Analytical and Numerical Results on Escape of Brownian Particles

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July 1, 2012

Ref: Analytical and Numerical Results for an Escape Problem
Caginalp and Chen
Archive for Rational Mechanics and Analysis, 203, 329-342 (2012)
Comptes Rendus Matematique 349, 191-194 (2011).

1. The problem and its applications

-Chemical process - Molecules A, B with $m_a >> m_b$ drift around. While B is moving, A essentially stationary.

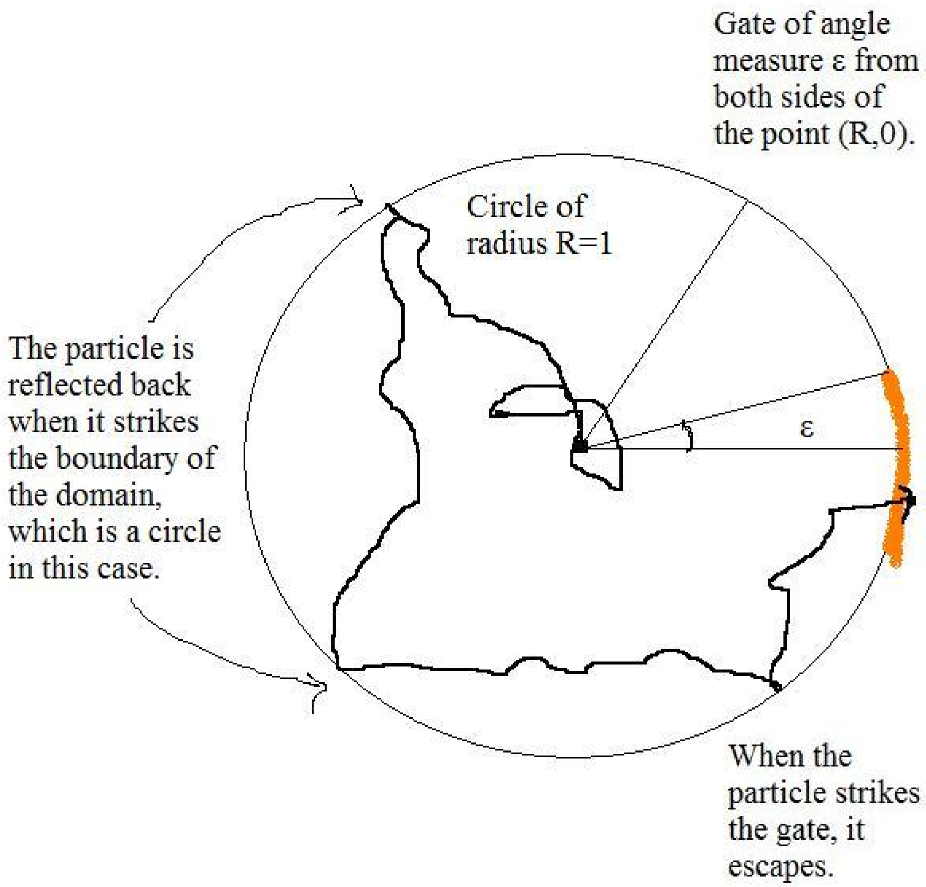
-Impurities diffusing through materials.

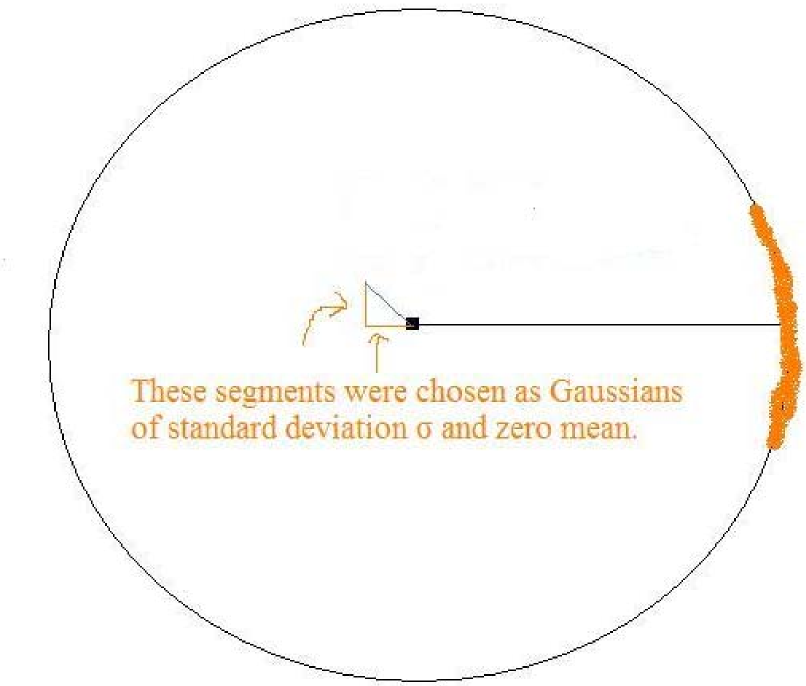
-Ion within a cell in a charged medium-reduction in electric gradient as more escape.

Biological process - Predator-prey systems

Financial mathematics -Triggering of stock options

The narrow escape problem involves a stochastic process where T is the time of first hitting a particular part of a boundary (escape) Γ_{ε}.





In my computer simulations, the motion of the particle is determined by a sequence small "steps." For each step, there was a displacement in each direction determined by a Gaussian function with a given mean and standard deviation.

