Séminaire de Mathématiques Appliquées du CERMICS

École des Ponts
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Simulation of Brownian motion's exit time from a domain

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6 décembre 2018

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December 6‹ 2018

Outline

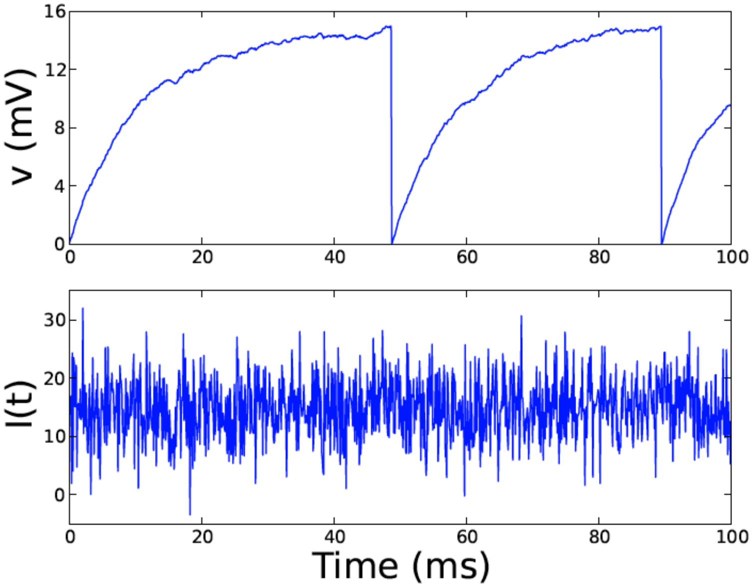
1. Introduction to the first-passage time (FPT) for a diffusion

Modeling biological or physical stochastic systems often requires to handle with diffusion processes.

Two types of information:

1. the marginal probability distribution function at a fixed time t.
2. the description of the whole paths (financial derivatives with barriers, ruin probability of an insurance fund, optimal stopping problems, neuronal sciences...)

Some Integrate and Fire models define the *spiking times* as the first hitting time of a threshold by the membrane potential. If the membrane potential $v(t)$ is described by a stochastic differential equation, the spiking times are the **first hitting times of the threshold v^{th} by such a diffusion.**


v (mV)
16
12
8
4
0
0
20
40
60
80
100
I(t)
30
20
10
0
0
20
40
60
80
100
Time (ms)

First-passage time τ_L

Let $(X_t,\ t \geq 0)$ be a one-dimensional diffusion process satisfying

$$dX_t = \sigma(X_t)dB_t + b(X_t)dt, \quad X_0 = x < L.$$

Aim: simulation of the FPT defined by $\tau_L := \inf\{t \geq 0 : X_t = L\}$.

Different tools for simulation purposes: explicit expression of the pdf, approximation of the stochastic process, rejection sampling...

Standard Brownian case ($B_0 = 0$):

The optional stopping thm applied to $M_t = \exp\{\lambda B_t - \frac{1}{2}\lambda^2 t\}$ leads to

$$\mathbb{E}[e^{-\lambda\tau_L}] = e^{-\sqrt{2\lambda}L}, \quad \lambda \geq 0.$$

Inversion of the Laplace transform:

$$\mathbb{P}(\tau_L \in dt) = \frac{1}{\sqrt{2\pi t^3}}\, e^{-\frac{L^2}{2t}}dt, \quad t > 0.$$

Hence $\tau_L \sim L^2/G^2$

where $G \sim \mathcal{N}(0,1)$.

Easy and exact simulation !

