The mean distance to the \( n \)th neighbour in a uniform distribution of random points: an application of probability theory

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Abstract

We study different ways of determining the mean distance \( \langle r_n \rangle \) between a reference point and its \( n \)th neighbour among random points distributed with uniform density in a \( D \)-dimensional Euclidean space. First, we present a heuristic method; though this method provides only a crude mathematical result, it shows a simple way of estimating \( \langle r_n \rangle \). Next, we describe two alternative means of deriving the exact expression of \( \langle r_n \rangle \): we review the method using absolute probability and develop an alternative method using conditional probability. Finally, we obtain an approximation to \( \langle r_n \rangle \) from the mean volume between the reference point and its \( n \)th neighbour and compare it with the heuristic and exact results.

1. Introduction

Consider random geometrical points, i.e., points with uncorrelated positions, distributed uniformly in a \( D \)-dimensional Euclidean space, with a density of \( N \) points per unit volume. A point is said to be the \( n \)th neighbour of another (the reference point) if there are exactly \( n - 1 \) other points that are closer to the latter than the former. We address the following problem: what is the mean distance \( \langle r_n \rangle \) between a given reference point and its \( n \)th neighbour, \( n < N \)? This is essentially a problem of geometrical interest. However, the quantity \( \langle r_n \rangle \) is relevant in certain physical and computational contexts: for example, in astrophysics it gives the mean distance between neighbouring stars distributed independently in a homogeneous model of the universe [1]. In optimization theory the values of \( \langle r_n \rangle \) help in estimating the optimal length of a closed path connecting a given set of points in space, as in the case of the travelling salesman...
problem [2–6]. It may also help in determining the statistical properties of complex networks [7].

In this paper, we study different ways of determining the mean $n$th neighbour distance. We first present a heuristic method of estimating $\langle r_n \rangle$ by using a physical picture. Next, we describe the derivation of the exact expression of $\langle r_n \rangle$ in two ways: we review the method using absolute probability and derive the result by an alternative method using conditional probability. The former method is comprehensive, while the latter is more analytic and explicitly illustrates the notion of ensemble average, i.e., the mean value of a macroscopic quantity calculated over all possible configurations of a system. Finally, we calculate the mean volume which separates the reference point from its $n$th neighbour and obtain an approximate expression of $\langle r_n \rangle$ from its radius. We find out how this approximation deviates from the exact expression of $\langle r_n \rangle$.

For the students of elementary probability, this problem offers a natural geometric context to look at absolute and conditional probabilities; for the students of elementary statistical mechanics, it introduces the method of ensemble average in the treatment with conditional probabilities; and for the advanced students it shows the use of scaling argument to very good effect.

2. A heuristic method

We begin with a heuristic approach to find the mean first neighbour distance. Consider a unit volume of the space described in the introduction, say, in the form of a hypersphere or a hypercube containing exactly $N$ random points including the reference one. Let us divide this unit volume into $N$ equal parts. Since the $N$ random points are distributed uniformly over the unit volume, each part is expected to contain just one of these. The mean distance $\langle r_1 \rangle$ between any point and its first neighbour is naively given by the linear extent of each part. Since the volume of each part is $1/N$, we expect

$$\langle r_1(N) \rangle \approx \left(\frac{1}{N}\right)^{1/D}.$$  \hfill (1)

We extend the above result for the first neighbour to the $n$th neighbour by the following heuristic argument. We choose any one of the points as the reference and locate its $n$th neighbour, $n < N$. The expected distance between them is $\langle r_n(N) \rangle$. Keeping these two points fixed, we change the number of points in the unit volume to $N\alpha$ by adding or removing points at random; the factor $\alpha$ is arbitrary to the extent that $N\alpha$ and $n\alpha$ are natural numbers. Since the distribution of points is uniform, the hypersphere that had originally enclosed $n$ points is now expected to contain $n\alpha$ points. Therefore, what was originally the $n$th neighbour of the reference point is now expected to be the $n\alpha$th neighbour for which the expected distance from the reference point is now $\langle r_{n\alpha}(N\alpha) \rangle$. Since the two points under consideration are fixed, so is the distance between them. Consequently,

$$\langle r_n(N) \rangle \approx \langle r_{n\alpha}(N\alpha) \rangle.$$  \hfill (2)