(Redner 2001)

Background; stochastics to deterministic PDE

We start with the equation

$$d\vec{x} = \vec{b}dt + \boldsymbol{\sigma} d\vec{w} \tag{1.1}$$

where $\vec{w} = [w_1(t), \ldots, w_n(t)]^T$ is Brownian motion in n dimensions. Later, this will be approximated in the numerics by $\vec{x}(t+\Delta t) = \vec{x}(t) + \boldsymbol{\sigma}\vec{N}(0,1)\Delta t$.

Definition of Brownian Motion. A real-valued stochastic process $w(t,\omega)$ defined on $\mathbb{R}_+ \times \Omega$ is a mathematical Brownian motion if

(1) $w(0,\omega) = 0$ with probability 1.

(2) $w(t,\omega)$ is a continuous function of t almost everywhere.

(3) For every $t, s \geq 0,$ the increment $\Delta w(s) = w(t+s,\omega) - w(t,\omega)$ is independent of events prior to t, and is a zero mean Gaussian random variable with variance

$$Variance := E|\Delta w(s)|^2 = s.$$

2. Derivation of the PDEs from Stochastic Differential Equations

By Ito's formula (essentially chain rule for stochastics):

$$df(\vec{x}(t),t) = Lfdt + (\nabla f)^T \boldsymbol{\sigma} d\vec{w} \qquad (2.1)$$

Let $a_{ij} = (\boldsymbol{\sigma}\boldsymbol{\sigma}^T)_{ij};$ then

$$Lf = \frac{\partial f}{\partial t} + \vec{b} \cdot \nabla f + \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j} =: \frac{\partial f}{\partial t} + Mf$$

In our case, we consider $\vec{b} = 0$ and $\boldsymbol{\sigma} = \sigma_0 I,$ where σ_0^2 is the variance, so we have

$$df(\vec{x}(t),t) = Lfdt + \nabla_x f\sigma_0 I d\vec{w} \qquad (2.1')$$

and

$$Lf = \frac{\partial f}{\partial t} + \frac{1}{2}\sum_{i=1}^{n}\sigma_0^2\frac{\partial^2 f}{\partial x_i^2} = \frac{\partial f}{\partial t} + Mf.$$

Now let $\vec{x}(t)$ be the solution of (1.1) and $\tau_{x,s} = \inf\{t \geq s : \vec{x}(t) \in \partial\Omega,\ \vec{x}(s) = \vec{x}\}$ be the first exit time of $\vec{x}(t)$ from Ω. We want to find the expected escape time $\mathbb{E}\tau_{x,s}$.

So we define $u(\vec{x},t)$ as the solution of

$$\frac{\partial u}{\partial t} + Mu = -1,\ t \geq s,\ \vec{x} \in \Omega$$
$$u(\vec{x}, t) = 0, \quad \vec{x} \in \partial\Omega.$$

Now we apply Ito's Lemma (integral form of (2.1)) to the function $u(\vec{x}(t), t)$ and obtain

$$u(\vec{x}(t), t) = u(\vec{x}, s) + \int_s^t \left(\frac{\partial u}{\partial \tilde{t}} + Mu \right) d\tilde{t} + \int_s^t (\nabla u)^T \cdot \boldsymbol{\sigma} d\vec{w}(t') \tag{2.2}$$

for all $s \leq t \leq \tau_{x,s}$. Setting $t = \tau_{x,s}$ and taking the expectation value of both sides of equation (2.2), conditioned on $\vec{x}(s) = \vec{x}$, we have

$$\mathbb{E}\left[u(\vec{x}(\tau_{x,s}), \tau_{x,s}) \ | \vec{x}(s) = \vec{x} \right] = u(\vec{x}(s), s) + \mathbb{E} \int_s^{\tau_{\vec{x},s}} (-1) dt' + 0 \tag{2.3}$$

since $E(d\vec{w}(t')) = 0$. Therefore, since $\vec{x}(\tau_{\vec{x},s}) \in \partial\Omega$, the BC above imply $u(\vec{x}(\tau_{\vec{x},s}), \tau_{\vec{x},s}) = 0$, so LHS of (2.3) vanishes, yielding

$$0 = u(\vec{x}, s) - \mathbb{E}\tau_{\vec{x},s} + s \Rightarrow \mathbb{E}\tau_{\vec{x},s} = s + u(\vec{x}, s).$$

If $\vec{b}$ and $\boldsymbol{\sigma}$ are functions of only $\vec{x}$, and not t, as they are in our case, then $\mathbb{E}\tau_x = u(\vec{x})$, where $u(\vec{x})$ is the solution of the elliptic boundary value problem

$$Mu = -1 \text{ in } \Omega \tag{2.4}$$
$$u = 0 \text{ on } \partial\Omega.$$

3. Rigorous Asymptotic Analysis

Now consider domain in which there is reflection on $\partial\Omega \setminus \Gamma_\varepsilon$ and termination at Γ_ε.

