Estimating Using The Monte Carlo Simulation

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1 What is the Monte Carlo Estimation?

The Monte Carlo Simulation is a mathematical technique to estimate the possible outcomes of an uncertain event, using repeated random sampling to obtain numeral results. One of the basic and well-known example is to estimate the digits of pi using the Monte Carlo Simulation.

2 Estimating π at a 2D space

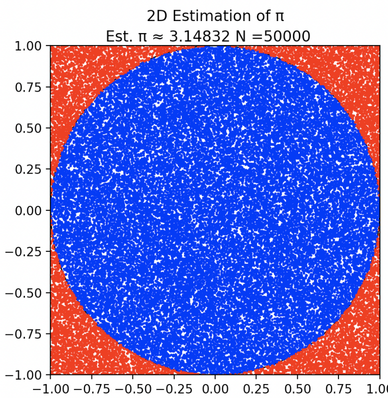
To estimate π at a Two-Dimensional Space, we would need to generate a square with $2r$ sides centering at $(0, 0)$). Within the region of the square, we will draw a circle with a radius of r, also centering at the origin $(0, 0)$. We will then generate many random points (x, y) with in the domain of the square. We then calculate the ratio of the points that lied inside the circle and the total points generated, and we would the ratio to estimate the digits of π.

The area of a square with $2r$ sides would be $4r^2$ and the area of the circle with a radius of r would be r^2. Thus, the ratio of the points that lied inside the circle and the total points generated would be:

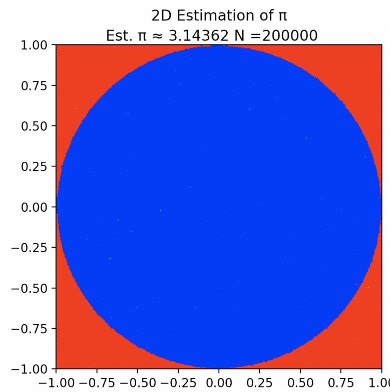
$$\frac{\pi r^2}{4r^2} = \frac{\pi}{4}$$

and π would be the ratio of points within the circle and the total of points generated $\times 4$.

Here is a visual representation of the 2D estimate with more than 200000 generated points (Figure 1). We can see that as more points are generated, the π estimation became more accurate, as the numbers diverged to the actual digits of π.



(a) 2D Estimation with 50000 points



(b) 2D Estimation with 200000 points

Figure 1: Comparison of 2D Estimation with different sample sizes (Click to see video)

3 Estimating π at a 3D space

After proving how we could estimate pi using the Monte Carlo Simulation in a two-dimensional surface, we wondered if the estimation also works in higher dimensions. We will determine if we could estimate π in a Three-Dimensional space using a unit sphere and a unit cube with a Monte Carlo Estimation.

First, we would need to evaluate the volume of a sphere and a cube. The cube is rather straightforward: given that the length of a cube is $2r$, the volume of the cube would become $(2r)^3$, being $8r^3$. The volume of the sphere could be found by using a triple integral with spherical coordinates with bounds on:

$$\begin{aligned}\rho &= [0, r]\\ \phi &= [0, \pi]\\ \theta &= [0, 2\pi]\end{aligned}$$

The integral expression would then be given as follows:

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{r} \rho^2 \sin(\phi)\, d\rho\, d\phi\, d\theta$$

By calculating the integral:

$$\begin{aligned}&= \int_0^{2\pi}\int_0^{\pi} \frac{\rho^3}{3}\bigg|_0^r \sin(\phi)\, d\phi\, d\theta\\ &= \int_0^{2\pi}\int_0^{\pi} \frac{r^3}{3} \sin(\phi)\, d\phi\, d\theta\\ &= \int_0^{2\pi} -\frac{r^3}{3}\cos(\phi)\bigg|_0^{\pi} d\theta\\ &= \int_0^{2\pi} \frac{2r^3}{3}\, d\theta\\ &= \frac{2r^3}{3}2\theta\bigg|_0^{2\pi}\\ &= \frac{4}{3}\pi r^3\end{aligned}$$