The above relation is approximate as the change in the density of points does not always convert the $n$th neighbour of the reference point to exactly its $n\alpha$th neighbour. Now we take $\alpha = 1/n$, so that

$$\langle r_n(N) \rangle \approx \left(\frac{1}{N}\right)^{1/D}.$$  \hfill (3)

which shows that the mean $n$th neighbour distance for a set of $N$ random points distributed uniformly is approximately given by the mean first neighbour distance for a depleted set of
The mean distance to the \( n \)th neighbour in a uniform distribution of random points is derived for such values of \( n \) that divide \( N \) exactly; however, this approximate relation may be used for any value of \( n \) when \( N \gg n \), by replacing \( N/n \) with the integer nearest to it. Using the expression of \( \langle r_1(N) \rangle \) from equation (1), we get

\[
\langle r_n(N) \rangle \approx \left( \frac{n}{N} \right)^{1/D}
\]  

which, therefore, requires as a necessary condition that \( N \gg n \). This heuristic method depicts a scaling approach. Though the results of equations (1) and (4) are extremely crude approximations, these provide us with a clear picture of the mean \( n \)th neighbour distance.

3. The method of absolute probability

We now review the derivation of the exact expression of \( \langle r_n \rangle \) by using the theory of \emph{absolute probability} [8]. The method described is similar to that followed in [6]. Consider the system of random points described at the beginning of the introduction. If the unit volume under consideration is part of an infinite space containing \( N \) points distributed randomly and uniformly in every unit volume, boundary effects will not appear in considering any particular unit volume. However, in practical cases the unit volume may be isolated and the effect of boundaries will appear; in such cases \( n \ll N \) should necessarily be observed to avoid the boundary effects. Alternatively, boundary effects may be ignored by imposing periodic boundary conditions. Assuming a certain random point as the reference there will be \( N-1 \) other random points within a \( D \)-dimensional hypersphere of unit volume with the reference point at its centre. For a given reference point, the absolute probability of finding its \( n \)th neighbour \((n < N)\) at a distance between \( r_n \) and \( r_n + d r_n \) from it is given by the probability that out of the \( N-1 \) random points (other than the reference point) distributed uniformly within the hypersphere of unit volume, exactly \( n-1 \) points lie within a concentric hypersphere of radius \( r_n \) and at least one of the remaining \( N-n \) points lies within the shell of internal radius \( r_n \) and thickness \( d r_n \):

\[
P(r_n) \, d r_n = \left( \frac{N-1}{n-1} \right) V_n^{n-1} \sum_{q=1}^{N-n} \left( \frac{n-1}{q} \right) (1 - V_n)^n \, (d V_n)^q,
\]

where

\[
V_n = \frac{\pi^{D/2} / \Gamma(D/2 + 1)}{r_n^D}
\]

and

\[
\left( \frac{N-1}{n-1} \right) = \frac{(N-1)!}{(n-1)! (N-n)!}, \quad \left( \frac{n-1}{q} \right) = \frac{(N-n)!}{q! (N-n-q)!}
\]

are binomial coefficients. Ignoring differentials of order higher than the first \((q = 1)\) in equation (5), as they are negligible compared to the first, we get

\[
P(r_n) \, d r_n = \left( \frac{N-1}{n-1} \right) (N-n) V_n^{n-1} (1 - V_n)^{N-n-1} \, d V_n.
\]

Since the \( n \)th neighbour \((n < N)\) must certainly lie within a unit volume centred at the reference point, its mean distance from the reference point is given by

\[
\langle r_n \rangle = \int_0^R r_n P(r_n) \, d r_n,
\]
Next, we develop an alternative way of deriving the exact expression of \( r_n \). The method of conditional probability and the complete asymptotic expression of the mean \( n \)

\[
R = \frac{\left[ \Gamma \left( \frac{D}{2} + 1 \right) \right]^{1/D}}{\pi^{1/2}}.
\]

