Numerical Differentiation and Integration

Cody Maxwell

November 2023

1 Introduction

Numerical differentiation and numerical integration are used in Numerical Analysis for approximating derivatives at some point x_0 and integrals on some interval $[a, b]$. Approximations of derivatives and integrals are often necessary, since many functions that are important to several fields of study often do not have easy or elementary derivatives or antiderivatives. Other times times, in the case of derivatives, may not have access to the function and only points that lie on the function. In either case, the only viable option is to employ numerical approximations. To illustrate the numerical methods in this paper we will implement them in two problems.

For numerical differentiation, we will approximate the first derivative of the function

$$f(x) = \frac{\sin(x)}{1 + e^x}$$

at $x = 0.4$ using step sizes $h = 0.1, 0.05, 0.025, 0.0125, 0.00625$, and 0.003125 with the methods in Section 2.

For numerical integration, we will approximate the integral

$$\int_0^\pi \sin(x)\, dx$$

using $n = 2, 4, 8, 16, 32$, and 64 intervals with the methods in Section 3.

1.1 Applications - Physics

One obvious application of both numerical integration and numerical differentiation is a field of study we often turn to for math applications, Physics. In Physics, one often generates a discrete set of data points via experimentation. For numerical differentiation, suppose we are driving a vehicle and we log the speed of the vehicle every 2 seconds. Given this data, we may approximate the acceleration of the vehicle in any numbers of ways depending on how many measurements were made. If we logged our speed at $t = \{0, 2, 4, 6, 8, 10\}$ and we wish to approximate our acceleration at $t = 4$, so of the methods we have at our disposal are Two-Point Backward Difference, Three-Point Central Difference, Five-Point Central Difference and many more.

On the other hand, for numerical integration, we have the following problem. Suppose we want to calculate the Work down on some mass as it is moved through a force field. We will assume the path is $y = x$ to simplify the integral for this example, but it is worth noting that this method is more broadly applicable to this type of problem. Note that P and Q are the starting and ending points of the path taken respectively through the force field F. Work is given as

$$W = \int_P^Q F \cdot dr = \int_P^Q (F_x, F_y) \cdot (dx, dy)$$

or as

$$W = \int_{x_0}^{x_1} (a(x, x) + b(x, x))dx$$

after factoring in our assumptions and noting that F_x is the x-component of the 2D force field. And assuming that $F(x, y) = \langle a(x, y), b(x, y)\rangle$.
From this point we may approximate this definite integral with as little error as our heart desires or within the limitations of the hardware we decide to use. Usually the force field is given as a function F is given as a function that has an elementary anti-derivative, but when that is not the case, the numerical integration techniques discussed in this paper as well as several others may be used to ensure an adequate amount of accuracy in problems like the one we have just discussed.

2 Numerical Methods - Differentiation

Two-point Backward Difference:
An $O(h)$ numerical differentiation scheme that makes use of two points.

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

Three-point Backward Difference:
An $O(h^2)$ numerical differentiation scheme that makes use of three points.

$$f'(x) = \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} + \frac{h^2}{3}f'''(\xi)$$

Three-point Central Difference:
An $O(h^2)$ numerical differentiation scheme that makes use of three points.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}f'''(\xi)$$

Five-point Central Difference:
An $O(h^4)$ numerical differentiation scheme that makes use of five points.

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{h^4}{30}f^{(5)}(\xi)$$

3 Numerical Methods - Integration

Midpoint Rule:
An $O(h^2)$ numerical integration scheme which sums over n subintervals, using the a linear combination of the midpoints of each subinterval.

$$\int_a^b f(x)dx = h\sum_{k=1}^{n} f\left(\frac{x_{k-1} + x_k}{2}\right) + \frac{h^2}{24}(b-a)f''(\xi)$$

Trapezoidal Rule:
An $O(h^2)$ numerical integration scheme which sums over n subintervals, using the a linear combination of the endpoints of each subinterval.

