Calculating mathematical constants with Monte Carlo simulations

A project submitted to
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by

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Project by

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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.

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Abstract

This project primarily serves to showcase Monte Carlo simulations. We first derive the naïve Monte Carlo estimator for numerical integration. Following which we use Monte Carlo simulations to estimate a few well known mathematical constants. Variance reduction techniques and Quasi-Monte Carlo integration 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 naïve numerical Monte Carlo integration.
- Using various Monte Carlo simulations to calculate π, e, γ_n, ϕ, and $\zeta(3)$.
- Describing variance reduction techniques for Monte Carlo integration.
- Demonstrating Quasi Monte Carlo integration and comparing it with naïve numerical Monte Carlo integration.

The Mathematica notebook (comprising of all code used for computations and plots) and LaTeX source code for this document 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 naïve [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* $\int_{[0,1]^s} f(x)\ dx$

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

$$\mathcal{I}[f] = \int_{[0,1]^s} f(x)\ dx$$

The approximation of $\mathcal{I}[f]$ is given by the expectation of $f(x)$.

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

Let X_i denote iid uniformly distributed random variates over $[0,1]^s$. We estimate $\mathcal{I}[f]$ with the mean of the function evaluated at N uniformly distributed random points

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

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 "naïve" since it utilizes uniformly distributed random variates, more sophisticated methods are discussed in the last section of this project.

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

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

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

In general, for a function $f(x)$ over any domain Ω (open connected subset) in $\mathbb{R}^s$ we can say [4],

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

Where $\lambda_s(\Omega)$ denotes the s dimensional Lebesgue measure [5]. 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 Standard error of Naïve Monte Carlo integration

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

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

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

Since X_i are iid uniform r.v., the variance of the sum is equal to the sum of the variance.

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

$\square$

This implies that, in naïve 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 in the last section of this project. For the rest of this project however, we will only utilize naïve Monte Carlo integration that we implement using pseudo-random numbers.

2.4 An example of naïve 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.

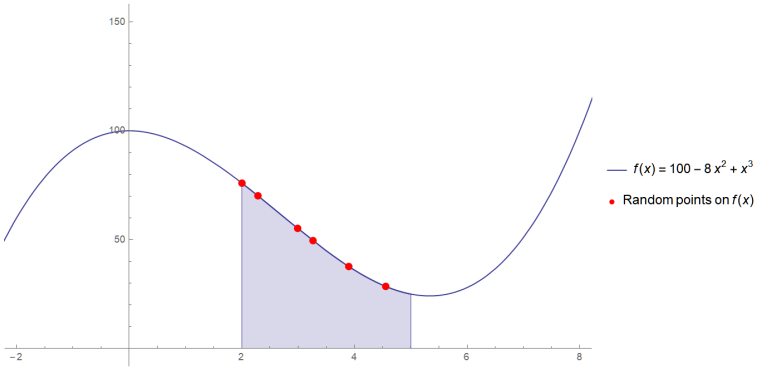

Figure 1: The plot of f(x) and 6 random points plotted on it.

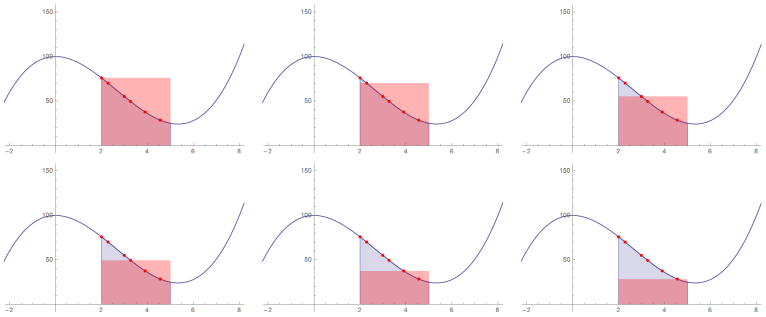

Figure 2: Rectangles of width $(b - a)$ with height corresponding to the random points.

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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 application of Monte Carlo techniques for estimating the value of pi.

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 $A_{\text{box}} = r^2 = 1$ and the area of the unit circle inscribed in the square is $A_{\text{circle}} = \pi r^2 = \pi$. 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.

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

An example of a single experiment is shown below.

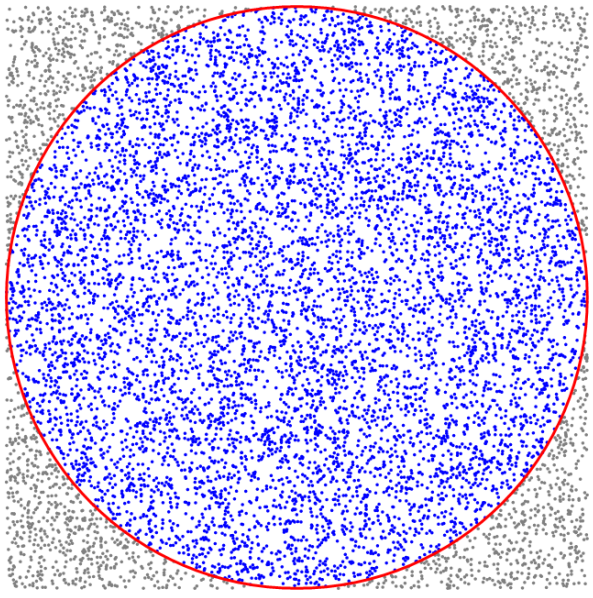

Figure 3: Experiment with 10,000 points, $N_{\text{circle}}/N_{\text{box}} = 3.1512$

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.

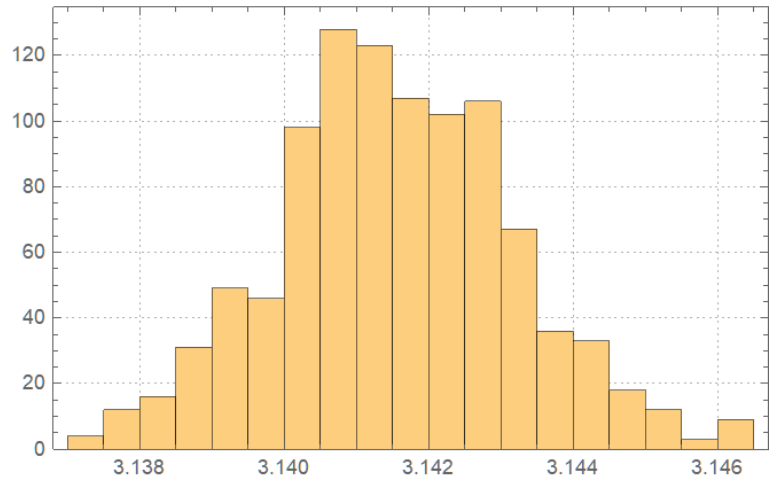

Figure 4: Histogram of experiment with 10^6 points, repeated 10^3 times.

