Lecture F. Homework 6

Covered Contents: Numerical Differentiation and Integration, (Lec 15 - 18)

Deadline: 11/12/2021, 23:59 PST

Total points: Pen-and-Paper $(10 + \overline{10 + 25 + 10 + 15} = 70) + \text{Coding } (30) = 100.$ Submit "hw6.zip"

Pen and Paper

F.1. 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?

F.2. 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

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \left(\frac{h^2}{6}f'''(x_0) + \frac{h^4}{120}f^{(5)}(\xi)\right) \tag{*}$$

 $(true\ value = approximation - error)$

(a similar expression was derived in lecture assuming only $f \in C^3([a,b])$.)

- (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 $f'(x_0)$.
- **F.3.** This exercise will derive the quadrature formula known as Simpson's rule using Taylor's theorem. Suppose $f \in C^4([a,b])$ and consider three equispaced points $\{x_0, x_1, x_2\}$ with $x_0 = a, x_1 = a + h$ and $x_2 = b$, where h = (b a)/2.
- (a) Use Taylor's theorem to write f(x) as a third order polynomial plus a remainder term using the point of expansion x_1 .
- (b) Insert the experssion for f(x) from (a) into the expression $\int_{x_0}^{x_2} f(x) dx$ and explicitly compute the integral of each term in the Taylor polynomial to derive

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx$$

(hint: two of the integrals will vanish identically because of parity, i.e., because they are antisymmetric functions)

(c) Justify using the weighted Mean Value Theorem from lecture for the remainder term, and obtain:

$$\frac{1}{24} \int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx = \frac{f^{(4)}(c)}{60} h^5$$

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

(d) Recall the centered difference formula for the second derivative shown in HW5, Q3:

$$f''(x_1) = \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2} - \frac{h^2}{12}f^{(4)}(\zeta)$$

(note: this is a slightly different expression than the one derived; the $f^{(4)}$ terms have been combined using the IVT. Also note $x_2 = x_1 + h$ and $x_0 = x_1 - h$). Insert both this expression and your answer from part (c) into the result from part (b) to conclude:

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{12} \left(\frac{1}{3} f^{(4)}(\zeta) - \frac{1}{5} f^{(4)}(c) \right).$$

The right hand side consists of Simpson's rule and a $O(h^5)$ error term.

- (e) Based on the error term, what is the degree of exactness of Simpson's rule?
- **F.4.** The Traperzoidal 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)?
- **F.5.** Determine the weights w_1 and w_2 and nodes x_1 and x_2 such that the quadrature formula

$$\int_{-1}^{1} f(x)dx \approx w_1 f(x_1) + w_2 f(x_2)$$

is exact for $f(x) = 1, x, x^2$ and x^3 . Then show that the formula is not exact for $f(x) = x^4$ and conclude that the degree of exactness is N = 3.

Coding

Please read "rate of convergence note.pdf" before starting on this part. (30 points).

- (a) Download and run the script 'diffapp.m'. Modify the script so that estimates of the rates of convergence of the centered difference approximation are also computed, and then record them.
- (b) Modify the script to calculate an approximation to f'(p) using Richardson Extrapolation (use your answer for problem 2 part (b), and compute the new rates of convergence and record them. (Hint: Suppose L is the exact solution of a numerical problem, $\Phi(h)$ and $\Phi(h/2)$ are two numerical approximations with "accuracy" h and h/2 respectively. You can compute the rate of convergence with the error $E(h) = |\Phi(h) L|$ and $E(h/2) = |\Phi(h/2) L|$. For part (a), $\Phi(h)$ is the centered difference, which is a linear combination of $f(p \pm h)$; For part (b), $\Phi(h)$ should be a combination of $f(p \pm h)$ and $f(p \pm h/2)$.)