

PATHS AND CHAINS OF RANDOM STRAIGHT-LINE SEGMENT

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Classical problems associated with paths composed of straight line segments with independent orientations, which have a continuous distribution, are discussed. Moment formulas are obtained for the distance between initial and terminal points, and a new approximation discussed. The Rayleigh approximation is used to derive approximations to other characteristics of the random path.

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1. Introduction and Historical Outline

The motion of a point traveling along a succession of straight-line segments of equal length (see Figure 1, section 2), but randomly and independently oriented, has been studied, in various contexts, by a considerable number of workers over a considerable period of time. Rayleigh (1880, 1899, 1905, 1919 a,b) studied such motions, firstly in a plane and later in three dimensions (and also in one dimension). In the 1880 paper, he obtained appropriate formulas for the distribution of the distance between the initial and terminal points of a path of N segments. In 1919 he gave exact explicit distributions (for the three dimensional problem) for some small values of N . The two-dimensional problem was posed, in connection with the study of random migration, by K. Pearson (1905) who also noted the relevance of Rayleigh's solution (K. Pearson (1905, 1906) also Rayleigh (1905)). In response to this statement of the problem, Rayleigh (1905) gave an outline of his analysis, and an exact solution, in the form of an integral, was obtained by Kluyver (1905). Numerical evaluation of this integral was not effected, however, until the work of Greenwood and Durand (1955). An exact explicit general solution for the three-dimensional case was given by R. A. Fisher (1953). This expresses the probability integral of the distribution of distance in terms of a set of polynomials, each polynomial corresponding to a different interval of values of the distance.

At about the same time that Pearson and Kluyver were working on the two-dimensional problem, Smoluchowski (1906) was working on the three-dimensional problem, in connection with the study of Brownian motion (with finite time between changes of path direction). He also considered the rather more difficult problem in which the angle between successive segments is fixed (though orientation in three dimensions is assumed random, subject to this constraint). Smoluchowski stated that his attention was drawn to the problem by two papers by Einstein (1905, 1906). However, the methods used by the latter were of a different nature, being based on continuous variation with each coordinate of the traveling point varying accordingly to a Wiener process (as it would now be called).

Kuhn (1934), apparently independently, initiated study of the three-dimensional problem, regarding the "path" as a chain composed of links of fixed length, but independent random orientations, which he proposed as a model for certain kinds of chain molecules. Kuhn's paper was followed by later papers by Kuhn and Grün (1942, 1946) and Kuhn (1946). In these papers a number of problems were solved approximately, including the problem studied by Smoluchowski, in which the angle between successive links (here regarded as the "valence angle") is fixed.

The accuracy of approximate solutions has been discussed, for the two-dimensional case, by Horner (1946), Slack (1946, 1947) and, in considerable detail, by Greenwood and Durand (1957). Lord (1948) commented generally on accuracy of approximation, pointing out that accuracy might be expected to increase with number of dimensions. Stephens (1962 a,b) has studied the accuracy of approximations for both two- and three-dimensional cases.

The case of fixed unequal segment lengths was discussed by Rayleigh (1919 a). A formal system of analysis (based on a method ascribed to

A. A. Markov), applicable to random varying (though independent) segment lengths was developed by Chandrasekhar (1943). This was found to lead to simple explicit results in certain special cases, such as the case of segment vectors with independent, identically normally distributed components. Grosjean (1960) allowed for random variation in segment length, and for a general orientation distribution, though he retained the assumptions of independence between segments, and between length and orientation of the same segment.

Apart from the distribution of distance between the initial and terminal points, the distribution of relative orientation of segments of the path has been the object of study. Kuhn and Gr^un (1942) considered the distribution (in three dimensions) of the angle between a randomly chosen link and the "terminal axis" joining the initial and terminal points of the chain. It is interesting to note that the approximate distribution they obtained had been introduced (in the study of magnetism) by Langevin (1905) about the time that Pearson, Kluyver and Smoluchowski were working on the distribution of distance between initial and terminal points. Statistical properties of the Langevin distribution were studied by R. A. Fisher (1953). Recently, a number of statistical procedures based on this distribution have been developed by G. S. Watson and co-workers (Watson and Williams (1956), Watson (1960), Stephens (1962 b)).

The corresponding two-dimensional distribution, described by Mises (1918), has been discussed and named the "circular normal" distribution by Gumbel et al. (1953). It also has recently been used as the basis for statistical procedures developed by Watson and Williams (1956), Watson (1961, 1962) and Stephens (1962 a). Breitenberger (1963) has discussed ways of describing the genesis of both the two- and three-dimensional distributions.

In this paper, relatively simple methods will be used to study random paths and chains. These methods can be adapted, in a straightforward fashion, to cases where the segments (or links) have lengths which are randomly distributed (and even correlated). We will, at first, be particularly concerned with the distribution of distance between initial and terminal points, but some other, related problems will be discussed later. We will not, here, be directly concerned with the development of tests of significance, and other statistical procedures connected with these problems.

