Math/Phys/Engr 428, Math 529/Phys 528
Numerical Methods - Fall 2020

Homework 5
Due: **Wednesday, November 18, 2020**

REVIEW section 5.6, READ sections 6.1-6.7, 6.9.

1. **(Natural Splines)**

   Find the natural cubic spline $S(x)$ satisfying

   $$S(0) = 0, \qquad S(1/2) = 1, \qquad S(1) = 0\,.$$

   Your answer will be 2 cubic polynomials, $S_0(x)$, $S_1(x)$. **Verify** that your answer satisfies all the necessary conditions (interpolation, continuity of 1st and 2nd derivatives, boundary conditions).

2. The following data describe the shape of a car called “Buggy”:

x=[0.0 0.5 1.0 1.5 1.7 1.85 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 5.75 6.0];
y=[0.0 0.9 1.2 1.35 1.4 1.7 1.95 2.3 2.35 2.4 2.35 2.25 1.8 1.0 0.7 0.0];

v=[0.0 0.5 1.0 1.25 1.5 1.75 2.0 2.25 2.5 2.75 3.0 3.25 3.5 3.75 4.0
4.25 4.5 4.75 5.0 5.25 5.5 5.75 6.0];

w=[0.0 0.0 0.0 0.0 0.0 0.45 0.6 0.45 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.45 0.6 0.45 0.0 0.0 0.0 0.0 0.0];

   Points (x, y) describe the upper part of the car while points (v, w) give the lower part of the car.

   Approximate the shape of the car using

   (a) polynomial interpolant;
   (b) cubic spline interpolant with “not-a-knot” boundary conditions.

   Which approximation is more accurate? Why?

   Note. The Matlab commands “polyfit”, “polyval” and “spline” may be useful.

3. **(Newton–Cotes).** Suppose that f is a function with four continuous derivatives on the interval $[a, b]$. Recall that the error bound for the composite trapezoidal rule $T(h)$ with panel width h is

   $$T(h) - \int_a^b f(x)dx = \frac{(b-a)\,h^2}{12} f''(\xi)$$

for some $\xi \in [a, b]$. The error in the composite Simpson's rule $S(h)$ with panel width h is

$$S(h) - \int_a^b f(x)dx = \frac{(b-a)\,h^4}{180} f^{(4)}(\xi)$$

for some (different) $\xi \in [a, b]$.

(a) A quadrature rule has degree of precision n if it correctly integrates all polynomials of degree n. Use these error bounds to demonstrate that the composite trapezoidal rule has precision of degree one and that the composite Simpson's rule has precision of degree three.

(b) Let $f(x) = \mathrm{e}^{-x} \sin x$. For the composite trapezoidal rule and the composite Simpson's rule, find the number of panels n required to integrate f on the interval $[0, 2\pi]$ with error at most 10^{-4}. Recall that $h = 2\pi/n$. How many function evaluations are required in each case?

(c) Using the number of panels determined in the last part of the problem, use each rule to approximate the integral numerically. Compare your results with the actual value of the integral. For your information, an antiderivative of f is

$$\int \mathrm{e}^{-x} \sin x dx = -0.5\ \mathrm{e}^{-x}(\sin x + \cos x).$$

4. **(Richardson Extrapolation Applied to Differentiation).**

(a) Suppose that $N(h)$ is an approximation to M for every $h > 0$ and that

$$M = N(h) + K_1 h^1 + K_2 h^2 + K_3 h^3 + \ldots$$

for some constants K_1, K_2, K_3, ... Use the values $N(h)$, $N(\frac{h}{3})$, and $N(\frac{h}{9})$ to produce an $\mathcal{O}(h^3)$ approximation to M.

(b) Recall that

$$\frac{df(x_0)}{dx} = \frac{f(x_0 + h) - f(x_0)}{h} + \sum_{i=2}^{\infty} \frac{h^{i-1}}{i!} f^{(i)}(x_0)\ .$$

Use the formula you constructed in part (a) to construct an $O(h^3)$ approximation to $\frac{df(x_0)}{dx}$.

5. Consider the definite integral $\int_a^b \sin(\sqrt{\pi x})\, dx$. Numerically determine the rate of convergence of the composite trapezoid rule for each of the following integration intervals. (See problem # 22, pg. 481 from Section 6.5, including discussion of Periodic Integrands)

(a) $[a,b] = [0,1]$

(b) $[a,b] = [\pi/4, 9\pi/4]$

(c) $[a,b] = [\pi, 2\pi]$

(d) Explain any variation among the rates of convergence obtained in parts (a), (b), and (c).

