



Practice Session: Numerical Methods

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Give motivations and/or derivations for your answers.

1. Integration and Differential equations

- (a) Explain the trapezoidal rule.
- (b) Explain how to obtain the Euler method and the Runge-Kutta 4 method, and their differences.
- (c) Given the integral

$$\int_0^1 e^{x^2} dx, \quad (1)$$

approximate the result to 4 significant digits, using Simpson's 1/3 rule with 4 subintervals.

- (d) What are the true and relative errors in the approximation, with respect to the literature value of 1.4626?

Solution:

- (a) Pick a step-size ($\Delta x = |x_i - x_{i-1}|$), compute the difference in function value at the one point and at a new point a step-size away ($f(x_{i-1})$ and $f(x_i)$), and multiply the difference between these with the step-size divided by 2. Sum this in the interval $[a, b]$ and you have an approximation for the integral.
- (b) The Euler and RK4 method work based on a Taylor expansion approximation. For Euler's method, only one other point is used while RK4 makes use of four intervals and averages to calculate the next point.
- (c) First, we decompose the interval $[0, 1]$ into 4 subintervals. Each subinterval needs to have width $h = \frac{(b-a)}{4} = \frac{1}{4}$. We then have as endpoints of the subintervals:

$$x_0 = 0, \quad x_1 = \frac{1}{4}, \quad x_2 = \frac{1}{2}, \quad x_3 = \frac{3}{4}, \quad x_4 = 1$$

We can now apply Simpson's 1/3 rule:

$$\begin{aligned} \int_{x_0}^{x_4} f(x) dx &= \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)] = \\ &= \frac{1}{12} \left[e^0 + 4e^{\frac{1}{16}} + 2e^{\frac{1}{4}} + 4e^{\frac{9}{16}} + e^1 \right] \approx 1.4637 \end{aligned} \quad (2)$$

- (d) The true error in the approximation is:

$$\text{True Error} = |\text{True Value} - \text{Approximate Value}| \approx 0.0011$$

The relative error is:

$$\text{Relative Error} = \frac{\text{True Error}}{\text{True Value}} \approx 0.00075 = 0.075\%$$



2. Numerical Linear Algebra

Solve for $\mathbf{A}\vec{x} = \mathbf{b}$, where

$$\mathbf{A} = \begin{bmatrix} 8 & 2 & 2 & 2 \\ 4 & 7 & 3 & 3 \\ 4 & 4 & 8 & 4 \\ 2 & 2 & 4 & 8 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} 14 \\ 17 \\ 20 \\ 16 \end{pmatrix} \quad (3)$$

(a) Using Doolittle's decomposition.

(b) Now determine the condition number of matrix $\mathbf{A}$ using the *row-sum norm* and

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{11}{72} & -\frac{1}{36} & -\frac{1}{54} & -\frac{1}{54} \\ -\frac{5}{72} & \frac{7}{36} & -\frac{1}{27} & -\frac{1}{27} \\ -\frac{1}{24} & -\frac{1}{12} & \frac{7}{36} & -\frac{1}{18} \\ 0 & 0 & -\frac{1}{12} & \frac{1}{6} \end{bmatrix}. \quad (4)$$

(c) Is matrix $\mathbf{A}$ ill-conditioned?

Solution:

(a) Doolittle's decomposition decomposes matrix $\mathbf{A}$ in a lower triangular matrix $\mathbf{L}$ and an upper triangular matrix $\mathbf{U}$ such that $\mathbf{A} = \mathbf{L}\mathbf{U}$, and

$$[\mathbf{L} \setminus \mathbf{U}] = \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ L_{21} & U_{22} & U_{23} & U_{24} \\ L_{31} & L_{32} & U_{33} & U_{34} \\ L_{41} & L_{42} & L_{43} & U_{44} \end{bmatrix}. \quad (5)$$

To obtain $\mathbf{U}$, we proceed by using row elimination

$$\begin{aligned} \mathbf{A} = \begin{bmatrix} 8 & 2 & 2 & 2 \\ 4 & 7 & 3 & 3 \\ 4 & 4 & 8 & 4 \\ 2 & 2 & 4 & 8 \end{bmatrix} &\xrightarrow{\substack{r_2 - \frac{1}{2}r_1 \\ r_3 - \frac{1}{2}r_1 \\ r_4 - \frac{1}{4}r_1}} \begin{bmatrix} 8 & 2 & 2 & 2 \\ 0 & 6 & 2 & 2 \\ 0 & 3 & 7 & 3 \\ 0 & \frac{3}{2} & \frac{7}{2} & \frac{15}{2} \end{bmatrix} \xrightarrow{\substack{r_3 - \frac{1}{2}r_2 \\ r_4 - \frac{1}{4}r_2}} \begin{bmatrix} 8 & 2 & 2 & 2 \\ 0 & 6 & 2 & 2 \\ 0 & 0 & 6 & 2 \\ 0 & 0 & 3 & 7 \end{bmatrix} \\ &\xrightarrow{r_4 - \frac{1}{2}r_3} \begin{bmatrix} 8 & 2 & 2 & 2 \\ 0 & 6 & 2 & 2 \\ 0 & 0 & 6 & 2 \\ 0 & 0 & 0 & 6 \end{bmatrix} = \mathbf{U}. \end{aligned} \quad (6)$$

Now, $\mathbf{L}$ can be recovered, noting that the *factors* ($\frac{\text{row } x - \text{factor} \times \text{row } y}{\text{row } x}$) correspond to the entries $L_{21} = L_{31} = \frac{1}{2}$, $L_{41} = L_{42} = \frac{1}{4}$, $L_{32} = L_{43} = \frac{1}{2}$ following the order of operations used to obtain $\mathbf{U}$. This gives

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & 1 \end{bmatrix} \quad (7)$$



To solve for $\vec{x}$, we first solve $\mathbf{L}\vec{y} = \mathbf{b}$ (e.g., by forward substitution), and from that solve $\mathbf{U}\vec{x} = \vec{y}$ through back substitution.

$\vec{y}$ can be calculated noting that $y_1 = b_1$ and using

$$y_k = b_k - \sum_{j=1}^{k-1} L_{kj} y_j, \quad k = 2, 3, \dots, n, \quad (8)$$

leading to

$$\begin{aligned} y_1 &= 14, \\ y_2 &= 17 - \frac{1}{2}(14) = 10, \\ y_3 &= 20 - \frac{1}{2}(14) - \frac{1}{2}(10) = 8, \\ y_4 &= 16 - \frac{1}{4}(14) - \frac{1}{4}(10) - \frac{1}{2}(8) = 6 \end{aligned} \quad (9)$$

Subsequently, $\mathbf{x}$ is solved through back substitution

$$\begin{aligned} U_{44}x_4 &= y_4 & x_4 &= \frac{y_4}{U_{44}} = \frac{6}{6} = 1 \\ U_{33}x_3 + U_{34}x_4 &= y_3 & x_3 &= \frac{y_3 - U_{34}x_4}{U_{33}} = \frac{8 - 2(1)}{6} = 1 \\ U_{22}x_2 + U_{23}x_3 + U_{24}x_4 &= y_2 & x_2 &= \dots = \frac{10 - 2(1) - 2(1)}{6} = 1 \\ U_{11}x_1 + U_{12}x_2 + U_{13}x_3 + U_{14}x_4 &= \dots = y_1 & x_1 &= \dots = \frac{14 - 2(1) - 2(1) - 2(1)}{8} = 1 \end{aligned} \quad (10)$$

Thus, $\vec{x} = (1 \ 1 \ 1 \ 1)^\top$.

