Computer Simulations assignment 1: Numerical differentiation

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Aim and Abstract

The aim of this computational investigation was to write a python code, which utilises the central difference method to compute the second derivative of cos(x). The analytical results, which yield an exact value, and the numerical results, which yield an approximate solution through a process of trial and error (the Central difference method), were compared within a range of 0 to 4π. The variation in the absolute error within this range was then deduced.
It was found that the numerical method yielded a reasonably accurate result, for instance, the value for the second derivative at x=nπ was approximately 0.992, compared to the analytical result of 1. The value of the step size at which the relative error for the Central Difference approximation was found to be 0.000225, producing a relative error value of 0.85x10^{-8}. Outside this value of h, it was found that the relative error increases exponentially on either side.
An amended version of this approximation is the Subtractive Central difference approximation and yielded a minimum value of the relative error to be 0.7x10^{-8}, and a lower h value of 0.000175. We found that this version was more suitable in producing accurate results for the second derivative of cos(x).

Background

The equation below is the Central Difference approximation for the second derivative of a function.

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} + O(h^2)$$

The term O(h) is the error, a quadratic in h, and will increase with h. We can analyse the accuracy of the numerical method results by calculating the absolute and relative error (which is an indication of the uncertainty of the result relative to its size).

$$absolute\ error = |true\ value - approximate\ value|$$

$$relative\ error = \left|\frac{true\ value - approximate\ value}{true\ value}\right|$$

We can do the same for the result obtained through the Subtractive Central difference method, for which the equation is shown below. This is a variation of the initial method used in this investigation and may produce more accurate results. As when machines are performing numerical calculations, an error known as subtractive cancellation can occur, whereby the number of significant figures is undesirably reduced.

$$f''(x) = \frac{\big(f(x+h) - f(x)\big) - (f(x) - f(x-h))}{h^2}$$

Method

Within the code, both the function (cos(x)) and the analytical result for the second derivative were simply defined: f= -1*np.cos(x). This analytical result was compared with the result obtained when one uses the Central Difference approximation, plotted for x ranging from 0 to 4π. The initial result for the Central Difference approximation was plotted with a fixed h (step size) value of π/10.

The value of h was then tested within a range of values which decreased successively. This was to determine the limit of machine accuracy, whereby a further reduction in the value of h would result in an inaccurate result for the plot of the second derivative, due to rounding errors. By plotting the variation in the relative error with a decreasing h, the most accurate result was obtained and the specific value of h at which this occurs.

After doing so, the same plot for the same range in h was graphed for the Subtractive Central Difference approximation, and the results for each type of approximation were compared. From this, we can see which method is more suitable for this code.

