Math 5601 Homework 4

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Question 1.

(a) We want to derive a finite difference formula for $f'(t_j)$ involving the sample values $f(t_j - 2h)$, $f(t_j - h)$, $f(t_j + h)$, and $f(t_j + 2h)$. Expanding f at these sample values with Taylor's Theorem (centered at t_j) gives

$$\begin{aligned}
f(t_j - 2h) &= f(t_j) - 2hf'(t_j) + \frac{4h^2}{2}f''(t_j) - \frac{8h^3}{6}f'''(t_j) + \frac{16h^4}{24}f''''(t_j) + O(h^5), && (1)\\
f(t_j - h) &= f(t_j) - hf'(t_j) + \frac{h^2}{2}f''(t_j) - \frac{h^3}{6}f'''(t_j) + \frac{h^4}{24}f''''(t_j) + O(h^5), && (2)\\
f(t_j + h) &= f(t_j) + hf'(t_j) + \frac{h^2}{2}f''(t_j) + \frac{h^3}{6}f'''(t_j) + \frac{h^4}{24}f''''(t_j) + O(h^5), && (3)\\
f(t_j + 2h) &= f(t_j) + 2hf'(t_j) + \frac{4h^2}{2}f''(t_j) + \frac{8h^3}{6}f'''(t_j) + \frac{16h^4}{24}f''''(t_j) + O(h^5). && (4)
\end{aligned}$$

Therefore,

$$\begin{aligned}
f(t_j - 2h) - 8f(t_j - h) + 8f(t_j + h) - f(t_j + 2h) &= (1 - 8 + 8 - 1)f(t_j)\\
&\quad + (-2 + 8 + 8 - 2)hf'(t_j)\\
&\quad + (4 - 8 + 8 - 4)\frac{h^2}{2}f''(t_j)\\
&\quad + (-8 - 8 + 8 + 8)\frac{h^3}{6}f'''(t_j) \qquad (5)\\
&\quad + (16 - 8 + 8 - 16)\frac{h^4}{24}f''''(t_j)\\
&\quad + O(h^5)\\
&= 12hf'(t_j) + O(h^5).
\end{aligned}$$

Dividing both sides by $12h$ yields the finite difference formula

$$f'(t_j) = \frac{1}{12h}\left[f(t_j - 2h) - 8f(t_j - h) + 8f(t_j + h) - f(t_j + 2h)\right] + O(h^4). \qquad (6)$$

(b) Let $\tilde{f}_j$ be the number actually stored in computer memory as an approximation of $f_j = f(t_j)$, and suppose that $f_j = \tilde{f}_j + e(t_j)$, where, for some $\varepsilon > 0$, the round-off error e satisfies the estimate $|e(t)| \le \varepsilon |f(t)|$ for all t.

Then the error between $f'(t_j)$ the approximation computed by the computer using the finite difference formula from (a) is given by

$$
\begin{aligned}
E(t_j) &= \left| f'(t_j) - \frac{\tilde{f}_{j-2} - 8\tilde{f}_{j-1} + 8\tilde{f}_{j+1} - \tilde{f}_{j+2}}{12h} \right| \\
&\le \left| f'(t_j) - \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h} \right| \\
&\quad + \frac{1}{12h} \left| \tilde{f}_{j-2} - f_{j-2} - 8(\tilde{f}_{j-1} - f_{j-2}) + 8(\tilde{f}_{j+1} - f_{j+1}) - (\tilde{f}_{j+2} - f_{j+2}) \right| \\
&\le O(h^4) + \frac{\varepsilon}{12h}(f_{j-2} + 8f_{j-1} + 8f_{j+1} + f_{j+2})
\end{aligned}
\tag{7}
$$

(c) The following Python script computes the numerical derivative $\ln'(3) = \frac{1}{3}$ using the formula from (a) for various values of h.

```
from math import log
fprime = 1/3
for n in range(1, 21):
    h = 10 ** (-n)
    fprime_approx = (log(3-2*h) - 8 * log(3-h) + 8*log(3+h) - log(3+2*h))/(12*h)
    print(f'h = 10^{-n}, error = {abs(fprime - fprime_approx)}')
```

Here is what was printed when I ran this script.

```
h = 10^-1, error = 3.3052928644083934e-07
h = 10^-2, error = 3.293260109060725e-11
h = 10^-3, error = 1.8207657603852567e-14
h = 10^-4, error = 1.0734746425100639e-12
h = 10^-5, error = 4.034106382277969e-12
h = 10^-6, error = 2.8088975589923848e-11
h = 10^-7, error = 2.0258236199666158e-09
h = 10^-8, error = 9.427310487808427e-09
h = 10^-9, error = 4.60838407434494e-08
h = 10^-10, error = 2.1261729443722288e-07
h = 10^-11, error = 1.8779518313749577e-06
h = 10^-12, error = 8.51446786782617e-05
h = 10^-13, error = 8.138877501551178e-05
h = 10^-14, error = 0.012686176008173844
h = 10^-15, error = 0.0002664259457863527
h = 10^-16, error = 0.14829616256247388
h = 10^-17, error = 1.517038374375261
h = 10^-18, error = 18.17038374375261
h = 10^-19, error = 184.7038374375261
h = 10^-20, error = 1850.0383743752611
```

