Separations inside a cube

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Abstract

Two points are randomly selected inside a three-dimensional euclidian cube. The value \( l \) of their separation lies somewhere between zero and the length of a diagonal of the cube. The probability density \( P(l) \) of the separation is constructed analytically. Also a Monte Carlo computer simulation is performed, showing good agreement with the formulas obtained.

1 Introduction

An important problem in geometry and statistics is: given a convex compact space endowed with a metric, and randomly choosing two points in the space, find the probability density \( P(l) \) that these points have a specified separation \( l \). The study of this problem has a long history [1], and recently gained considerable impetus from researchers in cosmic crystallography [2]-[19].

In a recent paper the functions \( P(l) \) corresponding to 2D disks and rectangles were obtained [20]. The methodology introduced in that work is here extended to a 3D euclidian cube.

2 Preliminaries

An euclidian cube with side \( a \) is assumed, occupying the location \( 0 < x, y, z < a \) in a cartesian frame. Randomly choosing two points \( A \) and \( B \) in the cube, we want the probability \( P(l)dl \) that the separation between the points lie between \( l \) and \( l + dl \). The probability density \( P(l) \) has to satisfy the normalization condition

\[
\int_0^{\sqrt{3}a} P(l)dl = 1. \tag{1}
\]

The calculation can be shortened if one considers the symmetries of the cube. Really, if the points \( A \) and \( B \) have been chosen, imagine the oriented segment \( A'B' \) parallel to

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$AB$, with the tip $A'$ coinciding with the origin $O$. The other tip $B'$ then lies inside a larger cube, with side $2a$. Since the probability density $\mathcal{P}(l)$ clearly does not depend on which octant of the large cube contains $B'$, there is no loose in generality in restricting the calculation to the cases where $B'$ is in the octant $0 < x, y, z < a$.

With this assumption, the point $B'$ has cartesian coordinates

$$B' = (l \cos \theta \cos \phi, l \cos \theta \sin \phi, l \sin \theta),$$

where both angles $\theta, \phi$ are bound to the interval $[0, \pi/2]$; here $\phi$ is the azimuthal angle, while $\theta$ is the polar angle measured from the $z = 0$ plane. The corresponding tip $B$ in the original segment must lie inside a parallelepiped with sides (see figure 1)

$$l_x := a - l \cos \theta \cos \phi, \quad l_y := a - l \cos \theta \sin \phi, \quad l_z := a - l \sin \theta. \quad (2)$$

![Figure 1](image)

The probability $\mathcal{P}(l, \theta, \phi)dl \, d\theta \, d\phi$ that the segment $AB$ has length between $l$ and $l + dl$, azimuth between $\phi$ and $\phi + d\phi$, and polar angle between $\theta$ and $\theta + d\theta$ is then

$$\mathcal{P}(l, \theta, \phi)dl \, d\theta \, d\phi = k l_x l_y l_z \cos \theta dl \, d\theta \, d\phi, \quad (3)$$

where $k$ is a constant and where the assumption $0 < \phi, \theta < \pi/2$ stands. Performing the angular integrations we shall obtain

$$\mathcal{P}(l) = \int \int \mathcal{P}(l, \theta, \phi) d\theta \, d\phi, \quad (4)$$

and we finally fix $k$ using the condition \([\text{II}].\)

To calculate $\mathcal{P}(l)$, three cases need be separately considered, depending on the value of $l$ relative to $a$: namely the cases $0 < l < a$, $a < l < \sqrt{2}a$, and $\sqrt{2}a < l < \sqrt{3}a$.

### 3 The case $0 < l < a$

As is seen in the figure 2, in this case we effectively have $\phi_{\text{min}} = \theta_{\text{min}} = 0$, and $\phi_{\text{max}} = \theta_{\text{max}} = \pi/2$. Then

$$\mathcal{P}(l < a) = k l^2 \int_0^{\pi/2} l_z \cos \theta d\theta \int_0^{\pi/2} l_x l_y d\phi \quad (5)$$
where \( k = 8/a^6 \) as will be fixed later on.

\[
= \frac{k l^2}{8} \left[ 4\pi a^3 - 6\pi a^2 l + 8al^2 - l^3 \right], \quad (6)
\]

\( \text{Figure 2} \) The triangular intersection of the 2D sphere with radius \( l \) and centre \( O \) with the 3D cube having side \( a > l \).

4 The case \( a < l < \sqrt{2}a \)

In this case the intersection of the 2D sphere (with radius \( l \)) with the 3D cube (with side \( a \)) is an hexagonal surface as in figure 3.

\( \text{Figure 3} \) The hexagonal intersection of a 2D sphere with radius \( l \) and centre \( O \) with a 3D cube with a vertex in \( O \) and having side \( a \) such that \( a < l < \sqrt{2}a \).

We note that the arcs of circle drawn on the faces \( x, y, z = 0 \) have radius \( l \), while those drawn on the faces \( x, y, z = a \) have radius \( \sqrt{l^2 - a^2} \).

For convenience of integration we divide the intersection into two regions. In region I we have \( \cos^{-1}(a/l) < \theta < \sin^{-1}(a/l) \) and \( 0 < \phi < \pi/2 \).

