UNCERTAIN DARCY'S PROBLEM AND THE STOCHASTIC PARTICLE TRANSPORT

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1 Expected exit time from a domain

We aim to estimate the exit time of a particle driven by a deterministic transport field and a stochastic diffusion from a domain $D \subset \mathbb{R}^d$. Given a vector $W(t)$ of m independent Brownian motions and two functions $f\colon \mathbb{R}^d \to \mathbb{R}^d, g\colon \mathbb{R}^d \to \mathbb{R}^{d\times m}$, we consider the following stochastic differential equation (SDE)

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases} \tag{1}$$

The problem is completed with two different types of boundary conditions, namely

i. *killing boundaries*: if the particle exits D the process is stopped,

ii. *reflecting boundaries*: the particle trajectory is reflected normally inside D when it touches the boundary ∂D.

Our aim is to estimate numerically the first exit time of the solution $X(t)$ from D, *i.e.*, the quantity

$$\tau = \min\{\min\{t\colon X(t) \notin D\}, T\}. \tag{2}$$

Let us remark that the parameter τ is meaningful only if there exists a portion of the boundary $\Gamma_k \subset \partial D$ that is endowed with killing boundary conditions. Otherwise, the process $X(t)$ will stay in D for the whole time interval, giving as a result $\tau = T$ for each realisation of $X(t)$. In the case of general f, g and for a d-dimensional SDE, there is no closed form for τ. Therefore, we approximate the value of τ by means of two numerical schemes, briefly presented in the following.

1.1 Numerical Methods

1.1.1 Discrete Euler-Maruyama

Given $N \in \mathbb{N}$ let us define a partition of $[0, T]$ as $P_h = \{t_i\}_{i=0}^N, t_i = ih, h = T/N$. The Discrete Euler-Maruyama method (DEM) for problem (1) is defined as follows

$$\begin{cases} X_h^d(t_{i+1}) = f(X(t_i))h + g(X(t_i))(W(t_{i+1}) - W(t_i)), \\ X_h^d(0) = X_0. \end{cases} \tag{3}$$

The exit time τ is approximated with the quantity τ_h^d defined as

$$\tau_h^d = \min\{\min\{t_i \colon X_h^d(t_i) \notin D\}, T\}. \tag{4}$$

Let us define the error as

$$err_h^d = |\tau_h^d - \tau|. \tag{5}$$

It is possible to show [1] that err_h^d is $O(h^{1/2})$.

1.1.2 Continuous Euler-Maruyama.

Let us consider the partition P_h of $[0, T]$ as above. The Continuous Euler-Maruyama (CEM) method is defined as

$$\begin{cases} X_h^c(t) = f(X(t_i))h + g(X(t_i))(W(t_{i+1}) - W(t_i)), & t_i < t \leq t_{i+1}, \\ X_h^c(0) = X_0. \end{cases} \tag{6}$$

Let us remark that in case the particle does not exit the domain, $X_h^c(t_i) = X_h^d(t_i)$ for all $t_i \in P_h$. It is possible to compute the probability that a particle has exited the domain at a time t between two consecutive timesteps t_i, t_{i+1} when D is an half-space with the following formula [1]

$$\mathbb{P}(\exists t \in [t_i, t_{i+1}] \quad X_h^d(t) \notin D | X_h^d(t_i) = x_i, X_h^d(t_{i+1}) = x_{i+1}) = p(x_i, x_{i+1}, h), \tag{7}$$

with $p(x_i, x_{i+1}, h)$ given by

$$p(x_i, x_{i+1}, h) = \exp\Big(-2\frac{[n \cdot (x_i - z_i)][n \cdot (x_{i+1} - z_i)]}{hn \cdot (gg^T(x_i)n)}\Big), \tag{8}$$

where z_i is the projection of x_i on ∂D and n is the normal to ∂D in z_i. At each timestep t_{i+1} we compute the probability $p(x_i, x_{i+1}, h)$, and then simulate a variable U distributed uniformly in the interval $[0, 1]$, thus obtaining a realization u. Hence, we counclude that the particle has left the domain for a time t in (t_i, t_{i+1}) if u is smaller than p. Therefore, we approximate the exit time as

$$\tau_h^c = \min\{T, \min\{t_i = hi \colon X_h(t_i) \notin D\}, \min\{t_i = hi \colon u < p(x_{i-1}, x_i, h)\}\}, \tag{9}$$

