ABSTRACT

CORRELATED WALKS IN $\mathbb{R}^1$ AND $\mathbb{R}^2$

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This thesis is concerned with certain Markovian correlated walks. The earliest references to such processes which we have been able to find in the literature were the applications by Fürth (1920) in his study of the movement of Infusoria, i.e. some microscopic living organisms, and Tchen (1950) in his study of polymer configurations.

The binomial random walk and certain discrete correlated walks in $\mathbb{R}^1$ and $\mathbb{R}^2$ are represented by Markov chains. A more general formulation of the correlated walk in $\mathbb{R}^2$ is considered. This formulation allows the discussion of the discrete random walks and correlated walks as special cases and at the same time provides a basis model for the description of the movement of biological cells in the plane.

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CHAPTER I

RANDOM WALKS IN $\mathbb{R}^1$ AND $\mathbb{R}^2$

§1 The Binomial Random Walk

Let $\{X_i\}$ $i=1,2,\cdots$ be a sequence of independent and identically distributed random variables each having the Bernoulli distribution: at every trial, i.e., at every step in the terminology of random walks, the random variables X_i assumes the values $+1$ and -1 with constant probabilities p and q respectively. For such a process,

$$E(X_i) = (-1)q + (+1)p \tag{1.1}$$

$$= p-q$$

We define $\lambda = p-q$

$$E(X_i^2) = 1 \tag{1.2}$$

$$\operatorname{var}(X_i) = 1-\lambda^2 \tag{1.3}$$

The partial sums $\{S_n\}$, $n=1,2,\cdots$ where

(1.4) $$S_n = \sum_{k=1}^{n} X_k$$

describe a binomial random walk on the integers and

(1.5) $$\therefore \quad E(S_n) = E(X_1) + E(X_2) + \cdots + E(X_n)$$

$$= n(p-q)$$

$$= n\lambda$$

(1.6) Now: $$\mathrm{var}(S_n) = \mathrm{var}\,X_1 + \mathrm{var}\,X_2 + \cdots + \mathrm{var}\,X_n$$

$$= n\,\mathrm{var}\,X_1$$

$$= n(1-\lambda^2)$$

(1.7) $$E(S_n^2) = \mathrm{var}(S_n) + E^2(S_n)$$

(1.8) $$= n - n\lambda^2 + n^2\lambda^2,$$

the expression for the mean square displacement in terms of n and λ.

§ 2 Pearson Walk

Consider in the plane a walk where the steps $\vec{r}_0, \vec{r}_1, \cdots$ form a sequence of independent 2-vectors whose lengths are fixed (though not necessarily equal) and whose directions Φ_i (w.r.t. the x-axis) are independent, uniformly distributed random variables. $\{\vec{r}_i\}\ i=0,1,2\cdots$ is a Pearson walk, after Karl Pearson (1905a,b) who first formulated the problem in the plane (the drunkard walk) in this fashion. The case of equal step lengths (Rayleigh, 1880; Rayleigh, 1905) leads to the result that the mean square displacement is proportional to the number of steps, n. Fig. 1 illustrates four steps of a Pearson walk.

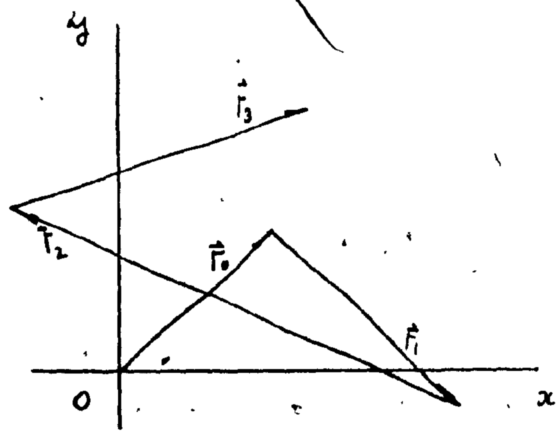

Fig. 1

<u>Theorem</u>: Let $\{X_i\}\ i=1,2,\cdots$ stand for a sequence of mutually independent two dimensional random variables with a common distribution F. Suppose that the expectations are zero and that the covariance matrix for the components $(X_i^{(x)}, X_i^{(y)})$ of X_i is given by

$$C = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \tag{1.10}$$

where $\rho = \rho(X_i^{(x)}, X_i^{(y)})$; $\sigma_1^2 = var(X_i^{(x)})$; $\sigma_2^2 = var(X_i^{(y)})$.

As $n \to \infty$ the distribution of $\dfrac{X_1 + X_2 + \cdots X_n}{\sqrt{n}}$ tends to the bivariate normal distribution with zero expectation and covariance matrix C, (Feller 2, 1971, p. 260).

In the above theorem, let the X_i have directions φ_i prescribed by the random variable $\Phi = \mathcal{U}(-\pi, \pi)$, i.e. $\{\Phi_i\}\ i = 0, 1, \cdots$ is a sequence of independent and uniformly distributed random variables. Let the lengths $l_i = |X_i|$ be given by a random variable L, and let $E(L^2) = 1$. $\{L_i\}\ i = 0, 1, \cdots$ is a sequence of independent and identically distributed random variables with a common density $g(l)$. Let L and Φ be independent. The covariance matrix for the components $(X_i^{(x)}, X_i^{(y)})$ of X_i, is given by $C = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ since the $\mathrm{cov}(X_i^{(x)}, X_i^{(y)}) = 0$ and $\sigma_{ix}^2 = \sigma_{iy}^2 = \frac{1}{2}$, by independence of Φ and L and by symmetry. The distribution of the normalized sum $\frac{S_n}{\sqrt{n}}$ where, $S_n = \sum_{i=0}^{n} X_i$ tends to the normal bivariate distribution Z with covariance matrix C. The distribution of the squared length of the vector $\frac{S_n}{\sqrt{n}}$ therefore tends to the distribution of the sum of the squares of two independent normal random variables, say $[Z^{(x)}]^2$ and $[Z^{(y)}]^2$ i.e. to a χ_2^2 distribution (Feller 2, 1971, p. 261).

§ 3 General Description of the Class of Walks We Study

Let $\{\vec{r}_i\}\ i = 0, 1, \cdots$ be a sequence of 2-vectors in the plane. Let the vectors $\vec{r}_i$ and $\vec{r}_{i+1}$ make an angle θ_{i+1}, the relative angle w.r.t. each other. Let each vector $\vec{r}_i$ make an angle φ_i with the reference x-axis. Fig.2 illustrates 3 steps of such a walk.

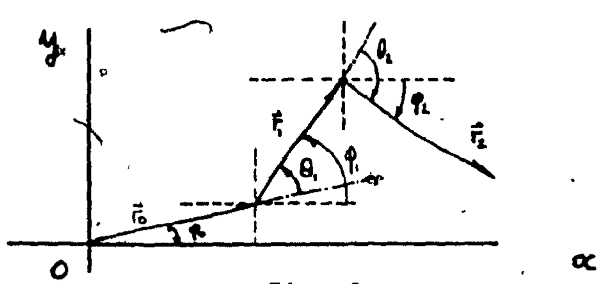

Fig. 2

Let Θ_{i+1} be a random variable which assigns a relative angle θ_{i+1} to the step $\vec{r}_{i+1}$, for each $i = 0, 1, 2, \cdots$. Let $\mathbb{R}_i$ be a random variable which assigns a length $r_i = |\vec{r}_i|$ to the step $\vec{r}_i$ for each $i = 0, 1, 2, \cdots$. Let Φ_0 be the random variable which assigns an angle φ_0 w.r.t. the reference x-axis to the initial step. We require that:

$\{\mathbb{R}_i\}$ $i = 0, 1, 2 \cdots$ be a sequence of independent and identically distributed random variables with a common density $g(r)$,

$\{\Theta_{i+1}\}$ $i = 0, 1, 2, \cdots$ be a sequence of independent and identically distributed random variables with a common, <u>even</u> density $f(\theta)$.

$\{\mathbb{R}\}$ and Θ be independent,

Φ_0 have an arbitrary density and be independent of Θ_{i+1} and $\{\mathbb{R}_i\}$.

In chapter II we focus on the representation of discrete correlated walks in $\mathbb{R}^1$ and $\mathbb{R}^2$ by Markov chains where the states are the directions rather than the positions. In chapter III the four assumptions mentioned above are taken up again for our general formulation of the correlated walk in the plane; we consider the discrete correlated walks in $\mathbb{R}^1$ and $\mathbb{R}^2$ as special cases. In chapter IV the works of Gail and Boone (1970), Nossal and Weiss (1974a,b) and Hall (1977) are discussed in connection with the application of correlated walks in the plane to theories of biological cell motion.

CHAPTER II

MARKOV REPRESENTATION OF DIRECTION DEPENDENT WALKS

§. 1 The Binomial Random Walk

The binomial random walk given by eq.(I-1.4) can be modeled by a two state stationary Markov chain in which the states are the positive and negative directions, which we denote by state 1 and state 2, respectively. The random variables $X_i, i = 1, 2, \cdots$ defined on these two states have identical Bernoulli distributions and assume as before the values $+1$ and -1 with constant probabilities p and q, respectively. Hence, we have

$$(1.1) \qquad P(X_{i+1} = k \mid X_i = h) = P(X_{i+1} = k) = p_k \quad h, k \in \{-1, 1\}$$

which is independent of h.

The four probabilities given by eq.(1.1) can be written in matrix form

$$(1.2) \qquad P = \begin{pmatrix} p & q \\ p & q \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(1+\lambda) & \frac{1}{2}(1-\lambda) \\ \frac{1}{2}(1+\lambda) & \frac{1}{2}(1-\lambda) \end{pmatrix},$$

where $\lambda = p - q$.

