PYU33C01

Assignment 2: Numerical Differentiation

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1 Introduction, and theory

In this assignment, I investigated the Richardson extrapolation scheme for reduction of error in the calculation of the numerical derivative. In our case we I analysed $f(x) = xe^x$, with second derivative, $f''(x) = xe^x + 2e^x$, both illustrated below in figure 1.1. The scheme takes advantage of the fact that for different multiples of step size h, we get different values of error for the derivative, $f'(x)$. From this difference in error, we can then eliminate the leading term of error of each successive approximation. Each successive approximation of the derivative is found using formula (1).

$$D_{n+1}(h) := \frac{2^{2n}D_n(h) - D_n(2h)}{2^{2n} - 1} \tag{1.1}$$

Where the first term is in our case is

$$D_1(h) = \frac{f'(x+h) - f'(x-h)}{2h}$$

which finds the second derivative using the central difference method, which was discussed in the last homework. The error is of $O(h^2)$, and it only contains even powers of h. For $D(2)$ this leading error is of order $O(h^4)$. The error continues to be eliminated in this fashion, as n increases.

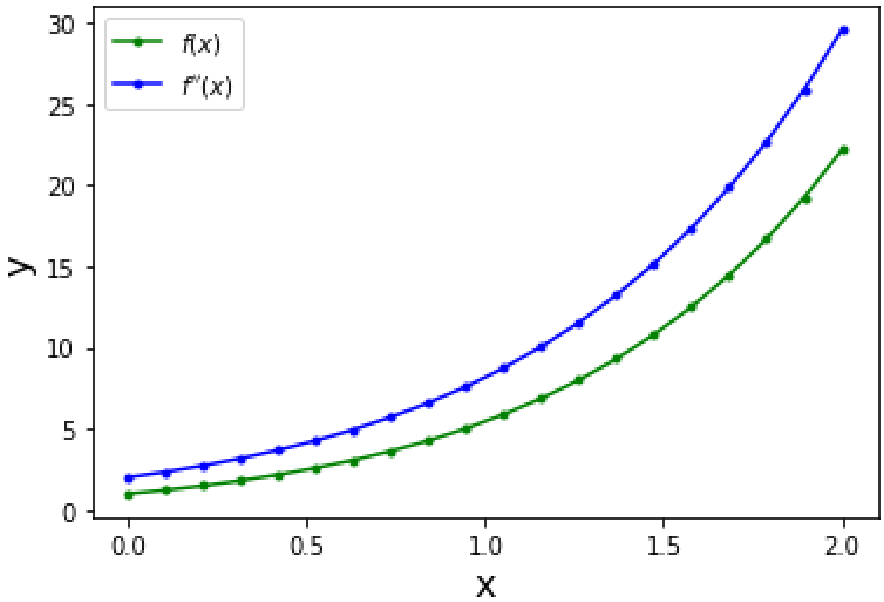

Figure 1.1: Plot of $f(x)$, and $f''(x)$ for $x \in [0, 2]$

2 Table of values obtained via Richardson extrapolation

Below is a table of values for approximations D_1 (standard central difference), D_2, D_3, and D_4. The second derivative was evaluated at $x = 2$,with analytical value $\frac{d^2f}{dx^2}|_{x=2} =$ 29.5562243957226. From this table we see that for a smaller step correlates with a higher accuracy of approximation, which is as to be expected. What is also evident, is that as the order of approximation increases, the accuracy at a larger step size h also increases.

h	D_1	D_2	D_3	D_4
0.001	29.55623178477751	29.556224395719255	29.556224395721365	29.556224395721404
0.1	29.630164231749205	29.556027060804823	29.556225337305438	29.55622438562351
0.2	29.852575744582353	29.553052913295577	29.556285293266885	29.556221739291917
0.3	30.225240238708544	29.540048927839482	29.556930311102317	29.55615315511096
0.4	30.75114423844268	29.504567213725995	29.560289193689908	29.555465867843633

3 using richardson extrapolation find $\frac{d^2f}{dx^2}|_{x=2}$ to the highest possible accuracy

Here we note from the table in section 2, that our approximation $D_4(h)$ is, as expected, the best approximation for the second derivative. So in order to find the highest accuracy possible, it is natural analyse $D_4(h)$. Using the while loop

```
while rel_error_numD4(p,k)>=rel_error_numD4(p,k-0.001):
    k=k-0.001
```

I found the the value of h, corrosponding to the minimum value of relative error to be $h = 0.02899$, which yields the most accurate value of relative error to be 1.27432×10^{-14}. An incredibly accurate result. Below in figure 3.1, I have illustrated the error around that point below.