$$\int_a^b f(x)dx = \frac{h}{2}\sum_{k=1}^{n}(f(x_{k-1}) + f(x_k)) - \frac{h^2}{12}(b-a)f''(\xi)$$

Simpson's Rule:
An $O(h^2)$ numerical integration scheme which sums over n subintervals, using the a linear combination of the endpoints and midpoints of each subinterval.

$$\int_a^b f(x)dx = \frac{h}{6}\sum_{k=1}^{n}\left(f(x_{k-1}) + 4f\left(\frac{x_{k-1} + x_k}{2}\right) + f(x_k)\right) - \frac{h^4}{2880}(b-a)f^{(4)}(\xi)$$

Boole's Rule:
An $O(h^4)$ numerical integration scheme which sums over n subintervals, using the a linear combination of the endpoints and other other points in each subinterval.

$$\int_a^b f(x)dx = \frac{h}{90}\sum_{k=1}^{n}\left(7f(x_{k-1}) + 32f\left(\frac{3x_{k-1}+x_k}{4}\right) + 12f\left(\frac{x_{k-1}+x_k}{2}\right) + 32f\left(\frac{x_{k-1}+3x_k}{4}\right) + 7f(x_k)\right) + \text{error term}$$

4 Numerical Results - Differentiation

4.1 Tables of Errors and Approximations

For the following tables we find the Absolute Error by using the exact answer found using standard derivative rules. That exact value is 0.276071201354 given to the precision of the program I used for the calculations.

Two-Point Backward Difference:

h	Approximate Value of $f'(0.4)$	Absolute Error
0.1	0.305175507689	$2.910430633517 \cdot 10^{-2}$
0.05	0.290609206343	$1.453800498882 \cdot 10^{-2}$
0.025	0.283334061239	$7.262859884921 \cdot 10^{-3}$
0.0125	0.279700775559	$3.629574205277 \cdot 10^{-3}$
0.00625	0.277885484878	$1.814283523882 \cdot 10^{-3}$
0.003125	0.276978212289	$9.070109350430 \cdot 10^{-4}$

Exact Order of Accuracy: 1

Estimated Order of Accuracy
1.001403327464853
1.001219652724978
1.000737435989671
1.000400383819446
1.000208078755238

Three-Point Backward Difference:

h	Approximate Value of $f'(0.4)$	Absolute Error
0.1	0.276129977146	$5.877579234687 \cdot 10^{-5}$
0.05	0.276042904996	$2.829635752671 \cdot 10^{-5}$
0.025	0.276058916135	$1.228521897700 \cdot 10^{-5}$
0.0125	0.276067489880	$3.711474366619 \cdot 10^{-6}$
0.00625	0.276070194196	$1.007157512833 \cdot 10^{-6}$
0.003125	0.276070939700	$2.616537962963 \cdot 10^{-7}$

Exact Order of Accuracy: 2

Estimated Order of Accuracy
1.054605729913330
1.203692779689015
1.726859263160298
1.881703075832623
1.944558232971566

Three-Point Central Difference:

h	Approximate Value of $f'(0.4)$	Absolute Error
0.1	0.276209015527	$1.378141732190 \cdot 10^{-4}$
0.05	0.276105877374	$3.467601960722 \cdot 10^{-5}$
0.025	0.276079884284	$8.682930084492 \cdot 10^{-6}$
0.0125	0.276073372957	$2.171603125212 \cdot 10^{-6}$
0.00625	0.276071744309	$5.429551542813 \cdot 10^{-7}$
0.003125	0.276071337096	$1.357421509640 \cdot 10^{-7}$

Exact Order of Accuracy: 2

Estimated Order of Accuracy
1.990714057695103
1.997684431582367
1.999421502011523
1.999855517433377
1.999964263356975

Five-Point Central Difference:

h	Approximate Value of $f'(0.4)$	Absolute Error
0.1	0.276075919716	$4.718362306755 \cdot 10^{-6}$
0.05	0.276071497989	$2.966350698408 \cdot 10^{-7}$
0.025	0.276071219921	$1.856691023150 \cdot 10^{-8}$
0.0125	0.276071202515	$1.160805396250 \cdot 10^{-9}$
0.00625	0.276071201426	$7.249839617529 \cdot 10^{-11}$
0.003125	0.276071201358	$4.486133686754 \cdot 10^{-12}$

