HW1 Computational Physics

9/10

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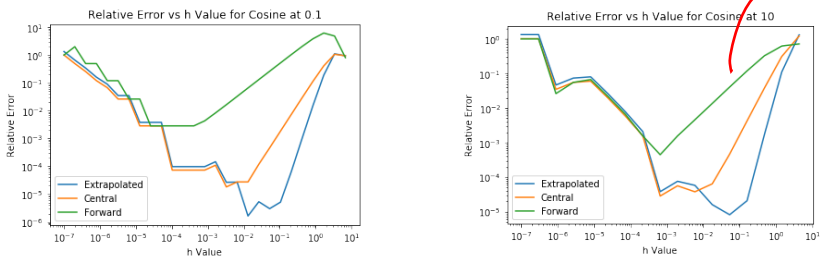
1 Introduction

In this homework, we analyzed numerical methods of integration and differentiation. We started by creating algorithms that implement the forward, central, and extrapolated methods of finding the derivative in single precision, and compared there relative errors. We then did the same thing for integration, using the midpoint, trapezoidal, and Simpson's rules. Finally, we applied these techniques and understandings to integrate power spectra in k space. This gave us a continuous correlation function with respect to comoving distance.

2 Problem 1

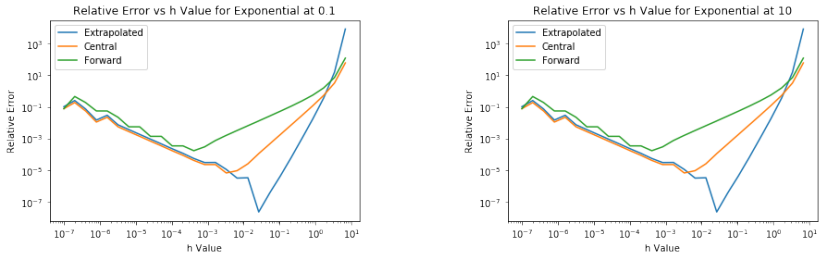
To start off with, we compared the results of using several different methods of numerical derivation. The first method that we used was the forward derivative. This method approximates the derivative at a point to be $\frac{df}{dx}_a = \frac{f(a+h)-f(a)}{h}$ for some small parameter h. Next, we used the central derivative. This method approximated $\frac{df}{dx}_a = \frac{f(a+h/2)-f(a-h/2)}{h}$. This method proves to provide much better accuracy as it is centered on a, rather than on a point a+h. Finally, we used a method called the extrapolated derivative. This method uses a Taylor expansion to reduce the error even further and gives an approximation $\frac{df}{dx}_a = \frac{8f(a+h)-8f(a-h)+f(x+2h-f(x-2h)}{12h}$. This result is even more accurate than the earlier methods. In practice, in single precision, we found that the forward derivative tended to reach a minimum relative error of around 10^{-3} at an h value of around10^{-4}. We also found that the central method had a minimum relative error around 10^{-4} with an optimal h of 10^{-3}. Finally, the extrapolated derivative had a minimum relative error of around 10^{-6} with an optimal h of 10^{-2}. Optimal hs are defined to be such that if we increase the step size of h, we start to see an increase in relative error due to round off error, but if we decrease the size of h, we will see see an increase in relative error due to truncation.

→ Put these as numbered equations, not in the text.



(a) (b)

Figure 1: Plots of different differentiation methods of cosine evaluated at 0.1 (a) and 10 (b)



(a) (b)

Figure 2: Plots of different differentiation methods of an exponential function evaluated at 0.1 (a) and 10 (b)

3 Problem 2

The first method that we used was the midpoint method which approximated the area under a section with $x = [a, a + h]$ to be equal to $h * f(x + h/2)$. This method is not particularly accurate as it approximates a function to be instantaneously constant. The second method that we used was the trapezoidal method. This approximates the area under a section with $x = [a, a + h]$ to be equal to $h/2 * (f(a) + f(a + h))$. This approximation, assumes that the function is linear in the area. However, it actually turns out to be slightly less accurate than the midpoint method, despite being of higher order. The third method that we used was Simpsons rule, which approximates a given section to be quadratic and uses the formula:

$$\int_a^b f(x) = h/3[f(a) + f(b) + \Sigma_{i=1,3,5\ldots N-1} 4 * f(a + hi) + \Sigma_{i=2,4,6\ldots N-2} 2 * f(a + ih)$$

Unfortunately, our calculations of Simpsons rule do not make a lot of sense and we have been unable to determine why. However, the behavior of trapezoidal rule and midpoint rule work very much as we would expect, almost identically,

with midpoint gaining an order two advantage in relative error at a given number of steps. We can also see that at very large number of steps, truncation error begins to become a problem for all of our methods, even the broken Simpsons method, increases until we approach machine precision.

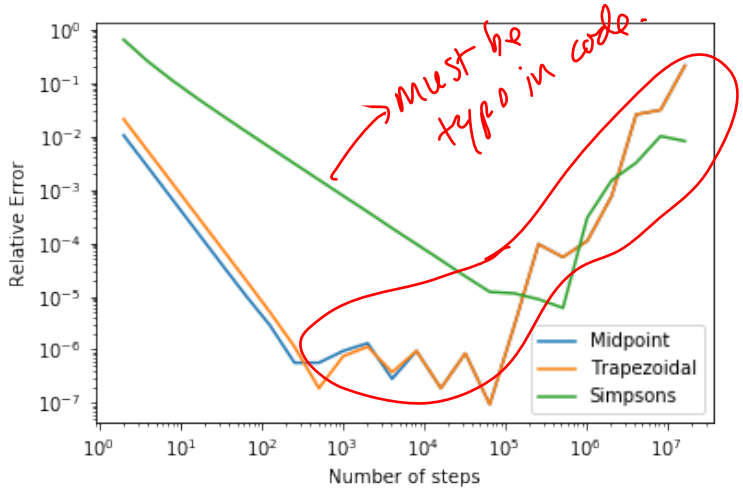
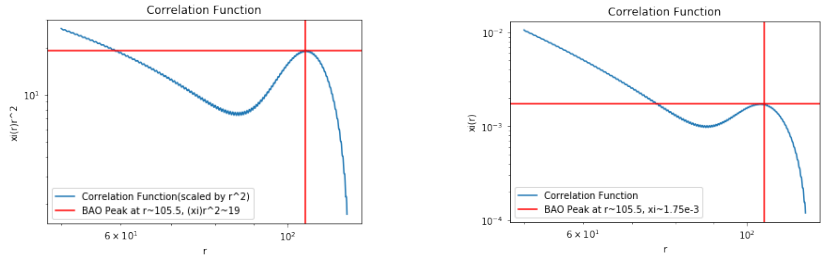


Figure 3

4 Problem 3

In problem 3, we applied the understanding that we gained in problem 2 to a real life problem in astrophysics, finding the correlation function from a set of power spectra in k space. We took all of the points given to us from the data and used cubic spline to interpolate them into a continuous and thus more easily integrable function. After that, took a much higher number of points to perform the integration than would have been possible given the number of data points we were initially given. Having started with around 400 data points, we ended up integrating the function with respect to 5000 points on the interpolated function of power spectrum.



(a) (b)

Figure 4: Plots of the correlation function, both scaled by r^2 (a) and unscaled (b)