

Computing the Volume of High-Dimensional Balls and Cubes

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1 Introduction

In this project, we study methods of computing the volume of high-dimensional convex bodies. We begin by analyzing the volume of a ball in \mathbb{R}^n by interpreting its theoretical volume as the sum of infinitely thin cross-sectional areas using integrals. However, we show that the deterministic methods used to describe the ball's volume fail when n becomes large, and then we turn to the use of Monte-Carlo algorithms. We then analyze the unit hypercube using Monte-Carlo methods and ultimately compute the volume of the unit ball in high dimensions.

2 Background

In this project we will frequently be discussing balls and cubes. The inside of a sphere in any dimension is referred to as a ball. All balls with radius r in \mathbb{R}^n are defined to be

$$B_n(r) = \{\mathbf{x} \in \mathbb{R}^n; \|\mathbf{x}\| \leq r\} \quad (1)$$

Cubes are the inside of a cube in any dimension. All cubes with face length l in \mathbb{R}^n , centered at the origin are defined to be

$$K_n(l) = \{\mathbf{x} = [\mathbf{x}_1 \dots \mathbf{x}_n] \in \mathbb{R}^n; \|\frac{-1}{2} \leq \mathbf{x} \leq \frac{1}{2}\|\} \quad (2)$$

We define the terms length, area, and volume as follows: The word *volume* is used for a set $A \subset \mathbb{R}^n$, and we write $\text{vol}(A)$ to denote the

Length: the volume of a set A for A on the real line ($n = 1$).

Area: the volume of a set A for A in the plane ($n=2$)

Volume: the volume of a set A for $A \in \mathbb{R}^n$ where $n \geq 3$.

3 The volume of a ball in \mathbb{R}^n

3.1 $V(B_1(1))$ and $V(B_2(1))$

The ball of radius r in \mathbb{R}^n is defined as

$$B_n(r) = \{x \in \mathbb{R}^n; \|x\| \leq r\} \quad (1)$$

From this we have the $V(B_1(1)) = 1$ and $V(B_2(1)) = \pi$ since the volume of $B_1(r)$ is the length of the set which is just equal to r , and the volume of $B_2(r)$ is the area of the circle of radius r .

3.2 A proof

From Cavalier's Principle, we have

$$V(B_n(1)) = V(B_{n-1}(1)) \int_0^\pi \sin^n(\theta) d\theta \quad (2)$$

Using this, we can say that the volume of an object in \mathbb{R}^n can be expressed as an integral of the cross sectional areas of the object. This gives us

$$V(B_n(1)) = \int_{-1}^1 V(B_{n-1}(\sqrt{1-x_n^2})) dx_n \quad (3)$$

We know

$$V(B_n(r)) = r^n V(B_n(1)) \quad (4)$$

We notice comparing (3) and (4) that we have $r = \sqrt{1-x_n^2}$ and thus

$$V(B_n(1)) = \int_{-1}^1 \left(\sqrt{1-x_n^2}\right)^{n-1} V(B_{n-1}(1)) dx_n \quad (5)$$

$V(B_{n-1}(1))$ is a constant, so it can be brought outside of the integral.

$$V(B_n(1)) = V(B_{n-1}(1)) \int_{-1}^1 \left(\sqrt{1-x_n^2}\right)^{n-1} dx_n \quad (6)$$

Now, we set $x_n = \cos(\theta)$ which gives us $dx_n = -\sin(\theta)d\theta$ and therefore

$$V(B_n(1)) = V(B_{n-1}(1)) \int_\pi^0 -\left(\sqrt{1-\cos^2(\theta)}\right)^{n-1} \sin(\theta) d\theta \quad (7)$$

From the identity $\cos^2(\theta) + \sin^2(\theta) = 1$, we get

$$V(B_n(1)) = V(B_{n-1}(1)) \int_0^\pi \sin^n(\theta) d\theta \quad (8)$$

Which is exactly the same as (2) so we have shown by direct proof that the statement is true.