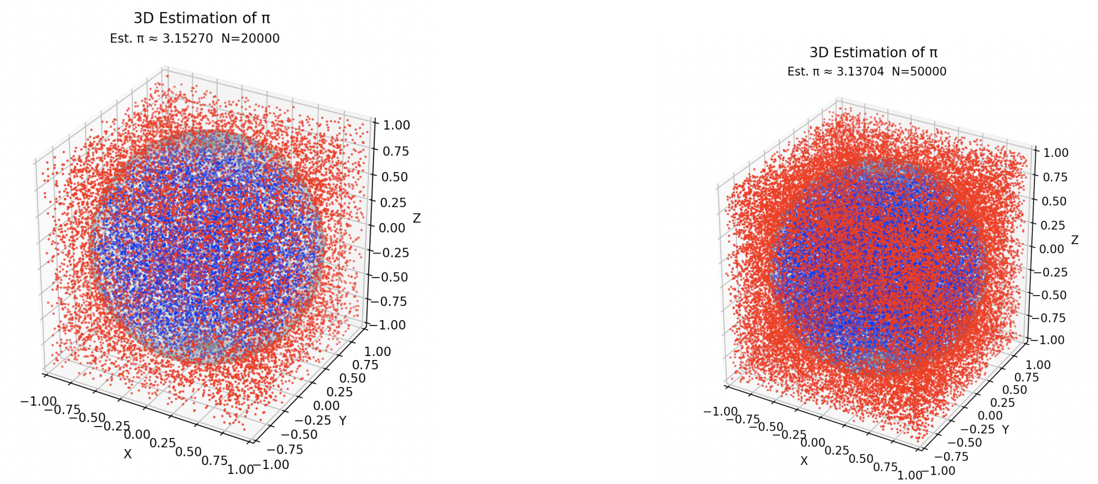
With the volume of a sphere with radius r, we can find the ratio between the sphere and the cube, which is:

$$\frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi r^3}{6r^3} = \frac{\pi}{6}$$

After knowing the ratio of the volume of a sphere with radius r and the volume of a cube with sides $2r$, we can use a unit sphere and a cube with radius 1 and sides 2, respectively. Thus, the ratio would be $\frac{\pi}{6}$, and π would equal the ratio $\times$ 6.

In theory, if we generate random points within the domain of a cube with sides 2, the ratio of the points that lay in the unit sphere and the total generated points would be $\frac{\pi}{6}$. To prove this, a computer program generated random points (x, y, z), $x, y, z \in [-1, 1]$, and calculated the ratio of the points that were within the sphere to the total generated points.

This is a visual representation of the Monte Carlo Estimation in a Three-Dimensional space (Figure 2).



(a) 3D Estimation with 20000 points

(b) 3D Estimation with 50000 points

Figure 2: Comparison of 3D Estimation with different sample sizes (Click image to see video)

4 Estimating π at a 4D space

Consider the n-sphere and a hypercube in both 4 dimensions. By finding both the volume of the hypercube and the n-sphere and finding the ratio of points as the amount of points approaches infinity, the theoretical equation for the Monte-Carlo estimation to find π can be found. For the volume of a hypercube, a quadruple integral of dx_1, dx_2, dx_3 and dx_4, the axis for the 4th dimension cube. To make calculations easier for the n-sphere that we will be integrating later, a hypercube of length $2r$ will be used. The equation for the volume of the hypercube can be considered as follows:

$$\int_0^{2r}\int_0^{2r}\int_0^{2r}\int_0^{2r} 1\, dx_1\, dx_2\, dx_3\, dx_4$$

The calculations of the integral are as follows:

$$\begin{aligned}
&= \int_0^{2r}\int_0^{2r}\int_0^{2r} x_1\Big|_0^{2r}\, dx_2\, dx_3\, dx_4 \\
&= \int_0^{2r}\int_0^{2r}\int_0^{2r} 2r\, dx_2\, dx_3\, dx_4 \\
&= \int_0^{2r}\int_0^{2r} 2rx_2\Big|_0^{2r}\, dx_3\, dx_4 \\
&= \int_0^{2r}\int_0^{2r} 2r^2\, dx_3\, dx_4 \\
&= \int_0^{2r} 4r^2x_3\Big|_0^{2r}\, dx_4 \\
&= \int_0^{2r} 8r^3\, dx_4 \\
&= 8r^3x_2\Big|_0^{2r} \\
&= 16r^4
\end{aligned}$$

By this, we have calculated the volume of the hypercube that we will be using for our Monte-Carlo estimation.