2. Distribution of Terminal Distance when Segment Lengths are Fixed

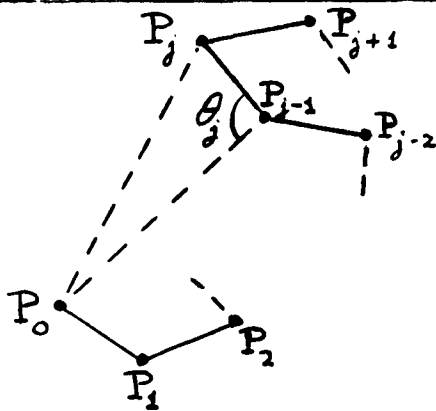


FIGURE 1

In Figure 1, P_0 represents the initial position of the point (or beginning of the chain) and $P_{j-1}P_j$ represents the j th straight line segment. It is supposed that the j th segment is of length l_j , which may be fixed or may be represented by a random variable.

Figure 1 is applicable, whatever the number ($\nu > 1$) of dimensions, though the distribution of the angle $\theta_j (\equiv \angle P_0 P_{j-1} P_j)$ depends on ν . The distance P_0P_j between the initial point and the end of the j th segment will be represented by r_j .

From the triangle $P_0 P_{j-1} P_j$

$$r_j^2 = r_{j-1}^2 - 2r_{j-1} l_j \cos \theta_j + l_j^2$$

or, equivalently

$$(1) \quad r_j^2 = r_{j-1}^2 + r_{j-1} l_j u_j + l_j^2$$

where the l_j 's and u_j 's are mutually independent random variables, and r_j is independent of l_i and u_i for $i > j$, but not for $i \leq j$. Each u_j has the same distribution, taking values in the interval $-2 \leq u_j \leq 2$. The probability density function of u_j when $\nu = 2$ (two dimensions) is

$$p(u_j) = [\pi \sqrt{4-u_j^2}]^{-1} ;$$

when $\nu = 3$, it is

$$p(u_j) = \frac{1}{4} , \text{ and generally } p(u_j) = \frac{\Gamma(\nu-1)}{4^{\nu-2} \{\Gamma(\frac{1}{2}(\nu-1))\}^2} (4-u_j^2)^{\frac{1}{2}(\nu-3)} .$$

In each case the formula applies for the interval $-2 \leq u_j \leq 2$ only. Whatever the value of ν , u_j is distributed symmetrically about zero, so $E(u_j^s) = 0$ if s be odd.

Adding together $(N-1)$ equations like (1) (with $j = 2, 3, \dots, N$), and noting that r_1 equals l_1 , we obtain

$$(2) \quad r_N^2 = \sum_{j=2}^N r_{j-1} l_j u_j + \sum_{j=1}^N l_j^2 .$$

We now proceed to evaluate the moments of r_N^2 , conditional on the l_j 's having fixed values. Since $E(u_j^s) = 0$ if s be odd,

$$(3) \quad E(r_N^2 | \{l\}) = \sum_{j=1}^N l_j^2$$

where $\{l\}$ denotes the set of fixed values l_1, l_2, \dots, l_N . The s th conditional central moment of r_N^2 is

$$\mu_s(r_N^2 | \{l\}) = E([\sum_{j=2}^N r_{j-1} l_j u_j]^2 | \{l\}) .$$

Putting $s = 2$,

$$\begin{aligned}
 \mu_2(r_N^2 | \{l\}) &= \sum_{j=2}^N l_j^2 E(r_{j-1}^2 | \{l\}) E(u_j^2) \\
 (4) \qquad \qquad \qquad &= E(u^2) \sum_{i < j}^N \sum_{i < j}^N l_i^2 l_j^2 \quad (\text{using } (3))
 \end{aligned}$$

where $E(u^2) = E(u_j^2)$ (for any j), and $\sum_{i < j}^N \sum_{i=1}^{N-1} \sum_{j=i+1}^N$ means $\sum_{i=1}^{N-1} \sum_{j=i+1}^N$. In later formulas, higher order summations will be introduced, using similar conventions.

The calculations for $s=3$ and $s=4$ follow similar lines. Thus

$$\begin{aligned}
 \mu_3(r_N^2 | \{l\}) &= 3E[\sum_{i < j}^N \sum_{i-1}^{l_i u_i} (r_{j-1} l_j u_j)^2 | \{l\}] \\
 &= 3E(u^2) \sum_{i < j}^N \sum_{i-1}^{l_i} l_j^2 E(r_{j-1}^2 | r_{i-1}, u_i, \{l\}) \{l\}.
 \end{aligned}$$

$$\text{Now } E(r_{j-1}^2 | r_{i-1}, u_i, \{l\}) = r_{i-1}^2 + r_{i-1} l_i u_i + \sum_{h=i}^{j-1} l_h^2,$$

and so

$$\begin{aligned}
 \mu_3(r_N^2 | \{l\}) &= 3[E(u^2)] \sum_{i < j}^N \sum_{i-1}^{l_i} l_j^2 E(r_{i-1}^2 | \{l\}) \quad (\text{since } E(u_i) = 0) \\
 (5) \qquad \qquad \qquad &= 3[E(u^2)]^2 \sum_{h < i < j}^N l_h^2 l_i^2 l_j^2.
 \end{aligned}$$

