Math 151A Homework #6

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Problem 0.1.

(a) For any $x \in [a, b]$, there exists $\xi \in [x_0, x]$ such that

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \frac{f'''(x_0)}{6}(x - x_0)^3 + \frac{f''''(\xi)}{24}(x - x_0)^4.$$

(b)

$$\begin{aligned}
f(x_0 + h) &= f(x_0) + f'(x_0)h + \frac{f''(x_0)h^2}{2} + \frac{f'''(x_0)h^3}{6} + \frac{f''''(\xi_1)h^4}{24} \\
f(x_0 - h) &= f(x_0) - f'(x_0)h + \frac{f''(x_0)h^2}{2} - \frac{f'''(x_0)h^3}{6} + \frac{f''''(\xi_2)h^4}{24} \\
\frac{f(x_0 - h) + f(x_0 + h) - 2f(x_0)}{h^2} &= f''(x_0) + \frac{h^2}{24}\left(f''''(\xi_1) + f''''(\xi_2)\right) \\
&= f''(x_0) + \frac{h^2}{24} f^{(4)}(\xi_3).
\end{aligned}$$

(c) As h goes to zero, $f''''(\xi_1)$ and $f''''(\xi_2)$ both approach a constant, so when calculating $f''(x_0)$, the error term is $O(h^2)$.

Problem 0.2.

The total error bound is

$$\left|-\frac{h^2 M}{6}\right| + \left|\frac{\varepsilon}{h}\right| = \frac{h^2 M}{6} + \frac{\varepsilon}{h},$$

since h and ε are both positive. If we treat ε and $|M|$ as constants, then the total error is a smooth function of $h \in (0, \infty)$, meaning we can calculate the minima and maxima by looking at the points where the derivative of the error bound with respect to h is zero.

$$\frac{\partial}{\partial h}\left(\frac{h^2 M}{6} + \frac{\varepsilon}{h}\right) = \frac{hM}{3} - \frac{\varepsilon}{h^2} = 0,$$

so $h^3 M/3 = \varepsilon$, so $h = \sqrt[3]{3\varepsilon/M}$. This is the only real solution to the equation above, and the second derivative of the error bound with respect to h is always positive, so $h = \sqrt[3]{3\varepsilon/M}$ minimizes the error bound.

Note that I have assumed ε does not depend on h, because the expression we are given is an upper bound on the error, not an exact value of the error. Because of that, I assumed ε_1 and ε_2 are upper bounds on the roundoff errors, not exact values of the roundoff errors.

Problem 0.3.

(a)

$$f'(x_0) = \frac{f(x_0+h/2)-f(x_0-h/2)}{h} - \left(\frac{h^2}{24}f'''(x_0) + \frac{h^4}{1920}f^{(5)}(\xi_1)\right).$$

(b) For some $\xi_3 \in [x_0-h, x_0+h]$,

$$\begin{aligned}
4f'(x_0) &= 4\cdot\frac{f(x_0+h/2)-f(x_0-h/2)}{h} - \left(\frac{h^2}{6}f'''(x_0) + \frac{h^4}{480}f^{(5)}(\xi_1)\right)\\
f'(x_0) &= \frac{f(x_0+h)-f(x_0-h)}{2h} - \left(\frac{h^2}{6}f'''(x_0) + \frac{h^4}{120}f^{(5)}(\xi_2)\right)\\
3f'(x_0) &= \frac{f(x_0+h)+8f(x_0+h/2)-8f(x_0-h/2)-f(x_0-h)}{2h} - \frac{h^4}{480}\left(f^{(5)}(\xi_1)+4f^{(5)}(\xi_2)\right)\\
&= \frac{f(x_0+h)+8f(x_0+h/2)-8f(x_0-h/2)-f(x_0-h)}{2h} - \frac{h^4}{480}\left(5f^{(5)}(\xi_3)\right)\\
f'(x_0) &= \frac{f(x_0+h)+8f(x_0+h/2)-8f(x_0-h/2)-f(x_0-h)}{6h} - \frac{h^4}{288}f^{(5)}(\xi_3).
\end{aligned}$$

Therefore the new error is only

$$-\frac{h^4 f^{(5)}(\xi_3)}{288}$$

(for some $\xi_3 \in [x_0-h, x_0+h]$).

