Calculating mathematical constants with Monte Carlo simulations

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Department of Statistics
St. Xavier's College (Autonomous), Mumbai
by

Bhoris Dhanjal
Khushi Chauhan

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St. Xavier's College (Autonomous), Mumbai
Department of Statistics
Project by

Sr. No.	Name of Student	Class	UID	Roll No.
1	Bhoris Dhanjal	SYBSc	202020	314
2	Khushi Chauhan	SYBSc	202019	313

Title of the Project:
Calculating mathematical constants with Monte Carlo simulations

Declaration by the Student

We hereby declare that the project entitled "Calculating mathematical constants with Monte Carlo simulations" was completed and written by us is the result of original project work and has not formed earlier the basis for the certificate (any award) or similar title of this or any other school/college or examining body.

Date: July 10, 2021
Name and Signature of Student:

Bhoris Dhanjal

Khushi Chauhan

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Calculating mathematical constants with Monte Carlo simulations

Bhoris Dhanjal
Khushi Chauhan

July 10, 2021

Abstract

This project primarily serves to showcase Monte Carlo simulations. We first derive the crude Monte Carlo estimator for numerical integration. Following which we will use MC simulations to estimate a few well known mathematical constants. Quasi-Monte Carlo integration and importance sampling as methods of reducing integration variance will be examined at the end.

1 Introduction

In this project we will explore Monte Carlo simulations. The objectives of this project are as follows:

- Provide a conceptual overview of the Monte Carlo method.
- Describing and demonstrating a naive numerical MC integration algorithm.
- Using various MC simulations to calculate π, e, γ_n and, ϕ.
- Demonstrating Quasi-Monte Carlo integration and comparing it with naive numerical MC integration.

The Mathematica notebook (comprising of all code used for computations and plots) and LaTeX source code can be viewed at GitHub with the following link.
https://github.com/BhorisDhanjal/MonteCarloMathsConstants

2 Numerical Monte Carlo integration

In this section we will describe the algorithm for numerical Monte Carlo integration. Before this we will provide a short overview of the concept of Monte Carlo simulations.

2.1 Overview of Monte Carlo method

Monte Carlo simulations are a general class of computational algorithms that rely on random number sampling [1]. They are used to estimate numerical results for problems for which analytical solutions are either very difficult to obtain or impossible.

2.2 Naive Monte Carlo integration

We can demonstrate the theory behind naive [2] Monte Carlo integration in a simplified manner as below [1, 2].

Theorem 2.1. $\frac{1}{N}\sum_{i=1}^{N} f(X_i)$ *is an unbiased estimator for* $\int_\Omega f(x)\,dx$

For points $x = (x_1, x_2, \ldots, x_d)$ consider a function $f(x)$ over the unit hypercube ($\Omega = [0,1]^d$) in $\mathbb{R}^d$.

$$\mathcal{I}[f] = \int_\Omega f(x)\,dx$$

The approximation of $\mathcal{I}[f]$ is given by the expectation of $f(X)$ for some uniformly distributed random variable X.

$$\mathcal{I}[f] = E[f(X)] = E$$

Where an estimation for expectation is given by the sample mean,

$$\widehat{\mathcal{I}} = \frac{1}{N}\sum_{i=1}^{N} f(X_i)$$

By the Law of Large numbers [3] we can state that,

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} f(X_i) \to \mathcal{I}[f]$$

[1] Note that for the majority of this project we will be utilizing pseudo-random numbers.

[2] We call it "naive" since it utilizes uniformly distributed random variates, more sophisticated methods are discussed in the last section of this project.

Furthermore we can state that $\widehat{\mathcal{I}}$ is an unbiased estimator since $E[\widehat{\mathcal{I}}] = \mathcal{I}[f]$ for all N

Therefore, we can estimate $\mathcal{I}[f]$ with,

$$\mathcal{I}[f] \approx \widehat{\mathcal{I}} = \frac{1}{N}\sum_{i=1}^{N} f(X_i) \qquad \square$$

In general, for a function $f(x)$ over any volume V in $\mathbb{R}^n$ we can say [4],

$$\mathcal{I}[f] = \int_V f(x)\, dx \approx V\frac{1}{N}\sum_{i=1}^{N} f(X_i) \tag{2.1}$$

We can simplify the above expression for the case of a one dimensional integral over some closed interval $[a, b]$ where $a, b \in \mathbb{R}^1$ as,

$$\int_a^b f(x)\, dx \approx (b-a)\frac{1}{N}\sum_{i=1}^{N} f(X_i) \tag{2.2}$$

2.3 Error of Naive Monte Carlo integration

Theorem 2.2. *The standard error of the estimator is inversely proportional to the square root of random points chosen.*

Consider the variance for above described estimator $\widehat{\mathcal{I}}$,

$$\begin{aligned}
\sigma^2_{\widehat{\mathcal{I}}} &= \sigma^2\left(\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right) \\
&= \frac{1}{N^2}\sigma^2\left(\sum_{i=1}^{N} f(X_i)\right)
\end{aligned}$$

