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Estimation Of Boundary Properties Using Stochastic Differential Equations

A. Atalla A. Jeremic

Department of Electrical and Computer Engineering
McMaster University

presented by
Aleksandar Jeremic

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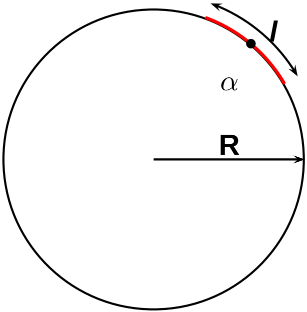
Inverse Problems in Diffusion

- It has many applications in thermal, biomedical, financial ... etc.
- Estimation of medium properties (diffusivity).
- Estimation of source properties (location, intensity, and release time).
- Estimation of boundary properties.

Problem description

- Circular region with radius *R* centered at origin.
- Boundary is divided into two segments:
    - Absorbing with a length of *l* and centered at α.
    - The rest of the boundary is reflecting.
- The main goal here is to estimate the parameters of the absorbing boundary (i.e. *l* and α).



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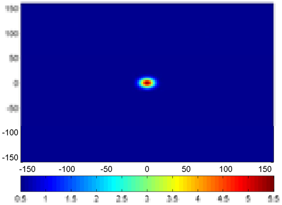
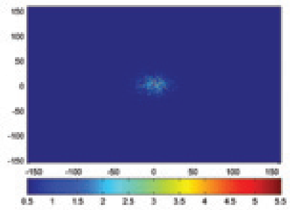
Stochastic vs Classical Approach

Let us assume

- When the number of particles is large, macroscopic approach corresponding to the Fick's law of diffusion is adequate.
- When their number is small, a microscopic approach corresponding to SDE is required.





Stochastic Differential Equation (SDE)

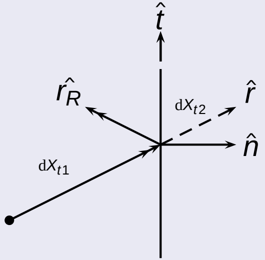
The SDE process for the transport of particle is given by

$$\mathrm{d}X_t = \mu(X_t, t)\mathrm{d}t + \sigma(X_t, t)\mathrm{d}W_t \quad (1)$$

Boundary conditions

- Absorbing: the displacement remains constant ($\mathrm{d}X_t = 0$).
- Reflecting: the new displacement over a small time step τ is:

$$\mathrm{d}X_t = \mathrm{d}X_{t1} + |\mathrm{d}X_{t2}| \cdot \hat{r_R} \quad (2)$$



Fokker Planck Equation

The probability density function of one particle occupying space around $\boldsymbol{r}$ at time t is given by the solution of

$$\frac{\partial f(\boldsymbol{r},t)}{\partial t} = \left[-\sum_{i=1}^{3} \frac{\partial}{\partial x_i} D_i^1(\boldsymbol{r}) + \sum_{i=1}^{3}\sum_{j=1}^{3} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}^2(\boldsymbol{r}) \right] f(\boldsymbol{r},t) \quad (3)$$

Along with the initial condition at $t = t_0$ is given by

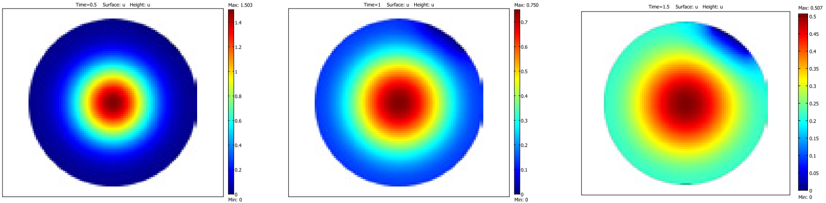
$$f(\boldsymbol{r},t_0) = \delta(\boldsymbol{r} - \boldsymbol{r}_0) \quad (4)$$

And the boundary conditions

$$f(\boldsymbol{r},t) = 0 \qquad \text{for absorbing boundaries} \quad (5)$$

$$\frac{\partial f(\boldsymbol{r},t)}{\partial n} = 0 \qquad \text{for reflecting boundaries} \quad (6)$$