3.3 Another proof

We wish to prove that

$$I_n = \frac{n-1}{n} I_{n-2}, \quad n \geq 3 \quad (9)$$

Where

$$I_n = \int_0^\pi \sin^n(\theta) d\theta \quad (10)$$

We start by showing the base case:

$$I_2 = \int_0^\pi \sin^2(\theta) d\theta \quad (11)$$

$$I_2 = \int_0^\pi \frac{1 - \cos(2\theta)}{2} d\theta$$

Breaking the integral apart gives us

$$I_2 = \frac{1}{2} \int_0^\pi 1 d\theta - \frac{1}{2} \int_0^\pi \cos(2\theta) d\theta$$

Let $u = 2\theta$. Thus, $du = 2d\theta$ which gives us

$$\begin{aligned} I_2 &= \frac{1}{2} \int_0^\pi 1 d\theta - \int_0^{2\pi} \cos(u) d\theta \\ I_2 &= \frac{1}{2} \left[\theta \right]_{\theta=0}^{\theta=\pi} - \left[\sin u \right]_{u=0}^{u=2\pi} \\ I_2 &= \frac{\pi}{2} \end{aligned}$$

We now check if (9) holds true for the base case.

$$\begin{aligned} I_2 &= \frac{(2-1)}{2} I_{(2-2)} \\ I_2 &= \frac{1}{2} I_0 \end{aligned} \quad (12)$$

Check I_0 :

$$I_0 = \int_0^\pi 1 d\theta = \left[\theta \right]_0^\pi = \pi \quad (13)$$

This gives us $I_2 = \frac{\pi}{2}$ which is the same as was found by solving (11), so the base case is true.

We now assume that (9) is true for n and check that it will hold for $n+1$. First, we manipulate the integral form of I_n from (10). Performing integration by parts setting $u = \sin^{n-1}(\theta)$ and $dv = \sin(\theta)$ gives us

$$I_n = \left[\sin^{n-1}(\theta) \cos(\theta) \right]_0^\pi + \int_0^\pi (n-1) \sin^{n-2}(\theta) \cos^2(\theta) d\theta \quad (14)$$

$$I_n = (n-1) \int_0^\pi \sin^{n-2}(\theta) (1 - \sin^2(\theta)) d\theta$$

$$I_n = (n-1)(I_{n-2} - I_n) \quad (15)$$

Which yields

$$I_n = \frac{n-1}{n} I_{n-2}, \quad n \geq 3 \quad (16)$$

And thus, we have shown that this is true by direct proof.

3.4 One More Proof

We wish to prove that, for $n \geq 1$,

$$I_{2n-1} I_{2n} = \frac{2\pi}{2n} \quad (17)$$

$$I_{2n} I_{2n+1} = \frac{2\pi}{2n+1} \quad (18)$$

First we will prove (17). From (9) we have

$$I_{2n-1} = \frac{2n-2}{2n-1} I_{2n-3} \quad (19)$$

$$I_{2n-3} = \frac{2n-4}{2n-3} I_{2n-5}$$

$$I_{2n-5} = \frac{2n-6}{2n-5} I_{2n-7}$$

⋮

Putting these together will give us

$$I_{2n-1} = \left(\frac{2n-2}{2n-1} \right) \left(\frac{2n-4}{2n-3} \right) \left(\frac{2n-6}{2n-5} \right) \cdots \left(\frac{1}{2} \right) I_1 \quad (20)$$

We also get

$$I_{2n} = \frac{2n-1}{2n} I_{2n-2} \quad (21)$$

$$I_{2n-2} = \frac{2n-3}{2n-2} I_{2n-4}$$

$$I_{2n-4} = \frac{2n-5}{2n-4} I_{2n-6}$$

⋮

Putting these together will give us

$$I_{2n} = \left(\frac{2n-1}{2n}\right) \left(\frac{2n-3}{2n-2}\right) \left(\frac{2n-5}{2n-4}\right) \cdots \left(\frac{2}{3}\right) I_0 \quad (22)$$

We now multiply (20) and (22) to get

$$I_{2n-1}I_{2n} = \left(\frac{2n-2}{2n-1}\right) \left(\frac{2n-4}{2n-3}\right) \cdots \left(\frac{1}{2}\right) I_1 \left(\frac{2n-1}{2n}\right) \left(\frac{2n-3}{2n-2}\right) \cdots \left(\frac{2}{3}\right) I_0 \quad (23)$$

Reordering gives us

$$I_{2n-1}I_{2n} = \left(\frac{2n-1}{2n}\right) \left(\frac{2n-2}{2n-1}\right) \left(\frac{2n-3}{2n-4}\right) \cdots \left(\frac{2}{3}\right) \left(\frac{1}{2}\right) I_1 I_0 \quad (24)$$