Since X_i are uniformly distributed random variables, we can say they are independent. Therefore, the variance of the sum is the same as the sum of the variance.

$$\begin{aligned}
&= \frac{1}{N^2}\sum_{i=1}^{N} \sigma^2(f(X_i)) \\
&= \frac{1}{N^2} N\sigma^2_{\mathcal{I}} \\
\sigma^2_{\widehat{\mathcal{I}}} &= \frac{\sigma^2_{\mathcal{I}}}{N} \\
\sigma_{\widehat{\mathcal{I}}} &= \frac{\sigma_{\mathcal{I}}}{\sqrt{N}} \\
\sigma_{\widehat{\mathcal{I}}} &\propto \frac{1}{\sqrt{N}} \qquad \square
\end{aligned}$$

This implies that, in naive Monte Carlo integration, reducing the error by half requires increasing the number of random points by a factor of 4.

We will explore variable reduction methods (i.e. quasi-random Monte Carlo, importance sampling etc.) in the last section of this project. For the rest of this project however, we will only utilize naive Monte Carlo integration that we implement using pseudo-random numbers.

2.4 An example of naive Monte Carlo Integration

In order to better motivate Monte Carlo integration we will provide a simple visualization.

Example 1. Estimating $\int_2^5 100 - 8x^2 + x^3 \, dx$ with 5 random points.

We begin by generating 6 random real numbers between 2 and 5. We will evaluate these points in $f(x) = 100 - 8x^2 + x^3$ and plot it.

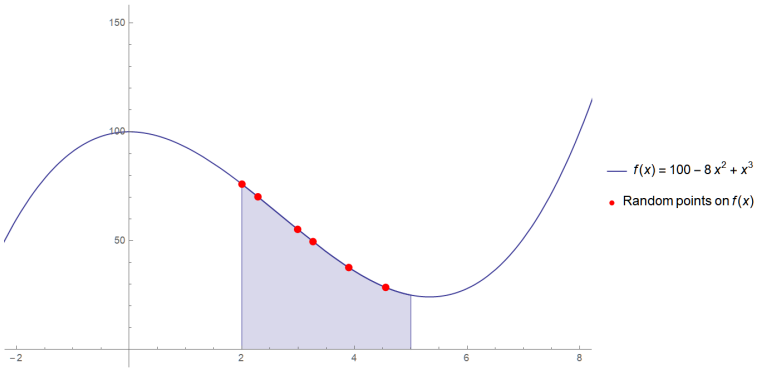

Figure 1: The plot of f(x) and 6 random points plotted on it.

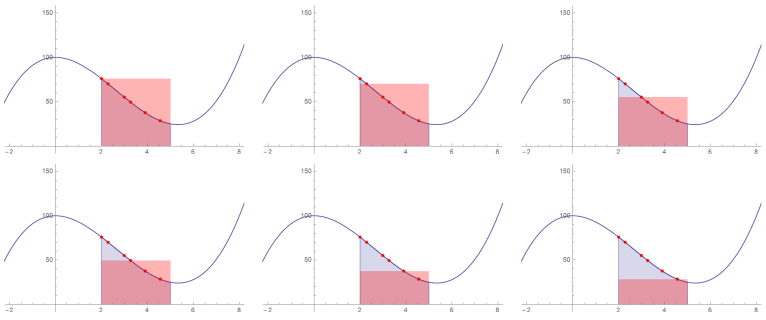

Figure 2: Rectangles of width $(b - a)$ with height corresponding to the random points.

Recall eq. 2.2, the multiplication of the $(b - a)$ term can be visualized as rectangles of width $(b - a)$ as above. It is now clear to see that taking the mean of these rectangle areas will give us an approximation to the integral that improves with the addition of more points.

3 Estimating Pi

In this section we will discuss the concepts of the Monte Carlo technique for estimating the value of pi(π).

3.1 Elementary Method

In order to estimate the value of pi using Monte Carlo simulations we will estimate the area of a unit circle inscribed in a unit square.

The experiment is conducted by taking random sample points in the region of the unit square. For an unbiased estimator of area of the circle it is assumed that the random sample points are uniformly distributed.

The bounding box area is $A_{box} = r^2 = 1$ and the area of the unit circle inscribed in the square is $A_{circle} = \pi r^2 = \pi$. With N_{box} total sample points and N_{circle} is the total sample points lying inside the unit circle.

Since the sample points are uniformly distributed within the bounding box, the ratio of the circle to the area of the bounding box is approximately equal to the ratio of the number of sample points falling in the circle to the number of points falling in the bounding box.

$$\frac{A_{pi}}{A_{box}} = \frac{\pi r^2}{r^2} = \pi \approx \frac{N_{pi}}{N_{box}} \tag{3.1}$$

An example of a single experiment is shown below.