To find the volume of the n-sphere, a higher-dimensional form of the spherical coordinates needs to be used, where a new variable ϕ_2 is used to measure the degree of the higher dimension axis to Rho. The domain and range for ρ, ϕ, ϕ_2, and θ is as follows:

$$\begin{aligned} \rho &= [0, \infty) \\ \phi &= [0, \pi] \\ \phi_2 &= [0, \pi] \\ \theta &= [0, 2\pi] \end{aligned}$$

And that:

$$\begin{aligned} x_1 &= \rho \cos\phi \\ x_2 &= \rho \sin\phi \cos\phi_2 \\ x_3 &= \rho \sin\phi \sin\phi_2 \cos\theta \\ x_4 &= \rho \sin\phi \sin\phi_2 \sin\theta \end{aligned}$$

A new integral expression is also needed in order to find the volume of the sphere. Specifically, the determinant for the quadruple integral needs to be calculated in order to find the volume. This can be found with a Jacobian matrix with the partial derivatives of x_1, x_2, x_3, x_4 all terms of ρ, ϕ, ϕ_2 and θ. The reason for this is because the Jacobian matrix and determinant express the change of unit area as one switches from a coordinate, say Cartesian, to another coordinate, say spherical. After finding the change of the unit area, the quadruple integral would then sum up these units in spherical coordinates and therefore get the total volume of what we are trying to find. The Jacobian matrix equation is given as follows:

$$\frac{\partial(x_1, x_2, x_3, x_4)}{\partial(\rho, \phi, \phi_2, \theta)} = \begin{bmatrix} \frac{\partial x_1}{\partial \rho} & \frac{\partial x_1}{\partial \phi} & \frac{\partial x_1}{\partial \phi_2} & \frac{\partial x_1}{\partial \theta} \\ \frac{\partial x_2}{\partial \rho} & \frac{\partial x_2}{\partial \phi} & \frac{\partial x_2}{\partial \phi_2} & \frac{\partial x_2}{\partial \theta} \\ \frac{\partial x_3}{\partial \rho} & \frac{\partial x_3}{\partial \phi} & \frac{\partial x_3}{\partial \phi_2} & \frac{\partial x_3}{\partial \theta} \\ \frac{\partial x_4}{\partial \rho} & \frac{\partial x_4}{\partial \phi} & \frac{\partial x_4}{\partial \phi_2} & \frac{\partial x_4}{\partial \theta} \end{bmatrix}$$

By plugging in each partial derivative, the matrix becomes such:

$$\begin{bmatrix} \cos\phi & -\rho\sin\phi & 0 & 0 \\ \sin\phi\cos phi_2 & \rho\cos\phi\cos\phi_2 & -\rho\sin\phi\sin\phi_2 & 0 \\ \sin\phi\sin\phi_2\cos\theta & \rho\cos\phi\sin\phi_2\cos\theta & \rho\sin\phi\cos\phi_2\cos\theta & -\rho\sin\phi\sin\phi_2\sin\theta \\ \sin\phi\sin\phi_2\sin\theta & \rho\cos\phi\sin\phi_2\sin\theta & \rho\sin\phi\cos\phi_2\sin\theta & \rho\sin\phi\sin\phi_2\cos\theta \end{bmatrix}$$

After this, the determinant of the matrix needs to be found in order to find the determinant to the quadruple integral. In this step a matrix calculator was used, and the end result yields the following:

$$J(\rho, \phi, \phi_2, \theta) = \rho^3 \sin^2\phi \sin\phi_2$$

giving the determinant for the quadruple integral.

The quadruple integral for the volume of the n-sphere with radius r can be set up with 4-Dimension spherical coordinates:

$$\int_0^{2\pi} \int_0^{\pi} \int_0^{\pi} \int_0^{r} 1\, \rho^3 \sin^2\phi \sin\phi_2 \, d\rho \, d\phi \, d\phi_2 \, d\theta$$

