CS6210: Homework 6

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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:
In the general case, we can use Legendre Polynomials. Were first we can find x with respect to t as being

$$x = \frac{2t - a - b}{b - a} = \frac{2t - 0 - 3}{3 - 0} = \frac{2t - 3}{3} = \frac{2}{3}t - 1$$

Giving us our parameters to be

$$\begin{aligned}
\phi_0 &= 1\\
\phi_1 &= x = \frac{2}{3}t - 1\\
\phi_2 &= \frac{1}{2}\left(3x^2 - 1\right) = \frac{1}{2}\left(3\left(\frac{2}{3}t - 1\right)^2 - 1\right) = \frac{2}{3}t^2 - 2t + 1\\
\phi_3 &= \frac{1}{27}\left(20t^3 - 90t^2 + 114t - 36\right)\\
c_0 &= \frac{\int_0^3 e^{-3t}\mathrm{d}t}{\int_0^3 \mathrm{d}t} = \frac{1 - e^{-9}}{9}\\
c_1 &= \frac{\int_0^3 \left(\frac{2}{3}t - 1\right)e^{-3t}\mathrm{d}t}{\int_0^3 \left(\frac{2}{3}t - 1\right)^2\mathrm{d}t} = \frac{-7 - 11e^{-9}}{27}\\
c_2 &= \frac{\int_0^3 \left(\frac{2}{3}t^2 - 2t + 1\right)e^{-3t}\mathrm{d}t}{\int_0^3 \left(\frac{2}{3}t^2 - 2t + 1\right)^2\mathrm{d}t} = \frac{65 - 245e^{-9}}{243}\\
c_3 &= \frac{\int_0^3 \left(\frac{1}{27}\left(20t^3 - 90t^2 + 114t - 36\right)\right)e^{-3t}\mathrm{d}t}{\int_0^3 \left(\frac{1}{27}\left(20t^3 - 90t^2 + 114t - 36\right)\right)^2\mathrm{d}t} = \frac{-413 - 5299e^{-9}}{2187}
\end{aligned}$$

We can then put ϕ_i and c_i into our approximation of the formua:

$$v(x) = \sum_{j=0}^{n} c_j \phi_j(x)$$

By using $n = 2$ we get $q_2(x)$ and by using $n = 3$ we get $q_3(x)$.

(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:

In general, for lower power polynomial expressions the higher polynomial that is used, the more accurate the result. Therefore $q_3(t)$ would provide the better approximation since it is $n = 3$ compared to $n = 2$ for $q_2(x)$, and the powers are not high enough to produce high oscillations.

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:

We can use the following four equations:

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f^{(3)}(x_0) + \frac{h^4}{24} f^{(4)}(x_0) + \frac{h^5}{120} f^{(5)}(\xi_1)$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f^{(3)}(x_0) + \frac{h^4}{24} f^{(4)}(x_0) - \frac{h^5}{120} f^{(5)}(\xi_1)$$

$$f(x_0 + 2h) = f(x_0) + 2hf'(x_0) + 2h^2 f''(x_0) + \frac{8h^3}{6} f^{(3)}(x_0) + \frac{16h^4}{24} f^{(4)}(x_0) + \frac{32h^5}{120} f^{(5)}(\xi_1)$$

$$f(x_0 - 2h) = f(x_0) - 2hf'(x_0) + 2h^2 f''(x_0) - \frac{8h^3}{6} f^{(3)}(x_0) + \frac{16h^4}{24} f^{(4)}(x_0) - \frac{32h^5}{120} f^{(5)}(\xi_1)$$

After subtracting the first two equations and using the intermediate value theorem:

$$f(x_0+h)-f(x_0-h)=2hf'(x_0)+\frac{h^3}{3}f^{(3)}(x_0)+\frac{h^5}{60}f^{(5)}(\eta_1)$$

Finding $f'(x_0)$

$$\begin{aligned}
2hf'(x_0)&=f(x_0+h)-f(x_0-h)-\frac{h^3}{3}f^{(3)}(x_0)-\frac{h^5}{60}f^{(5)}(\eta_1)\\
f'(x_0)&=\frac{1}{2h}\left(f(x_0+h)-f(x_0-h)-\frac{h^3}{3}f^{(3)}(x_0)-\frac{h^5}{60}f^{(5)}(\eta_1)\right)
\end{aligned}$$