Results and Discussion

Figure 1.1

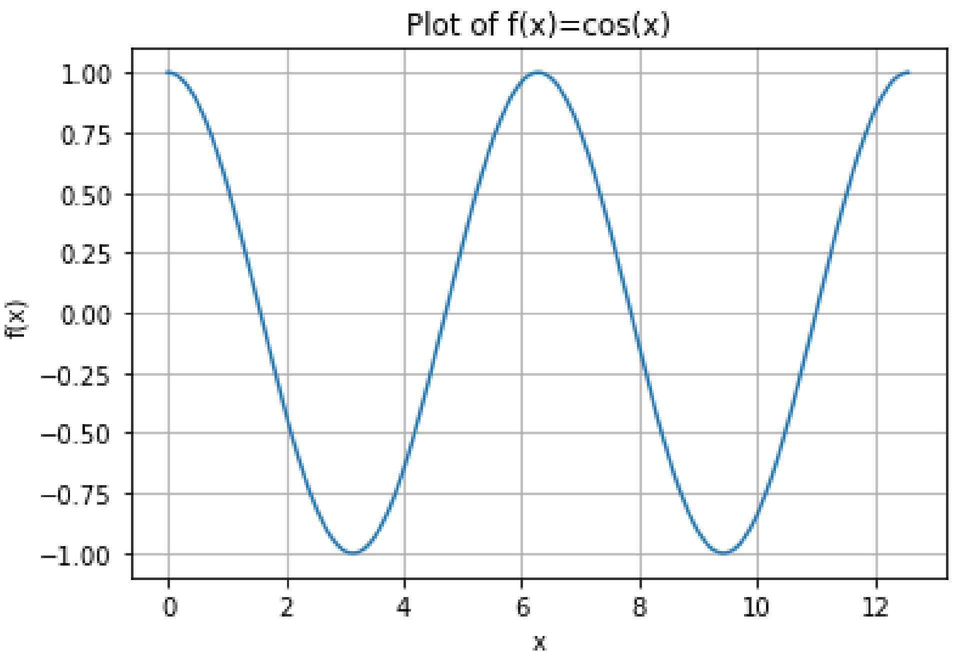


Figure 1.1 is a plot of the function upon which we will perform a second derivative.

Figure 1.2

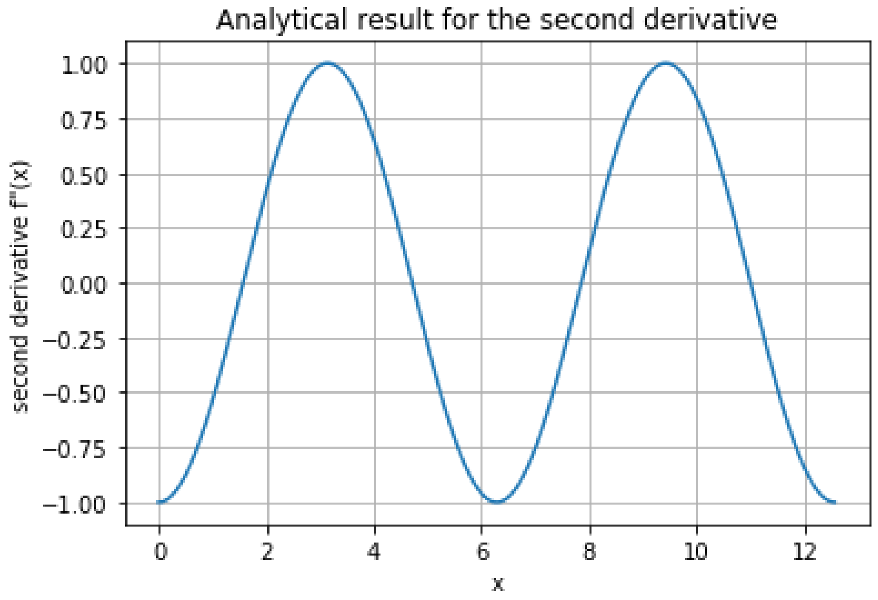


Figure 1.2 shows the graph of the function f”(x)=-cos(x), i.e. the analytical second derivative of the original function. We can see that the result is exactly as expected, for x ranging from 0 to 4π.

Figure 1.3

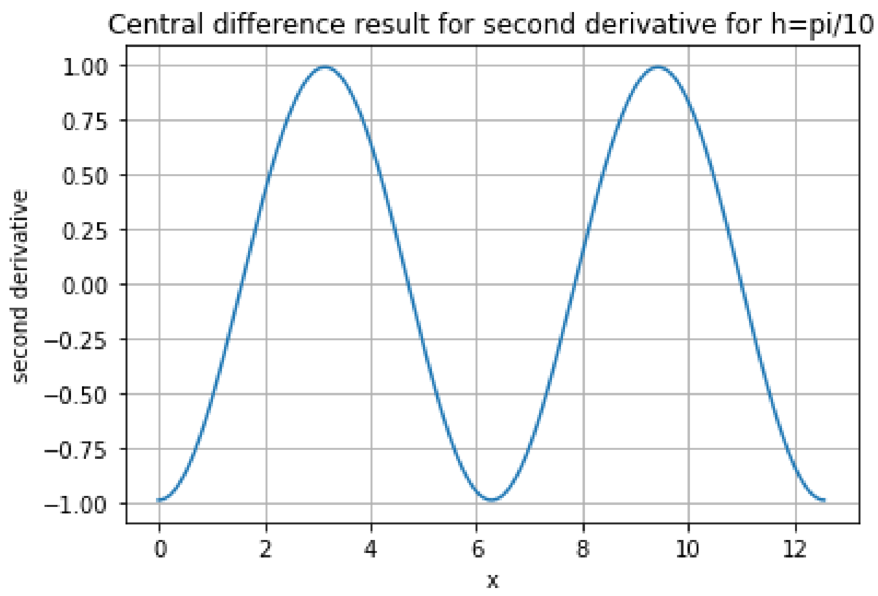


Figure 1.3 shows the result upon computing the second derivative using the Central Difference Approximation within the same range of x as 1.2.