(b) The *row-sum norm* is defined as,

$$\|\mathbf{A}\| = \max_{1 \leq i \leq n} \sum_{j=1}^n |A_{ij}| = \text{the largest sum of absolute values along the rows.} \quad (11)$$

And the *matrix condition number* is defined as,

$$\text{cond}(\mathbf{A}) = \|\mathbf{A}\| \|\mathbf{A}^{-1}\|. \quad (12)$$

We get

$$\begin{aligned} \text{row 1} &: 8 + 2 + 2 + 2 = 14 \\ \text{row 2} &: 4 + 7 + 3 + 3 = 17 \\ \text{row 3} &: 4 + 4 + 8 + 4 = 20 = \|\mathbf{A}\| \\ \text{row 4} &: 2 + 2 + 4 + 8 = 16, \end{aligned} \quad (13)$$

and

$$\begin{aligned} \text{row 1} &: \frac{11}{72} + \left|-\frac{1}{36}\right| + \left|-\frac{1}{54}\right| + \left|-\frac{1}{54}\right| = \frac{47}{216} \approx 0.218 \\ \text{row 2} &: \left|-\frac{5}{72}\right| + \frac{7}{36} + \left|-\frac{1}{27}\right| + \left|-\frac{1}{27}\right| = \frac{73}{216} \approx 0.338 \\ \text{row 3} &: \left|-\frac{1}{24}\right| + \left|-\frac{1}{12}\right| + \frac{7}{36} + \left|-\frac{1}{18}\right| = \frac{3}{8} = 0.375 = \|\mathbf{A}^{-1}\| \\ \text{row 4} &: 0 + 0 + \left|-\frac{1}{12}\right| + \frac{1}{6} = \frac{1}{4} = 0.25. \end{aligned} \quad (14)$$

Therefore, the condition number is $\|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| = 20 \cdot \frac{3}{8} = \frac{15}{2}$.



- (c) Generally, a matrix is ill-conditioned if its condition number is very large, reaching infinity if it is singular. So in this case $\mathbf{A}$ is not ill-conditioned.

3. Interpolation and extrapolation

- (a) Why is extrapolating data much more ‘risky’ than interpolating data?
- (b) Using (bi)linear interpolation between the set of data points $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$. What properties does the interpolation have at these data points?
- (c) Explain how quadratic and cubic splines work.
- (d) Consider the following data points

$$(x_0, y_0) = (0, 0), \quad (x_1, y_1) = (1, 1), \quad (x_2, y_2) = (2, 0). \quad (15)$$

Construct the natural cubic spline $S(x)$ interpolating these points. The “natural” means $S''(x_0) = S''(x_2) = 0$ in this case. Set up and solve for the second derivatives M_0, M_1, M_2 at the knots and write the piecewise cubic polynomials on $[0, 1]$ and $[1, 2]$.

- (e) Now construct a Lagrange polynomial that interpolates the points given in (d)
- (f) Is the Lagrange polynomial the same as the cubic splines over their respective intervals? Why (not)?
- (g) Why would you use a cubic spline instead of using a Lagrange polynomial?

Solution:

- (a) Unlike interpolation, the method of extrapolation has no previous and next data points to fit a polynomial locally. The effect is that extrapolation becomes increasingly inaccurate (and thus more unlikely to fit the data) for increasing iterations.
- (b) Linear interpolation methods suffer from discontinuous 1st derivatives at the known data points.

(c) Quadratic splines

A quadratic polynomial ($f(x) = a + bx + cx^2$) is fitted in between the data points x_i and x_{i+1} for the whole data set of length N . The fits are continuous at each data point so that $f_k(x_{i+1}) = f_{k+1}(x_{i+1})$, where f_k is the local fit in between x_i and x_{i+1} and f_{k+1} the local fit in between x_{i+1} and x_{i+2} . The derivatives of f_k are also continuous so that $f'_k(x_{i+1}) = f'_{k+1}(x_{i+1})$.

Cubic splines

A cubic polynomial ($f(x) = a + bx + cx^2 + dx^3$) is fitted in between the data points x_i and x_{i+1} for the whole data set of length N . It shares the same criteria as a quadratic spline *plus* the fact that the second derivative must also be continuous: $f''_k(x_{i+1}) = f''_{k+1}(x_{i+1})$.



- (d) A “natural” cubic spline on $[x_0, x_2]$ with knots at x_0, x_1, x_2 imposes that the second derivatives at the two endpoints vanish:

$$M_0 = S''(x_0) = 0, \quad M_2 = S''(x_2) = 0. \quad (16)$$

We have three knots, so second derivatives M_0, M_1, M_2 . Natural conditions give $M_0 = 0, M_2 = 0$. Only M_1 is unknown. Let $h_0 = x_1 - x_0 = 1 - 0 = 1$, and $h_1 = x_2 - x_1 = 2 - 1 = 1$.

The standard tridiagonal system for a natural cubic spline with uniform spacing is, for the interior knot x_1 :

$$h_0 M_0 + 2(h_0 + h_1)M_1 + h_1 M_2 = 6 \left(\frac{y_2 - y_1}{h_1} - \frac{y_1 - y_0}{h_0} \right). \quad (17)$$

We substitute values:

- $M_0 = 0, M_2 = 0$,
- $h_0 = h_1 = 1$, and
- $y_0 = 0, y_1 = 1, y_2 = 0$.

Right-hand side becomes

$$\frac{y_2 - y_1}{h_1} - \frac{y_1 - y_0}{h_0} = \frac{0 - 1}{1} - \frac{1 - 0}{1} = (-1) - (1) = -2. \quad (18)$$

Thus,

$$1 \cdot 0 + 2(1 + 1)M_1 + 1 \cdot 0 = 6 \times (-2) \implies 4M_1 = -12 \implies M_1 = -3. \quad (19)$$

Hence, we can say that the knots would be

$$M_0 = 0, \quad M_1 = -3, \quad M_2 = 0. \quad (20)$$

For each subinterval $[x_i, x_{i+1}]$ with $h_i = x_{i+1} - x_i$, the cubic spline can be written in Hermite-like form using second derivatives:

$$\begin{aligned} S_i(x) = & \frac{M_i}{6h_i}(x_{i+1} - x)^3 + \frac{M_{i+1}}{6h_i}(x - x_i)^3 \\ & + \left(y_i - \frac{M_i h_i^2}{6} \right) \frac{x_{i+1} - x}{h_i} + \left(y_{i+1} - \frac{M_{i+1} h_i^2}{6} \right) \frac{x - x_i}{h_i}. \end{aligned} \quad (21)$$

For interval $[0, 1]$ ($i = 0$), we have

- $x_0 = 0, x_1 = 1, h_0 = 1$.
- $M_0 = 0, M_1 = -3$.
- $y_0 = 0, y_1 = 1$.



Therefore, on $[0, 1]$, the cubic spline is

$$S_0(x) = -\frac{1}{2}x^3 + \frac{3}{2}x. \quad (22)$$

For interval $[1, 2]$ ($i = 1$), we have

- $x_1 = 1, x_2 = 2, h_1 = 1.$
- $M_1 = -3, M_2 = 0.]$
- $y_1 = 1, y_2 = 0.$

Hence, on $[1, 2]$, the cubic spline is

$$S_1(x) = -\frac{1}{2}(2-x)^3 + \frac{3}{2}(2-x). \quad (23)$$

Thus, the cubic spline is

$$S(x) = \begin{cases} -\frac{1}{2}x^3 + \frac{3}{2}x, & 0 < x \leq 1 \\ -\frac{1}{2}(2-x)^3 + \frac{3}{2}(2-x), & 1 < x \leq 2 \end{cases} \quad (24)$$

(e) Using the formula for a Lagrange polynomial.

$$P(x) = \sum_{i=0}^n y_i \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \quad (25)$$

Then filling in the points gives:

$$\begin{aligned} P(x) &= \left(0 \cdot \left(\frac{x-1}{0-1} \cdot \frac{x-2}{0-2}\right)\right) + \left(1 \cdot \left(\frac{x-0}{1-0} \cdot \frac{x-2}{1-2}\right)\right) + \left(0 \cdot \left(\frac{x-0}{2-0} \cdot \frac{x-1}{2-1}\right)\right) \\ P(x) &= \left(\frac{x-0}{1-0} \cdot \frac{x-2}{1-2}\right) = x \cdot (2-x) = -x^2 + 2x \end{aligned} \quad (26)$$

- (f) The Lagrange polynomial is not the same as the cubic spline over $[0; 1]$ or $[1; 2]$. Reasons for this are: - the Lagrange polynomial does not have the derivative constraints and therefore behaves differently - the Lagrange polynomial is a global interpolation while splines are local, this causes behaviour to differ
- (g) You should use cubic splines instead of Lagrange polynomials if you need your interpolation to have local behaviour or appear to be visibly smooth (C_2 continuous). Additionally, you could answer that a cubic spline has more stable behaviour with many points.

4. Root Finding

- (a) Describe how the bisection and the Newton-Rhapson methods work.



- (b) Find the root of the following equation

$$f(x) = e^{\sin(0.2x^2-1)} - 2 \quad \text{with} \quad f'(x) = \frac{1}{5} \left[2xe^{\sin\left(\frac{x^2}{5}-1\right)} \cos\left(\frac{x^2}{5}-1\right) \right] \quad (27)$$

in the interval $[2.5, 4]$ analytically.

- (c) And using bisection twice.
 (d) And using two Newton-Raphson iterations starting with $x_0 = 3.4$.
 (e) In addition, estimate how many bisection iterations would be necessary to reach a relative tolerance of $\varepsilon = 10^{-7}$?
 (f) And roughly how many Newton-Raphson iterations would it take to reach this same tolerance?
 (g) Describe why you would use Newton-Raphson or Bisection. Which one is generally preferred?
 (h) How can you find a maximum by root finding? what does this require of the function?

Solution:

- (a) The bisection method starts with evaluating the function at two points, one of the two points should result in a negative number. The function is then evaluated at the point in between the two boundaries, if the result is positive the positive boundary is replaced by the halfway point, and if the value is negative the negative boundary is replaced by the halfway point. Repeating this converges on the root.

Newton-Raphson only needs one starting point, it then uses the derivative of the function to extrapolate the slope out to a point where the slope crosses zero, this point is then the next point of evaluation. Again this is iterated.

- (b)

$$\begin{aligned} e^{\sin(0.2x^2-1)} - 2 &= 0 \longrightarrow e^{\sin(0.2x^2-1)} = 2 \\ \sin\left(\frac{1}{5}x^2 - 1\right) &= \ln(2) \\ \longrightarrow \frac{1}{5}x^2 - 1 &= \arcsin(\ln(2)) + 2k\pi \text{ for } k \in \mathbb{N} \\ x &= \begin{cases} \sqrt{5[\arcsin(\ln(2)) + 1 + 2k\pi]} \\ -\sqrt{5[\arcsin(\ln(2)) + 1 + 2k\pi]} \end{cases} \end{aligned} \quad (28)$$

Note that there are multiple solutions due to the square root, $\pm$, and $\arcsin$'s periodicity. The solution within the interval is $x = \sqrt{5[\arcsin(\ln(2)) + 1]} \approx 2.97140 \approx 3$.

- (c) The root is estimated to be the middle of the interval.

1st iteration: $\text{mid} = \frac{a+b}{2} = \frac{2.5+4}{2} = 3.25$. The next iteration is determined by determining new bounds through $a = \text{mid}$ if $f(a) \times f(\text{mid}) > 0$ otherwise $b = \text{mid}$.

$f(2.5) \times f(3.25) \approx -0.32495 < 0 \longrightarrow b = \text{mid}$.

2nd iteration: $\text{mid} = \frac{2.5+3.25}{2} = 2.875$, which is the root after two iterations.



- (d) The Newton-Raphson method defines the root x_{i+1} as,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}. \quad (29)$$

For the first iteration, $x_0 = 3.4$ and we get $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \approx 3.4 - \frac{0.6292}{0.9151} \approx 2.7124$.

And for the second iteration, the estimate for the root becomes $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \approx 2.7124 + \frac{-0.4252}{1.5222} \approx 2.9917$.

- (e) $n_{\text{bisection}} = \log_2 \left(\frac{|a - b|}{\varepsilon} \right) = \log_2 \left(\frac{|2.5 - 4|}{10^{-7}} \right) = 23.838459164932694 \rightarrow 24$ steps.

