote the derived process by \( y_t \). By Ito’s Lemma, the derived process \( y_t \) satisfies the following stochastic differential equation

\[ dy_t = \frac{1}{2} y_t (1 - y_t)(1 - 2y_t) dt + y_t (1 - y_t) dW_t, \quad y_0 = Y_0, \quad 0 < t < T, \quad (4.4) \]

where \( W_t \) is the standard Wiener process. The derived process has a state space \((0, 1)\) as the Wright-Fisher diffusion assuming inaccessible boundaries at 0 and 1. This suggests the derived process \( y_t \) as a good candidate for the reference process in our rejection sampling for the Wright-Fisher diffusion if its transition density is known in a closed form.

However, noting that \( y_t \) is a bijective transformation of a Gaussian process under \( g \), its transition density can be obtained by the transformation Theorem which we state shortly in the following paragraph, a detailed proof of which is found for example in Gut (2009) Chapter 1. Following Gut (2009), the transformation theorem is stated as follows,
Theorem 4.1. (Transformation theorem)
Let $X$ be an $n$-dimensional, continuous, random variable with density $f_X(x)$, and suppose that $X$ has its mass concentrated on a set $S \subset \mathbb{R}^n$. Let $g = (g_1, g_2, \ldots, g_n)$ be a bijection from $S$ to some set $T \subset \mathbb{R}^n$, and consider the $n$-dimensional random variable

$$Y = g(X).$$

Assume that $g$ and its inverse are both continuously differentiable. The density of $Y$ is given by

$$f_Y(y) = \begin{cases} f_X(h_1(y), h_2(y), \ldots, h_n(y)) |J| & \text{for } y \in T \\ 0 & \text{otherwise} \end{cases}$$

(4.5)

where $h$ is the inverse of $g$ and $|J|$ is the Jacobian.

Denote the transition density of (4.4) by $P_1$. By the transformation theorem 4.1, the transition density of the derived process equation (4.4) is obtained from the Gaussian density of a Brownian bridge and thus, given by

$$P_1(s, y_s, t, y_t) = \frac{1}{\sqrt{2\pi(t-s)}} \exp\left(\frac{-(y_t - y_s)^2}{2(t-s)}\right), \quad y_t \in (0, 1),$$

(4.6)

where $\beta_t = \log \left(\frac{y_t}{1-y_t}\right)$.

We now embark on sampling from the Wright-Fisher process using the process (4.4) as a reference process. Note that both processes share the same state space, however, their diffusion terms are different.

Thus, to employ our method, the diffusion (4.1) has to be transformed into a diffusion with the same diffusion coefficient as equation (4.4). In this regard, consider the map

$$f(x) = \frac{1}{1 + e^{-\sin^{-1}(2x-1)}}.$$

(4.7)

Under this transformation, (4.1) is transformed into an Ito process given by the following stochastic differential equation,

$$dy_t = \frac{1}{2} y_t(1-y_t)(1-2y_t - \tan \beta_t + \gamma \cos(\beta_t))dt + y_t(1-y_t)dW_t, \quad y_0 = Y_0$$

(4.8)
where $\beta_t = \log\left(\frac{y}{1-y}\right)$.

Now, we use the process given by equation (4.4) as the reference process in our sampling algorithm to obtain samples from the transition density of the stochastic process given by equation (4.8). The obtained samples are later transformed into samples from the Wright-Fisher process equation (4.1) by the inverse map $f^{-1}(x)$.

Observe that both processes (4.8) and (4.4) have bounded drift functions on $(0,1)$ and the diffusion coefficient is non degenerate over the same set. Hence, the two processes satisfy Aronson’s bound (theorem 3.2) so that the assumption A1 holds.

Thus, by theorem 3.1, the partial differential equation satisfied by the ratio of transition densities is given by

$$
\frac{\partial V}{\partial t} = \frac{1}{2} \left( \gamma \sin \beta + \sec^2 \beta + \frac{(\beta - \beta_0)(\gamma \cos \beta - \tan \beta)}{t} \right)V + \frac{1}{2} y(1-y)(1-2y + 2\frac{\beta_0 - \beta}{t} + \tan \beta - \gamma \cos \beta) \frac{\partial V}{\partial y} + \frac{(y(1-y))^2}{2} \frac{\partial^2 V}{\partial y^2}, \quad t > 0,
$$

where $\beta(y) = \log\left(\frac{y}{1-y}\right)$, $V(y, t) = \frac{P_2}{P_1}(y, t)$ and $P_2$ is the transition density to the transformed Wright-fisher Process (4.8). The PDE is subjected to initial conditions $\frac{P_2}{P_1}(y, 0) = 1$ and boundary conditions $\frac{P_2}{P_1}(y_{\text{min}}, t) = 1$, $\frac{P_2}{P_1}(y_{\text{max}}, t) = 1$.