General one-dimensional diffusion processes:

We define the generator associated to the diffusion $(X_t,\ t \geq 0)$ by

$$Lf(x) = \frac{\sigma^2(x)}{2}\frac{d^2 f}{dx^2}(x) + b(x)\frac{df}{dx}(x), \quad \text{for } x \in \mathbb{R}.$$

Then the Laplace transform of the FPT is the unique solution of the following Sturm-Liouville boundary value problem on $]-\infty, L[$:

$$\begin{cases} Lu(x) = \lambda u(x), \\ u\,|_{x=L} = 1 \\ \lim_{x\to-\infty} u(x) = 0. \end{cases}$$

The following property holds:

$$\mathbb{E}_x[e^{-\lambda \tau_L}] = \frac{\psi_\lambda(x)}{\psi_\lambda(L)}$$

Here ψ_λ stands for the unique increasing positive solution of $Lu = \lambda u$.

Approximation of the pdf:

- by inversion of the Laplace transform
- by solving a Voltera-type integral equation when the transition probabilities of (X_t) have an explicit expression (see Buonocore, Nobile, Ricciardi).

- General method: time discretization

Instead of considering the approximation of the pdf, it is possible to deal directly with an approximation of the diffusion process (Euler scheme).

$$X_{(n+1)\Delta} = X_{n\Delta} + \Delta b(X_{n\Delta}) + \sqrt{\Delta}\,\sigma(X_{n\Delta}) G_n, \quad n \geq 0,$$

where (G_n) stands for a sequence of independent Gaussian distributed r.v.

Let τ_L^Δ be the FPT of the **discrete-time process.**

Overestimation of the FPT: $\tau_L \underset{st}{\leq} \tau_L^\Delta$

Important to improve the algorithm:

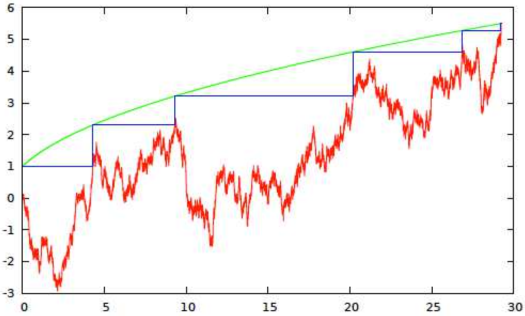
1. a shift of the boundary (Broadie-Glasserman-Kou, Gobet-Menozzi)
2. computation of the probability for a Brownian bridge to hit the boundary during a small time interval (Giraudo-Saccerdote-Zucca)

Advantage: rough description the paths. **But:** bounded time interval !

2. Simulation of the FPT: an iterative approach

Let us assume that X_t (solution of the SDE) satisfies $X_t = f(t, B_{\rho(t)})$ then τ_L is related to $\tau_\varphi^B := \inf\{t \geq 0 : \ B_t = \varphi(t)\}$.
Examples: linear or geometric diffusions.

- Approximate sequentially τ_φ^B for non decreasing functions φ.
- Simulate *simple* random variables (G_n standard gaussian r.v.)
- Stop the algorithm with an ϵ layer procedure



Initialization:

- $T_1 = 0$
- $T_2 = (\varphi(0)/G_0)^2$
- $\mathcal{N}^\epsilon = 1$

Evolution

- $T_1 \leftarrow T_2$
- $T_2 \leftarrow T_2 + (\varphi(T_2) - \varphi(T_1))^2 / G^2_{\mathcal{N}_\epsilon}$
- $\mathcal{N}_\epsilon \leftarrow \mathcal{N}_\epsilon + 1$

Stopping condition:

- $\varphi(T_2) - \varphi(T_1) \le \epsilon$

Outcome:

- $\tau_\varphi^{\epsilon,B} \leftarrow T_2$ and $\mathcal{N}_\epsilon$.

Theorem (H.-Tanré)

1. Assumptions:

$\varphi(0) > 0$ and $\limsup_{t\to\infty} \frac{\varphi(t)}{\sqrt{2t\log\log t}} < 1 \quad \Rightarrow \tau_\varphi$ is a.s. finite.

2. Convergence:

Let φ be an increasing $\mathcal{C}^1$-function + suitable conditions.

$$\text{Then } \tau_\varphi^{\epsilon,B} \Rightarrow \tau_\varphi^B \text{ as } \epsilon \to 0.$$

Theorem (H.-Tanré).

