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The Correlated Random Walk with Exclusion

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Introduction

The correlated random walk is a random walk in which the probability of moving in a particular direction is dependent on the direction in which the agent last moved. This model has applications in many fields, particularly biology; for example, moving cells are likely to have a persistence of direction where they are more likely to move in the direction they are facing, and thus this makes the correlated random walk model more accurate than a simple random walk model for the same system.

This process without exclusion has been studied by various authors; in particular, Renshaw and Henderson (1981, 1984) have shown that for a single walker the process is equivalent to a diffusion process in both one and two dimensions, with the diffusion coefficient based on the probability of moving in each direction relative to the last move. However, most such analysis has been based on a single walker or one whose movement is unobstructed.

The objective of this paper is to consider the case in which many such random walkers are moving on a one-dimensional lattice and interact with each other through simple exclusion, in other words any attempts to move into occupied lattice spaces are aborted. This captures an important aspect of multi-agent systems where agents are often unable to move into the immediate vicinity of other agents due to volume or other constraints.

Analysis

The base discrete model used in this paper considers agents occupying sites of a one-dimensional lattice. The possible location of an agent is given by a single integer coordinate i. Reflecting boundaries are imposed on the lattice.

Let p_f be the probability that the agent moves in the same direction it last moved if it has the opportunity, and p_b be the probability that it moves in the opposite direction. To simplify calculations, and noting that on conversion to a continuous system a time step will be introduced that can be varied depending on the number of moves desired per time unit, it is assumed that $p_f + p_b = 1$.

Define $p_{n,l}(i)$ to be the probability that there is an agent in lattice space i at time n whose last move was left, and $p_{n,r}(i)$ to be the probability that there is an agent in lattice space i at time n whose last move was right. Define $p_n(i) = p_{n,l}(i) + p_{n,r}(i)$.

A conservation-of-agent statement for the probability of position i being occupied after n time steps under the correlated random walk with simple exclusion is:

$$\begin{aligned}
p_{n+1,l}(i) &= p_{n,l}(i)\left[1 - p_f(1 - p_n(i-1)) - p_b(1 - p_n(i+1))\right] && (1)\\
&\quad + (1 - p_n(i))(p_f p_{n,l}(i+1) + p_b p_{n,r}(i+1)) && (2)\\
p_{n+1,r}(i) &= p_{n,r}(i)\left[1 - p_n(1 - p_n(i-1)) - p_f(1 - p_n(i+1))\right] && (3)\\
&\quad + (1 - p_n(i))(p_b p_{n,l}(i-1) + p_f p_{n,r}(i-1)) && (4)
\end{aligned}$$

The red terms have been derived through mean-field arguments by assuming independence between the occupancy of adjacent sites, and represent the probability that the space that the agent is attempting to move into is open, since moves are only allowed if this is true.

Continuum limit

The ultimate goal of this analysis is to derive a partial differential equation description of the system. To this end we convert the discrete model into a continuous model by introducing a unit of length Δ called the lattice spacing and a unit of time τ called the time step. Let $x = \Delta i$ and $t = n\tau$. Let $\mathbf{c}(x,t) = \begin{pmatrix} p_{n,l}(i) \\ p_{n,r}(i) \end{pmatrix}$ and $c(x,t) = [1 \quad 1]\mathbf{c}(x,t)$. Substituting into the above equations results in the following:

$$\begin{aligned}
\mathbf{c}(x, t+\tau) &= \left(c(x+\Delta, t) \begin{bmatrix} p_b & 0 \\ 0 & p_f \end{bmatrix} + c(x-\Delta, t) \begin{bmatrix} p_f & 0 \\ 0 & p_b \end{bmatrix} \right) \mathbf{c}(x,t) \\
&\quad + (1 - c(x,t)) \left(\begin{bmatrix} p_f & p_b \\ 0 & 0 \end{bmatrix} \mathbf{c}(x+\Delta, t) + \begin{bmatrix} 0 & 0 \\ p_b & p_f \end{bmatrix} \mathbf{c}(x-\Delta, t) \right) \quad (5)
\end{aligned}$$