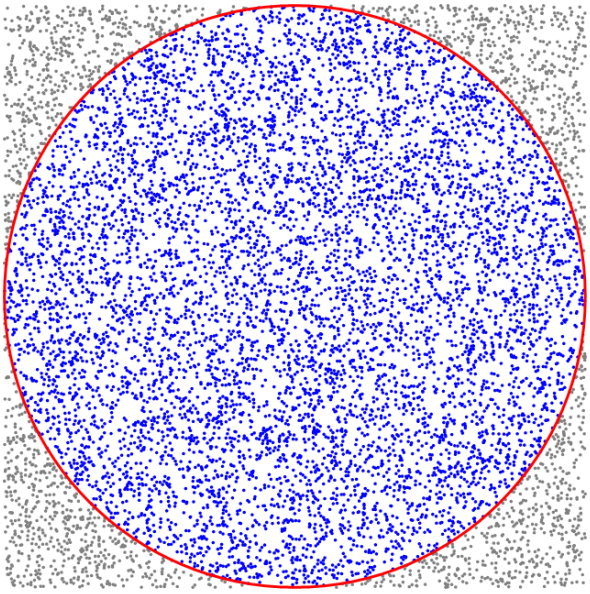

Figure 3: Experiment with 10,000 points, $N_{pi}/N_{box} = 3.1512$

We now repeat the experiment 10^3 times with 10^6 points. Taking the mean of these 10^3 experiments gives us the following approximation. $\pi \approx 3.14154 \pm 0.00165$, with $-1.696 \cdot 10^{-3}$ % error.

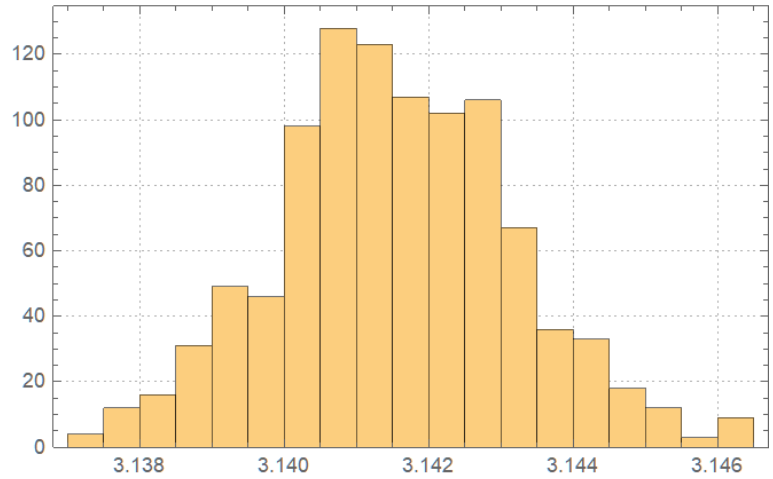

Figure 4: Histogram of experiment with 10^6 points, repeated 10^3 times.

3.2 Buffon's Needle

"A large plane area is ruled with equidistant parallel lines, the distance between two consecutive lines of the series being a. A thin needle of length $l < a$ is tossed randomly onto the plane. What is the probability that the needle will intersect one of the lines?"

This forms the basis of the Buffon's Needle problem. Which can be solved using elementary integral calculus [5]. Based on this analytical solution, the experiment can be used to approximate π using Monte Carlo simulations.

Theorem 3.1. *The probability of a needle intersecting a line is given by* $p = \frac{2l}{a\pi}$.

For a given needle of length "l" we model the dropping of the needle on the ruled plane with parallel lines "a" units apart as follows.

Let x be the distance from the center of the needle to the nearest line and θ be the acute angle between the needle and the lines. Let x be a uniform random variable over the interval

The uniform probability density function of x between 0 and $\frac{t}{2}$ is

$$\begin{cases} \frac{2}{a} & 0 \leqslant x \leqslant \frac{a}{2} \\ 0 & \text{otherwise} \end{cases}$$

and θ a uniform random variable over the interval $\left(0, \frac{\pi}{2}\right)$ with the probability density function:

$$\begin{cases} \frac{2}{\pi} & 0 \leqslant x \leqslant \frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases}$$

The two random variables, x and θ, are independent Therefore the joint probability density function of (x, θ)

$$\begin{cases} \frac{4}{a\pi} & 0 \leqslant x \leqslant \frac{a}{2} \text{ and } 0 \leqslant x \leqslant \frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases}$$

for the short needle case $(l \leqslant a)$ A needle intersects a line if

$$\left(x \leqslant \frac{l}{2} \sin\theta\right)$$

The probability that the needle will intersect a line is

$$p = \int_0^{\frac{\pi}{2}} \int_0^{\frac{l}{2}\sin\theta} f(x,\theta)\, dx\, d\theta = \int_0^{\frac{\pi}{2}} \int_0^{\frac{l}{2}\sin\theta} \frac{4}{a\pi}\, dx\, d\theta = \frac{2l}{a\pi}$$

$$p = \frac{2l}{a\pi} \qquad \square$$

The p value can be estimated through Buffon's needle experiment. If the experiment contains n needles and there are m needles intersect lines, then the probability p can be estimated by the proportion

$$\widehat{p} = \frac{m}{n}$$

π can therefore be estimated by

$$\widehat{\pi} = \frac{2nl}{ma} \tag{3.2}$$

An example of a single experiment with 1000 needles is shown below. We then repeat the experiment 10^3 times with 10^6 needles. Taking the mean of these 10^3 experiments gives us the following approximation. $\pi \approx 3.14018 \pm 0.04510$, with $-4.481 \cdot 10^{-2}$ % error.

