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A NOTE ON THE ASYMPTOTIC PROPERTIES OF CORRELATED RANDOM WALKS

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Abstract

We describe a simple relation between the asymptotic behavior of the variance and of the expected number of distinct sites visited during a correlated random walk. The relation is valid for multistate random walks with finite variance in dimensions 1 and 2. A similar relation, valid in all dimensions, exists between the asymptotic behavior of the variance and of the probability of return to the origin.

MULTISTATE RANDOM WALKS; VARIANCE, RANGE AND RETURN PROBABILITY

1. Introduction

In a recent paper, Henderson et al. [6] discussed a two-dimensional random walk in which, at each stage, the direction of the next step is correlated to that of the previous step. They found that in the asymptotic expressions for the variance and the expected number of distinct sites visited (henceforth denoted as *range*), there occurs the same multiplying factor. Accordingly the question was raised whether this relation applied only to their particular correlated random walk or whether it is of a more general validity. This question is answered in the affirmative in Section 2. There we also show that a similar relation exists between the asymptotic expressions for the variance and the probability of return to the origin.

As far as we know, a general relation between the variance and the probability of return to the origin or the range of a random walk was first conjectured by Shuler [9] in the context of random walks on inhomogeneous periodic lattices, i.e. lattices which consist of a periodically repeated unit cell, where each unit cell contains a number of non-equivalent sites. He argued that the range and the probability of return to the origin should be proportional, or inversely proportional respectively, to (in dimension 2) the 'area' $[E(x_n^2)E(y_n^2)]^{1/2}$ covered by the

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walker, where x_n and y_n are the displacements in the horizontal and vertical directions, respectively, after n steps. These conjectures were subsequently investigated within the context of multistate random walks, i.e. random walks where the walker can be in a number of internal states which affect his motion (Roerdink and Shuler [7], [8]). A similar study was recently reported by Bender and Richmond [2], but the precise relation between the variance and the probability of return to the origin or the range was not discussed by them.

In Section 2 we present the general results for the probability of return to the origin and the range of a correlated random walk. We restrict ourselves here to correlated random walks on homogeneous periodic lattices, but the extension to correlated walks on inhomogeneous periodic lattices is straightforward. It is also assumed that the correlations extend over a *finite* number of previous steps. In Section 3 we briefly indicate some applications of these results by means of two examples, the one of Henderson et al. [6], as well as its d-dimensional analogue, studied by Gillis [4] (see also Barber and Ninham [1], p. 52).

2. Theory

Consider a multistate random walk on a d-dimensional uniform lattice [3] (a uniform lattice is a lattice where all sites are equivalent, i.e. there is the same set of vector steps at each point). The position of the walker on the lattice is specified by a vector $\boldsymbol{r}$, where

$$\boldsymbol{r} = \sum_{i=1}^{d} l_i \boldsymbol{a}_i. \tag{2.1}$$

The $\{l_i\}$ are integers, and $\{\boldsymbol{a}_i\}$ is a set of so-called fundamental translation vectors, i.e. the lattice is mapped onto itself when translated along any of the vectors $\{\boldsymbol{a}_i\}$. A special case is that of hypercubic lattices, for which $\{\boldsymbol{a}_i\}$ are d orthonormal unit vectors $\{\boldsymbol{e}_i\}$, which generate the integer lattice $\mathbb{Z}^d$. The internal states of the walker are labeled by Greek indices, running from 1 to m, where m is the total number of internal states. A '*state*' of the walker is defined by his *position* $\boldsymbol{l}$ and his *internal state* α.