After subtracting the second two equations and using the intermediate value theorem for the error terms:

$$f(x_0+2h)-f(x_0-2h)=4hf'(x_0)+\frac{8h^3}{3}f^{(3)}(x_0)+\frac{32h^5}{60}f^{(5)}(\eta_2)$$

Finding $f'(x_0)$:

$$\begin{aligned}
4hf'(x_0)&=f(x_0+2h)-f(x_0-2h)-\frac{8h^3}{3}f^{(3)}(x_0)-\frac{32h^5}{60}f^{(5)}(\eta_2)\\
f'(x_0)&=\frac{1}{4h}\left(f(x_0+2h)-f(x_0-2h)-\frac{8h^3}{3}f^{(3)}(x_0)-\frac{32h^5}{60}f^{(5)}(\eta_2)\right)
\end{aligned}$$

After subtracting these two equations for $f'(x_0)$ and solving for $f^{(3)}(x_0)$, we have

$$\begin{aligned}
\frac{6h^3}{2}f^{(3)}(x_0)&=\frac{1}{4h}\left(f(x_0+2h)-f(x_0-2h)+2f(x_0-h)-2f(x_0+h)-\frac{1}{2}h^5f^{(5)}(\eta)\right)\\
f^{(3)}(x_0)&=\frac{1}{8h^3}\left(f(x_0+2h)-f(x_0-2h)+2f(x_0-h)-2f(x_0+h)-\frac{1}{2}h^5f^{(5)}(\eta)\right)
\end{aligned}$$

We used the intermediate value theorem to find η.

(b) Use your formula to provide approximations to $f^{(3)}(0)$ for the function $f(x)=e^x$ employing values $h=\{10^{-1},10^{-2},\dots,10^{-9}\}$, 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:

$\widetilde{f}(x)$ is the approximation for $f(x)$:

$\widetilde{f}(x) + f(x) + e_r(x)$

We do the same calculations on page 422

$$\left|f'(x_0) - \widetilde{D}\right| = \left|(f'(x_0) - D) + (D - \widetilde{D})\right| \leq |f'(x_0) - D| + \left|D - \widetilde{D}\right|$$

As we calculated in part a

$$|f'(x_0) - D| = \frac{1}{16}h^2 f^{(5)}(\eta)$$

And if M is a maximum for $f^{(5)}(x)$ on its whole domain, then

$$|f'(x_0) - D| \leq \frac{1}{16}h^2 M$$

As an upper bound for $\left|D - \widetilde{D}\right|$ we have $6\epsilon/h^3$ because: two ϵ for points $x_0 + h$ and $x_0 - h$ and two 2ϵ for $x_0 + 2h$ and $x_0 - 2h$

$$\left|D - \widetilde{D}\right| = \frac{6\epsilon}{h^3}$$

Puttin these two together

$$\left|f'(x_0) - \widetilde{D}\right| = \left|(f'(x_0) - D) + (D - \widetilde{D})\right| \leq |f'(x_0) - D| + \left|D - \widetilde{D}\right| \leq \frac{1}{16}h^2 M + \frac{6\epsilon}{h^3}$$

(d) How would you go about obtaining a forth order formula for $f^{(3)}(x_0)$ 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:

We can use seven points: x_0, $x_0 + h$, $x_0 - h$, $x_0 + 2h$, $x_0 - 2h$, $x_0 + 3h$, $x_0 - 3h$, and do similar computations for the fourth order as we did above.

