Numerical analysis(SI211)$_{\textbf{Fall 2021-22}}$ Homework 2

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Acknowledgements:

1. Deadline: **2021-12-10 11:59:00**, no late submission is allowed.
2. No handwritten homework is accepted. You should submit your homework in Blackboard with PDF format, we recommend you use LaTeX.
3. Giving your solution in English, solution in Chinese is not allowed.
4. Make sure that your codes can run and are consistent with your solutions, you can use any programming language.
5. Your PDF should be named as "your_student_id+HW2.pdf", package all your codes into "your_student_id+_Code2.zip" and upload. Don't put your PDF in your code file
6. All the results from your code should be shown in pdf but please do not inset your code into LaTeX.
7. Plagiarism is not allowed. Those plagiarized solutions and codes will get 0 point. If the results on the pdf are inconsistent with the results of code, your coding problem will get 0 point.

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1. **Numerical differentiation**(10 points.) Assume $f(x) \in C^3$, there are 3 points $f(x_0-\alpha h), f(x_0), f(x_0+h)$ with $\alpha > 0$.

   (a) use Lagrange Polynomials to construct an approximation for $f''(x_0)$

   (b) evaluate the approximation error and find the approximation order

   Solution:

   (a) The interpolation polynomial in the Lagrange form is

$$\begin{aligned}P(x) =& f(x_0-\alpha h)\frac{(x-x_0)(x-x_0-h)}{(x_0-\alpha h-x_0)(x_0-\alpha h-x_0-h)}\\ &+f(x_0)\frac{(x-x_0+\alpha h)(x-x_0-h)}{(x_0-x_0+\alpha h)(x_0-x_0-h)}\\ &+f(x_0+h)\frac{(x-x_0)(x-x_0+\alpha h)}{(x_0+h-x_0)(x_0+h-x_0+\alpha h)}\\ =&f(x_0-\alpha h)\frac{(x-x_0)(x-x_0-h)}{\alpha(\alpha+1)h^2}\\ &-f(x_0)\frac{(x-x_0+\alpha h)(x-x_0-h)}{\alpha h^2}\\ &+f(x_0+h)\frac{(x-x_0)(x-x_0+\alpha h)}{(\alpha+1)h^2},\end{aligned}$$

   $P''(x) = f(x_0-\alpha h)\frac{2}{\alpha(\alpha+1)h^2} - f(x_0)\frac{2}{\alpha h^2} + f(x_0+h)\frac{2}{(\alpha+1)h^2}$

   (b) Taylor expansion for $f(x_0-\alpha h)$ and $f(x_0+h)$ are

$$\begin{aligned}f(x_0-\alpha h) &= f(x_0) - \alpha h f'(x_0) + \frac{f^{(2)}(x_0)}{2}(-\alpha h)^2 + \frac{f^{(3)}(\xi_1)}{6}(-\alpha h)^3\\ f(x_0+h) &= f(x_0) + hf'(x_0) + \frac{f^{(2)}(x_0)}{2}h^2 + \frac{f^{(3)}(\xi_2)}{6}h^3,\end{aligned}$$

   where ξ_1 and ξ_2 are coefficients within $(x_0-\alpha h, x_0)$ and (x_0, x_0+h) respectively. Define an approximation for the second derivative

$$f''(x) \approx Af(x_0-\alpha h) + Bf(x_0) + Cf(x_0+h).$$

   Substitute the Taylor expansion for $f(x_0-\alpha h)$ and $f(x_0+h)$. We arrive at the system of three linear equations to determine A, B, C,

$$\begin{cases} A+B+C=0\\ -\alpha hA + hC = 0\\ \frac{A}{2}(\alpha h)^2 + \frac{C}{2}h^2 = 1,\end{cases}$$

solution of the system is $A = \frac{2}{h^2(\alpha^2+\alpha)}, B = -\frac{2}{\alpha h^2}, C = \frac{2}{h^2(1+\alpha)}$. Putting together,

$$f''(x_0) \approx \frac{2}{h^2(\alpha^2+\alpha)} f(x_0 - \alpha h) - \frac{2}{\alpha h^2} f(x_0) + \frac{2}{h^2(1+\alpha)} f(x_0 + h).$$