-Seek solution $T_\varepsilon(z)$ in 2D to the equations

$$-\Delta T = |\Omega|^{-1} \text{ in } \Omega \qquad (3.1)$$
$$T = 0 \text{ on } \Gamma_\varepsilon$$
$$\partial_n T = 0 \text{ on } \partial\Omega \setminus \Gamma_\varepsilon$$

-Singer, Schuss, Holcman:

$$T(z) = \frac{|\Omega|}{4\pi}\left[\ln\left(\frac{1}{\varepsilon}\right) + O(1)\right]$$

-Xinfu Chen and Avner Friedman (2010) use conformal mappings

Unit Circle→Upper Half-Plane→Even Reflection across →Half-Plane

where gate is mapped from

Part of unit circle→Negative real axis→Imaginary axis

obtain approximation $T_\varepsilon^{app}(z)$ s.t.

$$|T_\varepsilon^{app}(z) - T_\varepsilon(z)| \leq C\varepsilon$$

for $\varepsilon < \varepsilon_0$ and $|1 - z| > \delta(\varepsilon)$, C indepedent of ε and z.

$$T_\varepsilon^{app}(z) = \frac{1 - |z|^2}{4\pi} + \frac{1}{\pi}\ln\frac{2|1 - z|}{\varepsilon} + O(\varepsilon) + \frac{O(\varepsilon^2)}{dist(z, \Gamma_\varepsilon)}$$

$$\bar{T} = \frac{1}{8\pi} + \frac{1}{\pi}\ln\frac{2}{\varepsilon} + O(\varepsilon)$$

4. An exact solution for arbitrary size gate.

Theorem A Closed Formula (CC&XC) In 2-D, with points identified by complex numbers, let

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

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

$$T(z) = \frac{1-|z|^2}{2} + 2\log\left|\frac{1-z+\sqrt{(1-ze^{-i\varepsilon})(1-ze^{i\varepsilon})}}{2\sin\frac{\varepsilon}{2}}\right|. \tag{4.1}$$

Idea of Proof. Need to show: T given in (4.1) satisfies (3.1). For this, we use $\Re(z)$ and $\Im(z)$ to denote the real and imaginary part of a complex number z. For $z \in \Omega$ we have

$$\Re\left\{1-z+\sqrt{(1-ze^{-i\varepsilon})(1-ze^{i\varepsilon})}\right\}$$

$$= \Re(1-z) + \Re\sqrt{(1-ze^{-i\varepsilon})(1-ze^{i\varepsilon})} > 0.$$

Hence, the function

$$f(z) := 2\log\frac{1-z+\sqrt{(1-ze^{-i\varepsilon})(1-ze^{i\varepsilon})}}{2\sin\frac{\varepsilon}{2}}$$

is analytic in $\bar{\Omega} \setminus \{e^{i\varepsilon}, e^{-i\varepsilon}\}$ and continuous on $\bar{\Omega}$. Consequently, its real part, $\Re(f)$, is harmonic in Ω. Hence,

$$\Delta T(z) = \Delta\frac{1-|z|^2}{2} + \Delta\Re(f(z)) = \Delta\frac{1-|z|^2}{2} = -2 \quad \forall z \in \Omega.$$

We want to calculate
$\arg(1-e^{i(\theta-\varepsilon)})(1-e^{-i(\theta+\varepsilon)}) = \arg(1-e^{i(\theta-\varepsilon)}) + \arg(1-e^{-i(\theta+\varepsilon)})$
and then take square root.

Case (i) $|\theta| < \varepsilon$. Here the first angle, $\theta-\varepsilon$, is negative, while the second, $\theta+\varepsilon$, is positive. Hence, the first case (of the diagram) applies in the first and the second in the second. We have

$\arg(1-e^{i(\theta-\varepsilon)}) + \arg(1-e^{-i(\theta+\varepsilon)})$
$= \left(\frac{\pi}{2} + \frac{\theta-\varepsilon}{2}\right) + \left(-\frac{\pi}{2} + \frac{\theta+\varepsilon}{2}\right) = \theta.$

Case (ii) $\theta \in (\varepsilon, 2\pi - \varepsilon)$. Here the first angle $\theta - \varepsilon$ and the second angle $\theta + \varepsilon$ are both positive, so the second case applies in both parts and we have

$\arg(1-e^{i(\theta-\varepsilon)}) + \arg(1-e^{-i(\theta+\varepsilon)})$
$= \left(-\frac{\pi}{2} + \frac{\theta-\varepsilon}{2}\right) + \left(-\frac{\pi}{2} + \frac{\theta+\varepsilon}{2}\right) = -\pi + \theta.$

Next, for $z \in \Gamma$, we can write $z = e^{\mathbf{i}\theta}$ with $|\theta| \leqslant \varepsilon$. Note $\sqrt{\square} = \rho e^{i\gamma}$ $\rho := \sqrt{|\sin^2(\varepsilon/2) - \sin^2(\theta/2)|}$ and $\gamma = \arg\sqrt{\square}$

