Inverse Functions for Monte Carlo Simulations with applications to hitting time distributions

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Abstract

Random sampling is a ubiquitous tool in simulations and modeling in a variety of applications. There are efficient algorithms for these for several known distributions, but in general, one must resort to computing or approximating the inverse to the distribution to generate random samples, given a random number generator for a uniform distribution. In certain physical and biomedical applications with which we have been particularly concerned, it has proven to be more efficient to provide random times for a walk of a fixed length, rather than the conventional random step lengths in a given time step for the walker. For these, the hitting-time distributions which have to be sampled have been computed, and proved to be complicated expressions with no efficient method to compute the inverse. In this paper, we explore a well known probability (the F-ratio distribution) – whose inverses are efficiently computable – as an alternative to generating look-up tables and interpolations to obtain the required time samples. We find that this distribution approximates the hitting-time distribution well, and report on error measures for both the approximation to the desired, and the error in the generated time samples. Future Monte Carlo simulations in a number of fields of application may benefit from methods such as we report here.

Keywords: Random sampling, Hitting Time Distributions, F-distributions, Monte Carlo simulations.

1 Introduction

Simulations of random processes are used very widely, and it is important then to have efficient methods of generating random samples. In our work, we encountered this need in computational biomedicine; for example, in modeling transport of molecules, from water to proteins, in tissue [4, 6]. For reasons spelled out in the cited papers, we chose to use probabilistic representations of solutions of the elliptic and the parabolic partial differential equations that are required for those applications. The coefficients of the differential operators in these equations represent physical phenomena such as, for example, diffusion, advection, and loss of a drug molecule that is being transported in tissue after being injected therein in suspension in saline solution. In the cases of interest, these are all inhomogeneous, *i.e.*, the coefficients vary spatially. The general representations of the solutions have been long known to mathematicians, and we used the clear statements of these in the monograph of Freidlin [2]. An essential component of such solvers is the random walk that needs to be simulated to accumulate the solution to a specific problem. These random walks in general, besides being dependent on the specified diffusivity, also have a deterministic component that arises from the carrier fluid velocity ("drift") as well as an extinction rate due to losses, binding and degradation. The well-known Feynman-Kac formula is required to accommodate these last phenomena, as is described in detail in Freidlin's monograph.

It has also been known, and discussed in a previous publication [3], that efficient simulations of random walks require a perspective different from the most direct method which would be to select a time step Δt and then to select a random step length and direction to place the walker. The step length distribution is the Gaussian familiar from studies on random walk, and there are efficient simulations for these. However, to avoid excessive increase in the number of samples, we would select the maximum step length possible, given the medium inhomogeneities, and then select a random place on the sphere for placement and a random hitting-time of arrival there. This method has been popularized by Russian workers under the name "walk on spheres" method, see for example [7]. Therefore, instead of the Gaussian distribution, we have to simulate the hitting-time distributions (the hitting place offers no difficulty) and these are much more complicated than the elementary Gaussian. We refer to the already cited [4] and [6], as well as to [3] for background and motivation on all these issues, as well as the detailed derivations for series representations of the hitting-time distributions.

As mentioned, the application for our random number generation has been adequately motivated and described in the cited publications. In brief, the probabilistic representation of solutions to many partial differential equations (with non-constant and spatially varying coefficients) of interest in applications are useful in producing numerical solutions. Such methods demand simulations of random walks, and efficient simulations require one to produce random times (from a probability distribution given in Section 2.2 below) for a walk of given length. However, it is clear that there are an increasing number of applications having nothing to do with our interests where it would be useful to generate samples from increasingly complicated distributions. Even the very particular distribution that we computed in [3] is germane to applications where a random walk combined with a deterministic velocity requires to be simulated, which should be widely useful. Besides that, there are many other applications where a complicated distribution is given either in series, or other non-invertible form. It is customary to indicate several methods to generate random numbers from a specified distribution. See, e.g., [9]: (i) inversion of the distribution; (ii) transformation of the variable; (iii) acceptance/rejection and Monte Carlo methods; and (iv) approximating with known and easily sampled distributions. As can be seen from Section 2.2 below, our distributions are given in the form of an infinite series, which are not readily numerically tractable even for direct evaluation. Indeed, as we noted in our previous publication [3], we found it beneficial to use Mathematica$^{\text{TM}}$ (Wolfram Research, Inc., Version 10) in our evaluation. Mathematica has apparently some built-in algorithms to accumulate exponents in various factors before evaluation: thus large positive and negative exponents are allowed to cancel each other. Providing the same formulas to Matlab$^{\text{TM}}$ (The MathWorks, Inc.), for example, immediately resulted in numerical instability and overflow/underflow problems. We would have to do a lot more preparatory work to bring even the direct evaluation of the distributions into serviceable form in an application environment other than Mathematica$^{\text{TM}}$. In any case, inversion of this distribution is not available in analytic form. In [3], we used extensive numerical testing to provide an ad-hoc but quite efficient set of interpolating approximations to the inverse of the distribution, allowing fast generation of samples. In this paper, we explore the last approach (iv) listed above. As for the other remaining approaches, there is no transformation of variable apparent that could reduce the complicated formulas for the distributions to a known distribution. The acceptance-rejection method would run into intractable problems because it would require one to evaluate the distributions (to check against a random variable with uniform distribution over the unit interval). We have not developed methods for automatic checking of convergence or numerical stability of the series evaluation (we did it "by hand" for the cases where we checked against the approximate distribution). Thus we must treat our distribution essentially as a numerical distribution, and we employed the last approach, in particular, the F-ratio distribution well known in statistics, as the approximating distribution for reasons described below.