3.2 Buffon's Needle

"A large plane area is ruled with equidistant parallel lines, the distance between two consecutive lines is '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 [6]. with the help of 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

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

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

If experiment has n needles out of which m needles intersect lines, then the value of p can be estimated as

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

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.

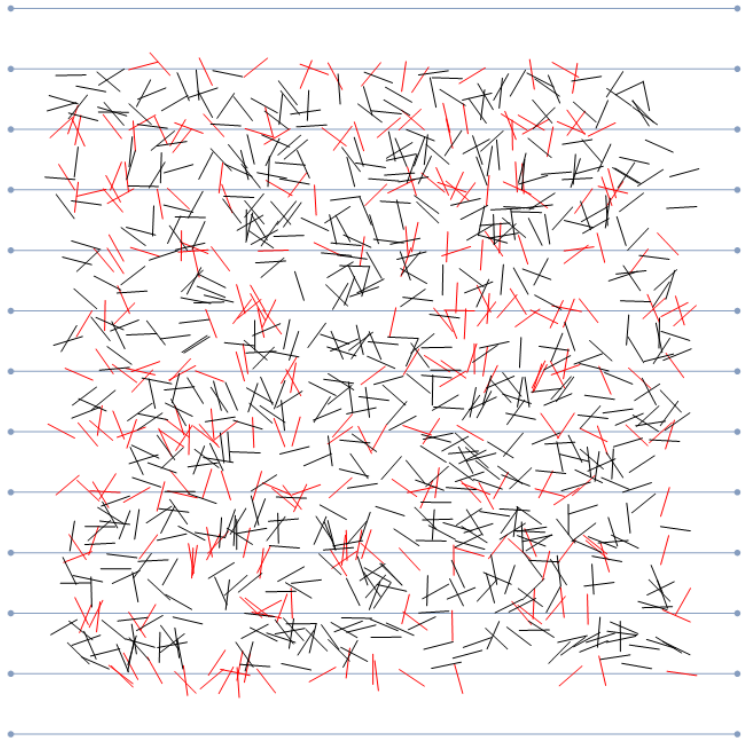

Figure 5: Experiment with 1000 needles, $\widehat{\pi} = 3.14465$

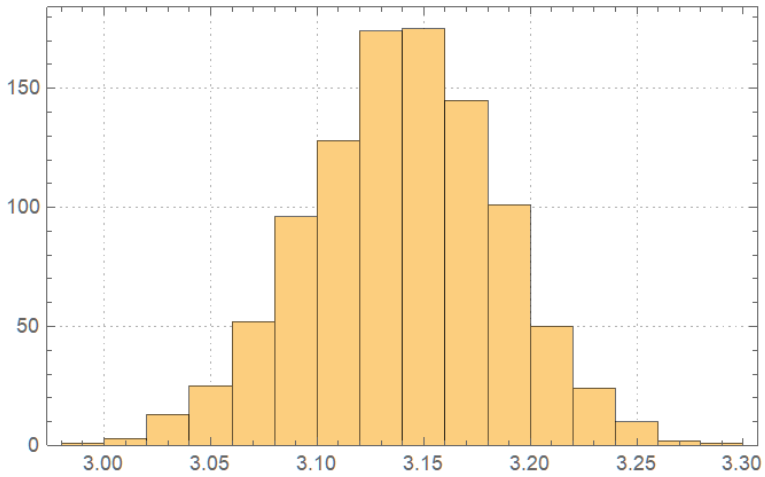

Figure 6: Histogram of Buffon's needle experiment with 10^4 needles, repeated 10^3 times.

3.3 Buffon's Noodle

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

For straight needle N there are n line crossing for n intersection of needles with the infinite grid and thus 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 [7].

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 take into consideration the fact that, a noodle due to its shape could cross a line in more than one spot. 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 equivalent to a noodle.

Consider a sequence of polygonal lines $L_1, L_2, \ldots, L_m$ which approaches the curve of the noodle N uniformly. Let $L_{i_1}, L_{i_2}, \ldots, L_{im}$ be the segments of the line L_i, such that $L_i = L_{i1} + L_{i2} + \cdots + L_{im}$. Let t_{ij} be the length of L_{ij} such that $t_{ij} < d$ for all i and j.

The expectation of line crossing the grid be E$[L_{ij}]$ hence E$[L_{ij}]$ =$2t/\pi d$ Now letting t_i be the length of L_i, we know that t_i approaches t as i tends to infinity. Hence, if $E[L_i] = E[L_j] + \cdots + E[L_n]$for all i, then

$$E[L_i] = \sum_{i=j}^{n} \frac{2t_i}{\pi d} = \frac{2}{\pi d} \sum_{i=j}^{n} t_i = \frac{2t}{\pi d} \tag{3.3}$$

hence in the limit

$$E[N] = \frac{2t}{\pi d} \qquad \square$$

3.3.1 A note on the simulation of noodles

Simulating a "noodle" isn't a very straightforward task computationally, since "noodles" aren't very well defined. Here, 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 a $+1.418$ % error.