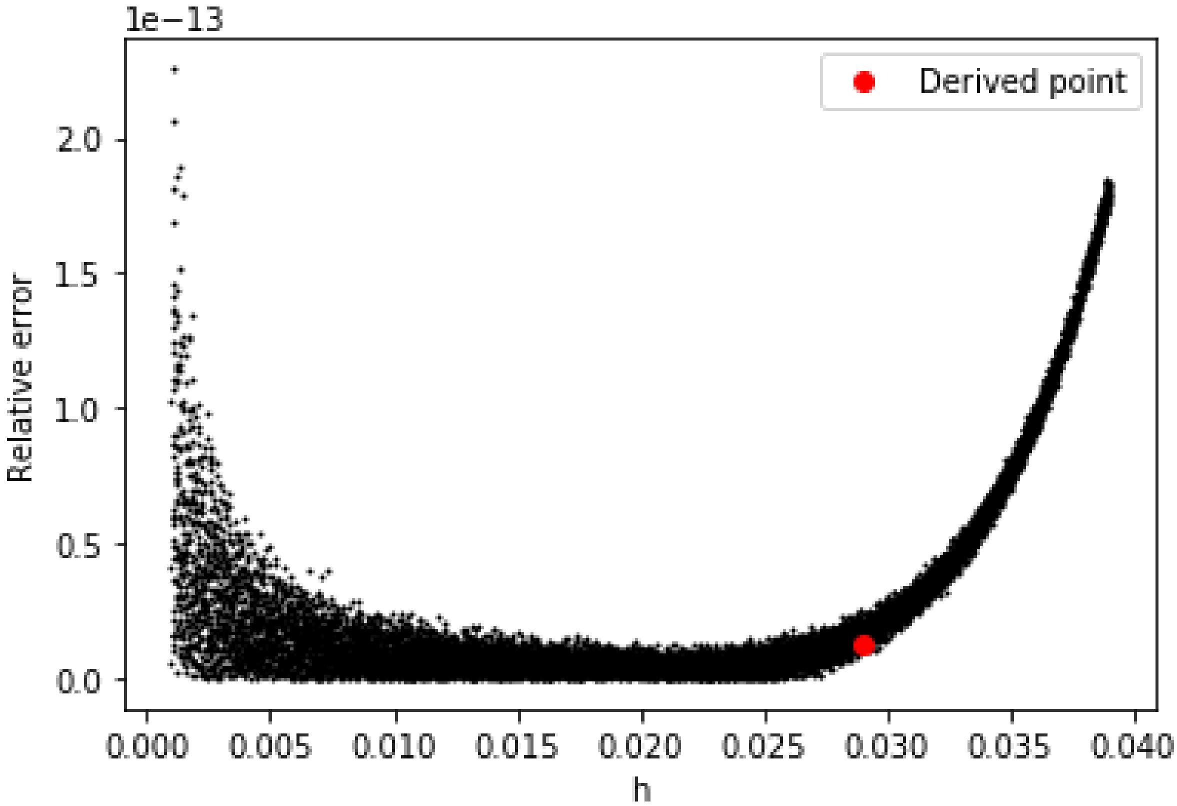

Figure 3.1: Relative error about the point of minimum error

This figure suggest that I have indeed found the most accurate value of relative error achievable. We also note the shape of the plot, which seems to be exponentially rising as h increases, and as h decreases about $h = 0.02$.