1.1 Outline of paper

This paper presupposes a lot of material either well-known or previously published. We therefore have chosen to quickly recapitulate these materials so that this paper is self-contained for reading, although some motivations will be unclear without the background. In Section 2, we summarize formulas from our previous paper to exhibit the distributions (and some associated expressions such as the moment generating functions) according to which we need to generate samples. Similarly, Section 3 begins with introducing the well-known F-distribution, and how we select the parameters for it and a distribution obtained by an affine mapping of its argument, so that the first four moments of the desired distribution are matched. We also examine an undesired cutoff that is forced by the affine mapping, and examines its potential consequences for limiting the applicability of our method. Section 4 summarizes our results: we characterize the distributions themselves (the approximating and the desired) using the Cramer–von Mises distance between the two; and finally the error in generating the time samples themselves. We have previously argued [3] that an L^1 error seems the most appropriate, and we evaluate this error for both our current and our previously published *ad-hoc* approximations. A concluding

Table 1: Glossary of Symbols

Symbol	Meaning
T_H	First hitting-time to a sphere from origin; $T_H \in]0, \infty[$
X_H	Hitting place on the sphere at time T_H
$\mathbf{v}, v, \mathbb{D}, D$	Drift vector field, $v = \|v\|$, diffusion tensor field, isotropic diffusion coefficient
V	Dimensionless drift speed
$p_V(.), P_V(.)$	Probability density function (pdf), (cumulative) probability distribution of T_H for drift speed V
$E[\circ]$	Expected value of random variable defined in the parentheses
$m_i(V), i = 1, 2, 3, 4$	First four moments of T_H, i.e., for the distribution with density p_V
$M(V), \mathcal{V}(V), S(V), K(V)$	Mean, variance, skewness, and kurtosis of the distribution with density p_V
$\overset{F}{M}(V), \overset{F}{\mathcal{V}}(V), \overset{F}{S}(V), \overset{F}{K}(V)$	Corresponding quantities for the F-distribution with parameters a, b
$\overleftarrow{t}_V(.)$	(Exact) inverse function to P_V; maps the unit interval onto the positive real line
$\widehat{p}$, $\widehat{P}$, $\widehat{T}$, $\widehat{t}$	Approximations to $p, P, T, \overleftarrow{t}$, respectively, with subscripts as for the unhatted symbols
$\tau \in\ ]0, \infty[$	(Dimensionless) argument of the hitting-time distributions
$u \in]0, 1[$	(Dimensionless) argument of the inverse functions
P_n	Legendre polynomial of order n

section discusses the utility of an approach such as the one we have here, as well as questions we have left for the future.

To avoid excessive typography, we do not indicate the random variable in the distributions: this must always be understood to be the hitting-time T_H unless otherwise specified (see below). Table 1 summarizes the symbols used in the paper. We note that hatted symbols are used for the approximations, whereas unhatted symbols are reserved for the exact or "true" distributions and functions.