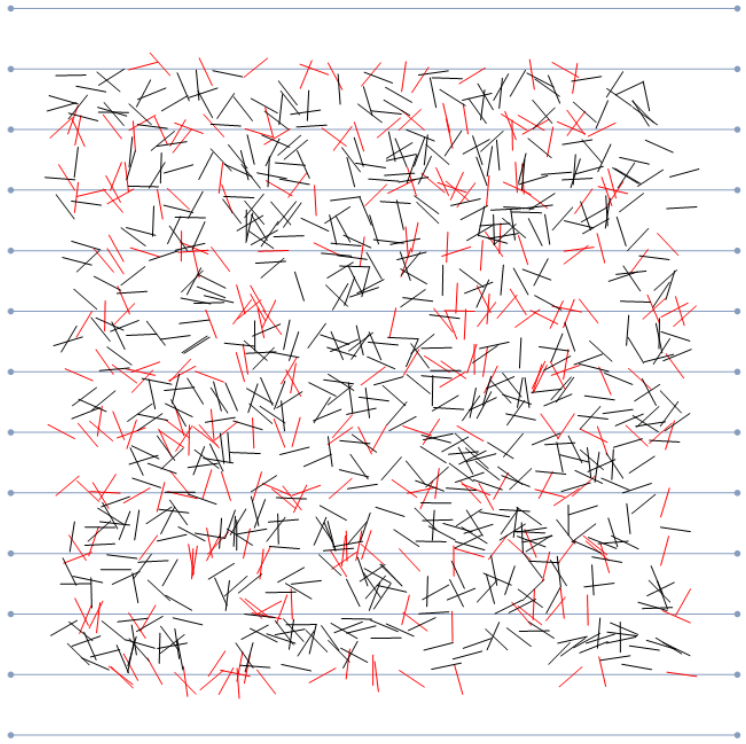

Figure 5: Experiment with 1000 needles, $\widehat{\pi} = 3.14465$

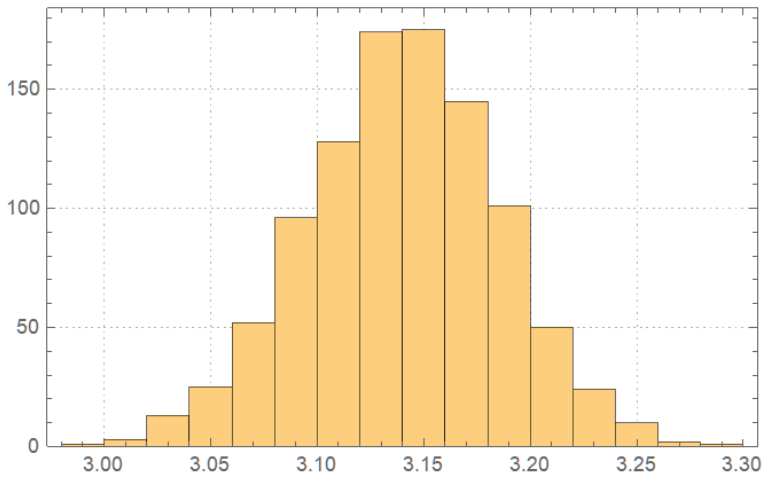

Figure 6: Histogram of Buffon's needle experiment with 10^4 needles, repeated 10^3 times.

3.3 Buffon's Noodle

In this case we will estimate π using Buffon's noodle problem. Buffon's noodle poses the question, "What is the expected number of crossings if we don't drop rigid needles but rather a flexible noodle?".

For straight needle N there are exactly n line crossing for exactly n intersection of needles with the infinite grid giving us the expectation of line crossing as $E(N) = \frac{2a}{\pi d}$. where a is the length of needle. using the corollary of this result that E(N) is a function of the length of the needle only, not its shape [6].

Theorem 3.2. *Let N be a noodle of length 't' thrown at random onto an infinite grid of parallel lines with common distance d between them. Then the expected number of line-crossings E(N) is given by E(N) =* $\frac{2t}{\pi d}$.

