CME 108/MATH 114
Introduction to Scientific Computing
Summer 2018

Problem Set 6

Due: Thursday, August 16 at 5:00pm

Warm-up Questions

1. *(Bradie, 6.2.4.)* Derive the following difference approximation for the first derivative:
$$f'(x_0) = \frac{f(x_0 + 2h) - f(x_0 - h)}{3h} + O(h)$$

2. *(Bradie, 6.2.11.)* Verify that each of the following difference approximations for the first derivative provides the exact value fo the derivative, regardless of h, for the functions $f(x) = 1$, $f(x) = x$, $f(x) = x^2$, but not for the function $f(x) = x^3$.

   (a) $f'(x_0) \approx \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$

   (b) $f'(x_0) \approx \frac{f(x_0+h)-f(x_0+h)}{2h}$

3. *(Verifying Gaussian D.O.P.)* Consider the 2-point Gaussian quadrature, which is defined by:
$$I = \int_a^b f(x)dx \approx \frac{b-a}{2}\left[f\left(\frac{b+a}{2} - \sqrt{\frac{1}{3}}\frac{b-a}{2}\right) + f\left(\frac{b+a}{2} + \sqrt{\frac{1}{3}}\frac{b-a}{2}\right)\right]. \quad (1)$$
Show that, with only two function evaluations, the quadrature given in (1) can integrate polynomials of degree at most 3 exactly.

   Hint: Consider first applying the change of variables $x = \frac{b-a}{2}t + \frac{b+a}{2}$ to transform I to an integral over a symmetric interval. Further, recall that the definite integral is linear and that every polynomial of degree at most 3 is a linear combination of terms of the form x^j, for $j = 0, 1, 2, 3$.

4. *(Using quadrature rules.)*

(a) Use the trapezoidal rule to approximate the value of $\ln 2$, noting that

$$\ln 2 = \int_1^2 \frac{1}{x}\,dx.$$

(b) Use the 2-point Gaussian quadrature rule to approximate the value of π, noting that

$$\pi = 2\int_{-1}^1 \frac{1}{1+x^2}\,dx.$$

5. *(Orthogonal polynomials).* Recall the Legendre polynomial P_n of degree n, which is defined by the recursion:

$$P_n(x) = \frac{2n+1}{n+1} x P_{n-1}(x) - \frac{n}{n+1} P_{n-2}(x),$$

with $P_0(x) = 1$ and $P_1(x) = x$.

(a) Verify that

$$P_n(x) = 2^n \sum_{k=0}^n \binom{n}{k} \binom{\frac{n+k-1}{2}}{n} x^k.$$

(b) Prove that

$$\int_{-1}^1 P_i(x) P_j(x)\,dx = 0,$$

whenever $i \neq j$.

Assignment problems

Remark. We say that the function $g(h)$ is *little-o* of h^k, written $g(h) = o(h^k)$ if

$$\lim_{h\to 0} \left| \frac{g(h)}{h^k} \right| = 0.$$

When discussing finite difference schemes and quadrature rules, we say that the scheme is of *order* k if the error in the approximation is $o(h^k)$. Therefore, a scheme of order k has an error term which is proportional to $h^{k+\alpha}$, for some $\alpha > 0$.

1. (15 points) Let f be a smooth function. Using Taylor exansion, develop a fourth order central difference approximation to $f''(x)$ of the form

$$f''(x_j) = \alpha_{-2} f_{j-2} + \alpha_{-1} f_{j-1} + \alpha_0 f_j + \alpha_1 f_{j+1} + \alpha_2 f_{j+2} + O(h^5),$$

where the α_k are coefficients to be determined and as usual we assume a uniformly spaced grid and we let $f_{j+b} = f(x_j + bh)$.

Report each α_k as a rational multiple of an integer power of h.

2. (15 points) *(Product central difference.)* Consider the central finite difference operator, $\frac{\delta}{\delta x}$, defined as

$$\frac{\delta}{\delta x}(f_j) = \frac{f_{j+1} - f_{j-1}}{2h}.$$

   (a) The product rule for differentiation in calculus guarantees the equality,

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}.$$

   Does the analogous finite difference equality hold? That is, is it true that

$$\frac{\delta}{\delta x}(u_j v_j) = u_j \frac{\delta}{\delta x}(v_j) + v_j \frac{\delta}{\delta x}(u_j)?$$

   (b) Show that

$$\frac{\delta}{\delta x}(u_j v_j) = \bar{u}_j \frac{\delta}{\delta x}(v_j) + \bar{v}_j \frac{\delta}{\delta x}(u_j),$$

   where the overbar indicates averaging over nearest neighbors:

$$\bar{u}_j = \frac{u_{j+1} + u_{j-1}}{2}.$$

3. (10 points) *(NC quadrature.)* Find the weights w_i of the closed Newton-Cotes quadrature rule using $n + 1 = 4$ abscissas.

4. (15 points) *(Convergence of Simpson's rule.)* Verify numerically that the absolute error of the composite Simpson's rule is proportional to h^4 by approximating $I = \int_0^{\frac{\pi}{2}} \cos(x)dx$ using $h = \pi/4, \pi/8, \ldots, \pi/256$.

   Hint: Consider the ratio of successive errors. For visual confirmation, use a `loglog` plot.

5. (15 points) *(Gaussian quadrature.)* Use the method of undetermined coefficients to derive the 3-point Gaussian quadrature rule. That is, find w_i and x_i such that the D.O.P. of the quadrature rule

$$\int_a^b f(x)\,dx \approx I_3(f) = \sum_{k=1}^{3} w_i f(x_i)$$

   is $2(3) - 1$.

   Note: There is no need to derive the error term for this problem, and you may use the Legendre polynomial **only to verify** your calculation.

   Hint: Note the symmetry in the relevant equations.

6. (10 points) *(Newton minimization.)* Implement the Newton minimization algorithm for single-variable functions in MATLAB.

   Use your code to find a minimum of the humps function

$$f(x) = \frac{1}{(x-0.3)^2 + 0.01} + \frac{1}{(x-0.9)^2 + 0.04} - 5.$$

   Use $p_0 = 0.5$ as the initial guess.

7. (10 points) (*Summer correlation.*) We would like to study how well ice cream sales correlate with sunglass sales during the summer. We are given the following data points from last June:

$$(0, 3.5),\ (2, 11),\ (3.2, 12.7),\ (5, 19.4),\ (6.2, 22),\ (10, 34).$$

   Each ordered pair corresponds to a city in the Bay Area, and in each pair the first coordinate denotes the number of pairs of sunglasses sold (in hundreds) and the second coordinate denotes the number of ice cream cones sold (in hundreds).

   Use MATLAB to compute the line of best fit through the given data and report your results.