Exact Order of Accuracy: 4

Estimated Order of Accuracy
3.991525126016958
3.997883513600172
3.999535716241731
4.001033241102422
4.014404561398578

4.2 Graph of Errors with respect to h

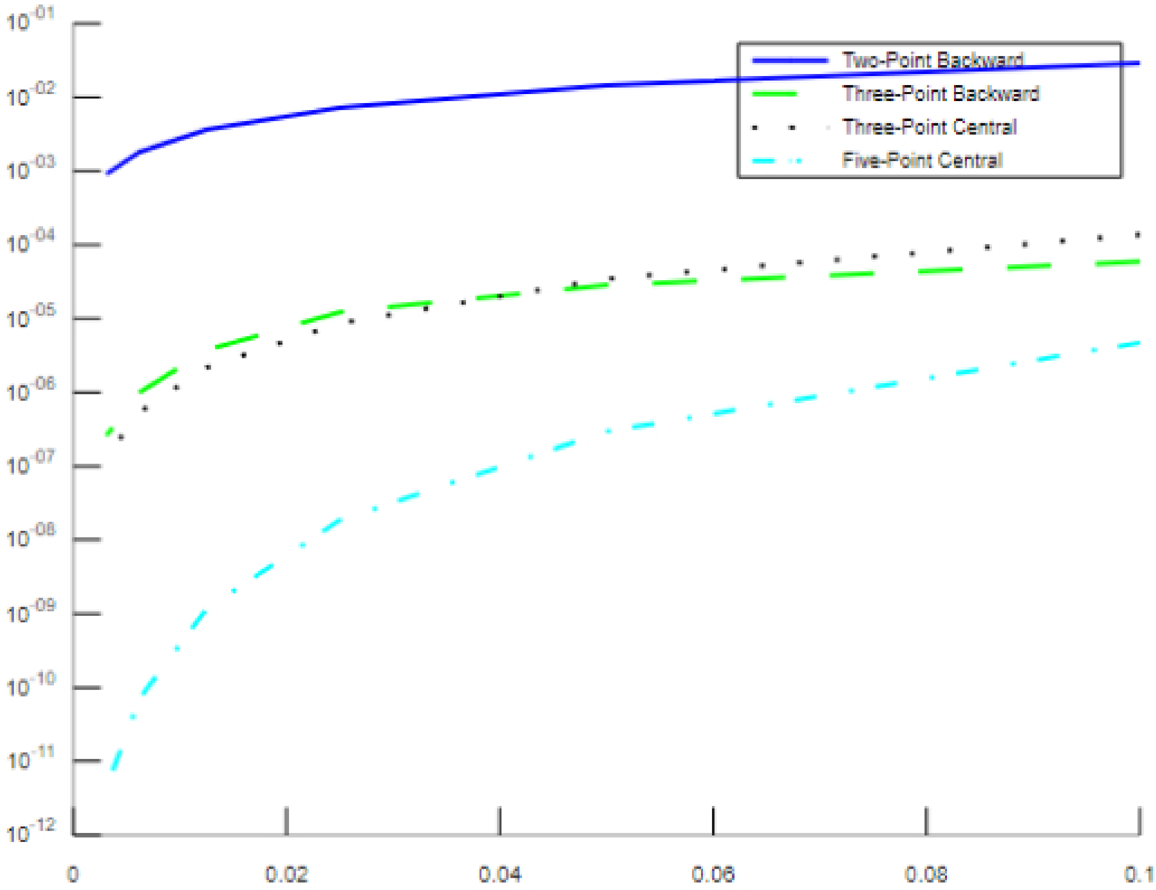

Figure 1: Errors against h

In the above plot, I graphed the errors of the methods against h, so we can see as h increases, so does the error. However it is also true that as h decreases the error also decreases. It's also worth noting that the estimation of the Order of accuracy agrees with the exact order of accuracy.

