ESC407 Lab 1

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1. Central Differences for Numerical Differentiation

   (a) The derivative of $f(x) = e^{2x}$ was calculated numerically at $x = 0$, using central differences. Table 1 lists the numerically computed value of $f'(0)$ for different step sizes h between 10^{-16} and 1.

h	10^{-16}	10^{-15}	10^{-14}	10^{-13}	10^{-12}	
$f'(0)$	1.11022302	2.10942375	1.99840144	1.99951167	2.00006678	
h	10^{-11}	10^{-10}	10^{-9}	10^{-8}	10^{-7}	10^{-6}
$f'(0)$	2.00000017	2.00000017	2.00000005	1.99999999	2.	2.
h	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{0}
$f'(0)$	2.	2.	2.00000033	2.00003333	2.003335	2.35040239

Table 1: Derivative of $f(x) = e^{2x}$ at $x = 0$ for different h values

The raw output from the code is

```
1 a) errors:  [1.11022302 2.10942375 1.99840144 1.99951167 2.00006678 2.00000017
2.00000017 2.00000005 1.99999999 2.         2.         2.
2.         2.00000033 2.00003333 2.003335   2.35040239]
```

   (b) The minimum in error and the corresponding step size matches the expected value, calculated using $C = 10^{-16}$. The calculated error as a function of h is shown in fig 1. The estimated optimal step size is 6.7×10^{-6}, with a corresponding error of 4.48×10^{-11}.

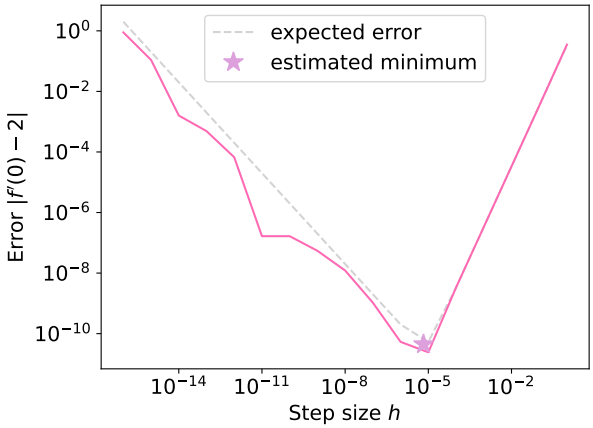

Figure 1: Calculated error vs h

(c) The first 10 derivatives of $f'(x)$ at $x = 0$ calculated using central differences with the optimal step size (which is the same for all derivatives of $f(x)$) are listed in table 2. The raw output from the

m	1	2	3	4	5
$f'(0)$	2	4	7.77	-2.21×10^{5}	8.26×10^{9}
	6	7	8	9	10
	2.22×10^{16}	-3.69×10^{20}	-2.12×10^{27}	2.06×10^{31}	2.0×10^{38}

Table 2: Approximate values for $f^m(0)$ computed using central differences

code is:

```
1 c) derivatives:  [2.0000000000234888, 4.000001933007014, 7.77155789571232,
    -221126.08039335813, 8258210993.557659, 2.2204420456714464e+16,
    -3.68559504405105e+20, -2.1195518363153336e+27, 2.05607099203305e+31,
    1.971716534777767e+38]
```

2. Integrating the Dawson Function Again

(a) Fig 2 shows the Dawson function at $x = 4$ evaluated using trapezoidal rule, Simpson's rule and gaussian quadrature for varying integration slices N. The function calculated using gaussian quadrature converges much more quickly than integration schemes using Newton-Cotes formulae.

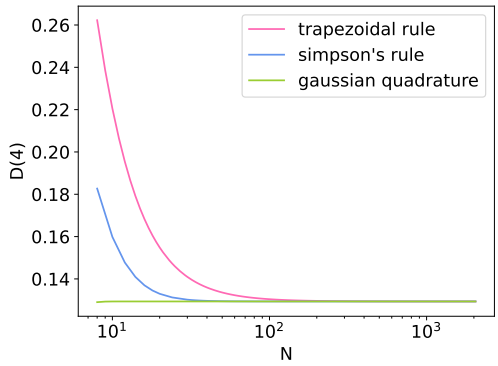

Figure 2: Dawson function $D(x)$ at $x = 4$ calculated numerically vs number of integration slices N

(b) The error on $D(4)$ using gaussian quadrature, $I_{2N} - I_N$ for the values of N in 2a) are plotted in fig 3. The error decreases quickly from $N = 8$ to around $N = 20$, and then remains around the machine precision limit.