The error of the second derivative approximation

$$\begin{aligned}
E =& f''(x_0) - \frac{2}{h^2(\alpha^2+\alpha)} f(x_0 - \alpha h) - \frac{2}{\alpha h^2} f(x_0) + \frac{2}{h^2(1+\alpha)} f(x_0 + h) \\
=& - A\frac{f^{(3)}(\xi_1)}{6}(-\alpha h)^3 - C\frac{f^{(3)}(\xi_2)}{6} h^3 \\
=& \frac{\alpha^2 h}{3(1+\alpha)} f^{(3)}(\xi_1) - \frac{h}{3(1+\alpha)} f^{(3)}(\xi_2) = O(h)
\end{aligned}$$

The approximation is only first order.

2. **Richardson extrapolation**(10 points.) The $f'(x_0)$ can be expressed as

$$f'(x_0) = \frac{1}{h}(f(x_0+h) - f(x_0)) - \frac{h}{2} f''(x_0) - \frac{h^2}{6} f'''(x_0) + O(h^3). \tag{1}$$

Use idea of Richardson extrapolation to derive a 3 point formula for $f'(x_0)$ with $O(h^2)$ error. (Hint:Replace step size h with $2h$.)
Solution:
Replacing h in 1 with 2h gives the new formula

$$f'(x_0) = \frac{1}{2h}(f(x_0+2h) - f(x_0)) - hf''(x_0) - \frac{4h^2}{6} f'''(x_0) + O(h^3). \tag{2}$$

Multiplying equation 1 by 2 and subtracting equation 2, we obtain:

$$f'(x_0) = \frac{2}{h}(f(x_0+h) - f(x_0)) - \frac{1}{2h}(f(x_0+2h) - f(x_0)) - \frac{h^2}{3} f'''(x_0) + \frac{2h^2}{3} f'''(x_0) + O(h^3) \tag{3}$$

Rewriting this equation, we get an $O(h^3)$ formula for $f'(x_0)$:

$$f'(x_0) = \frac{-f(x_0+2h) + 4f(x_0+h) - 3f(x_0)}{2h} + \frac{h^2}{3} f'''(x_0) + O(h^3). \tag{4}$$

Then we have the conclusion

$$f'(x_0) = \frac{-f(x_0+2h) + 4f(x_0+h) - 3f(x_0)}{2h} + O(h^2).$$

3. **Elements of Numerical Integration**(20 points.) For the integral $\int_2^6 \frac{1}{1+x} dx$, use numerical integration methods to approximate.

(a) Given only the values of $f(x)$ at $x = 2$,3,4, 5 and 6, use the Midpoint Rule, the Trapezoidal rule to approximate with the smallest step size possible.

(b) Use Romberg integration to compute $R_{3,3}$.

(c) Use Gaussian quadrature with $n = 2$ to approximate the integral.

Solutions:

(a) Midpoint Rule:$h = 2$,$\int_2^6 \frac{1}{1+x}dx \approx \int_2^4 \frac{1}{1+x}dx + \int_4^6 \frac{1}{1+x}dx = hf(3) + hf(5) = 5/6 \approx 0.83333$

Trapezoid Rule:$h = 1$,$\int_2^6 \frac{1}{1+x}dx \approx \int_2^4 \frac{1}{1+x}dx + \int_4^6 \frac{1}{1+x}dx = \frac{1}{3}h(f(2) + 4f(3) + f(4)) + \frac{1}{3}h(f(4) + 4f(5) + f(6)) \approx 0.8548$

(b) (See Example in textbook Section 4.5, Example 1)
$R_{1,1} = 0.952381, R_{2,1} = 0.876190, R_{3,1} = 0.854762, R_{2,2} = 0.850793, R_{3,2} = 0.847619, R_{3,3} = 0.847408$

