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Harmonic Analysis/Numerical Analysis

Analytical and numerical results for first escape time in 2D

Les résultats analytiques et numériques pour la première évasion de temps en 2D

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A R T I C L E   I N F O

A B S T R A C T

We consider the problem of a particle subject to Brownian motion in a 2D circular domain with reflecting boundaries except for an absorbing gate. An exact solution for the mean first escape time is given for a gate of any size. Also obtained is the exact probability density of the location of an exiting particle. Numerical simulations of the stochastic process with finite step size are compared with the exact solution to the Brownian motion (the limit of zero step size). The difference between the two appears to decrease with diminishing step size.

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R É S U M É

Nous considérons le problème d'une particule soumise au mouvement brownien dans un domaine 2D circulaire avec frontiers refletantes, sauf pour une porte d'absorption. Une solution exacte pour le moment première évasion moyenne est donnée pour une porte de n'importe quelle taille. En outre obtenu est la densité de probabilité exacte de l'emplacement d'une particule sortant. Des simulations numériques du processus stochastique avec un pas finis sont comparés avec la solution exacte pour le mouvement brownien (la limite de taille nulle étape). La différence entre les deux semble diminuer avec l'étape de diminution de la taille.

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1. Introduction

Many physical, chemical, and biological processes can be formulated in terms of a Brownian motion with reflection at most of the domain boundary and absorption from a small part. In chemical processes [8], particle A may move around randomly while B is essentially stationary, and a reaction occurs when A touches B. In cell biology, an ion drifts about within a cell, is reflected when it hits the membrane, which is most of the boundary of the cell, and escapes when it hits a small pore, thereby altering the electrostatic balance in and out of the cell. When predators are hunted by prey, a prey dies when it encounters a predator [5].

These applications thus lead to a mathematical problem of a particle in an n-dimensional domain Ω in which the particle is reflected from $\Omega \setminus \Gamma$ and absorbed at Γ. This problem has been studied by several authors ([5,2,3,7,4] and references therein), most recently, Chen and Friedman [1] who obtained mathematically rigorous results. In particular, they considered a two-dimensional circular domain and obtained rigorous asymptotic results for a gate of a small width ε.

In this paper, we obtain an exact solution for this problem which is crucial for understanding the difference between the computations and the true Brownian motion. First, there is an error due to the statistical sampling of a large number of particles. Even if one used an astronomical number of particles, the step size is necessarily finite, so that a second difference (that one might call "error") arises due to the finite step instead of the continuum process. This second source of error is better understood with numerics utilizing different step sizes. With an exact solution for the particular case of the circle, one can then obtain empirical results as step size and gate size vary. Thus, a careful comparison of the exact solution with the numerical solution illuminates the distinction between finite step random motion and Brownian motion. The comparison between the exact solution and the asymptotic solution determines the range of applicability and error of the asymptotic solutions. In particular, there are the questions of how large ε can be and how large the constant multiplying the error term can be.

2. Main theorems

Our starting point is the following theorem, which formulates the stochastics as elliptic equations. The equation for the mean time is a standard result [6], while the expression for the variance is new.

Theorem 1. *Let $\Omega \in \mathbb{R}^n$ be a bounded domain with smooth boundary $\partial\Omega$ and Γ be a closed subset of $\partial\Omega$. For each $x \in \Omega$, let τ_x be the first time of a particle hitting Γ, assuming that the particle starts from x, is subject to Brownian motion in Ω, and reflects from $\partial\Omega$. Then, the mean first hitting time (or exit time), $T(x) := \mathbb{E}[\tau_x]$, and its variance, $v(x) := \mathbb{E}[(\tau_x - T(x))^2]$, are solutions of the following boundary value problems:*

$$-\Delta T = 2 \quad \text{in } \Omega, \qquad T = 0 \quad \text{on } \Gamma, \qquad \partial_n T = 0 \quad \text{on } \partial\Omega \setminus \Gamma;$$
$$-\Delta v = 2|\nabla T|^2 \quad \text{in } \Omega, \qquad v = 0 \quad \text{on } \Gamma, \qquad \partial_n v = 0 \quad \text{on } \partial\Omega \setminus \Gamma.$$

Here $\partial_n := n \cdot \nabla$ is the derivative in the direction n, the exterior normal to $\partial\Omega$.
Consequently, the average of the variance can be calculated from the formula

$$\bar{v} := \frac{1}{|\Omega|} \int_{\Omega} v(x)\, dx = \frac{1}{|\Omega|} \int_{\Omega} T^2(x)\, dx =: \overline{T^2}.$$

Now, we will provide a closed formula for the mean exit time of a special case that has attracted much attention and been the subject of many theoretical investigations in the past; see [1,3,7] and the references therein.