Changing the variable of integration in equation (9) from radius to volume (by the relation \( V_n = \frac{\pi^{D/2}}{\Gamma(1 + D/2)} N^{D/2} \)), we get the exact result for the mean \( n \)th neighbour distance:

\[
\langle r_n(N) \rangle = \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \frac{(N - 1)}{(n - 1) \Gamma(1 + D/2)} \int_0^1 V_n^{n+1/(1+D)} (1 - V_n)^{N-n-1} dV_n
\]

\[
= \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \frac{(N - 1)}{(n - 1) \Gamma(1 + D/2)} B \left( n + 1, N - n \right)
\]

\[
= \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \frac{(n + 1)}{\Gamma(n + 1)} \frac{\Gamma(N)}{\Gamma(N + 1)}.
\]

Here, \( B(x, y) \) is the beta function defined as \( B(x, y) = \int_0^1 t^{x-1}(1 - t)^{y-1} dt \) and \( \Gamma(z) \) is the complete gamma function: \( \Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \). These functions are related by the formula [9]: \( B(x, y) = \Gamma(x) \Gamma(y)/\Gamma(x + y) \).

For large values of \( N \), we get by using Stirling’s approximation [10] for the gamma function: \( \Gamma(N + 1/D)/\Gamma(N) \sim N^{1/D} \); therefore, for large density \( N \), equation (11) reduces to the following asymptotic form:

\[
\langle r_n(N) \rangle \sim \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \frac{(n + 1)}{\Gamma(n + 1)} \frac{\Gamma(N)}{\Gamma(N + 1)} \right]^{1/D}.
\]

(12)

If the neighbour index \( n \) is also large (but \( n \ll N \)), we have \( \Gamma(n + 1/D)/\Gamma(n) \sim n^{1/D} \) and the complete asymptotic expression of the mean \( n \)th neighbour distance is given by

\[
\langle r_n(N) \rangle \sim \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \frac{(n + 1)}{\Gamma(n + 1)} \frac{\Gamma(N)}{\Gamma(N + 1)} \right]^{1/D}.
\]

(13)

The above equation shows that the expression of \( \langle r_n(N) \rangle \) obtained by heuristic means (equation (4)) has the correct asymptotic dependence on \( N \) and \( n \).

4. The method of conditional probability

Next, we develop an alternative way of deriving the exact expression of \( \langle r_n \rangle \) by using the theory of conditional probability [8]. We proceed by asserting that we look for the \( n \)th neighbour of a reference point only after its first \( n - 1 \) neighbours have been located. In that case the reference point and its first \( n - 1 \) neighbours are considered as given; now the probability \( P(r_n) \) of finding the \( n \)th neighbour of the reference point at a distance between \( r_n \) and \( r_n + dr_n \) from it is a conditional probability as the \( n \)th neighbour must certainly lie outside the hypersphere of radius \( r_{n-1} \):

\[
P(r_n) \ dr_n = \sum_{q=1}^{N-n} \binom{N-n}{q} \left[ 1 - \frac{V_n - V_{n-1}}{1 - V_{n-1}} \right]^{N-n-q} \left[ \frac{dV_n}{1 - V_{n-1}} \right]^q.
\]

(14)

Here, \( V_n \) is the volume of the \( D \)-dimensional hypersphere of radius \( r_n \) centred at the reference point (equation (6)). Ignoring differentials of order higher than the first (\( q = 1 \), as they are negligible compared to the first, in equation (14), we get

\[
P(r_n) \ dr_n = \left[ 1 - \frac{V_n - V_{n-1}}{1 - V_{n-1}} \right]^{N-n-1} \frac{(N-n) dV_n}{1 - V_{n-1}}.
\]