The simulated solution to the PDE is shown in Figure 1 with a corresponding accepted path in Figure 2.
Figure 1: **Fig.1** Numerical solutions of the PDE for $\gamma = 1$ at points on the proposed transformed Brownian path

In addition, we observe that paths that spend a significant time near the right boundary are rejected since PDE yields mostly zero values including negative values at some points that carry no physical meaning, see for instance Figure 3.

Figure 2: **Fig.2** Accepted transformed Brownian motion path

Figure 3: **Fig.3** Rejected path with corresponding numerical solutions of the PDE for $\gamma = 1$

Since statistical inference of diffusion processes assumes observed data, the accepted paths in our case are transformed into Brownian bridges. Figure 4 shows the Brownian bridges corresponding to accepted paths.
4.1.2 The 2-dimensional Wright-Fisher diffusion with selection.

In this section we investigate the performance our rejection sampling method in higher dimensions by considering the 2–dimensional Wright-Fisher diffusion with selection. Referring to the work of Aurell et.al (2019)\cite{4} where the 2-dimensional Wright-Fisher diffusion with selection only is given by the stochastic differential equation,

\[
\begin{align*}
    dx_t^{(1)} &= hx_t^{(1)}(1 - x_t^{(1)})x_t^{(2)} dt + \sqrt{x_t^{(1)}(1 - x_t^{(1)})}dW_t^{(1)}, \\
    dx_t^{(2)} &= hx_t^{(2)}(1 - x_t^{(2)})x_t^{(1)} dt + \sqrt{x_t^{(2)}(1 - x_t^{(2)})}dW_t^{(2)},
\end{align*}
\]

(4.10)

where $h$ is the selection coefficient, $W_t^{(i)}$, $i = 1, 2$ are 1dimensional independent Wiener process and initial conditions $(x_0^{(1)}, x_0^{(2)}) = (x, y)$.

Similar to the 1–dimensional case, we consider the transformation of each component of the 2-dimensional standard Wiener process by the sigmoid function equation (4.3). By Ito’s Lemma, the derived processes is given by the following SDE,

\[
\begin{align*}
    dy_t^{(1)} &= \frac{1}{2}y_t^{(1)}(1 - y_t^{(1)})(1 - 2y_t^{(1)})dt + y_t^{(1)}(1 - y_t^{(1)})dW_t^{(1)} \\
    dy_t^{(2)} &= \frac{1}{2}y_t^{(2)}(1 - y_t^{(2)})(1 - 2y_t^{(2)})dt + y_t^{(2)}(1 - y_t^{(2)})dW_t^{(2)},
\end{align*}
\]

(4.11)

with initial conditions $(y_0^{(1)}, y_0^{(2)}) = (X, Y)$.

Using the transformation theorem of random variables, it can be shown that the transition density of the process (4.11) is given by
where $\beta_i = \log \left( \frac{y_i^{(i)}}{1-y_i^{(i)}} \right)$ for $i = 1, 2$ and $\rho$ is the correlation coefficient.

Now, considering the process given by equation (4.10), under the multivariate transformation $y_i = \frac{1}{1+e^{-\sin^{-1}(2x_i^{(i)} - 1)}}$, we obtain a SDE satisfied by the transformed Wright-Fisher process.

\[
P_1(t, y_0^{(1)}, y_0^{(2)}; t, y_t^{(1)}, y_t^{(2)}) = \exp \left\{ \frac{1}{2 \pi t - t_0} \sqrt{1 - \rho^2} \right\} \left( \frac{1}{y_0^{(1)} y_t^{(2)} (1-y_0^{(1)})(1-y_t^{(2)}))} \times \frac{1}{\sqrt{(\beta_1^{(1)} - \beta_0^{(1)})^2 + (\beta_1^{(2)} - \beta_0^{(2)})^2 - 2(\beta_1^{(1)} - \beta_0^{(1)}) \beta_1^{(2)} - \beta_0^{(2)}}} \right) \right\}
\]

(4.12)

