UNIVERSITY OF AMSTERDAM

Assignment 1: Estimating the area of the Mandelbrot set using Monte Carlo integration

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Course:
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1 Introduction

The Monte Carlo method is generally considered any approach that leads to a solution to a population-based problem by using a random sequence of numbers to represent a sample of the total population (Halton 1970). It is a widely used method in the study of stochastic processes, like the behaviour of neutron chain reactions in fission devices (Eckhardt 1987) or the determination of efficiencies in gamma-ray detectors (Raeside 1976). The Monte Carlo method can also serve as a numerical integration technique to solve problems that are not necessarily stochastic. Compared to deterministic numerical integrators, such as the trapezoidal rule, the Monte Carlo integration method has a convergence rate independent of the dimensionality of the problem, indicating that it is a better technique for high-dimensional problems (James 1980).

Since the Monte Carlo integration method uses a random number generator, it is a non-deterministic method. Therefore, determining the quality as an estimator of the solution must be done statistically by looking at the variance. Adding more sample points would reduce the variance and yield a better estimator, but this also increases the computational cost (James 1980). Other techniques to reduce the variance, for example, stratified sampling and importance sampling, have been developed (James 1980; Kroese and Rubinstein 2012).

To study the Monte Carlo integration method and the different variance reduction techniques in more detail, we will use them to estimate the area of the Mandelbrot set. The Mandelbrot set is the set of values in the complex plane for which the sequence,

$$z_{n+1} = z_n^2 + c \tag{1}$$

with z_0 equal to zero, remains bounded (Ewing and Schober 1992). Until now, there is no analytical expression to calculate the area of the Mandelbrot set, so the exact value of the area remains unknown (Bittner et al. 2017). However, because the fraction of samples inside the Mandelbrot set is related to the area of the Mandelbrot set relative to the total sampling area, we can use the Monte Carlo integration technique to estimate the area.

In this process, there are two main approximations. The first one is the number of iterations for which we check if the sequence is bounded. For a value to be in the Mandelbrot set, equation 1 should be bounded for every n, but we can only check this for a finite sequence. The second approximation is the number of sample points for which we check if the sequence is bounded. A particularly interesting question is how the estimate of the area changes if we vary the number of iterations or the number of sampling points.

Additionally, we can look at the effect of using stratified sampling techniques on the convergence rate. With Latin hypercube sampling (Loh 1996) and orthogonal sampling, the idea is to subdivide the total sampling area into subareas to get a more homogeneous sampling strategy. As these are known ways to reduce the variance, we can assume that the estimate of the area of the Mandelbrot set would improve compared to pure random sampling.

In the final part, we will test if a combination of stratified and importance sampling can further improve the convergence rate.

2 Theory

2.1 Mandelbrot set

The Mandelbrot set is defined by a simple equation in which the resulting value is inserted into the equation again. $f(z) = z^2 + c$ with z, c $\in \mathbb{C}$. For some values in $\mathbb{C}$, the absolute value of the series $(z_{i+1} = f(z_i))$ diverges towards infinity and for others it does not. It is known however, that for all numbers with $\|z\| > 2$ this value diverges. For $\|c\| < 2$, $let\ \|z_i\| = 2 + \epsilon => \|z_i^2\| = \|z_i\|^2 = (2+\epsilon)^2 = 4 + 2\epsilon + \epsilon^2 => \|z_{i+1}\| = \|z^2 + c\| > \|z^2\| - \|c\| > (4-2) + 2\epsilon + \epsilon^2$. Therefore, the rate at which the value increases is at least constant and the series diverges. For a similar reason, we find values of $\|c\| > 2$ to be unimportant. This can be used to create a criterion to stop a recursive function determining the divergence with a given starting point. In 2001, Kerry Mitchel analysed the area of the Mandelbrot set and found it to be around 1.506484, with a 95% confidence interval of 4.35 10^{-6} (Mitchell 2001).