Rate of convergence. Let F (resp. F_ϵ be the cumulative distribution function of τ_φ (resp. τ_φ^ϵ). Then $F_\epsilon(t-\epsilon) - \frac{3\sqrt{\epsilon}}{\sqrt{2\pi}} \le F(t) \le F_\epsilon(t), \quad t \ge \epsilon$.

Number of steps: $\mathbb{E}[\mathcal{N}_\epsilon] \le C\sqrt{|\log \epsilon|}$.

Example: $\varphi(t) = \sqrt{1+t}$

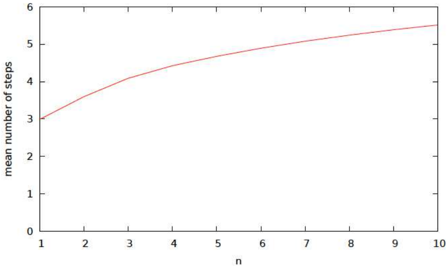
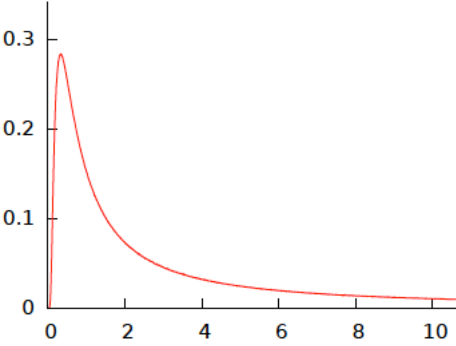


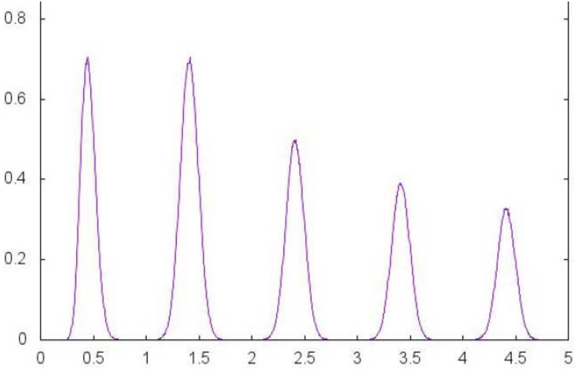
Figure: $\mathbb{E}(\mathcal{N}_\epsilon)$: mean number of steps for $\epsilon = 0.5^n$ as a function of n



Extention to general curved boundaries φ.

Application:
Ornstein-Uhlenbeck process
(LIF neuron model)

$$\begin{cases} dX_t = dB_t - \lambda X_t\, dt, \\ X_0 = x_0. \\ L(t) = \alpha + \beta \cos(\omega t). \end{cases}$$



We use the classical transformation to link both the O-U process and the Brownian motion: the same distribution as

$$Y_t := e^{-\lambda t}(x_0 + B_{\rho(t)}) \quad \text{with} \quad \rho(t) := \frac{1}{\lambda}(e^{2\lambda t} - 1).$$

Here $\varphi(t) = L(\frac{1}{2\lambda}\log(1 + \lambda t))\sqrt{1 + \lambda t} - x_0$.

Quite restrictive method: linear or geometric diffusion

3. Exact simulation of a diffusion FPT (acceptance-rejection method)

Principal idea: Let f and g two probability distribution functions, such that $h(x) := f(x)/g(x)$ is upper-bounded by a constant $c > 0$.
Aim: simulation of X with pdf f.

1. Generate a rv Y with pdf g.
2. Generate U uniformly distributed (independent from Y).
3. If $U \le h(Y)/c$, then set $X = Y$; otherwise go back to 1.

Important: h should be bounded and have an explicit expression !
Application to the FPT: Girsanov's transformation permits to

- link the distribution of $(X_t,\ t \ge 0)$ to $(B_t,\ t \ge 0)$.
- give an expression of the function h.

