Estimation Of Boundary Properties Using Stochastic Differential Equations

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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 $\alpha$.
  - The rest of the boundary is reflecting.
- The main goal here is to estimate the parameters of the absorbing boundary (i.e. $l$ and $\alpha$).
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.
The SDE process for the transport of particle is given by

\[ dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t \]  \hspace{1cm} (1)

**Boundary conditions**

- **Absorbing:** the displacement remains constant \( (dX_t = 0) \).
- **Reflecting:** the new displacement over a small time step \( \tau \) is:

\[ dX_t = dX_{t1} + |dX_{t2}| \cdot \hat{r}_R \]  \hspace{1cm} (2)
The probability density function of one particle occupying space around $r$ at time $t$ is given by the solution of

$$\frac{\partial f(r, t)}{\partial t} = \left[ - \sum_{i=1}^{3} \frac{\partial}{\partial x_i} D_1^i(r) + \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial^2}{\partial x_i \partial x_j} D_2^i_j(r) \right] f(r, t) \quad (3)$$

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

$$f(r, t_0) = \delta(r - r_0) \quad (4)$$

And the boundary conditions

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

$$\frac{\partial f(r, t)}{\partial n} = 0 \quad \text{for reflecting boundaries} \quad (6)$$
Fokker Planck Equation
Modeling procedure

- Simulating initial number of particles \((n_0 = 1000)\).
- The simulation is repeated 5000 times.
- The average percentage number of absorbed particles \((n_{\text{absorbed}}/n_0)\) 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

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

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 $l$. 

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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 rotation angle $\phi$ and time.
The average number of particles per sector shows a local minimum near $\alpha$. The relation between $\alpha$ and the minimum of $n/n_0$ can be represented as follows

$$\alpha = \arg \min_{\phi} \frac{n}{n_0}$$

(8)
Step 1

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

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

The estimated segment length is taken to be

$$\bar{l} = \frac{1}{k} \sum_{j=1}^{k} l_j$$
Step 2

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 ($\alpha_j$) can be estimated for each time step by

$$\alpha_j = \alpha(\arg \min_i y_{i,t_j})$$  \hspace{1cm} (11)

The estimated $\alpha$ is taken to be

$$\bar{\alpha} = \frac{1}{k} \sum_{j=1}^{k} \alpha_j$$  \hspace{1cm} (12)
Numerical Examples

Parameters

- Source strength of $n_0 = 500$ particles.
- Initially at $r_0 = 0$ 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 $\alpha = \pi/2$. 
## Numerical Examples

### Results

<table>
<thead>
<tr>
<th></th>
<th>$\pi/3$</th>
<th>$\pi/6$</th>
<th>$\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>absorbing length</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>% error in $l$</td>
<td>$1.23e-2$</td>
<td>$1.04e-2$</td>
<td>$1.34e-2$</td>
</tr>
<tr>
<td>% error in $\alpha$</td>
<td>$4.2e-2$</td>
<td>$3.91e-2$</td>
<td>$4.02e-2$</td>
</tr>
</tbody>
</table>

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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!