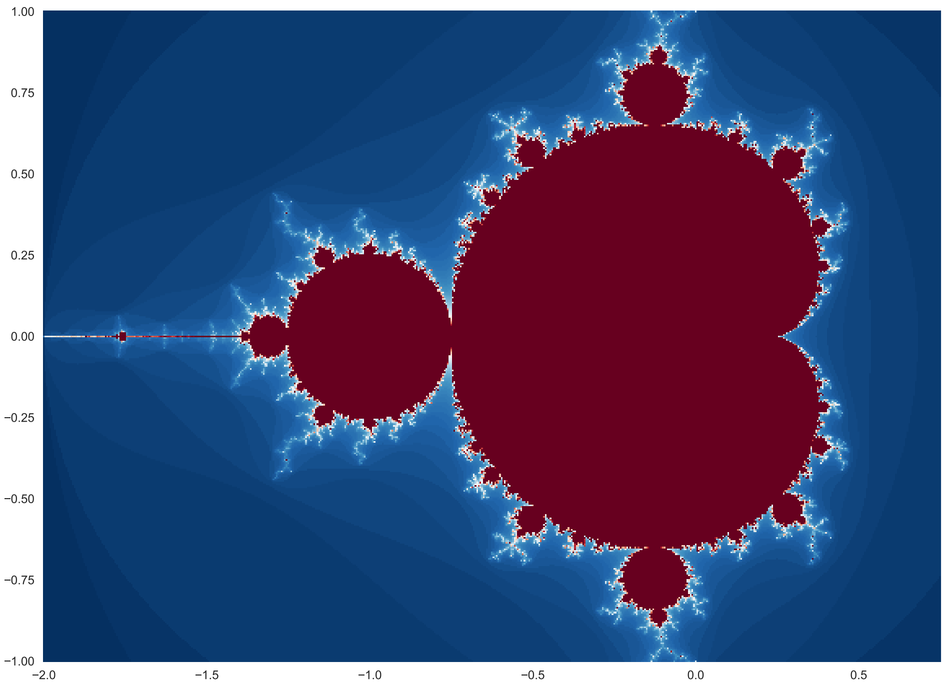


Figure 1: Fractal image of the Mandelbrot set.

2.2 Monte Carlo Method

The name Monte Carlo Method originated supposedly from Nikolai Metropolis (Nicholas Metropolis 1949) referring to the Monte Carlo Casinos in which everything was dependent on chance. In computational simulations, this method refers to a (pseudo)-random experiment being performed several times to extract data from models to find answers to posted questions. In this specific instance, the Monte Carlo method is used to pick random samples in a predefined area in the complex realm to determine if they are in the Mandelbrot set. That way we can estimate the area of the Mandelbrot set by multiplying the searched area by the probability of a sample in the area being inside the Mandelbrot set. Based on the number of samples used in the experiment, we also get a confidence interval for how confident we are that the true value will lie in a specified interval around the calculated value.

2.3 Accuracy vs Precision

For this specific experiment, there are two main variables of interest to determine the true area of the Mandelbrot set. First of all, to determine whether a specific value diverges or converges, we have to run a number of iterations of the Mandelbrot equation 1. It is unfeasible to test for infinite iterations if a sample is in the set or not. Therefore, we set a limit to the number of iterations. However, this will impact the accuracy of the result since we allow more values to be considered part of the Mandelbrot set than there are. The resulting area will be bigger than expected. Furthermore we expect the variance of the calculated area to decrease with increasing amount of samples used for calculating the area. The sample variance of the result in repeated experiments is defined as

$$S = 1/(n-1)\sum_{i=1}^{n}(x_i-\mu)^2, \tag{2}$$

with x_i being the estimated area with a fixed amount of samples and n the number of experiments used to calculate the variance. The variable μ in this equation is the average estimated area, which is defined as

$$\mu = 1/n\sum_{i=1}^{n}(x_i). \tag{3}$$

If we observe a lower variance for the same amount of samples with our devised method, we can declare it to converge faster.

