Assignment 1 - Solutions
MATH 3423 - Numerical Methods 2
Acadia University

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1 Requirements

I expected well presented papers with computer generated graphics and title pages. All of you met my standards so you all receive 5/5 for presentation. If you want a real challenge, try LaTeX in the future (not required).

A couple of students who will remain nameless did hand in an assignment without properly binding the sheets together. Since I actually read all of your work and go over it several times, this is very inconvenient. Please consider more robust binding.

2 Numerical Differentiation

2.1 Basic applications

1. [6 marks] For the following problems, approximate the specified derivative.

   (a) Using the forward-difference formula.

   (b) Using the backward-difference formula.

   (c) Using the central-difference formula.

   (d) Using Richardson extrapolation to improve (once) your central-difference result.

   Question 1. Approximate $y'(1.0)$ if $x = [0.8\,0.9\,1.0\,1.1\,1.2]$ and $y = [0.992\,0.999\,1.000\,1.001\,1.008]$.
   Solution: (a) 0.01 (b) 0.01 (c) 0.01 (d) several answers are possible, try $\frac{-f(-1.2)+4f(1.1)-3f(1)}{2(0.1)} = -0.02$.♣

   Question 2. Approximate $y'(1)$ if $x = [-1\,0\,1\,2\,3]$ and $y = [1/3\,1\,3\,9\,27]$.
   Solution: (a) 6 (b) 2 (c) 4 (d) several answers are possible, try $\frac{-f(3)+4f(2)-3f(1)}{2(1)} = 0$.♣

2. [5 marks] The altitude of a helicopter at three different instants is found to be $h_1 = 445.98$ at $t_1 = 0.20$, $h_2 = 471.85$ at $t_2 = 0.30$, and $h_3 = 503.46$ at $t_3 = 0.41$. Taylor expanding twice the altitude $h(t)$ of the helicopter about $t = 0.30$, find dh/dt at $t = 0.30$ using all of the available data. (HINT: do not try to plug in a formula... work out the math...)
   Solution: The proper way to do this problem is to Taylor expand "forward" and then "backward". Firstly,

$$h(t_3) = h(t_2) + h'(t_2)(t_3 - t_2) + \frac{(t_3 - t_2)^2 h''(t_2)}{2} + error,$$

   secondly

$$h(t_1) = h(t_2) + h'(t_2)(t_1 - t_2) + \frac{(t_1 - t_2)^2 h''(t_2)}{2} + error.$$

Plugging the numbers, these equations

$$503.46 - 471.85 = 0.121h''(t_2) + 0.11h'(t_2) + \ldots$$
$$445.98 - 471.85 = 0.01h''(t_2) - 0.1h'(t_2) + \ldots$$

Solving this set of equations in order to cancel out the $h''(t_2)$ terms should give you $h'(t_2) \cong 272.35$. You have to stop at this point and read the solution over. Make sure you understand it since this is pretty deep stuff. This is a perfect prototype for a test question!♣

2.2 Theory

1. [4 marks] Observe that the sum of all the coefficients of the functions values appearing in the numerator of all finite-difference derivatives seen in class is 0. Give at least 4 examples to justify this claim. Prove that it must always be so.
   Solution: Examples: $\frac{f_{i+1}-f_i}{\Delta x}, \frac{f_i - f_{i-1}}{\Delta x}, \frac{f_{i+1}-f_{i-1}}{2\Delta x}$, and $\frac{f_{i+1}-2f_i+f_{i-1}}{(\Delta x)^2}$. To prove the result, choose $f(x) = 1$, then $f_k = 1$ for all $k's$. Therefore, given a formula such as $\frac{\sum_i w_i f_i}{(\Delta x)^n} \simeq f^{(n)}$ for some derivative, we have that $0 = f^{(n)} = \frac{\sum_i w_i}{(\Delta x)^n}$ hence $\sum_i w_i = 0$. ♣

2. [6 marks] Give the order of accuracy ($O(\Delta x), O((\Delta x)^2), \ldots$) for the following formulas. Briefly justify your answer (do not guess!).**Solution:** In this question, 3 of the examples were, on purpose, flawed. I was expecting you to object when you were given an incorrect formula! ♣

   (a) $f_i' = \frac{f_{i+1}-f_i}{\Delta x}$
   Solution: Taylor series expansion leads to $O(\Delta x)$ (forward difference). See examples in class. ♣