In region II we have \( \theta_{\text{min}} = 0 \) and \( \theta_{\text{max}} = \cos^{-1}(a/l) \). To have \( \phi_{\text{min}}(\theta) \) we note that the circle drawn on the face \( x = a \) satisfies the equation \( \cos \phi \cos \theta = a/l \), so

\[
\phi_{\text{min}}(\theta) = \cos^{-1}\left( \frac{a}{l \cos \theta} \right) =: \phi_1(\theta). \quad (7)
\]
On the other hand, the circle drawn on the face $y = a$ satisfies $\sin \phi \cos \theta = a/l$, so we have

$$\phi_{\text{max}}(\theta) = \sin^{-1} \left( \frac{a}{l \cos \theta} \right) =: \phi_2(\theta).$$  \hspace{1cm} (8)

We then find

$$\mathcal{P}(a < l < \sqrt{2}a)$$

$$= \frac{k}{8} l^2 \left[ \int_{\cos^{-1}(a/l)}^{\sin^{-1}(a/l)} \cos \theta d\theta \int_{0}^{\pi/2} \cos \theta d\phi + \int_{0}^{\cos^{-1}(a/l)} \cos \theta d\theta \int_{\phi_1(\theta)}^{\phi_2(\theta)} d\phi \right] l_x l_y l_z \hspace{1cm} (9)$$

$$= \frac{k}{8} l^2 \left[ 2l^4 + 6a^2 l^2 - a^4 - 2\pi a^3 (4l - 3a) - 8a(2l^2 + a^2)\sqrt{l^2 - a^2} \right.$$  

$$\left. + 24a^2 l^2 \cos^{-1}(a/l) \right], \hspace{1cm} (10)$$

where $k = 8/a^6$ as will be fixed later on.

5 The case $\sqrt{2}a < l < \sqrt{3}a$

In this case the 2D sphere with radius $l$ intersects the 3D cube with side $a$ in the triangular surface shown in figure 4.

![Figure 4](image_url)

**Figure 4** The triangular intersection of a 2D sphere with radius $l$ and centre $O$ with a 3D cube with a vertex in $O$ and having side $a$ such that $\sqrt{2}a < l < \sqrt{3}a$.

As before, the circles drawn on the faces $x, y, z = a$ have radius $\sqrt{l^2 - a^2}$. The azimuthal integration is performed between $\phi_1(\theta)$ and $\phi_2(\theta)$ as in the region $II$ of the preceding case, and again $\sin \theta_{\text{max}} = a/l$; but now $\cos \theta_{\text{min}} = \sqrt{2}a/l$. We then find

$$\mathcal{P}(\sqrt{2}a < l < \sqrt{3}a) = \frac{k}{8} l^2 \int_{\cos^{-1}(\sqrt{2}a/l)}^{\sin^{-1}(a/l)} l_z \cos \theta d\theta \int_{\phi_1(\theta)}^{\phi_2(\theta)} l_x l_y d\phi \hspace{1cm} (11)$$

$$= \frac{k}{8} l^2 \left[ 8a(l^2 + a^2)\sqrt{l^2 - a^2} - (l^2 + a^2)(l^2 + 5a^2) + 2\pi a^2 (3l^2 - 4al + 3a^2) \right.  $$

$$\left. + 24a^3 l \sec^{-1}(l^2/a^2 - 1) - 24a^2 (l^2 + a^2) \sec^{-1} \sqrt{l^2/a^2 - 1} \right], \hspace{1cm} (12)$$
where \( k = 8/a^6 \).

This value for the constant \( k \) derives from the normalization condition (5), namely,

\[
\int_0^a P(l < a)dl + \int_a^{\sqrt{2}a} P(a < l < \sqrt{2}a)dl + \int_{\sqrt{2}a}^{\sqrt{3}a} P(\sqrt{2}a < l < \sqrt{3}a)dl = 1. \tag{13}
\]

6 Graphs of \( P(l) \)

In figure 5 we present a graph of the dimensionless function \( aP(l) \) against the dimensionless variable \( l/a \).

![Figure 5](image)

**Figure 5** The probability density \( P(l) \) of separation \( l \) of pairs of randomly distributed points inside a cube with side \( a \). The irregular curve is the output of a corresponding computer simulation.

We note that the function and its first derivative are continuous in the whole interval \( 0 < l < \sqrt{3}a \). Nevertheless the second derivative is discontinuous at \( l = a \), as discussed in the next section. In the figure a normalized histogram corresponding to 150,000 separations between pairs of points randomly selected in the cube is superimposed, for comparison; the agreement of the two curves evinces the correctness of the calculation.

7 Comments

The integration to find \( P(l) \) in eqs. (1)-(3) is almost trivial; however, not the same can be said about the two other cases, namely in going from (9) to (10) and from (11) to (12). A computer assistance appears paramount in these two cases, to confirm every short step in the calculation and simplification of expressions.

Similarly as in [21], the probability density \( P(l) \) and its first derivative are continuous throughout the entire range \( 0 < l < \sqrt{3}a \). But the second derivative shows a finite discontinuity at \( l = a \), although it is continuous at \( l = \sqrt{2}a \).

A remarkable feature of \( P(l) \) is its behaviour for large values of \( l \); really, near \( l = \sqrt{3}a \) we find

\[
aP(l) = \frac{9}{5}(\sqrt{3} - l/a)^5 + O((\sqrt{3} - l/a)^6), \tag{14}
\]
so $P(l)$ is essentially a fifth power of $\sqrt[3]{3} - l/a$. We find that 91% of the separations lie in the range $l \in (0, a)$, 9% lie in the interval $l \in (a, \sqrt{2}a)$, and only 0.04% have $l > \sqrt{2}a$.

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