2.4 Statistical tests

To compare both the precision and the accuracy we need to apply two different tests, the F test for equality of variances and the Welch's t-test for equality of mean. In the F test, the F-value is equal to S_x^2/S_y^2, with S_y^2 and S_x^2 being the variances of the two sample groups to compare. Under the Null-hypothesis, this F-value has a so-called F-distribution. In our experiment, the Null-Hypothesis describes the case that the two sample groups have the same variance, and all differences in the variance are up to random effects. In this report, we want to prove that our devised sampling method converges faster than the average Monte Carlo method for estimating the Mandelbrot area with orthogonal and Latin-hypercube sampling. So, we want to show that the variance of our method is significantly smaller than the variance of the compared method by $\frac{S^2_{Monte-Carlo}}{S^2_{Strategic-sampling}} >$

$F_{CriticalValue}$ (Chatfield 1980) This means that the likelihood of those two sample groups having the same variance is smaller than 5%(Fischer Constant/ significance level of 5%) with a degree of freedom of n-1 in both sample groups and a specific $F_{CriticalValue}$. The Welch's T-test is a version of the Students T-test in which the assumption that the two sample groups have a similar variance is dropped. We get the critical value that needs to be surpassed to reject the null hypothesis by

$$T_f^{-1}(\frac{p+1}{2}),$$

with

$$f = \frac{(\frac{S_x^2}{n} + \frac{S_y^2}{n})^2}{\frac{S_x^4}{n^2(n-1)} + \frac{S_y^4}{n^2(n-1)}}$$

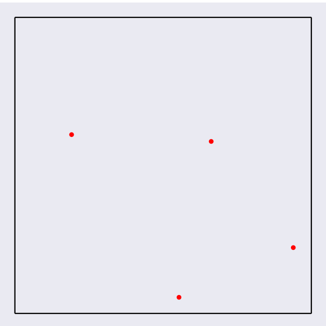
and the corresponding value obtained by the two samples to be

$$\|\frac{\overline{X} - \overline{Y}}{\sqrt{\frac{S_x^2}{n} + \frac{S_y^2}{n}}}\|.$$

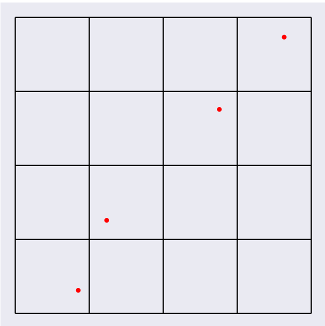
2.5 Latin hypercube/ orthogonal sampling

The most general sampling method is uniform sampling, where n samples are randomly drawn from the total sampling area (figure 2a). To improve on the sampling method to have a lower chance of samples only being generated in one area, a Latin hypercube sampling method or orthogonal sampling method can be used. With Latin hypercube sampling (LHS), the sample space is divided into n intervals in every dimension, where n is the number of samples. In every interval, a random value is taken as the coordinate of the sample point in that dimension. Then, the sample point is created by combining coordinates from every dimension. For the two-dimensional case, this comes down to having only one sampling point in every row and column of an n by n grid. An example of a Latin hypercube with four sampling points is shown in figure 2b.

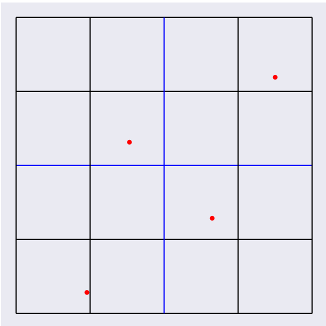
The orthogonal sampling method is similar to the Latin hypercube method, but it does have an additional constraint. The total sampling area is subdivided into n subareas and each of those subareas has to contain an equal number of samples. The orthogonal sampling method is depicted in figure 2c, where the blue lines indicate the four different subareas.



(a) Uniform



(b) Latin hypercube



(c) Orthogonal

Figure 2: Different sampling methods

2.6 Strategic sampling

The main idea of strategic sampling is to focus more on sampling in relevant areas. In the case of the Mandelbrot set, this means sampling more around the edges of the set because the regions completely inside or outside the set require less resolution(samples per unit of area) for an accurate result.

