Math 1B Project 2 Solutions.

Modifying Simpson's rule. Simpson's rule is a method to approximate the area under a given curve $f(x)$ in a subinterval $[x_0, x_2]$ (composed of two "panels" $[x_0, x_1]$ and $[x_1, x_2]$, each of width h), by constructing a quadratic polynomial $p(x)$ which fits three constraints: $p(x_0) = f(x_0)$, $p(x_1) = f(x_1)$, $p(x_2) = f(x_2)$

The three constraints determine a unique parabola $p(x)$, and $\int_{x_0}^{x_2} p(x)\,dx$ approximates $\int_{x_0}^{x_2} f(x)\,dx$. To improve accuracy, several parabolas may be placed end-to-end in contiguous subintervals, giving Simpson's rule with error term:

$$\int_{x_0}^{x_{2m}} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + \cdots + 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m}] - \frac{(x_{2m} - x_0)h^4 f^{(4)}(\mu)}{180}$$

for some $\mu \in (x_0, x_{2m})$. As the number of subintervals increases (and more parabolas are used to approximate $f(x)$), the size of h decreases; this decrease in h reduces the error dramatically since the error is proportional to h^4.

Here is a modification of Simpson's rule. The coefficients are altered, two derivative terms are added, and–most importantly–the error term is improved. The method is analagous to the trapezoidal rule with endpoint correction[1].

Suppose we build a polynomial $q(x)$ by imposing the three constraints of Simpson's rule plus two additional constraints:

$$q(x_0) = f(x_0), q(x_1) = f(x_1), q(x_2) = f(x_2), q'(x_0) = f'(x_0), \text{ and } q'(x_2) = f'(x_2)$$

Think of the two additional constraints as "clamping" the approximating polynomial $q(x)$ to $f(x)$ at the endpoints x_0 and x_2. As we'll see, these five constraints can be used to define a quartic polynomial which, expeanded about the midpoint of the subinterval, has the form

$$q(x) = a_4(x - x_1)^4 + a_3(x - x_1)^3 + a_2(x - x_1)^2 + a_1(x - x_1) + a_0$$

1. (10 points) Simplify

$$\int_{x_0}^{x_2} q(x)\,dx$$

in terms of h, a_0, a_2, and a_4.

Solution: The odd-powered terms will integrate to zero since they have odd symmetry about the midpoint, x_1, of the interval of integration. That leaves

$$\int_{x_0}^{x_2} q(x)\,dx = \int_{x_0}^{x_2} a_4(x - x_1)^4 + a_2(x - x_1)^2 + a_0\,dx = \frac{a_4(x - x_1)^5}{5} + \frac{a_2(x - x_1)^3}{3} + a_0 x\Big|_{x_0}^{x_2} = \frac{2h^5}{5}a_4 + \frac{2h^3}{3}a_2 + 2ha_0$$

2. (10 points) Use the five constraints to set up a system of five equations in the five unknowns, a_0, a_1, a_2, a_3, a_4, then solve these to find formulas for a_0, a_2, and a_4 in terms of the parameters $y_0 = f(x_0), y_1 = f(x_1), y_2 = f(x_2)$ and $y_0' = f'(x_0), y_2' = f'(x_2)$

Solution: Here is the system:

$$\begin{aligned}
q(x_0) &= a_4h^4 - a_3h^3 + a_2h^2 - a_1h + a_0 &= y_0\\
q(x_1) &= a_0 &= y_1\\
q(x_2) &= a_4h^4 + a_3h^3 + a_2h^2 + a_1h + a_0 &= y_2\\
q'(x_0) &= -4a_4h^3 + 3a_3h^2 - 2a_2h + a_1 &= y_0'\\
q'(x_2) &= 4a_4h^3 + 3a_3h^2 + 2a_2h + a_1 &= y_2'
\end{aligned}$$

Substituting $a_0 = y_1$ and adding the first and third and the fourth and fifth we get a 2×2 system in a_2 and a_4:

$$\begin{aligned}
2a_4h^4 + 2a_2h^2 &= y_2 - 2y_1 + y_0\\
8a_4h^3 + 4a_2h &= y_2' - y_0'
\end{aligned}$$

[1] Samuel D. Conte and Carl de Boor, Elementary Numerical Analysis, McGraw-Hill, New York, 1980.