(15)
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For a given reference point and its first \( n - 1 \) neighbours, the mean \( n \)th neighbour distance is thus obtained as

\[
\langle r_n \rangle^{(\text{conditional})} = \int_{r_{n-1}}^R r_n P(r_n) \, dr_n, \tag{16}
\]

where, as before, \( R \) is the radius of a \( D \)-dimensional hypersphere of unit volume. The quantity \( \langle r_n \rangle^{(\text{conditional})} \) is a function of the particular \( r_{n-1}, r_{n-2}, \ldots, r_1 \) which are the distances of the first \( n - 1 \) neighbours of the reference point. To remove the dependence of the mean \( n \)th neighbour distance on the particular set of values of the first \( n - 1 \) neighbour distances, the quantity \( \langle r_n \rangle^{(\text{conditional})} \) must be averaged successively over the probability distributions of each of the first \( n - 1 \) neighbours:

\[
\langle r_n \rangle = \int_{r_{n-1}}^R dr_{n-1} P(r_{n-1}) \langle r_n \rangle^{(\text{conditional})}, \tag{17}
\]

where the probability distribution of the \( i \)th neighbour distance is given by equation (15) with \( i \) replacing \( n \). This step is equivalent to an ensemble average in statistical mechanics [11]. After changing all the variables of integration in equation (17) from radii to the corresponding volumes (by the relation of equation (6)) and changing the order of the integrals such that the integral with respect to \( V_n \) has to be evaluated last, we get

\[
\langle r_n(N) \rangle = \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{D/2}} \right]^{1/D} \frac{(N-1)(N-2)(N-n)}{\Gamma(n)} \int_0^1 dV_n V_n^{1/D} (1 - V_n)^{N-n-1} V_n \int_{V_n}^1 dV_1 \int_{V_1}^1 dV_2 \cdots \int_{V_{n-1}}^1 dV_{n-2} \int_{V_{n-1}}^1 dV_{n-1}, \tag{18}
\]

which gives the final form of the mean \( n \)th neighbour distance:

\[
\langle r_n(N) \rangle = \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{D/2}} \right]^{1/D} \frac{(N-1)(N-n)}{\Gamma(n)} \int_0^1 V_n^{(n+1/D)-1} (1 - V_n)^{N-n-1} dV_n.
\]

This is identical to the result of equation (11) obtained in the previous section.

5. The mean volume estimate

Instead of calculating the mean distance to the \( n \)th neighbour, we now calculate the mean volume \( \langle V_n \rangle \) separating the reference point from its \( n \)th neighbour. The volume separating a reference point from its \( n \)th neighbour located at a distance \( r_n \) from it is defined as the volume of the hypersphere of radius \( r_n \) and centred at the reference point. Therefore, from equation (6), we get

\[
\langle V_n \rangle = \frac{\pi^{D/2}}{\Gamma \left( \frac{D}{2} + 1 \right)} \langle r_n^D \rangle. \tag{20}
\]

Using the absolute probability distribution of equation (8), we get

\[
\langle r_n^D \rangle = \int_0^R r_n^D P(r_n) \, dr_n. \tag{21}
\]
where \( R \) is defined in equation (10). Consequently, we get from the above two equations

\[
\langle V_n \rangle = \left( \frac{N - 1}{n - 1} \right) \left( N - n \right) \int_0^1 V_n^n (1 - V_n)^{N-n-1} dV_n
\]

\[
= \left( \frac{N - 1}{n - 1} \right) \left( N - n \right) B(n + 1, N - n)
\]

\[
= \frac{\Gamma(n + 1)}{\Gamma(n)} \frac{\Gamma(N)}{\Gamma(N + 1)} = \frac{n}{N}.
\]

(22)

Now we may estimate the mean \( n \)th neighbour distance by using the following approximation:

\[
\langle r_n \rangle \approx \langle r_D \rangle^{1/D}.
\]

(23)

From equations (20) and (22), we get

\[
\langle r_D \rangle^{1/D} = \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \left( \frac{n}{N} \right)^{1/D} - \langle r_n \rangle.
\]

(24)

The above result is the same as the asymptotic expression of \( \langle r_n \rangle \) obtained in equation (13) and thus equation (23) is valid as \( N \to \infty \) and \( n \to \infty, n \ll N \). Comparison with equation (4) shows that this approximation is a better estimate of \( \langle r_n \rangle \) than the result obtained by heuristic means.