We do this by dividing the area into subareas in an iterative way. Each subarea has its own specific sampling probability. In every iteration, we perform Latin hypercube sampling in every subarea. The sampling probability in subareas where all the sampling points are either inside or outside the Mandelbrot set is reduced in the next iteration. On the other hand, subareas that have sampling points both inside and outside of the set get an increased sampling probability because they are located on the edge of the Mandelbrot set. Doing this for a few iterations should yield a better resolution of the true Mandelbrot area with fewer overall samples and also reduce the variance.

3 Methodology

3.1 Varying the number of iterations and sample points

We can study the effect of changing the number of iterations by keeping all the other parameters in the calculation of the area constant. First, we generate 1000 random sample points, uniformly distributed in the total sampling area ($[-2, 2] + [-2i, 2i]$). Using these sample points, we calculate the estimated area of the Mandelbrot set with the number of iterations varying from 2^1 to 2^{15}.

For the effect of changing the number of sample points, we set the number of iterations fixed to 500 and calculate the average estimated area over 100 runs. We do this calculation with the number of sample points varying from 2^3 to 2^{12}.

3.2 Effect of stratified sampling

To see whether the stratified sampling methods, Latin hypercube sampling and orthogonal sampling reduce the variance of the estimated area compared to uniform sampling, we run 100 calculations using each sampling method. During these calculations, we set the number of iterations equal to 500 and we also perform these calculations using different numbers of sample points. That way we can check if the difference in the variance between the sampling methods depends on the number of sampling points.

To test if the difference between the average estimated area with different sampling methods is significant, we can use Welch's t-test. For the difference in the variance, we will use an F-test to see if this difference is significant.

3.3 Strategic sampling to improve the convergence rate

We used strategic sampling of the area $\mathbb{C} \supset \{[-2, 2] + [-2i, 2i]\}$(see Mandelbrot set in theory part for reason) to calculate the area of the Mandelbrot set and compared the results to the orthogonal/Latin hypercube sampled Monte Carlo Method in the same area. The basic idea was to focus more on the areas where it cannot a-priory be inferred whether the samples will belong to the Mandelbrot set or not. For this purpose we devised a sub-spacing algorithm, taking into account the first $x_k = x_{k-1} + 128 * (2^k)$ samples, with k being the iterator for that specific cycle, and determining if a specific subspace contains only samples that are in the set or out. The samples inside each subarea were generated through Latin hypercube sampling. The area was divided into $sa_k = 16 * (4^(k/2))$(with

k/2 being rounded down) sub-spaces with a corresponding value for sample probability and test-iterations in the subarea. In that case, future samples will be less likely taken out of that area. This is supposed to increase the precision of the result in the areas where there are both samples in the Mandelbrot set and outside. The number of samples in a subspace is set deterministic by the total number of samples required and the sample probability of that subspace. In each cycle, we increased the number of samples x_k and in the strategic sampling version the number of subareas sa_k. The resulting subareas will be added to the total area by their relative size.
We ran 100 experiments for the Monte Carlo method with orthogonal sampling, Latin hypercube sampling and the strategic sampling method, with 6 cycles each. Resulting in the following configurations across the 6 Cycles.

Cycle	1	2	3	4	5	6
Samples per cycle(L.-H./Orth.)	256	784	1849	3844	8100	16129
Samples per cycle(Strat.)	256	768	1792	3840	7936	16128
Subdivisions(L.-H./Orth.)	1	1	1	1	1	1
Subdivisions(Strat)	16	64	64	256	256	1048

The amount of samples used for the comparison(Latin hypercube/Orthogonal sampling) was slightly different for practical reasons, but chosen to be as close as possible to the samples used in strategic sampling.. After running the 100 experiments with these parameters, we get an array of resulting area estimations. The statistical tests mentioned in the theory part were performed on these data points, resulting in hypothesis tests to infer whether we could reliably tell if the two methods show different or improved convergence rates in both accuracy and precision.
The following sequence of graphs shows how samples are selected in each cycle.