2 Hitting time distributions: summary of previous results

In this section, we summarize the formulas which will serve as the basis for simulating random walks of fixed step length and random times, in contrast to the conventional Gaussian process simulating the walk in a fixed time, with random step lengths. Of course, there are many applications for such Monte Carlo methods other than the few that we have examined. The detailed justification and derivation of the formulas quoted below are available in [3], while applications to Dirichlet problems are discussed in [4], and to Neumann problems in [5]. We quote only as much of the formulas as we need to proceed with discussion of the problem of computing the inverse distribution for generating samples. The distributions we focus on are for the times at which the random walk reaches the boundary of a sphere of given length; it turns out (*loc cit*) that the place on the sphere has a readily invertible distribution so that generating the target points on the sphere is not a problem. Only the time distribution offers a difficulty in that its inverse cannot be expressed by an analytic function or simple reversion of the series for the distributions. We first quote the Poisson summation formula which we need for evaluating the distributions; after that, to make contact with our previous work, we use dimensionless variables corresponding to the time and the deterministic drift of the random walk. This is of no importance for this particular paper, which proceeds on the basis of only these dimensionless variables for efficiency of presentation, the application being of no consequence here. All the equations can be easily reconverted in terms of the physical parameters.

2.1 The Poisson resummation

The Poisson summation formula is often used to improve the convergence of a series in certain ranges. We quote this formula here as follows. Define the Fourier transform

$$F(x) := \int_{-\infty}^{\infty} dy \exp(-i2\pi xy) f(y) \tag{1}$$

Then for 'nicely' behaved functions

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} F(k) \tag{2}$$

(Any text or online source may be consulted for the conditions for validity of the Poisson summation.)

2.2 Dimensionless variables

We define the dimensionless time and speed variables:

$$\tau := \frac{D}{R^2} T; \quad V := \frac{1}{2} \frac{vR}{\pi^2 D} \tag{3}$$

where D is the isotropic diffusion coefficient of the random walk with dimension length^2/time, v is the magnitude of the deterministic drift velocity, R is the step length that is taken, and T is the time, the distribution of which needs to be computed. This distribution depends on the dimensional variables D, T, R, and v only through these two dimensionless combinations. We are considering isotropic diffusion, so R is the radius of a hitting sphere. The density function (since it is not dimensionless itself) also depends on the Jacobian, which in this case just means using the chain rule. For the development henceforth, we may just take as given that we have a family of distributions for the dimensionless hitting-time (the argument for this being denoted τ), while the family is parametrized by V. In applications, this is the speed of a particle with a given (vector) velocity and isotropic diffusion coefficient D. It turns out that the hitting-time distributions can be fully characterized in terms of these two parameters. In applications, we have allowed the dimensionless speed V to be either vanishing (pure diffusion) or in the range from $e^{-5} \sim 0.007$ to $e^{5} \sim 150$. We now summarize results we have obtained previously for the hitting-time distributions.

2.3 Summary of hitting-time distributions

The zero speed cumulative distribution is

$$P_0(\tau) = 1 + 2\sum_{n=1}^{\infty}(-1)^n \exp(-n^2\pi^2\tau) = \sum_{n=-\infty}^{\infty}(-1)^n \exp(-n^2\pi^2\tau) \tag{4}$$

Its Poisson resummed form (indicated by the superscript PS) is

$$\overset{PS}{P}_0(\tau) = \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{\pi\tau}} \exp[-(2k-1)^2/4\tau] \tag{5}$$

The distribution for non-zero speed is

$$P_V(\tau) = 1 + 2N \exp[-\pi^4 V^2 \tau] \sum_{n=1}^{\infty}(-1)^n \frac{n^2}{n^2+\pi^2V^2} \exp(-\pi^2\tau n^2) \tag{6}$$

and its Poisson-resummed form

$$\begin{aligned}\overset{PS}{P}_V(\tau) = {} & \frac{\sinh(\pi^2 V)}{\pi^2 V} \exp[-\pi^4 V^2 \tau] \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{\pi\tau}} \exp[-(2k-1)^2/4\tau] \\ & + \frac{1}{2}\sinh(\pi^2 V) \sum_{k=-\infty}^{\infty} \left\{ \exp[-|2k-1|\pi^2 V] \mathrm{erfc}\left[\frac{|2k-1| - 2\pi^2\tau V}{2\sqrt{\tau}}\right] \right. \\ & \left. - \exp[|2k-1|\pi^2 V] \mathrm{erfc}\left[\frac{|2k-1| + 2\pi^2\tau V}{2\sqrt{\tau}}\right] \right\}\end{aligned} \tag{7}$$