Evidently, the error decreases at first as h gets smaller, achieving a minimum for $h = 10^{-3}$, then it increases again as h gets even smaller. This is consistent with the estimate from part (b). This estimate involves two terms; the first decreases rapidly as $h \to 0$, and the second blows up as $h \to 0$. If the relative error ε is small enough compared to h, then the total error $E(t_j)$ should be small at first because the $O(h^4)$ term goes to zero so quickly, but as h gets even smaller, the total error could (and in this case does) increase in inverse proportion to h. In fact, each time h *decreases* by a factor of 10 below 10^{-5}, the total error roughly *increases* by a factor of 10, consistent with the $\frac{1}{h}$ relationship in the estimate.

Furthermore, we can see that the point where the error changes from decreasing to increasing is different if we use a different level of precision. Here we do the same experiment using 30 decimal digits of relative precision ($\varepsilon \approx 10^{-30}$) instead of Python's default 64-bit floating point representation ($\varepsilon \approx 10^{-15}$).

```python
from mpmath import mp, mpf, log
mp.dps = 30

fprime = mpf(1) / 3
for n in range(1, 21):
    h = mpf(10) ** (-n)
    fprime_approx = (log(3-2*h) - 8*log(3-h) + 8*log(3+h) - log(3+2*h)) / (12*h)
    print(f'h = 10^{-n}, error = {abs(fprime - fprime_approx)}')
```

This results in the following output.

```
h = 10^-1, error = 0.000000330529287394316004402906803334
h = 10^-2, error = 3.29231171680679755975451845909e-11
h = 10^-3, error = 3.2921823763803376195465228809e-15
h = 10^-4, error = 3.29218108325886682162187340946e-19
h = 10^-5, error = 3.29215652897465049577434955075e-23
h = 10^-6, error = 8.68735537064968066371557994169e-26
h = 10^-7, error = 1.12928697564002534249710051324e-24
h = 10^-8, error = 4.12978564366037573305902685826e-24
h = 10^-9, error = 1.02737398845590657985838335357e-22
h = 10^-10, error = 3.73866064741871909975852085448e-22
h = 10^-11, error = 1.23711256649616585150871196032e-20
h = 10^-12, error = 3.2002300253720255539322612194e-20
h = 10^-13, error = 8.86601614243133276799836453504e-19
h = 10^-14, error = 9.46719776678264666922910096583e-18
h = 10^-15, error = 2.59017999588870428473712539715e-17
h = 10^-16, error = 3.35659448267410067502208722659e-16
h = 10^-17, error = 1.36337524150213406861996890051e-14
h = 10^-18, error = 9.31911618336573413130731564024e-14
h = 10^-19, error = 1.36893268855804435281782277331e-13
h = 10^-20, error = 1.39419591102235110300363359764e-11
```

As we can see, the value of h where the error is minimal is now $h = 10^{-6}$. Furthermore, for the smallest value of $h = 10^{-20}$ (at which point the $O(h^4)$ error term should be completely irrelevant), the error has decreased by a factor of $\sim 10^{-15}$, that is, in proportion to ε, as the estimate for $E(t_j)$ suggests.

Question 2.

Suppose that

$$f'(t_j) = \frac{1}{h}\left[\alpha_1 f(t_j) + \alpha_2 f(t_j + h) + \alpha_3 f(t_j + 2h) + \alpha_4 f(t_j + 3h) + \alpha_5 f(t_j + 4h)\right] + O(h^4) \tag{8}$$

for some constants $\{\alpha_i\}$. Expanding f about t_j using Taylor's Theorem, we have, for $i \in \{0, 1, 2, 3, 4\}$,

$$f(t_j + ih) = f(t_j) + \sum_{k=1}^{4} \frac{(ih)^k}{k!} f^{(k)}(t_j) + O(h^5). \tag{9}$$