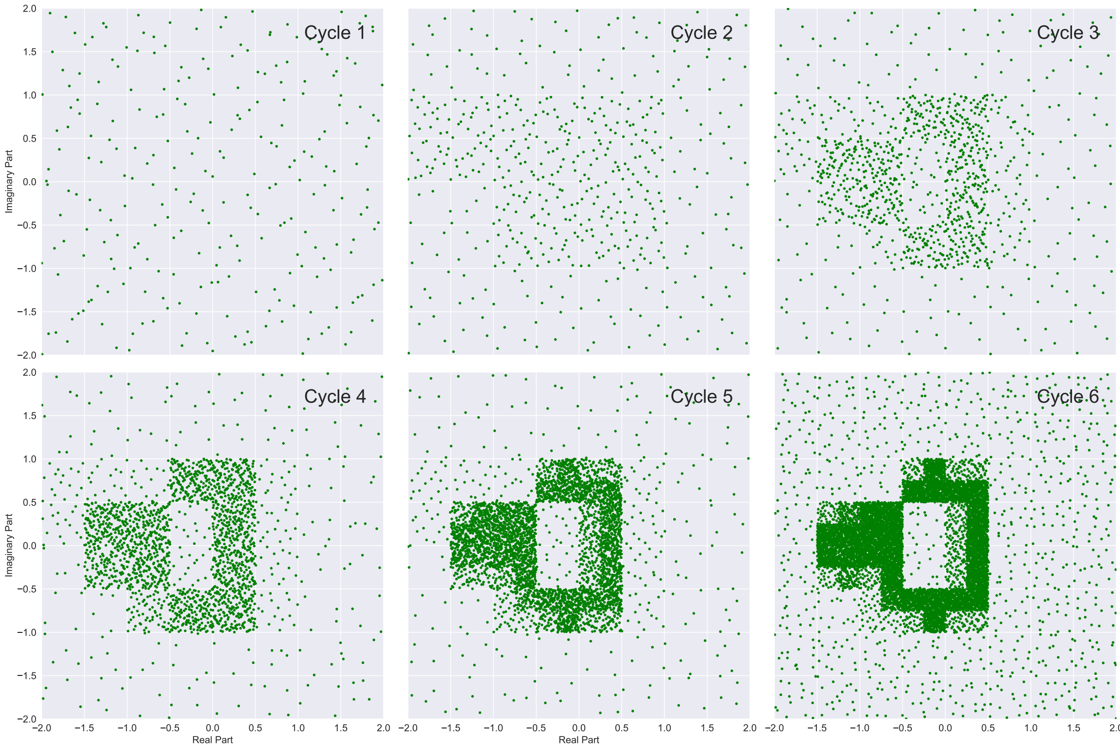


Figure 3: The samples taken in Strategic sampling while progressing through cycles.

4 Results and discussion

4.1 Varying the number or iterations and sample points

The left graph in figure 4 shows the estimated area of the Mandelbrot set as a function of the number of iterations, where the area is corrected with respect to the estimated area for the maximal number of iterations. At low iterations, we see that the area of the Mandelbrot set is highly overestimated. This is because many sample points are considered inside the Mandelbrot set because the value has a magnitude below 2 during the first few iterations of the sequence. Increasing the number of iterations will lead to a reduction of the estimated area because values for which it takes a while before the sequence starts to diverge are correctly assigned as outside the set. This means that increasing the number of iterations will lead to higher accuracy of the estimation.

In the right graph of figure 4, we keep the number of iterations constant and plot the average estimated area over 100 simulations as a function of the number of sample points. The edges of the coloured area represent the average area ± the sample variance. When using very few sample points, the average area is slightly underestimated because the sampling area is much bigger than the Mandelbrot area. Increasing the number of sample points leads to a significant reduction in the variance between different simulations.

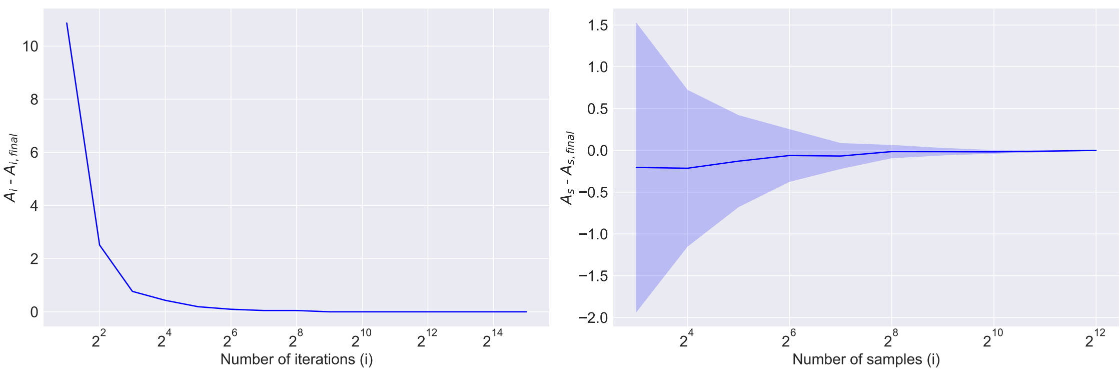


Figure 4: Estimate of the area of the Mandelbrot set as a function of the number of iterations and samples.

4.2 Effect of stratified sampling

Figure 5 shows the average estimated area and the sample variance as a function of the number of sampling points. When using a low number of sampling points, the Latin hypercube sampling method will have a higher estimated area compared to Latin hypercube and uniform sampling. Looking at the left graph 6, the difference in the average area between uniform and Latin hypercube / Latin hypercube and orthogonal sampling is only significant for the lowest number of sampling points. Increasing the number of sampling points shows that all three sampling methods converge towards the same estimated area.

In the right graph of figure 5, the sample variance is plotted as a function of the number of sampling points. The sample variance is clearly the highest for uniform sampling and orthogonal sampling results in the lowest variance. The results of an F-test, shown in the right graph of figure 6, indicate that the difference in the variance is significant for all the number of sampling points. This indicates that orthogonal sampling is the better technique compared to Latin hypercube sampling to improve the variance reduction.

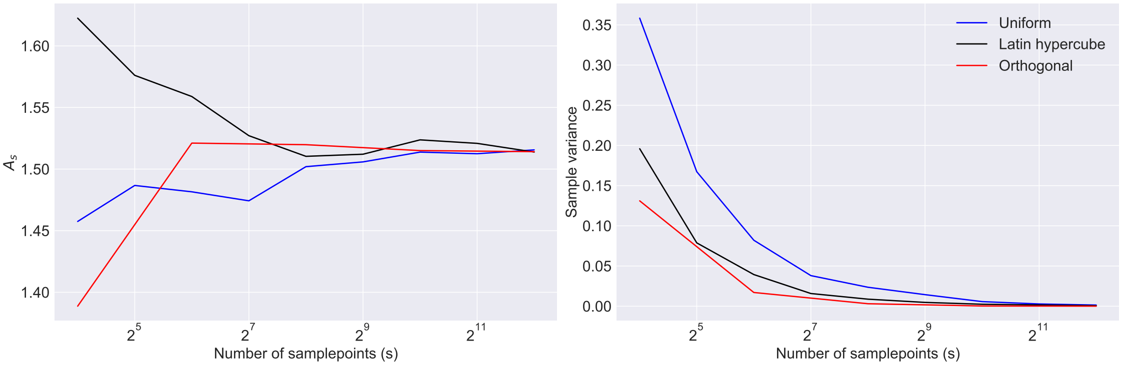


Figure 5: Estimate of the area of the Mandelbrot set using different sampling strategies.