Problem 0.4.

```
import math

def f(x):
    return math.sin(x)
def f_prime_exact(x):
    return math.cos(x)
def f_prime_approx(x, h):
    return (f(x) - f(x - h)) / h

x = math.pi / 3
print(f"{x=:.8f}  {f_prime_exact(x)=:.8f}\n")
for h in [.1, .01, .001]:
    absolute_error = abs(f_prime_exact(x) - f_prime_approx(x, h))
    print(f"{h=:.3f}  {f_prime_approx(x, h)=:.8f}  {absolute_error=:.8f}")
```

```
x=1.04719755  f_prime_exact(x)=0.50000000

h=0.100  f_prime_approx(x, h)=0.54243228  absolute_error=0.04243228
h=0.010  f_prime_approx(x, h)=0.50432176  absolute_error=0.00432176
h=0.001  f_prime_approx(x, h)=0.50043293  absolute_error=0.00043293
```

The absolute error is decreasing linearly, and for sufficiently small h, it appears to be $\approx 0.43 \cdot h$. This matches our expectations because

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + \frac{f''(\xi)h}{2}$$

for some $\xi \in [x_0 - h, x_0]$, and if h is approaching zero, then we can say $\xi \approx x_0 = \pi/3$. Therefore the error term is

$$\frac{f''(\xi)h}{2} \approx -\frac{\sin(\pi/3)h}{2} = -\frac{\sqrt{3}}{4} \cdot h \approx -0.433h.$$

Problem 0.5.

From problem 1(b), we have

$$f''(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} + \frac{h^2}{24} f^{(4)}(\xi).$$

The exact value we want is $f'(1.3)$:

$$\begin{aligned} f'(x) &= 3(1 + x)e^x + \sin(x) \\ f''(x) &= 3(2 + x)e^x + \cos(x) \\ f''(1.3) &= 9.9e^{1.3} + \cos(1.3) \approx 36.593535838 \end{aligned}$$

and our approximations are

$$f'(1.3) \approx \frac{f(1.4) - 2f(1.3) + f(1.2)}{0.1^2} \approx 36.64195350413504$$

(relative error $= 0.001323$) when $h = 0.1$, and

$$f'(1.3) \approx \frac{f(1.31) - 2f(1.3) + f(1.29)}{0.01} \approx 36.594019792950405$$

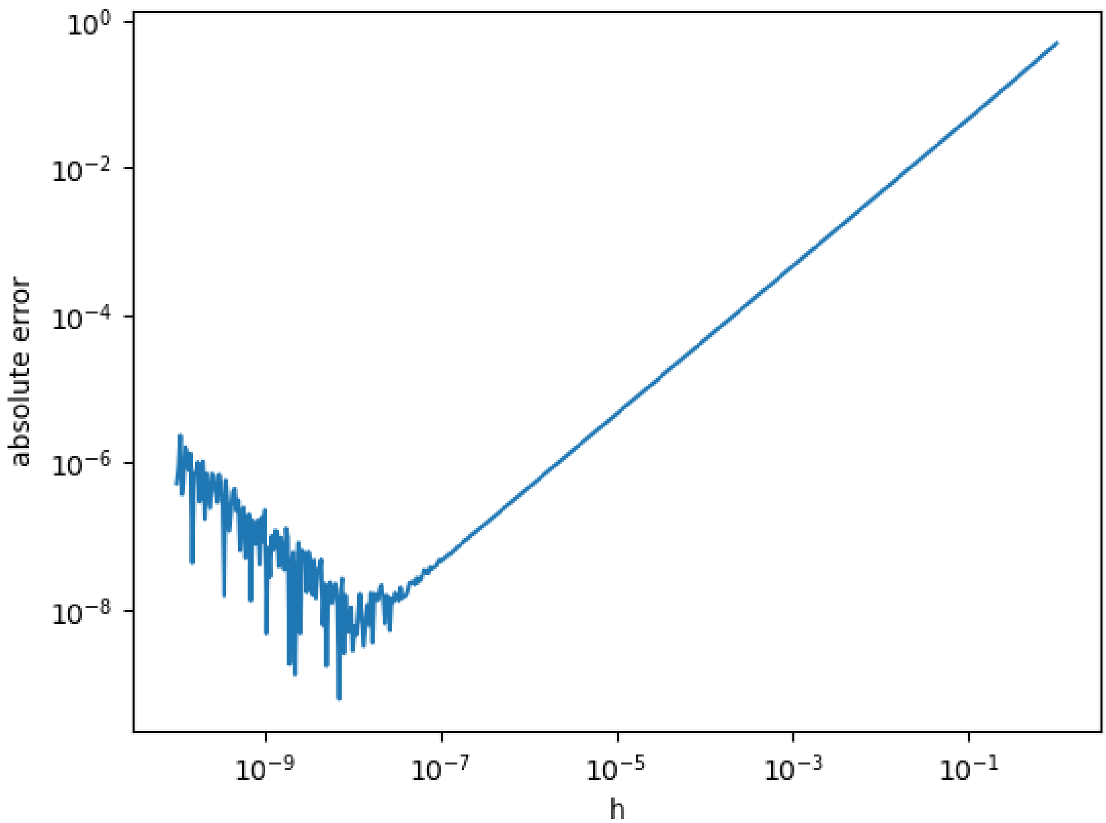
(relative error $= .00001322$) when $h = 0.01$.

```
>>> import math
>>> def f(x): return 3 * x * math.exp(x) - math.cos(x)
...
>>> (f(1.4) - 2 * f(1.3) + f(1.2)) / .01
36.64195350413504
>>> (f(1.31) - 2 * f(1.3) + f(1.29)) / .0001
36.594019792950405
```

Problem 0.6.