Multiplying the second equation by $-\dfrac{h}{4}$ and adding it to the first equation eliminates a_4 so we can solve for a_2:
$a_2 = \dfrac{1}{h^2}\left(y_2 - 2y_1 + y_0 - \dfrac{h}{4}(y_2' - y_0')\right) = \dfrac{y_2 - 2y_1 + y_0}{h^2} - \dfrac{y_2' - y_0'}{4h}$ and $a_4 = -\dfrac{y_2 - 2y_1 + y_0}{2h^4} + \dfrac{y_2' - y_0'}{4h^3}$

3. (10 points) Substitute these values for the coefficients of $q(x)$ to show that

$$\int_{x_0}^{x_2} q(x)\,dx = \frac{h}{15}\left(7f(x_0) + 16f(x_1) + 7f(x_2) + h[f'(x_0) - f'(x_2)]\right)$$

Solution:

$$\int_{x_0}^{x_2} q(x)\,dx = \frac{2h^5}{5}\left(-\frac{y_2 - 2y_1 + y_0}{2h^4} + \frac{y_2' - y_0'}{4h^3}\right) + \frac{2h^3}{3}\left(\frac{y_2 - 2y_1 + y_0}{h^2} - \frac{y_2' - y_0'}{4h}\right) + 2hy_1$$

$$-\frac{3h(y_2 - 2y_1 + y_0)}{15} + \frac{10h(y_2 - 2y_1 + y_0)}{15} + \frac{3h^2(y_2' - y_0')}{30} - \frac{5h^2(y_2' - y_0')}{30} + \frac{30hy_1}{15}$$

$$= \frac{h}{15}\left(7y_2 + 16y_1 + 7y_0 - h[y_2' - y_0']\right)$$

$$= \frac{h}{15}\left(7f(x_0) + 16f(x_1) + 7f(x_2) + h[f'(x_0) - f'(x_2)]\right)$$

4. (10 points) Simplify

$$\int_{x_0}^{x_{2m}} q(x)\,dx = \int_{x_0}^{x_2} q(x)\,dx + \int_{x_2}^{x_4} q(x)\,dx + \cdots + \int_{x_{2m-2}}^{x_{2m}} q(x)\,dx$$

in terms of the y-values, $y_i = f(x_i), i \in \{0, 1, \ldots 2m\}$ and the slopes $f'(x_0), f'(x_2), \ldots f'(x_{2m})$. How does this compare with Simpson's rule?

Solution: Except for the very first and last points in the partition, the endpoint values double up for the y-values at even indeces while the y' values telescope:

$$\int_{x_0}^{x_{2m}} q(x)\,dx = \frac{h}{15}\sum_{i=0}^{2n-2}(7y_i + 16y_{i+1} + 7y_{i+2}) + \frac{h^2}{15}\sum_{i=0}^{2n-2}(y_{i+2}' - y_i')$$

$$= \frac{h}{15}(7y_0 + 16y_1 + 7y_2 + 7y_2 + 16y_3 + 7y_4 + \cdots + 7y_{2n-2} + 16y_{2n-1} + 7y_{2n})$$

$$+\frac{h^2}{15}(y_2' - y_0' + y_4' - y_2' + \cdots + y_{2n-2}' - y_{2n-4}' + y_{2n}' - y_{2n-2}')$$

$$= \frac{h}{15}\left(7y_0 + 16y_1 + 14y_2 + 16y_3 + 14y_4 + \cdots + 14y_{2m-2} + 16y_{2m-1} + 7y_{2m} + h[f'(x_0) - f'(x_{2m})]\right)$$

This is similar to Simpson's rule except (1) the common multiplier is $\dfrac{h}{15}$ instead of $\dfrac{h}{6}$, the coefficients are $\{7, 16, 14, 16, 14, 15, \ldots, 14, 16, 7\}$ instead of $\{1, 2, 4, 2, 4, \ldots, 4, 2, 4, 1\}$ and there is extra term involving the derivatives: $\dfrac{h^2}{15}[f'(x_0) - f'(x_{2m}]$

5. (30 points) For each of the following integrals, complete a table of errors like this:

n	`Clamped Rule error`	`Simpson's Rule error`
2		
4		
8		
16		

(a) $\int_2^4 \frac{dx}{x}$

n	`Clamped Rule error`	`Simpson's Rule error`
2	2.34×10^{-6}	-1.07×10^{-4}
4	4.41×10^{-8}	-7.35×10^{-6}
8	7.30×10^{-10}	-4.72×10^{-7}
16	1.16×10^{-11}	-2.97×10^{-8}

(b) $\int_1^5 \ln(x)\,dx$

n	`Clamped Rule error`	`Simpson's Rule error`
2	-6.57×10^{-4}	5.71×10^{-3}
4	−2.24 × 1‘0−5	5.34×10^{-4}
8	-5.10×10^{-7}	3.98×10^{-5}
16	-9.16×10^{-9}	2.63×10^{-6}

(c) $\int_0^1 e^{-x^2}\,dx$

n	`Clamped Rule error`	`Simpson's Rule error`
2	1.17×10^{-7}	-3.12×10^{-5}
4	1.33×10^{-9}	-1.99×10^{-6}
8	1.91×10^{-11}	-1.25×10^{-7}
16	2.92×10^{-13}	-7.79×10^{-9}

There are a variety of ways to arrive at these error estimates. C++ code works well, if you can write it (Take CS7A in the fall!): Alternatively, write a little program for the TI85, like so:

```
PROGRAM:SIMPSON
:Prompt A
:Prompt B
:Prompt N
:(B-A)/N→H
:A→x
:y1→S
PAGE↓ PAGE↑ I/O CTL INSc

PROGRAM:SIMPSON
:7*y1→C
:x+H→x
:S+4*y1→S
:C+16*y1→C
:For(I,2,N-2,2)
:x+H→x
PAGE↓ PAGE↑ I/O CTL INSc

PROGRAM:SIMPSON
:S+2*y1→S
:C+14*y1→C
:x+H→x
:S+4*y1→S
:C+16*y1→C
:End
PAGE↓ PAGE↑ I/O CTL INSc

PROGRAM:SIMPSON
:B→x
:S+y1→S
:C+7*y1→C
:S*H/3→S
:nDer(y1,x)→D2
:A→x
PAGE↓ PAGE↑ I/O CTL INSc

PROGRAM:SIMPSON
:nDer(y1,x)→D1
:C-H*(D2-D1)→C
:C*H/15→C
:Disp "S=",S
:Disp "C=",C
:Disp ln 2-S
PAGE↓ PAGE↑ I/O CTL INSc
```

Then we can run the program with `y1=1/x` on Graph page to verify the errors we listed above:

```
A=?2    S=
B=?4              .693253968254
N=?4    C=
                   .69314484127
                -1.0678769406E-4
                  2.33929007E-6
                           Done

A=?2    S=
B=?4              .693154530655
N=?8    C=
                 .693147136428
                -7.35009459E-6
                   4.413154E-8
                          Done

A=?2    S=
B=?4              .693147652819
N=?16   C=
                 .69314717983
                -4.7225949E-7
                   7.3001E-10
                         Done

S=
                 .69314721029
C=
                .693147180548
                -2.972993E-8
                   1.147E-11
                        Done
```

For the error in the estimation

$$\int_{x_0}^{x_{2m}} f(x)\,dx \approx \int_{x_0}^{x_{2m}} q(x)\,dx$$

we can prove the following theorem:
Theorem. *If $f^{(6)}(x)$ is continuous on $[x_0, x_{2m}]$, then for some $v \in (x_0, x_{2m})$:*

$$\int_{x_0}^{x_{2m}} f(x)\,dx = \frac{h}{15}\left(7y_0 + 16y_1 + 14y_2 + 16y_3 + 14y_4 + \cdots + 14y_{2m-2} + 16y_{2m-1} + 7y_{2m} + h[f'(x_0) - f'(x_{2m})]\right)$$

$$+\frac{(x_{2m}-x_0)h^6 f^{(6)}(v)}{9450}$$

To determine the error, start by constructing the fifth degree polynomial

$$t(x) = q(x) + k(x-x_0)^2(x-x_1)(x-x_2)^2$$

which has the same integral as $q(x)$ on $[x_0, x_2]$ but allows for sharper estimates.

6. Explain why $\int_{x_0}^{x_2} k(x-x_0)^2(x-x_1)(x-x_2)^2\,dx = 0$

   Solution: The integrand has odd symmetry around the point $(x_1, 0)$ and the interval of integration is centered on $x = x_1$ so that the signed area in $x_0 \le x \le x_1$ is the opposite of that in $x_1 \le x \le x_2$. To be sure, the substitution $u = x - x_1$ yields $\int_{-h}^{h} k(u+h)^2u(u-h)^2\,du = k\int_{-h}^{h} u(u^2-h^2)^2\,du = 0$

7. (10 points) Show that $t(x)$ satisfies all the constraints of the clamped $q(x)$ and that if we take $k = (f'(x_1) - q'(x_1))/h^4$ then $t'(x_1) = f'(x_1)$.

   Solution:

$$t(x_0) = q(x_0), t(x_1) = q(x_1), t(x_2) = q(x_2)$$

$$t'(x) = q'(x) + 2k(x-x_0)(x-x_1)(x-x_2)^2 + k(x-x_0)^2(x-x_2)^2 + 2k(x-x_0)^2(x-x_1)(x-x_2)$$

so that

$$t'(x_0) = q'(x_0) = f'(x_0), \text{ and } t'(x_2) = q'(x_2) = f'(x_2)$$

Now

$$t'(x_1) = q'(x_1) + k(x_1-x_0)^2(x_1-x_2)^2 = q'(x_1) + kh^4 = f'(x_1) \Leftrightarrow k = \frac{f'(x_1) - q'(x_1)}{h^4}$$

does the trick, as desired. We leave the completion of the proof for the above theorem for another time.

8. (10 points) It is known that

$$2\int_0^\infty \frac{\cos x}{1+x^2}\,dx = \int_{-\infty}^{\infty} \frac{\cos x}{1+x^2}\,dx = \frac{\pi}{e} \approx 1.1557273497909217.$$

Investigate how the Clamped rule and Simpson's rule compare for approximating this integral as

$$2\int_0^{10,000} \frac{\cos x}{1+x^2}\,dx = 2\int_0^{10} \frac{\cos x}{1+x^2}\,dx + 2\int_{10}^{100} \frac{\cos x}{1+x^2}\,dx + 2\int_{100}^{1000} \frac{\cos x}{1+x^2}\,dx + 2\int_{1000}^{10,000} \frac{\cos x}{1+x^2}\,dx$$

for $n = 2, 4, 8, 16$.

Solution:

Using Mathematica, I find that $2\int_0^{10} \frac{\cos x}{1+x^2}\,dx \approx 0.57423915985756283000385890837367349472114644869057$

interval	n	integral	Clamped Rule error	Simpson's Rule error
$0 \le x \le 10$	32	0.5742391598575628	6.1275×10^{-10}	3.3488×10^{-8}
$10 \le x \le 100$	512	0.003572191617775706	-2.7726×10^{-11}	-4.8639×10^{-8}
$100 \le x \le 1000$	4096	0.00005314916913240810	-5.0963×10^{-13}	-6.0145×10^{-10}
$1000 \le x \le 10000$	8192	$-8.288032494498435 \times 10^{-7}$	1.8243×10^{-10}	7.8569×10^{-9}
$10000 \le x \le 100000$	65536	$3.057816242998889 * 10^{-9}$	-2.82×10^{-12}	-7.75×10^{-11}