Eq.(1.1) and the identical rows in eq.(1.2) indicate that the random variables are independent and the constant matrix P, that the Markov chain is stationary.

When $\lambda = 0$, we get from eq.(1.2)

(1.3) $$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = P^n$$ for all positive integers n.

Hence we have a Markov chain which describes a symmetric random walk with the state space the direction rather than the position.

When $\lambda = +1$ or $\lambda = -1$, we get from eq.(1.2)

$$P = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} = P^n$$ for all positive integers n

or $$P = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} = P^n$$ for all positive integers n,

where P^n is the n^{th} power of the matrix P.

In either case, $\lambda = +1$ or, $\lambda = -1$, the system does not change state and, looking at it from the point of view of a random walk, the particle executing the walk goes steadily to $+\infty$ or $-\infty$.

§ 2 Markov Dependent Bernoulli Trials

We consider now a sequence $\{X_i\}$ $i = 1, 2, \cdots$ of identically distributed random variables, each having the Bernoulli distribution as in §1, with, in addition, the following four conditional transition probabilities

(2.1) $$P\left(X_{i+1} = k \mid X_i = h\right) = p_{hk} \qquad h, k \in \{-1, 1\}$$

which are independent of i. We thus have a sequence of Markov dependent repeated Bernoulli trials, (Parzen, 1960, p. 129). The conditional probabilities in eq.(2.1) together with the initial distribution

(2.2) $$\pi = \left(p_1^{(1)},\ p_2^{(2)}\right) = (\pi_1, \pi_2)$$

determine this Markov chain. As an example we consider the following four, one step, conditional transition probabilities given by eq.(2.1) which we write in matrix form,

(2.3) $$P = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(1+\lambda) & \frac{1}{2}(1-\lambda) \\ \frac{1}{2}(1-\lambda) & \frac{1}{2}(1+\lambda) \end{pmatrix} = \begin{pmatrix} p & q \\ q & p \end{pmatrix}$$

where $|1 - p_{11} - p_{22}| < 1$ and $\lambda = p - q$.

The n-step conditional transition probabilities are given by

(2.4) $$P^n = \begin{pmatrix} p_{11}^{(n)} & p_{12}^{(n)} \\ p_{21}^{(n)} & p_{22}^{(n)} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(1+\lambda^n) & \frac{1}{2}(1-\lambda^n) \\ \frac{1}{2}(1-\lambda^n) & \frac{1}{2}(1+\lambda^n) \end{pmatrix}$$

It follows from eq's.(2.1), (2.2), (2.3), (2.4) that the unconditional probabilities of finding the system in state 1 and 2 at any step n are given by

(2.5a) $$\pi P^n = p^{(n)}$$

where the components of $p^{(n)}$ are given by

(2.5b) $$p_1^{(n)} = \pi_1 p_{11}^{(n)} + \pi_2 p_{21}^{(n)}$$

(2.5c) $$p_2^{(n)} = \pi_1 p_{12}^{(n)} + \pi_2 p_{22}^{(n)}$$

Let $\pi_1 = \frac{1}{2}(1+\varepsilon)$ and $\pi_2 = \frac{1}{2}(1-\varepsilon)$. Then from eq's.(2.4) and (2.5b,c) we get

(2.6) $$\begin{aligned} p_1^{(n)} &= \tfrac{1}{4}\left[(1+\varepsilon)(1+\lambda^n) + (1-\varepsilon)(1-\lambda^n)\right] \\ &= \tfrac{1}{4}\left(1+\cancel{\varepsilon}+\cancel{\lambda^n}+\varepsilon\lambda^n+1-\cancel{\varepsilon}-\cancel{\lambda^n}+\varepsilon\lambda^n\right) \\ &= \tfrac{1}{2}(1+\varepsilon\lambda^n) \end{aligned}$$

And similarly for $p_2^{(n)}$, we obtain

(2.7) $$p_2^{(n)} = \tfrac{1}{2}(1-\varepsilon\lambda^n)$$

Hence we can write

(2.8) $$\begin{aligned} E(X_i) &= (-1)\,p_2^{(i)} + (+1)\,p_1^{(i)} \\ &= -\tfrac{1}{2} + \tfrac{\varepsilon}{2}\lambda^i + \tfrac{1}{2} + \tfrac{\varepsilon}{2}\lambda^i \\ &= \varepsilon\lambda^i \end{aligned}$$

(2.9) $$\begin{aligned} E(X_i^2) &= (-1)^2\,p_2^{(i)} + (+1)^2\,p_1^{(i)} \\ &= 1 \end{aligned}$$

The partial sums $\{S_n\}$ $n=1,2,\cdots$, where $S_n = \sum_{i=1}^{n} X_i$ do not in general form a random walk on the integers since the X_i may not be independent. But the relation

$$X_i = S_i - S_{i-1} \tag{2.10}$$

exists; so that $\{S_n\}$ is a process with stationary increments, (Feller 2, 1971 p. 97). But in eq.(2.3) we have a constant matrix $\mathbf{P}$. Therefore the Markov chain is stationary.

From eq.(2.8) we get

$$\begin{aligned} E(S_n) &= \sum_{i=1}^{n} E(X_i) \\ &= \varepsilon \sum_{i=1}^{n} \lambda^i \\ &= \varepsilon \left(\frac{1-\lambda^{n+1}}{1-\lambda} - 1 \right) \\ &= \varepsilon \lambda \left(\frac{1-\lambda^n}{1-\lambda} \right) \end{aligned} \tag{2.11}$$

(2.12) Now: $E(S_n^2) = \sum_{i=1}^{n} E(X_i^2) + 2 \sum_{i=0}^{n-1} \sum_{j=i+1}^{n} E(X_i X_j)$

$$\begin{aligned} E(X_i X_j) &= \sum_{h,k} hk\, P(X_i = h, X_j = k) \qquad h,k \in (-1,1) \\ &= \sum_{h,k} hk\, P(X_i = h) P(X_j = k \mid X_i = h) \\ &= \left(p_1^{(i)} p_{11}^{(j-i)} + p_2^{(i)} p_{22}^{(j-i)} - p_1^{(i)} p_{12}^{(j-i)} - p_2^{(i)} p_{21}^{(j-i)} \right) \end{aligned} \tag{2.13}$$

Now from eq's.(2.3) and (2.4) we get

$$(2.14) \qquad P_{hk}^{j-i} = \begin{pmatrix} p_{11}^{(j-i)} & p_{12}^{(j-i)} \\ p_{21}^{(j-i)} & p_{22}^{(j-i)} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(1+\lambda^{j-i}) & \frac{1}{2}(1-\lambda^{j-i}) \\ \frac{1}{2}(1-\lambda^{j-i}) & \frac{1}{2}(1+\lambda^{j-i}) \end{pmatrix}$$

$h, k \in (1,2)$

Hence from eq's.(2.6), (2.7), (2.13) and (2.14) we get

$$(2.15) \qquad E(X_i X_j) = \frac{1}{4}\Big[(1+\varepsilon\lambda^i)(1+\lambda^{j-i}) + (1-\varepsilon\lambda^i)(1+\lambda^{j-i})$$

$$- (1+\varepsilon\lambda^i)(1-\lambda^{j-i}) - (1-\varepsilon\lambda^j)(1-\lambda^{j-i})\Big]$$

$$= \frac{1}{4}\Big(1 + \lambda^{j-i} + \varepsilon\lambda^i + \varepsilon\lambda^j + 1 + \lambda^{j-i} - \varepsilon\lambda^i - \varepsilon\lambda^j$$

$$-1 + \lambda^{j-i} - \varepsilon\lambda^i + \varepsilon\lambda^j - 1 + \lambda^{j-i} + \varepsilon\lambda^i - \varepsilon\lambda^j\Big)$$

$$= \lambda^{j-i},$$ (see also Feller 2, 1971, p. 97).

For $i = 1$, $\sum_{j=2}^{n} \lambda^{j-i} = \lambda + \lambda^2 + \cdots + \lambda^{n-3} + \lambda^{n-2} + \lambda^{n-1}$

For $i = 2$ $\sum_{j=3}^{n} \lambda^{j-i} = \lambda + \lambda^2 + \cdots + \lambda^{n-3} + \lambda^{n-2}$

For $i = n-1$ we get λ.

Hence, summing up, we get

$$(2.16) \qquad \sum_{i=0}^{n-1} \sum_{j=i+1}^{n} \lambda^{j-i} = (n-1)\lambda + (n-2)\lambda^2 + \cdots + [n-(n-1)]\lambda^{n-1}$$

$$= n\lambda + n\lambda^2 + \cdots + n\lambda^{n-1} - (\lambda + 2\lambda^2 + \cdots + (n-1)\lambda^{n-1})$$

$$= \frac{n(1-\lambda^n)}{1-\lambda} - n - \lambda \frac{d}{d\lambda}\left(\frac{1-\lambda^n}{1-\lambda}\right)$$

$$= \frac{\lambda}{1-\lambda}\left(n - \frac{1-\lambda^n}{1-\lambda}\right)$$

and from eq's. (2.9), (2.12), (2.16) we get

(2.17a) $$E(S_n^2) = n + \frac{2\lambda}{1-\lambda}\left(n - \frac{1-\lambda^n}{1-\lambda}\right)$$

(2.17b) $$= \left(\frac{1+\lambda}{1-\lambda}\right) n - \frac{2\lambda}{(1-\lambda)^2} + \frac{2\lambda^{n+1}}{(1-\lambda)^2}$$

a result which will be derived in chapter III by another method. asymptotic expression for the mean square displacement in eq.(2.17b) when $n \to \infty$ is given by

(2.18) $$E(S_n^2) \simeq \left(\frac{1+\lambda}{1-\lambda}\right) n - \frac{2\lambda}{(1-\lambda)^2}$$

where the r.h.s. of eq.(2.18), the asymptote to $E(S_n^2)$ in eq.(2.17b), has slope α and n-intercept β given by

(2.19) $$\alpha = \frac{1+\lambda}{1-\lambda} \qquad \beta = \frac{2\lambda}{1-\lambda^2}$$

Eq's.(2.17b) and (2.18) differ by the factor $\frac{2\lambda^{n+1}}{(1-\lambda)^2}$ and

(2.20) $$\lim_{n\to\infty} \frac{2\lambda^{n+1}}{(1-\lambda)^2} = 0 \qquad \text{when} \qquad |\lambda| < 1$$

From eq.(2.4) and the fact that P is aperiodic and irreducible, the stationary distribution exists and is unique.