Finally, we estimate the error

$$err_h^c = |\tau_h^c - \tau|, \tag{10}$$

For this numerical scheme, the error is expected to be $O(h)$ [1].

1.1.3 Reflecting boundaries

The reflecting boundaries are treated in the same way for both DEM and CEM. Let us denote by Γ_k and Γ_r the killing and reflecting subsets of ∂D, *i.e.*

$$\Gamma_r \cup \Gamma_k = \partial D, \quad \Gamma_r \cap \Gamma_k = \emptyset \tag{11}$$

In case the particle approaches Γ_k the exit is treated as above. If for a timestep of $t_i \in P_h$, $X(t_i)$ is not in D and has crossed Γ_r at a time $t_{i-1} < t < t_i$, we update the solution to be the normal reflection inside D of $X(t_i)$.

1.2 One-Dimensional Case

We consider problem (1) in case $d = 1$. Given $f, g\colon \mathbb{R} \to \mathbb{R}$, an interval $D = [l, r]$ and a Brownian motion $W(t)$, let us consider the following one dimensional SDE

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases} \tag{12}$$

In this case, the boundary of D consists of the two points $\{l, r\}$. In order for the problem of the determination of τ to be meaningful, at least one of the two points should be endowed with a killing boundary condition.

1.2.1 Analytical expression of the exit time

In this simple frame, it is possible to deduce an analytical formulation of the expectation of τ as a function of $X_0 = x$. Let us consider the boundary condition at $x = l$ fixed as *killing* and vary the boundary condition at $x = r$. Since the scope is deducing the exit time of a particle from D, this assumption is plausible. It is possible to show [2, 3] that the expected exit time $\bar{\tau} = \mathbb{E}(\tau | X_0 = x)$ is in the one-dimensional case the solution of the following boundary value problem

$$\begin{cases} f(x)\bar{\tau}'(x) + \frac{1}{2}g^2(x)\bar{\tau}''(x) = -1, & l < x < r, \\ \bar{\tau}(l) = 0, & \\ \bar{\tau}(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{killing}, \\ \bar{\tau}'(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{reflecting}. \end{cases} \tag{13}$$

The solution of (13) is given by

$$\bar{\tau}(x) = -2\int_l^x \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy + c_1 \int_l^x \exp(-\psi(y))dy + c_2, \tag{14}$$

where the function ψ is defined as

$$\psi(x) = \int_l^x \frac{2f(y)}{g^2(y)} dy, \tag{15}$$

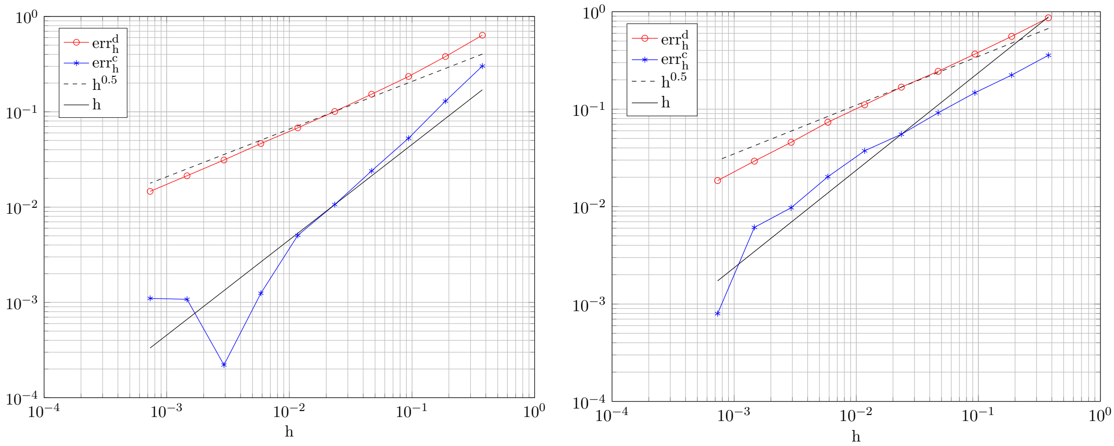
and the constants $c_1, c_2 \in \mathbb{R}$ depend on the boundary conditions as follows