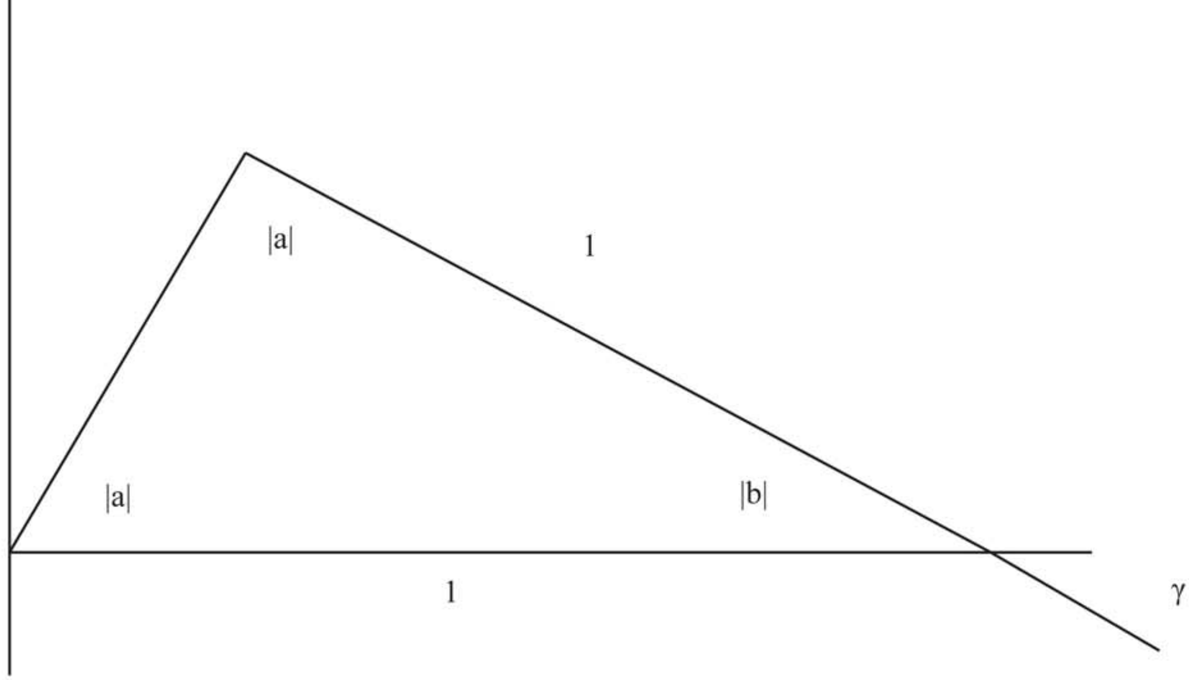
$f(e^{\mathbf{i}\theta}) :=$	$\lim_{r\nearrow 1} 2\log \dfrac{1 - re^{\mathbf{i}\theta} + \sqrt{(1-re^{\mathbf{i}[\theta-\varepsilon]})(1-re^{\mathbf{i}[\theta+\varepsilon]})}}{2\sin\frac{\varepsilon}{2}}$
	(now factor out $e^{i\theta/2}$)
	$= 2\log\left\{ e^{\mathbf{i}\theta/2} \dfrac{\sqrt{\sin^2\frac{\varepsilon}{2} - \sin^2\frac{\theta}{2}} - \mathbf{i}\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}} \right\}$
	$= \mathbf{i}\left\{\theta - 2\arcsin\dfrac{\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}}\right\} \quad \forall\,\theta \in [-\varepsilon, \varepsilon].$

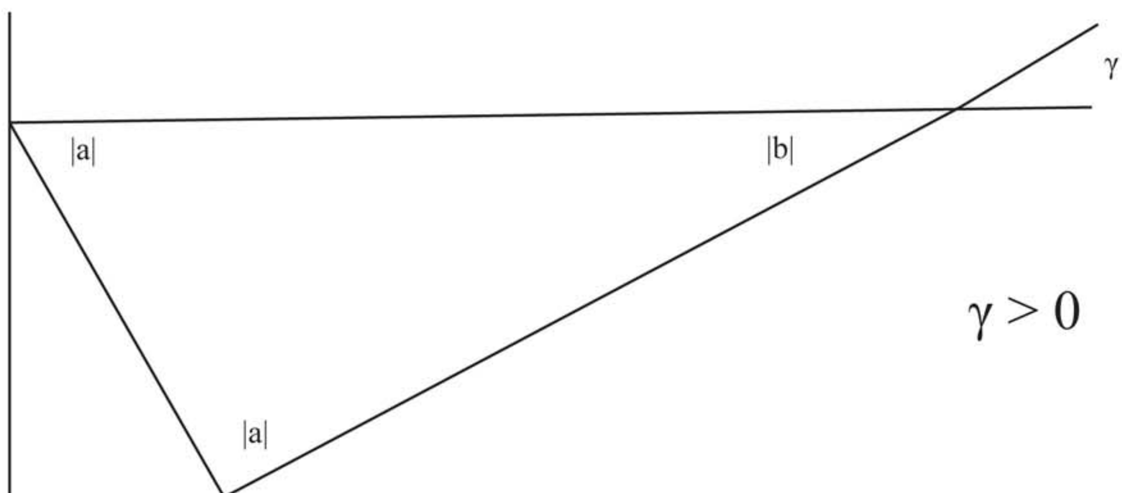
Thus, $\Re(f(z)) = 0$ when $z \in \Gamma$. Consequently, $T(z) = 0$ on Γ.