Denote by $P_1$ and $P_2$ the transition densities of the processes (4.13) and (4.11) respectively. Let $V(y_1, y_2, t) = \frac{P_2}{P_1}(y_1, y_2, t)$. By theorem 3.1, the ratio of transition densities $V$ satisfies the following partial differential equation,\[
\left\{ \begin{array}{ll}
\frac{dy_t^{(1)}}{dt} = \frac{1}{2} y_t^{(1)} (1 - y_t^{(1)}) (1 - 2y_t^{(1)} - \tan \beta_t^{(1)}) + \\
\frac{h}{2} (1 + \sin \beta_t^{(2)}) \cos \beta_t^{(1)} dt + y_t^{(1)} (1 - y_t^{(1)}) dW_t^{(1)} \\
\frac{dy_t^{(2)}}{dt} = \frac{1}{2} y_t^{(2)} (1 - y_t^{(2)}) (1 - 2y_t^{(2)} - \tan \beta_t^{(2)}) + \\
\frac{h}{2} (1 + \sin \beta_t^{(1)}) \cos \beta_t^{(2)} dt + y_t^{(2)} (1 - y_t^{(2)}) dW_t^{(2)}.
\end{array}
\right.
\]

(4.13)

\[
\frac{\partial V}{\partial t} = a(y_1, y_2, t) V + b_1(y_1, y_2, t) \frac{\partial V}{\partial y_1} + b_2(y_1, y_2, t) \frac{\partial V}{\partial y_2} + c_1(y_1, y_2) \frac{\partial^2 V}{\partial y_1^2} + c_2(y_1, y_2) \frac{\partial^2 V}{\partial y_2^2}, \quad t > 0,
\]

(4.14)

where

\[
a(y_1, y_2, t) = \frac{1}{2} \left\{ \begin{array}{l}
\sec^2 \beta_1 + \sec^2 \beta_2 + \frac{h}{2} (\sin \beta_1 + \sin \beta_2 + 2 \sin \beta_1 \sin \beta_2) + \\
\frac{\beta_1 - \beta_0^{(1)} - 2(\beta_1 - \beta_0^{(2)} ) \rho}{t(1- \rho^2)} (\frac{h}{2} (1 + \sin \beta_2) \cos \beta_1 - \tan \beta_1) + \\
\frac{\beta_2 - \beta_0^{(2)} - 2(\beta_2 - \beta_0^{(1)} ) \rho}{t(1- \rho^2)} (\frac{h}{2} (1 + \sin \beta_1) \cos \beta_2 - \tan \beta_2),
\end{array}
\right.
\]

\[
b_i(y_1, y_2, t) = \frac{1}{2} y_i (1 - y_i)(1 - 2y_i) + \frac{2[\beta_0^{(i)} - \beta_i + 2(\beta_j - \beta_0^{(j)} ) \rho]}{t(1- \rho^2)} + \tan \beta_i - \frac{h}{2} (1 + \sin \beta_j) \cos \beta_i \]

for $i \neq j$, $i, j = 1, 2$.\]

13
\[ c_i(y_1, y_2) = \frac{y_i^2(1 - y_i)^2}{2} \quad i = 1, 2. \]

Due to the non existence of numerical methods for solving a general two dimensional parabolic partial differential equation Mohanty & Jain (1996)\[16\], the following change of coordinates is employed to obtain a PDE with non variable diffusion coefficients.

Let \( x = x(y_1, y_2) = \beta_1 \) and \( y = y(y_1, y_2) = \beta_2 \). Under this change of coordinates, equation (4.14) is transformed into

\[
\frac{\partial V}{\partial t} = 2 \epsilon(x, y, t)V + c(x, y, t) \frac{\partial V}{\partial x} + d(x, y, t) \frac{\partial V}{\partial y} + \frac{1}{2} \frac{\partial^2 V}{\partial x^2} + \frac{1}{2} \frac{\partial^2 V}{\partial y^2}, \quad t > 0,
\]