6. **(Gram-Schmidt Orthogonalization Method).**

   (a) Apply the Gram-Schmidt orthogonalization method to find the 4th degree Legendre polynomial $P_4(x)$. The first 3 were derived in class and are:

$$P_0 = 1, \qquad P_1 = x$$
$$P_2 = x^2 - \frac{1}{3}, \qquad P_3 = x^3 - \frac{3}{5}x$$

   (b) Express x^4 as a linear combination of the first four Legendre polynomials $\{P_0, P_1, P_2, P_3, P_4\}$.

7. **(Gaussian Integration).** Consider the integral,

$$\int_0^1 x \exp^{-x^2} dx \ .$$

   (a) Use the 4-point Gaussian quadrature rule to approximate the integral (after changing variables to obtain an integral over $[-1,1]$).

   The points and weights are:

$$\begin{array}{ll} x_1 = -0.861136311594053 & c_1 = 0.347854845137454 \\ x_2 = -0.339981043584856 & c_2 = 0.652145154862546 \\ x_3 = -x_2 & c_3 = c_2 \\ x_4 = -x_1 & c_4 = c_1 \end{array}$$

   (b) What value of n would be needed to obtain the same accuracy if the compound Trapezoid rule were used?

8. **(Gauss-Laguerre Quadrature).**

   The first three Laguerre polynomials are $L_0(x) = 1$, $L_1(x) = 1 - x$, and $L_2(x) = x^2 - 4x + 2$.

   (a) Show that these polynomials are orthogonal over the interval $(0, \infty)$ with respect to the weight function $w(x) = e^{-x}$.

(b) It is easily seen that the roots of $L_2(x)$ are $x_{1,2} = 2 \pm \sqrt{2}$. Using the method of undetermined coefficients, and the fact the 2-point Gauss-Laquerre quadrature rule

$$\int_0^\infty f(x) e^{-x}\, dx \approx c_1 f(x_1) + c_2 f(x_2)$$

is exact for all polynomials of degree ≤ 3, derive the weights $c_{1,2}$. (They are $c_{1,2} = x_{2,1}/4$.)

9. **(Gauss-Legendre Quadrature).** We proved in class that Gauss-Legendre Quadrature rule

$$(*) \qquad \int_{-1}^{1} f(x)\, dx \approx \sum_{j=1}^{n} c_j f(x_j)$$

is **exact** for polynomials of degree $\leq 2n$–1, where $\{x_j\}_{j=1}^n$ are the n distinct roots of the Legendre polynomial $p_n(x)$ of degree n, and $\{c_j\}_{j=1}^n$ the corresponding weights. Show that indeed this is the best we can expect by **proving** that $(*)$ is **not exact** for

$$f(x) = \prod_{i=1}^{n} (x - x_i)^2 ,$$

a polynomial of degree $2n$. (Hint: Compute the approximation for any n).

Suggested / Additional problems for Math 529 / Phys 528 students:

10. **(Clamped Splines)**

In the case of the clamped spline, the column vector of unknowns is $m = (a_0, a_1, \ldots, a_{n-1}, a_n)^T$. Note that the equations for a_0 and a_n are no longer $a_0 = 0$ and $a_n = 0$, so that the tridiagonal matrix B will change slightly. One can write down the matrix and right hand side for the linear system $Bm = f$ which determines m. The matrix B is invertible, and hence the clamped cubic spline exits and is unique. (Matrix B is strictly diagonal dominant, hence, it is non-singular.)

Determine the clamped cubic spline $S(x)$ that interpolates the data $f(0) = 0$, $f(1) = 1$, $f(2) = 2$ and satisfies $S'(0) = S'(2) = 1$. Again, your answer will consist of 2 cubic polynomials, $S_0(x)$, $S_1(x)$. **Verify** all the necessary conditions and note that the boundary conditions for the clamped spline are different from those for the natural spline. Plot the spline over the interval $[0, 2]$.

11. (**Integration Quadrature**)

(a) Construct the quadrature formula for $\int_a^b f(x)dx$ using a second order polynomial approximation to $f(x)$. The polynomial should pass through the points $x_0 = a$, $x_1 = a + h + \varepsilon$, and $x_2 = a + 2h$, where $h = \frac{b-a}{2}$ and $\varepsilon \in (-\frac{a+b}{2}, \frac{a+b}{2})$.

(b) Show that for any choice of ε other than $\varepsilon = 0$, the method is $O(h^4)$ instead of being $O(h^5)$.

Note: symbolic software like Maple, Maxima or Matlab symbolic toolbox should be useful.

12. **(Romberg Integration (see Section 6.7))**

(a) Starting with only one subinterval, construct the four row Romberg integration table for $\int_3^{3.5} \frac{x}{\sqrt{x^2-4}} dx$ (see problem # 8, pg. 503).

(b) What is the error estimate for the final approximation? How does this compare with the actual error?

(c) How many subintervals would have been necessary to achieve the same accuracy using the composite trapezoid rule without extrapolation?