The Laplace transform, equivalent to the moment generating function, is

$$M_V(\alpha) := E[(-\alpha\tau)]_{p_V(\tau)} = \frac{\sinh(\pi^2 V)}{\pi^2 V} \frac{\sqrt{\alpha + \pi^4 V^2}}{\sinh(\sqrt{\alpha + \pi^4 V^2})} \tag{8}$$

from which the moments are obtained by differentiation (and paying attention to the sign). Since we will be matching the first four moments, we give the expressions for these, obtained by successive differentiation of the moment generating function above:

$$m_1(V) = \frac{\pi^2 V \coth(\pi^2 V) - 1}{2\pi^4 V^2} \tag{9}$$

$$m_2(V) = \frac{\pi^4 V^2 \coth^2(\pi^2 V) + \pi^4 V^2 \mathrm{cosech}^2(\pi^2 V) - \pi^2 V \coth(\pi^2 V) - 1}{4\pi^8 V^4} \tag{10}$$

$$\begin{aligned} m_3(V) &= \left(8\pi^{12} V^6\right)^{-1} \\ &\times \left\{\pi^2 V \coth\left(\pi^2 V\right)\left[5\pi^4 V^2 \mathrm{cosech}^2\left(\pi^2 V\right) - 3\right] + \pi^6 V^3 \coth^3\left(\pi^2 V\right) - 3\right\} \end{aligned} \tag{11}$$

$$\begin{aligned} m_4(V) = &\left(16\pi^{16} V^8\right)^{-1} \\ &\times \left\{3\pi^4 V^2 \coth^2\left(\pi^2 V\right)\left[6\pi^4 V^2 \mathrm{cosech}^2\left(\pi^2 V\right) - 1\right]\right. \\ &+ 5\pi^2 V \coth\left(\pi^2 V\right)\left[2\pi^4 V^2 \mathrm{cosech}^2\left(\pi^2 V\right) - 3\right] \\ &+ 5\pi^8 V^4 \mathrm{cosech}^4\left(\pi^2 V\right) - 3\pi^4 V^2 \mathrm{cosech}^2\left(\pi^2 V\right) + \pi^8 V^4 \coth^4\left(\pi^2 V\right) \\ &\left. + 2\pi^6 V^3 \coth^3\left(\pi^2 V\right) - 15\right\} \end{aligned} \tag{12}$$

The values of these moments for the pure diffusive process ($V = 0$) are

$$\begin{array}{ll} m_1(0) = 1/6; & m_2(0) = 7/180; \\ m_3(0) = 31/2520; & m_4(0) = 127/25200 \end{array} \tag{13}$$

The above expressions for the moments are not suitable for small V because they result in ∞/∞ expressions resulting in numerical instability. However, it is easy enough to find the Taylor series for the moments, and we use the following expressions for small V (the constant term in each has been given immediately above):

$$m_1(V) - m_1(0) = -\frac{\pi^4 V^2}{90} + \frac{\pi^8 V^4}{945} + \cdots \tag{14}$$

$$m_2(V) - m_2(0) = -\frac{11\pi^4 V^2}{1890} + \frac{\pi^8 V^4}{1260} + \cdots \tag{15}$$

$$m_3(V) - m_3(0) = -\frac{113\pi^4 V^2}{37800} + \frac{677\pi^8 V^4}{1247400} + \cdots \tag{16}$$

$$m_4(V) - m_4(0) = -\frac{1073\pi^4 V^2}{623700} + \frac{671003\pi^8 V^4}{1702701000} + \cdots \tag{17}$$

The Taylor expansion above is used for the first three moments for $V \leq 0.01$ while that for the fourth moment is used for $V \leq 0.02$. We also introduce calligraphic fonts

$$\mathcal{M}(V),\ \mathcal{V}(V),\ \mathcal{S}(V),\ \mathcal{K}(V) \tag{18}$$

to denote the mean, the variance, the skewness, and the kurtosis, respectively, of the density function p_V. For convenience, we reproduce the relationship of these quantities to the moments (henceforth we drop the argument V for the moments and the related quantities, the argument V being understood):

$$\begin{aligned}\mathcal{M} &= m_1 \\ \mathcal{V} &= m_2 - m_1^2 \\ \mathcal{S} &= [m_3 - 3m_1m_2 + 2m_1^3]/\mathcal{V}^{3/2} \\ \mathcal{K} &= [m_4 + m_1(-4m_3 + m_1(6m_2 - 3m_1^2))]/\mathcal{V}^2\end{aligned} \tag{19}$$

For example, the variance of the distribution is thus seen to be

$$\mathcal{V} = \frac{\pi^4V^2\,\mathrm{cosech}^2(\pi^2V) + \pi^2V\coth(\pi^2V) - 2}{4\pi^8V^4} \tag{20}$$