The error in this estimate of \( \langle r_n \rangle \) by equation (23) is given by \( \langle r_D \rangle^{1/D} - \langle r_n \rangle \). From equations (11) and (24), we get

\[
\pi^{1/2} \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \left( \frac{n}{N} \right)^{1/D} - \langle r_n \rangle \right] = \left( \frac{n}{N} \right)^{1/D} - \frac{\Gamma \left( \frac{n + 1}{D} \right)}{\Gamma(n)} \frac{\Gamma(N)}{\Gamma(N + 1/D)}.
\]

(25)

It is obvious that the error is zero for \( D = 1 \) and from the expression in equation (25) it is clear that the error is greater than zero for all finite dimensions \( D \geq 2 \). For large values of \( D \), we get

\[
\frac{\Gamma \left( \frac{n + 1}{D} \right)}{\Gamma(n)} \approx \Gamma \left( 1 + \frac{1}{D} \right) \left[ 1 + \frac{H_{n-1}}{D} \right]
\]

(26)

and a similar expression for \( \Gamma(N + 1/D) / \Gamma(N) \), where \( H_n = \sum_{k=1}^{n} 1/k \) are called harmonic numbers [10]. Consequently, equation (25) reduces to the form

\[
\pi^{1/2} \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \left( \frac{n}{N} \right)^{1/D} - \langle r_n \rangle \right] \approx \left( \frac{n}{N} \right)^{1/D} - \frac{1 + \frac{1}{D} H_{n-1}}{1 + \frac{1}{D} H_{n-1}}
\]

\[
\approx \left( \frac{n}{N} \right)^{1/D} - \left[ 1 + \frac{1}{D} \left( H_{n-1} - H_{N-1} \right) \right].
\]

(27)

Since \( \lim_{n \to \infty} (H_n - \ln n) = \gamma = \lim_{N \to \infty} (H_N - \ln N) \), where \( \gamma = 0.577 215 6649 \ldots \) is Euler’s constant [10], for large values of \( n \) and \( N \), equation (27) may be written as

\[
\pi^{1/2} \left[ \frac{\Gamma \left( \frac{D}{2} + 1 \right)}{\pi^{1/2}} \left( \frac{n}{N} \right)^{1/D} - \langle r_n \rangle \right] \approx \left( \frac{n}{N} \right)^{1/D} - \left[ 1 + \frac{1}{D} \ln \left( \frac{n}{N} \right) \right].
\]

(28)

The error is then practically zero, since, for large values of \( D \), we get

\[
\left( \frac{n}{N} \right)^{1/D} = \exp \left[ \frac{1}{D} \ln \left( \frac{n}{N} \right) \right] \approx 1 + \frac{1}{D} \ln \left( \frac{n}{N} \right).
\]

(29)
6. Concluding remarks

In this paper, we have studied two kinds of approaches to determine the mean rth neighbour distance in a system of uniformly distributed random points. In one kind of approach we construct the solution from a physical picture of the system; though it produces only an approximate mathematical result it helps to visualize the solution. The heuristic method of section 2 and the mean volume method of section 5 are of this kind. The other kind of approach is rigorous and produces the exact mathematical result, while the method of absolute probability used in section 3 is largely pedagogical, the method of conditional probability used in section 4 provides a detailed insight into the problem. Though the heuristic estimate of $\langle r_n \rangle$ is close to the exact result only for large values of $n$, $N$ and $D$, along with the condition $N \gg n$, the advantage of the heuristic method lies in its simplicity; however approximate, it gives an essence of $\langle r_n \rangle$. Therefore, in cases where the distribution of points in space is such that an exact evaluation of $\langle r_n \rangle$ is not possible [12], heuristic constructions similar to this one may be useful.

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