4 Examination of scaling relations

It seems that the error as h decreases is a sort of exponential relationship. To test this hypothesis, I have plotted log-log plots of the absolute error of each of the expressions D_i. In order to avoid any input from rounding errors, I started with $h = 0.028$, as any lower and the input from rounding error means the error doesn't reduce further.

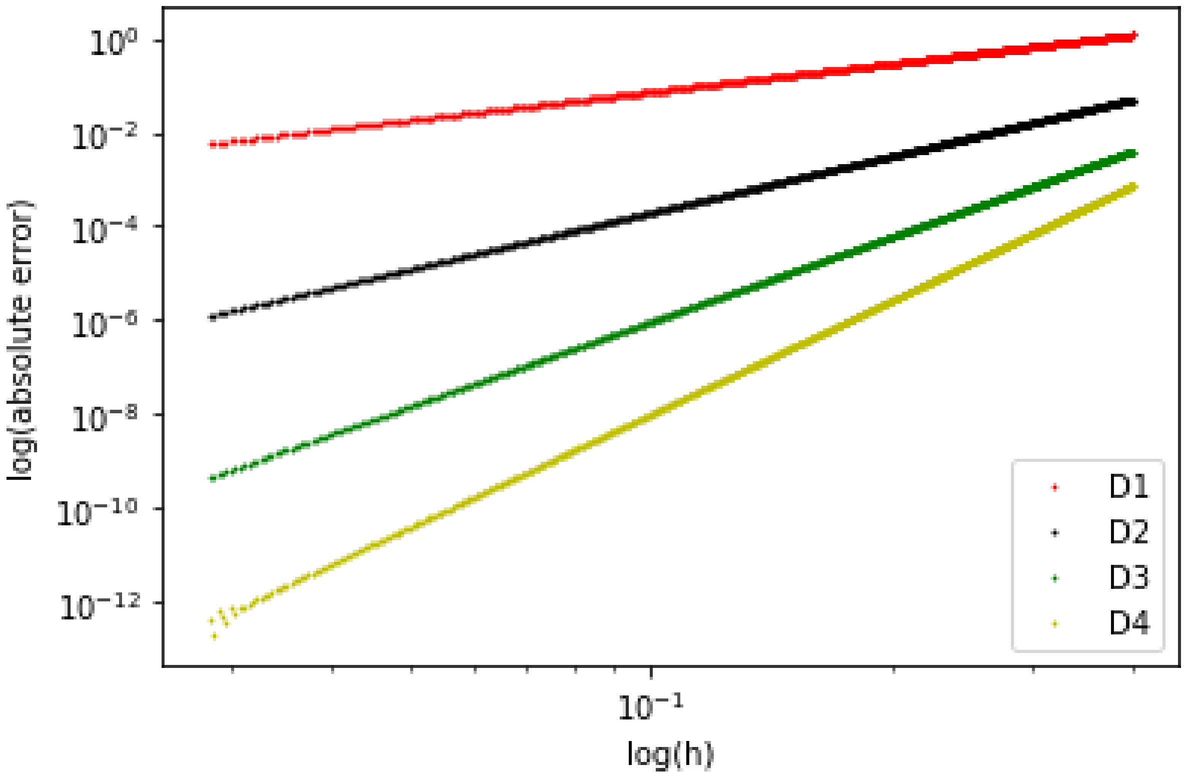

Figure 4.1: Log-log plot of the scaling relations

Clearly each D_i exhibit unique linear relations, and thus the absolute error increases exponentially in h. This agrees perfectly with theory. Also, the slope of D_4 is the steepest, as it corresponds to a higher order of h present in the theoretically derived error. This is consistent with throughout, with the slope of the successive expression being greater then the previous.

Now from theory our error should be of order $2i$, where i is the order of approximation. I took the slope of graph 4.1, and found the values

$$D_1 \ \ slope = 2.0042,$$

$$D_2 \ \ slope = 4.0093,$$

$$D_3 \ \ slope = 6.0219,$$

$$D_4 \ \ slope = 8.061,$$

which all agree within reason with the hypothesis that the error is of order $2i$.