The density functions themselves for $V = 0$ are as follows:

$$p_0(\tau) = \sum_{n=-\infty}^{\infty}(-1)^{n+1}n^2\pi^2\exp(-\pi^2\tau n^2) = \sum_{n=-\infty}^{\infty}\frac{d}{d\tau}[\exp(i\pi n)\exp(-\pi^2\tau n^2)] \tag{21}$$

$$\overset{PS}{p}_0(\tau) = \sum_{k=-\infty}^{\infty}\frac{d}{d\tau}\left[\frac{1}{\sqrt{\pi\tau}}\exp[-(2k-1)^2/4\tau]\right] \tag{22}$$

and, for non-zero speeds, the density is given by

$$p_V(\tau) = N\exp[-\pi^4V^2\tau]p_0(\tau) \tag{23}$$

where the normalization

$$N = 2\frac{\sinh(\pi^2V)}{\pi^2V} \tag{24}$$

Thus, using the Fourier transform and integrating by parts, the Poisson resummed density is immediate:

$$\overset{PS}{p}_V(\tau) = N\exp[-\pi^4V^2\tau]\sum_{k=-\infty}^{\infty}\frac{d}{d\tau}\left[\frac{1}{\sqrt{\pi\tau}}\exp[-(2k-1)^2/4\tau]\right] \tag{25}$$

2.3.1 Summary

The distributions have been computed above: the direct ones converge for large arguments, while the Poisson resummed ones are needed for smaller arguments, which in fact comprise most of the useful range. We use $\overleftarrow{t}_V(u)$ to denote the inverse function to the distribution. Then if u is generated with uniform distribution in its range on the unit interval, the mapping by the inverse function will generate samples with the desired distribution in time. The objective of this paper is to generate such random samples. (The transition time above which one should use the direct series and below which one should use the Poisson resummed one, for stable and fast evaluation of the respective series, depends on the speed V, see [3].) It is obvious, as mentioned in the last paragraph of the introduction, that one cannot find a readily expressible inverse function to the distribution. In our previous work [3], we used an *ad-hoc* approach which divided the range of V in logarithmic increments of 0.1 in the exponent from -5 to 5, that is, from $V = \exp(-5)$ to $\exp(+5)$ in addition to $V = 0$. A table of parameters and interpolation functions based upon them was then used to describe the inverse as detailed previously. We now explore approximating it with a F-distribution which is well-studied in statistics with robust numerical schemes for inversion.

3 F-distributions

We here explore an alternative approach to generating samples, namely by approximating the desired distribution by standard and well-studied statistical distributions. We refer to Chapter 6 of [8] for justifying our taking this approach. Briefly, we seek to find a family of distributions that can 'satisfactorily' represent the given hitting-time distribution computed above, and then seek the best fit to a distribution within the family. We will demand that the distribution fits the first four moments exactly, so as to capture enough of the non-Gaussian nature of the distribution. Using more moments of course adds accuracy for the fit, but drastically introduced complexity.

Figure 1(a) illustrates the reason for our choice. In this figure we show a parametric plot of the skewness and kurtosis for a variety of distributions [8] as indicated in the legend. Different functions have different relationships between skewness and kurtosis. For some functions the skewness and the kurtosis are dependent as is the case for a lognormal density function whose representation in the Pearson system (skewness squares-vs-kurtosis) is a line, the normal probability density function (pdf) is a point (zero skewness, and kurtosis of 3), and for some other functions the skewness is independent of the kurtosis, and the function spans a range of values in the Pearson chart. In addition, a scatter plot of data points obtained from the true hitting-time distributions for a number of values for $V \leq 100$ are shown. We find that the skewness and kurtosis fall within the family distribution given by Pearson type VI. Thus, all arbitrary functions that produce a given pair (skewness, kurtosis) can be described by Pearson type VI. The Pearson type VI can be represented by the F-distribution (given in Mathematica by FRatioDistribution) or by a Beta distribution of the second kind. We choose (for convenience) the F-distribution. We do not need to display the line that obtains for this distribution, since as discussed immediately above, it has been constructed to fit all the first four moments exactly and hence will go through the data points shown. It would appear that we will need a four-parameter family but we choose the two parameter (central) F-distribution, which we first describe. We shall later return to discussing why we did not choose a distribution with more paramaters. We denote the F-ratio distribution and density respectively, for some non-negative random variable X, the relation of which to the hitting-time we shall specify below, as