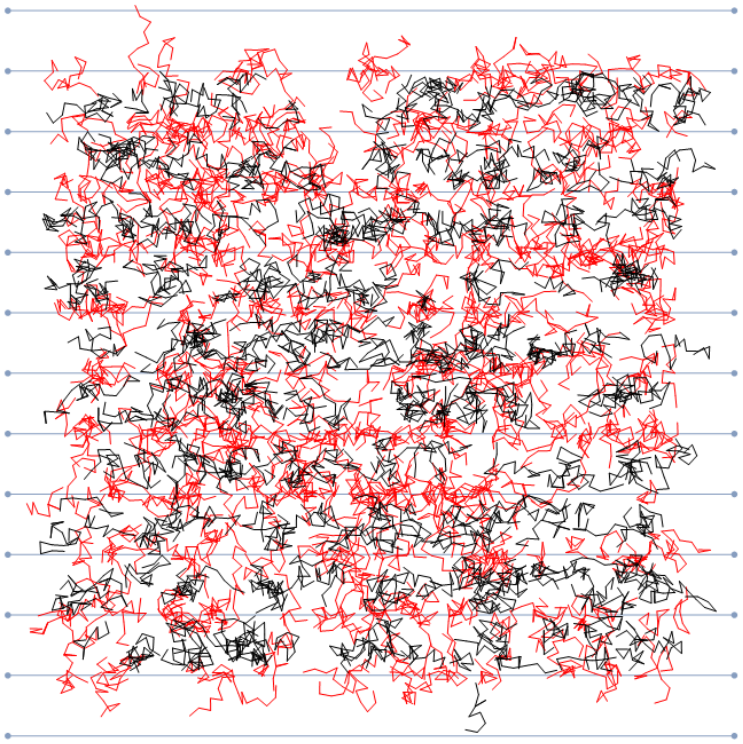

Figure 7: Experiment with 1000 noodles, $\widehat{\pi} = 3.36984$

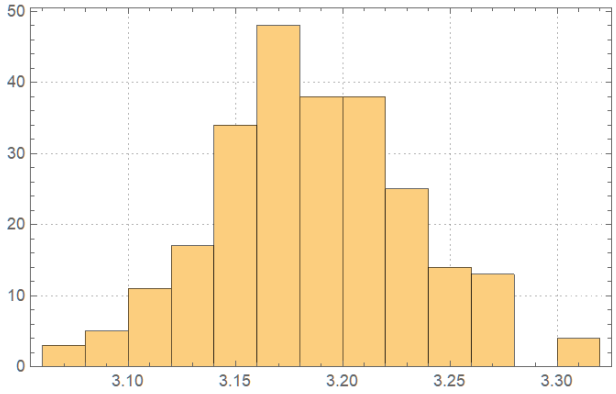

Figure 8: Histogram of Buffon's noodle experiment with 10^4 needles, repeated 250 times.

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 [8]. For this section we will be drawing from two papers written by K. G. Russel on this topic [9, 10].

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,

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

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 [11].

The Irwin-Hall distribution is defined as, the sum of n independent and identically distributed, uniform distributions 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 [10].

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.

[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.

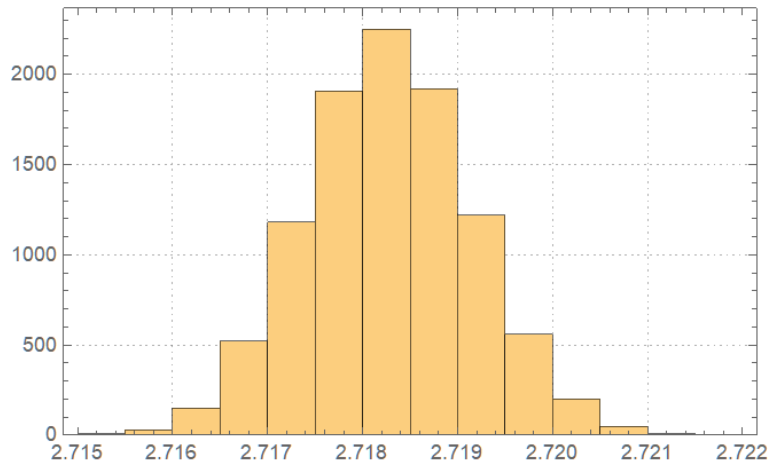

Figure 9: Histogram of e experiment with 10^6 numbers, repeated 10^4 times.

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 [12].

$$\zeta(z) = \frac{1}{z-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n (z-1)^n \tag{5.3}$$

The coefficients for the Laurent series expansion can be derived by the following expression of the Riemann Zeta function [13, Pg. 215, eq. 60],

$$\zeta(-n) = (-1)^n \frac{n!}{2\pi i} \int_C \frac{z^{-n-1}}{e^z - 1}\, dz$$

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 examine this.

5.1 Euler-Mascheroni constant

We will estimate the Euler-Mascheroni constant by first approximating the Gumbel distribution [14].

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.

$$Q(p) = \log\left(-\log\left(p\right)\right) \tag{5.4}$$

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.

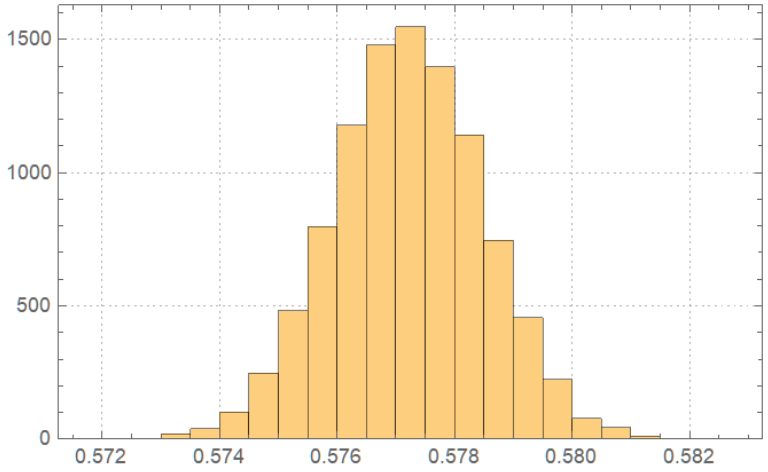

Figure 10: Histogram of experiment with 10^6 points, repeated 10^4 times.

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 [12] (see eq.12). Extensive work has also been done in implementing fast algorithms to compute Stieltjes constants with high accuracy [15].

In this project we will approximate a few Stieltjes constants using a define integral representation of the Stieltjes constants.

Theorem 5.1. $\gamma_n = \dfrac{(-1)^n n!}{2\pi} \displaystyle\int_0^{2\pi} e^{niz} \zeta(e^{iz}+1)\, dz$

We begin with the Laurent series expansion of $\zeta(z)$ around 1(eq. 5.3)

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

Consider the typical Taylor series expansion of a function $f(x)$ around x_0,

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!} (x-x_0)^n$$

Comparing the Laurent series and the typical Taylor series we can conclude the following,

$$(-1)^n \gamma_n = \frac{d^n}{dz^n} \left(\zeta(z) - \frac{1}{z-1} \right) \Big|_{z=1} \tag{5.5}$$

We now apply the Higher-order Cauchy integral formula which is stated as follows [13, Pg. 120, eq. 24]

$$, f^{(n)}(z_0) = \frac{n!}{2\pi i} \int_C \frac{f(z)}{(z-z_0)^{n+1}}\, dz$$

Where $\int_C$ denotes the complex integral over some closed rectifiable curve C. We will now apply the Cauchy integral formula on eq. 5.5. Which gives us,

$$\begin{aligned}(-1)^n\gamma_n &= \frac{n!}{2\pi i}\int_C \frac{1}{(z-1)^{n+1}}\left(\zeta(z)-\frac{1}{z-1}\right)dz \\ &= \frac{n!}{2\pi i}\left(\int_C \frac{\zeta(z)}{(z-1)^{n+1}}\,dz - \int_C \frac{1}{(z-1)^{n+2}}\,dz\right)\end{aligned}$$