We remark that our definition of line-crossing demands that we count as distinct crossings in the event that the noodle crosses the same line in different places In general if a needle intersects n times in m attempts, then a combination of "a" such needles is expected to be intersected "na" times in m attempts If this combination is formed by infinitesimally small needles , then it will become noodle

Lets choose a sequence of polygonal lines L_1 L_2,$\cdots$ that approaches the curve N uniformly. The segments of the line L_i we shall denote as L_i1, L_i2, $\cdots$, L_in and we shall write $L_i = L_i1 + L_i2 + \cdots + L_in$ letting a_ij be the length of L_{ij} such that $a_{ij} < d$ for all i and j so that e(L_ij) is just the probability that L_ij crosses a line, e(L_ij) =$2a/\pi d$ Now letting a_i be the length of L_i, we know that a_i approaches a as i tends to infinity. Hence, if $e(L_i) = e(L_j) + \cdots + e(L_n)$for all i, then

$$e(L_i) = \sum(2a_i/\pi d) = (2/\pi d)\sum(a_ij) = (2/\pi d)a_i \tag{3.3}$$

hence in the limit

$$e(N) = \frac{2a}{\pi d} \tag{3.4}$$

3.3.1 A note on the simulation of noodles

Simulating a "noodle" isn't very straightforward computationally, since "noodles" aren't very well defined. We choose to simulate it by considering a line of length l divided into a random number of segments (between 5 and 10), and then randomizing the angles between the segments. One could also choose the make smooth noodles, by using bezier curves instead.

An example of a single experiment with 1000 noodles is shown below. We now repeat the experiment 250 times with 10^4 noodles. Taking the

mean of these 250 experiments gives us the following approximation. $\pi \approx 3.18615 \pm 0.04602$, with $+1.418\ \%$ error.

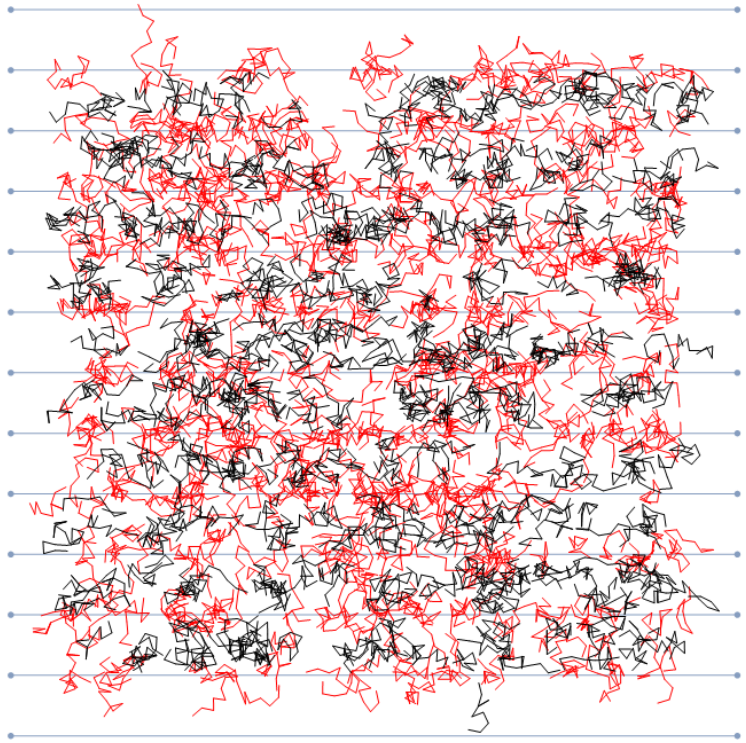

Figure 7: Experiment with 1000 noodles, $\widehat{\pi} = 3.36984$

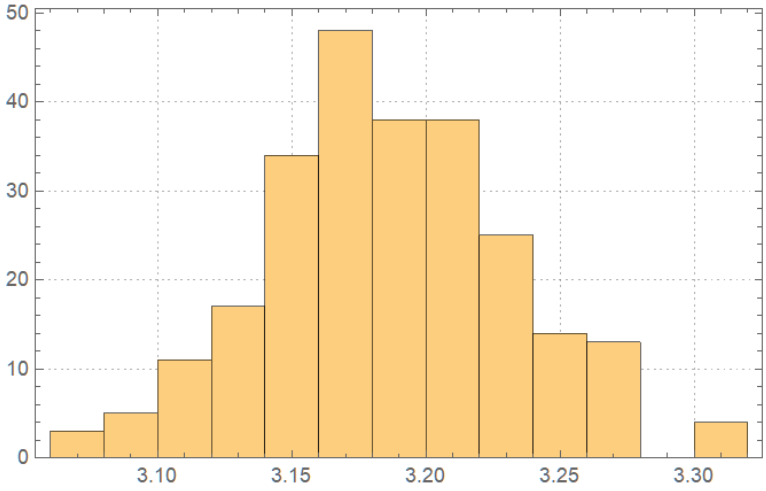

Figure 8: Histogram of Buffon's noodle experiment with 10^4 needles, repeated 250 times.