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At this point we apply partial Taylor expansions to derive a partial differential equation. The Taylor expansions are taken to the first order in τ and the second order in Δ.

$$\begin{aligned}
&\mathbf{c} + \tau\frac{\partial \mathbf{c}}{\partial t} + o(\tau) \\
=\ & \left((c + \frac{\Delta^2}{2}\frac{\partial^2 c}{\partial x^2} + o(\Delta^2))\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + (\Delta\frac{\partial c}{\partial x})\begin{bmatrix} p_b - p_f & 0 \\ 0 & p_f - p_b \end{bmatrix}\right)\mathbf{c} \\
& +(1-c)\left(\begin{bmatrix} p_f & p_b \\ p_b & p_f \end{bmatrix}(\mathbf{c} + \frac{\Delta^2}{2}\frac{\partial^2 \mathbf{c}}{\partial x^2} + o(\Delta^2)) + \begin{bmatrix} p_f & p_b \\ -p_b & -p_f \end{bmatrix}\Delta\frac{\partial \mathbf{c}}{\partial x}\right) \qquad (6)
\end{aligned}$$

To simplify the system into a system of scalars, we introduce a new variable $\phi(x,t) = [1 \quad -1]\mathbf{c}(x,t)$. The introduction of this variable means that we have now decomposed the variable $\mathbf{c}$ into symmetric and anti-symmetric components (c and ϕ respectively). In particular,

$$\mathbf{c} = \frac{1}{2}\left(c\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \phi\begin{bmatrix} 1 \\ -1 \end{bmatrix}\right). \qquad (7)$$

After substituting this into (5), some simplification, dropping the $o(\cdot)$ terms and equating the coefficients of $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$ we eventually derive the following system of equations:

$$\begin{aligned}
\frac{\partial c}{\partial t} &= \frac{\Delta}{\tau}\frac{\partial c}{\partial x}\phi(p_b - p_f) + (1-c)(p_f - p_b)\frac{\Delta}{\tau}\frac{\partial \phi}{\partial x} + \frac{\Delta^2}{2\tau}\frac{\partial^2 c}{\partial x^2} \qquad (8) \\
\frac{\partial \phi}{\partial t} &= -2p_b(1-c)\phi + \frac{\Delta^2}{2\tau}\frac{\partial^2 c}{\partial x^2}\phi + \frac{\Delta}{\tau}\frac{\partial c}{\partial x}(1 - 2p_f c) + (1-c)\frac{\Delta^2}{2\tau}\frac{\partial^2 \phi}{\partial x^2}(p_f - p_b) \qquad (9)
\end{aligned}$$

In these equations' current state we cannot take the continuum limit as $\Delta \to 0$ and $\tau \to 0$, because the ratio of $\frac{\Delta^2}{\tau}$ needs to be held constant, but there are many terms which will disappear when the limit is taken which is not a sensible limit. For this reason another step needs to be taken before the limit can be applied. The method used here is to scale the variable ϕ so that it disappears in the continuum limit, in other words let $\phi = \Delta\Phi$.

After bringing τ back to the left-hand side in (8) we take the continuum limit and simplify. We then find that the model reduces to the following one-dimensional partial differential equation:

$$\frac{\partial c}{\partial t} = D\frac{\partial}{\partial x}\left(\left(\frac{1}{2} - c(p_f - p_b)\right)\frac{\partial c}{\partial x}\right), \text{ where } D = \lim_{\Delta,\tau\to 0}\frac{\Delta^2 p_f}{\tau p_b} \qquad (10)$$

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This corresponds to a non-linear diffusion equation, which indicates that the system behaves as a system of particles diffusing at a rate dependent on the concentration.