(2.21) $$\lim_{n\to\infty} P^n = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

i.e. $$\lim_{n\to\infty} p_j^{(n)} = \frac{1}{2} \; ; j = 1,2 ;$$ (see eq's.(2.6) and (2.7))

And we also get from eq.(2.17b)

(2.22) $$\lim_{n\to\infty} \frac{E(S_n^2)}{E(S_n^2)_{\lambda=0}} = \lim_{n\to\infty} \frac{E(S_n^2)}{n}$$
$$= \left(\frac{1+\lambda}{1-\lambda}\right).$$

Sufficient conditions for the convergence of $\frac{E(S_n^2)}{n}$ according to Montroll (1950) is that the correlation function between the steps be decreasing as fast as $\frac{A}{s^{1+\varepsilon}}$ where A is a constant of proportionality, $s = |j-i|$ and ε an arbitrarily small positive constant. We see that from eq.(2.15), $\lambda^{j-i} = E(X_i X_j)$ has that property.

As an example, let in eq.(2.3) P be given by

(2.23) $$P = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

an irreducible aperiodic matrix of transition probabilities. 1 is an eigenvalue of P and $\lambda = p - q = \frac{1}{2}$ is the other.

$$(2.24)\qquad P^n = \begin{pmatrix} \frac{1}{2}\left(1+\frac{1}{2^n}\right) & \frac{1}{2}\left(1-\frac{1}{2^n}\right) \\ \frac{1}{2}\left(1-\frac{1}{2^n}\right) & \frac{1}{2}\left(1+\frac{1}{2^n}\right) \end{pmatrix},$$

(see eq's.(2.4) and (2.14). For the Markov chain with transition matrix P given by eq.(2.23), we obtain the asymptotic form from eq.(2.18), i.e.

$$(2.25)\qquad E(S_n^2) \simeq \left(\frac{1+\lambda}{1-\lambda}\right)n - \frac{2\lambda}{(1-\lambda)^2}$$

$$= 3n - 4$$

Fig.3 illustrates how $E(S_n^2)$ approaches the asymptote given by the r.h.s. of eq.(2.25), as n gets larger.

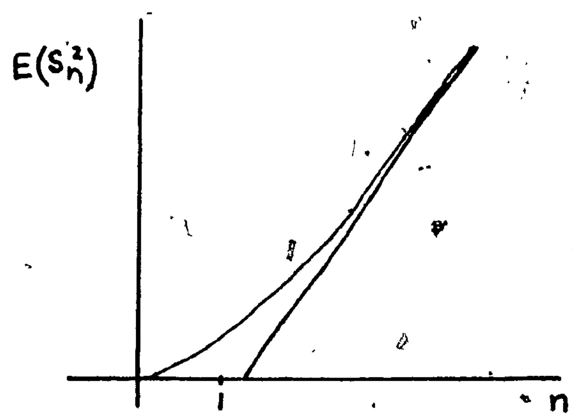

Fig. 3

§ 3 The Two Dimensional Case

In extending these results to $\mathbb{R}^2$, we will consider special cases. The 16 conditional probabilities corresponding to eq.(2.1) are given by

$$(3.1) \qquad P\left(X_{i+1} = k \,\middle|\, X_i = h\right) = p_{hk} \qquad h,k \in \{(1,0),(-1,0),(0,1),(0,-1)\}$$

where the X_i's take value in $\{(1,0),(-1,0),(0,1),(0,-1)\}$, corresponding to the states i.e. the 4 directions on the x and the y axes. For example, in matrix form, we consider eq.(3.1) to be given by

$$(3.2) \qquad P = \begin{pmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{pmatrix} = \begin{pmatrix} p & q & \ell & r \\ q & p & r & \ell \\ r & \ell & p & q \\ \ell & r & q & p \end{pmatrix}$$

From eq.(3.2) we read, for example, the probability that the next step will be in the negative y-direction given that it is now in the positive x-direction, is r.

As in eq.(2.5a) we have

$$(3.3a) \qquad \pi P^n = p^{(n)}$$

where the components of $p^{(n)}$ are given by $p_j^{(n)}$, $j = 1,2,3,4$.

$$(3.3b) \qquad p_1^{(n)} = \pi_1 p_{11}^{(n)} + \pi_2 p_{21}^{(n)} + \pi_3 p_{31}^{(n)} + \pi_4 p_{41}^{(n)}$$

$$p_2^{(n)} = \pi_1 p_{12}^{(n)} + \pi_2 p_{22}^{(n)} + \pi_3 p_{32}^{(n)} + \pi_4 p_{42}^{(n)} .$$

$$p_3^{(n)} = \pi_1 p_{13}^{(n)} + \pi_2 p_{23}^{(n)} + \pi_3 p_{33}^{(n)} + \pi_4 p_{43}^{(n)}$$

$$p_4^{(n)} = \pi_1 p_{14}^{(n)} + \pi_2 p_{24}^{(n)} + \pi_3 p_{34}^{(n)} + \pi_4 p_{44}^{(n)}$$

and where $\pi = (\pi_1, \pi_2, \pi_3, \pi_4)$, the initial probability vector.

P in eq.(3.2) is doubly stochastic. And from eq's.(3.3a) and (3.3b) we can compute $E(X_i)$ and $E(X_i X_j)$, $i,j = 1,2,\cdots$.

(3.4)
$$E(X_i) = \sum_h h P(X_i = h)$$
$$= (1,0)p_1^{(i)} + (-1,0)p_2^{(i)} + (0,1)p_3^{(i)} + (0,-1)p_4^{(i)}$$

(3.5)
$$E(X_i X_j) = \sum_{h,k} hk P(X_i = h, X_j = k)$$
$$= \sum_{h,k} hk P(X_i = h) P(X_j = k | X_i = h)$$

$$h,k \in \{(1,0), (-1,0), (0,1), (0,-1)\}$$

As special cases of this example we consider the following matrices

a)

(3.6)
$$P = \begin{pmatrix} p & q & 0 & 0 \\ q & p & 0 & 0 \\ 0 & 0 & p & q \\ 0 & 0 & q & p \end{pmatrix}$$

$\mathbf{P}$ consists of two submatrices $\begin{pmatrix} p & q \\ q & p \end{pmatrix}$. Hence the result of eq.(2.17b) for the mean square displacement holds.

b) Let $\mathbf{P}$ be given by

(3.7) $$\mathbf{P} = \begin{pmatrix} 0 & p & 0 & q \\ q & 0 & p & 0 \\ 0 & q & 0 & p \\ p & 0 & q & 0 \end{pmatrix}$$

The entries of $\mathbf{P}^n$ are given by

(3.8) $$p_{hk}^{(n)} = \frac{1}{4}\left\{ 1 + (q-p)^n i^{h-k-n} \right\}\left\{ 1 + (-1)^{h+k-n} \right\}$$

(Feller 1, 1968, p.434)

Let the initial probability vector be given by

(3.9) $$\pi = \left(p_1^{(1)},\ p_2^{(1)},\ p_3^{(1)};\ p_4^{(1)}\right) = \left(\pi_1, \pi_2, \pi_3, \pi_4\right)$$

(3.10) where $\pi_1 = \pi_3 = 0$

and $\pi_4 - \pi_2 = \varepsilon$

and $\pi_4 = \frac{1}{2}(1+\varepsilon)$; $\pi_2 = \frac{1}{2}(1-\varepsilon)$.

Now, as in eq.(2.5b), we get

(3.11) $$p_1^{(n)} = \pi_2 p_{21}^{(n)} + \pi_4 p_{41}^{(n)}$$

$$p_2^{(n)} = \pi_2 p_{22}^{(n)} + \pi_4 p_{42}^{(n)}$$

$$p_3^{(n)} = \pi_2 p_{23}^{(n)} + \pi_4 p_{43}^{(n)}$$

$$p_4^{(n)} = \pi_2 p_{24}^{(n)} + \pi_4 p_{44}^{(n)}$$

By using eq's.(3.4), (3.5), (3.8) and (3.11) and taking into account the periodicity of $\mathbf{P}$, we could find the mean square displacement for this walk, in terms of $\lambda = q - p$.

Consider the following restricted walk on a square lattice where steps in the reverse direction are prohibited. The probability of each step depends on the preceding step. We are dealing here with a stationary 4-state Markov chain whose transition matrix is given by

$$(3.12) \qquad \mathbf{P} = \begin{pmatrix} 1-2p & 0 & p & p \\ 0 & 1-2p & p & p \\ p & p & 1-2p & 0 \\ p & p & 0 & 1-2p \end{pmatrix}$$

again a doubly stochastic matrix.