4 Estimating Euler's number

If $U_1, U_2 \cdots U_n$ are some independent and uniformly distributed random variables over (0,1). Let $S_n = \sum_{i=1}^{n} U_i$ and if N is the minimum value of n for which $S_n > 1$. The expectation of N is in fact equal to e.

This problem originated from as a exercise from a famous Russian textbook by Gnedenko [7]. For this section we will be drawing from two papers written by K. G. Russel on this topic [8, 9].

Theorem 4.1. *For iid uniform r.v. $U_1, U_2 \cdots U_n$ over (0,1), with $S_n = \sum_{i=1}^{n} U_i$ and if N is the minimum value of n for which $S_n > 1$, then $E[N] = e$.*

Note that our goal is to show that

$$E[N] = \sum_{n=2}^{\infty} nP(N = n) = e \tag{4.1}$$

If we can show that $P(N = n) = \frac{n-1}{n!}$, then we are done. Hence we continue as follows,

$$\begin{aligned} P(N = n) &= P(S_n > 1 \cap S_{n-1} < 1) \\ &= P(S_n > 1)P(S_{n-1} < 1) = P(S_{n-1} < 1) - P(S_n < 1) \end{aligned}$$

We have further simplified our problem, now all that remains is to show that $P(S_n < 1) = \frac{1}{n!}$. This would complete the proof. We use the CDF of the Irwin-Hall distribution [10].

The Irwin-Hall distribution is simply defined as, the sum of n independent and identically distributed, uniform distributions defined on the unit interval. The CDF of Irwin-Hall distribution is given as [3],

$$F(x) = \frac{1}{n!} \sum_{k=0}^{\lfloor x \rfloor} (-1)^k \binom{n}{k} (x - k)^n$$

For x=1

$$F(1) = P(S_n < 1) = \frac{1}{n!} \sum_{k=0}^{1} (-1)^k \binom{n}{k} (1 - k)^n = \frac{1}{n!} \qquad \square$$

The astute reader may ask what is $E[N]$ if we consider $S_n > a$ for any real number a? This general form is answered in the paper by Russell [9].

[3] This can be derived by integrating the pdf, which is in turn derived by induction by taking the convolution of $f_n * f$ to prove the $n + 1^{th}$ case.

We now continue with the simulation to predict e by choosing 10^6 random uniform numbers between (0,1) and counting the average number of times it takes for the sum to cross 1.

We now repeat the experiment 10^4 times with 10^6 numbers per experiment. Taking the mean of these 10^4 experiments gives us the following approximation. $e \approx 2.71827 \pm 0.00087$, with $-3.405 \cdot 10^{-4}$ % error.

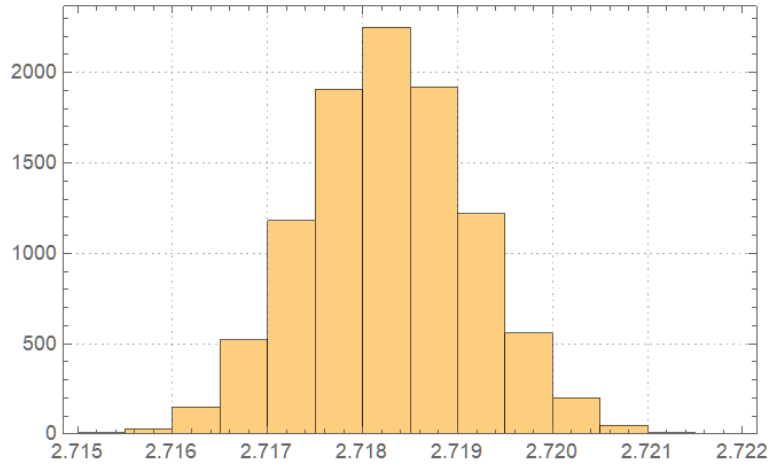

Figure 9: Histogram of e experiment with 10^6 numbers, repeated 10^4 times.

5 Estimating Euler-Mascheroni constant and Stieltjes constants

We begin this section by defining the Euler-Mascheroni constant and Stieltjes constants.

The Euler Mascheroni Constant (γ) is defined as the limiting difference between the harmonic series and the natural logarithm, i.e.

$$\begin{aligned} \gamma &= \lim_{n\to\infty} (H_n - \log n) \\ &= \lim_{n\to\infty} \left(\sum_{k=1}^{n} \frac{1}{k} - \log n \right) \end{aligned} \tag{5.1}$$

Stieltjes constants can be thought of as a generalization of the Euler-Mascheroni constant, defined as,

$$\gamma_n = \lim_{m\to\infty} \left(\sum_{k=1}^{m} \frac{(\log k)^n}{k} - \frac{(\log m)^{n+1})}{n+1} \right) \tag{5.2}$$

It is clear to see that $\gamma_0 = \gamma$. It is interesting to note that Stieltjes constants were originally discovered in the Laurent series expansion (about 1) of the Riemann Zeta function [11].

$$\zeta(z) = \frac{1}{z-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n (z-1)^n$$

We can in fact further generalize Stieltjes constants by considering the Laurent series of the Hurwitz-Zeta function instead of Riemann zeta. However, we will not further examine this.