Every term's numerator is canceled by the following terms denominator leaving us with

$$I_{2n-1}I_{2n} = \frac{I_1 I_0}{2n} \quad (25)$$

Now, we simply calculate I_1 and I_0 .

$$I_1 = \int_0^\pi \sin(\theta) d\theta = \left[-\cos(\theta)\right]_0^\pi = 2 \quad (26)$$

$$I_0 = \int_0^\pi 1 d\theta = \left[\theta\right]_0^\pi = \pi \quad (27)$$

Thus, we have proven

$$I_{2n-1}I_{2n} = \frac{2\pi}{2n} \quad (28)$$

Now we will prove (18). From (9) we have

$$I_{2n+1} = \frac{2n}{2n+1} I_{2n-1} \quad (29)$$

$$I_{2n-1} = \frac{2n-2}{2n-1} I_{2n-3}$$

$$I_{2n-3} = \frac{2n-4}{2n-3} I_{2n-5}$$

⋮

Putting these together will give us

$$I_{2n+1} = \left(\frac{2n}{2n+1}\right) \left(\frac{2n-2}{2n-1}\right) \left(\frac{2n-4}{2n-3}\right) \cdots \left(\frac{1}{2}\right) I_1 \quad (30)$$

We now multiply (22) and (30) to get

$$I_{2n}I_{2n+1} = \left(\frac{2n-1}{2n}\right)\left(\frac{2n-3}{2n-2}\right)\cdots\left(\frac{2}{3}\right)I_0\left(\frac{2n}{2n+1}\right)\left(\frac{2n-2}{2n-1}\right)\cdots\left(\frac{1}{2}\right)I_1 \quad (31)$$

Reordering gives us

$$I_{2n}I_{2n+1} = \left(\frac{2n}{2n-1}\right)\left(\frac{2n-1}{2n}\right)\left(\frac{2n-2}{2n-1}\right)\cdots\left(\frac{2}{3}\right)\left(\frac{1}{2}\right)I_1I_0 \quad (32)$$

Every term's numerator is canceled by the following terms denominator leaving us with

$$I_{2n}I_{2n+1} = \frac{I_1I_0}{2n+1} \quad (33)$$

We know that $I_1 = 2$ and $I_0 = \pi$ (see (26) and (27)). Thus we have proven that,

$$I_{2n}I_{2n+1} = \frac{2\pi}{2n+1} \quad (34)$$

3.5 Conclusion from proofs

We wish to draw a conclusion from the proofs performed in the last 3 sections.

We know now from (2) that

$$V(B_{2n}(1)) = V(B_{2n-1}(1)) \int_0^\pi \sin^{2n}(\theta)d\theta \quad (35)$$

$$V(B_{2n}(1)) = V(B_{2n-1}(1))I_{2n}$$

$$V(B_{2n}(1)) = V(B_{2n-2}(1))I_{2n} \int_0^\pi \sin^{2n-1}(\theta)d\theta$$

$$V(B_{2n}(1)) = V(B_{2n-3}(1))I_{2n}I_{2n-1} \int_0^\pi \sin^{2n-1}(\theta)d\theta$$

⋮

$$V(B_{2n}(1)) = V(B_1(1))I_{2n}I_{2n-1}\cdots I_2I_1 \quad (36)$$

From section 3.1 we know that that $V(B_1(1)) = 1$ and from (17) that $I_{2n}I_{2n-1} = \frac{\pi}{n}$ thus we have

$$V(B_{2n}(1)) = \frac{\pi^n}{n!} \quad (37)$$

We can also draw a similar conclusion for $V(B_{2n+1}(1))$.

$$V(B_{2n+1}(1)) = V(B_{2n}(1)) \int_0^\pi \sin^{2n+1}(\theta)d\theta \quad (38)$$

$$\begin{aligned}
V(B_{2n+1}(1)) &= V(B_{2n}(1))I_{2n+1} \\
V(B_{2n+1}(1)) &= V(B_{2n-1}(1))I_{2n+1} \int_0^\pi \sin^{2n}(\theta)d\theta \\
V(B_{2n+1}(1)) &= V(B_{2n-2}(1))I_{2n+1}I_{2n} \int_0^\pi \sin^{2n}(\theta)d\theta \\
&\vdots \\
V(B_{2n+1}(1)) &= V(B_1(1))I_{2n+1}I_{2n} \dots I_2I_1 \tag{39}
\end{aligned}$$