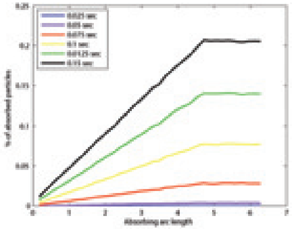
Fokker Planck Equation

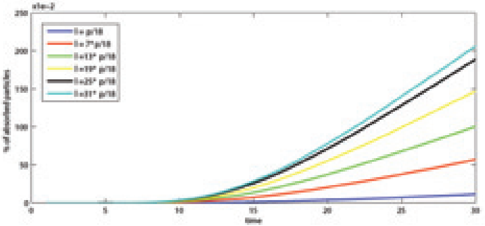


Modeling the Total Absorption

Modeling procedure

- Simulating initial number of particles ($n_0 = 1000$).
- The simulation is repeated 5000 times.
- The average percentage number of absorbed particles ($n_{absorbed}/n_0$) is plotted as a function of t and l.





Modeling the Total Absorption

Result

The relation between the percentage number of absorbed particles, time and l is given by

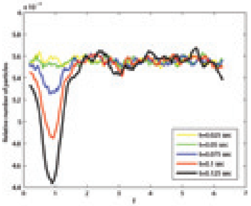
$$n_{absorbed}/n_0 = (2/\pi)\arctan(a(l)t^3 + b(l)t^2 + c(l)t + d(l)) \quad (7)$$

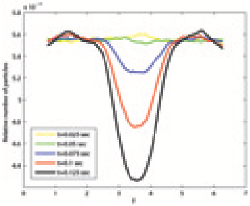
where a, b, c, and d are functions of l and can be fitted using cubic polynomials in order to have a smooth behavior with respect to l.

Modeling the Total Absorption

Modeling procedure

- Circular geometry is divided into S sectors.
- Simulating initial number of particles ($n_0 = 1000$).
- The simulation is repeated 5000 times.
- The average number of particles in each sector is plotted as a function the rogation angle ϕ and time.





Modeling the Total Absorption

Result

The average number of particles per sector shows a local minimum near α. The relation between α and the minimum of n/n_0 can be represented as follows

$$\alpha = \arg\min_{\phi} n/n_0 \tag{8}$$

Estimation Algorithm

Step1

Let y_{t_j} to be the measured number of particles at time t_j, where $j = 1, \ldots, k$ and k is the total number of time samples. Then, the corresponding segment length l_j can be estimated by

$$l_j = \arg\min_{l} |y_{t_j} - g(l, t_j)| \tag{9}$$

The estimated segment length is taken to be

$$\bar{l} = \frac{1}{k} \sum_{j=1}^{k} l_j \tag{10}$$

Estimation Algorithm

Step2

Let y_{i,t_j} to be the measured number of particles at sector i and time $t = t_j$ where $i = 1, \ldots, S$ and S is the total number of sectors. The corresponding boundary center (α_j) can be estimated for each time step by

$$\alpha_j = \alpha(\arg\min_i y_{i,t_j}) \tag{11}$$

The estimated α is taken to be

$$\bar{\alpha} = \frac{1}{k}\sum_{j=1}^{k} \alpha_j \tag{12}$$

Numerical Examples

Parameters

- Source strength of $n_0 = 500$ particles.
- Initially at $\boldsymbol{r}_0 = 0$ and $t_0 = 0$.
- Bounded by a circular domain of radius $R = 1$.
- The number of time samples is $k = 30$.
- The results are carried out for absorbing regions of ($l = \pi/3, \pi/6, \pi$) a centered at $\alpha = \pi/2$.

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Numerical Examples

Results

absorbing length	$\pi/3$	$\pi/6$	π
% error in l	$1.23e-2$	$1.04e-2$	$1.34e-2$
% error in α	$4.2e-2$	$3.91e-2$	$4.02e-2$

Summary

- In this paper we propose a preliminary algorithm for the estimation of the boundary properties
- The accuracy of this method is reasonable compared to the computational effort required for the estimation
- This algorithm can be used in applications where the estimation time has higher priority with acceptable margin of error

Thank You!