Similar calculations lead to

$$\begin{aligned}
 \mu_4(r_N^2 | \{l\}) &= 18[E(u^2)]^2 [1+E(u^2)] \sum_{g < h < i < j}^N \sum_{g}^N \sum_{h}^N \sum_{i}^N \sum_{j}^N l_g^2 l_h^2 l_i^2 l_j^2 \\
 (6) \qquad \qquad \qquad &+ 6[E(u^2)]^2 \sum_{h \neq i, h \neq j, i < j}^N \sum_{h}^N \sum_{i}^N \sum_{j}^N l_h^4 l_i^2 l_j^2 + E(u^4) \sum_{i < j}^N \sum_{i}^N \sum_{j}^N l_i^4 l_j^4
 \end{aligned}$$

The second term on the right-hand side of (6) is actually

$$\{6[E(u^2)]^2 \sum_{h<i<j}^N \sum_{i<h<j}^N + E(u^4) [2+E(u^2)] \sum_{i<j<h}^N\} \ell_h^4 \ell_i^2 \ell_j^2$$

but, for our purposes, it can be written in the form shown, since $E(u^2) = 4v^{-1}$ and $E(u^4) = 48[v(v+2)]^{-1}$ and so $6[E(u^2)]^2 = E(u^4)[2+E(u^2)]$.

If each straight-line segment is of the same fixed length ℓ , then (using ℓ in place of $\{\ell\}$ to denote $\ell_1 = \ell_2 = \dots = \ell_N = \ell$).

$$(7) \quad E(r^2 | \ell) = N \ell^2$$

$$(8) \quad \text{var}(r_N^2 | \ell) = \frac{1}{2} E(u^2) N(N-1) \ell^4$$

$$(9) \quad \mu_3(r_N^2 | \ell) = \frac{1}{2} [E(u^2)]^2 N(N-1)(N-2) \ell^6$$

$$(10) \quad \mu_4(r_N^2 | \ell) = \left\{ \frac{3}{4} [E(u^2)]^2 [1+E(u^2)] N(N-1)(N-2)(N-3) \right. \\ \left. + 3[E(u^2)]^2 N(N-1)(N-2) + \frac{1}{2} E(u^4) N(N-1) \right\} \ell^8 .$$

In two dimensions

$$(11) \quad \text{var}(r_N^2 | \ell) = N(N-1) \ell^4$$

$$(12) \quad \mu_3(r_N^2 | \ell) = 2N(N-1)(N-2) \ell^6$$

$$(13) \quad \mu_4(r_N^2 | \ell) = 3N(N-1)(3N^2 - 11N + 11) \ell^8 .$$

In three dimensions

$$(14) \quad \text{var}(r_N^2 | \ell) = \frac{2}{3} N(N-1) \ell^4$$

$$(15) \quad \mu_3(r_N^2 | \ell) = \frac{8}{9} N(N-1)(N-2) \ell^6$$

$$(16) \quad \mu_4(r_N^2 | \ell) = \frac{4}{45} N(N-1)(35N^2 - 115N + 108) \ell^8$$

3. Approximations to Distribution of r_N^2

For the case of constant segment length the asymptotic distributions of $(\nu/(N\ell^2))r_N^2$, as N increases, is that of χ^2 with ν degrees of freedom. (Rayleigh (1880), Pearson (1905), Kluyver (1906), Smoluchowski (1906), Kuhn (1934) etc.) This result can be obtained (see Stephens (1962 a, pp. 473-4) by introducing Cartesian coordinates x_{tN} ($t = 1, 2, \dots, \nu$) for P_N , with $x_{t0} = 0$ for all t , so that P_0 is at the origin of coordinates, and noting that

(i) x_{tN} is the sum of independent, identically distributed random variables $v_j^{(t)}$ (the projections of links $P_{j-1} P_j$ on the x_t axis) which each have a finite range of variation, expected value zero and variance ℓ^2/ν , and (ii) $x_{1N}, x_{2N}, \dots, x_{\nu N}$ are uncorrelated (though not independent).

It may be noted that a similar argument applies also when the ℓ_j 's are independent random variables with identical distributions with finite expected value and standard deviation. The only modification is the replacement of ℓ^2 by $E(\ell^2)$.

Horner (1946), Slack (1946, 1947) and Greenwood and Durand (1955) found that the asymptotic distribution did not give very good results for N less than 10 when $\nu = 2$ (i.e., in two dimensions). However, as Lord (1948) pointed out, the approximation would be expected to be better as ν increases. Rayleigh (1919 a, b), Pearson (1906) and Kuhn (1934) investigated possible improvements of the χ^2 approximation, and various methods of approximation (in the case $\nu=2$) were compared by Durand and Greenwood (1957).

For relatively small values of N , a natural method of approximation is to use a Pearson Type I curve with the same first two moments as r_N^2 , and the same range of variation (from 0 to $(N\ell)^2$). This gives exactly correct results when $N = 2$.