From section 3.1 we know that that $V(B_1(1)) = 1$ and from (18) that $I_{2n+1}I_{2n} = \frac{2\pi}{2n+1}$ thus we have

$$V(B_{2n+1}(1)) = \frac{2^{n+1}\pi^n}{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n+1)} \tag{40}$$

Which is the same as

$$V(B_{2n+1}(1)) = \frac{\pi^n}{(\frac{1}{2}) \cdot (\frac{3}{2}) \cdot (\frac{5}{2}) \cdot \dots \cdot (n + (\frac{1}{2}))} \tag{41}$$

3.6 A Theoretical Ratio

The theoretical ratio of points generated inside a hypercube $[-1, 1]^n$ that randomly fall in the ball of dimension in $(B_n(1))$ will be equal to

$$\lim_{n \rightarrow \infty} \frac{vol(B_n(1))}{vol([-1, 1]^n)} \tag{42}$$

We have not yet found a specific formula for $V(B_n(1))$ but it can be approximated by the average of $V(B_{2n}(1))$ and $V(B_{2n+1}(1))$

In section 3.5 we found that these are

$$V(B_{2n}(1)) = \frac{\pi^n}{n!} \tag{43}$$

$$V(B_{2n+1}(1)) = \frac{\pi^n}{(\frac{1}{2}) \cdot (\frac{3}{2}) \cdot (\frac{5}{2}) \cdot \dots \cdot (n + (\frac{1}{2}))} \tag{44}$$

Averaging these yields

$$V(B_{2n}(1))V(B_{2n+1}(1)) = \frac{\pi^{2n}}{n! \left((\frac{1}{2}) \cdot (\frac{3}{2}) \cdot (\frac{5}{2}) \cdot \dots \cdot (n + (\frac{1}{2})) \right)} \tag{45}$$

The volume of a cube in \mathbb{R}^n with side length two is simply 2^n so (42) becomes

$$\lim_{n \rightarrow \infty} \frac{2^n \pi^{2n}}{n! \left(\left(\frac{1}{2}\right) \cdot \left(\frac{3}{2}\right) \cdot \left(\frac{5}{2}\right) \cdot \dots \cdot \left(n + \left(\frac{1}{2}\right)\right) \right)} \quad (46)$$

Which evaluates to 0.

4 The Hypercube in High Dimensions

4.1 Pairwise Distances in the Hypercube

Within the world that humans can intuitively interpret, points in space can be represented by a set of coordinates. In one-dimensional space, representing a coordinate only requires a single value, which can be intuitively described as the x -coordinate. To then represent a coordinate in a dimension one step higher, in the two-dimensional coordinate plane, it only requires one additional value, making the coordinate a set of two values. Humans are fortunate enough to be able to visualize space up to the third-dimension, but higher dimensions than those are outside the limits of human intuition. However, mathematically, the foundations of coordinates remain exactly the same in higher dimensions, and points resting in a higher dimensions only require a set of values whose size is equal to the dimension in which it rests, which can then be generalized to $X_n = \{a_1, a_2, \dots, a_n\}$ with n being our desired dimension. Then, when generating a collection of random points within a hypercube, each set of coordinate values becomes a subset within the set of points, giving us a set of $H_N = \{X_1, X_2, \dots, X_N\}$ where N is equal to the desired number of samples. Since H is our set of subsets, the entire set of points and coordinate values can be stored in a matrix of size n by N , where each row contains the coordinates of its respective point. MATLAB's `rand()` function makes the generation process incredibly easy. The function generates a matrix of random real numbers on a domain of $x \in [0, 1]$, and we can define its size to be equal to our desired dimension of 100 and number of samples at 400. Then, to transform the randomly generated values to fit our domain, it's as simple as multiplying them by the difference in the upper and lower bounds and then adding the lower bound. Since our desired domain still has a length of 1, we don't really need to include it, but by subtracting $\frac{1}{2}$ from the randomly generated values, we end up with our points properly on the domain of $x \in \left[-\frac{1}{2}, \frac{1}{2}\right]$.

