RobertRash_MATH3316_Project4

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0.1 Project 4 - Numerical Integration

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0.2 Introduction

0.2.1 Project Structure

```
In [1]: %ls ..
MATH3316-Project4.xcodeproj/ lib/
Makefile res/
bin/ src/
doc/
```

Excluding the .xcodeproj file, which was used for integration with the Xcode IDE, debugging, and profiling purposes, each item in the project directory serves the following purpose:

- Makefile: GNU Make project build automation definitions.
- bin/: compiled binaries. Make will put binaries here by default.
- doc/: directory containing all documentation, including this report.
- lib/: reused libraries that are not part of this project specifically. Contains a rewrite of the Matrix library (phrz/matrix).
- res/: where calculated data is stored after program execution. Files are .txt files containing real numbers, space delimited to denote row items, and newline delimited to denote new rows. For this project, the .txt files are also organized into separate res/part{1..3}/ directories.
- src/: contains the C++ implementations of the calculations described in this report.

0.2.2 Using this Project

Prerequisites

- A Unix or Unix-like OS (e.g. macOS or Linux)
- A compiler with support for C++14 (LLVM or GNU toolchain)
- Python 3.5
- The latest Jupyter distribution
 - matplotlib

- LaTeX with pdflatex
- GNU Make 3.81

Building this project make all (default) - will compile binaries, execute them to generate data files, execute Jupyter notebooks with new data files, and convert them to PDFs in res/reports/.

make all_bin - will compile binaries for part 1 and 2 of this project.

make all_data - will compile binaries and execute them to generate data files.

make clean - will delete all compiled binaries, generated data, executed notebook copies (but not the original notebooks), and report PDFs.

0.3 Part 1 - Trapezoidal Rule and Simpson's Rule

This portion of the project involves approximating the definite integral of a polynomial function and a trigonometric function using both the composite trapezoidal rule and the composite Simpson's rule.

0.3.1 Background

Composite Trapezoidal Rule One method for finding the area under a curve y = f(x) over the interval [a, b] is by approximating the area using a series of trapezoids over the intervals $\{[x_k, x_{k+1}]\}$.

Let the interval [a, b] be divided into n subintervals $[x_k, x_{k+1}]$ of width h = (b - a) / n using the equally spaced nodes $x_k = a + kh$, k = 0, 1, ... n. The composite trapezoidal rule can then be expressed as

$$T(f) = \frac{h}{2}(f_0 + 2f_1 + \dots + 2f_{n-1} + f_n)$$

This approximates the the integral of f(x) over the interval [a, b]

$$\int_a^b f(x) dx \approx T(f) = \frac{h}{2} (f_0 + 2 f_1 + \dots + 2 f_{n-1} + f_n)$$

Generally speaking, the absolute error |f(x) - T(f)| decreases as n increases. That is to say, the higher the "resolution", the better the approximation of the integral.

Composite Simpson's Rule Another method for finding the area under a curve is by approximating the area using a series of quadratic interpolants over the intervals $\{[x_k, x_{k+1}]\}$.

Let the interval [a, b] be divided into n subintervals $[x_k, x_{k+1}]$ of width h = (b - a) / n using the equally spaced nodes $x_k = a + kh$, k = 0, 1, ... n. This rule only works when n is an even number. The composite Simpson's rule can then be expressed as

$$S(f) = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + \dots + 2f_{n-2} + 4f_{n-1} + f_n)$$

This approximates the the integral of f(x) over the interval [a, b]

$$\int_{a}^{b} f(x) dx \approx S(f) = \frac{h}{3} (f_0 + 4 f_1 + 2 f_2 + \dots + 2 f_{n-2} + 4 f_{n-1} + f_n)$$

Similarly to the composite trapezoidal rule, the composite Simpson's rule tends to provide a better approximation given a higher value n.

Additionally, it can be shown that the composite Simpson's rule is exact for polynomials of degree $\in [0,3]$. The error formula for the composite Simpson's rule is known to be

$$E_S(f) = \frac{-f^{(4)}(\xi)}{180}(b-a) h^4$$

 $E_S(f)$ is proportional to $f^{(4)}(\xi)$, and the fourth derivative of any polynomial of degree $\in [0,3]$ is zero at all points. Thus, the error for any polynomial of degree $\in [0,3]$ will be zero (i.e. the results are exact).

0.3.2 Implementation

Implementation entails the creation of two functions composite_trapezoid and composite_simpson. Each of these functions has been included in the interface for a class NumericalIntegrator.

composite_trapezoid performs the composite trapezoidal rule for a given function Fcn over the bounds a and b using a number of subintervals n.

Accordingly, composite_simpson performs the composite Simpson's rule for a given function Fcn over the bounds a and b using a number of subintervals n.

Testing The above functions are tested in the file test_basic_rules.cpp by approximating the integral of a polynomial function

$$I_{f poly} = \int_{-1}^{2} 6x^2 - 4x + 1 \, dx = 15$$

and a trigonometric function

$$I_{f trig} = \int_{-1}^{1} \sin(\pi x) \exp(x) dx = \frac{\pi(e - \frac{1}{e})}{1 + \pi^2}$$

The absolute error $|f(x) - I_f|$ is also calculated and output for each test case.

When approximating the integral of the polynomial function, the value n is set at 1000. The results for the polynomial can be seen below.

```
In [2]: import subprocess
```

```
res = subprocess.run(["../bin/Project4_Part1_1"], stdout=subprocess.PIPE)
output = res.stdout.decode("UTF-8")
print('\n'.join(output.split('\n')[:11]))
```

True Integral (polynomial) = 1.5000000000000000e+01

Simpson's Rule Polynomial test (f(x) = $6x^2 - 4x + 1$): n I_f abs err

.----

1000 1.5000000000000000000020e+01 2.0e-14

Trapezoid Rule Polynomial test $(f(x) = 6x^2 - 4x + 1)$:

The error for both types of approximations are reasonable. For the composite Simpson's rule, we can see that, as predicted earlier, the result is exact barring a little bit of floating point error. Predictably, the composite trapezoidal rule is less accurate given the number of subintervals, though it gets remarkably close to the true value of the antiderivative, with an absolute error value of only ~ 0.051 .

For the trigonometric function, the two methods of approximation were tested using the subintervals $n = \{20, 40, 80, 160, 320, 640\}$. In addition, the convergence rate

$$C_n = \frac{\log(E_{n-1}(f)) - \log(E_n(f))}{\log(h_{n-1}) - \log(h_n)}$$

is output for values $n \in \{40, 80, 160, 320, 640\}$. The results can be seen below.

In [3]: import subprocess

```
res = subprocess.run(["../bin/Project4_Part1_1"], stdout=subprocess.PIPE)
output = res.stdout.decode("UTF-8")
print('\n'.join(output.split('\n')[15:]))
```

True Integral (trig function) = 6.7932618340209472e-01

Simpson Rule approximation:

	n	I_f	abs err	conv rate
-	 20	6.7935437830861389e-01	2.8e-05	
	40	6.7932794496229432e-01	1.8e-06	4.000509
	80	6.7932629348720586e-01	1.1e-07	4.000163
	160	6.7932619028221009e-01	6.9e-09	4.000043
	320	6.7932618383209908e-01	4.3e-10	4.000010
	640	6.7932618342896989e-01	2.7e-11	4.000006

Trapezoid Rule approximation:

	n	I_f	abs err	conv rate
_	20	5.9715988223642913e-01	8.2e-02	
	40	6.5756270293473129e-01	2.2e-02	1.916638
	80	6.7374136764046710e-01	5.6e-03	1.962328
	160	6.7791261630888933e-01	1.4e-03	1.982169
	320	6.7897066314063759e-01	3.6e-04	1.991337
	640	6.7923703997387375e-01	8.9e-05	1.995731

0.4 Part 2 - Application

In this section, we focus on interpolation using the Newton form in addition to the resulting error analysis relative to the function as calculated using the built-in function.

0.4.1 Background

0.4.2 Implementation

0.4.3 Analysis

Populating the interactive namespace from numpy and matplotlib

```
In [5]: names = [ 'carbon_1', 'carbon_2', 'carbon_10', 'carbon_40' ]
        data = {name: loadtxt('../res/part2/'+name+'.txt') for name in names}
        data['x'] = linspace(0,3,200)
In [6]: # plot C(x, t) versus x for each specified value of t
        # and overlay the four curves (corresponding to four
        # values of t) in one figure
        pylab.plot(data['x'], data['carbon_1'])
        pylab.plot(data['x'], data['carbon_2'])
        pylab.plot(data['x'], data['carbon_10'])
        pylab.plot(data['x'], data['carbon_40'])
        pylab.title('Concentration of carbon C(x,t) in a piece of steel, x \in [0, 3], t \in [0, 3]
        pylab.xlabel('$x$')
        pylab.ylabel('$C(x,t)$')
        pylab.grid()
        pylab.legend(('$C(x,1)$',
                      '$C(x,2)$',
                      '$C(x,10)$',
```

Out[6]: <matplotlib.legend.Legend at 0x10f7ed588>

'\$C(x,40)\$')

Concentration of carbon C(x, t) in a piece of steel, $x \in [0, 3], t \in \{1, 2, 10, 40\}$