Figure 1.4 below shows the subtle difference in the two results and the slight inaccuracy when using the numerical method.

Figure 1.4

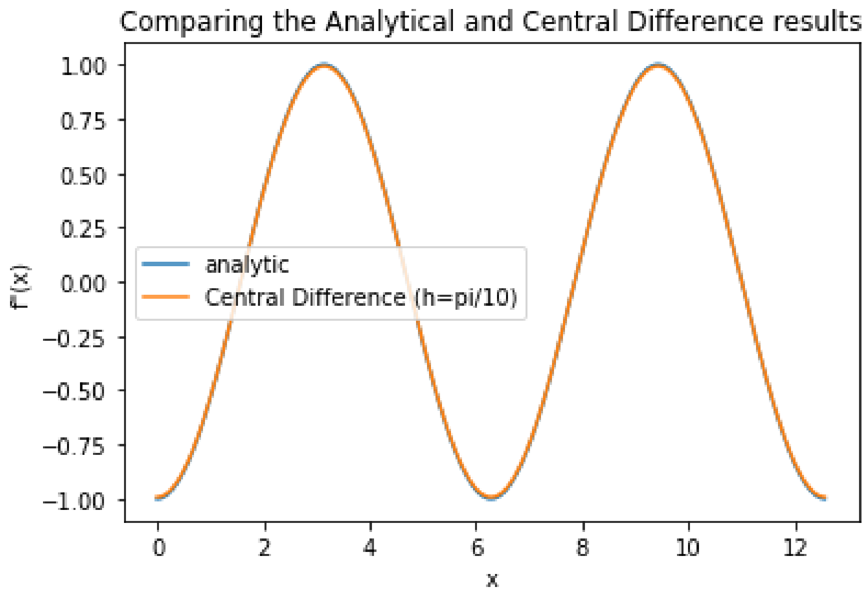


Figure 1.5

This plot is a magnified version of figure 1.4, where x ranges from 0 to 0.3. Here the difference in the two methods is much more apparent, where the Central difference approximation has a minimum value approximately 0.01 units less negative than expected for x=0. This is seen within the code, whereby the precision of the result is tested- the result for the second derivative evaluated at x=π and h=π/10 was: 0.9918023401109021 for the Central difference approximation, whereas the analytical result yields 1.