Similarly, for $z \in \partial\Omega \setminus \Gamma$, we write $z = e^{\mathbf{i}\theta}$ with $\theta \in (\varepsilon, 2\pi - \varepsilon)$ to obtain

(Case A) Consider 1 - exp(iγ) where $\gamma<0$
Geometry --> $2|a|+|b|=\pi$, or
$|a| = \pi/2 - |\gamma| /2 = \pi /2 + \gamma /2$
$\arg \{1 - \exp(i\gamma)\}=|a|= \pi /2 + \gamma /2$

$\gamma < 0$





(Case B) Consider 1 - exp(iγ) where $\gamma>0$
Geometry --> $2|a|+|b|=\pi$, or
$|a| = \pi/2 - |\gamma| /2 = \pi /2 - \gamma /2$
$\arg \{1 - \exp(i\gamma)\}= - |a| = - \pi /2 + \gamma /2$

$$\lim_{r\nearrow 1} \arg\sqrt{(1-re^{\mathbf{i}[\theta-\varepsilon]}))(1-re^{\mathbf{i}[\theta+\varepsilon]})}$$

$$= \frac{1}{2}\left\{-\frac{\pi}{2}+\frac{\theta-\varepsilon}{2}\right\} - \frac{1}{2}\left\{\frac{\pi}{2}-\frac{\varepsilon+\theta}{2}\right\} = \frac{\theta-\pi}{2}.$$

Hence,

$$f(e^{\mathbf{i}\theta}) := \lim_{r\nearrow 1} f(re^{\mathbf{i}\theta}) = 2\log\left\{e^{\mathbf{i}(\theta-\pi)/2}\frac{\sin\frac{\theta}{2}+\sqrt{\sin^2\frac{\theta}{2}-\sin^2\frac{\varepsilon}{2}}}{\sin\frac{\varepsilon}{2}}\right\}$$

$$= (\theta-\pi)\mathbf{i} + 2\ \operatorname{arccosh}\frac{\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}} \quad \forall\,\theta\in[\varepsilon, 2\pi-\varepsilon].$$

Here $\operatorname{arccosh} : [1,\infty) \to [0,\infty)$ is defined by $\operatorname{arccosh} z := \log[z+\sqrt{z^2-1}\,]$ for $z \geqslant 1$. It then follows from the Cauchy-Riemann equation that in the polar coordinates (r,θ),

$$\frac{\partial}{\partial r}\Re(f(e^{\mathbf{i}\theta})) = \frac{\partial}{\partial\theta}\Im(f(e^{\mathbf{i}\theta})) = 1 \quad \forall\,\theta\in(\varepsilon, 2\pi-\varepsilon).$$

Hence, for $z \in \partial\Omega\setminus\Gamma$,

$$\partial_n T(z) = \frac{\partial}{\partial r}\frac{1-|z|^2}{2} + \frac{\partial}{\partial r}\Re(f(z)) = 0.$$

Therefore, by the uniqueness of the solution of problem (3.1), T is given by the formula (4.1). ///

Theorem. (CC&XC) The average of the variance, $v(x) := \mathbb{E}[(\tau_x - T(x))^2]$, can be calculated from the formula

$$\bar{v} := \frac{1}{|\Omega|}\int_\Omega v(x)dx = \frac{1}{|\Omega|}\int_\Omega T^2(x)dx =: \overline{T^2}. \qquad (4.2)$$

Theorem. (CC&XC) The probability density of the location of a particle at time of its exit is given by

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

That is, 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

$$P(\gamma) = \int_\gamma \bar{j}(y)dS_y$$

where dS_y is the surface element of $\partial\Omega$ at $y \in \partial\Omega$.

5. Numerial Computation

Use

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \boldsymbol{\sigma}\vec{N}(0,1)\Delta t$$

to approximate

$$d\vec{x} = \vec{b}dt + \boldsymbol{\sigma}d\vec{w}$$

Motivation:

1- Effect of $\Delta x, \Delta t$ instead of $dx, dt,$ i.e. finite step size effect.

2- Does small gate exaggerate this effect?

3- In general, are C, ε_0 in the asymptotics such that formula is useful?

4- Develop numerical methodology to deal with arbitrary regions.

5- Can compare numerical result with exact solution, asymptotic approx, to find relationship between error, step size.

Paths $\{X_i^t\}_{t\geq 0}, i = 1, 2, \ldots, 400000$ start at center: $X_i^0 = (0, 0)$.

$Y_i^{t+\Delta t} = X_i^t + \eta_{it}\sqrt{\Delta t}, X_i^{t+\Delta t} = \dfrac{Y_i^{t+\Delta t}}{\max\left\{1, \lvert Y_i^{t+\Delta t}\rvert^2\right\}}$
for $t \in T = \{\Delta t, 2\Delta t, \ldots, 10^8 \Delta t\}$

The sample mean and sample standard deviation are

calculated by

$$\hat{T} = \frac{1}{n}\sum_{i=1}^{n} T_i, \qquad \hat{\sigma} = \left\{\frac{1}{n-1}\sum_{i=1}^{n}(T_i - \hat{T})^2\right\}^{1/2}.$$

Denote by $T_{\Delta t} = \lim_{n\to\infty}\hat{T}$. Then by the Central Limit Theorem, for $n \geqslant 10$, we can present our conclusion from a Monte-Carlo simulation as $\hat{T} \approx T_{\Delta t} + N(0, \hat{\sigma}^2/n)$, or simply

