Homework #4: Numerical Differentiation

Solutions

1 Fourth Order Central Difference (first derivative)

It is possible to combine the following two-point central difference approximations for the first derivative $f'(x)$ (one using the values $f(x \pm \Delta x)$ and the other using the values $f(x \pm 2\Delta x)$)

$$f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x^2) \quad \textbf{and} \quad f'(x) = \frac{f(x+2\Delta x) - f(x-2\Delta x)}{4\Delta x} + O(\Delta x^2)$$

to obtain an even more accurate approximation (at least as Δx becomes small) as follows

$$f'(x) = \frac{4}{3}\left(\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}\right) - \frac{1}{3}\left(\frac{f(x+2\Delta x) - f(x-2\Delta x)}{4\Delta x}\right) + O(\Delta x^4).$$

Show how these strategic combination weights of $\frac{4}{3}$ and $-\frac{1}{3}$ arise, as well as why the error term now becomes $O(\Delta x^4)$, by manipulating the following system of Taylor series expansions according to the procedure outlined in class. (For full credit, don't just substitute these expansions into the equation above to verify that it true, but demonstrate the process by which the above equation is obtained.)

$$\begin{aligned}
f(x+2\Delta x) &= f(x) + 2\Delta x\, f'(x) + 2\Delta x^2 f''(x) + \frac{4}{3}\Delta x^3 f'''(x) + \frac{2}{3}\Delta x^4 f^{(4)}(x) + O(\Delta x^5) \\
f(x-2\Delta x) &= f(x) - 2\Delta x\, f'(x) + 2\Delta x^2 f''(x) - \frac{4}{3}\Delta x^3 f'''(x) + \frac{2}{3}\Delta x^4 f^{(4)}(x) + O(\Delta x^5) \\
f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \frac{1}{2}\Delta x^2 f''(x) + \frac{1}{6}\Delta x^3 f'''(x) + \frac{1}{24}\Delta x^4 f^{(4)}(x) + O(\Delta x^5) \\
f(x-\Delta x) &= f(x) - \Delta x\, f'(x) + \frac{1}{2}\Delta x^2 f''(x) - \frac{1}{6}\Delta x^3 f'''(x) + \frac{1}{24}\Delta x^4 f^{(4)}(x) + O(\Delta x^5)
\end{aligned}$$

Solution:

Subtracting the first two equations from each other and subtracting the last two equations from each other yield the following two expansions with only odd-powered terms.

$$\begin{aligned}
f(x+2\Delta x) - f(x-2\Delta x) &= 4\Delta x\, f'(x) + \frac{8}{3}\Delta x^3 f'''(x) + O(\Delta x^5) \\
f(x+\Delta x) - f(x-\Delta x) &= 2\Delta x\, f'(x) + \frac{1}{3}\Delta x^3 f'''(x) + O(\Delta x^5)
\end{aligned}$$

Next, we eliminate the third derivative terms on the right hand side by subtracting a multiple of 8 times the bottom equation from the top equation.

$$\left(f(x+2\Delta x) - f(x-2\Delta x)\right) - 8\left(f(x+\Delta x) - f(x-\Delta x)\right) = -12\Delta x\, f'(x) + O(\Delta x^5)$$

Finally, dividing by $12\Delta x$ and rearranging yields the following derivative approximation for $f'(x)$ which is equivalent to the combination of two-point central differences presented in the problem statement.

$$f'(x) = \frac{8\left(f(x+\Delta x) - f(x-\Delta x)\right) - \left(f(x+2\Delta x) - f(x-2\Delta x)\right)}{12\Delta x} + O(\Delta x^4)$$

2 Fourth Order Central Difference (second derivative)

Now develop a fourth order approximation for the second derivative using the sample values $f(x), f(x\pm\Delta x), f(x\pm2\Delta x)$. You should find the same four Taylor series expansions above helpful. (HINT: You will need to extend these same expansions, however, by one additional term in order to demonstrate the fourth-order nature of your final derivative approximation.)

Solution

First we extend the expansions from the previous problem to explicitly show the fifth-derivative terms.

$$\begin{aligned}
f(x+2\Delta x) &= f(x) + 2\Delta x\, f'(x) + 2\Delta x^2 f''(x) + \frac{4}{3}\Delta x^3 f'''(x) + \frac{2}{3}\Delta x^4 f^{(4)}(x) + \frac{4}{15}\Delta x^5 f^{(5)}(x) + O(\Delta x^6)\\
f(x-2\Delta x) &= f(x) - 2\Delta x\, f'(x) + 2\Delta x^2 f''(x) - \frac{4}{3}\Delta x^3 f'''(x) + \frac{2}{3}\Delta x^4 f^{(4)}(x) - \frac{4}{15}\Delta x^5 f^{(5)}(x) + O(\Delta x^6)\\
f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \frac{1}{2}\Delta x^2 f''(x) + \frac{1}{6}\Delta x^3 f'''(x) + \frac{1}{24}\Delta x^4 f^{(4)}(x) + \frac{1}{120}\Delta x^5 f^{(5)}(x) + O(\Delta x^6)\\
f(x-\Delta x) &= f(x) - \Delta x\, f'(x) + \frac{1}{2}\Delta x^2 f''(x) - \frac{1}{6}\Delta x^3 f'''(x) + \frac{1}{24}\Delta x^4 f^{(4)}(x) - \frac{1}{120}\Delta x^5 f^{(5)}(x) + O(\Delta x^6)
\end{aligned}$$