Comparison with simulation, discussion and conclusions

There are many ways to simulate random walk models of agent motility. The one used in this analysis is where there are N agents present, and in each update N move attempts occur, each of which is made by a random independently chosen agent. This is known as random sequential update (Chowdrury et al. 2005). An agent is selected once on average but may be selected more than once or not at all.

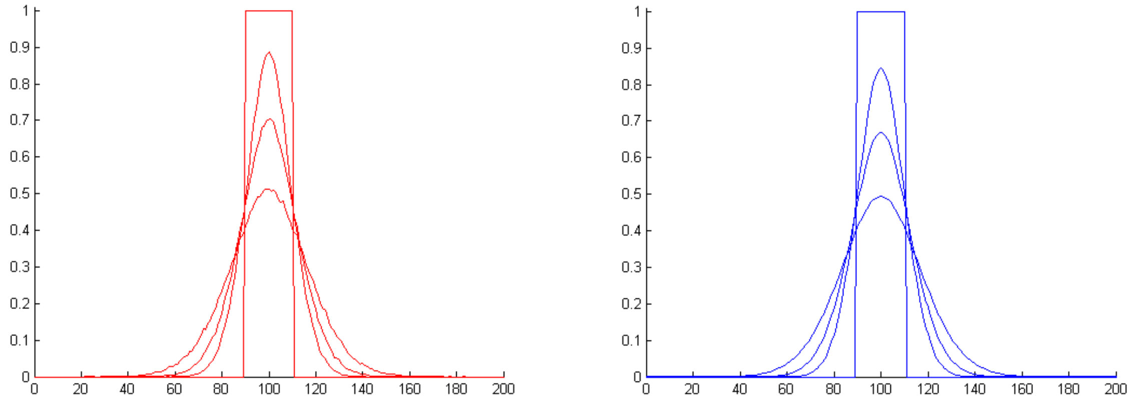

Figure 1: Red: Average of 10000 simulations. The state of the system is shown at times $n = 0, 50, 100, 200$. The horizontal axis denotes position and the vertical axis denotes concentration. Blue: PDE approximation. The state of the system is shown at times $n = 0, 50, 100, 200$. The horizontal axis denotes position and the vertical axis denotes concentration.

Simulations were performed on a one-dimensional lattice of width 201 sites, with $0 \leq i \leq 200$. The left diagram displays the average of 10000 simulations at times $n = 0, 50, 100, 200$ for $p_f = 0.6$. The right diagram shows the numerical solution of (10) for the initial condition where sites $90 \leq i \leq 110$ are occupied and all other sites are vacant. It can be seen that the PDE approximation is a reasonable though not perfect fit with the simulation data, particularly at the centre where the agents

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are initially most concentrated. Conversely, further away from this point the fit is almost perfect. Reasons for the discrepancy may include correlation effects between site occupancy, or effects caused by the simplification due to the scaling.

It should be noted that the partial differential equation description fails whenever p_f is above 0.75 and the concentration is sufficiently large, since the effective diffusion coefficient in that case becomes negative. As a result, attempting to solve the PDE in this case results in the concentration diverging at the edges of the initial block of agents, as well as turning negative in some regions. Resolving this problem is left to future research.

AMSI Experience

The vacation scholarship program was an enjoyable experience that gave me a taste of independent academic research and an opportunity to apply my mathematical knowledge to a useful problem. I met with challenges along the way, but thanks to the guidance of my supervisors I was able to overcome them, and the feeling when I find a solution to a problem is exhilarating. I now have a better understanding of how research works and have learned new problem solving techniques, as well as gained practice for presentation skills, as a result. The CSIRO Big Day In allowed me to meet a range of like-minded students, learn about a variety of projects on the cutting-edge of scientific research, and gain an insight into the wider mathematics and scientific community and what sort of questions currently interest mathematicians and scientists in these fields.

I would like to thank my supervisors Professor Barry Hughes and Professor Kerry Landman for the guidance and support they provided over the course of my research, and the University of Melbourne, AMSI and CSIRO for providing me with the opportunity to participate in this program.

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