This method is equivalent to approximating the probability density function of $y_N = (r_N/(N\ell))^2$ by

$$(17) \quad \bar{p}(y_N) = [B(\alpha, \beta)]^{-1} y_N^{\alpha-1} (1-y_N)^{\beta-1} \quad (0 \leq y_N \leq 1)$$

with
$$\alpha = \frac{1}{2} \nu - N^{-1}; \quad \beta = (N-1) \left(\frac{1}{2} \nu - N^{-1} \right) .$$

The third and fourth central moments of r_N^2 corresponding to the approximating distribution (17) are

$$\bar{\mu}_3(r_N^2 | \ell) = \frac{4N^2(N-1)(N-2)\ell^6}{\nu \left(\frac{1}{2} \nu N + 1 \right)}$$

$$\bar{\mu}_4(r_N^2 | \ell) = \frac{6N^3(N-1) \left[(N-1) \left(\frac{1}{2} \nu - 7 \right) + 2N^2 \right] \ell^8}{\nu \left(\frac{1}{2} \nu N + 1 \right) \left(\frac{1}{2} \nu N + 2 \right)} .$$

The ratios of approximating to exact values of the third and fourth central moments are

$$\frac{\bar{\mu}_3(r_N^2 | \ell)}{\mu_3(r_N^2 | \ell)} = \frac{N\nu}{N\nu + 2} ; \quad (\text{for } N > 2).$$

$$\frac{\bar{\mu}_4(r_N^2 | \ell)}{\mu_4(r_N^2 | \ell)} = \frac{N^2 \nu^2}{(N\nu + 2)(N\nu + 4)} \times \frac{(\nu + 4)N^2 - (\nu + 14)N + 14}{(\nu + 4)N^2 - (\nu + 20)N + \frac{4(5\nu + 12)}{\nu + 2}} .$$

Some values of these ratios are shown in Table 1. In assessing these ratios as indices to the accuracy of approximation it should be borne in mind (see Pearson (1963)) that variation in high order moments may have little effect on computed probabilities. (It may be more informative to consider the "standardized" ratios $\sqrt[3]{\bar{\mu}_3/\mu_3}$ and $\sqrt[4]{\bar{\mu}_4/\mu_4}$.)

Table 1

Ratios of Approximate to Exact Central Moments of r^2_N

N	Third Moment		Fourth Moment	
	$v=2$	$v=3$	$v=2$	$v=3$
3	0.750	0.818	0.900	0.933
4	0.800	0.857	0.818	0.896
5	0.833	0.882	0.806	0.888
7	0.875	0.913	0.823	0.895
10	0.909	0.937	0.856	0.915
20	0.952	0.968	0.910	0.950

Application of this approximation requires the evaluation of the incomplete beta function ratio $I_x(\alpha, \beta)$ with $x = (r/(Nl))^2$. Lower percentage points can be obtained (using linear harmonic interpolation) from the recently published tables of Vogler (1964). This is, unfortunately, not so for the upper percentage points, so no direct comparison has been made with the upper 5% and 1% points given by Greenwood and Durand (1955). Special calculations gave the following comparisons with exact values of the probability integral of r , for $N = 7$ and $v = 2$ given by these authors

Table 2

Probability Integral of $r_7(v=2)$

R/(Nl)	Pr[$r_7 \leq R$]		
	Exact	χ^2_2 approx.	Type I approx.
1.0	0.125	0.133	0.145
2.0	0.418	0.435	0.425
3.0	0.714	0.724	0.704
4.0	0.900	0.898	0.895
6.0	0.9979	0.9942	0.9992

For small values of R the present approximation is not even as good as the χ^2 approximation, but the approximation improves for larger values of R .

The χ^2 approximation may also be used in obtaining approximations to other properties of random paths and chains (see, e.g., Stephens (1962 a,b)). In section 5 of this paper there will be found some applications of this kind. The accuracy of these approximations depends closely on that of the χ^2 approximation on which they are based; they improve as ν and/or N increase.

4. Variable Segment Length

If the ℓ 's are not constants, but random variables, the moments about zero of r_N^2 can be obtained by finding the expected values of the corresponding conditional moments,

$$\mu'_s(r_N^2) = E(\mu'_s(r_N^2 | \{\ell\})).$$

(The corresponding relationship for central moments is, of course, not generally true.)

If the ℓ^2 's are mutually independent and identically distributed, with finite moments (about zero) μ'_s , then the moments of r_N^2 can be expressed in terms of these μ'_s 's.

