Numeric Differentiation Report

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11 February 2022

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1 Introduction

This report details various numerical methods of taking the derivative of the function:

$$y(t) = e^{-t^2} \tag{1}$$

The various methods detailed in further parts will be compared based on the RMS error, which for N points can be computed as

$$RMS = \sqrt{\frac{\sum \left| x_f^2 - x_n^2 \right|}{N}} \tag{2}$$

where x_n represents the calculated version of the derivative and x_f represents the empirical functional form of the derivative

$$y'(t) = -2te^{-t^2} (3)$$

1.1 Various Notes

In this project, all code was completed in Python and all plots were generated with Matplotlib. Because of the use of Python, no issues with floating point arithmetic were detected as h was decreased. In addition, an RMS error of 1×10^{-3} was classified as the threshold for good evaluation. Finally, all computations were done in the range [-10, 10].

1.2 Sample Plots

Fig. 1 depicts a graph of y(t) with 100 sample points, which will serve as a benchmark for the derivatives that will be estimated in the further parts of this project.

2 Slope Derivative

For the slope derivative, the derivative in each interval (t, t + h) was calculated as

$$y' = \frac{y(t+h) - y(t)}{h} \tag{4}$$

Specifically, three locations for assigning y' were explored. In the left sided case, the calculated derivative in the interval was assigned to y'(t) and in the right sided case, the derivative in the interval was assigned to y'(t+h). In the mid-sided case, the derivative was assigned to $y'(t+\frac{h}{2})$. In all cases, the RMS error was computed with n-1 points because with n sampling locations, there would be n-1 pairs of adjacent points and thus n-1 intervals to sample.

Table 1 depicts the RMS Error in Slope Derivatives against the number of iterations, with left-sided and right-sided derivatives reaching "good" results in around 4400 iterations and middle-sided

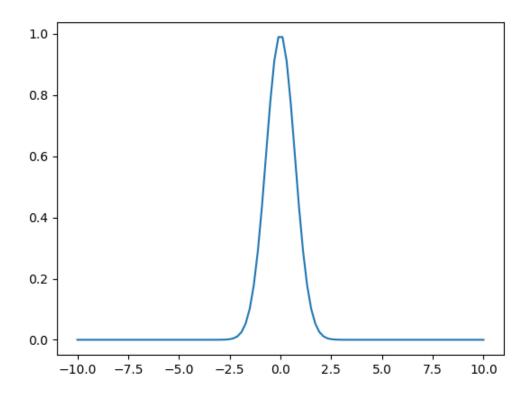


Figure 1: Figure 1 depicts a sample graph of y(t) taking a sample of 100 points.

Table 1: RMS Error in Slope Derivatives

# Iterations	Left-Sided	Middle-Sided	Right-Sided
20	0.21087	0.01953	0.21087
50	0.08647	0.00663	0.08647
100	0.04354	0.00164	0.04354
130	0.03349	0.00097	0.03349
200	0.02175	0.00041	0.02175
500	0.00868	6.4885 e - 05	0.00868
1000	0.00434	1.6190e-05	0.00434
2000	0.00217	4.0437e-06	0.00217
4400	0.00099	8.3503e-07	0.00099
5000	0.00087	6.4661e-07	0.00087

derivative reaching "good" results in around 130 iterations. In addition, the RMS Error for left-sided and right-sided derivative converges approximately linearly as the number of iterations increases. However, the RMS Error for the middle-sided derivative converges approximately quadratically as the number of iterations increases.

Thus, I would recommend choosing the assignment point at the middle of the interval (x, x + h), because it reaches "good" results by far the fastest and also has the highest rate of convergence.