(4.15)

where

\[
\epsilon(x, y, t) = \frac{1}{4} \left\{ \sec^2 x + \sec^2 y + \frac{h}{2}(\sin x + \sin y + 2 \sin x \sin y) + \right.
\left. \frac{x - \beta_0^{(1)} - 2(y - \beta_0^{(2)})}{t(1 - \rho^2)} \left( \frac{h}{2} (1 + \sin y) \cos x - \tan x \right) \right. \\
\left. + \frac{y - \beta_0^{(2)} - 2(x - \beta_0^{(1)})}{t(1 - \rho^2)} \left( \frac{h}{2} (1 + \sin x) \cos y - \tan y \right) \right\},
\]

\[
c(x, y, t) = \frac{\beta_0^{(1)} - x + 2(y - \beta_0^{(2)})}{t(1 - \rho^2)} + \frac{1}{2} \tan x - \frac{h}{4} (1 + \sin y) \cos x,
\]

\[
d(x, y, t) = \frac{\beta_0^{(2)} - y + 2(x - \beta_0^{(1)})}{t(1 - \rho^2)} + \frac{1}{2} \tan y - \frac{h}{4} (1 + \sin x) \cos y.
\]

Following Karaa (2009)\[13\] for the numerical solution to (4.15), define difference operators in the coordinate directions \( x \) and \( y \) as follows,

\[
A_x = -\left[ \alpha + \frac{\Delta x^2}{12} \left( \frac{c^2}{\alpha} - \epsilon - 2 \delta_x c \right) \right] \delta_x^2 + \left[ c + \frac{\Delta x^2}{12} \left( \delta_x^2 c - \frac{c}{\alpha} \delta_x c + 2 \delta_x \epsilon - \frac{c \epsilon}{\alpha} \right) \right] \delta_x + \left[ \epsilon + \frac{\Delta x^2}{12} \left( \delta_x^2 \epsilon - \frac{c}{\alpha} \delta_x \epsilon \right) \right],
\]

\[
L_x = \left[ 1 + \frac{\Delta x^2}{12} (\delta_x^2 - \frac{c}{\alpha} \delta_x) \right]
\]

14
and

\[ A_y = -\left[ \alpha + \frac{\Delta y^2}{12} \left( \frac{d^2}{d} - \epsilon - 2\delta_y d \right) \right] \delta_y^2 + \left[ d + \frac{\Delta y^2}{12} \left( \delta_y^2 d - \frac{d}{\alpha} \delta_y + 2\delta_y \epsilon - \frac{d \epsilon}{\alpha} \right) \right] \delta_y + \left[ \epsilon + \frac{\Delta y^2}{12} \left( \delta_y^2 \epsilon - \frac{d}{\alpha} \delta_y \epsilon \right) \right], \]

\[ L_y = \left[ 1 + \frac{\Delta y^2}{12} \left( \delta_y^2 - \frac{d}{\alpha} \delta_y \right) \right]. \]

Here, \( \alpha \) is the diffusion coefficient in the parabolic PDE which in this case is equal to \( \frac{1}{2} \). \( \delta_x \) and \( \delta_y \) are the central difference operators for the approximation of the second and first derivatives in the respective directions, \( \Delta x \) and \( \Delta y \) are respectively the spatial step length in the \( x \) and \( y \) direction.

In addition, denote the length of time step by \( \Delta t \).

Under the assumption \( \Delta t \leq \min(\Delta x, \Delta y) \), Karaa (2009)\(^{13}\) showed that, the Cranck-Nicolson scheme for the parabolic PDE \((4.15)\) is given by

\[
\left( L_x + \frac{\Delta t}{2} A_x \right) \left( L_y + \frac{\Delta t}{2} A_y \right) V_{i,j}^{n+1} = \left( L_x - \frac{\Delta t}{2} A_x \right) \left( L_y - \frac{\Delta t}{2} A_y \right) V_{i,j}^n, \tag{4.16}
\]

where \( V_{i,j} \) is the approximate solution to \( V \) at the point \((x_i, y_j)\) at time step \( n \). In implementing the numerical scheme \((4.16)\), it is split into the alternating direction implicit (ADI) scheme

\[
\left( L_x + \frac{\Delta t}{2} A_x \right) V^* = \left( L_x - \frac{\Delta t}{2} A_x \right) \left( L_y - \frac{\Delta t}{2} A_y \right) V_{i,j}^n, \tag{4.17}
\]

\[
\left( L_y + \frac{\Delta t}{2} A_y \right) V_{i,j}^{n+1} = V_{i,j}^*, \tag{4.18}
\]

where \( V^* \) is the approximate solution at an intermediate time step between \( t = n \) and \( t = n + 1 \).

Utilising the the above ADI scheme, the normalised numerical solution \( V \) to the PDE at different time steps are shown in Figures 5.