   (b) $f_i' = \frac{f_{i+1}-f_{i-1}}{2\Delta x}$
   Solution: Taylor series expansion leads to $O((\Delta x)^2)$ (centered difference). See examples in class. ♣

   (c) $f_i'' = \frac{f_{i+2}-2f_{i+1}+f_i}{(\Delta x)^2}$
   Solution: Taylor series expansion leads to $O(\Delta x)$ (forward difference). See examples in class. ♣

   (d) $f_i'' = \frac{f_{i+1}-2f_i+f_{i-1}}{\Delta x^2}$
   Solution: The new trick here is that instead of having $(\Delta x)^2$ in the numerator, we have Δx^2. Does that matter? Suppose that $x = k\Delta x$, then $x^2 = k^2(\Delta x)^2$ and $\Delta x^2 = (k+1)^2(\Delta x)^2 - k^2(\Delta x)^2 = (2k+1)(\Delta x)^2$. Therefore Δx^2 is incorrect here. However, I took off few marks if you gave the answer $O((\Delta x)^2)$ (centered difference) by assuming that the formula was $f_i'' = \frac{f_{i+1}-2f_i+f_{i-1}}{(\Delta x)^2}$. ♣

   (e) $f_i''' = \frac{f_{i+3}-3f_{i+2}-3f_{i+1}-f_i}{\Delta x^3}$
   Solution: The real answer was to say that this is not a proper formula for several reasons (trick question). However, if you assumed that the formula was $f_i''' = \frac{f_{i+3}-3f_{i+2}+3f_{i+1}-f_i}{(\Delta x)^3}$ and said that since this is a centered difference formula, it must be $O((\Delta x)^2)$, then you are also correct.♣

   (f) $f_i' = \frac{f_{i+1}-f_i}{2\Delta x}$
   Solution: The real answer was to say that this is not a proper formula(trick question). I wouldn't accept $O(\Delta x)$ (forward difference) as an answer here. This formula is clearly flawed (compare with part a). The only valid answer was to say that the formula was incorrect.♣

3. [5 marks] Recall that $\|f-g\|_{L^\infty(S)} = \max\{|f(x)-g(x)|, x \in S\}$. Give the formulas for two families of real-valued functions f, g with a parameter a (for example $\sin ax$) over the real numbers such that $\|f-g\|_{L^\infty}$ can be made as small as we want (by a change of parameter) while $\|f'-g'\|_{L^\infty} \geq 1$. Suppose now that you have a sampling of two functions f_i, g_i for some x values (x_i), use your example to show that while the values f_i, g_i might be very close, and thus their numerical derivatives, their actual derivatives might be very different.
   Solution: Take $f = 0$ and $g = \frac{\sin ax}{a}$ defined over $S = [0, 2\pi]$ then $\|f-g\|_{L^\infty(S)} = 1/a \to 0$ as $a \to \infty$. On the other hand, $g' = \cos ax$ and hence $\|f'-g'\|_{L^\infty} = 1$.♣

2.3 Problem

You are working for NASA. The American government has spotted an UFO and you must process the collected data. Write a computer program to estimate the speed as a function of time of the object and its acceleration (one real number per time sample for both speed and acceleration). You must do this work for accuracy orders $O(\Delta x), O((\Delta x)^2)$, and $O((\Delta x)^4)$. You must hand in the computer program you wrote, a brief explanation of the formulas you used and two plots for each order of accuracy: speed vs time and acceleration vs time.

Data (in format $[x,y,z,t]$) : [0.84, 1.71, 1.0], [4.0, 1.81, 5.38, 2.0], [9.0, 0.42, 17.08, 3.0], [16.0, - 3.02, 50.59, 4.0], [25.0, - 4.79, 143.41, 5.0], [36.0, - 1.67, 397.42, 6.0], [49.0, 4.59, 1089.63, 7.0], [64.0, 7.91, 2972.95, 8.0], [81.0, 3.70, 8094.08, 9.0], [100.0, - 5.44, 22016.46, 10.0], [121.0, - 10.99, 59863.14, 11.0], [144.0, - 6.43, 162742.79, 12.0], [169.0, 5.46, 442400.39, 13.0], [196.0, 13.86, 1202590.28, 14.0], [225.0, 9.75, 3269002.37, 15.0],[256.0, - 4.60, 8886094.52, 16.0].