2.1 Sample Plots

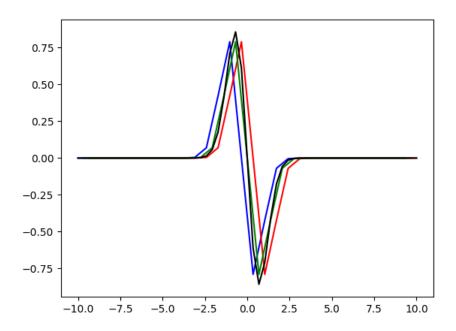


Figure 2: Figure 2 depicts a sample graph of y'(t) with the left-sided slope derivative in blue, mid-sided in green, and right-sided in red, taking a sample of 30 points.

Fig. 2 depicts the graphs of y'(t) with the left-sided slope derivative in blue, mid-sided in green, and right-sided in red, taking a sample of 30 points. As seen, the mid-sided derivative is closest to the actual value, reaching a much lower RMS value.

3 Three-Point Derivative

For the three point derivative, the midpoint slope derivative was first calculated. Then, the threepoint derivative was calculated as the average of the two midpoint derivatives on the edges of the interval observed. Contextualizing the values in terms of y and h, the three-point derivative was calculated as

$$y'(t) = \frac{y(t+h) - y(t-h)}{2h}$$
 (5)

In this case, n-2 points were generated and used to calculate the convergence of RMS error.

Table 2: RMS Error in Three-Point Derivatives

# Iterations	RMS Error
20	0.16280
50	0.02568
100	0.00653
200	0.00163
260	0.0097
500	0.00026

As shown in Table 2, the three-point derivative reaches "good" results in around 260 iterations and converges approximately quadratically as the number of iterations increases.

3.1 Sample Plots

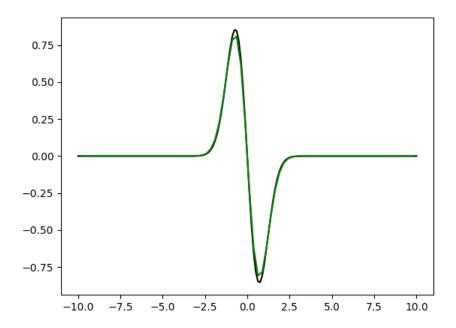


Figure 3: Figure 3 depicts a sample graph of y'(t) with the three-point derivative in green, taking a sample of 80 points.

Fig. 3 depicts the graph of y'(t) with the three-point derivative in green, taking a sample of 80 points. As seen, the three-point derivative looks similar to the mid-sided derivative.

4 Parabola Fit

For the parabola fit, the three adjacent points (t_1, y_1) , (t_2, y_2) , and (t_3, y_3) were fit to the parabola $y = at^2 + bt + c$. Then, the derivative at the middle point was calculated as

$$y'(t_2) = 2at_2 + b (6)$$

For the two endpoints, a similar procedure was used, except at the edges of the interval, resulting in the creation of n derivative points.

To calculate the fit, the system of equations

$$\begin{cases} at_1^2 + bt_1 + c = y_1 \\ at_2^2 + bt_2 + c = y_2 \\ at_3^2 + bt_3 + c = y_3 \end{cases}$$
(7)

was solved. The first step was eliminating the term c, which was achieved by subtracting the second equation from the first and the third equation from the second to derive

$$\begin{cases}
 a(t_1^2 - t_2^2) + b(t_1 - t_2) = (y_1 - y_2) \\
 a(t_2^2 - t_3^2) + b(t_2 - t_3) = (y_2 - y_3)
\end{cases}$$
(8)

With these two equations, the first equation was multiplied by $(t_3 - t_2)$ and the second equation was multiplied by $(t_1 - t_2)$. Then, the two equations were added to reach

$$a\left((t_1^2 - t_2^2)(t_3 - t_2) + (t_2^2 - t_3^2)(t_1 - t_2)\right) = (y_1 - y_2)(t_3 - t_2) + (y_2 - y_3)(t_1 - t_2) \tag{9}$$

Finally, this equation can be solved to find

$$a = \frac{(y_1 - y_2)(t_3 - t_2) + (y_1 - y_3)(t_1 - t_2)}{(t_1 - t_2)(t_2 - t_3)(t_3 - t_1)}$$

$$(10)$$

Substituting into the equation $a(t_1^2 - t_2^2) + b(t_1 - t_2) = (y_1 - y_2)$, this equation can be solved to find

$$b = \frac{(y_1 - y_2) - a(t_1^2 - t_2^2)}{(t_1 - t_2)} \tag{11}$$

In the code, these expressions were used to compute a and b, which can be substituted into the expression for the numerical value of the derivative, which were evaluated for RMS error over n points.