Thus

$$(18) \quad \mu'_1(r_N^2) = E\left(\sum_{j=1}^N \ell_j^2\right) = N \mu'_1$$

$$(19) \quad \begin{aligned} \mu'_2(r_N^2) &= E\left(E(u^2) \sum_{i<j}^N \ell_i^2 \ell_j^2 + \left(\sum_{j=1}^N \ell_j^2\right)^2\right) \\ &= E\left([2+E(u^2)] \sum_{i<j}^N \ell_i^2 \ell_j^2 + \sum_{j=1}^N \ell_j^4\right) \\ &= \left[1 + \frac{1}{2}E(u^2)\right]N(N-1)\mu_1'^2 + N \mu_2' \end{aligned}$$

In a similar fashion we obtain

$$(20) \quad \mu'_3(r_N^2) = \frac{1}{2}[1+E(u^2)][2+E(u^2)]N(N-1)(N-2)\mu_1'^3 \\ + 3[1+E(u^2)]N(N-1)\mu_2'\mu_1' + N\mu_3'$$

and

$$(21) \quad \mu'_4(r_N^2) = \frac{1}{4}[1+E(u^2)][2+E(u^2)][2+3E(u^2)]N(N-1)(N-2)(N-3)\mu_1'^4 \\ + 3[1+E(u^2)][2+3E(u^2)]N(N-1)(N-2)\mu_2'\mu_1'^2 + \frac{1}{2}[E(u^4)+12E(u^2)+6]N(N-1)\mu_2'^2 \\ + 2[2+3E(u^2)]N(N-1)\mu_3'\mu_1' + N\mu_4' .$$

Expressing equations (19)-(21) in terms of central moments (for both r_N^2 and ℓ^2), we find

$$(22) \quad \mu_2(r_N^2) = \frac{1}{2} E(u^2) N(N-1) \mu_1'^2 + N \mu_2$$

$$(23) \quad \mu_3(r_N^2) = \frac{1}{2}[E(u^2)]^2 N(N-1)(N-2) \mu_1'^3 + 3E(u^2) N(N-1) \mu_2\mu_1' + N \mu_3$$

$$(24) \quad \mu_4(r_N^2) = [\frac{1}{2}E(u^4) + \frac{3}{4}\{E(u^2)\}^3(N-2)(N-3) + \frac{3}{4}\{E(u^2)\}^2(N+1)(N-2)]N(N-1)\mu_1'^4 \\ + [E(u^4) + 9\{E(u^2)\}^2(N-2) + 3E(u^2)N] N(N-1) \mu_2\mu_1'^2 \\ + \frac{1}{2}[E(u^4) + 12E(u^2) + 6]N(N-1) \mu_2^2 + 6E(u^2)N(N-1)\mu_3\mu_1' + N\mu_4 .$$

So, in two dimensions

$$(26) \quad \mu_2(r_N^2) = N(N-1) \mu_1'^2 + N \mu_2$$

$$(26) \quad \mu_3(r_N^2) = 2N(N-1)(N-2) \mu_1'^3 + 6N(N-1) \mu_2\mu_1' + N\mu_3$$

$$(27) \quad \mu_4(r_N^2) = 3N(N-1)(3N^2-11N+11) \mu_1'^4 + 6N(N-1)(7N-11) \mu_2 \mu_1'^2 \\ + 18N(N-1) \mu_2^2 + 12N(N-1) \mu_3 \mu_1' + N \mu_4$$

and in three dimensions

$$(28) \quad \mu_2(r_N^2) = \frac{2}{3} N(N-1) \mu_1'^2 + N \mu_2$$

$$(29) \quad \mu_3(r_N^2) = \frac{8}{9} N(N-1)(N-2) \mu_1'^3 + 4N(N-1) \mu_2 \mu_1'^2 + N \mu_3$$

$$(30) \quad \mu_4(r_N^2) = \frac{4}{45} N(N-1)(35N^2-115N+108) \mu_1'^4 + \frac{4}{5} N(N-1)(25N-36) \mu_2 \mu_1'^2 \\ + \frac{63}{5} N(N-1) \mu_2^2 + 8N(N-1) \mu_3 \mu_1' + N \mu_4 .$$

It can be seen that, for sufficiently large N , the most important term in $\mu_s(r_N^2)$ is that containing $\mu_1'^s$. This term can be obtained from the corresponding formula for fixed $\ell_1 = \ell_2 = \dots = \ell_N = \ell$, by replacing ℓ^s by $\mu_1'^s$. It is to be expected that r_N^2 will tend to its asymptotic distribution (that of $(\frac{N\mu_1'}{\nu}) \times (\chi^2$ with ν degrees of freedom)) more rapidly when μ_2, μ_3, μ_4 are small compared with μ_1' .

The moments of r_N^2 can be evaluated in a similar way when the ℓ^2 's are not independent. If the ℓ^2 's all have the same moments, and the correlations among them are

$$\rho(\ell_j^2, \ell_{j+1}^2) = \rho; \quad \rho(\ell_j^2, \ell_i^2) = 0 \quad \text{if} \quad |i-j| > 1$$

then

$$(31) \quad \mu_2(r_N^2) = \frac{1}{2} E(u^2)N(N-1)\mu_1'^2 + \{N + \rho[2+E(u^2)](N-1)\} \mu_2 ;$$

while if $\rho(\ell_j^2, \ell_i^2) = \rho^{|i-j|}$, then

$$(32) \quad \mu_2(r_N^2) = \frac{1}{2}E(u^2)N(N-1)\mu_1'^2 + \left\{N + \frac{\rho}{1-\rho}[N-1 - \frac{\rho(1-\rho^{N-1})}{1-\rho}]\right\}[2+E(u^2)]\mu_2.$$

In these two cases the limiting values of the moment-ratios as the same (as N increases) as when there is no correlation. If, however, all ℓ_j^2 's have the same correlation, that is $\rho(\ell_i^2, \ell_j^2) = \rho$ for all $i \neq j$.

$$(33) \quad \mu_2(r_N^2) = \frac{1}{2} N(N-1) \{E(u^2)\mu_1'^2 + \rho[2+E(u^2)]\mu_2\} + N\mu_2$$

and the limiting value of the variance of v_N^2/N is increased in the ratio.

$$1 + \rho \left[\frac{2}{E(u^2)} + 1 \right] \frac{\mu_2}{\mu_1'^2}.$$

The other moments are affected also.