5 Examination of rounding error as h decreases

Again, from examining figure 3.1, I suspect an exponential relationship for the increase of rounding error as h decreases. So I plotted a log-log of the four relations error again, but this time, up to $h = 0.28$, where in 3.1 we see rounding error creep in.

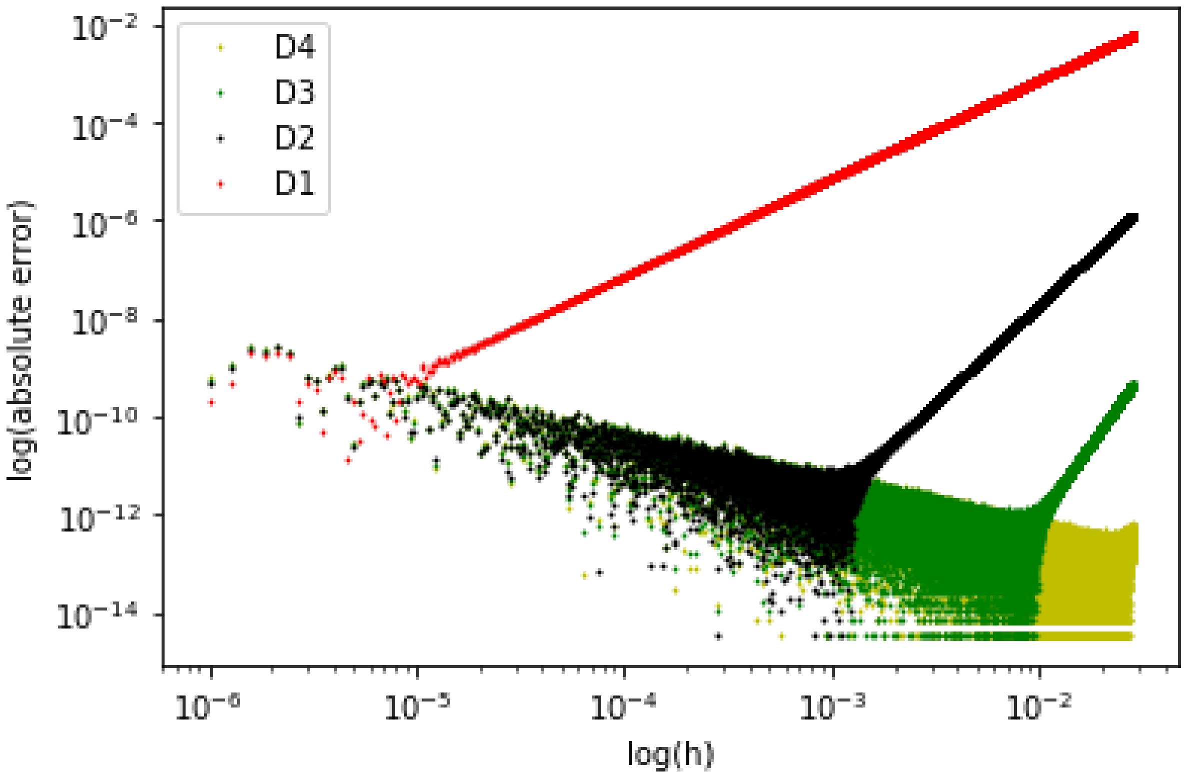

Figure 5.1: Log-log plot of the rounding error relation

From this figure, we see that the error starts rises exponentially, after a critical point in each D_i, as h decreases. At this point, the rounding error takes over, and the further reduction of h has the opposite effect. What I found surprising, was that each of these four critical points are co-linear (in this log-log representation). This line acts as an upper limit on how un-accurate each approximation can be when it goes under the critical value of h. Another interesting observation of this dataset, is that we see that the difference in the minimum error decreases as i increases. This leads me to believe that eventually when that creating a higher order of D_i will eventually lead to to no real benefit in reduction of error.

I found the slope of this line to be

$$\textit{Rounding error slope} = -1.002,$$

which corresponds to the slope of the rounding error being of order -1.