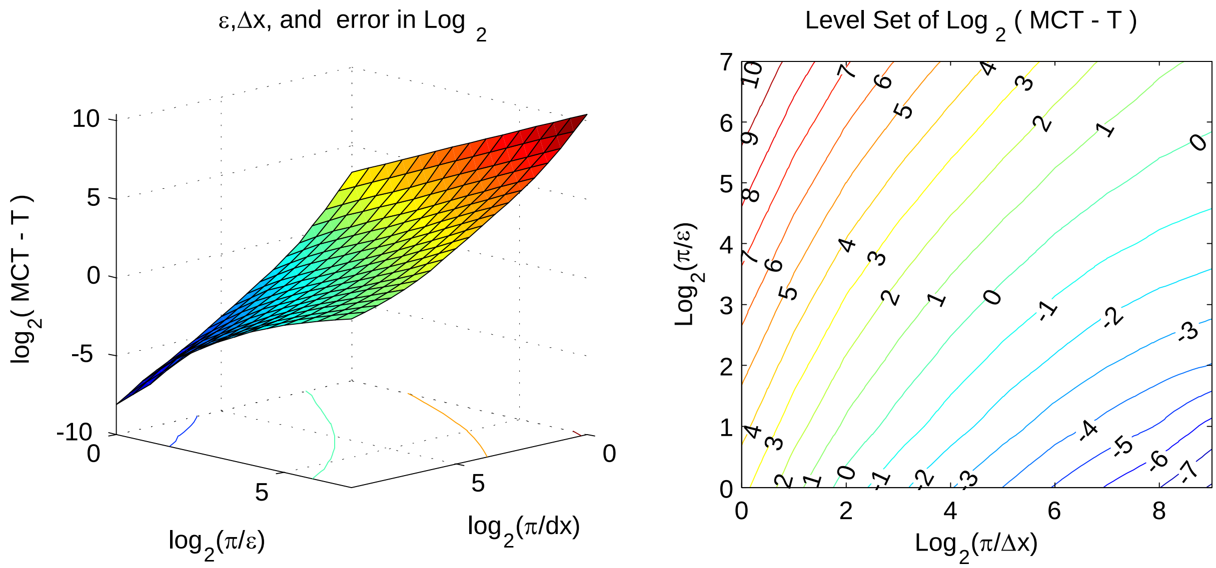
$$T_{\Delta t} = \hat{T} \pm \frac{\hat{\sigma}}{\sqrt{n}}, \qquad T_{\Delta t} = \hat{T} \pm \frac{3\hat{\sigma}}{\sqrt{n}}$$

In our simulations, we take $n = 400,000$ particles, so the Central Limit Theorem can be reasonably applied.

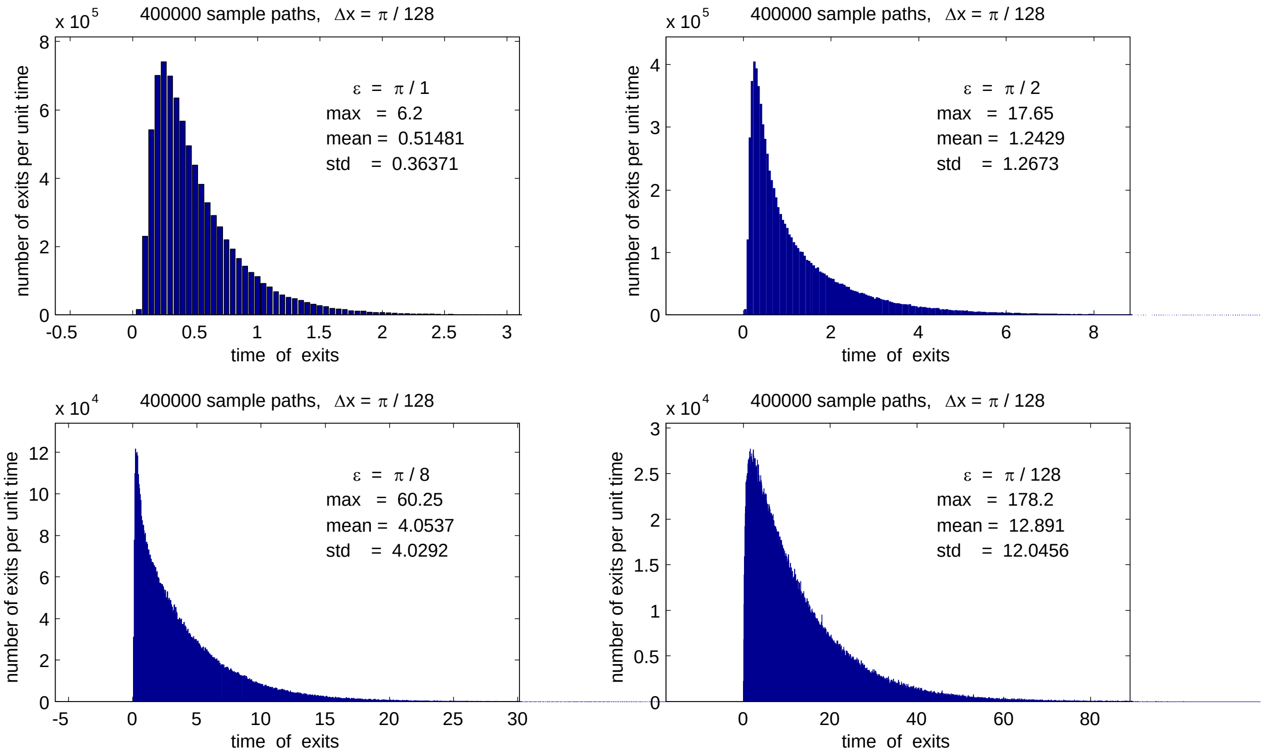
Parameters: $N = 400,000$, Δx varying from π to $\frac{\pi}{2^9}$, $\Delta t = (\Delta x)^2$ and ε varying from π (the whole circle) to $\frac{\pi}{2^7}$.