Therefore, the approximation in (8) can be estimated by

$$
\begin{aligned}
\frac{1}{h}\sum_{i=0}^{4}\alpha_{i+1}f(t_j+ih) &= \sum_{i=0}^{4}\alpha_{i+1}\left[f(t_j)+\sum_{k=1}^{4}\frac{i^k}{k!}f^{(k)}(t_j)h^{k-1}\right]+O(h^4) && (10)\\
&= \left(\sum_{i=0}^{4}i\alpha_{i+1}\right)f'(t_j)+\sum_{i=0}^{4}\alpha_{i+1}\left[f(t_j)h^{-1}+\sum_{k=2}^{4}\frac{i^k}{k!}f^{(k)}(t_j)h^{k-1}\right]+O(h^4) && (11)\\
&= \left(\sum_{i=1}^{5}(i-1)\alpha_i\right)f'(t_j)+\left(\sum_{i=1}^{5}\alpha_i\right)f(t_j)h^{-1} && (12)\\
&\quad+\sum_{k=2}^{4}f^{(k)}(t_j)\frac{h^{k-1}}{k!}\left(\sum_{i=1}^{5}\alpha_i(i-1)^k\right)+O(h^4).
\end{aligned}
$$

So, to obtain (8), we would need the coefficient of $f'(t_j)$ in (12) to be 1, and we would need the rest of the coefficients of h^k to be zero when $k<4$, since otherwise we would not have an error of $O(h^4)$. That is, $\{\alpha_i\}$ must satisfy the system of equations

$$
\begin{bmatrix}1&1&1&1&1\\0&1&2&3&4\\0&1&4&9&16\\0&1&8&27&64\\0&1&16&81&256\end{bmatrix}\begin{bmatrix}\alpha_1\\\alpha_2\\\alpha_3\\\alpha_4\\\alpha_5\end{bmatrix}=\begin{bmatrix}0\\1\\0\\0\\0\end{bmatrix}. \tag{13}
$$

Thus, $\alpha_1=-\sum_{i=2}^{5}\alpha_i$, and the remaining $\{\alpha_i\}_{i=2}^{5}$ must satisfy

$$
\begin{bmatrix}1&2&3&4\\1&4&9&16\\1&8&27&64\\1&16&81&256\end{bmatrix}\begin{bmatrix}\alpha_2\\\alpha_3\\\alpha_4\\\alpha_5\end{bmatrix}=\begin{bmatrix}1\\0\\0\\0\end{bmatrix}. \tag{14}
$$

Then $\alpha_2=1-\sum_{i=3}^{5}(i-1)\alpha_i$, and the last three rows are equivalent to

$$
\begin{bmatrix}4&9&16\\8&27&64\\16&81&256\end{bmatrix}\begin{bmatrix}\alpha_3\\\alpha_4\\\alpha_5\end{bmatrix}=-\alpha_2\begin{bmatrix}1\\1\\1\end{bmatrix}. \tag{15}
$$

Let A be the matrix on LHS(15). Then

$$
\det(A)=4(27\cdot256-64\cdot81)-9(8\cdot256-64\cdot16)+16\cdot(8\cdot81-27\cdot16)=1152.
$$

Using Cramer's Rule, the solution of $Ax=[1\quad 0\quad 0]^T$ is

$$
\frac{1}{\det(A)}\left[\begin{vmatrix}27&64\\81&256\end{vmatrix}\quad -\begin{vmatrix}8&64\\16&256\end{vmatrix}\quad \begin{vmatrix}8&27\\16&81\end{vmatrix}\right]^T=\frac{1}{1152}\begin{bmatrix}1728\\-1024\\216\end{bmatrix}, \tag{16}
$$

the solution of $Ax=[0\quad 1\quad 0]^T$ is

$$
\frac{1}{\det(A)}\left[-\begin{vmatrix}9&16\\81&256\end{vmatrix}\quad \begin{vmatrix}4&16\\16&256\end{vmatrix}\quad -\begin{vmatrix}4&9\\16&81\end{vmatrix}\right]^T=\frac{1}{1152}\begin{bmatrix}-1008\\768\\-180\end{bmatrix}, \tag{17}
$$

and the solution of $Ax = [0 \quad 0 \quad 1]^T$ is

$$\frac{1}{\det(A)}\begin{bmatrix}\begin{vmatrix}9 & 16\\27 & 64\end{vmatrix} & -\begin{vmatrix}4 & 16\\8 & 64\end{vmatrix} & \begin{vmatrix}4 & 9\\8 & 27\end{vmatrix}\end{bmatrix}^T = \frac{1}{1152}\begin{bmatrix}144\\-128\\36\end{bmatrix}. \tag{18}$$

Therefore,

$$A^{-1} = \frac{1}{1152}\begin{bmatrix}1728 & -1008 & 144\\-1024 & 768 & -128\\216 & -180 & 36\end{bmatrix}. \tag{19}$$