A basic quantity for these walks is the probability $P_{\alpha\beta}^{(n)}(\boldsymbol{l}-\boldsymbol{l}_0)$ that after n steps the walker is at site $\boldsymbol{l}$ and internal state α, given that he started at site $\boldsymbol{l}_0$ in internal state β. (The components of $\boldsymbol{l}$ are the integers l_i in (2.1).) The fact that only the difference $\boldsymbol{l}-\boldsymbol{l}_0$ appears is due to the translational invariance of the lattice. The evolution of the probability distribution is described by the Chapman–Kolmogorov equation

$$P_{\alpha\beta}^{(n+1)}(\boldsymbol{l}-\boldsymbol{l}_0) = \sum_{\boldsymbol{l}',\gamma} T_{\alpha\gamma}(\boldsymbol{l}-\boldsymbol{l}')P_{\gamma\beta}^{(n)}(\boldsymbol{l}'-\boldsymbol{l}_0) \tag{2.2}$$

where $T_{\alpha\gamma}(\boldsymbol{l}-\boldsymbol{l}')$ is the single-step transition probability from site $\boldsymbol{l}'$ and the internal state γ to site $\boldsymbol{l}$ and internal state α. A fundamental role is played by the $m \times m$ matrix $\mathbf{T}$, with matrix elements defined by

$$T_{\alpha\gamma} = \sum_{\boldsymbol{l}} T_{\alpha\gamma}(\boldsymbol{l}). \tag{2.3}$$

By the normalization of transition probabilities, $\Sigma_\alpha T_{\alpha\gamma} = 1$, so $\mathbf{T}$ is a stochastic matrix, which we assume to be *irreducible*. That is, $\mathbf{T}$ has a *simple* maximal eigenvalue $\lambda_0 = 1$ with associated right eigenvector $\boldsymbol{\pi}$, which is normalized, $\Sigma_{\alpha=1}^m \pi_\alpha = 1$. The matrix $\mathbf{T}$ governs the evolution of an m-state Markov chain, which describes the transitions between the m internal states. The asymptotic occupation probability of internal state α is π_α.

In order to state our results, we further define a set of *diffusion coefficients* D_{ij} $(i, j = 1, 2, \cdots, d)$ as follows:

$$D_{ij} = \lim_{n\to\infty} \frac{1}{2}\frac{1}{n} \{E[r_i(n) r_j(n)] - E[r_i(n)]E[r_j(n)]\} \tag{2.4}$$

where $\boldsymbol{r}(n)$ is the displacement of the walker after n steps with components $r_i(n) = \boldsymbol{r}(n) \cdot \boldsymbol{e}_i$ $(i = 1, 2, \cdots, d)$, where the $\{\boldsymbol{e}_i\}$ are defined above. The limit exists if the single-step distribution $T_{\alpha\gamma}(\boldsymbol{l} - \boldsymbol{l}')$ in (2.2) has finite means and variances for all α and γ, as will be assumed in the following. An algorithm to calculate the diffusion coefficients is given by Roerdink and Shuler [7] but will not be discussed here.

Having defined the matrix $\mathbf{T}$ and associated eigenvector $\boldsymbol{\pi}$ and the diffusion coefficients D_{ij}, we are in a position to state our results on the probability of return to the origin and the range of correlated random walks. These results have been derived for multistate random walks on inhomogeneous periodic lattices (Roerdink and Shuler [7]), and only some minor modifications are necessary for the present case of correlated random walks, which can be viewed as multistate random walks where the internal states are determined by the previous step(s) (see Section 3). Therefore, the details of the derivation are omitted.

(i) *Probability of return to the origin.* We assume that the walk is irreducible (every state can be reached from every other state) and without drift, i.e. $E[r_i(n)] \sim 0$ $(n \to \infty)$ for all $i = 1, 2, \cdots, d$ $[f(x) \sim g(x)$ as $x \to c$ means $\lim_{x\to c} (f(x)/g(x)) = 1]$. First we consider the case of *primitive* walks, i.e. there exists a positive integer N such that a path of N steps exists between any pair of states of the walk. In this case the probability $P_{\alpha\beta}^{(n)}(\boldsymbol{o})$ that the walker returns to the origin $\boldsymbol{o}$ after n steps, with initial internal state β and final internal state α, is given asymptotically by [7]

$$P_{\alpha\beta}^{(n)}(\boldsymbol{o}) \sim \pi_\alpha \det(2\mathbf{D})^{-1/2} (\det \mathbf{A}) (2\pi n)^{-d/2} \qquad (n \to \infty). \tag{2.5}$$