Theorem 2 *(A closed formula for the mean exit time). In 2-D, with points identified by complex numbers, let*

$$\Omega := \big\{ re^{\mathbf{i}\theta} \,\big|\, 0 \leqslant r < 1,\ -\varepsilon \leqslant \theta \leqslant 2\pi - \varepsilon \big\}, \qquad \Gamma := \big\{ e^{\mathbf{i}\theta} \,\big|\, |\theta| \leqslant \varepsilon \big\}. \tag{1}$$

Then the mean exit time $T(z)$, for $z \in \bar{\Omega}$, is given by

$$T(z) = \frac{1 - |z|^2}{2} + 2\log \left| \frac{1 - z + \sqrt{(1 - ze^{-\mathbf{i}\varepsilon})(1 - ze^{\mathbf{i}\varepsilon})}}{2\sin\frac{\varepsilon}{2}} \right|.$$

For the rest of this paper, we will assume Ω and Γ are as in (1). This exact formula allows us to improve the result of Theorem 5.1 in [1] by the following.

Theorem 3. *The mean escape time T has the following properties:*

$$T(0) = \frac{1}{2} + 2\log \frac{1}{\sin\frac{\varepsilon}{2}}, \qquad T(e^{\mathbf{i}\theta}) = 2\operatorname{arccosh} \frac{\max\{\sin\frac{\varepsilon}{2}, |\sin\frac{\theta}{2}|\}}{\sin\frac{\varepsilon}{2}}, \quad \forall \theta \in \mathbb{R},$$
$$\bar{T} := \frac{1}{|\Omega|} \int_{\Omega} T(x)\, dx = \frac{1}{4} + 2\log \frac{1}{\sin\frac{\varepsilon}{2}} = T(0) - \frac{1}{4}.$$

In addition, setting $\hat{\varepsilon} = 2\sin\frac{\varepsilon}{2} = |e^{\mathbf{i}\varepsilon} - 1|$, we have, when $0 < \hat{\varepsilon} \leqslant |1 - z|$ and $z \in \bar{\Omega}$,

$$T(z) = \frac{1 - |z|^2}{2} + 2\log \frac{2|1-z|}{\hat{\varepsilon}} + \Re\left[\frac{z\hat{\varepsilon}^2}{2(1-z)^2} - \frac{3z^2\hat{\varepsilon}^4}{16(1-z)^4} \right] + \frac{O(1)z^3\varepsilon^6}{|1-z|^6}$$
$$= 2\log \frac{2|1-z|}{\varepsilon} + \frac{1 - |z|^2}{2} + \left(\frac{1}{12} + \Re\left[\frac{z}{2(1-z)^2} \right] \right)\varepsilon^2 + \frac{O(1)\varepsilon^4}{|1-z|^4},$$

where $O(1)$ is a quantity bounded by a universal constant.

Finally we consider the location of a particle when it exits.

Theorem 4. *The probability density of the location of an exit of a particle is given by*

$$\bar{j}(e^{\mathbf{i}\theta}) := -\frac{1}{2\pi}\frac{\partial}{\partial r}T(e^{\mathbf{i}\theta}) = \begin{cases} 0, & if\ \varepsilon < \theta < 2\pi - \varepsilon, \\ \frac{1}{2\pi}\frac{\cos\frac{\theta}{2}}{\sqrt{\sin^2\frac{\varepsilon}{2}-\sin^2\frac{\theta}{2}}}, & if\ |\theta| < \varepsilon. \end{cases}$$

Then for any (*Borel set*) $\gamma \subset \partial\Omega$, *the probability that a particle, starting either at the origin or uniformly distributed in Ω, making Brownian motion in Ω, reflecting when it hits $\partial\Omega \setminus \Gamma$, and escaping once it hits Γ, ends up escaping from γ is*

$$P(\gamma) = \int\limits_{\gamma} \bar{j}(y)\,\mathrm{d}S_y,$$

where $\mathrm{d}S_y$ is the surface element of $\partial\Omega$ at $y \in \partial\Omega$.