It is possible to investigate cases where individual ℓ_j^2 's have different distributions, using methods of the kind described above.

5. Uses of the Chi-Square Approximation to Distribution of Length

It can be seen from the results in the last section that the moment-ratios of the distribution of r_N^2 tend to those of χ^2 with ν degrees of freedom as N increases. Although the work of Greenwood and Durand (1955) indicated that this approximation is not completely satisfactory for values of N even as large as 20, it can be used with confidence for larger values of N (say 40-50 or more) and can provide useful insight into the nature of the distribution of the end-points of segments of the path or chain.

As an example, suppose we wish to consider the distribution of the distance d_n of P_n from the "terminal axis" P_0P_N joining the extremities of the (path or) chain ($n < N$). Assuming that there is no dependence between lengths of segments, and that each ℓ_j^2 has the same distribution we have

$$(34) \quad d_n^2 = \frac{r_n r'_{N-n} \sin^2 \phi}{r_n^2 - 2r_n r'_{N-n} \cos \phi + r_{N-n}^2}$$

where ϕ (the angle $P_{O_n} P_{N-n}$), r_n (P_{O_n}) and r'_{N-n} (P_{N-n}) are mutually independent random variables: $-2 \cos \phi$ has the same distribution as u , and r_n^2 , r_{N-n}^2 are distributed as r_N^2 with N replaced by n , $N-n$ respectively. We will now drop the prime in r'_{N-n} .

The distribution of d_n can be obtained by direct analyses. The following demonstration, for $\nu = 3$ dimensions, is particularly simple.

$$\begin{aligned} \Pr[d_n^2 > D^2 | r_n^2, r_{N-n}^2] &= \Pr\left[\frac{D^2 - \sqrt{(r_n^2 - D^2)(r_{N-n}^2 - D^2)}}{r_n r_{N-n}} \right. \\ &\quad \left. < \cos \phi < \frac{D^2 + \sqrt{(r_n^2 - D^2)(r_{N-n}^2 - D^2)}}{r_n r_{N-n}} \mid r_n^2, r_{N-n}^2 \right] \end{aligned}$$

provided $D < \min(r_n, r_{N-n})$. Otherwise the probability is zero.

Since (for $\nu = 3$) $\cos \phi$ is uniformly distributed between -1 and $+1$

$$\Pr[d_n^2 > D^2 | r_n^2, r_{N-n}^2] = \frac{\sqrt{(r_n^2 - D^2)(r_{N-n}^2 - D^2)}}{r_n r_{N-n}} \quad (\text{for } D < \min(r_n, r_{N-n}))$$

and

$$(35) \quad \Pr[d_n^2 > D^2] = \left(\int_{D^2}^{\infty} \frac{\sqrt{r_n^2 - D^2}}{r_n} p(r_n^2) dr_n^2 \right) \left(\int_{D^2}^{\infty} \frac{\sqrt{r_{N-n}^2 - D^2}}{r_{N-n}} p(r_{N-n}^2) dr_{N-n}^2 \right)$$

(since r_n^2 and r_{N-n}^2 are mutually independent). Now introducing the approximate probability density function (corresponding to the asymptotic χ^2 distribution)

$$(36) \quad p(r_N^2) \doteq \frac{(r_N^2)^{\frac{1}{2}} \exp\left[-\frac{3r_N^2}{2N\mu_1}\right]}{\sqrt{2\pi} \left(\frac{1}{3} N\mu_1\right)^{3/2}} \quad (0 < r_N^2)$$

we obtain from (35)

$$(37) \quad \Pr[d_n^2 > D^2] \doteq \exp\left(-\frac{3ND^2}{2n(N-n)\mu_1'}\right) .$$

(Note that $\int_{\theta}^{\infty} (z-\theta)^{\frac{1}{2}} e^{-Kz} dz = \frac{1}{2K} e^{-K\theta} K^{-\frac{3}{2}} \sqrt{\pi}$.)

From (37) we see that d_n^2 is approximately distributed as

$$\frac{1}{3}n(1-\frac{n}{N})\mu_1' \times (\chi^2 \text{ with two degrees of freedom}), \text{ as compared with}$$

$$\frac{1}{3}n\mu_1' \times (\chi^2 \text{ with two degrees of freedom})$$

for the distribution of the square of the distance of P_n from an arbitrary line through P_0 .