$$F_V(x \mid a, b), \qquad f_V(x \mid a, b) \tag{26}$$

We shall not give the explicit expression of the distribution or its density (these are readily available online) in terms of known special functions. However, again for convenience, we give the expression of the first four moments of the F-distribution in terms of the parameters:

$$\begin{aligned}
\overset{F}{\mathcal{M}} &= \frac{b}{b-2}, b > 2 \\
\overset{F}{\mathcal{V}} &= \frac{2b^2(a+b-2)}{a(b-2)^2(b-4)}, b > 4 \\
\overset{F}{\mathcal{S}} &= \frac{2a+b-2}{b-6}\frac{\sqrt{8(b-4)}}{\sqrt{a(a+b-2)}}, b > 6 \\
\overset{F}{\mathcal{K}} &= 3 + \frac{12[(b-2)^2(b-4)+a(a+b-2)(5b-22)]}{a(a+b-2)(b-6)(b-8)}, \qquad b > 8
\end{aligned} \tag{27}$$

We proceed as follows. We first fit the parameters of the distribution to skewness and the kurtosis of the actual density p_V, and obtained from its moment generating function, both given above. It may be shown that the desired relationships are

$$\begin{aligned}
a = &-2 + \frac{2(K+3)}{6-2K+3S^2} \\
&+ 6\sqrt{\frac{(K+3)^2S^2(S^2-K+1)^2}{(3S^2-2K+6)^2(S^2(K(K+78)-63)-32K(K-3)-36S^4)}}
\end{aligned} \tag{28}$$

$$b = 6 + \frac{4(K+3)}{2K-3(S^2+2)} \tag{29}$$

We now define the new random variable

$$T := cX + d \tag{30}$$

where we adjust the constants c, d to equate the mean and variance of the hitting-time distribution P_V and its Poisson-resummed form $\overset{PS}{P}_V$ of T from Section 2 to that of X. In effect, we are endowing the F-distribution with four parameters. This results in

$$c = \sqrt{\mathcal{V}/\overset{F}{\mathcal{V}}} \tag{31}$$

$$d = m_1 - c \times \overset{F}{m}_1 \tag{32}$$

We denote the transformed distribution and density as $\widehat{P}_V(\tau)$ and $\widehat{p}_V(\tau)$, respectively, the parameters a, b, c, d being understood as arguments of the approximating functions. It is understood that these parameters all depend on V, the dependence being obtained by matching these parameters to the moments obtained earlier. Thus, we now see that the first four moments of the distribution $\widehat{P}_V$ agree with the corresponding four moments of the desired distribution previousy denoted P_V. We therefore will now work with $\widehat{P}_V(\tau)$ and $\widehat{p}_V(\tau)$ as defined above to serve as our approximations to the true distributions. From the transformation (30), we easily see that

$$\widehat{p}_V(\tau) = \begin{cases} \frac{1}{c} f_V \left(\frac{\tau - d}{c} \middle| \, |a, b \right), & \tau \geq d \\ 0, & \tau < d \end{cases} \tag{33}$$

Thus, this density unlike the original density of a F-distribution is cut off at d: we shall evaluate this cutoff below and see that it is positive. Thus, a hitting-time s shorter than d does not occur in this approximation. By integration we see that

$$\widehat{P}_V(\tau) = \begin{cases} F_V \left(\frac{\tau - d}{c} \middle| \, |a, b \right), & \tau \geq d \\ 0, & \tau < d \end{cases} \tag{34}$$

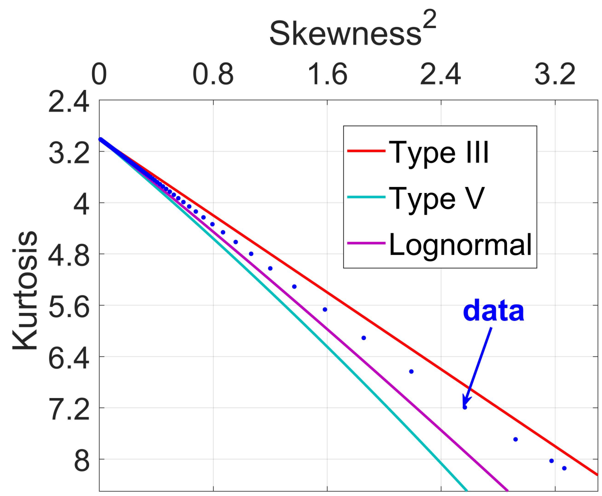
These then are the approximations to the true distributions we shall use. The F-distributions depend on the parameters a, b which are given by equations (28) and (29), while the independent variable in the distribution is now $(\tau - d)/c$ with c, d given as in equations (31) and (32). Thus for simulation, we use the inverse of the F-distributions and compare that to those of the true distributions. Our time sample generated is thus