Let the steps in the allowed directions have a constant length ℓ. Then the mean square displacement for such a walk (Volkenstein, 1963, p. 219) is given by

$$(3.13) \qquad E(S_n^2) = \sum_{i=0}^{n-1} \left[E(X_i^2) + E(Y_i^2)\right] + 2 \sum_{\substack{i<j \\ i=0}}^{n-1} \left[E(X_i X_j) + E(Y_i Y_j)\right]$$

where X_i and Y_i are the components of the vector step ℓ.

(3.14a) $$E(X_i^2) = \frac{\ell^2}{2}\left[1 + (1-2p)^{i+1}\right]$$

(3.14b) $$E(Y_i^2) = \frac{\ell^2}{2}\left[1 - (1-2p)^{i+1}\right]$$

(3.14c) $$E(X_i X_j) = \frac{\ell^2}{2}(1-2p)^{j-i}\left[1 - (1-2p)^{i}\right]$$

(3.14d) $$E(Y_i Y_j) = \frac{\ell^2}{2}(1-2p)^{j-i}\left[1 - (1-2p)^{i}\right]$$

Hence we get

(3.15) $$E(S_n^2) = n\ell^2 + 2\ell^2 \sum_{\substack{i<j \\ i=0}}^{n-1} (1-2p)^{j-i}$$
$$= \ell^2\left[n\frac{1-p}{p} + (1-2p)\frac{(1-2p)^n - 1}{p^2}\right]$$

We note that the eigenvalues of the matrix $\underset{\sim}{P}$ are

$$\lambda_1 = 1 ; \quad \lambda_2 = \lambda_3 = 1-2p$$

and $\lambda_4 = 1-4p$.

CHAPTER III

THE CORRELATED WALK IN $\mathbb{R}^2$

§ 1 Statement of Assumptions

$\{\vec{r}_i\}$ $i = 0, 1, 2, \cdots$ is a sequence of 2-dimensional random vectors.

$\{\mathbb{R}_i\}$ $i = 0, 1, 2, \cdots$ is a sequence of independent and identically distributed random variables with common density $g(r)$; $\mathbb{R}_i$ takes value $r_i = |\vec{r}_i|$.

$\{\Theta_{i+1}\}$ $i = 0, 1, 2, \cdots$ is a sequence of independent and identically distributed random variables with common, even density $f(\theta)$.

Φ_0 is the random variable which assigns the angle φ_0 to the initial step $\vec{r}_0$; Φ_0 is arbitrary and independent of Θ_{i+1} and $\mathbb{R}_i$.

$\mathbb{R}$ and Θ are independent.

§ 2 Description of the Walk

Let $\vec{r}_0, \vec{r}_1, \cdots$ be a sequence of 2-dimensional random vectors in the plane, where $|\vec{r}_i|$, $i = 0, 1, \cdots$ represent the step lengths of the correlated walk. The position of the walker at the end of the n^{th} step is given by the partial sums

$$\vec{R}_n = \sum_{i=0}^{n-1} \vec{r}_i \tag{2.1}$$

where $|\vec{R}_n|$ is the distance from the origin and $\vec{R}_n$ the resultant.

Each vector $\vec{r}_i$ makes an angle φ_i with the reference x-axis. The angle θ_i between two adjacent steps $\vec{r}_i$ and $\vec{r}_{i+1}$ $i=0,1,\cdots$ is the angle between the two adjacent vectors $\vec{r}_i$ and $\vec{r}_{i+1}$. (see fig.4). θ_i denotes the relative angle and its value is given by the p.d.f. $f(\theta)$ of the random variable $\Theta = \Theta_{i+1}$, where $\{\Theta_{i+1}\}$ $i=0,1,2,\cdots$ is the sequence of independent and identically distributed random variables defined above. The representation of a path of such a walk is illustrated in fig. 4

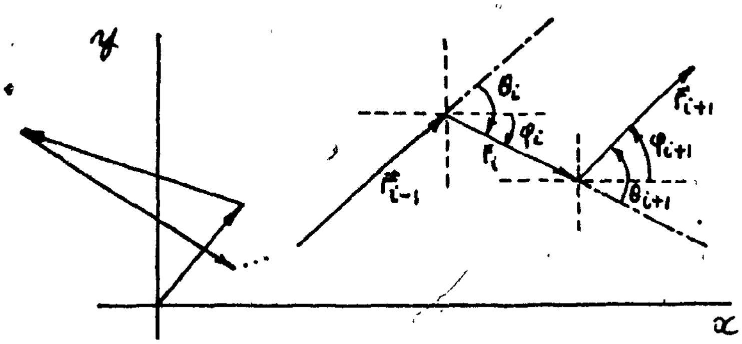

Fig. 4

A point on the path is given by

$$(X_i, Y_i) = (r_i \cos\varphi_i , r_i \sin\varphi_i) \tag{2.2}$$

For every i , the angle φ_i can be written as

$$\begin{aligned}
\varphi_i &= \varphi_0 + (\varphi_1 - \varphi_0) + \cdots + (\varphi_i - \varphi_{i-1}) \\
&= \varphi_0 + \theta_1 + \theta_2 + \cdots + \theta_i \\
&= \varphi_0 + \sum_{k=1}^{i} \theta_k
\end{aligned}$$

The relation

(2.4) $\theta_{i+1} = \varphi_{i+1} - \varphi_i$ with $\theta_i, \varphi_i \in [-\pi, \pi]$

indicates that the process $\{\varphi_i\}\ i = 0,1,2,\cdots$ has independent increments and therefore is a random walk. $\sum_{i=0}^{n-1} \theta_{i+1}$ and $\sum_{i=0}^{n-1} r_i$ are random walks. Now $\{\vec{R}_n\}$ and $\{\vec{r}_n\}$ are not random walks. But $\{\vec{r}_n\}$ is a Markov chain.

§ 3 <u>The Mean and the Variance of $\vec{r}_i$</u>

From eq.(2.2) we can write

(3.1) $$(X_i, Y_i) = \left[r_i \cos(\varphi_0 + \sum_{j=1}^{i} \theta_j),\ r_i \sin(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right]$$

(3.2) $$E(\vec{r}_i) = \left[E(X_i), E(Y_i)\right]$$

$$= \left\{E(r_i)\, E\left[\cos(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right],\ E(r_i)\, E\left[\sin(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right]\right\}$$

$$= E(r_i)\left\{E\left[\cos(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right],\ E\left[\sin(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right]\right\}$$

We take the expectation $E\left[\cos(\varphi_0 + \sum_{j=1}^{i} \theta_j)\right]$ with respect to the joint density of $\varphi_0, \theta_1, \theta_2, \cdots, \theta_i, r_0, r_1, \cdots, r_i$, namely,

(3.3) $$p(\varphi_0, \theta_1, \cdots, \theta_i, r_0, \cdots, r_i) = h(\varphi_0)\, f(\theta_1) \cdots f(\theta_i)\, g(r_0) \cdots g(r_i)$$

(3.4a) Let $\lambda_0 = E(\cos\varphi_0)$

(3.4b) $\lambda_0' = E(\sin\varphi_0)$

(3.4c) $\lambda = E(\cos\theta_j) \qquad j = 1, 2, \ldots, i$

(3.4d) $\lambda' = E(\sin\theta_j) = 0 \qquad j = 1, 2, \ldots, i$

(3.5) $E\left[\cos\left(\varphi_0 + \sum_{j=1}^{i}\theta_j\right)\right] =$

$$= E\left[\cos\varphi_0 \cos\left(\sum_{j=1}^{i}\theta_j\right) - \sin\varphi_0 \sin\left(\sum_{j=1}^{i}\theta_j\right)\right]$$

$$= E(\cos\varphi_0)\, E\left[\cos\theta_1 \cos\left(\sum_{j=2}^{i}\theta_j\right) - \sin\theta_1 \sin\left(\sum_{j=2}^{i}\theta_j\right)\right]$$

$$- E(\sin\varphi_0)\, E\left[\sin\theta_1 \cos\left(\sum_{j=2}^{i}\theta_j\right) + \cos\theta_1 \sin\left(\sum_{j=2}^{i}\theta_j\right)\right]$$

$$= \lambda_0 \left\{\lambda E\left[\cos\left(\sum_{j=2}^{i}\theta_j\right)\right] - \lambda' E\left[\sin\left(\sum_{j=2}^{i}\theta_j\right)\right]\right\}$$

$$- \lambda_0' \left\{\lambda' E\left[\cos\left(\sum_{j=2}^{i}\theta_j\right)\right] + \lambda E\left[\sin\left(\sum_{j=2}^{i}\theta_j\right)\right]\right\}$$

$$= \lambda_0 \lambda^{i-1} E(\cos\theta_i) - \lambda_0' \lambda^{i-1} E(\sin\theta_i)$$

$$= \lambda_0 \lambda^i$$

Similarly,

(3.6) $E\left[\sin\left(\varphi_0 + \sum_{j=1}^{i}\theta_j\right)\right] =$

$$= E\left[\sin\varphi_0 \cos\left(\sum_{j=1}^{i}\theta_j\right) + \cos\varphi_0 \sin\left(\sum_{j=1}^{i}\theta_j\right)\right]$$

$$= E(\sin\varphi_0)\, E\left[\cos\theta_1 \cos\left(\sum_{j=2}^{i}\theta_j\right) - \sin\theta_1 \sin\left(\sum_{j=2}^{i}\theta_j\right)\right]$$

$$+ E(\cos\varphi_0)\, E\left[\sin\theta_1 \cos\left(\sum_{j=2}^{i}\theta_j\right) + \cos\theta_1 \sin\left(\sum_{j=2}^{i}\theta_j\right)\right]$$

$$= \lambda_0'\left\{\lambda E\left[\cos\left(\sum_{j=2}\theta_j\right)\right] - \lambda' E\left[\sin\left(\sum_{j=2}^{i}\theta_j\right)\right]\right\}$$

$$+ \lambda_0\left\{\lambda' E\left[\cos\left(\sum_{j=2}^{i}\theta_j\right)\right] + \lambda E\left[\sin\left(\sum_{j=2}^{i}\theta_j\right)\right]\right\}$$

$$= \lambda_0' \lambda^{i-1} E(\cos\theta_i) + \lambda_0 \lambda^{i-1} E(\sin\theta_i)$$

$$= \lambda_0' \lambda^{i}$$

Now we let

$$\mu_r = \int_0^\infty r\, g(r)\, dr \tag{3.7}$$

$$= E(r)$$

$$= E(r_i)$$

Then we can write

(3.8) $$E(\vec{r}_i) = E(r_i)\left(\lambda_0\lambda^i,\ \lambda_0'\lambda^i\right)$$
$$= \mu_r\left(\lambda_0\lambda^i,\ \lambda_0'\lambda^i\right).$$