Here π_α is the αth component of the eigenvector $\boldsymbol{\pi}$ as defined above, $\mathbf{D}$ is the diffusion matrix defined in (2.4), and $\mathbf{A}$ is the matrix with elements

$$A_{ij} = \boldsymbol{a}_i \cdot \boldsymbol{e}_j.$$

For the case of a hypercubic lattice, $\boldsymbol{a}_i = \boldsymbol{e}_i$, $\|\boldsymbol{e}_i\| = 1$, so $\mathbf{A}$ is equal to the unit matrix, and the geometrical factor $\det \mathbf{A} = 1$. For correlated walks we want to know the total probability of return to the origin, independent of the internal state of the walker when he starts or returns. Therefore, we sum (2.5) over final internal states α and average over the initial distribution $\{p_\beta^{(o)}\}$ of the internal states to find

$$p_n(\boldsymbol{o}) \equiv \sum_{\alpha,\beta} P_{\alpha\beta}^{(n)}(\boldsymbol{o}) p_\beta^{(o)} \sim (\det 2\mathbf{D})^{-1/2} (2\pi n)^{-d/2} \qquad (n \to \infty) \tag{2.6}$$

where we have used that $\Sigma_\alpha \pi_\alpha = 1$ and put $\det \mathbf{A} = 1$. This formula clearly displays the connection between the probability of return to the origin and the diffusion coefficients or the corresponding (co)variances. The same prefactor $(\det 2\mathbf{D})^{-1/2}$ of course appears also in $p_n(\boldsymbol{r})$ for $\boldsymbol{r} \neq \boldsymbol{o}$.

For *periodic* (i.e. non-primitive) irreducible walks, the probability $p_n(\boldsymbol{o})$ is 0 for a subset of values of n. For example, for walks in which the walker can only return to the origin after an even number of steps, the results (2.5) and (2.6) have to be multiplied by a factor $[1 + (-1)^n]$.

(ii) *Range.* To calculate the asymptotic behavior of $S_{\alpha\beta}^{(n)}$, the range (or expected number of distinct sites visited) after n steps, with initial and final internal state given by β and α, respectively, the derivation given before in [7] has to be slightly modified by starting from Equation (2.2.2) of that paper, instead of Equation (2.2.1). The reason is that for the present case of correlated walks visits to the same site, but with different internal states of the walker during such a visit, are counted only once. The result, again for irreducible and driftless walks, is

$$S_{\alpha\beta}^{(n)} \overset{n\to\infty}{\sim} \pi_\alpha \frac{(\det 2\mathbf{D})^{1/2}}{\det \mathbf{A}} \begin{cases} \left(\dfrac{8n}{\pi}\right)^{1/2} & d = 1 \\ 2\pi n / \log n & d = 2. \end{cases} \tag{2.7}$$

In dimension $d \geqq 3$, $S_{\alpha\beta}^{(n)}$ is proportional to n for large n, where the proportionality constant depends on the value of the generating functions $G_{\alpha'\beta'}(\boldsymbol{o}, z) = \Sigma_{n=0}^{\infty} z^n P_{\alpha'\beta'}^{(n)}(\boldsymbol{o})$ at $z = 1$, so the dependence on the variance is not so simple as in dimension $d < 3$. Summing again over final internal states and averaging over initial internal states, we find, for the case $\det \mathbf{A} = 1$,

$$S_n \equiv \sum_{\alpha,\beta} S_{\alpha\beta}^{(n)} p_\beta^{(0)} \overset{n\to\infty}{\sim} (\det 2\mathbf{D})^{1/2} \begin{cases} \left(\dfrac{8n}{\pi}\right)^{1/2} & d = 1 \\ 2\pi n / \log n & d = 2. \end{cases} \tag{2.8}$$

Again the relation between S_n and the variances is clear through the presence of the diffusion matrix, and in fact the factor $(\det 2\mathbf{D})^{1/2}(\det \mathbf{A})^{-1}$ in (2.7) is the inverse of the multiplying factor in (2.5).