The numerical solution displays a decreasing behaviour for increasing values on both axes which is rather expected since for a fixed value of \( h \), there is an increasing divergence between the proposal process and the target process. A similar property of the solution is further displayed by the solution for increasing values of the parameter \( h \) shown in the appendix, which is explained by the same reason given in the previous line. Thus, a higher acceptance probability is expected for a process which spends a significant time near the left lower corner of the square \((0, 1) \times (0, 1)\) and counter behaviour at the right top corner, see second plot in Figure 6. This is explained by fact that the proposal process best approximates the target process for values near the zero point.
Figure 5: **Fig.5** Normalised numerical solution $V$ at time step 5, 10, 15, 20 respectively for $h = 1$

However, we observe a slightly different behaviour in the numerical solution for $h = 0$, see the left hand plot in Figure 6. Here, the proposal process differs from the target process by only terms $\tan(\beta(0))$ which influences the properties of the solution.
4.2 Unbounded Drift: The Ornstein-Uhlenbeck Process

Here, we implement the our method on particular processes with known explicit forms of transition densities and take a comparison between the approximated ratio values using the PDE and the theoretical values for processes. Particularly, we consider the Ornstein-Uhlenbeck Process whose drift is unbounded and hence its transition density Kusuoka (2017) \[14\]. We consider the Wiener process as the reference process in our rejection sampling.

Consider an Ornstein-Uhlenbeck process given the stochastic differential equation,

$$dX_t = -\beta X_t dt + \sigma dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T, \beta > 0.$$  \hspace{1cm} (4.19)

Suppose we require to sample from the conditional densities of the O-U process at different times using Wiener process as the reference process. We thus consider the Wiener process given by the SDE

$$dX_t = \sigma dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T.$$  \hspace{1cm} (4.20)

The Fokker-Planck equations associated with the equations (4.20) and (4.19) are respectively given by

$$\frac{\partial}{\partial t} P_1(x, t/x_0, t_0) = \frac{1}{2} \frac{\partial^2}{\partial x^2} [\sigma^2 P_1(x, t/x_0, t_0)],$$  \hspace{1cm} (4.21)

$$\frac{\partial}{\partial t} P_2(x, t/x_0, t_0) = \frac{\partial}{\partial x} [\beta x P_2(x, t/x_0, t_0)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [\sigma^2 P_2(x, t/x_0, t_0)],$$  \hspace{1cm} (4.22)

with initial condition $P_i(x, t_0/x_0, t_0) = \delta(x - x_0)$ $i = 1, 2$.

However, by Ito calculus, $P_2(x, t/x_0, t_0)$ is known to be a Gaussian density with mean $\mu_2(t) = x_0 e^{-\beta t}$ and variance $\sigma_2^2(t) = \frac{\sigma^2}{2\beta} (1 - e^{-2\beta t})$.

Similarly, $P_1(x, t/x_0, t_0) \in N(\mu_1(t), \sigma_1^2(t))$, where $\mu_1(t) = x_0$ and $\sigma_1^2(t) = \sigma^2 t$. 

Figure 6: Fig.6 Normalised numerical solution $V$ at time step 20 for $h = 0$
Proposition 4.1. The quotient of transition densities \( \frac{P_2}{P_1}(x,t/x_0,t_0) \) satisfies the parabolic partial differential equation (3.12).

Proof. \( \sigma(x) = \sigma^2 \), \( S_1(x) = 0 \), \( S_2(x) = -\beta x \), \( S'_1(x) = 0 \) and \( S'_2(x) = -\beta \), \( f(x,t) = \frac{\partial}{\partial x} \log P_1 \) implying \( f(x,t) = -\frac{x-\mu_1}{\sigma_1^2} \).

\[
a(x,t) = S'_1(x) - S'_2(x) + [S_1(x) - S_2(x)]f(x,t),
\]
implying that

\[
a(x,t) = \frac{\beta}{\sigma_1^2}\left\{ \sigma_1^2 - x(x - \mu_1) \right\}, \tag{4.23}
\]

\[
b(x,t) = \sigma(x)f(x,t) + \sigma'(x) - S_2(x),
\]

\[
b(x,t) = (\beta - \frac{\sigma_2^2}{\sigma_1^2})x + \frac{\sigma_1^2\mu_1}{\sigma_1^2}, \tag{4.24}
\]

and

\[
c(x,t) = \frac{\sigma_2^2}{2}. \tag{4.25}
\]

\[
\frac{\partial}{\partial x} \left[ \frac{P_2}{P_1} \right] = \frac{P_2}{P_1}\left\{ \frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2} \right\}x + \frac{\mu_2}{\sigma_2^2} - \frac{\mu_1}{\sigma_1^2}, \tag{4.26}
\]