Solution: [20 marks] The plots should show a roughly exponential increase in speed and acceleration. You were expected to use formulas such as

$$v(t) = \frac{\|\underline{X}(t+\Delta t) - \underline{X}(t)\|}{\Delta t}$$

and

$$a(t) = \frac{\|\underline{X}(t+\Delta t) - 2\underline{X}(t) + \underline{X}(t-\Delta t)\|}{(\Delta t)^2}.$$

And various, straight-forward generalizations.♣

3 Numerical Integration

3.1 Basic Applications

1. [4 marks] Use Gaussian quadrature with $n=3$ and exact arithmetic to approximate $\int_{-1}^{1} x^4 dx$. Compare your result with the expected value of the integral and discuss the two.
   Solution: The exact arithmetic answer is $2/5$. For $n=3$, you should get $2/5$ from the Gaussian quadrature formula since it is exact for polynomials of degree $2n-1 = 2(3)-1 = 5$ and x^4 is a polynomial of degree $4<5$.♣

2. [10 marks] Evaluate the integral $\int_0^{2\pi} \cos^2 x dx$ using the following methods with 6 function evaluations (give all of your computations):

   (a) Trapezoidal rule.
   Solution: Choosing the composite trapezoidal rule with nodes at $x = 0, \frac{2\pi}{5}, \frac{4\pi}{5}, \frac{6\pi}{5}, \frac{8\pi}{5}, 2\pi$, you get π. Please note that in this case, the number of function evaluation is exactly the same as the number of nodes. No marks were taken off if you only took 5 nodes because of the possible confusion in part b.♣

   (b) Simpson's rule (1/3)
   Solution: For this case, you had to recognize that it was impossible to use exactly 6 function evaluations. You could have chosen to use 7 function evaluations, but using 5 function evaluations was a fine alternative. You had to choose the nodes $x = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}, 2\pi$ and the answer is then $\frac{4\pi}{6}$.♣

   (c) Gauss quadrature formula
   Solution: Given the Matlab program I provided, on through any other mean, you had to find the weights and the nodes for the $n=6$ gaussian quadrature. You had to get values that look (roughly) like the following table.

weights	nodes
0.17	± 0.93
0.36	± 0.66
0.47	± 0.24

   From that point, it was easy to get 3.1 as an approximation. Of course, you had to do a change of variables to get the integral to be from -1 to 1 ($t = \frac{x-\pi}{\pi}$) and integrate

$$\frac{1}{\pi}\int_{-1}^{1} \cos^2(\pi t + \pi)\, dt$$

. It is interesting to point out that in this case, the exact answer is π and therefore the most accurate scheme is trapezoidal rule followed by the gaussian quadrature. Does that bother you that Simpson gives a worse result? Can you explain why? (HINT: I said in class that we don't necessarily want to always go for high order schemes because...) ♣

3.2 Theory

1. [5 marks] Show that the integral given by the trapezoidal rule is the average of the integrals given by the two rectangular rules.
Solution: Integrating f over $[a,b]$, the left-hand-side rectangular rule gives $f(a)(b-a)$ whereas the right-hand-side rule gives $f(b)(b-a)$, the average of the two is $\frac{f(a)+f(b)}{2}(b-a)$ which is the trapezoidal rule.♣

2. [10 marks] Use the definition of the Legendre polynomial $P_n(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}[(1-x^2)^n]$, $n \geq 1$ to find a relationship between $P_n'(x)$ and $P_{n+1}(x)$, and then show the equivalence of the following expressions for the coefficients for Gaussian quadrature: $c_i = \frac{-2}{(n+1)P_n'(x_i)P_{n+1}(x_i)}$ and $c_i = \frac{2(1-x_i^2)}{(n+1)^2 P_{n+1}^2(x_i)}$.
HINTS:
(a) The x_i's are the roots of P_n and thus $P_n(x_i) = 0$, however, $P_n'(x_i)$ is not zero in general, nor is $P_{n+1}(x_i)$. (Why?)
(b) You might want to use Leibnitz' rule which says that

$$\frac{d^n}{dx^n}uv = \sum_{k=0}^{n} \frac{n!}{(n-k)!k!}\frac{d^k}{dx^k}u\frac{d^{n-k}}{dx^{n-k}}u.$$

You don't have to prove Leibnitz' rule, but you should be clever enough to know how to prove it if your life depended on it!
Solution: In order to show that