$$\widehat{t}(u) = c\widehat{\tau}(u) + d \tag{35}$$

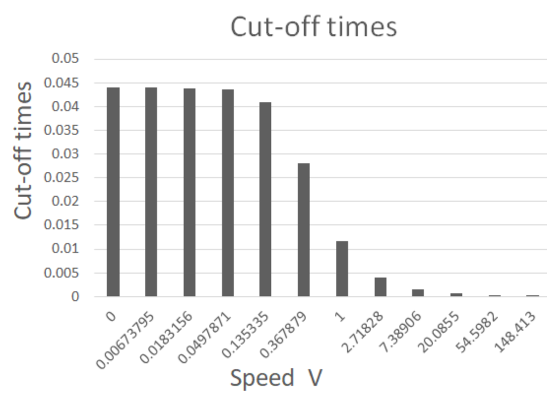
where $\widehat{\tau}$ denotes the inverse function to $\widehat{P}_V$ and is understood to depend on the parameters a and b as well. We now comment on our choice of distribution and on the cutoff d which prevents our approximation from generating sample times below the cutoff.

Figure 1(b) shows the cutoff times d, namely the (dimensionless) τ values which will fail to be generated by our approximation, due to the affine shift involved in the argument as discussed above. *However, an examination of the cutoff probabilities shows no cause for concern.* At $V = 0$, we find that the probability at the right-hand limit (that is, approaching the limiting τ value of $d = 0.04396$ from above), is 4.58×10^{-8}, and this is the worst case probability. That means that we encounter values below the cutoff at most one time in 100 million. This drops to the cumulative distribution value of 4×10^{-9} for $V = e^{-5}$, and down to 10^{-9} for $V = e^{-2}$. Beyond this, for larger values of V, the cumulative probability for encountering times below the cutoff are vanishingly small (for $V = 1/e$ it is $< 10^{-13}$ and continues to decline steeply). Thus, we may conclude that even for $V = 0$, the errors are small enough to be negligible for most applications. We now evaluate the actual performance of the approximation for generating time samples, and compare the approximating distribution to the actual.

We conclude by discussing the alternatives to the particular method we have discussed. It is difficult to improve the approximating distribution without substantial increase in complexity and numerical evaluations which will slow down



(a)



(b) The speeds V are just integer powers of e (the base of natural logs) from -5 to $+5$ in unit steps.

Figure 1: Characteristics of the F-distribution approximation

simulations. If we choose three-parameter distributions (such as the non-central F), then we cannot dispense with either the scale or the shift in equation (30), which will produce a cutoff to time samples from the approximating distribution. Thus, if we begin with equation (30), but eliminate the shift d, by matching the third parameter to the mean or to the variance, then the linear scaling c will alter these. If we eliminate the scale by matching to a third parameter, the shift, which results in the cutoff, remains. We could use a four-parameter distribution like the Beta Type II, but the numerical complexity of evaluating moments is excessive. The same remark applies to matching four moments by using, say, a maximum entropy distribution.

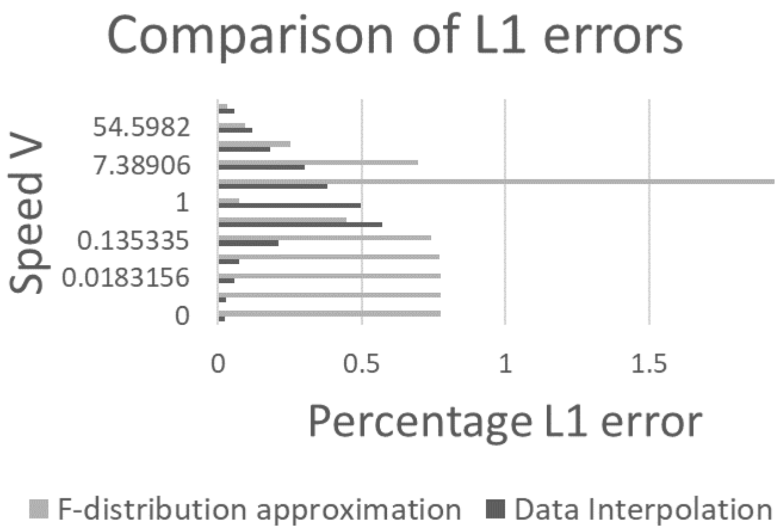
4 Evaluation of the F-distribution approximation