$$H(N, n) = \left(\frac{1}{2} + \frac{1}{2}\right) \cdot \text{rand}(N, n) - \frac{1}{2} \quad (1)$$

Once our set of points is organized into a matrix, calculation of the pairwise distances between each point becomes an easy task. In mathematics, regardless of the number of dimensions, the distance between each point is calculated by taking the square root of the total sum of each coordinate difference squared. This is a property that can be generalized by the equation below, with D_{ij} being the distance between any two points, i and j , in the set of H .

$$D_{ij} = \sqrt{\sum_{k=0}^n (H_{ik} - H_{jk})^2} \quad (2)$$

Since we want the pairwise distances for all given points on our set, a matrix in which each point is compared to one another is exactly what we want to use. By using simple `for()` loops in Matlab, we can script a program that cycles through all coordinates and calculates the distance between them, resulting in a matrix of size N by N that contains the pairwise distances between every single point. Then, while plotting the histogram, we simply need to omit any zero values that were calculated from a point comparing to itself, which is easily solved by utilizing Matlab's `nonzeros()` function. Once plotted, we end up with the histogram similar to the one below.

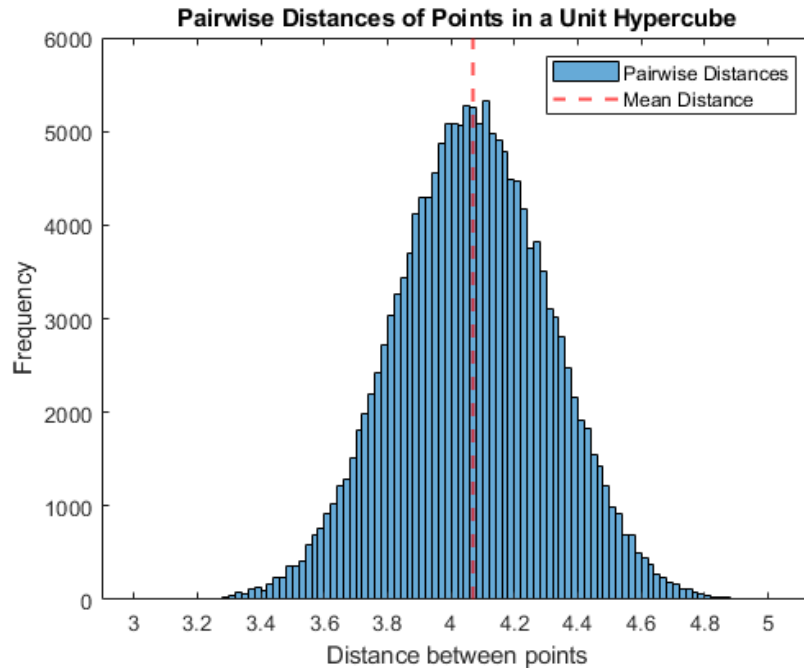


Figure 1: In higher dimensions, the mean distance between points is greater than the length of its domain.

The mean distance, represented by the red, dashed, vertical line, is easily calculable by dividing the total sum by the number of connected lines, representable by the equation below. Since self-referential points aren't counted as a line, the total number of lines is equal to our number of samples N multiplied by $N - 1$. The self-referential points have a distance equal to zero anyways, so their values aren't added when calculating the mean.

$$D_{avg} = \frac{\sum_{i=1}^N \sum_{j=1}^N D_{ij}}{N(N-1)} \quad (3)$$

For the histogram above, calculating the mean pairwise distance results in a value of 4.06852, which is far greater than the size of our specified domain. While a result like this might initially seem incorrect, a similar instance can already be found in both two and three dimensions. On a domain of $x \in [0, 1]$, the maximum possible distance between two points is equal to the square root of the dimension in which they are plotted, where the length in two dimensions and three dimensions is $\sqrt{2}$ and $\sqrt{3}$ respectively. So, in our unit hypercube of 100 dimensions, any length less than $\sqrt{100}$, and thus 10, is valid. Besides, since only a single square root is taken when determining distance regardless of dimension size, then having a larger sum inside the square root will only further increase the resulting value.