$$\begin{aligned} c_1 &= 2\frac{\int_l^r \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy}{\int_l^r \exp(-\psi(y))dy}, \text{ if for } x = r \text{ the boundary is } \textit{killing}, \\ c_1 &= 2\int_l^r \frac{\exp(-\psi(y))}{g(y)^2} dy, \text{ if for } x = r \text{ the boundary is } \textit{reflecting}, \\ c_2 &= 0. \end{aligned} \tag{16}$$

Let us remark that in case $f = -V'$ for some smooth function V and $g = \sigma \in \mathbb{R}$, the expression of ψ semplifies to

$$\psi(x) = 2\frac{V(l) - V(x)}{\sigma^2}. \tag{17}$$

The value for the expected exit time given by (14) will be used as a reference for verifying the order of convergence of the numerical methods.



(a) Killing boundary in $x = 1$

(b) Reflecting boundary in $x = 1$

Figure 1: Orders of convergence for DEM and CEM in the one-dimensional case.

1.2.2 Numerical experiments

We consider as a domain for (12) the interval $D = [-1, 1]$, final time $T = 3$ and the following functions

$$\begin{aligned} &f(x) = -V'(x), \text{ where } V(x) = 0.1(8x^4 - 8x^2 + x + 2),\\ &g(x) = \sigma = 1. \end{aligned} \tag{18}$$

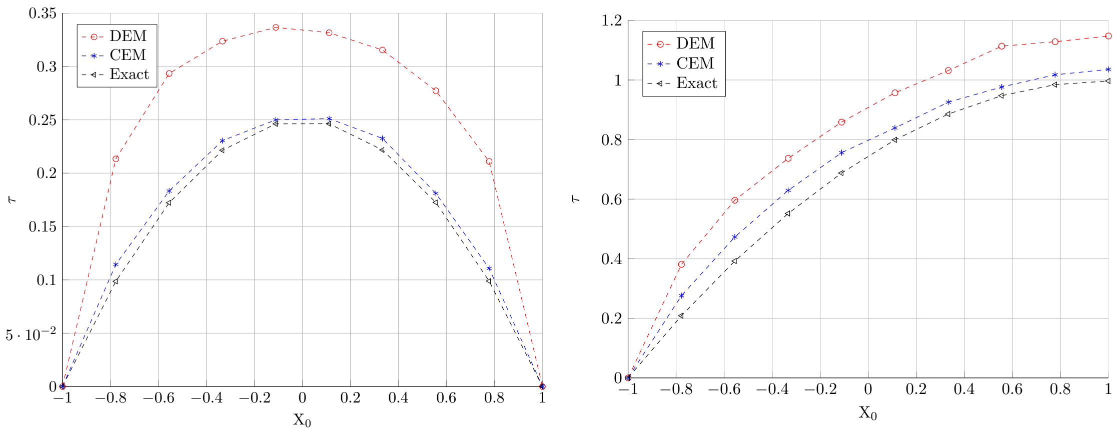
We approximate the value of τ with a Montecarlo simulation of τ_h^d and τ_h^c computed as in (4) and (9) from the solutions provided by DEM and CEM respectively. In order to verify the order of convergence of the methods, we let N vary in the set $2^i, i = 3, \ldots, 12$ and we fix the number of trajectories M to 10000. In this way, the error caused by the Montecarlo estimation should not spoil the order of convergence. In Figure 1 we show the errors obtained fixing $X_0 = -0.5$ in both the cases of killing and reflecting boundary conditions in $x = 1$. Moreover, in Figure 2 we show an approximation of τ obtained with the two methods with $h = T/128$ and $M = 1000$ for a set of 10 initial values equispaced along D. It is possible to remark that computing the probability of exit between two consecutive timesteps as in (8) allows correcting the overestimation of τ obtained simply using DEM.

