Stochastic Simulations

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Mini-project

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Stochastic modeling of pollutant transport in aquifers

Introduction

In this project we will analyze models describing the trajectories of particles of pollutants in groundwater. We consider an "infinite" homogeneous aquifer occupying the region $D = \mathbb{R}^2 \backslash B(0,R)$. The obstacle B represents a well from which drinking water is extracted with mass rate Q. The motion of the fluid can be described by the velocity field $\boldsymbol{u}(x,y) = (u_1(x,y), u_2(x,y)), \quad (x,y) \in D$ which satisfies the Darcy equation

$$\begin{aligned} &\nabla \cdot \boldsymbol{u} = 0 && \text{in } D, \\ &\boldsymbol{u} = -k\nabla p && \text{in } D, \\ &\int_{\partial B} \boldsymbol{u} \cdot n = q, && p \text{ constant on } \partial B, \end{aligned} \tag{1}$$

together with suitable conditions at infinity. Consider now a particle of contaminant released at position $\boldsymbol{X}(0) = (X_0, Y_0) \in D$ at time $t = 0$. The particle is drifted by the vector field $\boldsymbol{u}$ and diffused due to the porous nature of the soil. Its trajectory can then be described by the following system of stochastic differential equations (SDEs):

$$\begin{aligned} &dX(t) = u_1(X(t), Y(t))dt + \sigma dW_1(t), \quad 0 \le t \le T \\ &dY(t) = u_2(X(t), Y(t))dt + \sigma dW_2(t), \quad 0 \le t \le T \\ &X(0) = X_0, \quad Y(0) = Y_0, \quad X_0, Y_0 \in D, \end{aligned} \tag{2}$$

where $W_1(t)$, and $W_2(t)$ are two independent standard Brownian motions, and the scalar value σ represents the diffusion due to the porous medium. The aim is then to estimate the probability that the contaminant reaches the drinking well within a time horizon T. For a pollutant particle starting at $(X(0), Y(0))$, we define the first passage time of the particle through the well as $\tau = \inf(t \ge 0 : (X(t), Y(t)) \in B)$. Thus, we assume that a particle that enters B is contaminating the drinking well. From a modeling perspective, we consider this to be a *killing boundary,* as we stop the simulation once the particle has entered B. In addition we assume that a particle that has not entered B at a time T is not going to contaminate said well. In particular, we will examine the probability of the particle entering B before some time T. This quantity can be studied using stochastic or deterministic approaches, which are linked by the Feynman-Kac formulation, illustrated hereafter. Define the following differential operator

$$\mathcal{L}v := (\boldsymbol{u} \cdot \nabla)v + \frac{1}{2}(\sigma^2 \Delta v) \tag{3}$$

acting on functions $v(x,t) \in C^{2,1}(D \times (0,T))$. Then, we can state the following proposition relating the aforementioned exit probability to a deterministic process:

Proposition: *Let $\mathcal{L}$ be the differential operator defined in (3). Then, the exit probability by time T, is given by*

$$\mathbb{P}(\tau \leq T | \boldsymbol{X}(0) = (Y_0, Y_0)) = \varphi(\boldsymbol{X}(0), 0),$$

where $\varphi(\boldsymbol{x}, t)$ solves the backwards parabolic PDE

$$\begin{aligned} &\varphi_t + \mathcal{L}\varphi = 0 && \text{in } D \times [0,T] \\ &\varphi = 1 && \text{on } \partial B \times [0,T] \\ &\varphi(\boldsymbol{x}, t) \to 0, && \text{as } |\boldsymbol{x}| \to \infty, \\ &\varphi(\boldsymbol{x}, T) = 0 && \text{in } D. \end{aligned} \tag{4}$$

Thus, the escape probability can be computed either by Monte Carlo methods on (2) or by solving the PDE (4).

Remarks on implementation

I. In order to simulate the SDE (2), you will need to use a numerical method for the approximate solution of a SDE. For instance, you could use the Euler-Maruyama method, a simple generalization of the Euler method for ordinary differential equations to stochastic differential equations. The idea is to replace an SDE of the form of (2) with a discretized version. Partition the interval $[0,T]$ into N equal subintervals of width $\Delta t > 0$. Then, (2) can be discretized as

$$\begin{aligned} X_{k+1} &= X_k + u_1(X_k, Y_k)\Delta t + \sigma\sqrt{\Delta t} Z_k, \quad Z_k \sim N(0,1), \\ Y_{k+1} &= Y_k + u_2(X_k, Y_k)\Delta t + \sigma\sqrt{\Delta t} Z'_k, \quad Z'_k \sim N(0,1), \end{aligned} \tag{5}$$

with X_0, Y_0 given and Z_k, Z'_k independent. Notice that, clearly, the accuracy of the implementation will depend on the size of Δt.

II. To implement the numerical solution of the PDE (4), you can use, e.g, finite difference or finite element methods on a truncated domain. For instance, you could consider a sufficiently large ball around the well. We remark as well that there are various python libraries for the solution of PDEs, such as FEniCS (finite elements) and FiPy (finite volume). In particular, the implementation of the problems considered herein is relatively straightforward, however, please contact the assistants should you run into any issues with the numerical approximation of the PDE.