(c) Fig 4 shows the relative error on $D(4)$ calculated using gaussian quadrature compared to the true value (from Scipy) as a function of the number of integration slices. The behaviour of the relative error is the same as the estimated error from fig 3, while being around an order or magnitude larger than the estimated error.

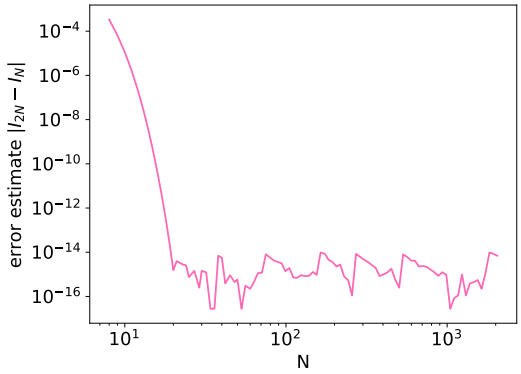

Figure 3: Error on $D(4)$ using gaussian quadrature vs number of integration slices

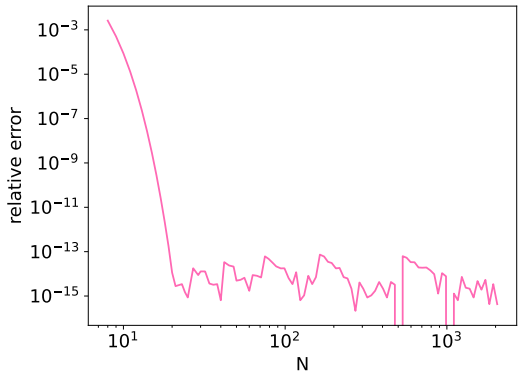

Figure 4: Relative error on $D(4)$ vs number of integration slices

3. Calculating potential energy of QM harmonic oscillator

   (a) A function $H(n, x)$ was written to calculate the n^{th} degree Hermite polynomial for a given x based on its recursion relation $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$.

   (b) Fig 5 shows the wave functions for the first 4 energy levels of a 1D quantum harmoniz oscillator.

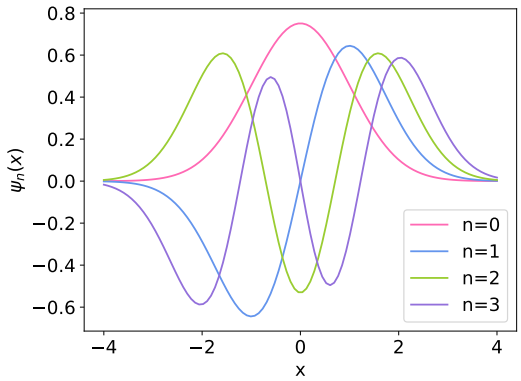

Figure 5: Harmonic oscillator wave functions

   (c) The potential energy for n from 0 to 10 computed using Gaussian quadrature using 100 points,

from the formula

$$PE = \frac{\langle x^2 \rangle}{2} = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 dx$$

The improper integral is calculated using the following transformation

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-\pi/2}^{\pi/2} \frac{f(\tan z)}{\cos^2 z} dz$$

The potential energies are listed in table 3

n	0	1	2	3	4	5	6	7	8	9	10
$\langle x^2 \rangle$	0.25	0.75	1.25	1.75	2.25	2.75	3.25	3.75	4.25	4.75	5.25

Table 3: Potential energies of the quantum harmonic oscillator

The raw output from the code is

```
0 0.24999999999999997
1 0.7500000000000119
2 1.2500000000003055
3 1.7499999999981126
4 2.249999999916142
5 2.7499999996902913
6 3.250000005587624
7 3.750000044358483
8 4.249999920351134
9 4.749998195042198
10 5.24999677662962
```