5 Numerical Results - Integration

5.1 Tables of Errors and Approximations

For the following tables, we make use of the fact that the integral discussed in Section 1 has an exact value of 2 in order to calculate the Absolute Error.

Midpoint Rule

n	Approximate Value	Absolute Error
2	2.221441469079	$2.214414690792 \cdot 10^{-1}$
4	2.052344305954	$5.234430595406 \cdot 10^{-2}$
8	2.012909085599	$1.290908559913 \cdot 10^{-2}$
16	2.003216378168	$3.216378167950 \cdot 10^{-3}$
32	2.000803416310	$8.034163099300 \cdot 10^{-4}$
64	2.000200811728	$2.008117283672 \cdot 10^{-4}$

Exact Order of Accuracy: 2

Estimated Order of Accuracy
2.080820905649389
2.019645795884853
2.004877865051498
2.001217387842432
2.000304217376749

Trapezoidal Rule

n	Approximate Value	Absolute Error
2	1.570796326795	$4.292036732051 \cdot 10^{-1}$
4	1.896118897937	$1.038811020630 \cdot 10^{-1}$
8	1.974231601946	$2.576839805445 \cdot 10^{-2}$
16	1.993570343772	$6.429656227661 \cdot 10^{-3}$
32	1.998393360970	$1.606639029856 \cdot 10^{-3}$
64	1.999598388640	$4.016113599608 \cdot 10^{-4}$

Exact Order of Accuracy: 2

Estimated Order of Accuracy
2.046729198400550
2.011258467611465
2.002789343254670
2.000695774267732
2.000173846255759

Simpson's Rule

n	Approximate Value	Absolute Error
2	2.004559754984	$4.559754984421 \cdot 10^{-3}$
4	2.000269169948	$2.691699483877 \cdot 10^{-4}$
8	2.000016591048	$1.659104793550 \cdot 10^{-5}$
16	2.000001033369	$1.033369412706 \cdot 10^{-6}$
32	2.000000064530	$6.453000178652 \cdot 10^{-8}$
64	2.000000004032	$4.032258971165 \cdot 10^{-9}$

Exact Order of Accuracy: 4

Estimated Order of Accuracy
4.082367050509514
4.020040429727343
4.004977022233515
4.001242210701076
4.000309861647120

Boole's Rule

n	Approximate Value	Absolute Error
2	1.999983130946	$1.686905401455 \cdot 10^{-5}$
4	1.999999752455	$2.475454277118 \cdot 10^{-7}$
8	1.999999996191	$3.809155879608 \cdot 10^{-9}$
16	1.999999999941	$5.929212676392 \cdot 10^{-11}$
32	1.999999999999	$9.257039579325 \cdot 10^{-13}$
64	2.000000000000	$1.332267629550 \cdot 10^{-14}$

Exact Order of Accuracy: 6

Estimated Order of Accuracy
6.090541959744963
6.022078164439768
6.005486971314586
6.001145845470761
6.118595061199871