The absolute error appears to be minimized when $h \approx 6.9773 \times 10^{-9}$, but there is a ton of noise in this function, so it's hard to tell where the actual minimum is. If you actually wanted to minimize the error, you would be better off deriving a theoretical upper bound on the absolute error, which would be a smooth function of h whose second derivative is always positive, then minimizing that function.

The reason the absolute error increases when h becomes sufficiently small is because the rounding/truncation error become proportionally much more significant.



```
import math
import numpy as np
import matplotlib.pyplot as plt

def f(x):
    return x * x * math.log(x)
def f_prime_approx(x, h):
    return (f(x + h) - f(x)) / h
def f_prime_exact(x):
    return 2 * x * math.log(x) + x
def absolute_error(x, h):
    return abs(f_prime_exact(x) - f_prime_approx(x, h)) / f_prime_exact(x)

x_vals = 10 ** np.linspace(-10, 0, 500)
y_vals = [absolute_error(2, h) for h in x_vals]

best_h = x_vals[y_vals.index(min(y_vals))]
print(f"Absolute error is minimized when h = {best_h}")

plt.plot(x_vals, y_vals)
plt.xlabel("h")
plt.ylabel("absolute error")
plt.xscale("log")
```

```
plt.yscale("log")
plt.show()
```

Math 151A
HW #6, due on Friday, November 22, 2024 at 11:59pm PST.

[1] [*Centered difference approximation of second derivative*]
Let $f \in C^4([a,b])$.

(a) Use Taylor's theorem to write f as a third order (cubic) Taylor polynomial plus a fourth order (quartic) remainder term. Expand about the point x_0.

(b) Use the result from (a) to evaluate $f(x)$ at the points $x = x_0 + h$ and $x = x_0 - h$. Add the two results together to derive the centered difference approximation to the second derivative:

$$\frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} = f''(x_0) + \frac{h^2}{4!}(f^{(4)}(\xi_1) + f^{(4)}(\xi_2))$$

(c) What is the order or this method in terms of big-O notation?

[2] In Lecture 18 we derived a formula for the error in the $O(h^2)$ approximation of f'. In particular we showed that if $\varepsilon_1, \varepsilon_2$ are the roundoff errors respectively in $f(x_0+h), f(x_0-h)$ and $\varepsilon = \max\{\varepsilon_1, \varepsilon_2\}$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \left| -\frac{h^2 M}{6} \right| + \left| \frac{\varepsilon}{h} \right|$$

Assume $h > 0$, $\varepsilon > 0$. Find a formula for the optimal h.

[3] [*Richardson extrapolation for a 2nd order accurate approximation*]
Using Taylor's theorem, it can be shown that if $f \in C^5([a,b])$, then the centered difference approximation formula for the first derivative is given by

$$\underbrace{f'(x_0)}_{\text{true value}} = \underbrace{\frac{f(x_0+h) - f(x_0-h)}{2h}}_{\text{approximation}} - \left(\underbrace{\frac{h^2}{6} f'''(x_0) + \frac{h^4}{120} f^{(5)}(\xi)}_{\text{error}} \right) \qquad (*)$$

(a) Re-write this formula using step size $h/2$ instead of h.

(b) Multiply your answer from (a) by 4, subtract $(*)$ from the result, and then divide everything by 3. We now should have an approximation to $f'(x_0)$ based on $f(x_0 + h,\ f(x_0 - h),\ f(x_0 + h/2)$ and $f(x_0 - h/2)$. What is the error in this new approximation $f'(x_0)$?

[4]
Let $f(x) = \sin(x)$. Use the backwards difference formula to approximate $f'(x = \pi/3)$ using $h = 0.1$, $h = 0.01$, and $h = 0.001$ and record the absolute error. By how much does the error decrease each time?

[5]
Let $f(x) = 3xe^x - \cos(x)$. Use the data below and your answer to exercise [1] to approximate $f''(1.3)$ with $h = 0.1$ and $h = 0.01$. Compare your results to the true $f''(1.3)$ using the relative error.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

[6] Computational Problem
Consider the function $f(x) = x^2 \ln(x)$. We want to numerically approximate the derivative of the function at the point $x = 2$.

(a) Use the first order forward difference scheme

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

to approximate $f'(2)$.

(b) Write a code to find the optimal h (the h for which the error is smallest) by numerical experimentation. Report your estimate of the optimal h.

(c) Create a graph that shows how the error decreases and then starts to increase as h continues to decrease. Why isn't the error always decreasing?

Hint: It might be helpful to use a `log-log` plot to visualize the error. Additionally when thinking about values of h to try you can try different increments, but a good starting place is incrementing by $1/10^n$ for $n = 1, \ldots$

Note: You can identify the "optimal" h as the value that gives the lowest error when using different h vectors. You can calculate the true derivative of f by hand.