Note that the second integral in holomorphic on any $C \setminus \{1\}$ and does not have a pole at 0, therefore with the Cauchy-Goursat theorem [13, Pg. 141, Th. 15], we can say that the second integral goes to zero. Hence we are left with,

$$(-1)^n\gamma_n = \frac{n!}{2\pi i}\int_C \frac{\zeta(z)}{(z-1)^{n+1}}\,dz = \frac{n!}{2\pi i}\int_C \frac{\zeta(z+1)}{z^{n+1}}\,dz$$

Now taking the unit circle contour $C : [0, 2\pi] \to \mathbb{C}$ where $C(t) = e^{it}$,

$$\gamma_n = \frac{(-1)^n n!}{2\pi}\int_0^{2\pi} e^{niz}\zeta(e^{iz}+1)\,dz \qquad \square$$

The reader should note that calculating Stieltjes constants with Monte Carlo integration is completely impractical due to the low accuracy. For practical approximations other forms of numerical integration techniques are used [15, 16].

The following table shows the results we achieved by estimating the integral representation.

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)

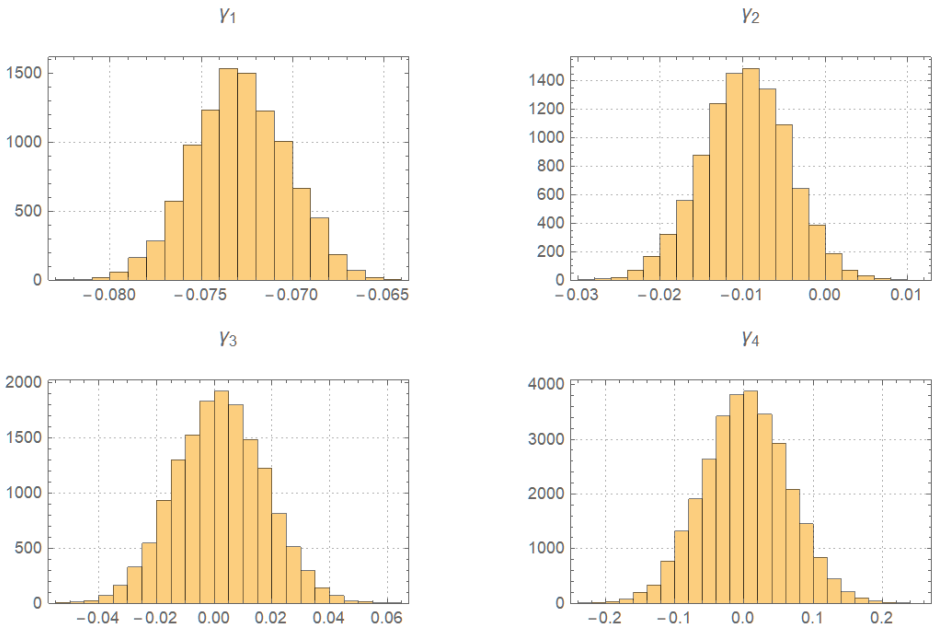

Figure 11: Histogram of the 4 experiments.

6 Estimating Phi

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

Since the golden ratio (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.

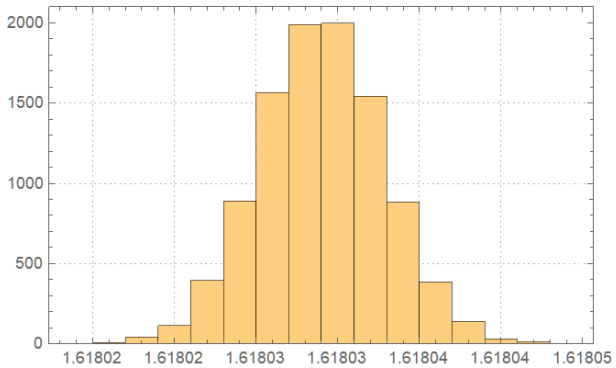

Figure 12: Histogram of experiment with 10^6 points, repeated 10^4 times.

7 Methods of integral variance reduction

Throughout the project so far we have only considered what is known as "naïve" Monte Carlo integration. We will now justify its nomenclature by listing out a few modified methods of Monte Carlo integration that are designed to reduce variability [1, 17].

To demonstrate the effectiveness of these methods we will be estimating the following integral,

$$f(x,y) = \int_0^1 \int_0^1 \frac{\sin x \sin y}{xy}\, dx\, dy \tag{7.1}$$

7.1 Antithetic variates

Antithetic variates is a technique for variance reduction, in which we use the antithetic pair of pre-obtained samples in the Monte Carlo simulation.

Consider the pre-obtained points $(x_1, \cdots x_s)$ in $[a_1, b_2] \times \cdots \times [a_s, b_s]$. The antithetic points are defined to be $(b_1 - x_1, b_2 - x_2, \cdots, b_s - x_s)$. Antithetic points are perfectly negatively correlated to the original set of points.

The advantage of this technique is that, it reduces the number of samples to be taken to generate N integration nodes, and thus, reduces the variance of the sample .

Theorem 7.1. *Using antithetic variates along with pre-obtained points reduces integration variance.*

Consider two random variables X and Y. Let Y be antithetic to X. The variance of the sum of X, Y is given by,

$$\mathrm{Var}\,[X+Y] = \mathrm{Var}(X) + \mathrm{Var}(Y) + 2\ \mathrm{Cov}(X,Y)$$

and since we know that,

$$\mathrm{Cov}(X,Y) = \rho\sqrt{\mathrm{Var}X}\sqrt{\mathrm{Var}Y}$$

where ρ is the correlation between X and Y. It can be seen that $\mathrm{Var}[X+Y]$ is minimised when $\rho = -1$ i.e if X and Y are perfectly negatively correlated.

□

Now we will compare antithetic variables vs naïve Monte Carlo with eq. 7.1.