Goals of the project

(a) Consider a steady flow $\boldsymbol{u}^{\text{steady}}(x,y) = (1,0)$ from left to right, which is locally perturbed due to the presence of the well. As a first approximation we can write the perturbed flow field as

$$\boldsymbol{u}(x,y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + q\nabla \frac{1}{2\pi} \log\left(\sqrt{x^2+y^2}\right). \tag{6}$$

Take $\sigma = 2$, $q = 1$ and $R = 1$, and consider different starting values, namely $\boldsymbol{X}_0^{(1)} = (1.2, 1.1)$, $\boldsymbol{X}_0^{(2)} = (3, 4)$, $\boldsymbol{X}_0^{(3)} = (2.5, 2.5)$. Determine the probability of the particle reaching the well on before time $T = 1$ by simulating SDE (2) for a sufficiently small time step Δt. Compare your results with the numerical solution of the equivalent parabolic PDE.

(b) A possible shortcoming of the previous method is that the exit probability is somewhat related to the step size Δt of the Euler-Maruyama scheme, as it is depicted in Figure 1. To overcome this, we can introduce some "adaptivity" on Δt. Propose an adaptive time step (i.e, take Δt_n as a function of the distance r between $(X_n(t), Y_n(t))$ and the well B, such that the time step decreases with distance) and repeat the simulations from the previous point. Compare your results.

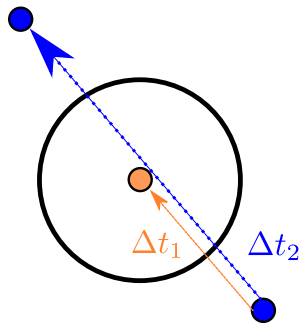

Figure 1: Path for two different time steps Δt_1 and Δt_2, with $\Delta t_1 < \Delta t_2$. The well is depicted by the black circle. Notice that when the step size is too large, the stochastic process might miss the well, thus affecting the exit probability.

(c) Consider the initial point $(2.5, 2.5)$. Propose a variance reduction technique to estimate $\mathbb{P}(\tau \leq T | \boldsymbol{X}(0) = (2.5, 2.5))$ and quantify the amount of variance reduction achieved. Justify your choice.

(d) Now suppose that the particle starts very far from the well. In this case, the probability of the particle reaching the well on a short time interval can be considered as a *rare event*. Simulation of rare events can be done, in theory, by standard Monte Carlo methods, however, this can be computationally challenging as this would typically require a large sample size. A possible alternative suitable for the problem at hand is given by the *splitting method*, where the probability of the rare event (i.e, reaching B in a time T starting at a (X_0, Y_0)) is written as the product of conditional probabilities, each of which can be estimated much more accurately than the rare event itself. More concretely, if we define a sequence of concentric circles $B = C_0 \subset C_1 \subset \cdots \subset C_m$ such that C_i has radius R_i, with $R_i < R_{i+1}$, and corresponding first passage time $\tau_j = \inf_{t \geq 0}\{(X(t), Y(t)) \in C_j\}$, then the probability $\mathbb{P}_B = \mathbb{P}_{\boldsymbol{X}_0}(\tau_0 \leq T)$ can be written as

$$\mathbb{P}_B = \mathbb{P}_{\boldsymbol{X}_0}(\tau_0 \leq T, \tau_1 \leq T, \ldots, \tau_m \leq T) = P_{\boldsymbol{X}_0}(\tau_m \leq T) \prod_{j=0}^{m-1} \mathbb{P}(\tau_j \leq T | \tau_{j-1} \leq T).$$

A depiction of the previous process is given in Figure 2. Review the splitting method (see chapters 2 and 3 in [2]) and implement it to compute the probability of the particle contaminating the well when $x_0 = (7.0, 7.0)$ and $T = 1$.

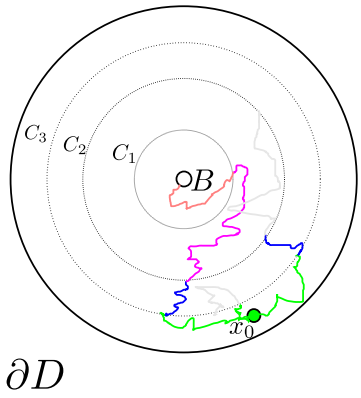

Figure 2: Sketch of the splitting method for different regions that are concentric with B. Starting at x_0, the idea is then to simulate paths that get absorbed at C_3. Based on the probability of reaching C_3 given that we started at x_0, we generate paths to compute the probability of reaching C_2, given that we started at x_0, written as a product of conditional probabilities, and so on until we reach B. Colored lines show samples that reach C_i starting at C_{i+1}. Gray lines show samples that did not reach C_i starting at C_{i+1}.

References

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[2] Garvels, Marnix Joseph Johann. "The splitting method in rare event simulation." *Doctoral thesis, University of Twente* (2000).

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