Integrating this expression gives the formula for the volume of the n-sphere:

$$
\begin{aligned}
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{\pi} \frac{\rho^4}{4}\sin^2\phi\sin\phi_2\bigg|_0^r d\phi_2\, d\phi\, d\theta \\
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{\pi} \frac{r^4}{4}\sin^2\phi\sin\phi_2\, d\phi_2\, d\phi\, d\theta \\
&= \int_0^{2\pi}\int_0^{\pi} -\frac{r^4}{4}\sin^2\phi\cos\phi_2\bigg|_0^{\pi} d\phi\, d\theta \\
&= \int_0^{2\pi}\int_0^{\pi} \frac{2r^4}{4}\sin^2\phi\ d\phi\, d\theta \\
&= \int_0^{2\pi}\int_0^{\pi} \frac{2r^4(1-\cos 2\theta)}{8}\sin^2\phi\, d\phi\, d\theta \\
&= \int_0^{2\pi}\int_0^{\pi} \frac{r^4(1-\cos 2\phi)}{4}\, d\phi\, d\theta \\
&= \frac{r^4}{4}\int_0^{2\pi}\int_0^{\pi} (1-\cos 2\phi)\, d\phi\, d\theta \\
&= \frac{r^4}{4}\int_0^{2\pi} \phi - \frac{\sin 2\phi}{2}\bigg|_0^{\pi} d\theta \\
&= \frac{r^4}{4}\int_0^{2\pi} \pi\, d\theta \\
&= \frac{r^4}{4}\pi\theta\bigg|_0^{2\pi} \\
&= \frac{r^4}{2}\pi^2
\end{aligned}
$$

Finally, by finding the volume for both the n-sphere and the hypercube, the ratio of the points inside the n-sphere and the total amount of points as the points approach infinity can be found by dividing the volume of the n-sphere by the volume of the hypercube:

$$\frac{\frac{1}{2}r^4\pi^2}{16r^4} = \frac{\pi^2}{32}$$

Thus, to calculate π, we need to multiply the ratio by 32, and take the square root of it:

$$\pi = \sqrt{\frac{\pi^2}{32} \times 32}$$

To prove whether we can estimate π in a four-dimensional space, we will use computer programming to simulate random points (x, y, z, w) and determine whether the calculated ratio diverges into the digits of π.

Here, we coded a program using Python to estimate π in a four-dimensional space:

```python
        INTERVAL = 100
        circle_points = 0
        square_points = 0

        for i in range(INTERVAL**3):

        rand_x = random.uniform(-1, 1)
        rand_y = random.uniform(-1, 1)
        rand_z = random.uniform(-1, 1)
        rand_w = random.uniform(-1, 1)

        if rand_x**2 + rand_y**2 + rand_z**2 + rand_w**2 <= 1:
            circle_points += 1
        square_points += 1

        pi = math.sqrt(32 * inside_sphere / total_points)

        print("Final Estimation of Pi=", pi)
```

```
Final Estimation of Pi= 3.14640620390947
Final Estimation of Pi= 3.1443409484341864
Final Estimation of Pi= 3.142747842255245
Final Estimation of Pi= 3.1433230823445433
Final Estimation of Pi= 3.1432161872833375
Final Estimation of Pi= 3.141108084736977
Final Estimation of Pi= 3.1417905722692594
Final Estimation of Pi= 3.138193110692839
Final Estimation of Pi= 3.142666383821229
Final Estimation of Pi= 3.138432729882863
```

In the simulation, we generated random one million random points (x, y, z, w), $x, y, z, w \in [-1, 1]$. If the distance between the point and the origin ≤ 1, then the point is located in the unit hypercube that is located at the origin. However, if the distance between the point and the origin > 1, then the point isn't located in the unit hypercube.

With the data, we calculate the ratio of the points that remained within the hypercube and the total points generated and $\times 32$. Then, we take the square root to calculate the estimated digits of π.

Looking at the output of 10 simulations, all simulations have their π estimations within [3.13, 3.15], and the average of the 10 simulations is around 3.1422. The average result of the simulations is extremely close to the actual digits of π which is 3.1415.

As we calculate the percentage error:

$$\frac{|3.1422 - 3.1415|}{3.1415} = 0.000222 = 0.222\%$$

Thus, with a 0.222% error, we are confident that the digits of π can be estimated in a four-dimensional space using a unit hypersphere and a hypercube.

All in all, with the Monte Carlo simulation performed in both 3D and 4D, it is proven that this estimation technique is also possible with higher-dimension surfaces. With this, the Monte Carlo estimation could be applied into a greater field of studies such as estimating higher dimension surface areas or even giving insight into probability in higher dimensions. This research also poses new possibilities into determining π with the addition of higher dimensions.

References

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