The approximate expected value of d_n^2 , calculated from (37), is $\frac{2n(N-n)}{3N} \cdot \mu_1'$. If N is even and $n = \frac{1}{2} N$, so that P_n is the mid-point of the path or chain, the approximate expected value is $\frac{1}{6} N\mu_1'$, or $\frac{1}{6} N\ell^2$ if each link is of length ℓ , agreeing with Kuhn and Grün (1942) and Kuhn (1946).

One further application may be noted here, though we shall not pursue the matter in great detail. It is possible to write down an approximate formula for the joint probability density function of $r_{N_1}^2, r_{N_2}^2, \dots, r_{N_s}^2$, where $N_1 < N_2 < \dots < N_s$ and $N_1, N_2 - N_1, \dots, N_s - N_{s-1}$ are each large enough for the χ^2 approximation to be useful.

We first consider the conditional distribution of $r_{N_2}^2$, given $x_{1N_1}, \dots, x_{vN_1}$. Using the random variables $u_j^{(t)}$ defined in section 4, we have

$$r_{N_2}^2 = \sum_{t=1}^v \left[\sum_{j=N_1+1}^{N_2} u_j^{(t)} + x_{tN_1} \right]^2 .$$

The conditional distribution of $r_{N_2}^2$ given $x_{1N_1}, \dots, x_{vN_1}$ is approximately that of

$\nu^{-1}(N_2 - N_1)\mu'_1$ x (Non-central χ^2 with ν degrees of freedom and non-centrality parameter $\nu r_{N_1}^2 [(N_2 - N_1)\mu'_1]^{-1}$).

Hence this is also the conditional distribution of $r_{N_2}^2$ given $r_{N_1}^2$, and using the χ^2 approximation to the distribution of $r_{N_1}^2$,

$$(38) \quad p(r_{N_1}^2, r_{N_2}^2) = p(r_{N_1}^2) p(r_{N_2}^2 | r_{N_1}^2)$$

$$= \frac{(r_{N_1}^2 r_{N_2}^2)^{\frac{1}{2}\nu-1} \exp\left[-\frac{\nu}{2(N_2 - N_1)\mu'_1} \left\{ \frac{N_2}{N_1} r_{N_1}^2 + r_{N_2}^2 \right\}\right]}{[4\nu^{-2} N_1 (N_2 - N_1)\mu'_1]^{\frac{1}{2}\nu}} \sum_{i=0}^{\infty} \frac{\left[\left(\frac{\nu}{2(N_2 - N_1)\mu'_1} \right)^2 r_{N_1}^2 r_{N_2}^2 \right]^i}{i! \Gamma\left(\frac{1}{2}\nu + i\right)}$$

The approximate joint distribution of $r_{N_1}^2$, $r_{N_2}^2$, and $r_{N_3}^2$ is obtained by multiplying (38) by the approximate conditional probability density function $p(r_{N_3}^2 | r_{N_2}^2)$ and so on. When $\nu = 3$ (three dimensions) the relationship

$$i! \Gamma\left(\frac{3}{2} + i\right) = 2^{-(2i+1)} (2i + 1)! \sqrt{\pi}$$

leads to considerable simplification, giving

$$(39) \quad p(r_{N_1}^2, \dots, r_{N_s}^2) = \frac{\exp\left[-\frac{3}{2\mu'_1} \sum_{j=1}^s a_j r_{N_j}^2\right]}{(2\pi)^{\frac{1}{2}s} \left(\frac{1}{3}\mu'_1\right)^{\frac{3}{2}s} N_1^{3/2}} \prod_{j=2}^s \left[\frac{\sinh\left(\frac{3\sqrt{r_{N_j}^2 r_{N_{j+1}}^2}}{N_{j+1} - N_j}\right)}{N_{j+1} - N_j} \right] \quad (0 \leq r_{N_j}^2)$$

where

$$a_1 = N_2 N_1^{-1} (N_2 - N_1)^{-1}; \quad a_j = (N_{j+1} - N_{j-1})(N_{j+1} - N_j)^{-1} (N_j - N_{j-1})^{-1}, \quad (2 \leq j \leq s-1);$$

$$a_s = (N_s - N_{s-1})^{-1}.$$

The right-hand side of (39) can be written as a weighted sum of terms of the form

$$(40) \quad \exp[\text{quadratic function of } r_{N_1}, \dots, r_{N_s}].$$

Approximate evaluation of the probability of a given class of configurations of the set of values $(r_{N_1}, \dots, r_{N_s})$ can be effected by term-by-term integration of expressions of type (40) with respect to $r_{N_1}^2, \dots, r_{N_s}^2$.

Among other interesting approximate results which can be obtained using the methods of this section may be mentioned the distribution of the distance between the terminal points P_N, P'_N of two independent chains with initial points a distance R apart. The square of this distance is approximately distributed as

$$\nu^{-1} (N\ell^2 + N'\ell'^2) \times (\text{non-central } \chi^2 \text{ with } \nu \text{ degrees of freedom and non-centrality parameter } \nu R^2 (N\ell^2 + N'\ell'^2)^{-1})$$

using an obvious notation.