Now our goal is to combine the results to leave the keep the second derivative term on the right and cancel everything else. We start by adding the first two equations together and adding the second two equations together to obtain the following two expansions with only even-powered terms.

$$\begin{aligned}
f(x+2\Delta x) + f(x-2\Delta x) &= 2f(x) + 4\Delta x^2 f''(x) + \frac{4}{3}\Delta x^4 f^{(4)}(x) + O(\Delta x^6)\\
f(x+\Delta x) + f(x-\Delta x) &= 2f(x) + \Delta x^2 f''(x) + \frac{1}{12}\Delta x^4 f^{(4)}(x) + O(\Delta x^6)
\end{aligned}$$

Next, in order to eliminate the fourth-derivative terms, we subtract a multiple of 16 times the bottom equation from the top equation.

$$\left(f(x+2\Delta x) + f(x-2\Delta x)\right) - 16\left(f(x+\Delta x) + f(x-\Delta x)\right) = -30f(x) - 12\Delta x^2 f''(x) + O(\Delta x^6)$$

Finally, dividing by $12\Delta x^2$ and rearranging yields the following second derivative approximation formula.

$$f''(x) = \frac{16\left(f(x+\Delta x) - 2f(x) + f(x-\Delta x)\right) - \left(f(x+2\Delta x) - 2f(x) + f(x-2\Delta x)\right)}{12\Delta x^2} + O(\Delta x^4)$$

(Notice that this is the same weighted combination, weights of $\frac{4}{3}$ and $-\frac{1}{3}$, as in part one, but this time applied to the second derivative central differences based on the $\pm\Delta x$ neighbors and the $\pm 2\Delta x$ neighbors respectively.)

3 Third Order Forward Difference (first derivative)

Using $f(x)$ and three sample values $f(x+\Delta x)$, $f(x+2\Delta x)$, $f(x+3\Delta x)$ all in the forward direction, develop a third order approximation for the first derivative $f'(x)$.

Solution

We start by developing the three Taylor series expansions of the forward samples up to $O(\Delta x^4)$ as follows.

$$
\begin{aligned}
f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \frac{1}{2}\Delta x^2 f''(x) + \frac{1}{6}\Delta x^3 f'''(x) + O(\Delta x^4) \\
f(x+2\Delta x) &= f(x) + 2\Delta x\, f'(x) + \frac{4}{2}\Delta x^2 f''(x) + \frac{8}{6}\Delta x^3 f'''(x) + O(\Delta x^4) \\
f(x+3\Delta x) &= f(x) + 3\Delta x\, f'(x) + \frac{9}{2}\Delta x^2 f''(x) + \frac{27}{6}\Delta x^3 f'''(x) + O(\Delta x^4)
\end{aligned}
$$

The goal is to combine these three expansions to eliminate the third and second derivative terms from the right hand side. Subtracting a multiple of 8 times the first equation from the second equation and a multiple of 27 times the first equation from the third equation yields the following two new equations without the third derivative term.

$$
\begin{aligned}
f(x+2\Delta x) - 8f(x+\Delta x) &= -7f(x) - 6\Delta x\, f'(x) - 2\Delta x^2 f''(x) + O(\Delta x^4) \\
f(x+3\Delta x) - 27f(x+\Delta x) &= -26f(x) - 24\Delta x\, f'(x) - 9\Delta x^2 f''(x) + O(\Delta x^4)
\end{aligned}
$$

Next, subtracting $\frac{9}{2}$ the top equation from the bottom equation will eliminate the second derivative term.

$$
\left(f(x+3\Delta x) - 27f(x+\Delta x)\right) - \frac{9}{2}\left(f(x+2\Delta x) - 8f(x+\Delta x)\right) = \frac{11}{2}f(x) + 3\Delta x\, f'(x) + O(\Delta x^4)
$$

Finally, dividing by $3\Delta x$ and rearranging yields the following first derivative approximation formula.

$$
f'(x) = \frac{2f(x+3\Delta x) - 9f(x+2\Delta x) + 18f(x+\Delta x) - 11f(x)}{6\Delta x} + O(\Delta x^3)
$$