Table 3: RMS Error in Parabola Derivatives

# Iterations	RMS Error
20	0.27218
50	0.10195
100	0.04772
130	0.03600
200	0.02283
500	0.00886
1000	0.00438
2000	0.00218
4400	0.00099
5000	0.00087

As shown in Table 3, the parabola derivative achieves "good" results in around 4400 iterations and converges approximately linearly as the number of iterations increases. This amount is approximately the same as that for the left and right-sided slope derivative but much worse than the midpoint slope derivative and the three-point derivative, meaning that the parabola derivative is not a good solution.

4.1 Sample Plots

Fig. 4 depicts a sample graph of y'(t) with the parabola derivative in red, taking a sample of 50 points. As seen in the graph, the parabola derivative is similar to the left-sided slope derivative.

5 Five-Point Stencil

In the five-point stencil, the derivative is calculated using a set of five points chosen using the third-order Taylor series approximations of the function y(t). Contextualizing the values in terms of y and h, the five-point stencil was calculated,

$$y'(t) = \frac{y(t-2h) - 8y(t-h) + 8y(t+h) - y(t+2h)}{12h}$$
(12)

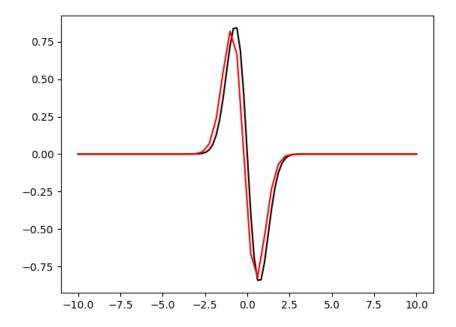


Figure 4: Figure 4 depicts a sample graph of y'(t) with the parabola derivative in red, taking a sample of 50 points.

In this case, n-4 derivative points were generated and used to calculate the convergence of RMS error.

Table 4: RMS Error in Five-Point Stencil

# Iterations	RMS Error
20	0.14456
50	0.00595
80	0.00099
100	0.00041

As shown in Table 4, the five-point stencil achieves "good" results in around 80 iterations and converges approximately quartically as the number of iterations increase. These results cement the five-point stencil as the best derivative scheme, as they have the least number of points required to produce "good" results and also have the fastest convergence rate.

5.1 Sample Plots

Fig. 5 depicts a sample graph of y'(t) with the five-point stencil in blue, taking a sample of 50 points.

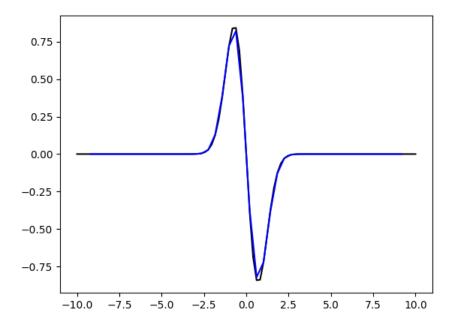


Figure 5: Figure 5 depicts a sample graph of y'(t) with the five-point stencil in blue, taking a sample of 50 points.

6 Conclusion

Thus, through this analysis, the five-point stencil emerged as the best derivative algorithm, converging and reaching "good" results the fastest. Conversely, the left-sided slope, the right-sided-slope, and parabola derivatives were the slowest, with the mid-sided slope and three-point derivatives in the middle.