1.3 Two-dimensional case

We are interested in estimating the exit time of a particle from a domain $D \subset \mathbb{R}^2$. Given $W(t)$ a vector of two independent Brownian motions, we consider the equation (1). In this case, $f\colon \mathbb{R}^2 \to \mathbb{R}^2, g\colon \mathbb{R}^2 \to \mathbb{R}^{2\times 2}$. We show an analytical expression of the expected exit time from the domain D and the results given by the two numerical schemes in this case.

1.3.1 Analytical exit time in the general case

Let us denote by Γ_k, Γ_r the killing and reflecting subsets of ∂D. It is possible to show that for the d-dimensionional case the expectation of τ, denoted as above as $\bar{\tau}$, is the solution



(a) Killing boundary in $x = 1$

(b) Reflecting boundary in $x = 1$

Figure 2: Approximation of τ for the discrete and continuous EM method in the one-dimensional case.

of the following partial differential equation [2, 3]

$$\begin{cases} f \cdot \nabla\bar{\tau} + \frac{1}{2} g g^T : \nabla\nabla\bar{\tau} = -1, & \text{in } D, \\ \bar{\tau} = 0 & \text{on } \Gamma_k, \\ \nabla\bar{\tau} \cdot n = 0 & \text{on } \Gamma_r. \end{cases} \tag{19}$$

Let us remark that this problem reduces to (13) if $d = 1$. Unlike the one-dimensional case, there exists no analyitcal solution of (19). It is possible to approximate the solution $\bar{\tau}$ with a function $\bar{\tau}_h$ obtained with a classical method for solving PDE's, such as finite differences or the Finite Elements Method.

1.3.2 Numerical experiments

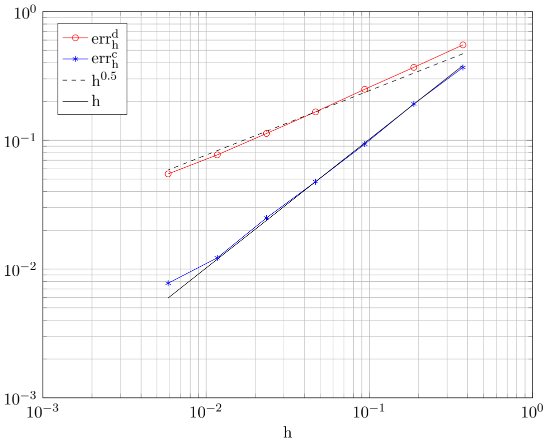
Killing boundary conditions. We consider a simple case of (1) in $D = [-1, 1] \times [-1, 1]$, where

$$f = 0 \in R^2, \; g = \sigma I \in R^{2\times 2}, \sigma \in \mathbb{R}.$$

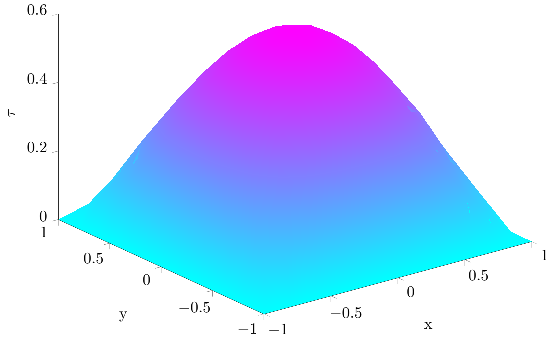
Moreover, we consider ∂D to be a killing boundary. The solution in this case is a Brownian motion. In this case, the partial differential equation (19) reduces to

$$\begin{cases} -\sigma^2 \Delta\bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \partial D. \end{cases} \tag{20}$$