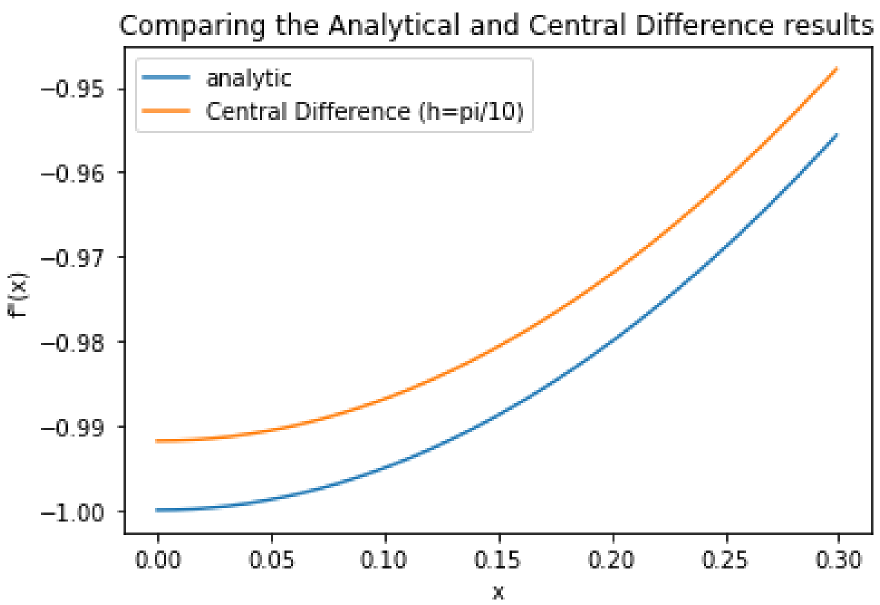


Figure 2.1

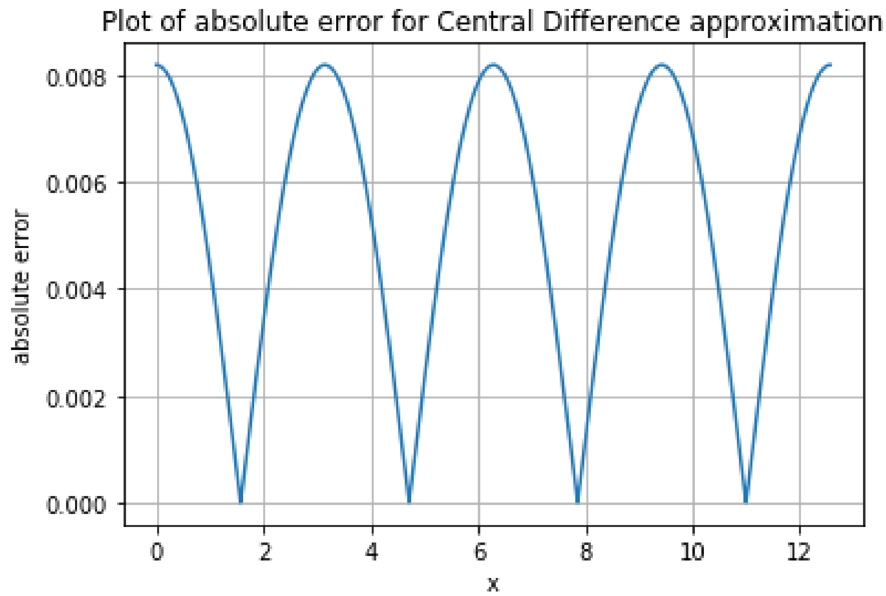


Figure 2.1 shows the variation of the absolute error in the Central difference approximation for x ranging from 0 to 4π, for a fixed value of h (π/10). Here we can see that the maximum error occurs at x=nπ (n=0,1,2,3...) and the minimum error occurs at x=(n/2)π (n=1,2,3...). The maximum error is approximately equal to 0.0082 and the minimum error appears to be 0.

Figure 3.1

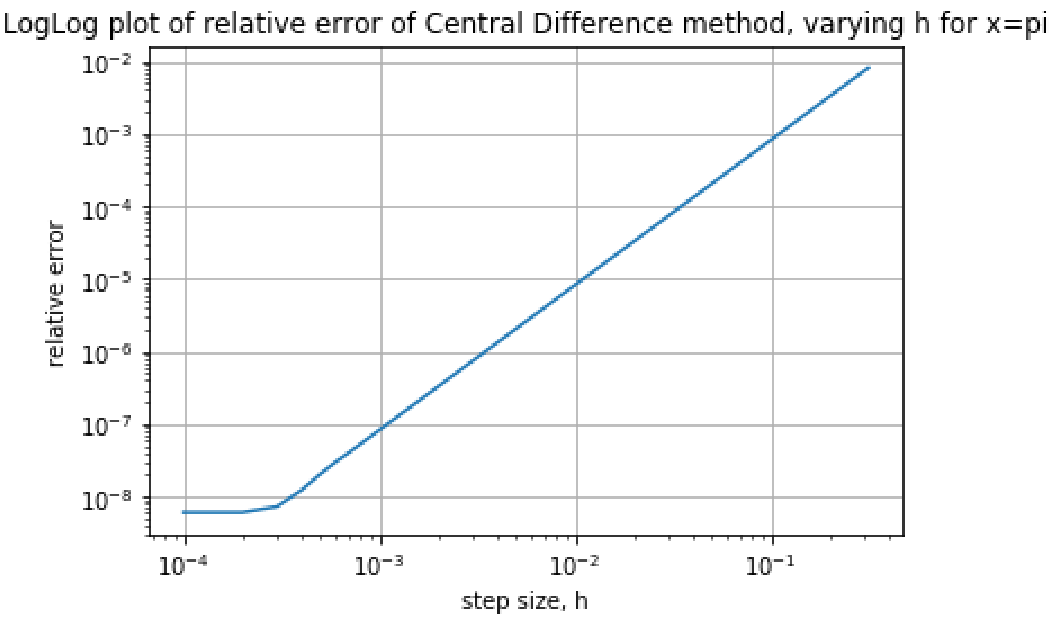


Figure 3.1 is a plot of the logarithm of the relative error versus the logarithm of the step size, h, where h is varying from 0 to π/10. Here we can see a horizontal line at around h=1x10^{-4}, and onwards the relative error begins to rise. We then see a direct proportionality between increasing step size and an increasing relative error.