3. Examples

(i) Henderson et al. [6] discuss a random walk on the square lattice, where the walker has probabilities f, b, r and l to take a step forward, backward, to the right and to the left, with respect to his previous step, respectively. They defined four states, $E_1, \cdots, E_4$, according to whether the previous step was in the positive x-, negative x-, positive y-, or negative y-direction, respectively. They found (we take $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ to be the unit vectors in the positive x- and y-direction, respectively),

$$(3.1) \qquad 2D_{11} = 2D_{22} = \frac{\frac{1}{2}[1-(f-b)^2-(r-l)^2]}{[1-(f-b)]^2+(r-l)^2} \qquad D_{12} = D_{21} = 0.$$

Although this result was derived for a special initial condition, it remains correct as long as the matrix $\mathbf{T}$ is irreducible.

From (2.6) we find that

$$(3.2) \qquad p_n(\boldsymbol{o}) \sim (2D_{11})^{-1}(2\pi n)^{-1}[1+(-)^n]$$

where the extra factor $1+(-)^n$ accounts for the periodicity of the walk. In the special case $f = b = 0$, $r = \frac{1}{2}(1+\alpha)$, $l = \frac{1}{2}(1-\alpha)$, the walker can only return to the origin after $4, 8, 12, \cdots$ steps, so

$$(3.3) \qquad p_n(\boldsymbol{o}) \sim \frac{2(1+\alpha^2)}{1-\alpha^2}(2\pi n)^{-1}[1+(-)^n+(i)^n+(-i)^n],$$

a result already derived by Gillis [5] via a different method.

From (2.8) and (3.1) we conclude that

$$S_n \sim 2D_{11} \cdot 2\pi n/\log n$$

in agreement with the result of Henderson et al. [6]. The advantage of our method is that the lengthy expansions of the generating function are avoided (the diffusion coefficients (3.1) can be calculated without using generating functions by the matrix algorithm in [7]).

(ii) A d-dimensional generalization of the previous example was treated by Gillis [4] and later by Domb and Fisher [3]. See also [1]. They considered a d-dimensional hypercubic lattice, where the walker steps with probabilities f and b in the forward and backward direction or takes any of the directions orthogonal to his previous step with probability r. For this walk the mean is asymptotically 0 and the (co)variances are (see [1], [3]) with $\delta = f - b$,

$$E[r_i^2(n)] \overset{n\to\infty}{\sim} n \cdot \frac{1}{d}\frac{1+\delta}{1-\delta}\,; \quad E[r_i(n)r_j(n)] \overset{n\to\infty}{\sim} 0 \qquad (i \neq j)$$

whence

$$\det 2\mathbf{D} = \prod_{i=1}^{d} 2D_{ii} = \left(\frac{1}{d}\frac{1+\delta}{1-\delta}\right)^{d}. \tag{3.4}$$

Gillis [4] found for the probability $R_n(\delta)$ of returning to the origin after n steps, as a function of δ,

$$R_n(\delta) \sim \left(\frac{1-\delta}{1+\delta}\right)^{d/2} R_n(o) \qquad (n \to \infty). \tag{3.5}$$

From (2.6) and the fact that return to the origin is only possible after an even number of steps, we find alternatively (we use (3.4)),

$$R_n(\delta) \sim \left(\frac{1}{d}\frac{1+\delta}{1-\delta}\right)^{-d/2} (2\pi n)^{-d/2}[1+(-)^n], \tag{3.6}$$

which is in agreement with (3.5).

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