MAF310 – Numerical modeling

Assignment 1 – Fall 2022

This assignment is due on Tuesday 27th Sept.

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(1) Briefly explain what the following terms mean:

- Singular matrix and conditioning number
  Singular matrix is a matrix that has a zero determinant. There is no unique solution to system of linear equations described by a singular. The conditioning number is a measure how much the solution to a system of linear equations changes if the input is changed a little. A singular matrix has an infinite condition number.

- Pivoting in the context of solving systems of linear algebraic equations
  In solving a system of linear equations using gauss-elimination, pivoting means reshuffling rows such that one avoids dividing by zero, or by a very small number. This is done to make the solution to by numerically stable.

- Interpolation, extrapolation and curve fitting
  Interpolation, extrapolation, and curve fitting are means to estimate a function based on knowledge of the function in a finite set of points. Interpolation refers to approximating the underlying function between the points with an approximate function that goes through all the points. Extrapolation refers to estimating the function beyond the domain where the function is known. Curve fitting refers to finding parameters of a model function that best represent the data, typically in least-squares sense.

- Spline
  A piecewise-defined polynomial function used in interpolation.

- Linear form in the context of curve fitting
  A model function that is linear in the unknown parameters that are optimized in curve fitting. Finding the best fit parameters (in the least-squares sense) of linear forms can be reduced to a linear-algebra problem.

(2) Systems of linear algebraic equations: Use Doolittle's decomposition to solve $\mathbf{Ax} = \mathbf{b}$, where

$$\mathbf{A} = \begin{pmatrix} -3 & 6 & -4 \\ 9 & -8 & 24 \\ -12 & 24 & -26 \end{pmatrix}, \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} -3 \\ 65 \\ -42 \end{pmatrix}.$$

Solution: $\mathbf{A} = \mathbf{LU}$, with

$$\begin{pmatrix} -3 & 6 & -4 \\ 9 & -8 & 24 \\ -12 & 24 & -26 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 4 & 0 & 1 \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} -3 & 6 & -4 \\ 0 & 10 & 12 \\ 0 & 0 & -10 \end{pmatrix}$$

(3) Interpolation: The points

x	-2	1	4	-1	3	-4
y	-1	2	59	4	24	-53

lie on a polynomial. Use (for example) the divided difference table of Newton's method to determine the degree of the polynomial.

i	x_i	y_i	∇y_i	$\nabla^2 y_i$	$\nabla^3 y_i$	$\nabla^4 y_i$	$\nabla^5 y_i$
0	-2	-1	–	–	–	–	–
1	1	2	1	–	–	–	–
2	4	59	10	3	–	–	–
3	-1	4	5	-2	1	–	–
4	3	24	5	2	1	0	–
5	-4	-53	26	-5	1	0	0

$$\nabla y_i = \frac{y_i - y_0}{x_i - x_0}, \quad \nabla y_1 = \frac{2-(-1)}{1-(-2)} = 1, \ldots$$

$$\nabla^2 y_i = \frac{\Delta y_i - \Delta y_1}{x_i - x_1}, \quad \nabla^2 y_2 = \frac{10-1}{4-1} = 3, \ldots$$

The polynomial is given by the diagonal elements of the tableau

$$\begin{aligned} & y_0 \\ & + \nabla y_1 (x - x_0) \\ & + \nabla^2 y_2 (x - x_0)(x - x_1) \\ & + \nabla^3 y_3 (x - x_0)(x - x_1)(x - x_2) \\ & + \nabla^4 y_4 (x - x_0)(x - x_1)(x - x_2)(x - x_3) + \ldots \\ & = -1 + 1(x - (-2)) + 3(x - (-2))(x - 1) + 1(x - (-2))(x - 1)(x - 4) \end{aligned} \tag{1}$$

That is, the polynomial that generated is of 3rd order.

(4) Curve fitting: Determine a and b so that function $f(x) = axe^{bx}$ fits the following data in the least-squares sense. (Note that the function $f(x)$ is not quite just an exponential function!).

x	0.5	1.0	1.5	2.0	2.5
y	0.541	0.398	0.232	0.106	0.052

The strategy here is to define a new variable $\tilde{y} = \log(\frac{y}{x})$ *that should be described by a linear function* $\tilde{y} = \tilde{a} + \tilde{b}x$, *with*

$$\tilde{a} = \log a \qquad \tilde{b} = b$$

Simplest solution: The simplest solution is to just fit a least squares line for the $\tilde{y}$.

x	0.5	1.0	1.5	2.0	2.5
$\tilde{y}$	0.0788	-0.921	-1.866	-2.937	-3.873

The linear fit to this data is given by

$$\tilde{a} = \frac{S_{\tilde{y}} S_{xx} - S_x S_{x\tilde{y}}}{S_1 S_{xx} - S_x^2} = 1.072 \tag{2}$$

$$\tilde{b} = \frac{S_{x\tilde{y}} S_1 - S_x S_{\tilde{y}}}{S_1 S_{xx} - S_x^2} = -1.983, \tag{3}$$

where the following sums where used:

$$S_1 = \sum_i 1 = 5 \tag{4}$$

$$S_x = \sum_i x_i = 7.5 \tag{5}$$

$$S_{xx} = \sum_i x_i^2 = 13.5 \tag{6}$$

$$S_{\tilde{y}} = \sum_i \tilde{y}_i = -9.51924 \tag{7}$$

$$S_{x\tilde{y}} = \sum x_i \tilde{y}_i = -19.2386 \tag{8}$$

This then leads to

$$a = \exp(\tilde{a}) = 2.91 \tag{9}$$

$$b = \tilde{b} = -1.983 \tag{10}$$