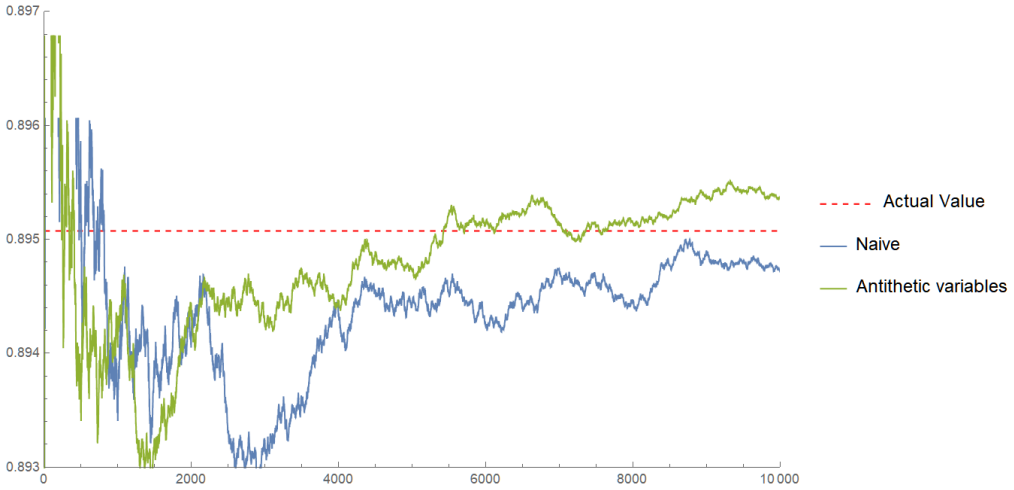

Figure 13: Comparison of estimating e.q. 7.1 with naïve Monte Carlo vs Monte Carlo with antithetic variables (for points ranging from 1 to 10,000).

7.2 Control variates

In this variance reduction technique, we use a known integral with a value approximately equal to the unknown integral to reduce the error in the estimate of unknown integral.

Theorem 7.2. $\mathcal{I}[f] \approx \frac{1}{N}\sum_{i=1}^{N}(f(X_i) - g(X_i)) + \theta$

Suppose we want to find $\mu = \int f$. We choose some $\theta = \int g$ where $g \approx f$, hence $\widehat{\mu} = \frac{1}{N}\sum_{i=1}^{N} f(X_i)$ and $\widehat{\theta} = \frac{1}{N}\sum_{i=1}^{N} g(X_i)$ for uniform iid r.v. X_i. We can estimate μ by the following estimator,

$$\widehat{\mu}_{\text{diff}} = \frac{1}{N}\sum_{i=1}^{N}(f(x_i) - g(x_i)) + \theta$$

This estimator is motivated due to the linearity of integrals. The expected value of $\widehat{\mu}_{\text{diff}} = \mu$, since $E[\widehat{\theta}] = \theta$.

$$\text{Var}(\widehat{\mu}_{\text{diff}}) = \frac{1}{N}\text{Var}(f(X) - g(X))$$

If $f(X) \approx g(X)$, then,

$$\text{Var}(f(X) - g(X)) < \text{Var}(f(X))$$

Hence, we use $(\widehat{\mu}_{\text{diff}})$ to reduce the variance. Here $g(X)$ is known as the control variate.

□

We will now compare Monte Carlo integration in estimating eq. 7.1 using both control variates as well as antithetic variables.

We obtain $g(x, y)$ using the Taylor series expansion of $f(x, y)$,

$$\frac{\sin x \sin y}{xy} \approx g(x, y) = 1 - \frac{x^2}{6} - \frac{y^2}{6} + \frac{x^2 y^2}{36}$$

We therefore use this approximation as $g(x, y)$,

$$\int_0^1 \int_0^1 g(x, y)\, dx\, dy = \int_0^1 \int_0^1 1 - \frac{x^2}{6} - \frac{y^2}{6} + \frac{x^2 y^2}{36}\, dx\, dy = \frac{289}{324} \tag{7.2}$$

Finding a Taylor series is obviously not practical for most integrands, but even very rough approximations will reduce variability.

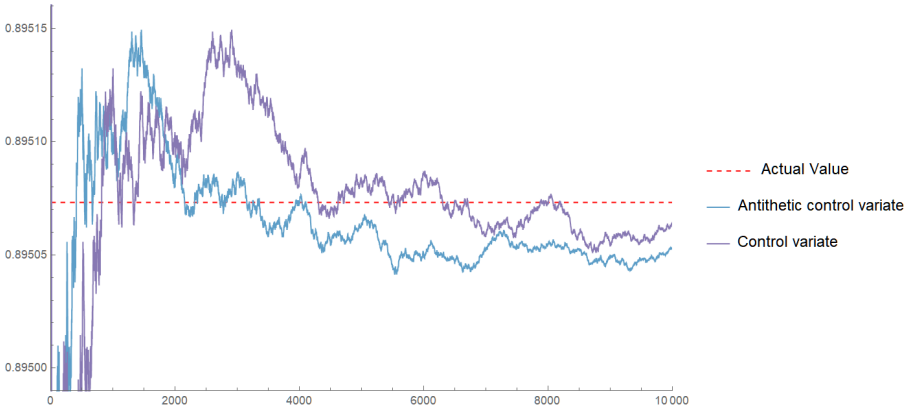

Figure 14: Comparison of estimating e.q. 7.1 with control variate vs antithetic + control variate (for points ranging from 1 to 10,000).

To put this the effectiveness of the control variate method in perspective we shall see it in comparison with the antithetic and the naïve method.

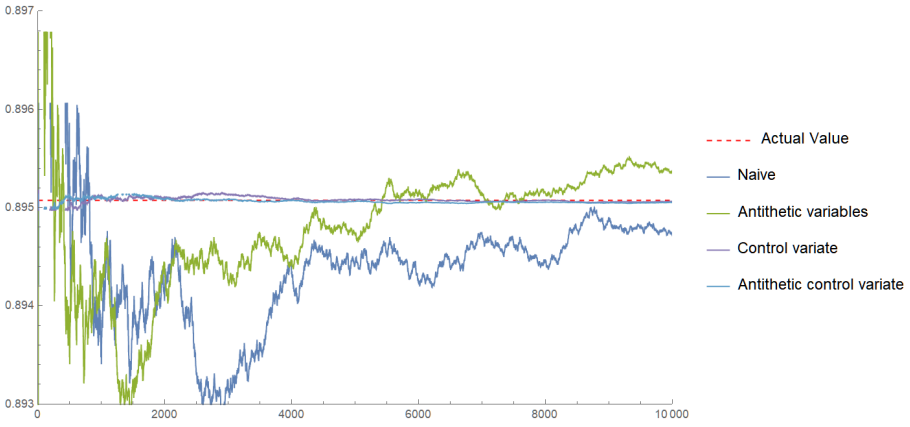

Figure 15: Comparison of the control variate with naïve Monte Carlo.

The reduction is variance is now much more striking.