Let \( A = \left( \frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2} \right)x + \frac{\mu_2}{\sigma_2^2} - \frac{\mu_1}{\sigma_1^2} \). Then,

\[
\frac{\partial^2}{\partial x^2} \left[ \frac{P_2}{P_1} \right] = \frac{P_2}{P_1}\left\{ A^2 + \frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2} \right\}. \tag{4.27}
\]

Considering the left hand term of equation (3.12)

\[
\frac{\partial}{\partial t} \left[ \frac{P_2}{P_1} \right] = \frac{P_2}{P_1}\left\{ \frac{\sigma_1'^2}{\sigma_1^2} - \frac{\sigma_2'^2}{\sigma_2^2} + \left( \frac{1}{\sigma_1} - \frac{\mu_1}{\sigma_1^2} \right)\left( -\frac{\sigma_2'}{\sigma_1^2} x + \frac{\mu_1'}{\sigma_1^2} + \frac{\mu_2'}{\sigma_2^2} \mu_1 \right) - \left( \frac{1}{\sigma_2} - \frac{\mu_2}{\sigma_2^2} \right)\left( -\frac{\sigma_2'}{\sigma_2^2} x + \frac{\mu_2'}{\sigma_2^2} + \frac{\mu_1}{\sigma_2^2} \mu_2 \right) \right\}. \tag{4.28}
\]
Let
\[ h(x,t) = a(x,t) + b(x,t).A + c(x,t)(A^2 + \frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2}). \]  \tag{4.29}

To check whether the partial differential equation (3.12) is satisfied, it is enough to check whether term in the right hand parenthesis of equation (4.28) is equal to equation (4.29) for all \((x,t)\).

However, equations (4.28) and (4.29) are quadratic polynomials in \(x\) with time dependent coefficients.

From the laws of algebra, any two polynomials are equal if and only if the coefficients are equal for all values \(t\). Thus, we check where the coefficients are equal and with some manipulations of the involved terms equality is established. For instance, comparing coefficients of the quadratic terms, from (4.28), this is given by
\[ \frac{-\sigma_1'}{\sigma_1^2} + \frac{\sigma_2'}{\sigma_2^2} = -\frac{1}{2\sigma_1^2} \sigma^2 + \frac{\sigma_1^2}{2\sigma_2^2} - \frac{\beta}{\sigma_2^2}. \]  \tag{4.30}

The derivatives in (4.30) are with respect to the time variable \(t\).

Similarly, from (4.29), the coefficient of the quadratic term is given by
\[ \frac{-\beta}{\sigma_1^2} + (\beta - \frac{\sigma^2}{\sigma_1^2})(\frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2}) + \frac{\sigma^2}{2}(\frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2})^2 = -\frac{1}{2\sigma_1^2} \sigma^2 + \frac{1}{2\sigma_2^2} \sigma^2 - \frac{\beta}{\sigma_2^2}. \]  \tag{4.31}

Similarly the coefficients for the other terms are also found to be equal and thus the PDE(3.12) is satisfied.

Consequently, \(\frac{P_2}{P_1}(x,t_0,0)\) evolves according to a second order linear parabolic partial differential equation whose coefficients are given by
\[ a(x,t) = \frac{\beta}{\sigma_1^2} \{ \sigma_1^2 - x(x - \mu_1) \}, \quad b(x,t) = (\beta - \frac{\sigma^2}{\sigma_1^2})x + \frac{\sigma^2 \mu_1}{\sigma_1^2}, \quad \text{and} \quad c(x,t) = \frac{\sigma^2}{2}. \]

We further check for the bound on quotient \(\frac{P_2}{P_1}\) since our proposed rejection method requires quotient \(\frac{P_2}{P_1}\) to be bounded for \(t \in [0,T]\).