(3.9) $$E^2(\vec{r}_i) = \mu_r^2\left(\lambda_0\lambda^i,\ \lambda_0'\lambda^i\right)^2$$
$$= \mu_r^2\left[(\lambda_0\lambda^i)^2 + (\lambda_0'\lambda^i)^2\right]$$

(3.10) Now: $$\vec{r}_i^{\,2} = \left[r_i\cos\left(\varphi_0+\sum_{j=1}^{i}\theta_j\right),\ r_i\sin\left(\varphi_0+\sum_{j=1}^{i}\theta_j\right)\right]^2$$
$$= r_i^2$$

(3.11) $$E(\vec{r}_i^{\,2}) = E(r^2) = \int_0^\infty r^2 g(r)\,dr$$
$$= \sigma_r^2 + \mu_r^2$$

(3.12) But: $$\sigma_r^2 = \operatorname{var} r$$
$$= \operatorname{var} r_i$$
$$= E(r_i^2) - E^2(r_i)$$
$$= E(r_i^2) - \mu_r^2$$

(3.13) $$\therefore\ \operatorname{var}\vec{r}_i \doteq E(\vec{r}_i^{\,2}) - E^2(\vec{r}_i).$$
$$= \sigma_r^2 + \mu_r^2 - \mu_r^2\lambda^{2i}(\lambda_0^2 + \lambda_0'^2)$$

§ 4 The Mean Square Displacement

(4.1a) $$\vec{R}_n^{\,2} = \left[\sum_{i=0}^{n-1} \vec{r}_i \right]^2$$

(4.1b) $$= \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} \left\{ \left[r_j \cos\left(\varphi_0 + \sum_{k=1}^{j} \theta_k\right),\ r_j \sin\left(\varphi_0 + \sum_{k=1}^{j} \theta_k\right) \right] \cdot \left[r_i \cos\left(\varphi_0 + \sum_{k=1}^{i} \theta_k\right),\ r_i \sin\left(\varphi_0 + \sum_{k=1}^{i} \theta_k\right) \right] \right\}$$

(4.1c) $$= \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} r_j r_i \left[\cos\left(\varphi_0 + \sum_{k=1}^{j} \theta_k\right) \cos\left(\varphi_0 + \sum_{k=1}^{i} \theta_k\right) + \sin\left(\varphi_0 + \sum_{k=1}^{j} \theta_k\right) \sin\left(\varphi_0 + \sum_{k=1}^{i} \theta_k\right) \right]$$

(4.1d) $$= \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} r_j r_i \cos\left[\left(\varphi_0 + \sum_{k=1}^{j} \theta_k\right) - \left(\varphi_0 + \sum_{k=1}^{i} \theta_k\right) \right]$$

(4.1e) $$= \sum_{i=0}^{n-1} r_i^2 + 2 \sum_{\substack{i<j \\ i=0}}^{n-1} r_j r_i \cos\left(\theta_{i+1} + \cdots + \theta_j\right)$$

As in eq.(3.10), we have

(4.2) $$\vec{R}_n^{\,2} = R_n^2$$

Hence,

(4.3) $$E\left(\vec{R}_n^{\,2}\right) = \sum_{i=0}^{n-1} E\left(r_i^2\right) + 2 \sum_{\substack{i<j \\ i=0}}^{n-1} E(r_i) E(r_j) E\left[\cos(\theta_{i+1} + \cdots \theta_j)\right]$$

which indicates the dependence of the walk on $\sum_{k=i+1}^{j} \theta_k$ i.e. on $\varphi_j - \varphi_i$.

Also, eq.(4.1d) shows, as expected, that the mean square distance does not depend on the distribution of φ_o .

$$(4.4)\qquad E\left[\cos(\theta_{i+1}+\cdots+\theta_j)\right] = E\left[\cos\left(\theta_{i+1}+\sum_{k=i+2}^{j}\theta_k\right)\right]$$

$$= E\left[\cos\theta_{i+1}\cos\left(\sum_{k=i+2}^{j}\theta_k\right) - \sin\theta_{i+1}\sin\left(\sum_{k=i+2}^{j}\theta_k\right)\right]$$

$$= \lambda E\left[\cos\left(\sum_{k=i+2}^{j}\theta_k\right)\right]$$

$$= \lambda^{j-i}$$

where we have used eq.(3.4d).

Now the summation $\sum_{\substack{i<j\\ i=0}}^{n-1}\lambda^{j-i}$ was obtained in eq.(II-2.16).

Hence from eq's.(4.3), (3.11) and (3.7) we have

$$(4.5)\qquad E(R_n^2) = nE(r^2) + 2\mu_r^2\sum_{\substack{i<j\\ i=0}}^{n-1}\lambda^{j-i}$$

$$(4.6)\qquad = nE(r^2) + 2\mu_r^2\frac{\lambda}{1-\lambda}\left(n-\frac{1-\lambda^n}{1-\lambda}\right)$$

$$(4.7)\qquad = \left(E(r^2) + 2\mu_r^2\frac{\lambda}{1-\lambda}\right)n - 2\mu_r^2\frac{\lambda}{(1-\lambda)^2} + 2\mu_r^2\frac{\lambda^{n+1}}{(1-\lambda)^2}$$

$$(4.8)\qquad \frac{E(R_n^2)}{E(r^2)} = \left(1 + 2s\frac{\lambda}{1-\lambda}\right)n - \frac{2s\lambda}{(1-\lambda)^2} + \frac{2s\lambda^{n+1}}{(1-\lambda)^2}$$

(4.9) where $$s = \frac{\mu_r^2}{E(r^2)}$$

We can write eq.(4.7) the following way

(4.10) $$E(R_n^2) = An + B + C^n$$

where $\lim_{n \to \infty} C^n = 0$ since $|\lambda| < 1$. The asymptote to $E(R_n^2)$ is given by

(4.11a) $$f(n) = An + B$$

We also have

(4.11b) $$\lim_{n \to \infty} \left[E(R_n^2) - f(n) \right] = 0$$

So how fast $E(R_n^2)$ approaches the asymptote depends on how fast C^n goes to zero, i.e. in eq.(4.7), on the rate of convergence of λ^{n+1} to zero, as $n \to \infty$. Fig. 5a illustrates this relationship for an asymptote with $A > 1$ and $\frac{B}{A} < 1$.

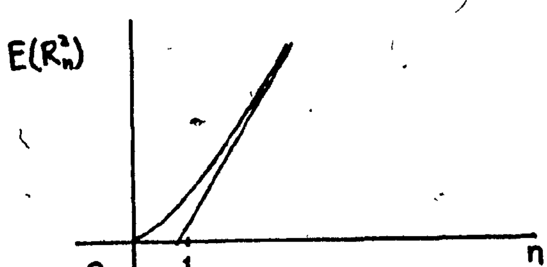

Fig. 5a

Let $\lambda = 0$. Then from eq.(4.6) we get

(4.12a) $$E(R_n^2) = n E(r^2)$$

which we represent in fig. 5b for $E(r^2) > 1$.

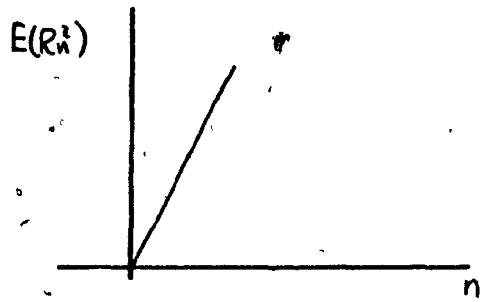

Fig. 5b

When $E(r^2) = 1$ eq.(4.12a) becomes

(4.12b) $$E(R_n^2) = n$$

the expression for the mean square displacement for a symmetric, drift free, random walk.

Let $|\lambda| < 1$ and $\lambda \neq 0$. Then, from eq.(4.7), we obtain an asymptotic expression for the mean square displacement, (see eq.4.4),

(4.13) $$E(R_n^2) \simeq \left[E(r^2) + 2\mu_r^2 \frac{\lambda}{1-\lambda} \right] n - 2\mu_r^2 \frac{\lambda}{(1-\lambda)^2}$$

and we also have

(4.14) $$\frac{E(R_n^2)}{E(r^2)} \simeq \left(1 + 2s \frac{\lambda}{1-\lambda} \right) n - 2s \frac{\lambda}{(1-\lambda)^2}$$

where $$s = \frac{\mu_r^2}{E(r^2)}$$

The r.h.s. of eq.(4.14) is a linear equation in n, the asymptote to which $E(R_n^2)$ in eq.(4.7) approches as $n \to \infty$, with slope α and n-intercept, t.