4.2 Mean Angle

While trying to find the angle between two vectors in either two or three dimensional space, it's always still possible fall back to the trusty protractor for answers. However, in higher dimensions, the inability for humans to intuit coordinates makes the previously handy dandy protractor completely useless. Fortunately, there exists a far more reliable method of calculating the angle between vectors, and it works not only in two and three dimensional space, but higher ones as well. That method is by using the definition of the dot product.

$$u = ||u|| ||v|| \cos(\theta) \quad (4)$$

↓

$$\theta = \cos^{-1} \left(\frac{u \cdot v}{||u|| ||v||} \right) \quad (5)$$

$$u \cdot v = u_1 v_1 + u_2 v_2 + \dots + u_n v_n \quad (6)$$

Since the dot product of two vectors is defined as the total sum of the products of each matching coordinate, then as long as two vectors have sets of equal length, the dot product between them can always be calculated. Then, since magnitude is simply a calculation of a vector's distance, we can find them by taking the square root of the sum of squared coordinates. To calculate all the pairwise angles found between vectors, we take a similar approach to how we calculated the pairwise distances between points, and that is by comparing all the vectors to one another and storing them in a matrix we'll label A. Since we're calculating vectors that extend from the origin, the coordinates from our existing set of points suffice for their values. While looping through all pairings of vectors, we take the dot product of each one and divide it by their multiplied magnitudes. Once we have this value, we take the inverse cosine of it to calculate our angles. For easier interpretation, the values were converted from radians to degrees.

$$A_{ij} = \cos^{-1} \left(\frac{H_i \cdot H_j}{\|H_i\| \|H_j\|} \right) \quad (7)$$

Now that we have our matrix of pairwise angles set up, we can actually calculate the mean angle in the exact same fashion we did for calculating the mean edge distance. To get our mean angle, we take the sum of all angles and divide it by the total number of pairings.

$$A_{avg} = \frac{\sum_{i=1}^N \sum_{j=1}^N A_{ij}}{N(N-1)} \quad (8)$$

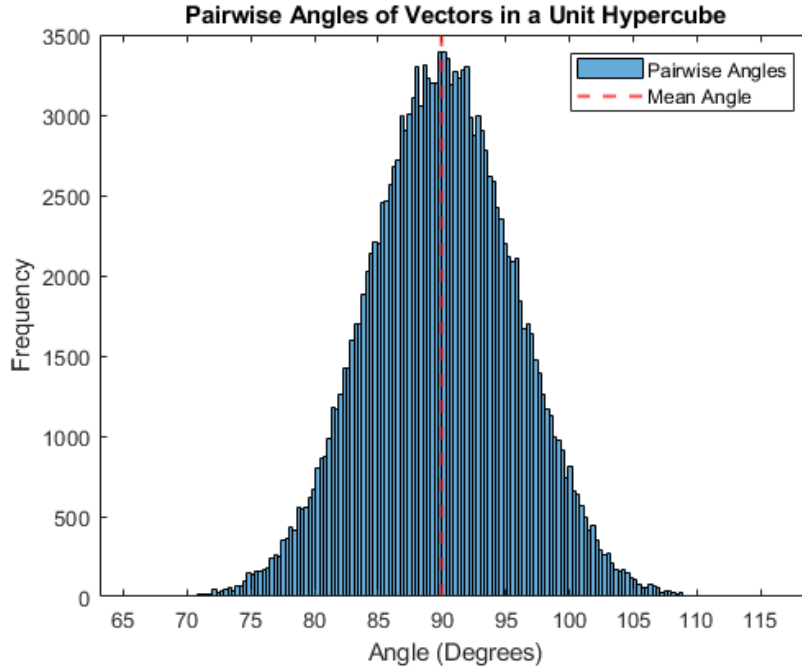


Figure 2: As the number of dimensions increases, the resulting range of pairwise angles tightens, but the mean angle stays roughly around 90° .

When calculating the mean angle of the data used in the histogram above, it gives us a value of 89.99856° . Given that the data nearly balances itself out on both sides of the histogram, it makes sense for the mean value to be close to 90° : an angle that lies directly in the middle of the domain of $\theta \in [0^\circ, 180^\circ]$. So, even though higher dimensions tightens the range of possible pairwise angles, the mean angle still stays close to the midpoint of the domain at 90° .

5 The Unit Ball in High Dimensions

In this section, we generate samples of points uniformly inside the unit ball in \mathbb{R}^n . This is equivalent to generating 10,000 vectors. If the norm of a given vector is less than one, we count it as inside the sphere.

