CS6210: Homework 6

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December 8, 2016

1. (a) Using an orthogonal polynomial basis, find the best least squares polynomial approximations, $q_2(t)$ of degree at most 2 and $q_3(t)$ of degree at most 3, to $f(t) = e^{-3t}$ over the interval $[0, 3]$.

   [Hint: For a polynomial $p(x)$ of degree n and a scalar $a > 0$ we have $\int e^{-ax} p(x) \mathrm{d}x = -\frac{e^{-ax}}{a} \left(\sum_{j=0}^{n} \frac{p^{(j)}(x)}{a^j} \right)$, where $p^{(j)}(x)$ is the j^{th} derivative of $p(x)$. Alternatively, just use numerical quadrature, e.g., the MATLAB function `quad`.]

   Solution:

   (b) Plot the error functions $f(t) - q_2(t)$ and $f(t) - q_3(t)$ on the same graph on the interval $[0, 3]$. Compare the errors of the two approximating polynomials. In the least squares sense, which polynomial provides the better approximation?

   [Hint: In each case you may compute the *norm* of the error, $\left(\int_a^b (f(t) - q_n(t))^2 \mathrm{d}t \right)^2$, using the MATLAB function `quad`]

   Solution:

   (c) Without any computation, prove that $q_3(t)$ generally provides a least squares fit, which is never worse than with $q_2(t)$.

   Solution:

2. Let $f(x)$ be a given function that can be evaluated at points $x_0 \pm jh$, $j = \{0, 1, 2, \ldots\}$ for any fixed value of h, $0 < h \ll 1$.

   (a) Find a second order formula (i.e., trunctation error $\mathcal{O}(h^2)$) approximating the third derivative $f'''(x_0)$. Give the formula, as well as an expression for the truncation error, i.e. not just its order

   Solution:

   (b) Use your formula to provide approximations to $f'''(0)$ for the function $f(x) = e^x$ employing values $h = \{10^{-1}, 10^{-2}, \ldots, 10^{-9}\}$, with the default `Matlab` arithmetic. Verify that for the larger values of h your formula is indeed second order accurate. Which value of h gives the closest approximation to $e^0 = 1$?

   Solution:

   (c) For the formual that you derived in (a), how does the roundoff error behave as a function of h, as $h \to 0$.

   Solution:

(d) How would you go about obtaining a forth order formula for $f'''(x_0)$ in general? (You don't have to actually derive it: just describe in one or two sentences.) How many points would this formula require?
Solution:

3. Consider the derivation of an approximate formula for the second derivative $f''(x_0)$ of a smooth function $f(x)$ using three points x_{-1}, $x_0 = x_{-1} + h_0$, and $x_1 = x_0 + h_1$, where $h_0 \neq h_1$.

   Consider the following two methods:

   i. Define $g(x) = f'(x)$ and seek a *staggered mesh*, centered approximiations as follows:

$$g_{1/2} = \frac{f(x_1) - f(x_0)}{h_1}; \quad g_{-1/2} = \frac{f(x_0) - f(x_{-1})}{h_0}$$
$$f''(x_0) \approx \frac{g_{1/2} - g_{-1/2}}{(h_0 + h_1)/2}$$

   The idea is that all of the differences are short(i.e., not long differences) and centered.

   ii. Using the second degree interpolating polynomial in Newton form, differentiated twice, define

$$f''(x_0) \approx 2f[x_{-1}, x_0, x_1]$$

   Here is where you come in:

   (a) Show that the above two methods are one in the same
   Solution:

   (b) Show that this method is only first order accurate in general
   Solution:

   (c) Run the two methods for the example depicted in Table 14.2 (but for the second derivative of $f(x) = e^x$). Report your findings
   Solution:

4. Continuing with the notation of Exercise 12 (page 437), one could define

$$g_{1/2} = \frac{f_1 - f_0}{h} \quad \text{and} \quad g_{-1/2} = \frac{f_0 - f_{-1}}{h}$$

   These approximate to second order the first derivative values $f'(x_0 + h/2)$ and $f'(x_0 - h/2)$, respectively. Then define

$$f_{pp_0} = \frac{g_{1/2} - g_{-1/2}}{h}$$

All three derivative approximations here are centered (hence second order), and they are applied to first derivatives and hence have roundoff error increeasing proportionally to h^{-1}, not h^{-2}. Can we manage to (partially) cheat the hangman way?!