(4.15) $$\alpha = \left(1 + \frac{2s\lambda}{1-\lambda}\right)$$

(4.16) $$t = \frac{2s\lambda}{(1-\lambda)^2} \cdot \frac{1-\lambda}{1-\lambda+2s\lambda} = \frac{2s\lambda}{(1-\lambda)[1-\lambda(1-2s\lambda)]}$$

where α and t are functions of the individual steps and of λ.

§ 5 Special Cases

In the cases we consider next, we let $g(r)$ and $f(\theta)$ have the densities of the following type

(5.1) $$g(r) = \sum_i m_i \, \delta(r - l_i)$$

(5.2) $$f(\theta) \doteq \sum_i m_i \, \delta(\theta - \alpha_i)$$

where $0 \leq m_i \leq 1$ and $\sum_i m_i = 1$. m_i, $i = 1, 2, \cdots$, is a probability weight attached to $\delta(r - l_i)$ or $\delta(\theta - \alpha_i)$ where $l_i \geq 0$ and $-\pi \leq \alpha_i \leq \pi$.

Fig. 6 indicates the probability mass distribution of the m_i's for a function of the type given in eq.(5.2) for example, where $m_1 = m_2 = m_3 = \frac{1}{3}$ and $\alpha_1 = \frac{\pi}{4}$; $\alpha_2 = -\frac{\pi}{4}$; $\alpha_3 = 0$; $m : \Theta \longrightarrow [0,1]$.

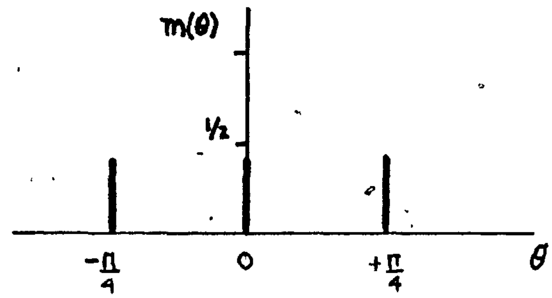

Fig. 6

A) <u>Cases where $\lambda = 0$</u>

1o) Let $g(r)$ be given by

$$g(r) = \delta(r - \ell) \tag{5.3}$$

Fig. 7 indicates the p. m. distribution of the unique m_r, $m(\ell) = 1$.

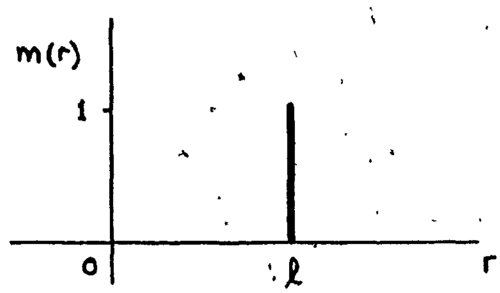

Fig. 7

$g(r)$ generates a walk by a sequence of fixed step lengths, ℓ .

Let $f(\theta)$ be given by

(5.4a) $$f(\theta) = \sum_i m_i \, \delta(\theta - \alpha_i)$$

where $m_1 = m_2 = \frac{1}{4}$; $m_3 = \frac{1}{2}$; $\alpha_1 = \pi$; $\alpha_2 = -\pi$; $\alpha_3 = 0$

(5.4b) i.e. $$f(\theta) = \frac{1}{4}\left\{ \delta(\theta - \pi) + \delta(\theta + \pi) \right\} + \frac{1}{2}\delta(\theta) .$$

We represent the p. m. distribution of the m_i's in fig. 8a. A section of the path of such a walk is illustrated in fig. 8b.

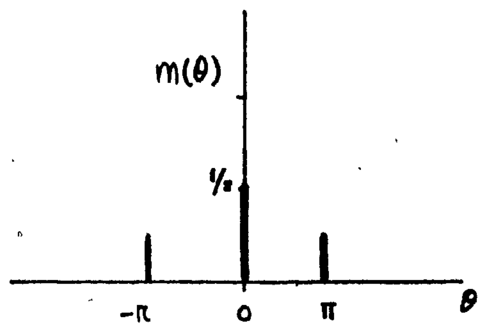

Fig. 8a

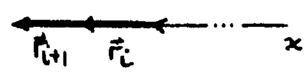

Fig. 8b

Looking at the steps $\vec{r}_i$ and $\vec{r}_{i+1}$ we see that $\theta_{i+1} = 0$ and $\varphi_{i+1} = \pi$. An angle θ assumes the values 0, π, or $-\pi$. Because of the relation $\theta_{i+1} = \varphi_{i+1} - \varphi_i$, the φ_i's will also take values 0, π, or $-\pi$.

$$(5.4c)\qquad \lambda = E(\cos\Theta)$$

$$= \int_{-\pi}^{\pi} \cos\theta \left\{ \frac{1}{4}\left[\delta(\theta-\pi) + \delta(\theta+\pi) + \frac{1}{2}\delta(\theta) \right\} d\theta\right.$$

$$= \frac{1}{4}\cos\pi + \frac{1}{4}\cos(-\pi) + \frac{1}{2}\cos 0$$

$$= 0$$

Now $E(\vec{r}_i^{\,2}) = \sigma_r^2 + \mu_r^2$ where, because of eq.(5.3), $\sigma_r^2 = 0$ and $\mu_r^2 = \ell^2$. Hence by eq's.(3.11) and (4.6)

$$(5.4d)\qquad E(R_n^2) = \ell^2 n$$

which is the expression for the mean square displacement in a one-dimensional symmetric random walk on the integer lattice, a Bernoulli walk where the walker takes steps in the positive x-direction with length $g(r) = \ell$ with probability $(\frac{1}{4} + \frac{1}{4}) = \frac{1}{2}$, since $-\pi$ and π represent the same direction on the x-axis. This formulation enhances the directional aspect of the walk rather than the positional one; it also shows the dependence of φ_{i+1} on φ_i.

2o) Let $g(r)$ be given by eq.(5.3) and $f(\theta)$ by

$$(5.5a)\qquad f(\theta) = \frac{1}{8}\left\{\delta(\theta-\pi) + \delta(\theta+\pi)\right\} + \frac{1}{4}\left\{\delta(\theta) + \delta(\theta-\tfrac{\pi}{2}) + \delta(\theta+\tfrac{\pi}{2})\right\}$$

where we represent the probability distribution of the m_i's in fig. 9a. A section of the path of such a walk is illustrated in fig. 9b, where, from the relation $\theta_{i+1} = \varphi_{i+1} - \varphi_i$ we see that $\theta_{i+1} = -\frac{\pi}{2}$ for the steps $\vec{r}_i$ and $\vec{r}_{i+1}$.

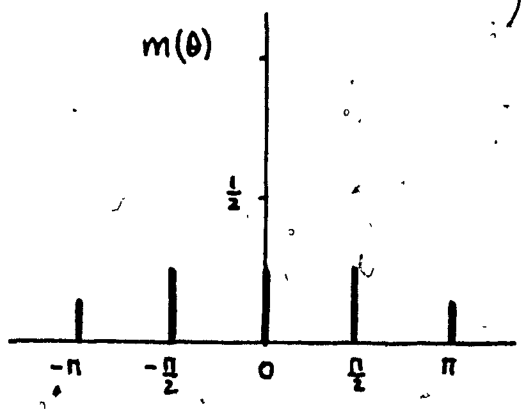

Fig. 9a

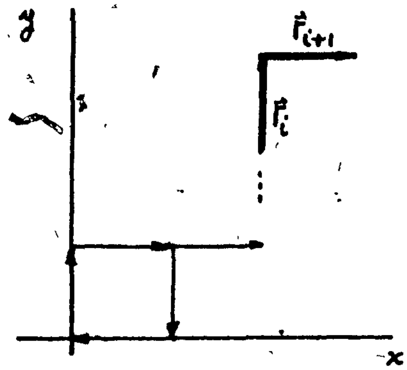

Fig. 9b

For $f(\theta)$ as in eq.(5.5a) we get

$$\lambda = \tfrac{1}{4} - \tfrac{1}{4} = 0$$

Hence we obtain from eq's.(3.11) and (4.6)

(5.5c) $$E(R_n^2) = \ell^2 n$$

the mean square displacement for a symmetric random walk in the plane with step length $\ell = 1$.

3o) Let $g(r)$ be given by eq.(5.3) and $f(\theta)$ by

(5.6a) $$f(\theta) = \tfrac{1}{2}\left\{ \delta\left(\theta - \tfrac{\pi}{2}\right) + \delta\left(\theta + \tfrac{\pi}{2}\right) \right\}$$

where the distribution of the m_i's is represented in fig. 10a and an illustration of this walk in fig. 10b, where, from the relation $\theta_{i+1} = \varphi_{i+1} - \varphi_i$ we see that $\theta_{i+1} = \frac{\pi}{2} - \pi = -\frac{\pi}{2}$.

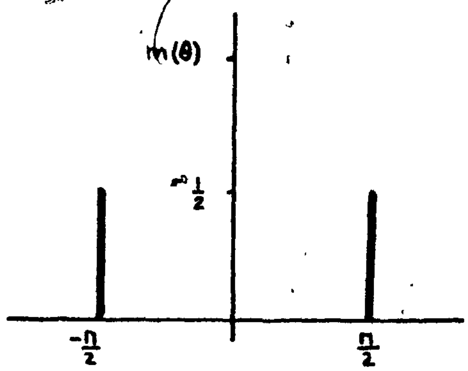

Fig. 10a

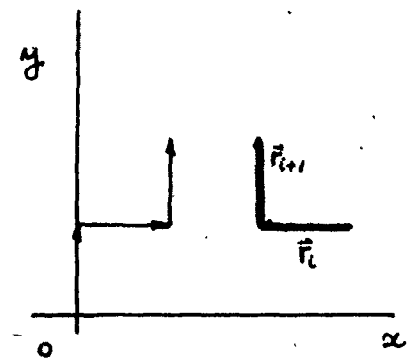

Fig. 10b

For this walk, we again get $E(R_n^2) = \ell^2 n$. It is a restricted walk on a square lattice where the walker must turn left or right with equal probability $\frac{1}{2}$. The restrictive aspect of the walk appears in the forbidden steps: reversal steps as well as those where the walker persists in the same direction.

B) <u>Cases when $|\lambda| < 1$ and $\lambda \neq 0$</u>

1o) Let $g(r)$ be given by eq.(5.3) and $f(\theta)$ by

(5.7a) $$f(\theta) = \frac{1}{2}\left\{\delta\left(\theta - \frac{\pi}{3}\right) + \delta\left(\theta + \frac{\pi}{3}\right)\right\}$$

Fig. 11a and fig. 11b represent the graph of the distribution of the m_i's for $f(\theta)$ and an illustration of this walk, respectively. From fig. 11b we see that $\theta_{i+1} = \frac{5\pi}{3} - \frac{4\pi}{3} = \frac{\pi}{3}$. We also have

(5.7b) $$\lambda = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$

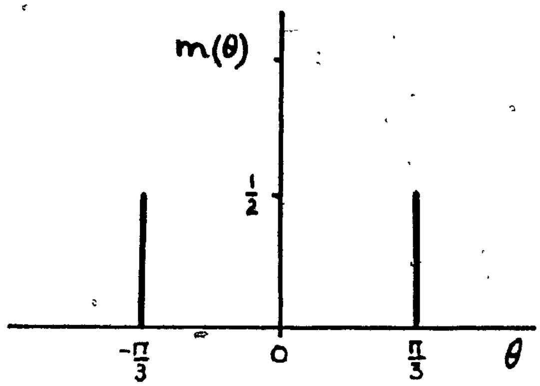

Fig. 11a

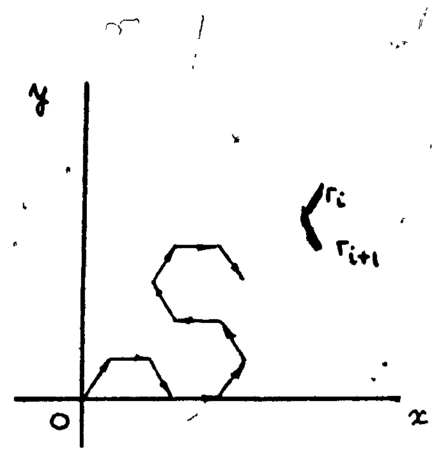

Fig. 11b

From eq. (4.13) and recalling that $f(\theta)$ is even, we have

(5.7c) $$E(R_n^2) \simeq \left(\sigma_r^2 + \mu_r^2 + 2\mu_r^2 \frac{\lambda}{1-\lambda}\right)n - \frac{2\mu_r^2 \lambda}{(1-\lambda)^2}$$

where $\sigma_r^2 = 0$ by eq.(5.3), and $\mu_r^2 = \ell^2$. Hence

(5.7d) $$E(R_n^2) \simeq \left(1 + \frac{2\lambda}{1-\lambda}\right)n\ell^2 - \frac{2\lambda\ell^2}{(1-\lambda)^2}$$

$$= 3n\ell^2 - 4\ell^2 \quad \text{for} \quad \lambda = \tfrac{1}{2}$$

(5.7e) Let $f(n) = 3n\ell^2 - 4\ell^2$

(5.7f) Then $\lim_{n\to\infty} \left[E(R_n^2) - f(n)\right] = 0$

Eq.(5.7e) is the asymptote toward which $E(R_n^2)$ approaches as $n \to \infty$. It has slope $3\ell^2$ and n-intercept 4/3. A slope $\alpha > \ell^2$ indicates that the walker undergoing this walk moves further than a walker undergoing a random walk.

2o) Let $g(r)$ be given by eq.(5.3) and $f(\theta)$ by

(5.8a) $$f(\theta) = \frac{1}{3}\left\{ \delta\left(\theta - \frac{\pi}{2}\right) + \delta\left(\theta + \frac{\pi}{2}\right) + \delta(\theta) \right\}$$

Fig. 12a and Fig. 12b show the graph of the probability distribution of the m_i's and an illustration of the path of such a walk, respectively.

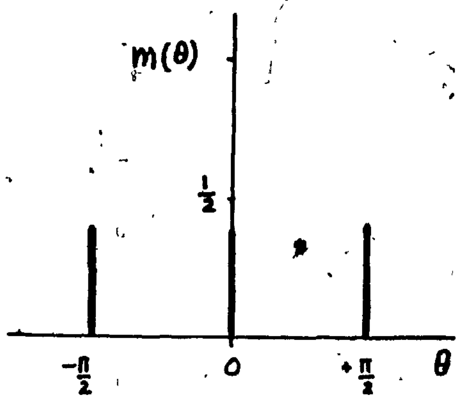

Fig. 12a

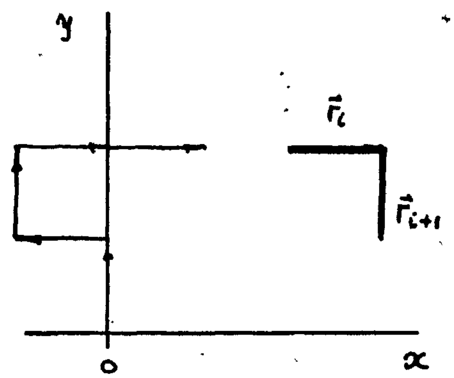

Fig. 12b

For this walk,

(5.8b) $$\lambda = \frac{1}{3}$$

This is a restricted walk on a square lattice where the restriction is expressed in the direct reversals which are forbidden. The steps remain as usual correlated since $\theta_{i+1} = \varphi_{i+1} - \varphi_i$. In fig. 12b, we see that $\theta_{i+1} = -\frac{\pi}{2}$. This is the walk that we have considered earlier in chapter II with the transition matrix given by eq.(II-3.12), for which we had found the asymptotic expression for the mean square displacement by another method, eq.(II-3.15).

From eq.(4.7)

(5.8c) $$E(R_n^2) = \left(\sigma_r^2 + \mu_r^2 + 2\mu_r^2 \frac{\lambda}{1-\lambda}\right) n - 2\mu_r^2 \frac{\lambda}{(1-\lambda)^2} + 2\mu_r^2 \frac{\lambda^{n+1}}{(1-\lambda)^2}$$

$$= \ell^2 \left\{ \left(1 + \frac{2\lambda}{1-\lambda}\right) n + 2\lambda \frac{(\lambda^n - 1)}{(1-\lambda)^2} \right\}$$

where $\sigma_r^2 = 0$ and $\mu_r^2 = \ell^2$ by eq.(5.3). We see that the equations (II-3.15) and (III-5.8c) are identical when $\lambda = 1 - 2p$. Now for $\lambda = \frac{1}{3}$, we express by

(5.8d) $$E(R_n^2) \simeq 2n - \frac{3}{2}$$

the fact that, as $n \to \infty$, $E(R_n^2)$ approaches the asymptote given by

(5.8e) $$f(n) = 2n - \frac{3}{2}$$

where, in eq.(5.8c), $\ell^2 = 1$.

(5.8f) i.e. $$\lim_{n \to \infty} \left[E(R_n^2) - f(n) \right] = 0$$

§ 6 Example of a Restricted Walk

This example is based on the representation of polymer formation (Montroll, 1950) by a Markov chain on an integer lattice in the plane. In this walk, the particle:

a) must turn left or right at a 90° angle from the previous step, with equal probability;

b) cannot revisit any lattice point in four steps, indicating that loops with the following forms (see fig. 13 below), i.e. 1st order loops, are not allowed.

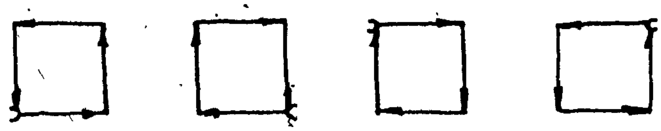

Fig. 13

The particle has a one step memory such that its n^{th} step is influenced by its $(n-2)^{nd}$ step. Such a walk is direction dependent by a) and position dependent by b). The Markov chain is a sequence $\{X_i\}$ $i = 0, 1, 2, \cdots$ of groups of 4 steps, of identically distributed random variables. 16 such groups of 4 steps can be formed. The 12 allowed groups are represented in Fig. 14., where the 1st step of each group illustrated takes either one of the two horizontal directions.

Let q be the probability that the walker, at the completion of the k^{th} step, be as far away as possible from the position he was in at the completion of the $(k-3)^{rd}$ step. Let p be the probability that the walker, at the completion of the k^{th} step, be

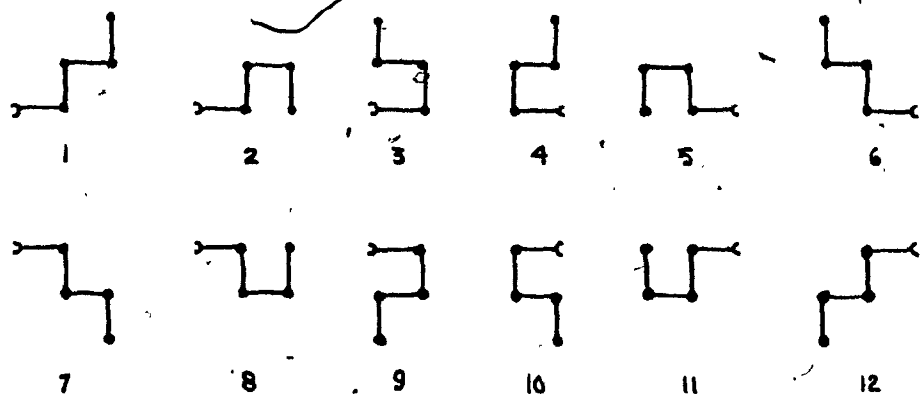

Fig. 14

as near as possible to the position he was in at the completion of the $(k-3)$rd step. There is a joint probability associated with each configuration. In particular, consider the first configuration which is drawn in fig. 15.