6. Distribution of Angle of Inclination to Terminal Axis

So far, we have been mainly concerned with the distance between the initial and terminal points P_O, P_N respectively. We now consider the distribution of the angle between a randomly chosen segment $P_{j-1}P_j$, and the terminal axis $P_O P_N$. This distribution will evidently depend on the length of $P_O P_N(r_N)$, and it is **this conditional** distribution that we will consider. We will confine our attention to the case of segments of constant length, ℓ , in three dimensions.

Since any ordering of the N segments, given a set of N orientations, leads to the same position for the terminal point; and since each such ordering is, under our assumptions, equally likely, it follows that the distribution of the angle between $P_{j-1}P_j$ and the terminal axis is the same for all values of j . It is convenient to consider the angle between the final segment, $P_{N-1}P_N$, and the terminal axis $P_O P_N$. Denoting this angle by ψ , we have from the triangle

$P_0^P P_N^P P_{N-1}^P$,

$$(41) \quad \cos \psi = \frac{r_N^2 + \ell^2 - r_{N-1}^2}{2r_N \ell}.$$

Hence the conditional distribution of $\cos \psi$, given r_N^2 , is directly derivable from that of r_{N-1}^2 , given r_N^2 . From the relation (see (1))

$$r_N^2 = r_{N-1}^2 + r_{N-1} \ell_N u_N + \ell^2$$

it can be seen that (in three dimensions)

$$p(r_N^2 | r_{N-1}^2) = (4r_{N-1} \ell)^{-1} \quad ((r_{N-1} - \ell)^2 \leq r_N^2 \leq (r_{N-1} + \ell)^2).$$

Hence
$$p(r_{N-1}^2, r_N^2) = (4r_{N-1} \ell)^{-1} p(r_{N-1}^2)$$

and
$$p(r_{N-1}^2 | r_N^2) = (4r_{N-1} \ell)^{-1} p(r_{N-1}^2) / p(r_N^2).$$

Hence, from (41)

$$(42) \quad p(\cos \psi | r_N^2) = \frac{1}{2} \left[\frac{r_N}{p(r_N^2)} \right] \left[\frac{p(r_{N-1}^2)}{r_{N-1}} \right]_{r_{N-1} = [r_N^2 + \ell^2 - 2r_N \ell \cos \psi]^{\frac{1}{2}}} \quad (-1 \leq \cos \psi \leq 1).$$

Now introducing the χ^2 approximation for the distribution of r_{N-1}^2 we find

$$(43) \quad p(\cos \psi | r_N^2) \propto \exp \left[\frac{3r_N}{(N-1)\ell} \cos \psi \right] \quad (-1 \leq \cos \psi \leq 1)$$

approximately.

Kuhn and Grün (1942) studied this problem, by dividing the range of variation of ψ into a large number of small intervals and maximizing the probability, among sets of ψ 's constrained to give a specified value of r_N . The limiting relative frequencies of different values of ψ , obtained in this way were found to lead to a distribution of the same type as (43) but with

$3r_N[(N-1)\ell]^{-1}$ replaced by the inverse Langevin function of $r_N/(N\ell)$; i.e., the value of β satisfying.

$$(44) \quad \coth \beta - \beta^{-1} = r_N/(N\ell) .$$

For small values of $r_N/(N\ell)$, (43) implies $\beta \doteq 3r_N/(N\ell)$. Since the expected value and standard deviation of r_N are both of order \sqrt{N} , the ratio $r_N/(N\ell)$ will usually be small when N is large. Our result is thus in quite good agreement with that of Kuhn and Gr \ddot{u} n.

7. Continually Varying Orientation as a Limiting Case

It would appear natural to try to approach the situation in which the point moves with a continuously varying orientation by considering the limit of the case considered in section 2 (with common fixed segment length ℓ) as N tends to infinity and ℓ to zero, $N\ell$ remaining constant. (If the point be imagined to move with a fixed velocity, $N\ell$ is proportional to the time the point is in motion.) However, from (7) and (8) we have

$$\lim E(r_N^2|\ell) = \lim \text{var}(r_N^2|\ell) = 0;$$

and in fact $\lim \mu_s(r_N^2|\ell) = 0$ for all $s > 1$. As the limit is approached the probability of the terminal point being in any neighborhood, however small, of the initial point tends to one.

A non-degenerate limit can be obtained by assuming (see Chandrasekhar (1943, p. 19), also Einstein (1905)) that $N\ell^2$ remains constant--equal to ϕ say. Then the limiting values of the moments of r_N^2 are

$$\lim E(r_N^2|\ell) = \phi; \quad \lim \mu_2(r_N^2|\ell) = \frac{1}{2} E(u^2)\phi^2;$$

$$\lim \mu_3(r_N^2|\ell) = \frac{1}{2} [E(u^2)]^2\phi^3$$

$$\lim \mu_4(r_N^2|\ell) = \frac{3}{4}[E(u^2)]^2[1+E(u^2)]\phi^4$$

and the limiting distribution of r_N^2 is that of $(\phi/\nu) \times (\chi^2$ with ν degrees of freedom). If the ℓ_j 's are independent identically distributed random variables and $\sqrt{N} \ell_j$ has a proper limiting distribution r_N^2 also has a proper limiting distribution, but it need not be of χ^2 form.

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