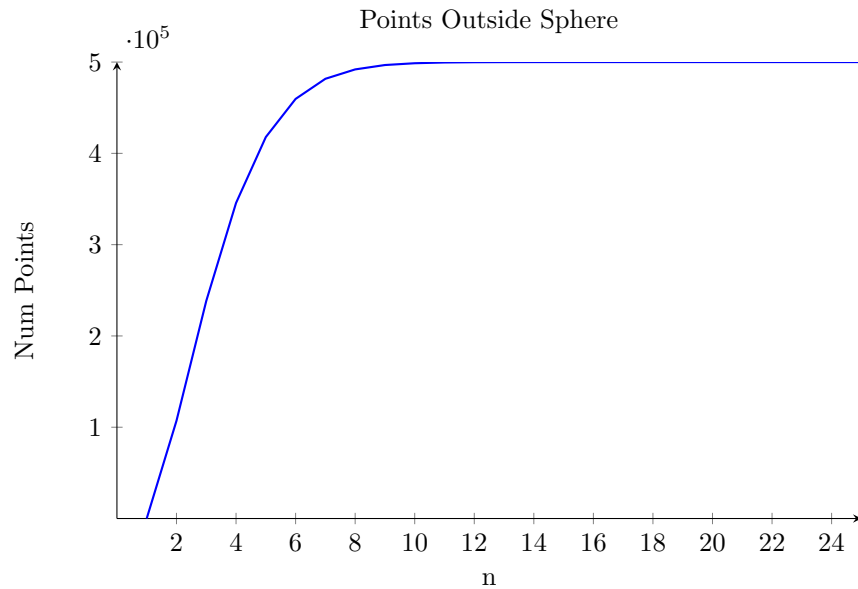


Figure 3: A plot of the number of points outside of the sphere as a function of dimension, n . The plot increases until $n=15$, at which point all of the points are outside of the sphere. We had a sample size of 500,000 points.

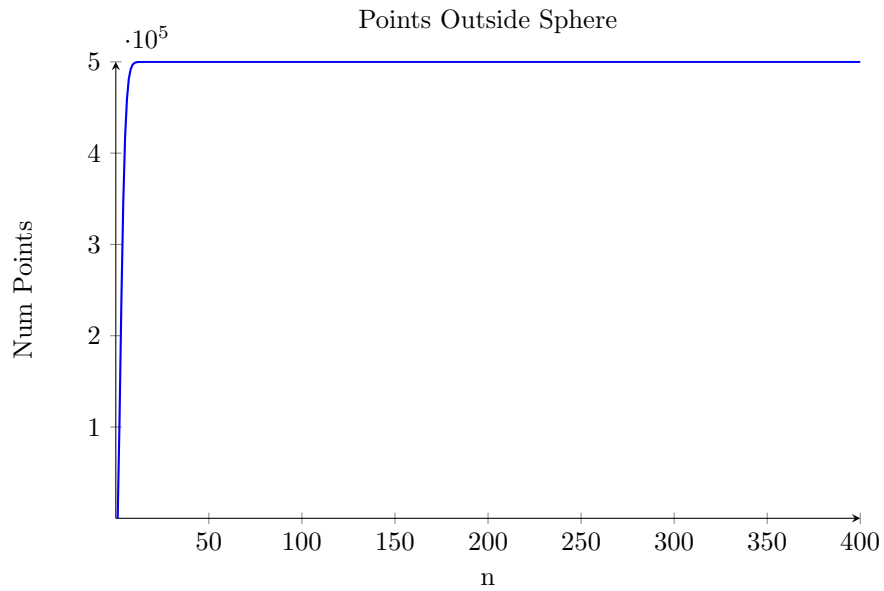


Figure 4: A plot of the number of points outside of the sphere as a function of dimension, n . The plot increases until $n=15$, at which point all of the points are outside of the sphere. We had a sample size of 500,000 points.

From the plot above, we show that the total number of points outside of the sphere increases as dimension increase. At $n=15$, all of the points are outside of the sphere, meaning that the volume of the sphere is zero.