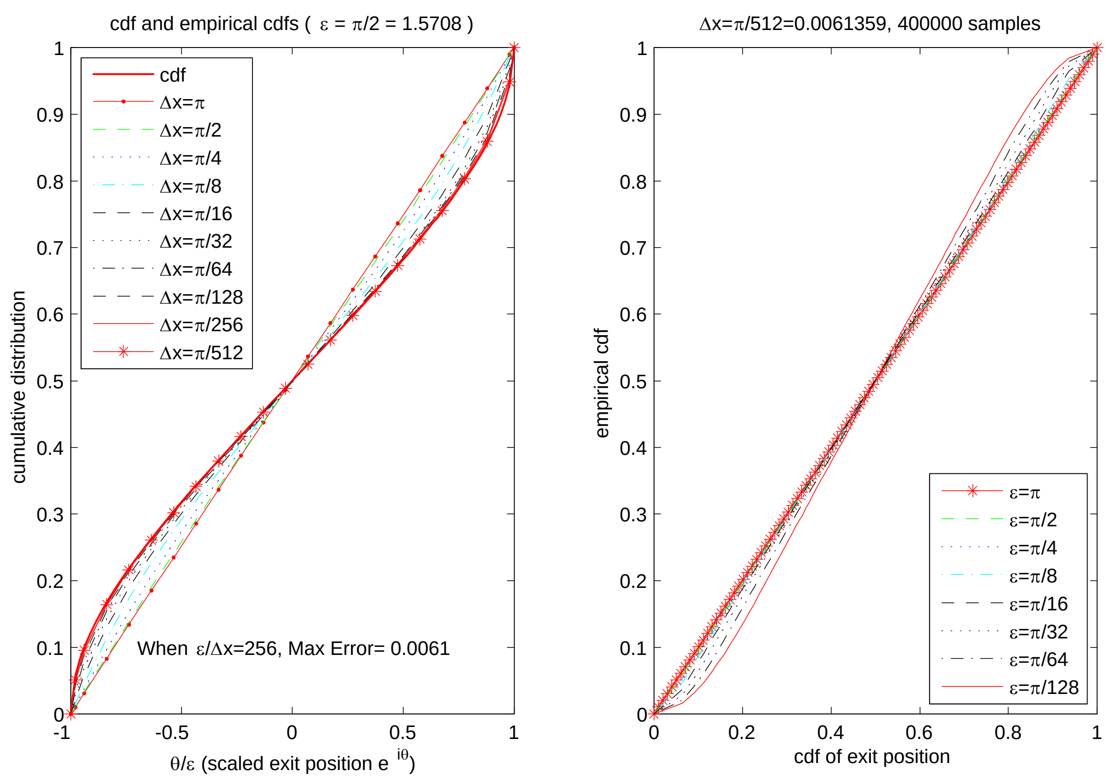
Typical standard deviation $\sigma^{\text{experimental}} \simeq T$ (empirical)

Discretization Error. Using the approximation $T_{\Delta t} \approx \hat{T} \pm \hat{\sigma}/\sqrt{n}$, we display the absolute error $T_{\Delta t} - T$ and relative error $T_{\Delta t}/T - 1$. From the Figure, one sees that $\log_2(T_{\Delta t} - T)$ is almost linear in $\log_2\varepsilon$ and in $\log_2\Delta x$. This suggests that



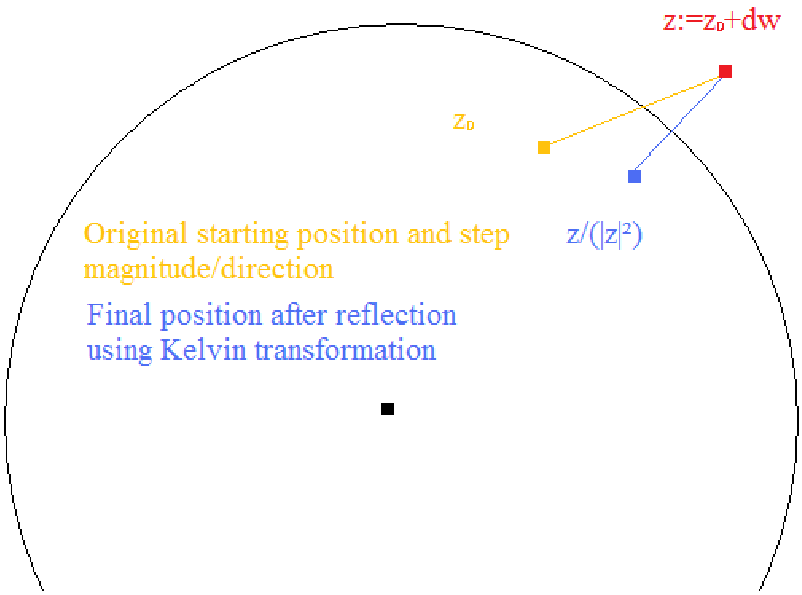
$$T_{\Delta t} - T \approx \frac{2\Delta x}{\varepsilon}, \qquad \frac{T_{\Delta t}}{T} - 1 \approx \frac{4\Delta x}{\varepsilon(1 + 4|\ln \sin \frac{\varepsilon}{2}|)} .$$