8 Quasi Monte-Carlo integration

Quasi-Monte Carlo integration, simply put, is Monte Carlo integration using quasi-random generated numbers to form the integration nodes (as opposed to pseudo-random in naïve integration) [18].

The reader should note that in this section, we will only provide a cursory overview of Quasi Monte-Carlo integration and its results. Detailed proofs will not be given as they are far beyond the scope of this project. A vast amount of the theory surrounding this topic has been carried out by H. Niederreiter in a series of papers [19, 20] and books [21] which we recommend for further reading.

8.1 Quasi-random sequences (low-discrepancy sequences)

Quasi-random numbers are numbers generated from quasi-random sequences, which are in turn defined as sequences with low discrepancy [22]. We will first define what is meant by discrepancy.

Discrepancy can be intuitively thought of as a measure of uniformity. We will now see the formal definition for discrepancy for a s-dimensional sequence [19].

Let $x_1, x_2, \cdots x_N$ be N numbers in $I = [0,1]^s$, let $E \subseteq I$. Define a function $A(E;N)$ such that, it counts the number of $n, 1 \leq n \leq N$, for $x_n \in E$. The discrepancy D_n of the N numbers in I is then given by,

$$D_n = \sup_J \left| \frac{A(J;N)}{N} - \lambda_s(J) \right| \tag{8.1}$$

Where, J is any sub-interval of I and $\lambda_s(J)$ denotes the s dimensional Lebesgue measure. The star discrepancy (D_N^*) is a more commonly used definition which is defined as follows,

$$D_N^* = \sup_{t \in [0,1]^s} \left| \frac{A([0,t);N)}{N} - \lambda_s([0,t)) \right| \tag{8.2}$$

D_n and D_n^* are related by the following inequality [19]

$$D_n^* \leq D_n \leq 2^s D_n^* \tag{8.3}$$

8.2 Error in Quasi Monte-Carlo integration

Niederreiter has shown [19] that for any dimension $s \geq 1$, there exists an infinite sequence of points in I^s such that, for some constant c_s only dependent on dimension,

$$D_N = O\left(c_s \frac{\log N^s}{N}\right)$$

The famous Koksma–Hlawka inequality states that [19],

$$\left|\frac{1}{N}\sum_{i=1}^{N} f(X_i) - \int_{[0,1]^s} f(x)dx\right| \leq V(f)D_N^*$$

Where, $V(f)$ denotes the bounded Hardy-Krause total variation of the function [4].

The Koksma-Hlawka inequality along with eq. 8.3 is used to show that the error of Quasi Monte-Carlo integration is given by $O\left(c_s \frac{\log N^s}{N}\right)$.

8.3 Examples of Quasi-Random sequences

We have so far restrained from giving any examples of methods used to generate quasi-random sequences. In this section we will describe a few important methods [5].

8.3.1 Van der Corput and Halton sequence

We begin by describing Van der Corput sequences [21, 23], which are conceptually the easiest to understand.

For any integer $n \geq 0$ as follows, we define the following function, known as the radical-inverse function,

$$\phi_b(n) = \frac{a_1}{b} + \frac{a_2}{b^2} \cdots \tag{8.4}$$

Where, $n = a_1 + a_2 b + a_3 b^2 + \ldots$, $b \in \mathbb{Z}$ and $b \geq 2$. The reader should note the similarity of this function with the base b representation of a number. $\phi_b(n)$ is contained in $[0, 1]$.

The Van der Corput sequence is then defined for $n \in \mathbb{N}_0$ as,

$$x_n = \phi_2(n) \tag{8.5}$$

With star discrepancy equal to,

$$D_N^* = O\left(\frac{\log N}{N}\right) \tag{8.6}$$

n	n_2	$\phi_2(n)$
0	0	0
1	1	$0.1_2 = 1/2_{10}$
2	10	$0.01_2 = 1/4_{10}$
3	11	$0.11_2 = 3/4_{10}$
4	100	$0.001_2 = 1/8_{10}$

Table 2: First 5 values of Van der Corput sequence

However, the limitation of Van der Corput should now be clear to see. Van der Corput sequences only generates single dimensional numbers.

Halton sequences [24] are a very natural extension of Van der Corput sequences for higher dimensions s, which we define as,

$$x_n^s = (\phi_{p_1}(n), \phi_{p_2}(n), \cdots, \phi_{p_s}(n)) \tag{8.7}$$

Where, $p_1, p_2 \cdots p_s$ are co-prime integers. It is common to simply use the p^{th} prime number at each stage. The reason for this specific selection of bases is to reduce the dimension dependent constant in the discrepancy.

The star discrepancy of Halton sequences is, as expected,

$$D_N^* = O\left(\frac{\log N^s}{N}\right) \tag{8.8}$$

It has been theorized that Van der Corput and Halton sequences have the lowest discrepancy of any quasi-random sequence. This is however not yet been proved. Nevertheless, Halton sequences are very rarely used for numeric integration due to its tendency of becoming overly predictable in higher dimensions.

An early fix for this problem was given by Faure [25] who proposed to use bases in the Halton sequence as the first prime number greater than dimension s, and further to re-order each element using certain permutations based on Pascal matrices.

Below we have displayed a 2-dimensional Halton sequence with 1500 points using base 2 and 3. To illustrate the predictable nature for high dimensions we will also display a 2-dimensional graph using the 10th and 11th prime respectively.

[4]Note that this is not variance. Discussing total variation rigorously is well beyond the scope of this project, it can be roughly thought of as a infinitesimal absolute value.

[5]We will not be proving the values of discrepancies of these examples.

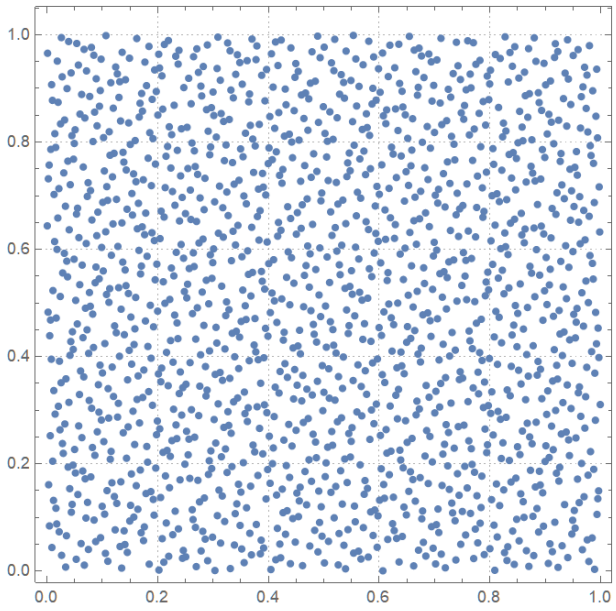

Figure 16: 2-D Halton sequence with 1500 points using 2^{nd} and 3^{rd} prime as bases.