This implies that

$$\begin{bmatrix}\alpha_3\\\alpha_4\\\alpha_5\end{bmatrix} = -\alpha_2 A^{-1}\begin{bmatrix}1\\1\\1\end{bmatrix} = -\frac{\alpha_2}{1152}\begin{bmatrix}1728-1008+144\\-1024+768-128\\216-180+36\end{bmatrix} = -\frac{\alpha_2}{1152}\begin{bmatrix}864\\-384\\72\end{bmatrix} = \frac{\alpha_2}{48}\begin{bmatrix}-36\\16\\-3\end{bmatrix}, \tag{20}$$

or $\alpha_3 = -\frac{3}{4}\alpha_2$, $\alpha_4 = \frac{1}{3}\alpha_2$, and $\alpha_5 = -\frac{1}{16}\alpha_2$. Next,

$$\alpha_2 = 1 - 2\alpha_3 - 3\alpha_4 - 4\alpha_5 = 1 + \frac{3}{2}\alpha_2 - \alpha_2 + \frac{1}{4}\alpha_2 \implies \alpha_2 = 4. \tag{21}$$

Thus, $\alpha_3 = -3$, $\alpha_4 = \frac{4}{3}$, and $\alpha_5 = -\frac{1}{4}$. Lastly, we get

$$\alpha_1 = -\alpha_2 - \alpha_3 - \alpha_4 - \alpha_5 = -4 + 3 - \frac{4}{3} + \frac{1}{4} = -\frac{25}{12}. \tag{22}$$

Therefore, the desired finite difference formula is

$$f'(t_j) = \frac{-25f(t_j) + 48f(t_j+h) - 36f(t_j+2h) + 16f(t_j+3h) - 3f(t_j+4h)}{12h} + O(h^4). \tag{23}$$

Question 3.

Let $f \in C^\infty(-\infty,\infty)$, and let $x \in \mathbf{R}$.

(a) Define

$$S_h = \frac{f(x+h) - f(x-h)}{2h}. \tag{24}$$

Then

$$S_h = f'(x) + \sum_{i=1}^{\infty} c_i h^{2i} \tag{25}$$

for constants c_i independent of h.

Proof. By Taylor's Theorem (assuming f is analytic in a neighborhood of x and h is sufficiently small),

$$f(x+sh) = \sum_{i=0}^{\infty}\frac{f^{(i)}(x)}{i!}s^i h^i, \tag{26}$$

where $s \in \{-1, 1\}$. Then

$$S_h = \frac{1}{2h}\left[\sum_{i=0}^{\infty}\frac{f^{(i)}(x)}{i!}h^i - \sum_{i=0}^{\infty}\frac{f^{(i)}(x)}{i!}(-1)^i h^i\right] = \frac{1}{2h}\sum_{i=0}^{\infty}\frac{f^{(i)}(x)}{i!}\left(1-(-1)^i\right)h^i. \tag{27}$$

Since $1 - (-1)^i = 0$ if i is even and 2 if i is odd, it follows that

$$S_h = \frac{1}{h}\sum_{i=0}^{\infty} \frac{f^{(2i+1)}(x)}{(2i+1)!}h^{2i+1} = f'(x) + \sum_{i=1}^{\infty} \frac{f^{(2i+1)}(x)}{(2i+1)!}h^{2i}. \tag{28}$$

The claim follows if we choose $c_i = \frac{f^{(2i+1)}(x)}{(2i+1)!}$. □

(b) Suppose that

$$\alpha_1 S_h + \alpha_2 S_{\frac{h}{2}} = f'(x) + O(h^4). \tag{29}$$

Using part (a), we see that

$$\alpha_1 S_h + \alpha_2 S_{\frac{h}{2}} = (\alpha_1 + \alpha_2)f'(x) + \sum_{i=1}^{\infty} c_i \left(\alpha_1 + \frac{\alpha_2}{2^{2i}}\right) h^{2i}. \tag{30}$$

Since $\sum c_i h^{2i}$ converges, the remainder of the infinite series starting from $i = 2$ is $O(h^4)$. The first term of the infinite series, however, is at best $O(h^2)$, so, in order to satisfy the assumption, we must choose α_1 and α_2 so that the coefficient of the h^2 term in the series is zero. We must also ensure that the coefficient of $f'(x)$ is 1. That is, α_1 and α_2 must solve the equations

$$\alpha_1 + \alpha_2 = 1, \tag{31}$$

$$\alpha_1 + \frac{1}{4}\alpha_2 = 0. \tag{32}$$

Then $\alpha_2 = -4\alpha_1$, so $-3\alpha_1 = 1$, and $\alpha_1 = -\frac{1}{3}$, and $\alpha_2 = \frac{4}{3}$. Then

$$\alpha_1 S_h + \alpha_2 S_{\frac{h}{2}} = \frac{4S_{\frac{h}{2}} - S_h}{3} = f'(x) + O(h^4). \tag{33}$$