This is the Poisson equation, hence it is possible to solve it numerically with the Finite Elements Method or the finite differences avoiding a high computational cost. We use the finite differences scheme with equal constant spacing in the x and y directions, obtaining a solution as in Figure 3b. In order to verify the orders of convergence of DEM and CEM, we set $T = 3$, $\sigma = 1$, $X_0 = (0, 0)^T$, with $M = 10000$ and $N = 2^i, i = 3, \ldots, 9$. We then compare the Montecarlo estimation we obtain with the value of $\bar{\tau}$ in $(0, 0)$, where we were careful with the choice of the mesh so that $(0, 0)$ is one of its vertices. The orders of convergence for this numerical experiment are shown in Figure 3a. The results confirm the theoretical orders of convergence for DEM and CEM, with an average order of 0.55 for DEM and 0.93 for CEM, which corrects to 0.98 if the last point is not taken into account.

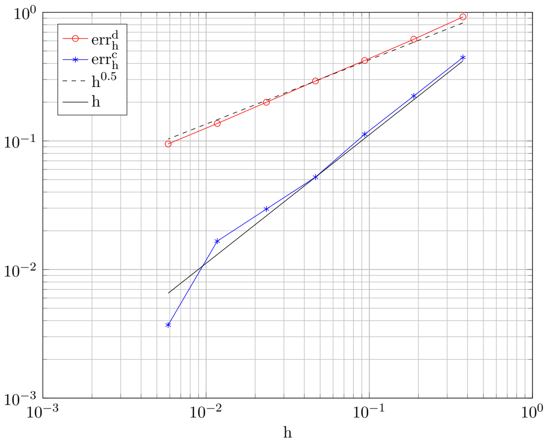


(a) Convergence of CEM and DEM.

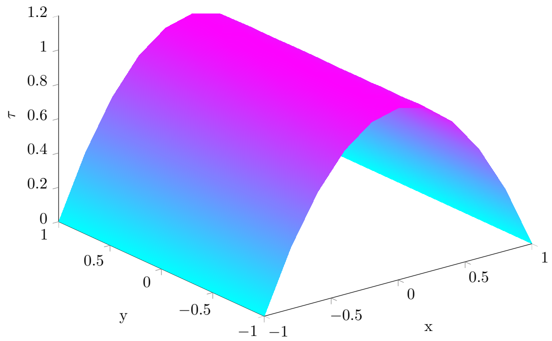


(b) Expectation of exit time.

Figure 3: Summary of the results for the two-dimensional case with pure killing boundary conditions.



(a) Convergence of CEM and DEM.



(b) Expectation of exit time.

Figure 4: Summary of the results for the two-dimensional case with mixed boundary conditions.

Mixed boundary conditions. We consider the same problem as above with mixed killing and reflecting boundary conditions. f and g are the same as above, so the SDE model does not change, but we consider the two left and right boundaries of D, defined by $x = \pm 1$, to be reflecting. We denote this portion of the boundary as Γ_r, and the rest as Γ_k. In this case, the equation for $\bar{\tau}$ becomes

$$\begin{cases} -\sigma^2 \Delta \bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \Gamma_k, \\ \partial \bar{\tau} \cdot n = 0 & \text{on } \Gamma_r. \end{cases} \tag{21}$$

The solution of this equation is shown in Figure 4b. We compute the expectation of τ with DEM and CEM with the same parameters as above. The results (Figure 4a), show that the theoretical orders of convergence are not spoilt by this choice of boundary conditions. The mean order for DEM in this case is 0.55, while for CEM it is 1.15.

References

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