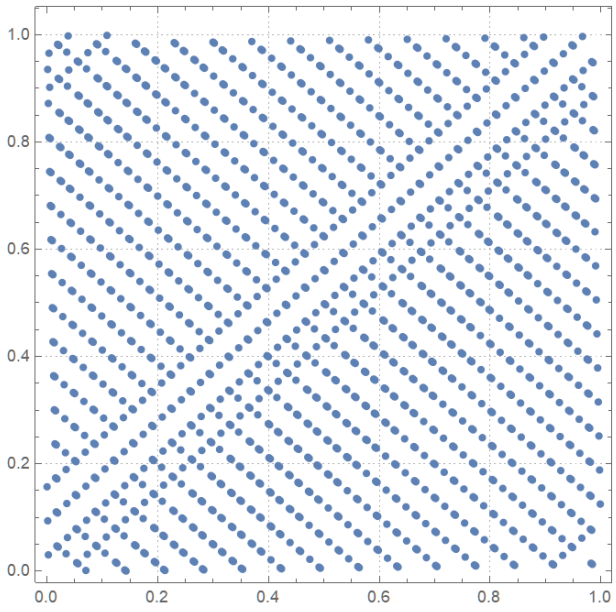

Figure 17: 2-D Halton sequence with 1500 points using 10^{th} and 11^{th} prime as bases. This helps visualize the problem of overly predictive points that occur in higher dimensions.

8.3.2 A cursory view of (t,s) sequences

Before expounding on a few other types of quasi-random sequences (namely, Sobol' and Niederreiter) we will first list out a few important definitions in a summarized manner. Throughout this section we will extensively refer to a paper by J. Dick and H. Niederreiter [26].

Recall the definition of the radical-inverse function (see e.q. 8.4). For some $\mathbf{x} \in [0,1]^s$ consider,

$$[\mathbf{x}]_{b,m} = (\phi_b(x^1), \cdots, \phi_b(x^s))$$

Here m is the upper bound of summation. Note the difference between the Halton sequence, here we use a fixed base b.

For integers $b \geq 2, s \geq 1$ and $t \geq 0$. Consider a sequence of points $x_0, x_1, \cdots$, in $[0,1]^s$. This sequence of points is called a ***(t, s)* sequence** in base b. If for all integers $k \geq 0$ and $m > t$, the set $\mathcal{P}_{k,m}$ consisting of the points $[x_n]_{b,m}$ with $kb^m \leq n < (k+1)b^m$ has the following property-
for every half-open sub-interval E of $[0,1]^s$ of the following form

$$E = \prod_{i=1}^{s} [a_i b^{-c_i}, (a_i + 1)b^{-c_i}) \tag{8.9}$$

for some integers $c_i > 0$ and $0 \leq a_i < b^{c_i}$ for $1 \leq i \leq s$ and volume b^{t-m}, there are exactly b^t points of $\mathcal{P}_{k,m}$ contained in E.

For the purposes of this project we are not providing detailed motivation for the concept of (t,s) sequences, we state it in a simplified definition since both Niederreiter and Sobol' sequences are in fact (t,s) sequences.

8.3.3 Niederreiter sequence

Niederreiter sequences are considered to be the best quasi-random sequence for numerical integration. Here we shall provide a very brief overview of Niederreiter sequences [20, 26] without going into details of the construction, with an example at the end.

Consider for some fixed dimension $s \geq 1$, consider a list of pairwise co-prime non-constant polynomials belonging to any finite field of order q,[6] with $e_i = \deg(p_i) \geq 1$ for $1 \leq i \leq s.$, i.e., $p_1, p_2, \cdots p_s \in \mathbb{F}_q$.

The generating matrices for the Niederreiter sequence are constructed using the constants of the Laurent series expansions over these polynomials and objects known as (t,m,s) nets [7].

For detailed construction of the Niederreiter sequence we recommend referring to the book by Niederreiter [21] and the book by Leobacher & Pillichshammer [23].

[6] With the ordinary restriction that q is a power of some prime.

[7] We have refrained from defining (t,m,s) nets as we are not providing the full proof. They are closely related to (t,s) sequences.

The matter of note is that the Niederreiter sequences in fact form (t,s) sequences with the exact value of t given as follows,

$$t = \sum_{i=1}^{s} (e_i - 1)$$

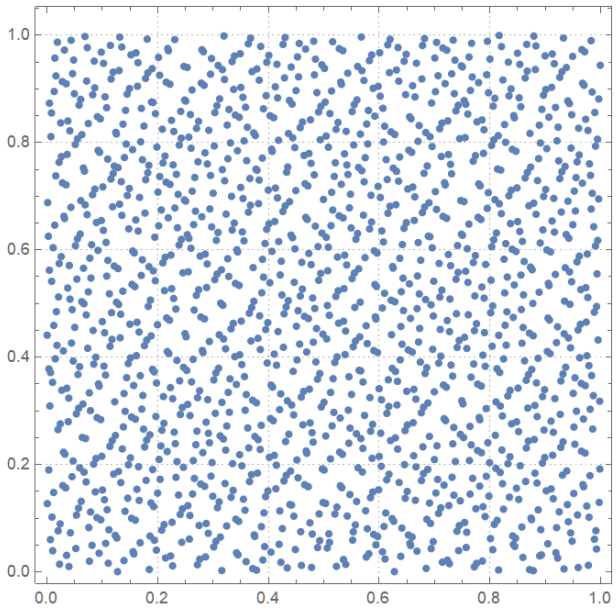

Figure 18: An example of a 2-Dimensional Niederreiter sequence with 1500 points.

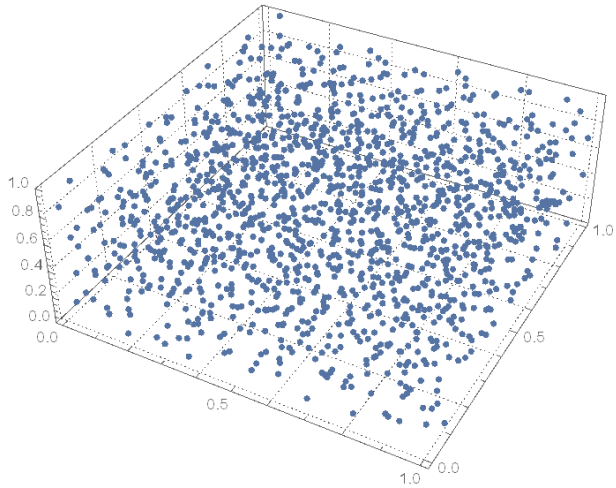

Figure 19: An example of a 3-Dimensional Niederreiter sequence with 1500 points.