Girsanov's transformation was already used for simulation purposes by Beskos and Roberts (exact simulation on some fixed interval $[0, T]$).

From now on, $\sigma = 1$ (diffusion coefficient). We assume that the drift term $b \in \mathcal{C}^1(]-\infty, L])$ and introduce $\beta(x) = \int_0^x b(y)dy$ and $\gamma := \frac{b^2+b'}{2}$.

Girsanov's transformation

For any bounded measurable function $\psi : \mathbb{R} \to \mathbb{R}$, we obtain

$$\mathbb{E}_{\mathbb{P}}[\psi(\tau_L)1_{\{\tau_L<\infty\}}] = \mathbb{E}_{\mathbb{Q}}[\psi(\tau_L)\eta(\tau_L)] \exp\left\{\beta(L) - \beta(x)\right\},$$

where $\mathbb{P}$ (resp. $\mathbb{Q}$) corresponds to X (resp. B) and

$$\eta(t) := \mathbb{E}\Big[\exp - \int_0^t \gamma(L - R_s)ds \Big| R_t = L - x\Big].$$

Here $(R_t,\ t \geq 0)$ stands for a 3-dimensional Bessel process with $R_0 = 0$.

- Under $\mathbb{Q}$, it is easy to generate τ_L.
- An appropriate situation for a rejection method, if $\tau_L < \infty$ under $\mathbb{P}$.
- difficulties: we assume $0 \leq \gamma(x) \leq \kappa$ since η is not explicit.

Algorithm

Step 1: *Simulate a r.v.* $T = (L - x)^2/G^2$ *with* $G \sim \mathcal{N}(0,1)$.

Step 2: *Simulate a 3-dimensional Bessel process* (R_t) *on the time interval* $[0, T]$ *with endpoint* $R_T = L - x$ *and define*

$$D_{R,T} := \Big\{(t, v) \in [0, T] \times \mathbb{R}_+ : \ v \le \gamma(L - R_t)\Big\}.$$

Step 3: *Simulate a Poisson point process* N *on the state space* $[0, T] \times \mathbb{R}_+$, *independent of the Bessel process, whose intensity measure is the Lebesgue one.*

Step 4: *If* $N(D_{R,T}) = 0$ *then set* $Y = T$ *otherwise go to Step 1.*

Theorem (theoretical viewpoint) H.-Zucca

Y and the FPT of the diffusion process τ_L are identically distributed. Moreover the number of iterations satisfies $\mathbb{E}[\mathcal{I}] \le \exp((L - x)\sqrt{2\kappa})$.

4. Introduction to the Brownian exit problem

Let $\mathcal{D}$ be a bounded domain in $\mathbb{R}^d$. We denote by $\tau_{\mathcal{D}}$ the first exit time of the Brownian motion from the domain.
Aim: to simulate $(\tau_{\mathcal{D}}, B_{\tau_{\mathcal{D}}})$. Application to Initial-Boundary Value Problem (IBVP) for the heat equation.

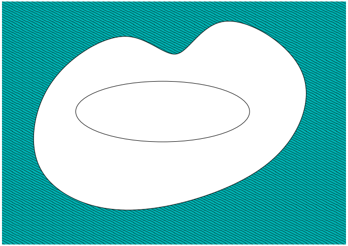
- *Historical background:* studies based on the Dirichlet problem for Laplace's equation:

$$\begin{cases} \Delta u(x) = 0, & \forall x \in \mathcal{D} \\ u(x) = f(x), & \forall x \in \partial\mathcal{D}, \end{cases}$$

  with the representation $u(x) = \mathbb{E}_x[f(B_{\tau_{\mathcal{D}}})]$.
- Idea: use the Monte-Carlo method and an accurate simulation of the exit location in order to approximate $u(x)$.
- Simulation of $B_{\tau_{\mathcal{D}}}$: Walk on Spheres algorithms WoS (Müller '56, Mascagni & Hwuang '03, Villa-Moralès '12 '16, Binder & Braverman '12) based on the mean-value formula and the martingale theory.