400000 sample paths, Δx = π / 128
x 10^5
number of exits per unit time
time of exits
ε = π / 1
max = 6.2
mean = 0.51481
std = 0.36371
400000 sample paths, Δx = π / 128
x 10^5
number of exits per unit time
time of exits
ε = π / 2
max = 17.65
mean = 1.2429
std = 1.2673
400000 sample paths, Δx = π / 128
x 10^4
number of exits per unit time
time of exits
ε = π / 8
max = 60.25
mean = 4.0537
std = 4.0292
400000 sample paths, Δx = π / 128
x 10^4
number of exits per unit time
time of exits
ε = π / 128
max = 178.2
mean = 12.891
std = 12.0456


cdf and empirical cdfs (ε = π/2 = 1.5708)
cdf
Δx=π
Δx=π/2
Δx=π/4
Δx=π/8
Δx=π/16
Δx=π/32
Δx=π/64
Δx=π/128
Δx=π/256
Δx=π/512
When ε/Δx=256, Max Error= 0.0061
cumulative distribution
θ/ε (scaled exit position e^iθ)
Δx=π/512=0.0061359, 400000 samples
ε=π
ε=π/2
ε=π/4
ε=π/8
ε=π/16
ε=π/32
ε=π/64
ε=π/128
empirical cdf
cdf of exit position

Some details of our program

Reflect with normal conditions



Instead of simulating one by one, do all N simultaneously using a matrix. As particles escape, delete and replace with new particles until last N are running, then wait for those to finish.

$$X = \begin{bmatrix} X_1^x & X_1^y \\ X_2^x & X_2^y \\ \dots & \dots \\ X_n^x & X_n^y \end{bmatrix}$$

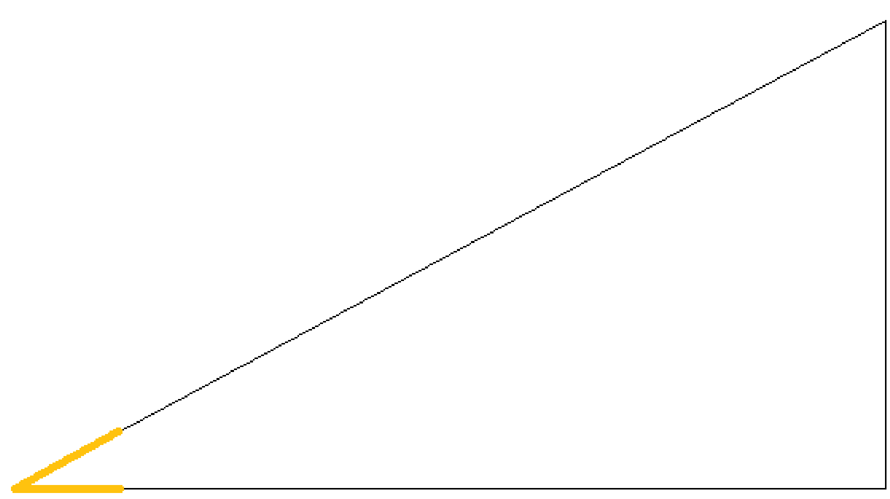
6. Future problems in Brownian motion

-Prove relation $T_{\Delta t} \approx T + \frac{2\sqrt{\Delta t}}{\varepsilon}$

-Design numerical scheme with smaller biased error, i.e.

$$T_{\Delta t} = T + \frac{O(\Delta t)}{O(\sqrt{\varepsilon}\,)}.$$

A. NARROW ESCAPE FOR A TRIANGULAR REGION.



We can use Schwarz-Christoffel transformation to map circle→triangle. Then need other ideas to transform solution.

Vertical side can be moved to ∞ to obtain limit of infinite wedge.

B. NONLINEARITY IN GATE SIZE AND SCALING RELATIONSHIPS. Let $\rho(x,y,t;\varepsilon)$:= survival probability of a particle starting from x and hitting y before gate of size ε.

When $x = 0$ we will omit it.

Let $S(t,\varepsilon) := \int_\Omega \rho(0,y,t;\varepsilon)dy.$ But now suppose that ε depends on $S,$ i.e.,

$$S(t,\varepsilon(S)) := \int_\Omega \rho(0,y,t;\varepsilon(S))dy.$$

In other words, the size of the gate becomes smaller as S becomes smaller. As more particles (charged ions) leave the cell the difference between the charge inside Ω and outside changes and results in pores that are smaller or larger (i.e., the gate size changes). For example, the gate size could be assumed to vary linearly with S :

$$\varepsilon(S) := aS + b.$$

A nonlinear problem is to examine how the mean escape time of a certain fraction of particles increases as a decreases, and to calculate the exponent of the increase. Other relationships beyond linearity can also be considered.

C. STOCHASTICS WITH DRIFT AND SCALING RELATIONSHIPS. Consider the usual stochastic process but add drift:

$$dX = bdt + \sigma dW$$

and assume we start at $X = 0.$ Let the domain be the unit circle with gate $\Gamma := \{e^{i\theta} : -\varepsilon < \theta < \varepsilon\}.$ Suppose the drift is in the negative or positive y direction (i.e., along the imaginary axis).

We can determine how the mean escape time (e.g., starting from 0) increases as we increase the magnitude of $b,$ and determine the exponent of this increase.

D. LET σ DEPEND ON THE RADIAL DISTANCE.

Suppose that the Brownian motion takes large steps near the center and smaller steps near the edge. For example,

$$\sigma(r) = e^{-a/|r-1|}.$$

Also, as $a \downarrow 0,\ T \to \infty$ by what exponent?

E. What is the differential equation satisfied by the finite random step problem (i.e., Δt as used in the numerics).