5.2 Graph of Errors with respect to n

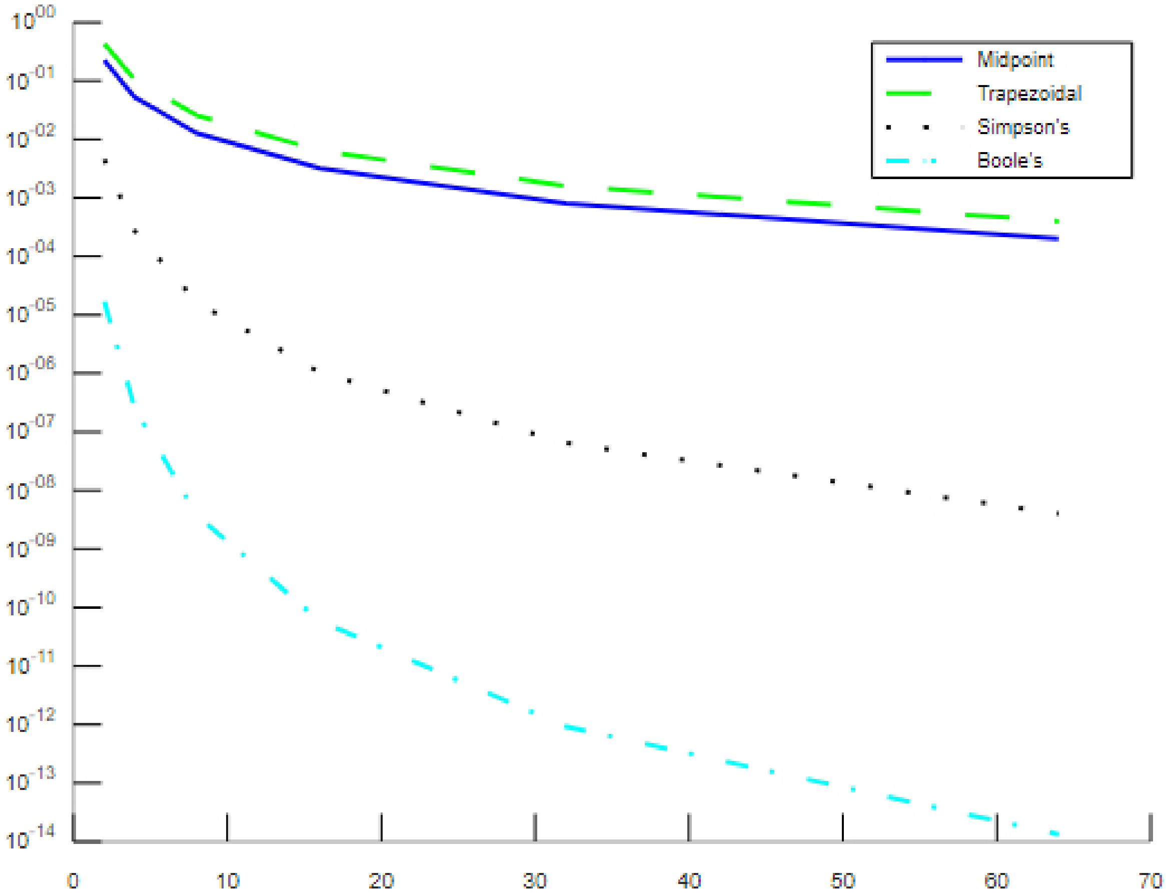

Figure 2: Errors against n

In the above graphic we see that as n increases, the error conversely decreases. And again, we should notice that the estimation of the order is appears to approach the true order of accuracy.

6 Conclusion and Discussion

In conclusion, numerical differentiation and numerical integration are vital to several fields of study, particularly in the sciences, such as physics, engineering and others. And since they are necessary, they must be studied carefully to understand the error bound, so that we known they are actually useful. To demonstrate how they can be used we looked at two problems. The first was, given

$$f(x) = \frac{\sin(x)}{1 + e^x}$$

find $f'(0.4)$ using the four numerical differentiation techniques. And the second problem was to approximate the integral

$$\int_0^\pi \sin(x)\, dx$$

using the four numerical integration techniques. However, one may ask, "Why do we need so many methods?"

The answer is fairly straightforward, we need this many methods, because there are many different kinds of problems and situations that we find ourselves in when we want answers. Depending on the information given and the tools at our disposal we may not be able to use just any method. For example, if we only have three points, we can't use the Five-point central difference. And similarly, if our machine has a small machine epsilon, there would be no point in using Boole's rule to calculate some definite integral. It may be clear to the reader at this point why developing such methods of approximation is a field of its own and is still actively being developed as it is quite interesting and useful for problem solving.

As a closing remark, I would like to acknowledge one last time that the estimated order of accuracy agree with the theoretical value and every numerical method we use involves some give and take. In general, to increase the order of any given method, you need more information.