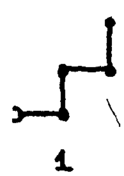

Fig. 15

The first step has probability $\frac{1}{2}$. The 2nd step has probability $\frac{1}{2}$ also, since the walker has taken a left step. The 3rd and 4th steps have, each, probability q since at the completion of the 3rd step, the walker is as far as he can be from the starting position; and at the completion of the 4th step, the walker is also as far as he can be from the 1st position. Hence we get

(6.1a) $$p_1 = P(X_i = 1) = \frac{1}{4} q^2$$

Similarly, we get for the 2nd configuration

(6.1b) $$p_2 = P(X_i = 2) = \frac{1}{4} pq$$

The probability vector of the 1st step of the Markov chain given by $\{X_i\}\ i = 1, 2, \cdots$ is

(6.2) $$p^{(1)} \doteq (p_1, p_2, p_3, \cdots, p_{10}, p_{11}, p_{12})$$

Montroll (1950) computed the 144 conditional probabilities

(6.3) $$p_{hk} = P(X_{i+1} = k \mid X_i = h) .$$

where $h, k \in (1, 2, 3, \cdots, 10, 11, 12)$

In particular, the conditional probability that the particle be in state 2 at the $(i+1)$th step given that it is in state 1 at the ith step is

(6.4a) $$p_{12} = P(X_{i+1} = 2 \mid X_i = 1)$$

Fig. 16 illustrates how the configurations 1 and 2 (see fig. 14), i.e. two links of the Markov chain, join. "a", "b", "c" and "d" in fig. 16 illustrate, in broken line, the formation of the 1st, 2nd, 3rd and 4th step, respectively, of configuration 2 which follows configuration 1. "e" in fig. 16 illustrates configurations 1 and 2 in succession.

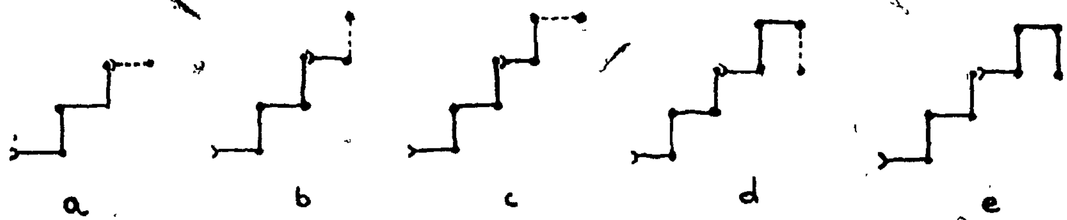

Fig. 16

The 1st step of conformation 2 in the making (i.e. broken segment in "a") has probability q since at the completion of that step, the walker will be as far away as possible from the 2nd position of configuration 1, i.e. the 3rd previous position. By similar reasoning, the 2nd and 3rd step, i.e. broken segments in "b" and "c", respectively, have each probability q, while the 4th step (see "d", fig. 16) has probability p.

(6.4b) Hence $$p_{12} = P(X_{i+1} = 2 \mid X_i = 1) = pq^3.$$

Let $\vec{R}_n$ be the vector which connects the two ends of the chain of groups of four steps. Montroll (1950) found that

(6.5) $$E(\vec{R}_n) = 0$$

(6.6) $$\lim_{n\to\infty} \frac{E(R_n^2)}{Na^2} = \left(\frac{1+p^2}{1-p^2}\right)\frac{1}{p}$$

where $N = 4n$ and a, the bond length.

(6.7) Let $$f(p) = \left[\left(\frac{1+p^2}{1-p^2}\right)\frac{1}{p}\right]^{1/2}$$

When 1st order overlaps are allowed, this walk becomes exactly that discussed in § 5-A-3o, eq's.(5.3) and (5.6a). And Montroll (1950) found

(6.8) $$\lim_{n \to \infty} \frac{E(R_n^2)}{Na^2} = \frac{q}{p} .$$

(6.9) Let $$f(p) = \left(\frac{q}{p}\right)^{1/2} .$$

Eq's (6.7) and (6.9) are the limiting expressions for the root mean square distance between the ends of the chain (very long) when 1st order overlaps are allowed and when they are not, respectively. Fig. 17 expresses the root mean square of the distance as function of ρ .

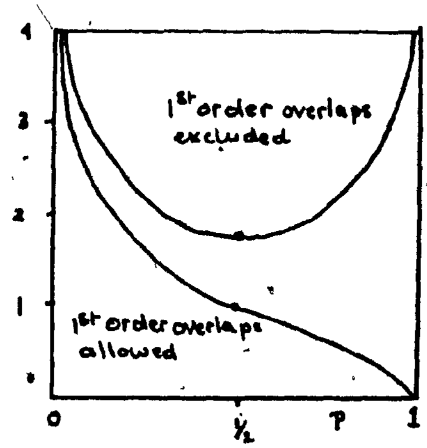

Fig. 17

When 1st order overlaps are allowed, $f(\rho) = 1$ when $p = \frac{1}{2}$, as expected, for a random case. When they are not allowed, Montroll (1950) has found that the average chain length has increased by a factor of 1.8, as indicated by fig. 17, even when $p = \frac{1}{2}$.

CHAPTER IV

CONCLUSION

Applications to Biological Cell Motion on Surfaces

Studies have been made of the planar cell motion of certain biological cells with and without chemotaxis (i.e., movement towards an attractive agent). Gail and Boone (1970), Nossal and Weiss (1974a,b) Nossal (1976) and Hall (1977) have dealt with the problem of modeling this cell motion as a correlated walk in $\mathbb{R}^2$. Salient aspects of their work will be mentioned here.

Gail and Boone (1970) studied the motion of mouse fibroblasts in tissue culture on surfaces, in the absence of chemotactic agents. They have observed the position of the cells at equal intervals of time and analyzed an idealization of the path formed by the sequence of 2-vectors joining these points. The resultant sum squared was assumed to have an exponential density given by

$$f(T^2) = \frac{1}{4Dt} e^{-\frac{T^2}{4Dt}} , \text{ for fixed } t > 0 \tag{1.1}$$

where D is the diffusion constant.

The mean square displacement for this walk is given by

$$E(T^2) = 4Dt \tag{1.2}$$

by the exponential property of $\mathcal{f}$. These authors have shown in theory that a "persisting" cell, like a random walker undergoes a mean square displacement proportional to time if suitably long intervals of time are chosen. Because these authors studied only the cell positions spaced at equal intervals of time, i.e. "equal-time step", they overlooked the detail of the actual trajectories of the cells in space. Fig. 17 shows an illustration for a path formed by a sequence of 2-vectors in the plane where the positions at equal intervals of time are indicated by dots and the "equal-time steps" by the dashes.

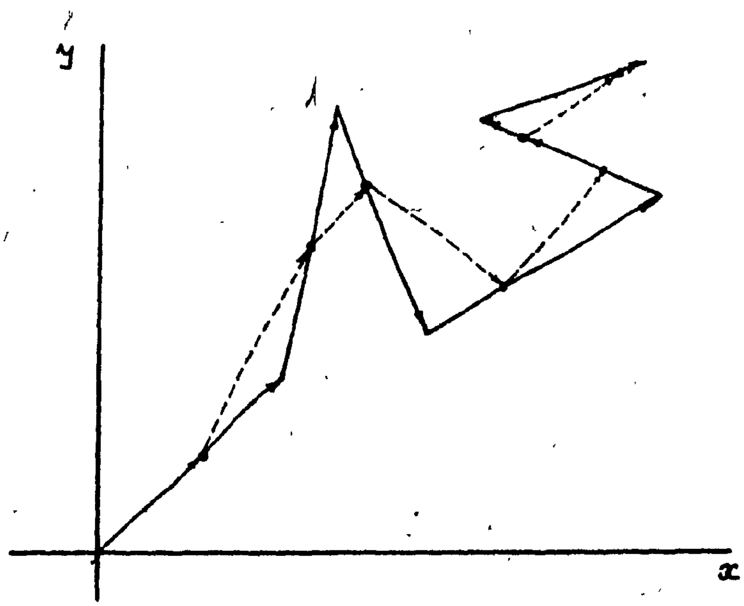

Fig. 18

A more detailed model for planar cell motion was constructed by Nossal and Weiss (1974b), who proposed a theory of planar cell motion in a chemotactic gradient. The correlation between the steps in this model is introduced by the way of the relative angles.

Hall (1977) has represented the motion of the amoeba Dictyostelium discoideum in the absence of chemotactic agents as a correlated walk with straight line steps of variable lengths. His assumption of independent relative angles θ_i and independent step lengths $\vec{r}_i$ were suggested by a detailed statistical analysis of the data. This led to the correlated walk model for cell trajectories he proposed. Hall (1977) raised the question of the difficulty which a representation by "time step" runs into if the time interval is chosen to be small. Taylor (1920) has presented a tentative theoretical analysis of the passage to the limit of vanishingly small steps for a correlated walk.

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