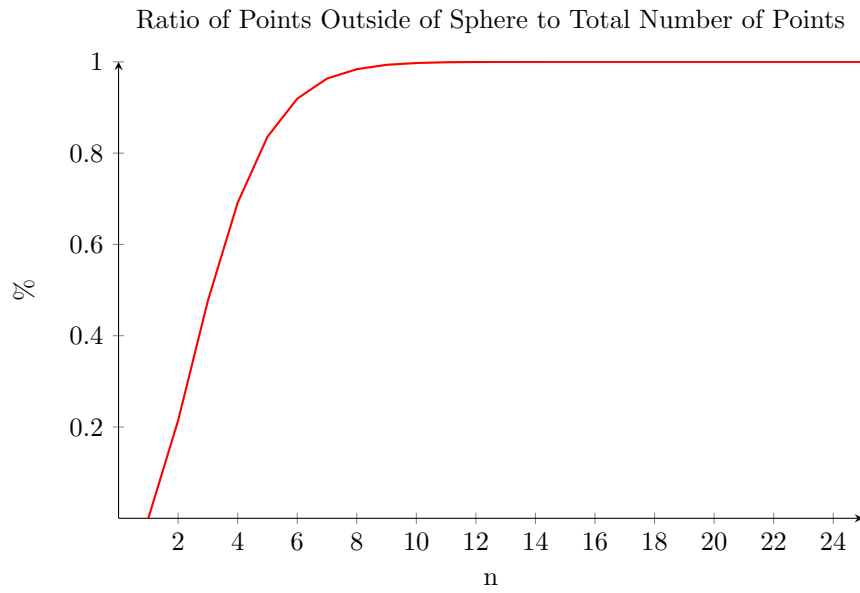


Figure 5: A plot of the number of points outside of the sphere as a function of dimension, n . The plot increases until $n=15$, at which point all of the points are outside of the sphere. We had a sample size of 500,000 points.

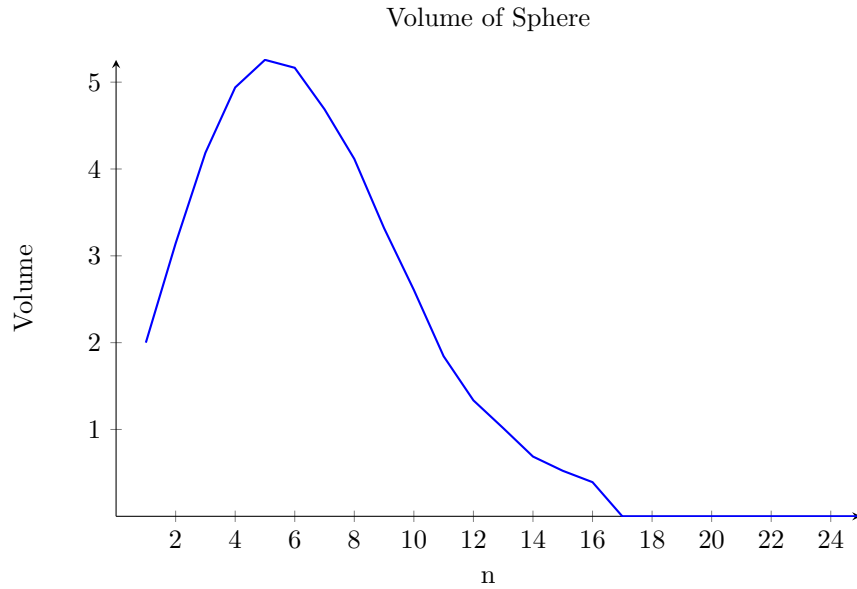


Figure 6: A plot of the volume of the sphere as a function of dimension. The volume of the sphere increases until $n=5$, and then decreases until $n=17$, at which point the volume of the sphere becomes zero.

Since the theoretical ratio and the Monte-Carlo approximation yield similar values, we conclude that the Monte-Carlo method is a practical method for finding the volume of a sphere in high dimensions.

6 Conclusion

In this project we worked through many steps to find an approximation for the theoretical ratio of the volume of the hyperball to the volume of the hypercube. We found that cubes in higher dimensions behave quite similarly to cubes in dimensions we can perceive. Both the theoretical calculations and the Monte-Carlo approximation predict that the volume of an n -dimensional unit sphere is zero as n goes to infinity. We conclude that the Monte-Carlo method is a very practical method for computing the volume of a sphere in high-dimension. This result holds for any convex body.