(a) Show that in exact arithmetic f_{pp_0} defined above and in Exercise 12 are one in the same

Solution:

(b) Implement this method and compare to the results of Exercise 12. Explain your observations

Solution:

5. Consider the numerical differentiation of the function $f(x) = c(x)e^{x/\pi}$ defined on $[0, \pi]$, where

$$c(x) = j, \quad \frac{1}{4}(j-1)\pi \leq x < \frac{1}{4}j\pi, \quad j = \{1, 2, 3, 4\}$$

(a) Contemplating a difference approximation with step size $h = n/\pi$, explain why it is a very good idea to ensure that n is an integer multiple of 4, $n = 4l$.

Solution:

(b) With $n = 4l$, show that the expression $h^{-1}c(t_i)\left(e^{x_{i+1}/\pi} - e^{x_i/\pi}\right)$ provides a second order approximation (i.e., $\mathcal{O}\left(h^2\right)$ error) of $f'(t_i)$, where $t_i = x_i + h/2 = (i + 1/2)h, i = \{0, 1, \ldots, n-1\}$

Solution:

6. The basic trapezoidal rule for approximating $I_f = \int_a^b f(x)\mathrm{d}x$ is based on linear interpolation of f at $x_0 = a$ and $x_1 = b$. The Simpson rule is likewise based on quadratic polynomial interpolation. Consider now a cubic Hermite polynomial, interpolating both$f$ and its derivative f' at a and b. The osculating interpolation formula gives

$$p_3(x) = f(a) + f'(a)(x-a) + f[a, a, b, b](x-1)^2(x-b)$$

and integrating this yields (after some algebra)

$$I_f \approx \int_a^b p_3(x)\mathrm{d}x = \frac{b-a}{2}[f(a) + f(b)] + \frac{(b-a)^2}{12}[f'(a) - f'(b)]$$

This formula is called the **corrected trapezoidal rule**

(a) Show that the error in the basic corrected trapezoidal rule can be estimated by

$$E(f) = \frac{f^{(4)}(\eta)}{720}(b-a)^5$$

Solution:

(b) Use the basic corrected trapezoidal rule to evaluate approximations for $\int_0^1 e^x \mathrm{d}x$ and $\int_{0.9}^1 e^x \mathrm{d}x$. Compare errors to those of Example 15.2. What are your observations?

Solution:

7. (a) Derive a formula for the *composite midpoint rule*. How many function evaluations are required?

   Solution:

   (b) Obtain an expression for the error in the composite midpoint rule. Conclude that this method is second order accurate

   Solution:

8. Suppose that the interval of integration $[a, b]$ is divided into equal subintervals of length h each such that $r = (b - a)/h$ is even. Denote by R_1 the result of applying the composite trapezoidal method with step size $2h$ and by R_2 the result of applying the same method with step size h. Show that one application of Richardson extrapolation, reading

$$S = \frac{4R_2 - R_1}{3}$$

   yields the composite Simpson method

   Solution:

9. Using Romberg integration, compute π to 8 digits (i.e. 3.xxxxxxxx) by obtaining approximations to the integral

$$\pi = \int_0^1 \left(\frac{4}{1 + x^2} \right) \mathrm{d}x$$

   Describe your solution approach and provide the appropriate Romberg table.

   Comapre the computational effort (function evaluations) of Romberg integration to that using the adaptive routine developed in Section 15.4 with `tol`$= 10^{-7}$.

   You may find for some of the rows of your Romberg table that only the first step of extrapolation improves the approximation. Explain this phenomenon.

   [Hint: Reconsider the assumed form of the composite trapezoidal method's truncation error and the effects of extrapolation for this particular integration]

   Solution: