Math 151A Homework #7

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Problem 0.1.

(a) Let $f(x) = x^2 e^{-x}$. Then

$$\begin{aligned}\int_0^1 f(x)\mathrm{d}x &= \frac{f(0)+f(1)}{2} \\ &= \frac{0}{2} + \frac{1^2}{2e} \\ &= \frac{1}{2e} \\ &\approx 0.1839\end{aligned}$$

This is fairly close to the actual answer, which is $2 - 5/e \approx 0.1606$

(b) Let $f(x) = 2x/(x^2-4)$. Then

$$\begin{aligned}\int_1^{1.6} f(x)\mathrm{d}x &= (1.6-1)\frac{f(1)+f(1.6)}{2} \\ &= 0.3\left(\frac{2}{1-4} + \frac{3.2}{2.56-4}\right) \\ &= 0.3\left(-\frac{2}{3} - \frac{20}{9}\right) \\ &= -0.2 - \frac{2}{3} \\ &= -0.8666\ldots\end{aligned}$$

The actual answer is $-0.7340\ldots$ which is not too far off.

Problem 0.2.

The trapezoidal rule says

$$2 \cdot \frac{f(0)+f(2)}{2} = 4,$$

and Simpson's rule says that

$$\frac{1}{3} \cdot (f(0) + 4f(1) + f(2)) = 2,$$

so $(1/3)(4 + 4f(1)) = 2$, which means $4(1 + f(1)) = 6$, so

$$f(1) = -\frac{1}{2}.$$

Problem 0.3.

The actual value of the integral is

$$\begin{aligned}\int_1^2 x\ln(x)\mathrm{d}x &= \left[\frac{x^2}{2}\ln(x)\right]_1^2 - \int_1^2 \frac{x^2}{2}\cdot\frac{1}{x}\mathrm{d}x \\ &= 2\ln(2) - \frac{1}{2}\ln(1) - \left[\frac{x^2}{4}\right]_1^2 \\ &= 2\ln(2) - \frac{3}{4} \\ &\approx 0.636294\end{aligned}$$

The composite trapezoidal rule gives 0.639900 (relative error of 0.00566737), and the composite Simpson's rule gives 0.636310 (relative error of 0.0000243106). Here is the code I used to calculate those:

```
>>> from math import log
>>> def f(x): return x * log(x)
...
>>> x_i = [1, 1.25, 1.5, 1.75, 2]
>>> w_i = [.125, .25, .25, .25, .125]
>>> sum([f(x_i[i]) * w_i[i] for i in range(5)])
0.639900477687986
>>> w_i = [1/12, 1/3, 1/6, 1/3, 1/12]
>>> sum([f(x_i[i]) * w_i[i] for i in range(5)])
0.6363098297969493
```

Problem 0.4.

We already know that the error for Simpson's rule is

$$E[f] = \sum_{j=1}^{n/2} \frac{h^5 f^{(4)}(\xi_j)}{90},$$

where each ξ_j is in $[a,b]$, and $nh = b-a$. By IVT, there is some $\xi \in [a,b]$ such that

$$\sum_{j=1}^{n/2} f^{(4)}(\xi_j) = \frac{n}{2} f^{(4)}(\xi),$$

so the error is

$$E[f] = \frac{h^4(b-a)}{180} f^{(4)}(\xi),$$

and the absolute error is the absolute value of that. Also, the given inequality is true by the triangle inequality.

Problem 0.5.

(a) If $f(x) = x\ln(x)$, then $f'(x) = \ln(x) + 1$, and $f''(x) = \frac{1}{x}$. Note that the domain of f is the set of positive real numbers, so the lowest posible upper bound for $f''(\mu)$ when $\mu \in (a,b)$ is $1/a$ (assuming

$a < b$). This means the absolute error is guaranteed to be less than $h^2(b-a)/(12a)$. If $a = 1$ and $b = 2$ and we want to guarantee that the absolute error is less than $\tau = 10^{-5}$, we need

$$\begin{aligned}
\frac{h^2}{12} &< \tau = 10^{-5} \\
h &< \sqrt{1.2 \times 10^{-4}} \approx 0.010954 \\
n = \frac{1}{h} &> 91.287 \\
n &\geq 92.
\end{aligned}$$

(b) With the composite Simpson's rule, the absolute error is

$$E[f] = \frac{h^4(b-a)}{180} \left| f^{(4)}(\xi) \right|$$

for some $\xi \in [a, b]$. We have the same f, a, b as before, so $f'''(x) = -1/x^2$ and $f^{(4)}(x) = 2/x^3$, meaning the upper bound on $\left| f^{(4)}(\xi) \right|$ is $2/a^3 = 2$. Therefore

$$\begin{aligned}
E[f] \leq \frac{h^4(b-a)}{180} \cdot 2 &< \tau = 10^{-5} \\
h^4 &< 9 \times 10^{-4} \\
h &< \sqrt[4]{9 \times 10^{-4}} \approx 0.1732 \\
n = \frac{1}{h} &> 5.7735 \\
n &\geq 6.
\end{aligned}$$

Problem 0.6.

This is equivalent to ensuring that whenever f is a degree 3 polynomial, the error for that quadrature rule is zero. If $f(x) = \alpha + \beta x + \gamma x^2 + \delta x^3$, then we have the following equations:

$$\begin{aligned}
f'(x) &= \beta + 2\gamma x + 3\delta x^2 \\
I := \int_{-1}^{1} f(x)\mathrm{d}x &= \left[\alpha x + \frac{\beta x^2}{2} + \frac{\gamma x^3}{3} + \frac{\delta x^4}{4}\right]_{-1}^{1} \\
I &= \left(\alpha + \frac{\beta}{2} + \frac{\gamma}{3} + \frac{\delta}{4}\right) - \left(-\alpha + \frac{\beta}{2} - \frac{\gamma}{3} + \frac{\delta}{4}\right) \\
I &= 2\alpha + \frac{2\gamma}{3} \\
f(-1) &= \alpha - \beta + \gamma - \delta \\
f(1) &= \alpha + \beta + \gamma + \delta \\
f'(-1) &= \beta - 2\gamma + 3\delta \\
f'(1) &= \beta + 2\gamma + 3\delta \\
I &= af(-1) + bf(1) + cf'(-1) + df'(1) \\
\begin{bmatrix} 2 \\ 0 \\ \frac{2}{3} \\ 0 \end{bmatrix} &= \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & -2 & 2 \\ -1 & 1 & 3 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \\
\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} &= \frac{1}{4} \begin{bmatrix} 2 & -3 & 0 & 1 \\ 2 & 3 & 0 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ \frac{2}{3} \\ 0 \end{bmatrix} \\
a &= 1 \\
b &= 1 \\
c &= \frac{1}{3} \\
d &= -\frac{1}{3}.
\end{aligned}$$

Problem 0.7.

(a) Given some initial guess x_0 for a solution to the equation, Newton's method says to iteratively apply

$$\begin{aligned}
x_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \\
&= x_n - \sqrt{2\pi} \cdot e^{x_n^2/2} \cdot f(x_n).
\end{aligned}$$

(b) The composite trapezoidal rule approximates $f(x)$ as

$$\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}} \int_0^x e^{-t^2/2}\mathrm{d}t - 0.45 \\
&= (-0.45) + \frac{1}{\sqrt{2\pi}} \sum_{j=1}^{N} \frac{x}{2N} \left(\exp\left(-\frac{((j-1)x/N)^2}{2}\right) + \exp\left(-\frac{(jx/N)^2}{2}\right)\right).
\end{aligned}$$

Plugging that back in to Newton's method gives

$$x_{n+1} = x_n + \exp\left(\frac{x_n^2}{2}\right)\left(0.45\sqrt{2\pi} - \frac{x}{2N}\sum_{j=1}^{N}\left[\exp\left(-\frac{((j-1)x_n/N)^2}{2}\right) + \exp\left(-\frac{(jx_n/N)^2}{2}\right)\right]\right).$$

(c) When I use $N = 50$ and $x_0 = 0.5$, the first guess to reach the desired tolerance is $x_4 = 1.644962$, but if I keep iterating, the method converges to $x \approx 1.645002$. However, when I use $N = 200$ (and $x_0 = 0.5$), it converges to 1.644863 instead, and if I reduce N to 20, it converges to 1.645782. We can assume that the higher N is, the closer we get to the actual root.

```
#!/usr/bin/env python3
from math import exp, sqrt, pi

x = 0.5
N = 50
def f(x):
    summation = 0
    for j in range(N):
        summation += exp(0 - (j     *x/N)**2 / 2)
        summation += exp(0 - ((j+1)*x/N)**2 / 2)
    return -0.45 + summation * x / (2 * N * sqrt(2 * pi))

for i in range(100):
    print(f"x_{i} = {x}")
    residual = f(x)
    if abs(residual) < 1e-15:
        break
    x -= sqrt(2 * pi) * exp(x**2 / 2) * residual
```

```
x_0 = 0.5
x_1 = 1.234349525548872
x_2 = 1.5487272386153916
x_3 = 1.6380320881922388
x_4 = 1.6449621080925367
```

Math 151A
HW #7, due on Friday, November 29, 2024 at 11:59pm PST.

[1] Approximate the following integrals using Trapezoidal rule.

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

(b) $\int_1^{1.6} \frac{2x}{x^2-4}\, dx$

[2] The Trapezoidal Rule applied to $\int_0^2 f(x)dx$ gives the value 4, and Simpson's rule gives the value 2. What is $f(1)$?

[3] [*Composite quadrature rules*]

Use the Composite Trapezoidal and Composite Simpson's rules to approximate the integral

$$\int_1^2 x\ln(x)dx$$

with $n = 4$ subintervals. What are the relative errors? (*Hint*: to compute the true value of the integral, integrate by parts.)

[4] Using Intermediate Value Theorem show that the error for Composite Simpson's Rule can be estimated by:

$$\left|\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)\right| \le \frac{h^4}{180}(b-a)|f^{(4)}(\xi)|$$

Hint: Use similar steps as for the error in composite Trapezoidal rule.

[5] [*Computational cost as a function of error tolerance*]

Recall from lecture that the error in the Composite Trapezoidal Rule (CTR) using n subintervals of width h is given by

$$\frac{-h^2}{12}(b-a)\, f''(\mu) \tag{1}$$

for some $\mu \in (a,b)$.

(a) Determine the values of n and h that are sufficient to approximate

$$\int_1^2 x \ln(x) dx \tag{2}$$

to within an error tolerance of $\tau = 10^{-5}$; that is, determine n and h so that the error when applying the CTR to (2) is smaller (in absolute value) that τ.

(b) Repeat part (a) for the case of Composite Simpson's Rule.

[**6**] Find constants a, b, c, d such that the quadrature rule below has degree of precision 3.

$$\int_{-1}^{1} f(x)\, dx = a\, f(-1) + b\, f(1) + c\, f'(-1) + d\, f'(1)$$

[**7**] **Computational exercise** Consider the nonlinear equation for x:

$$\int_0^x \frac{1}{\sqrt{2\pi}} e^{-t^2/2}\, dt = 0.45.$$

Note that t is just a 'dummy' variable of integration.

(a) Define

$$f(x) := \int_0^x \frac{1}{\sqrt{2\pi}} e^{-t^2/2}\, dt - 0.45.$$

Using the Fundamental Theorem of Calculus, write down Newton's method applied to f.

(b) Each step of Newton's method derived in (a) requires of an evaluation of $f(x)$. Rewrite the method you derived in (a) using Composite Trapezoidal Rule to estimate $f(x)$. Indicate with N the number of subintervals.

(c) Implement in MATLAB the method derived in part (b) to find the solution x to the equation $f(x) = 0$; terminate the iteration when the *residual* is smaller than $\tau = 10^{-5}$. Use $x_0 = 0.5$ as an initial guess and $N = 50$ for composite trapezoidal rule.