(c) (See Example in textbook Section 4.7, Example 1 and 2)
$\int_2^6 f(x)dx \approx 0.84507$

4. **Coding of Simpson's Rule**(20 points.) For integral:

$$\int_0^4 e^x dx, \tag{5}$$

we write it in the form:

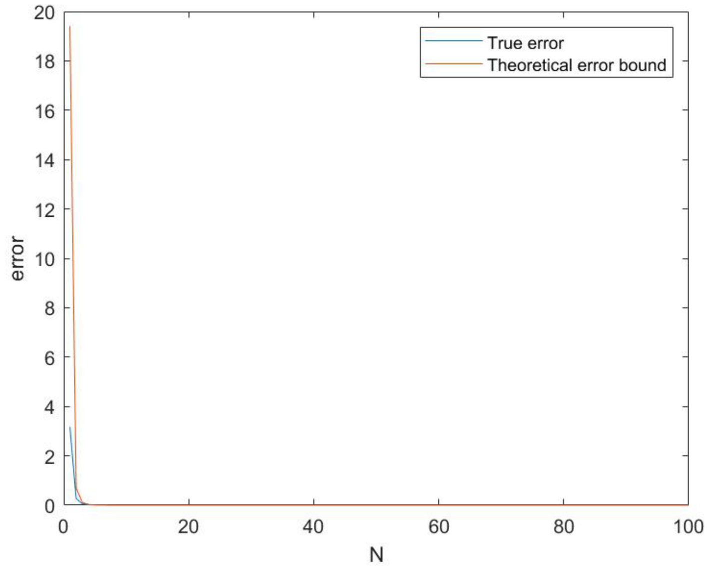
$$\int_0^4 e^x dx = \sum_{i=0}^{N-1} \{ \int_{4i/N}^{4(i+1)/N} e^x dx \}, \tag{6}$$

then apply Simpson's rule on each part separately and sum up the results. You need to:

- Plot the actual error of this integral approximation versus N for $N \in \{0, 1, 2 \ldots, 100\}$.
- Derive a theoretical bound on the integral approximation in dependence on N and plot this upper bound, too.

Solutions: The integral approximation of each part is:

$$\int_{4i/N}^{4(i+1)/N} e^x dx \approx \frac{h}{3}[f(\frac{4i}{N}) + 4f(\frac{4i+2}{N}) + f(\frac{4i+4}{N})], h = \frac{2}{N}$$



5. **Bonus Coding** **(Multiple Integrals)** (20 points.) For the

$$\iint_{\mathcal{D}} e^{-xy} \mathrm{d}x\mathrm{d}y \tag{7}$$

with $\mathcal{D} =: \{0 \leq x \leq 1.5, 0 \leq y \leq 2\}$.

- Use Composite Simpson's rule with $n = 6$ and $m = 8$, i.e., $h_x = \frac{1.5}{6}, h_y = \frac{2}{8}$ to approximate (7). (**Note:** your code should input the box range $\mathcal{D}$ and the integers n, m, you can use the Example.1 from the page-239 to debug).

Solution: Refer the page-237, 238 and page-240 of the text book.

- $$\int_0^{1.5}\int_0^{2} e^{-xy} \mathrm{d}y\mathrm{d}x \approx \int_0^{1.5} \frac{h_y}{3}\left[e^{xy_0} + 2\sum_{j=1}^{(m/2)-1} e^{-xy_{2j}} + 4\sum_{j=1}^{m/2} e^{-xy_{2j-1}} + e^{-xy_m}\right] \mathrm{d}x. \tag{8}$$

  Then use the Simpson's rule with $x_i = x_0 + ih_x$ with $h_x = \frac{1.5}{6}$ and $i = 1, 2, 3, 4, 5, 6$. Then we get the approximation of (7) as 1.688976836598060 .