The proofs of these theorems will be published elsewhere.

3. Monte Carlo simulations

We also perform Monte Carlo simulations for the motion of Brownian particles starting in Ω and bouncing back from $\partial\Omega$. From the Monte Carlo sample paths, we find the first time that a particle hits Γ, and from these first hitting times we calculate the related statistical quantities. The escape problem involves a stochastic process $\{x^t(p)\}_{t\geqslant 0, p\in D}$ where we approximate the stochastic process by particles 1 to k and let

$$X_i^0 = \eta_{i0}, \qquad \hat{X}_i^k := X_i^{(k-1)\Delta t} + \eta_{ik}\sqrt{\Delta t}, \qquad X_i^{k\Delta t} = \frac{\hat{X}_i^k}{\max\{1, |\hat{X}_i^k|^2\}}, \quad i = 1,\dots,n,\ k = 1,2,\dots,$$

where $\{\eta_{10},\dots,\eta_{n0}\}$ are the starting positions related to the initial distribution of the particle, and $\{\eta_{ik} \mid i = 1,\dots,n,\ k = 1,2,\dots\}$ are i.i.d. random variables with mean vector $(0,0)$ and covariance matrix equal to identity. Note that $\hat{X}_i^k$ is the would be position at time $k\Delta t$ of the discretized Brownian particle without bouncing from $\partial\Omega$. In our computations, we represent bouncing from the boundary $\partial\Omega$ by the Kelvin transformation $z \longrightarrow z/|z|^2$ for $|z| > 1$. Other reflection principles can also be used; for example, one can return the particle to its position before it took the final step causing reflection, or reflect the particle geometrically from the boundary without significant change in the results provided the step size is small. If we are simulating particles starting from a fixed point $z \in \Omega$, we simply take $\eta_{ij} = z$ for $i = 1,\dots,n$. In the computations below we take all particles starting from the center, $z = 0$. For exit times from random points, one can generate random starting points from CRNs.

The discretized Brownian motion. As long as $\{\eta_{ik}\}$ are i.i.d. random variables with mean vector $(0,0)$, covariance matrix $\mathbf{I}$ and finite fourth order momentum, the limit, as $\Delta t \searrow 0$, of the piecewise linear curve connected by points $\{(k\Delta t, X_i^{k\Delta t})\}_{k=0}^{\infty}$ is a Brownian motion path. There are two standard choices of the i.i.d. random variables $\{\eta_{ik}\}$:

(i) $\{\eta_{ik} \mid i = 1,\dots,n,\ k = 1,2,\dots\}$ are i.i.d. random variables with binary (in each component) distribution, i.e. a $\frac{1}{4}$ probability of moving either up, down, left, or right.

(ii) $\{\eta_{ik} \mid i = 1,\dots,n,\ k = 1,2,\dots\}$ are i.i.d. random variables with $N((0,0),\mathbf{I})$ Gaussian distribution. This is the method we use.

The first hitting time. For the ith particle path, $\{X_i^{k\Delta t}\}_{k=0}^{\infty}$, its time of first hitting Γ is defined as

$$T_i := k_i\Delta t, \qquad k_i := \min\{k \in \mathbb{N} \mid \arg(X_i^{k\Delta t}) \in [-\varepsilon, \varepsilon],\ |\hat{X}_i^k| \geqslant 1\}.$$

We terminate the simulation for the ith particle when we reach the time T_i.