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:

$$f''(x_0) = \frac{g_{1/2} - g_{-1/2}}{(h_0 + h_1)/2} = \frac{\frac{f(x_1)-f(x_0)}{x_1-x_0} - \frac{f(x_0)-f(x_{-1})}{x_0-x_{-1}}}{\frac{x_1-x_{-1}}{2}}$$
$$= \frac{\frac{f(x_1)-f(x_0)}{x_1-x_0} - \frac{f(x_0)-f(x_{-1})}{x_0-x_{-1}}}{x_1 - x_{-1}} = 2f[x_{-1}, x_0, x_1]$$

(b) Show that this method is only first order accurate in general
Solution:
We can use the Taylor expansion of f around x_1:

$$f(x_1) = f(x_0 + h_1) = f(x_0) + h_1 f'(x_0) + \frac{h_1^2}{2} f''(x_0) + \frac{h_1^3}{3!} f^{(3)}(\eta_1)$$

Now we can rewrite $g_{1/2}$ as

$$g_{1/2} = \frac{f(x_1) - f(x_0)}{h_1} = f'(x_0) + \frac{h_1}{2} f''(x_0) + \frac{h_1^2}{3!} f^{(3)}(\eta_1)$$

We can use the Taylor expansion of f around x_0:

$$f(x_0) = f(x_{-1} + h_0) = f(x_{-1}) + h_0 f'(x_{-1}) + \frac{h_0^2}{2} f''(x_{-1}) + \frac{h_0^3}{3!} f^{(3)}(\eta_2)$$

Now we can rewrite $g_{-1/2}$ as

$$g_{-1/2} = \frac{f(x_0) - f(x_{-1})}{h_0} = f'(x_{-1}) + \frac{h_0}{2} f''(x_{-1}) + \frac{h_0^2}{3!} f^{(3)}(\eta_2)$$

To prove that $f''(x_0)$ is first order accurate we just need to consider the last expression in $g_{1/2}$ and $g_{-1/2}$ in the formula $f''(x_0)$. The formula for $f''(x_0)$ is:

$$f''(x_0) = \frac{g_{1/2} - g_{-1/2}}{(h_0 + h_1)/2}$$

So we just consider the last expression in $g_{1/2}$ and $g_{-1/2}$:

$$f''(x_0) = 2 \frac{\frac{h_1^2}{3!} f^{(3)}(\eta_1) - \frac{h_0^2}{3!} f^{(3)}(\eta_2)}{h_0 + h_1}$$

we find η by using the intermediate value theorem:

$$\begin{aligned} f'' &= 2 \frac{\frac{h_1^2}{3!} f^{(3)}(\eta_1) - \frac{h_0^2}{3!} f^{(3)}(\eta_2)}{h_0 + h_1} \\ &= 2 \frac{\left(\frac{h_1^2}{3!} - \frac{h_0^2}{3!} \right) f^{(3)}(\eta)}{h_0 + h_1} \end{aligned}$$

The numerator is of $\mathcal{O}(h^2)$ while the denominator is $\mathcal{O}(h)$, so it's overall $\mathcal{O}(h)$.

(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:

$$pp_0 = \frac{g_{1/2} - g_{-1/2}}{h} = \frac{\frac{f_1 - f_0}{h} - \frac{f_0 - f_{-1}}{h}}{h}$$
$$= \frac{f_1 - f_0 - f_0 + f_{-1}}{h^2}$$

Which is equal to the expression in Exercise 12.

(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 $h = \pi/n$ [fixed from errata], explain why it is a very good idea to ensure that n is an integer multiple of 4, $n = 4l$.

Solution:

We can simply show what happens at one boundary point, and the same argument holds true for the other

$j = 1$:

$$0 \leq x \leq \frac{1}{4}\pi$$

$f(\pi/4) = e^{1/4}$

$j = 2$:

$$\frac{1}{4}\pi \leq x \leq \frac{2}{4}\pi$$

Where the value at $f(\pi/4)$ is $2e^{1/4}$, so the boundary points are discontinuous, which is the reason we want to split the interval to subintervals in which the boundary points are where the function is discontinuous.