Figure 3.2

Figure 3.2 shows the general trend that as step size increases, the relative error will also increase exponentially.

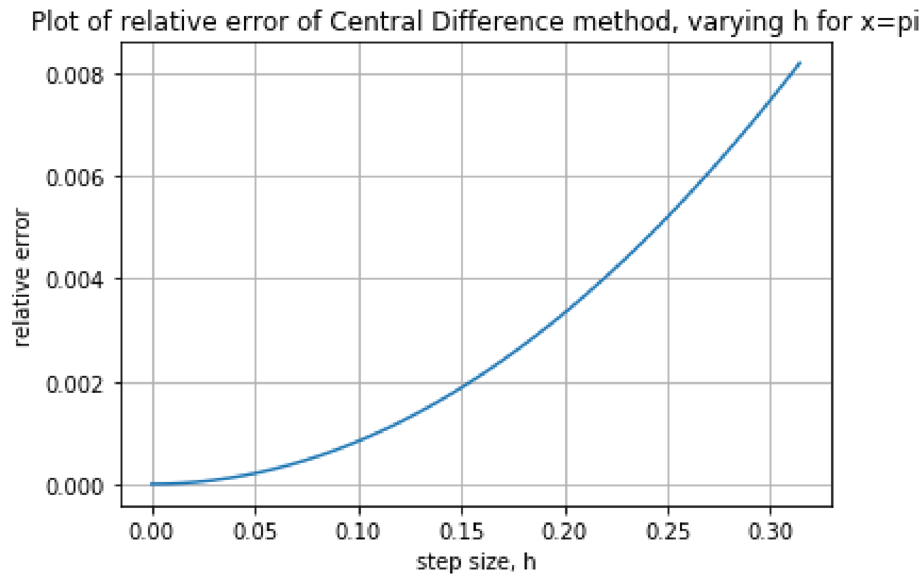


Figure 3.4

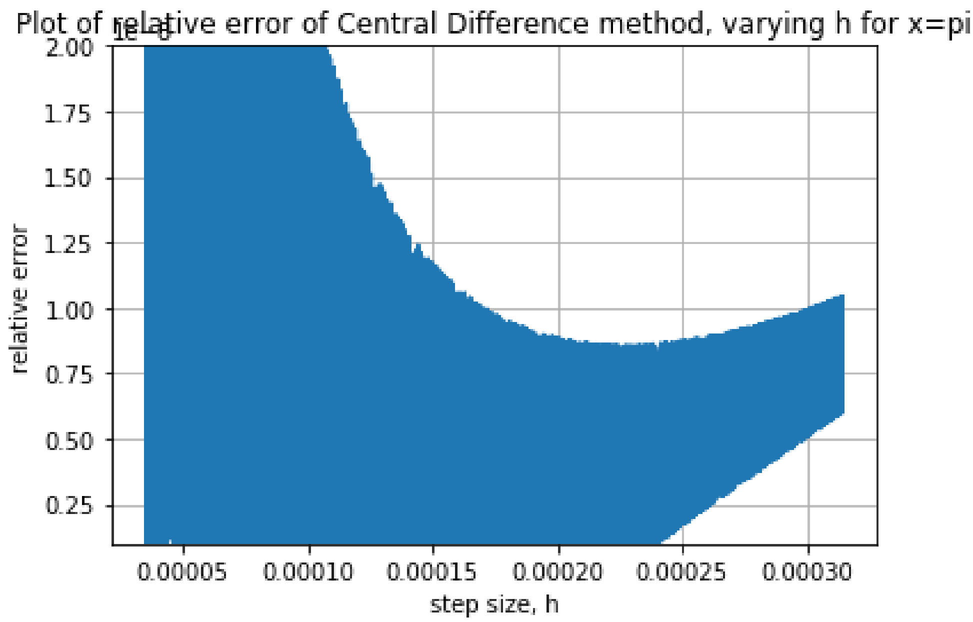


Figure 3.4 is a magnified version of the graph shown in figure 3.3 (where h and the y axis have been limited to a range shown in the code: h=np.arange(np.π/90000,np.π/10000,np.π/1000000000), plt.ylim(0.01e-7,0.2e-7)). This allows us to see the minimum value of the relative error and at which h value this occurs. Here we can see the step size at which the minimum occurs is approximately 0.000225, and this minimum has a value of $0.85\text{x}10^{-8}$.

From this graph, we can also see where the rounding error in machine accuracy begins to have an effect, as lower values of h (past 0.00020) lead to a significant exponential increase in the relative error.

Figure 4.1

This figure displays the results of the relative error for the Subtractive Central Difference approximation. At this range, the results for both methods seem to produce the same relative errors for a given range of h.