Consider the ratio of conditional densities \(P_1\) and \(P_2\),
\[
\frac{P_2}{P_1}(x, t|x_0, t_0) = \frac{\sigma_1}{\sigma_2} \exp \left( -\frac{1}{2} \left\{ \frac{(x - x_0 e^{-\beta t})^2}{\sigma_2^2 (1 - e^{-2\beta t})} - \frac{(x - x_0)^2}{\sigma_1^2 \beta (1 - e^{-2\beta t})} \right\} \right).
\] (4.32)

The ratio (4.32) is bounded above by a constant \(C\) that depends on \(\beta\).
That is,

\[
\frac{\sigma_1}{\sigma_2} \exp \left( -\frac{1}{2} \left\{ \frac{(x - x_0 e^{-\beta t})^2}{\sigma_2^2 (1 - e^{-2\beta t})} - \frac{(x - x_0)^2}{\sigma_1^2 \beta (1 - e^{-2\beta t})} \right\} \right) \leq C(\beta).
\] (4.33)

Hence for a fixed value of \(\beta\) an upper bound on ratio of conditional densities can be established. Moreover, such a bound for a ratio of conditional transition densities with unknown closed forms for diffusion processes described by SDEs can equally be established, see for instance, Downes (2008)\[9\] for a detailed discussion of bounds on transition densities of time-homogeneous diffusion processes described by stochastic differential equations.

Following the work of Downes(2008)\[9\] on bounds on transition densities, it can be shown that the upper bound \(C(\beta)\) on \(\frac{P_2}{P_1}\) in the case of the O-U process with Brownian motion as the reference process is given by

\[
C(\beta) = e^{\frac{\beta}{\sigma_1^2} (x_{\text{max}}^2 - x_0^2 + T)}.\]

Now suppose the closed form of \(P_2\) is unknown but available is the SDE (4.19) for the stochastic process or equally the Fokker-Planck equation for \(P_2\) equation (4.22) since to every Fokker-Planck equation we can associate a stochastic differential equation Gardiner (1985), chapter 5. In addition, let the Wiener process (4.20) be the proposal process in our rejection method. Thus, we require the solution to parabolic

\[
\frac{\partial}{\partial t} V(x, t) = \frac{\beta}{\sigma_1^2} \left\{ \sigma_1^2 - x(x - \mu_1) \right\} V(x, t) + \\
\left\{ \frac{(\beta - \frac{\sigma_1^2}{\sigma_2^2})}{\sigma_1^2} x + \frac{\sigma_2^2 \mu_1}{\sigma_1^2} \right\} \frac{\partial}{\partial x} V(x, t) + \frac{\sigma_1^2}{2} \frac{\partial^2}{\partial x^2} V(x, t),
\] (4.34)

where \(\mu_1 = x_0, \sigma_1^2 = \sigma^2 t\), subject to initial condition \(V(x, t_0) = 1\). Noting that equation (4.34) is a second order parabolic equation, for solution we further require that we specify the boundary conditions. However, the boundary conditions depend on the nature of the boundaries shared by both processes on the interval over which the processes are constrained over the time interval
[0, T]. According to Gardiner (1985)[11], the boundaries can take on any of the following forms; reflecting, absorbing, periodic or prescribed boundaries.

In this particular case, the boundaries are finite considering the time period [0, T] and these are assumed to be \( x = x_{\text{min}} \) and \( x = x_{\text{max}} \) and the boundary conditions are given by \( V(x_{\text{min}}, t) = 1 \) and \( V(x_{\text{max}}, t) = 1 \).

Considering the Cranck-Nicolson finite difference scheme for equation (4.34) as described in section 3.1, the numerical solutions for the PDE adjusted by \( C(\beta) \) for \( \beta = 25, 0.05, 0.005, 5 \times 10^{-20} \) with the corresponding simulated O-U processes are shown in the figure 1.

Figure 7: Fig.7 Normalised numerical solutions of the PDE for different \( \beta \) values with corresponding O-U processes

Figure 8: Fig.8 Proposal discretized Brownian motion paths with corresponding normalised numerical solutions of the PDE for different \( \beta \) values

The numerical solution to the PDE possesses the expected behaviour of \( V \) tending to unity as \( \beta \) tends to zero. Observe that, for large values of \( \beta \), \( V \) tends to zero indicating that \( P_1 \) is no longer enveloped in \( P_2 \) over the considered time interval. This is due to the fact that higher values of \( \beta \) introduce a trend in the paths of the diffusion model (4.19) and thus candidate paths with no trends can hardly be solutions. This is the case for \( \beta = 25 \) in which the solutions to the SDE constitutes a trend.

Whereas \( V \) tends to unity for very small \( \beta \) values, for extremely large values of \( \beta \) the approximate solution to the PDE remains bounded.