The sample mean and standard deviation of the first hitting time. In a given Monte Carlo simulation, $\{\eta_{ik}\}$ are generated from CRNs according the needed distribution. The sample mean and sample standard deviation are calculated by $\hat{T} = n^{-1}\sum_{i=1}^{n} T_i$ and $\hat{\sigma} = (n-1)^{-1/2}\{\sum_{i=1}^{n}(T_i - \hat{T})^2\}^{1/2}$. By the central limit theorem, for $n \geqslant 10$, we can present our conclusion from a Monte Carlo simulation as

$$T_{\Delta t} = \hat{T} \pm \frac{\hat{\sigma}}{\sqrt{n}} \quad \text{with 65\% confidence}, \qquad T_{\Delta t} = \hat{T} \pm \frac{2\hat{\sigma}}{\sqrt{n}} \quad \text{with 95\% confidence}.$$

In our simulation, we take $n = 90\,000$ particles, so the central limit theorem can be reasonably applied. Numerically, it may be preferable to use $\Delta x := \sqrt{\Delta t}$ as a parameter to address the accuracy of the approximation of the Brownian motion by discretization. The percent error in the computed time (compared with the exact result) is shown in Fig. 1(a).
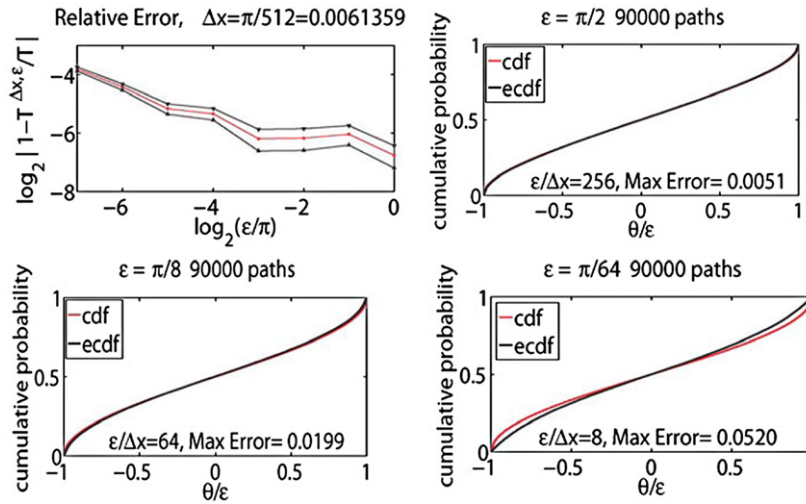
Fig. 1. Clockwise from top left: (a) Relative error for step size $\Delta x = \pi/512$; (b)–(d) True cumulative distribution function (cdf) (Brownian motion) compared with empirical cumulative distribution function (ecdf) for various ε.

Distribution of exits. Using the positions of the sample exits $\{X_i^{T_i}\}_{i=1}^n \subset \Gamma$, we can find the sample distribution of the exits along the gate and compare it with the theoretical density $\bar{j}(y)$, $y \in \Gamma$ from Theorem 4. The results are shown in Fig. 1(b), (c), (d), from which we can see that the error in the computed solution decreases as the step size becomes a large fraction of the gate.

References

[1] Xinfu Chen, Avner Friedman, Asymptotic analysis for the narrow escape problem, preprint.
[2] I.V. Grigoriev, Y.A. Makhnovskii, A.M. Berezhkovskii, V.Y. Zitserman, Kinetics of escape through a small hole, J. Chem. Phys. 116 (2002) 9574–9577.
[3] D. Holcman, Z. Schuss, Diffusion escape through a cluster of small absorbing windows, J. Phys. A: Math. Theory 41 (2008) 155001.
[4] S. Pillay, M.J. Ward, A. Peirce, R. Straube, T. Kolokolnikov, An asymptotic analysis of the mean first passage time for narrow escape problems, in press.
[5] S. Redner, A Guide to First Passage Time Processes, Cambridge Univ. Press, Cambridge, 2001.
[6] Z. Schuss, Theory and Applications of Stochastic Differential Equations: An Analytical Approach, Springer, New York, 2010.
[7] A. Singer, Z. Schuss, D. Holcman, Narrow escape, Part II: the circular disk, J. Stat. Phys. 122 (2006) 465–489.
[8] Z. Zwanzig, A rate process with an entropy barrier, J. Chem. Phys. 94 (1991) 6147–6152.