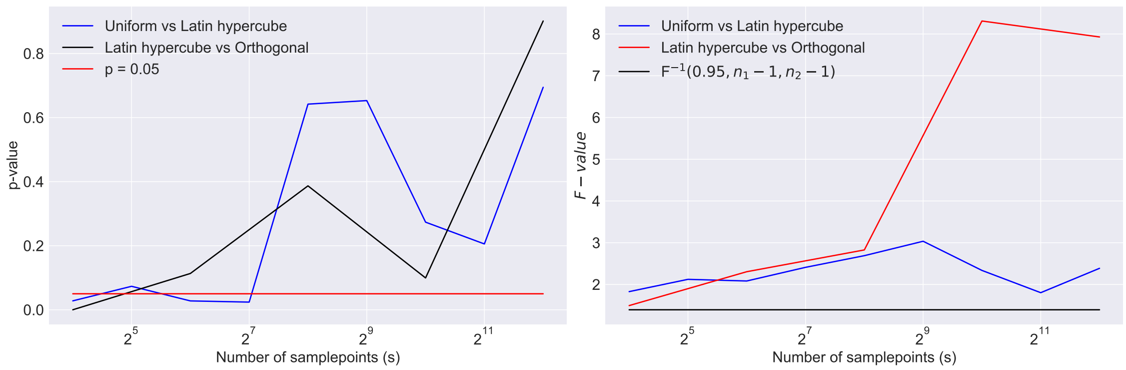


Figure 6: Left: p-values of a Welch t-test as a function of the number of sampling points. Right: F-values as a function of the number of sampling points.

4.3 Strategic sampling to improve the convergence rate

We compared the results of the Strategic sampling method against Latin hypercube/orthogonal sampling to determine whether the mean or variance is impacted by the choice of method. The exact Statistical tests were discussed in the Theory part. The Null Hypothesis was described as the results being virtually similar.

4.3.1 Accuracy

To determine if the accuracy of the results is affected we compared the means in figure 7 showing the overlap in confidence intervals. The confidence intervals were created by adding the standard deviation of the sample group to the mean in that cycle. For orthogonal sampling, the confidence intervals overlap neatly whereas for Latin hypercube sampling the confidence intervals show distinct areas. In each case, the averages of the samples lie inside the confidence intervals of both methods.

The Welch's T-test, shown in figure 8, compares the Welch's T-value in each cycle against the required critical value, to reject the null hypothesis. The orthogonal sampling

Figure 7: Mean comparison with 1-sigma confidence intervals using Latin hypercube(right) and orthogonal sampling(left) when compared with Strategic Sampling. The dashed green Line represents the measured value for the Mandelbrot set area from (Mitchell 2001)

method shows one distinct value in all the cycles, otherwise, the critical value is not surpassed.

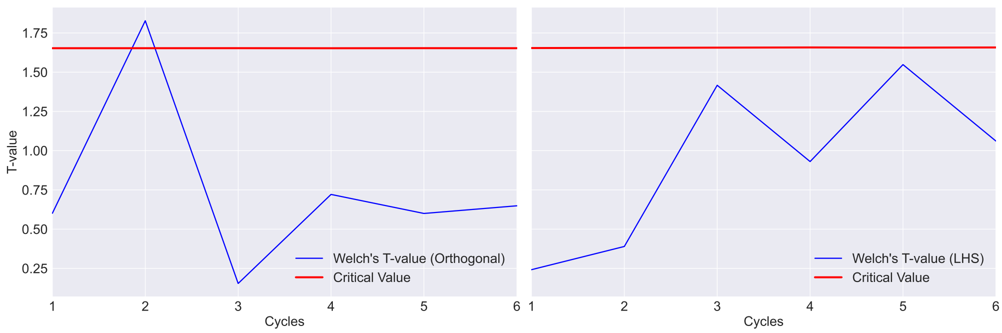


Figure 8: Welch's T-test comparing the mean distributions for Strategic sampling with Latin hypercube(right) and orthogonal sampling(left) with the critical T-value(red) with significance level 0.05

The T test shows that the mean values are not separate for the different values. The one outlier in figure 8 can be attributed to randomness since the experiment is repeated for several cycles and subsequent values are not affected. This suggests our method does not improve the accuracy of the results.

4.3.2 Precision

To find out if the precision of the result is affected by the method we compared the variances (figure 9) in the sample groups and performed a F-test (figure 10) which was compared against the corresponding critical F-value for significance. In figure 9, the variance of the Latin hypercube sampling method was constantly higher than the Strategic sampling method, whereas the variance of the orthogonal sampling method had very similar results to our applied method.