5.1 Euler-Mascheroni constant

We will estimate the Euler-Mascheroni constant by first approximating the Gumbel distribution [12].

The Gumbel distribution accepts two parameters, α and β. It is defined by the following probability density function,

$$\begin{aligned} P(x) &= \frac{1}{\beta} e^{\frac{x-\alpha}{\beta} - e^{\frac{x-\alpha}{\beta}}} \\ &= \frac{1}{\beta} \exp\left(\frac{x-\alpha}{\beta} - \exp\left(\frac{x-\alpha}{\beta}\right)\right) \end{aligned}$$

and the following cumulative distributive function,

$$F(x) = 1 - \exp\left(-\exp\left(\frac{x-\alpha}{\beta}\right)\right)$$

It can be seen using integral representation of γ that the mean of the Gumbel distribution is,

$$\mu = \alpha - \gamma\beta$$

Our goal is therefore to simulate a Gumbel distribution with parameters $\alpha = 0$ and $\beta = -1$. The mean of this would therefore be γ.

We simulate the Gumbel distribution by using its quantile function (i.e. inverse CDF).

Calculating the inverse function for F(x) with $\alpha = 0, \gamma = -1$ we get.

$$Q(p) = \log\left(-\log\left(p\right)\right) \tag{5.3}$$

Where p takes values between 0 and 1. Taking n random points p between 0 and 1, and taking the mean of their respective $Q(p)$ we approximate γ.

Taking 10^6 points and repeating the experiment 10^4 times gives us the following approximation $\gamma \approx 0.57721 \pm 0.00128$. With $-4.824 \cdot 10^{-4}\%$ error.

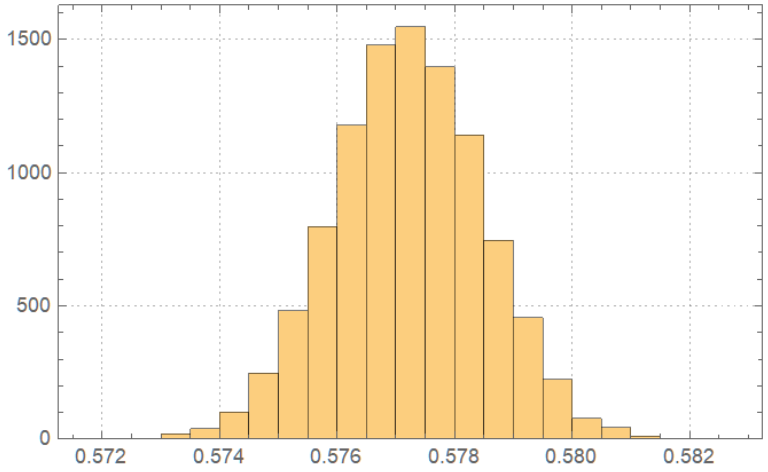

Figure 10: Histogram of experiment with 10^6 points, repeated 10^4 times.

5.2 Stieltjes constants

Calculating Stieltjes constants is not a trivial task, there exist many infinite series representations of Stieltjes constants which converge very slowly [11] (see eq.12). Extensive work has also been done in implementing fast algorithms to compute Stieltjes constants with high accuracy [13].

We will approximate a few Stieltjes constants by estimating the following integral definition.

$$\gamma_n = \frac{(-1)^n n!}{2\pi} \int_0^{2\pi} e^{nix} \zeta(e^{ix} + 1)\, dx \tag{5.4}$$

The above integral is derived by using Cauchy's differentiation formula on

$$(-1)^n \gamma_n = \frac{d^n}{dz^n} \left(\zeta(z) - \frac{1}{z-1} \right) \Bigg|_{z=1}$$

which is in turn derived by comparing the Laurent series of the Zeta function with a traditional Taylor series.

The reader should note that calculating Stieltjes constants with Monte Carlo integration is not at all practical due to the low accuracy. For practical approximations other forms of numerical integration techniques are used [13, 14].

We will estimate eq. 5.4 using the crude Monte Carlo integration described in the first section. The following table shows the results we achieved.