5. Exit problem: the classical walk on spheres (WoS)

1. Construct a random walk $(X_n)_{n\geq 0}$ starting from $X_0 = x$ which represents a simple squeleton of the Brownian paths
2. Find a martingale in order to prove the convergence of the WoS: $\lim_{n\to\infty} X_n = B_{\tau_{\mathcal{D}}}$ in distribution.
3. Describe the rate of convergence.

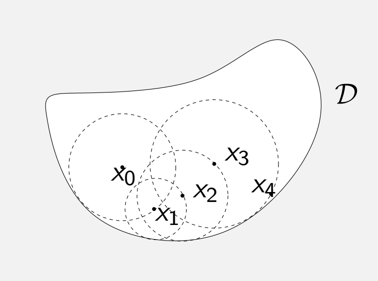


A simple remark:
in order to exit from the domain $\mathcal{D}$, the Brownian paths needs to exit from any smaller domain $\mathcal{D}'$ containing x.

The best choice:
the sphere centred in x (rotational invariance of BM). The exit location is then uniformly distributed on $\partial\mathcal{D}'$.

The procedure is then the following:

Let $\mathcal{S}^1$ the bigest sphere centred in x and included in $\mathcal{D}$, let X_1 the exit location of $\mathcal{S}^1$ for the BM. This point is then the *new initial point* and so on... We construct a MC: $(X_n,\ n \geq 0)$. V harmonic $\Rightarrow (V(X_n))_{n\geq 0}$ defines a martingale (mean-value formula).



X_n converges towards $X_\infty \in \partial\mathcal{D}$ (same distribution as $B_{\tau_\mathcal{D}}$)

An algorithm based on the chain (X_n) with a stopping procedure:

Stop as soon as $\boldsymbol{\delta(X_n, \partial\mathcal{D}) < \varepsilon}$ (Euclidian distance)

We denote by $\mathcal{N}_\varepsilon$ the number of steps of the algorithm

Rate of convergence (Binder & Braverman '12) $\mathbb{E}[\mathcal{N}_\varepsilon] = \mathcal{O}(|\log \varepsilon|)$.

6. Exit problem: the walk on spheroids.

1. Construct a simple random walk $(T_n, X_n)_{n\geq 0}$ starting from $(T_0, X_0) = (0, x)$ which represents a squeleton of the Brownian paths
2. Find a martingale in order to prove the convergence of the WoHB: $\lim_{n\to\infty}(T_n, X_n) = (\tau_{\mathcal{D}}, B_{\tau_{\mathcal{D}}})$ in distribution.
3. Describe the rate of convergence

Exit time and position for a **general domain** $\mathbb{R}_+ \times \mathcal{D}$**: too difficult !**

- A good idea: find a sequence of particular subdomains $\mathcal{D}'_n \subset \mathbb{R}_+ \times \mathcal{D}$ whose exit problem turns out to be simple !
- Let us start the random walk with $(T_0, X_0) = (0, x)$ and consider (T_1, X_1) the time and location of the exit problem associated to $\mathcal{D}'_1 \subset \mathbb{R}_+ \times \mathcal{D}$ and construct the Random Walk step by step.

Aim: choose $\mathcal{D}'_1$ in order to obtain a simple expression for (T_1, X_1).

First idea: the generic form of $\mathcal{D}'$ could be a cylinder $\mathbb{R}_+ \times \mathbb{S}$.

$$\mathbb{P}(\tau_{\mathbb{S}} > s) = \frac{1}{2^{\nu-1}\Gamma(\nu+1)} \sum_{k=1}^{\infty} \frac{j_{\nu,k}^{\nu-1}}{\mathcal{J}_{\nu+1}(j_{\nu,k})} e^{-\frac{j_{\nu,k}^2}{2}s}, \quad x > 0,\ \nu = d/2 - 1$$

$\mathcal{J}_\cdot$ is the Bessel function (first kind) and $j_{\cdot,k}$ its positive zeros.