In the F-test (figure 10), the F-value for the Latin hypercube sampling comparison is always above the critical value. The orthogonal Sampling comparison lies close to the crit-

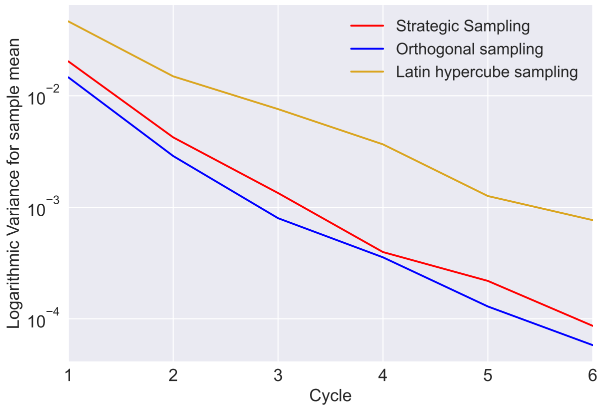


Figure 9: Difference in variance in between Strategic sampling(red) and Latin hypercube(yellow)/ orthogonal sampling(blue) as shown on a logarithmic scale

ical value for the most part but shows two occasions clearly surpassing the value in a cycle.

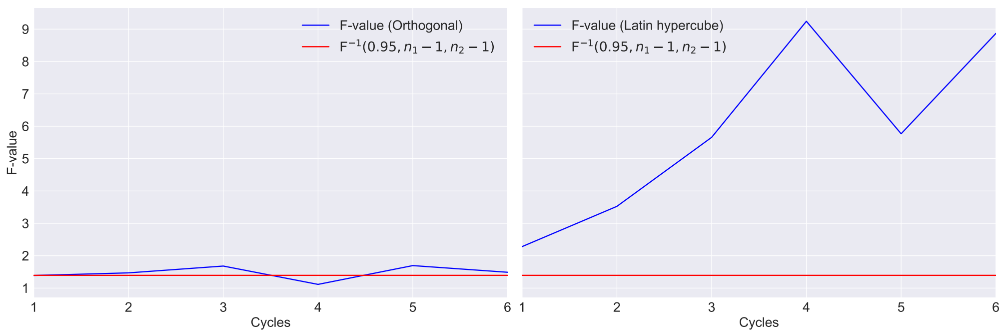


Figure 10: F-test comparing the variance distributions for Strategic sampling with Latin hypercube(right) and orthogonal sampling(left) with the critical F-value(red) with significance level 0.05 as shown on a logarithmic scale

This shows that our method improved the variance and therefore the precision compared to Latin hypercube sampling since the F-test suggests two differing variances while the variance is higher for Latin hypercube sampling (figure 9). On the other hand, orthogonal sampling still converges either similarly fast or even faster than Strategic sampling as suggested by their respective plots in figure 9 and 10.

5 Conclusions

In conclusion, we were able to show that increasing the number of iterations to check for divergence in the Mandelbrot set improved the overall accuracy of the result, specifically reduced the resulting area, while the number of samples used for calculating the result in a Monte Carlo simulation increased the precision/ decreased the variance in the resulting area estimations.

Also when comparing sampling methods uniform, Latin hypercube and orthogonal we found no evidence suggesting they affect the overall accuracy but found the Latin hypercube sampling method to improve the precision compared to uniform sampling and orthogonal sampling to improve the precision compared to Latin hypercube sampling.

Furthermore, we improved the precision of the Monte Carlo Method estimating the area of the Mandelbrot set using Strategic sampling compared to Latin hypercube sampling which it was based on, but could not affect the accuracy of the result similar to previous results. The orthogonal Sampling Method on the other hand was able either outperform or contest the Strategic Sampling approach by itself.

Future Precision improvements seem plausible when applying orthogonal sampling to the sampling methods in the subareas instead of Latin hypercube sampling. Due to time constraints, this approach could not be investigated in this report.

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