(a)

$$c_i = \frac{-2}{(n+1)P_n'(x_i)P_{n+1}(x_i)}$$

and

$$c_i = \frac{2(1-x_i^2)}{(n+1)^2 P_{n+1}^2(x_i)}$$

are equivalent formulas, you need to show that

$$\frac{-2}{(n+1)P_n'(x_i)P_{n+1}(x_i)} = \frac{2(1-x_i^2)}{(n+1)^2 P_{n+1}^2(x_i)}$$

or else,

$$-(n+1)P_{n+1}(x_i) = (1-x_i^2)P_n'(x_i). \tag{1}$$

Using Rodrigue's formula

$$P_n(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}[(1-x^2)^n],$$

equation 1 becomes

$$\frac{d^{n+1}}{dx^{n+1}}[(1-x_i^2)^{n+1}] = 2(1-x_i^2)\frac{d^{n+1}}{dx^{n+1}}[(1-x_i^2)^n] \tag{2}$$

subject to

$$\frac{d^n}{dx^n}[(1-x_i^2)^n] = 0.$$

Let $b(x) = x^2 - 1$, starting with the simple formula

$$(x^2-1)\frac{d}{dx}(x^2-1)^n - 2nx(x^2-1)^n = 0,$$

or

$$b\frac{d}{dx}b^n - 2nxb^n = 0$$

we differentiate n times using Leibnitz' rule (the computation only relies on Leibnitz' rule and some elementary algebra!)

$$\begin{aligned}
0 &= \frac{d^n}{dx^n}\left(b\frac{d}{dx}b^n - 2nxb^n\right) \\
&= n(n-1)\frac{d^{n-1}}{dx^{n-1}}b^n + 2nx\frac{d^n}{dx^n}b^n + b\frac{d^{n+1}}{dx^{n+1}}b^n \\
&\quad -2n^2\frac{d^{n-1}}{dx^{n-1}}b^n - 2nx\frac{d^n}{dx^n}b^n \\
&= - \quad (1-x^2)\frac{d^{n+1}b^n}{dx^{n+1}} - n(n+1)\frac{d^{n-1}b^n}{dx^{n-1}}.
\end{aligned}$$

Hence, we have

$$(1-x^2)\frac{d^{n+1}}{dx^{n+1}}[(1-x^2)^n] = -n(n+1)\frac{d^{n-1}}{dx^{n-1}}[(1-x^2)^n]$$

Using Leibnitz' rule again, we differentiate $(1-x^2)^{n+1}$, $n+1$ times

$$\begin{aligned}
\frac{d^{n+1}}{dx^{n+1}}[(1-x^2)^{n+1}] &= (1-x^2)\frac{d^{n+1}}{dx^{n+1}}[(1-x^2)^n] \\
&\quad -2(n+1)x\frac{d^n}{dx^n}[(1-x^2)^n] - (n+1)(n)\frac{d^{n-1}}{dx^{n-1}}[(1-x^2)^n].
\end{aligned}$$

The rest is left as an exercice. (HINT: combine the last two equations and evaluate at a root of P_n).♣

3. [5 marks] Suppose that the quadrature rule $\int_a^b f(x)dx \approx \sum_{i=1}^n w_i f(x_i)$ is exact for all constant functions. What does this imply about the weights w_i or the nodes x_i?
Solution: Choose $f = 1$, then $b - a = \int_a^b dx \approx \sum_{i=1}^n w_i$. ♣

3.3 Problem

[15 marks] Assuming that f is twice differentiable, prove that $\int_a^b f(x)dx = (b-a)f\left(\frac{b+a}{2}\right) + \frac{(b-a)^3}{24}f''(\xi)$ for some $\xi \in [a,b]$. The formula $\int_a^b f(x)dx \cong (b-a)f\left(\frac{b+a}{2}\right)$ is called the Midpoint formula. Write a computer program to implement the Midpoint formula and use it to integrate $\sin x$ between 0 and π using as many function evaluations as you need to properly estimate the integral starting with $2, 4, 8, 16, 32, 64...$ function evaluations. You must hand in the code of your computer program and a table with your results (function evaluations vs value). Plot your table. Briefly comment on your results (what is the apparent rate of convergence...what do you expect from the theory...).
Solution: Getting over the minor typo in the original question, the trick is to Taylor expand f about $\frac{b+a}{2}$,

$$f(x) = f\left(\frac{a+b}{2}\right) + \left(x - \frac{a+b}{2}\right)f'\left(\frac{a+b}{2}\right) + \frac{\left(x-\frac{a+b}{2}\right)^2}{2}f''(\xi)$$

and then you integrate. Clearly, the linear term goes to zero and you get the desired formula. The plot should show that the integral converges to 2 very quickly (consistent with $(\Delta x)^3$ convergence!)♣