We first discuss how to evaluate the performance in terms of the application, and then return to evaluating the distribution itself. When comparing the use of the approximate random variable $\widehat{t}_V(u)$ in favor of the exact $\overleftarrow{t}_V(u)$, where u is the uniform random variable in the unit interval, we note that the inverse has to return times in accordance with the actual distributions for all times, though of course at either end of the interval, larger relative errors can be tolerated. We have therefore chosen to use the relative error using the L^1 norm as our criterion. In other words, we define and compute

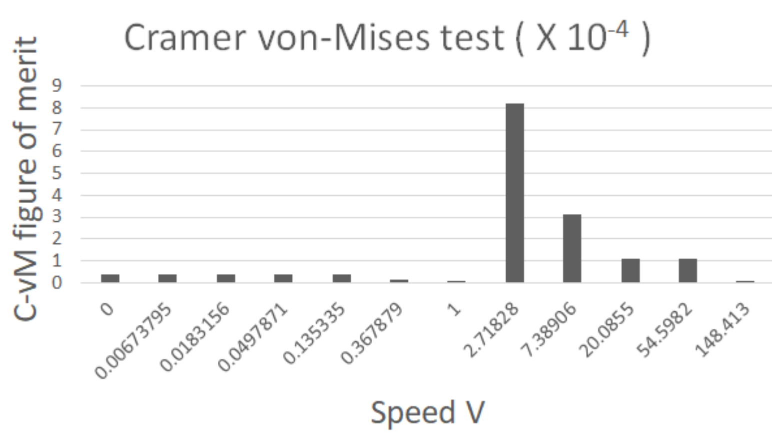
$$\text{L1err} := \frac{\int_0^1 |\overleftarrow{t}_V(u) - \widehat{t}_V(u)|du}{\int_0^1 \overleftarrow{t}_V(u)du} \times 100 \tag{36}$$

(the denominator on the right-hand side being the mean hitting-time) and display this as the percentage error. We have also computed the mean square error compared with the second moment, with errors that are even smaller, so we do not display these.

Figure 2(a) shows the result, and compares with our previous method which was entirely empirical and based on constructing tables and interpolating functions. The method we are illustrating in the paper uses standard software (in this case, Mathematica) to compute the inverse of the F-distributions for the purpose of generating samples. We admit that our previous *ad-hoc* approach does indeed perform well, though in both cases the errors are relatively small. The worst case for the performance of the present method, in this metric, is in fact for $V \sim e$ but this is precisely the range in which the drift as well as the diffusion behave comparably: the distribution is most sensitive to V around this region: for $V = 0$, it is purely diffusive, and for large V, one may estimate the hitting-time simply by $1/V$. (However, due to historical circumstances as discussed in [3], we introduced factors of π into the definitions of the dimensionless quantities, so that the hitting-time turned out to be $1/\pi^2 V$ for unimportant reasons.) In Figure 2(b) we evaluate the goodness of fit by computing the Cramer–von Mises (symmetric) distance [1] between the two distributions. This



(a)



(b)

Figure 2: Performance of the F-distribution approximation

distance is given by the expectation value of the difference squared between the two distributions (the expectation value may be taken with respect to either):

$$\mathcal{E}\left[\left(P_V - \widehat{P}_V\right)^2\right] \tag{37}$$

The figure shows this measure. If we want to compare this with some number, we may pick the expectation of the square of either distribution which would give us 1/3: we have not done so in the bar graph, but it is easy enough to multiply by 3. The goodness of the approximation is excellent.

5 Conclusion and discussion

Being able to simulate distributions with complicated expressions, not expressible in analytic form, is an increasingly frequent requirement. We encountered such needs in our own work in computational biomedicine. Faced with this requirement, one approach explored here is to approximate the desired distribution with a distribution within a canonical family of distributions and test if the desired accuracy is sufficient. The advantage of course is the body of knowledge and of software available for such distributions. We have given a detailed look at a distribution required for the solutions of partial differential equations encountered ubiquitously including in our prior work, and an approximation that matched the first four moments with a two-parameter F-distribution together with an affine transform of the random variable, effectively endowing the distribution with four parameters. Some error estimates were also computed and plotted, and seem adequately small for application. We hope that such methods, namely the use of canonical distributions for sampling, gain further notice in computational applications of random walk and Monte Carlo methods.

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