(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:

In order for the expression to be second order approximate, we need to find an approximation of $f'(x)$ of the form

$$f'(t_i) = c(t_i)\frac{e^{\left(t_i+\frac{h}{2}\right)/\pi} - e^{\left(t_i-\frac{h}{2}\right)/\pi}}{h} - \frac{h^2}{A}f^B(\xi)$$

For which, A and B are constants. We start with the Taylor Series about two points

$$f\left(t_i + \frac{h}{2}\right) = f(t_i) + \frac{h}{2}f'(t_i) + \frac{h^2}{2! \cdot 4}f''(t_i) + \frac{h^3}{3! \cdot 8}f^{(3)}(\xi_1)$$
$$f\left(t_i - \frac{h}{2}\right) = f(t_i) - \frac{h}{2}f'(t_i) + \frac{h^2}{2! \cdot 4}f''(t_i) - \frac{h^3}{3! \cdot 8}f^{(3)}(\xi_2)$$

In subtracting the two and solving for $f'(t_i)$ we get

$$f'(t_i) = \frac{f\left(t_i + \frac{h}{2}\right) - f\left(t_i - \frac{h}{2}\right)}{h} - \frac{h^2}{3! \cdot 4}f^{(3)}(\xi)$$

where we have from the posed quesiton

$$x_i = t_i - \frac{h}{2}$$
$$x_{i+1} = t_i + \frac{h}{2}$$

Using the above values for x_i with our equation for $f'(t_i)$

$$\begin{aligned}
f'(t_i) &= \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h^2}{3! \cdot 4}f^{(3)}(\xi) \\
&= \frac{c(x_{i+1})e^{x_{i+1}/\pi} - c(x_i)e^{x_i/\pi} - f(x_i)}{h} - \frac{h^2}{3! \cdot 4}f^{(3)}(\xi)
\end{aligned}$$

As the interval is on $[x_i, x_{i+1}]$, the function is constant in that subinterval since $c(x_{i+1}) = c(x_i) = c(t_i)$

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:
Page 320 from the text tells us that for the Hermite Cubic Interpolation we have $m_0 = m_1 = 1$. Using the formula on page 321, we get the repitition of the first interpolation point, a, is $m_0 + 1 = 2$. The second interpolation point b is $m_1 + 1 = 2$. From page 443, the interpolation error is:

$$f(x) - p_n(x) = f[x_0, x_1, \ldots, x_n, x] \prod_{i=0}^{n} (x - x_i)$$

We should use two a's and two b's as the interpolation points, giving

$$E(f) = \int_a^b f[a,a,b,b,x]\left((x-a)^2(x-b)^2\right)\mathrm{d}x$$

Since the integrand is always positive, we can use the intermediate value problem to find ξ in $[a,b]$ such that

$$E(f) = \int_a^b f[a,a,b,b,\xi]\left((x-a)^2(x-b)^2\right)\mathrm{d}x$$

where f can be taken out of the integral since it's now independent of x

$$E(f) = f[a,a,b,b,\xi]\int_a^b \left((x-a)^2(x-b)^2\right)\mathrm{d}x$$

Now we can separate the two and solve for their values, giving

$$\int_a^b \left((x-a)^2(x-b)^2\right)\mathrm{d}x = 0 - 2\frac{(a-b)^5}{3(4)5} = \frac{4(b-a)^5}{5!} \tag{1}$$

And from page 312 we have

$$f[a,a,b,b,\xi] = \frac{f^{(4)}(\eta)}{4!} \tag{2}$$

for some η in $[a,b]$. Putting Equations (1) and (2) together, we get

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

(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:

$$I_f = \frac{b-a}{2}(f(a)+f(b)) + \frac{(b-a)^2}{12}(f'(a)-f'(b))$$

For $a=0$ and $b=1$

$$I_f = \frac{1}{2}(1+e) + \frac{1}{12}(1-e) = 1.7160$$

For $a=0.9$ and $b=1$

$$I_f = \frac{1}{2}\left(e^{0.9}+e\right) + \frac{1}{12}\left(e^{0.9}-e\right) = 2.5674$$

According to Example 15.2, the actual value is given, so we can find the error by the corrected trapezoidal rule, for $a=0$ and $b=1$

$$E(f) = |1.7183 - 1.7160| = 0.0023$$

for $a=0.9$ and $b=1$

$$E(f) = |1.7183 - 2.5674| = 0.8491$$

In $[0,1]$, the corrected trapezoidal rule is more accurate than the regular trapezoidal rule and the midpoint rule, though it still underperforms when compared to Simpson's rule ($\xi = 0.0006$). However, in $[0.9,1]$ all of the methods are more accurate than the corrected trapezoidal rule.

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: