

Homework 5: CS321, Fall 2004

Due Date: 2:50pm, April 5, 2004

Please show all steps in your work. Please be reminded that you should do your homework independently.

1. (10 points) Find an approximate value of $\int_1^2 x^{-1} dx$ using composite Simpson's rule with $h = 0.25$. Give a bound on the error. Then calculate the exact value of the integration and compute the exact error to see if the error bound is accurate.

Solution. The composite Simpson's rule consists of using the basic Simpson's rule for each of the half intervals.

$$\begin{aligned}\int_1^2 x^{-1} dx &\approx \frac{h}{3} \left(\frac{1}{1} + \frac{4}{1.25} + \frac{2}{1.5} + \frac{4}{1.75} + \frac{1}{2} \right) \\ &\approx 0.693254\end{aligned}$$

The error bound for the composite Simpson's rule is

$$|e| = \left| \frac{b-a}{90} h^4 f^{(4)}(\xi) \right|$$

Since

$$|f^{(4)}(\xi)| = |24\xi^{-5}| \leq 24, \quad \text{for } x \in [1, 2]$$

We have

$$|e| \leq \frac{1}{90} \times 0.25^4 \times 24 = 5.2083 \times 10^{-4}$$

The exact solution is computed as

$$\int_1^2 2x^{-1} dx = \ln x \Big|_1^2 = \ln 2 \approx 0.693147$$

The error of the numerically approximated solution is

$$|0.693254 - 0.693147| = 1.05 \times 10^{-4}$$

We see that the error of the numerically approximated solution is smaller than the theoretical error bound. We can conclude that the theoretical error bound is accurate in predicting the accuracy of the approximate solution.

2. (10 points) A numerical integration scheme that is not as well known is the basic Simpson's $\frac{3}{8}$ rule over three intervals

$$\int_a^{a+3h} f(x) dx \approx \frac{3h}{8} [f(a) + 3f(a+h) + 3f(a+2h) + f(a+3h)].$$

Estimate the error term for this rule and explain why this rule is not as popular as the Simpson's rule.

Solution. Denote $f(a) = f$ and use Taylor expansion, we have

$$\begin{aligned} f(a+h) &= f + hf' + \frac{1}{2}h^2f'' + \frac{1}{6}h^3f''' + \frac{1}{24}h^4f^{(4)} + \dots \\ f(a+2h) &= f + 2hf' + 2h^2f'' + \frac{4}{3}h^3f''' + \frac{2}{3}h^4f^{(4)} + \dots \\ f(a+3h) &= f + 3hf' + \frac{9}{2}h^2f'' + \frac{9}{2}h^3f''' + \frac{27}{8}h^4f^{(4)} + \dots \end{aligned}$$

It follows that

$$\begin{aligned} f(a) + 3f(a+h) + 3f(a+2h) + f(a+3h) \\ = 8f + 12hf' + 12h^2f'' + 9h^3f''' + \frac{11}{2}h^4f^{(4)} + \dots \end{aligned}$$

and

$$\begin{aligned} \frac{3h}{8}(f(a) + 3f(a+h) + 3f(a+2h) + f(a+3h)) \\ = 3hf + \frac{9}{2}h^2f' + \frac{9}{2}h^3f'' + \frac{27}{8}h^4f''' + \frac{33}{16}h^5f^{(4)} + \dots \end{aligned}$$

The Taylor series for function $F(a+3h)$ is

$$F(a+3h) = F(a) + 3hF'(a) + \frac{9}{2}h^2F''(a) + \frac{9}{2}h^3F'''(a) + \frac{27}{8}h^4F^{(4)}(a) + \frac{81}{40}h^5F^{(5)}(a) + \dots$$

Define

$$F(x) = \int_a^x f(t) dt$$

By the Fundamental Theorem of Calculus, we have $F' = f$, $F'' = f'$, \dots , and

$$\int_a^{a+3h} f(x) dx = 3hf + \frac{9}{2}h^2f' + \frac{9}{2}h^3f'' + \frac{27}{8}h^4f''' + \frac{81}{40}h^5f^{(4)} + \dots$$

Subtracting the above two equations, we obtain

$$\begin{aligned} \int_a^{a+3h} f(x) dx - \frac{3h}{8}(f(a) + 3f(a+h) + 3f(a+2h) + f(a+3h)) \\ = \frac{33}{16}h^5f^{(4)} - \frac{81}{40}h^5f^{(4)} + O(h^6) \\ = \frac{3}{80}h^5f^{(4)}(\xi) \end{aligned}$$

Compared with the basic Simpson's rule, this $\frac{8}{3}$ has a larger error bound. It also has one more functional evaluation and is more expensive to compute.

3. (10 points) For what value of α does the straightforward Gaussian elimination produce erroneous answers for this system?

$$\begin{aligned}x_1 + x_2 &= 2 \\ \alpha x_1 + x_2 &= 2 + \alpha\end{aligned}$$

Explain what happens in the computer.

Solution. Straightforward Gaussian elimination lead to

$$(1 - \alpha)x_2 = 2 - \alpha$$

We solve

$$x_2 = \frac{2 - \alpha}{1 - \alpha}$$

Substituting x_2 into the first equation, we have

$$x_1 = -\frac{\alpha}{1 - \alpha}$$

We can see that if $\alpha \rightarrow 1$, both x_1 and x_2 approach infinity, causing computer to overflow. In fact, when $\alpha = 1$ the system

$$\begin{aligned}x_1 + x_2 &= 2 \\ x_1 + x_2 &= 3\end{aligned}$$

is inconsistent.

4. (10 points) Solve the following system using straightforward Gaussian elimination with forward elimination and back substitution. Carry four significant digits.

$$\begin{aligned}3x_1 + 2x_2 - 5x_3 &= 0 \\ 2x_1 - 3x_2 + x_3 &= 0 \\ x_1 + 4x_2 - x_3 &= 4\end{aligned}$$

Solution By eliminating x_1 from the last two equations, we have

$$\begin{aligned}3x_1 + 2x_2 - 5x_3 &= 0 \\ -x_2 + x_3 &= 0 \\ 5x_2 + 2x_3 &= 6\end{aligned}$$

After eliminating x_2 from the third equation, we get

$$\begin{aligned}3x_1 + 2x_2 - 5x_3 &= 0 \\ -x_2 + x_3 &= 0 \\ 4x_3 &= 4\end{aligned}$$

It follows that $x_3 = 1$. From

$$-x_2 + x_3 = 0,$$

we compute $x_2 = x_3 = 1$. Moreover, from the first equation

$$3x_1 + 2x_2 - 5x_3 = 0,$$

we obtain

$$x_1 = \frac{1}{3}(5x_3 - 2x_2) = 1$$

5. (10 points) Solve the following system using Gaussian elimination with scaled partial pivoting. Carry four significant digits.

$$\begin{aligned} 3x_1 + 2x_2 - x_3 &= 7 \\ 5x_1 + 3x_2 + 2x_3 &= 4 \\ -x_1 + x_2 - 3x_3 &= -1 \end{aligned}$$

Solution. Note that $l = [1 \ 2 \ 3]$ and $s = [3 \ 5 \ 3]$. To find out the first pivoting row, we examine

$$\left\{ \frac{|q_{l_i,1}|}{s_{l_i}} : l = 1, 2, 3 \right\} = \left\{ \frac{3}{3}, \frac{5}{5}, \frac{1}{3} \right\}$$

It follows that the first pivoting row should be the first row. After the first elimination, the system becomes

$$\begin{aligned} 3x_1 + 2x_2 - x_3 &= 7 \\ -\frac{1}{3}x_2 + \frac{11}{3}x_3 &= -\frac{23}{3} \\ \frac{5}{3}x_2 - \frac{10}{3}x_3 &= \frac{4}{3} \end{aligned}$$

Check the second pivoting row,

$$\left\{ \frac{|q_{l_i,2}|}{s_{l_i}} : l = 2, 3 \right\} = \left\{ \frac{1}{15}, \frac{5}{9} \right\}$$

So we choose the third row as the pivoting row. We now have

$$\begin{aligned} 3x_1 + 2x_2 - x_3 &= 7 \\ 3x_3 &= -\frac{37}{5} \\ \frac{5}{3}x_2 - \frac{10}{3}x_3 &= \frac{4}{3} \end{aligned}$$

The solution is $x_3 = -2.4667$, $x_2 = -4.1333$, $x_1 = 4.2667$.