One other choice for $\mathcal{D}'$ is the heat ball with the generic form:

$$\Gamma_{t,x} := \left\{(s,y) :\ \|y-x\| \le 2\sqrt{(s-t)\log((s-t)^{-d/2})} = 2\psi_d(s-t)\right\}$$

Result (method of images):

1. *p.d.f.* of the exit time τ_Γ: $p_d(s) = \frac{1}{\Gamma(d/2)}\ \frac{\psi_d^d(s)}{s} 1_{[0,1]}(s)$,

   thus $\quad \tau_\Gamma \sim e^{-G}$ where $G \sim \Gamma((d+2)/2, 2/d)$.
2. The location B_{τ_Γ} is uniformly distributed on $\partial B(x, 2\psi_d(\tau_\Gamma))$.

Using scaling prop., we define a r.w. on the boundaries of the heat balls.

At each step we choose the biggest heat ball which belongs to $[t, \infty] \times \mathcal{D}$.
Similar algorithms: Haji-Sheikh and Sparrow '66 introduced the Floating Random Walk (spheres), Sipin introduced the random walk on balloïds.

Consequences (Deaconu-H.)

- If h belongs to $\mathcal{C}^{1,2}(]0, \infty[\times\overline{\mathcal{D}})$ and if it is a temperature in $]0, \infty[\times\mathcal{D}$, then $\mathcal{M}_n := h(T_n, X_n)$ is a bounded martingale.
- The process $M_n = (T_n, X_n)$ converges almost surely as $n \to \infty$ to a limit (T_∞, X_∞) (same distribution as $(\tau_\mathcal{D}, B_{\tau_\mathcal{D}})$).

For numerical purposes, we need a ε-stopping procedure.

Efficiency result (Deaconu-H.).

Let $\mathcal{D}$ be a 0-thick domain (convex domains, domains with any cone condition, domains bounded by a smooth hypersurface). $\exists C > 0$ and $\varepsilon_0 > 0$ both independent of (t, x) such that the number of steps satisfies

$$\mathbb{E}[\mathcal{N}_\varepsilon] \leq C|\log \varepsilon|, \quad \text{for all} \quad \varepsilon \leq \varepsilon_0.$$

Application to the Initial-Boundary Value Problem (Deaconu - H.)

We consider the parabolic PDE:

$$\begin{cases} \partial_t u(t,x) = \Delta_x u(t,x), & \forall (t,x) \in \mathbb{R}_+ \times \mathcal{D}, \\ u(t,x) = f(t,x), & \forall (t,x) \in \mathbb{R}_+ \times \partial\mathcal{D}, \\ u(0,x) = f_0(x) & \forall\ x \in \mathcal{D}, \end{cases}$$

- f and f_0 being continuous functions.

Generic procedure

1. *Probabilistic representation:* We introduce $\tau_t = \tau_{\mathcal{D}} \wedge t$ then

$$u(t,x) = \mathbb{E}_x\Big[f(t-\tau_t, B_{\tau_t})1_{\{B_{\tau_t}\in\partial\mathcal{D}\}}\Big] + \mathbb{E}_x\Big[f_0(B_{\tau_t})1_{\{B_{\tau_t}\notin\partial\mathcal{D}\}}\Big].$$

2. *Monte-Carlo method:*

   A sequence of i.i.d r.v. $(\tau_n, Y_n)_{n\geq 0}$ (distributed as (τ_t, B_{τ_t})) leads to

$$u(t,x) \approx u_N(t,x) := \frac{1}{N}\sum_{n=1}^N f(t-\tau_n, Y_n)1_{\{Y_n\in\partial\mathcal{D}\}} + f_0(Y_n)1_{\{Y_n\notin\partial\mathcal{D}\}}.$$

The hypercube $\mathcal{D} =]0, L[^d$

$$\begin{cases} \partial_t u(t,x) - \Delta_x u(t,x) = 0, \\ u(t,x) = f(t,x), \text{ on } \mathbb{R}_+ \times \partial\mathcal{D}, \\ u(0,x) = f_0(x), \forall\ x \in \mathcal{D}. \end{cases}$$

We choose

$$f(t,x) = e^{-d\pi^2 t/L} \prod_{i=1}^{d} \sin(\pi x_i / L^2),$$

and $f_0(x) = f(0,x)$ for the compatibility assumptions.