- (f) As Newton-Raphson converges quadratically and bisection linearly, it reaches the tolerance in roughly $\sqrt{n_{\text{bisection}}} \approx 4$ steps.
- (g) The bisection method always works but is slow. The Newton-Raphson method is faster but the function needs to be differentiable.
- (h) A maximum can be found by finding the root(s) in the derivative. And I suppose you need to make sure the second derivative is positive. As long as you can compute the derivative, you can find the root.

5. Floating-point Error

Throughout this exercise, use base $b = 10$ and precision $p = 2$ (two significant digits in the significand), and the round-half-up convention.

The *fractional error* is defined as $E_f = \frac{|fl(x) - x_{\text{true}}|}{|x_{\text{true}}|}$.

For each operation below: express each operand in floating-point form, compute the floating-point result, and find E_f .

- (a) Compute $fl(48 + 77)$.
- (b) Compute $fl(576 - 560)$.
Why is E_f so much larger than in (a), even though the individual rounding error on $fl(576)$ is less than 1%?
- (c) Compute $fl(57 \times 78)$.
- (d) Compute $fl(1/7)$.

hint: for any real number x , the floating-point representation in base 10 is $fl(x) = s \times 10^e$ where $1 \leq s < 10$ and s is rounded to p significant digits.

**Solution:**

(a) Addition

$$fl(48) = 4.8 \times 10^1 \quad (\text{exact}), \quad fl(77) = 7.7 \times 10^1 \quad (\text{exact})$$

$$48 + 77 = 125 = 1.25 \times 10^2$$

The 3rd significant digit is $5 \geq 5$, so we round up:

$$fl(125) = 1.3 \times 10^2 = 130$$

$$E_f = \frac{|130 - 125|}{125} = \frac{5}{125} = \frac{1}{25} = 4\%$$

(b) Subtraction

$$fl(576) = 5.8 \times 10^2 = 580 \quad (3\text{rd digit} = 6 \geq 5, \text{ round up})$$

$$fl(560) = 5.6 \times 10^2 = 560 \quad (\text{exact})$$

$$fl(576) - fl(560) = 580 - 560 = 20$$

$$E_f = \frac{|20 - 16|}{16} = \frac{4}{16} = \frac{1}{4} = 25\%$$

Why is this so large? From the error propagation formula (for $y = a - b$):

$$E_f = \frac{\delta y}{y} = \frac{\delta a - \delta b}{a - b}$$

Here $\delta a = |580 - 576| = 4$, $\delta b = 0$, and $a - b = 16$. Even though the individual rounding error of $fl(576)$ is only $4/576 \approx 0.7\%$, dividing by the small difference $a - b = 16$ amplifies it to $4/16 = 25\%$.

This is catastrophic cancellation: when two nearly equal numbers are subtracted, the relative error in their difference can be far larger than the individual rounding errors. The closer $a \sim b$, the larger E_f becomes.

(c) Multiplication

$$fl(57) = 5.7 \times 10^1 \quad (\text{exact}), \quad fl(78) = 7.8 \times 10^1 \quad (\text{exact})$$

$$57 \times 78 = 4446 = 4.446 \times 10^3$$

The 3rd digit is $4 < 5$, round down:



$$fl(4446) = 4.4 \times 10^3 = 4400$$

$$E_f = \frac{|4400 - 4446|}{4446} = \frac{46}{4446} \approx 1\%$$

From error propagation for $y = a \times b$: $E_f \approx \delta a/a + \delta b/b$ (first order approximation), which is well-defined for any a, b . Multiplication does not suffer from catastrophic cancellation.

(d) Division

$$\frac{1}{7} = 0.142857 \dots = 1.42857 \dots \times 10^{-1}$$

The 3rd significant digit is $2 < 5$, round down:

$$fl(1/7) = 1.4 \times 10^{-1} = 0.14$$

$$E_f = \frac{|0.14 - \frac{1}{7}|}{\frac{1}{7}} = 7 \times \left| \frac{7}{50} - \frac{1}{7} \right| = 7 \times \frac{|49 - 50|}{350} = \frac{7}{350} = \frac{1}{50} = 2\%$$

Note: in iterative procedures, this 2% error could accumulate at every step depending on the algorithm