γ_n	No. of points chosen	No. of times repeated	Mean and Standard Deviation	Real values	Percentage Error
1	10^5	10^4	-0.0728663 ± 0.00258	-0.0728159	$-2.00069 \cdot 10^{-2}$
2	10^5	10^4	-0.00969426 ± 0.00524	-0.0096904	$+4.02199 \cdot 10^{-2}$
3	10^5	$1.5 \cdot 10^4$	$+0.00204329 \pm 0.01551$	$+0.0020538$	$-5.13216 \cdot 10^{-1}$
4	10^5	$3 \cdot 10^4$	$+0.00233049 \pm 0.06136$	$+0.0023253$	$+2.20283 \cdot 10^{-1}$

Table 1: Computed values of the first 4 Stieltjes constants (not including 0)

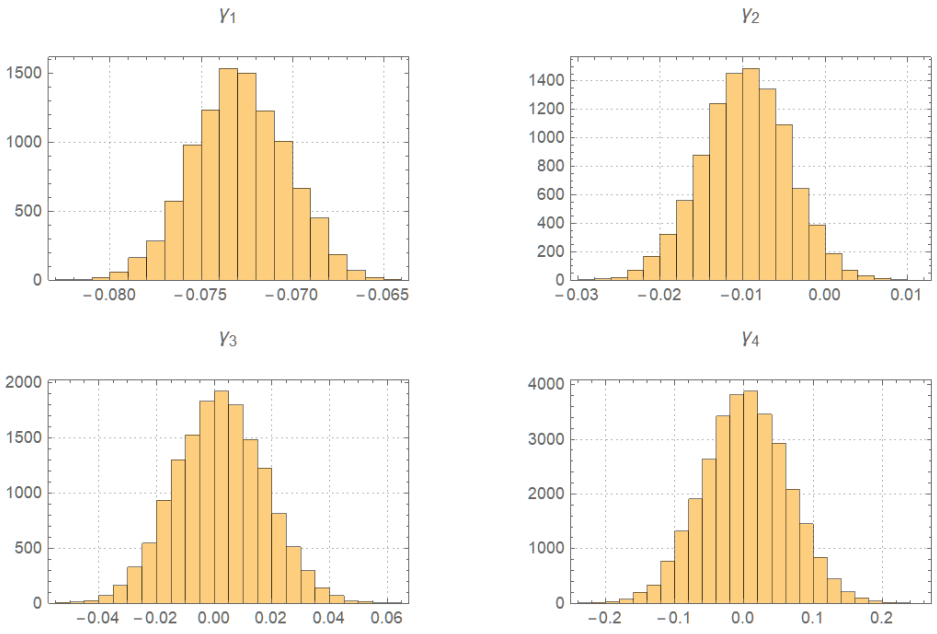

Figure 11: Histogram of the 4 experiments.

6 Estimating Phi

We conclude the estimation of mathematical constants on a lighter note.

Since φ is an algebraic number, estimating φ is very trivial. Since we know that $\varphi = \frac{1+\sqrt{5}}{2}$, we can simply choose an integral which evaluates to the desired result. We will choose $\int_4^5 \frac{3}{2} + \frac{1}{4\sqrt{x}}\, dx$ which is evidently equal to φ.

We estimate the integral with the method described in Section 1.

We repeat the experiment 10^4 times with 10^6 points per experiment. Taking the mean of these 10^4 experiments gives us the following approximation, $\varphi \approx 1.61803 \pm 3.79948 \cdot 10^{-}6$, with $6.544 \cdot 10^{-7}$ % error. In fact the approximation is correct up to 7 decimal places.

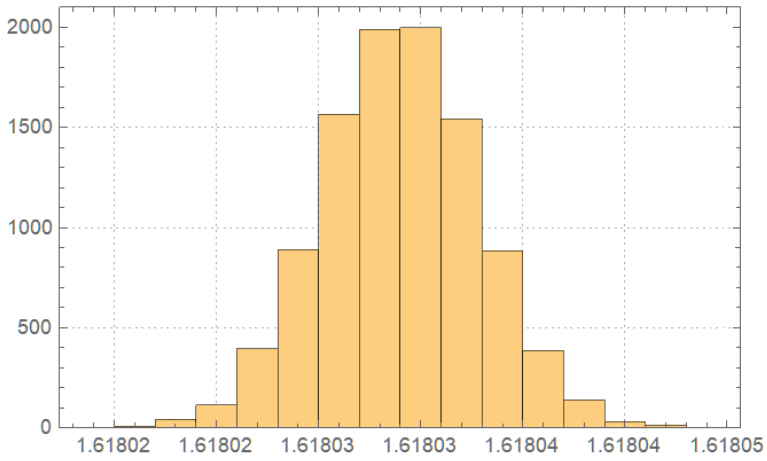

Figure 12: Histogram of experiment with 10^6 points, repeated 10^4 times.

7 Quasi-Monte Carlo integration

Throughout the project so far we have only considered what is known as "naive" Monte Carlo integration. We will now justify its nomenclature by listing out 2 modified methods of Monte Carlo integration that are so designed to reduce variability.

Quasi-Monte Carlo integration is simply, Monte Carlo integration using quasi-random generated numbers to form the integration nodes (as opposed to pseudo-random in naive integration) [15].

7.1 Quasi-random sequences (low-discrepancy sequences)

To make the above statement clearer, we will first define quasi-random numbers.

Quasi-random numbers are numbers generated from quasi-random sequences, which are in turn defined as sequences with low discrepancy [16].

8 Importance sampling

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