8.3.4 Sobol' sequence

Sobol' sequences can be thought of as a special case of the Generalized Niederreiter sequence [26, 27]. It also uses polynomials to generate the quasi-random sequence.

Sobol' sequences are a (t,s) sequences in base 2 that uses polynomials as such, $p_1(x) = x \in \mathbb{F}_2[x]$ and $p_2, \cdots, p_s$ being primitive polynomials of successive order arranged in non-decreasing degrees. The first primitive polynomial is used to pick a set odd natural numbers after which we expand the list of odd natural numbers via a recurrence relation that utilizes the other polynomials.

These odd natural numbers are used to define "direction numbers" which are finally multiplied with the coefficients of the base 2 expansions of any natural number. Applying the bitwise exclusive-or operator on each of these products we obtain one number in the Sobol' sequence.

Reusing the obtained direction numbers for different natural numbers allows us to quickly generate the Sobol' sequence for s dimensions. For a detailed construction of the Sobol' sequence we once again recommend referring to the book by Niederreiter [21] and the book by Leobacher & Pillichshammer [23].

Note the difference, Sobol' uses primitive polynomials in base 2 while Niederreiter uses any pairwise co-prime polynomials in any base.

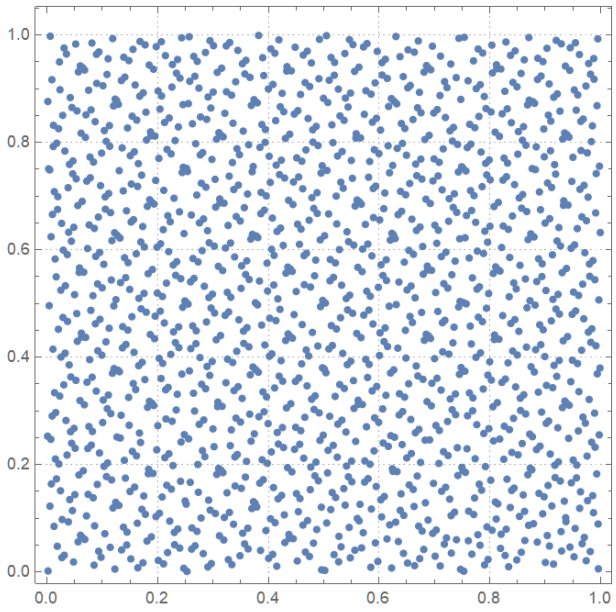

Figure 20: An example of a 2-Dimensional Sobol sequence with 1500 points.

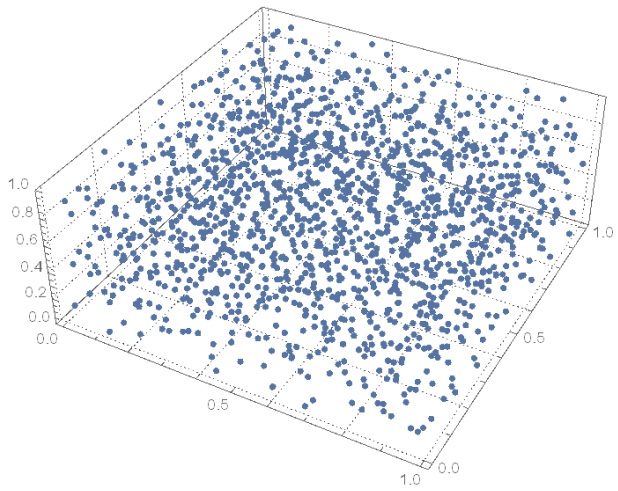

Figure 21: An example of a 3-Dimensional Sobol sequence with 1500 points.

8.4 Computing Apery's constant

We will end the project by computing a final example using Quasi Monte Carlo integration.

Apery's constant is $\zeta(3) = \sum_{n=0}^{\infty} \frac{1}{3^n}$. A simple integral representation of Apery's constant is given as follows,

$$\zeta(3) = \int_0^1 \int_0^1 \int_0^1 \frac{1}{1-xyz}\, dx\, dy\, dz$$

For comparisons sake we will estimate the integral with Quasi Monte-Carlo and naïve Monte Carlo to provide a direct comparison. This is shown in the graph below.

Repeating the experiment using the Niederreiter sequence with 10^6 points repeated 10^2 times we obtain the following results.

$\zeta(3) \approx 1.202055 \pm 3.095 \cdot 10^{-5}$, with a percentage error of $-1.514 \cdot 10^{-4}\%$.

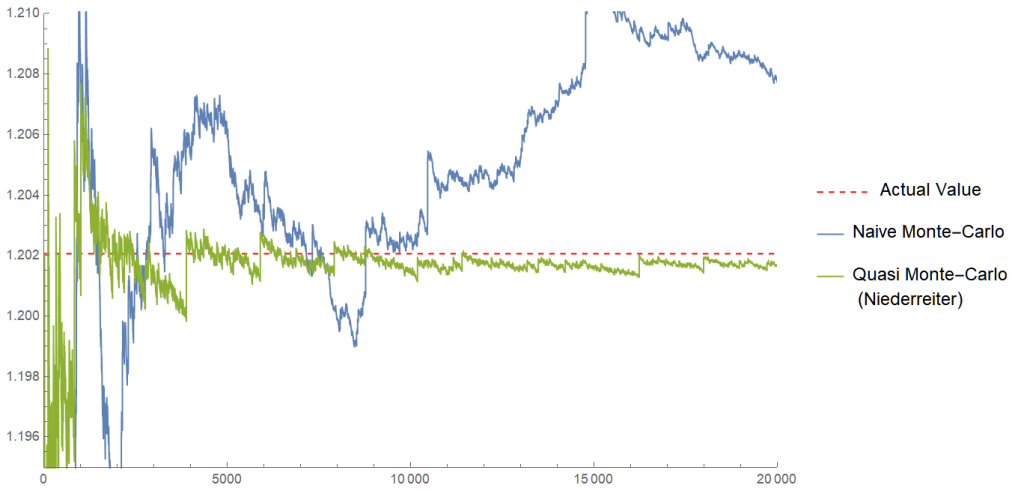

Figure 22: Quasi Monte Carlo vs naïve Monte Carlo estimates for Apery's constant (no. of points ranging from 1 to 20,000).

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