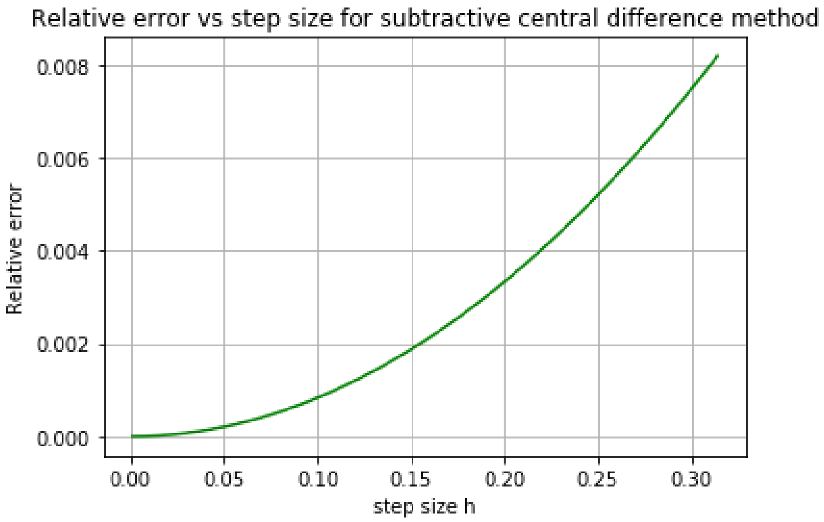


Figure 4.2

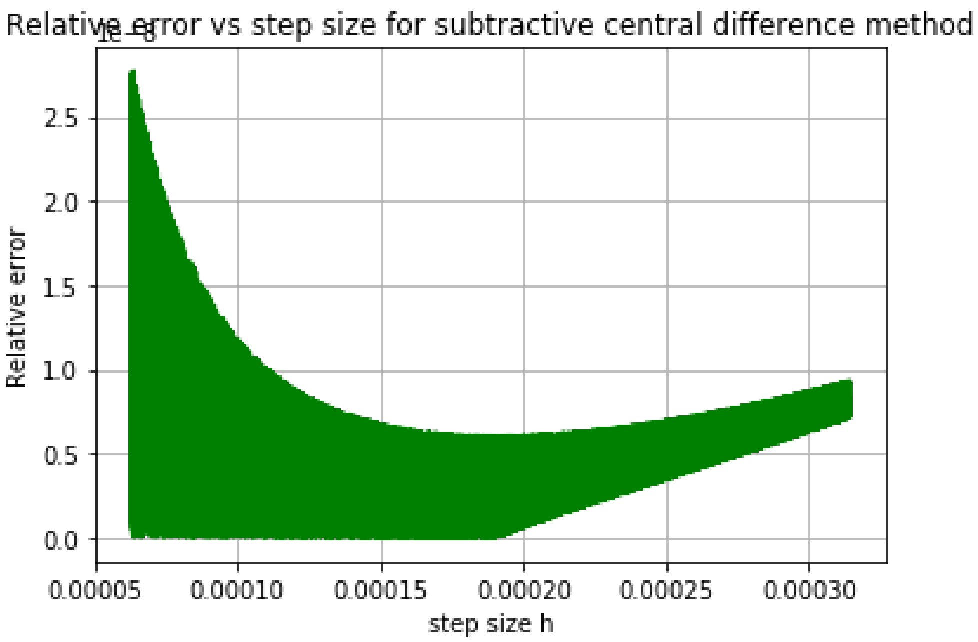
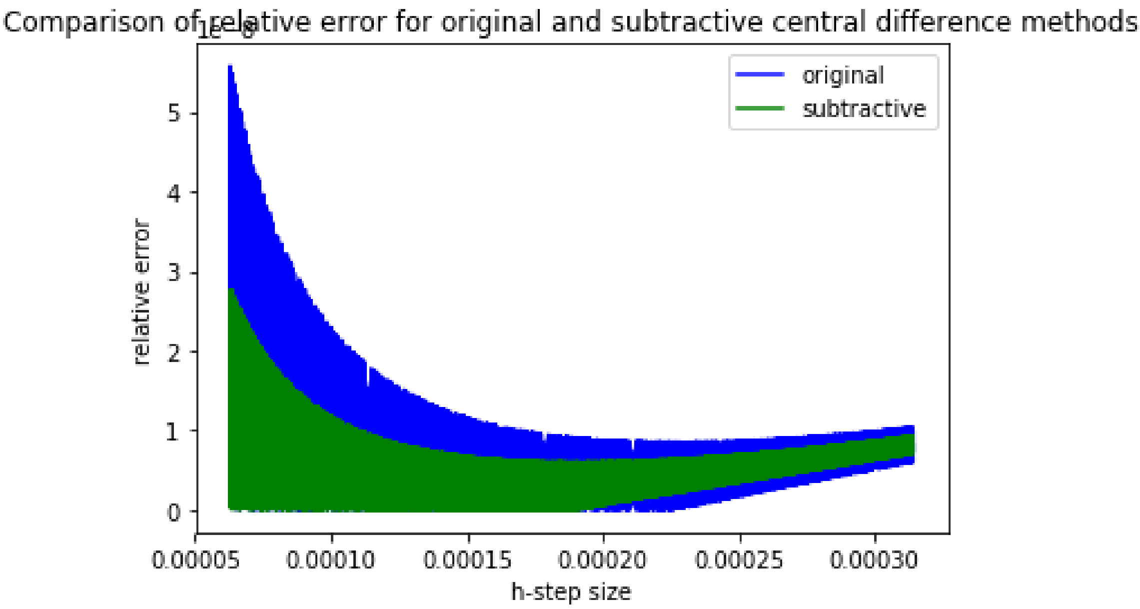


Figure 4.2 shows the minimum value for the relative error to be around $0.7\text{x}10^{-8}$ at a step size, h, of around 0.000175.

Figure 4.3



From this graph (4.3), we can more clearly see the difference in the original and subtractive Central Difference approximations. The subtractive method is more accurate for smaller step sizes (between step size values 0.00010 and 0.00015) and is less suspect to rounding errors at these smaller values. Whereas the original method becomes less accurate below h values of 0.00020. The original method has a higher minimum value than the Subtractive method- with values of $0.85\text{x}10^{-8}$ and $0.7\text{x}10^{-8}$ respectively.

Conclusion

From this investigation, it was established that, while the Central difference approximation does not yield the correct values, it was highly accurate in evaluating the second derivative of cos(x). This was seen in the calculation of the second derivative evaluated at x=π, yielding an answer of 0.992.

Upon plotting the absolute error of the Central difference approximation along the range of 0 to 4π, the expected result of a periodic function was obtained. It is clear from the graph that the minimum absolute error 0.0 at x=(n/2)π and the maximum absolute error is around 0.0082 at x=nπ.

It was then that the step size was varied in order to test the effect of rounding errors. It was found that for the Central Difference approximation, values of h below 0.00020 led to a significant rise in the relative error of the results. Furthermore, values beyond 0.00025 resulted in a rise of smaller gradient in the relative error.

The Subtractive Central Difference approximation was found to produce more accurate values (the relative error was around $0.15\text{x}10^{-8}$units less) and rounding errors occurred at smaller values of h (around 0.00015). This leads to a conclusion that the Subtractive method is ultimately more accurate and utilises machine precision more effectively.