The proposed paths figure 8 are rejected in the case of \( \beta = 5 \) for the reason similar to the case of \( \beta = 25 \) mentioned in the previous paragraph. However, for \( \beta = 0.005 \) some points on the path are rejected whereas others are accepted. Thus, the solution path can be constructed by interpolating.
between the accepted points by means of a diffusion bridge, a brownian bridge in this case. We further note that for the last two cases in figure 8, the proposed paths are accepted entirely and the solution at any other time points can similarly be obtained by Brownian bridges. Moreover, the numerical solution to the PDE converges to the theoretical values as $\beta$ becomes small. That is, the absolute error in the numerical solution reduces is small for smaller values of $\beta$, see Figure 9.

![Figure 9: Normalised numerical solutions of the PDE for different $\beta$ values with corresponding theoretical values](image)

5 Conclusion

In a nutshell therefore, we have proposed a new method of carrying out rejection sampling using transition densities including those that are unknown in closed form. The method has been tested on cases with known transition densities and the results are consistent with theoretical values. Thus the method provides a possibility of simulating paths for diffusions at discrete time points using associated transition densities even when they are unknown in closed form. We have provided a multidimensional extension of the method in addition, and we believe avails an opportunity for use of likelihood free inferential methods for numerous diffusion processes such as Approximately Bayesian computational (ABC) methods. Since by our method sampling from the transition density of multidimensional Wright-Fisher diffusion at discrete time points is possible, in the future, we embark on applying likelihood free methods in determining the interaction graphical networks in allele frequency data using coupled Wright-Fisher diffusion as the underlying model.
References

[1] Aït-Sahalia, Y. Maximum likelihood estimation of discretely sampled diffusions: a closed-form approximation approach. *Econometrica* 70, 1 (2002), 223–262.

[2] Aït-Sahalia, Y., et al. Closed-form likelihood expansions for multivariate diffusions. *The Annals of Statistics* 36, 2 (2008), 906–937.

[3] Aronson, D. G. Bounds for the fundamental solution of a parabolic equation. *Bulletin of the American Mathematical society* 73, 6 (1967), 890–896.

[4] Aurell, E., Ekeberg, M., and Koski, T. On a multilocus wright-fisher model with mutation and a svirezhev-shahshahani gradient-like selection dynamics. *arXiv preprint arXiv:1906.00716* (2019).

[5] Beskos, A., Papaspiliopoulos, O., and Roberts, G. O. A factorisation of diffusion measure and finite sample path constructions. *Methodology and Computing in Applied Probability* 10, 1 (2008), 85–104.

[6] Beskos, A., Papaspiliopoulos, O., Roberts, G. O., et al. Retrospective exact simulation of diffusion sample paths with applications. *Bernoulli* 12, 6 (2006), 1077–1098.

[7] Beskos, A., Roberts, G. O., et al. Exact simulation of diffusions. *The Annals of Applied Probability* 15, 4 (2005), 2422–2444.

[8] Bollback, J. P., York, T. L., and Nielsen, R. Estimation of 2nes from temporal allele frequency data. *Genetics* 179, 1 (2008), 497–502.

[9] Downes, A. N. Bounds for the transition density of time-homogeneous diffusion processes. *Statistics & probability letters* 79, 6 (2009), 835–841.

[10] Florens-Zmirou, D. Approximate discrete-time schemes for statistics of diffusion processes. *Statistics: A Journal of Theoretical and Applied Statistics* 20, 4 (1989), 547–557.

[11] Gardiner, C. W., et al. *Handbook of stochastic methods*, vol. 3. Springer Berlin, 1985.

[12] Gut, A. An intermediate course in probability, ed, 2009.

[13] Karaa, S. A high-order adi method for parabolic problems with variable coefficients. *International Journal of Computer Mathematics* 86, 1 (2009), 109–120.

[14] Kusuoka, S. Continuity and gaussian two-sided bounds of the density functions of the solutions to path-dependent stochastic differential equations via perturbation. *Stochastic Processes and their Applications* 127, 2 (2017), 359–384.

[15] Marques, C. N. Option pricing under variable volatility. Master’s thesis, Instituto Superior de Economia e Gestão, 2017.
Appendix

Figure 10: **Fig.10** Normalised numerical solution $V$ at time step 10 and 20 respectively for $h = 10$
Figure 11: Fig.11 Normalised numerical solution $V$ at time step 10 and 20 respectively for $h = 50$