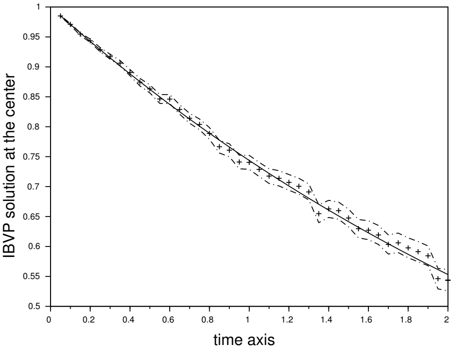
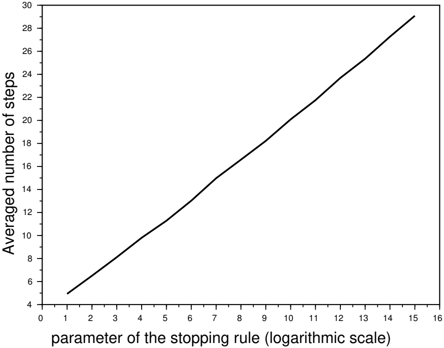
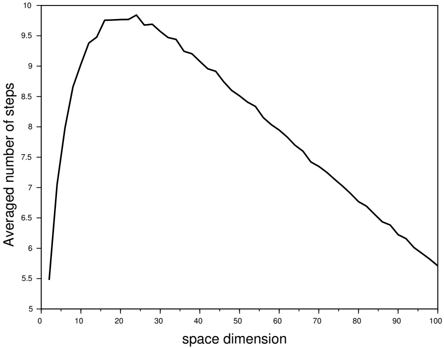


Figure: IBVP solution versus t. Exact solution (solid line), approximated solution $u_N^\varepsilon(t,x)$ (plus sign) and 95%-confidence interval, $L = 10$, $N = 1\,000$, $\varepsilon = 0.001$, $d = 3$.



Averaged number of steps versus n for $\varepsilon = 0.5^n$, 10 000 trials, $d = 3$, $t = 4$, $L = 10$.



Averaged number of steps versus the dimension d, $\varepsilon = 0.001$, 10 000 trials, $t = 4$, $L = 1$.

Summary and open questions

- Description of the efficiency for the Random Walk on Moving Spheres algorithm in order to simulate the Brownian exit time and location from a bounded domain in $\mathbb{R}^d$ (in order to solve the IBVP of the heat equation).
- General diffusions processes (application to IBVP for parabolic equations) ?

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Let us define:

$$R_{n+1} := \left(\Pi^U_{n+1}\right)^{2/d} \exp\Big\{ -(1-\frac{2}{d}\lfloor\frac{d}{2}\rfloor)G^2_{n+1}\Big\}$$

ALGORITHM

Initialisation: $(T_0, X_0) = (t, x)$.
Step n: The sequence is defined step by step as follows: for $n \geq 0$,

$$\begin{cases} T_{n+1} = T_n - \delta^2(X_n, \partial\mathcal{D})R_{n+1}, \\ X_{n+1} = X_n + 2\delta(X_n, \partial\mathcal{D})\psi_d(R_{n+1})V_{n+1}, \end{cases}$$

Stop If $\delta(X_n, \partial\mathcal{D}) \leq \varepsilon$ then $\mathcal{N}_\varepsilon = n$. Outcome $(T_\varepsilon, X_\varepsilon) := (X_{\mathcal{N}_\varepsilon}, T_{\mathcal{N}_\varepsilon})$.