Homework 4 Part 1: Evaluating the Error Function

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An algorithm was written to evaluate the error function using Simpson's method of integration.

1. INTRODUCTION

The error function,

$$E(x) = \int_0^x e^{-t^2}\, dt \tag{1}$$

represents the probability that a random variable with a normal distribution will fall within the range $[-x, x]$.[1, 2] There are no known methods to solve this integral analytically, so it has to be solved numerically. This is a good application of computational methods because the process of evaluating the error function by hand is tedious, while the computer is able to calculate the integral much more quickly and with higher precision than is realistic otherwise. The error function has applications in several physical contexts, including quantum mechanics and thermodynamics.

To evaluate the function, I chose to use Simpson's rule to approximate the the integral. By implementing Simpson's rule in an algorithm to solve the integral, I was able to evaluate the Eq. 1 over the range $0 \leq x \leq 3$ in increments of $h = 0.1$.

2. EXPERIMENT

Simpson's method of integration takes 3 evenly spaced points in a function and fits them to a parabolic curve to evaluate the integral of the function over that range.[1] It is a better method to approximate the integral of a function than the trapezoid method, because there are more degrees of freedom to get a closer fit to the curve than with the trapezoid method.[1] The equation for Simpson's method that was implemented for the algorithm is below:[1]

$$\int_a^b f(x)\, dx = \frac{h}{3}\Bigg[f(a) + f(b) + 4 \sum_{\substack{k_{odd} \\ 1 \ldots N-1}} f(a+kh) + 2 \sum_{\substack{k_{even} \\ 1 \ldots N-2}} f(a+kh)\Bigg] \tag{2}$$

The error associated with using the approximation of Simpson's rule is given by:[1]

$$\epsilon = \frac{h^4}{180}[f'''(a) - f'''(b)] \tag{3}$$

In order to implement these equations, I defined functions to calculate the integrand of the error function, the third derivative of the integrand of the error function, and the Simpson's rule evaluation of the error function.

FIG. 1: Pseudocode for a general version of Simpson's rule including the approximation error calculation

3. RESULTS

The value of the error function increases, leveling off at 1. This is consistent with expectations because the integrand is a normalized Gaussian. Because the total probability is one represented by the Gaussian is equal to one, we expect the error function to increase to approach one. The approximation error with using $N = 30$ is much

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Part 2: Apply Simpson's Rule code to Error Function

$E(x) = \int_0^x e^{-t^2} dt$

Argument of simpson's rule:

$f = e^{-t^2}$ $\quad f''' = \frac{d^3 f}{dt^3} = 4t e^{-t^2}(3-2t^2)$ $\quad a=0$ $\quad b=x$ $\quad N=?$

The problem says to evaluate E(x) from $0 \le x \le 3$ in increments of 0.1. That means N=30.

Steps:

↳ Define functions to calculate f and f'''

↳ Make list of x-values to calculate value of E(x).

↳ For each element in that list, calculate E(x) and the approximation error using Simpson's Rule.

Store these values in new lists so that we can graph them together.

Pseudocode:

```
def E(t):
 return exp(-t**2)
def E3d(t):
 return 4t E(t)(3-2t**2)
a =0
b =3
N = 30
x = np.linspace(a, b, 30, endpoints =True)
Erf = [] # initialize list to store error function vals as func of x.
err = [] # initialize list to store approximation error values as a function of x.
for i in x:
 I, ϵ = simpsons(E, E3d, a, x(i), N)
 Erf.append (I)
 err.append (ϵ)
```

Part 3: Make graph

```
- latex fonts ***
- plt.plot (x, Erf, 'k', label=r'Error function')
- plt.plot(x, err, 'r', label=r'Approximation Error')
- plt.xlabel(r'$x$', fontsize=16)
- plt.ylabel(r'$E(x)$', fontsize=24)
- plt.legend()
- plt.show()
```

FIG. 2: Pseudocode for calculating the integrand of the error function, calling the Simpson's rule and graphing.

less than 0.1, which is low enough not to impact the shape of the error function curve, so we know that this number of bins is appropriate for the function.

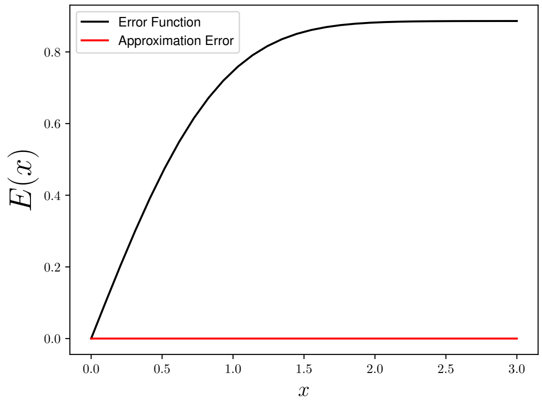

FIG. 3: The Error Function. The error function begins at zero, increasing logarithmically to converge at 1.

4. CONCLUSIONS

The algorithms for the Simpson's Rule evaluation of the error functions were successful in producing an accurate function and visualization of the data. The algorithm written would be easily used to evaluate the integral of different functions and to different levels of precision.

[1] M. Newman, *Computational Physics* (2013), revised and expanded ed., ISBN 978-1-4801-4551-1.

[2] *Error function*, https://en.wikipedia.org/wiki/Error_function.

Appendix A: Declaration of Collaborators

I collaborated with Woody on this assignment.

Appendix B: Survey Question

This assignment took me a much more reasonable amount of time, I was able to complete it in one day with 2 hours of writing pseudocode, 2.5 hours coding, and 2 hours of writing the report. The most interesting thing I learned about this assignment was the theory behind Simpson's rule and especially calculating the approximation error.