Solutions to Final Exam

Question 1: 20 points

Problem Statement. Recall from our class lectures that if $[A]$ is an $(n \times n)$ matrix then, in general, it can be factored into a product of lower and upper triangular matrices, i.e., $[A] = [L]\,[U]$ where $[L]$ and $[U]$ are also $(n \times n)$ matrices. Our case study programs with Python and sympy assume that the lower diagonal elements are unity (i.e., $L_{ii} = 1$), but this is only one way of enabling the factorization. A second possibility is to set the upper diagonal elements to unity (i.e., $U_{ii} = 1$). The key point here is that any set of constraints that reduces the total number of unknowns from $\left(n^2 + n\right)$ to n^2 might work.

Part [1a]. (10 pts). Calculate the LU decomposition for the matrix

$$[A] = \begin{bmatrix} 1 & 1 & 0 \\ a & 8 & 4 \\ 0 & 1 & 2 \end{bmatrix}. \tag{1}$$

by assuming that $U_{ii} = 1$. Show all of your working ...

Solution: With $U_{ii} = 1$, the LU decomposition can be written:

$$\begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} 1 & U_{12} & U_{13} \\ 0 & 1 & U_{23} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ a & 8 & 4 \\ 0 & 1 & 2 \end{bmatrix}. \tag{2}$$

We have 9 matrix terms and 9 unknowns.

Matching terms in the first row of L and columns of U gives:

$$1 \cdot L_{11} = 1, \longrightarrow L_{11} = 1. \tag{3}$$

$$L_{11} U_{12} = 1, \longrightarrow U_{12} = 1. \tag{4}$$

$$L_{11}U_{13} = 0, \longrightarrow U_{13} = 0. \tag{5}$$

Matching terms in the second row of L and columns of U gives:

$$L_{21}U_{11} = a, \longrightarrow L_{21} = a. \tag{6}$$

$$L_{21} + L_{22} = 8, \longrightarrow L_{22} = (8 - a)\,. \tag{7}$$

$$L_{22}U_{23} = 4, \longrightarrow U_{23} = frac48 - a. \tag{8}$$

Matching terms in the third row of L and U gives:

$$L_{31}U_{11} = 0, \longrightarrow L_{31} = 0. \tag{9}$$

$$L_{31} + L_{32} = 1, \longrightarrow L_{32} = 1. \tag{10}$$

$$L_{31}U_{13} + L_{32}U_{23} + L_{33}U_{33} = 2, \longrightarrow L_{33} = 2 - \frac{4}{8 - a}. \tag{11}$$

Collecting terms gives:

$$\begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 & 0 \\ a & 8 - a & 0 \\ 0 & 1 & 2 - \frac{4}{8-a} \end{bmatrix} \tag{12}$$

$$\begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & \frac{4}{8-a} \\ 0 & 0 & 1 \end{bmatrix} \tag{13}$$

Part [1b]. (3 pts). Hence, write down the det[A]?. Note: Do not calculate the determinate by the method of cofactors - there is a much faster way that is a one line calculation!

Solution: det(A) = det(L).det(U) = $(8-a)\left(2-\frac{4}{8-a}\right) = 12-2a$.

Part [1c]. (7 pts). Use forward and backward substitution to show that the general solution to $[L]\,[U]\,[x] = [1, 2, b]^T$. can be written:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} (-4-2b)/(a-6) \\ (a+2b-2)/(a-6) \\ (ab-a-8b+2)/(2a-12) \end{bmatrix}. \tag{14}$$

This is a hand calculation, so show all of your working.

Solution: Two steps:

Forward Substitution: Solve Lz = B, i.e.,

$$\begin{bmatrix} 1 & 0 & 0 \\ a & 8-a & 0 \\ 0 & 1 & 2-\frac{4}{8-a} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ b \end{bmatrix} \longrightarrow \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ (a-2)/(a-8) \\ (b(a-8)-a+2)/(2a-12) \end{bmatrix}. \tag{15}$$

Backward Substitution: Solve Ux = Z, i.e.,

$$\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & \frac{4}{8-a} \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} \longrightarrow \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} (-4-2a)/(a-6) \\ (a+2b-2)/(a-6) \\ ((a-8)b+2-a)/(2a-12) \end{bmatrix}. \tag{16}$$

Part [1d]. (3 pts). For what values (a,b) will the system have: (a) a unique solution, (b) zero solutions, (c) infinite solutions?

Solution: Unique solution: a $\neq$ 6. Infinite solutions: When a = 6, b = -2, rank(A) = rank(A | b) = 2. Otherwise, when a = 6, b $\neq$ -2, zero solutions.

Question 2: 10 points

Problem Statement. This question covers numerical computation of the roots to an equation (i.e., f(x) = 0) using a novel implementation of Newton Raphson iteration. Preliminary work indicates that $f(x)$ has multiple roots at a and, thus, can be factored:

$$f(x) = (x-a)^m h(x). \tag{17}$$

Here $m \geq 2$. Our test equation for this question is:

$$f(x) = x^4 - 12x^3 + 47x^2 - 66x + 18. \tag{18}$$

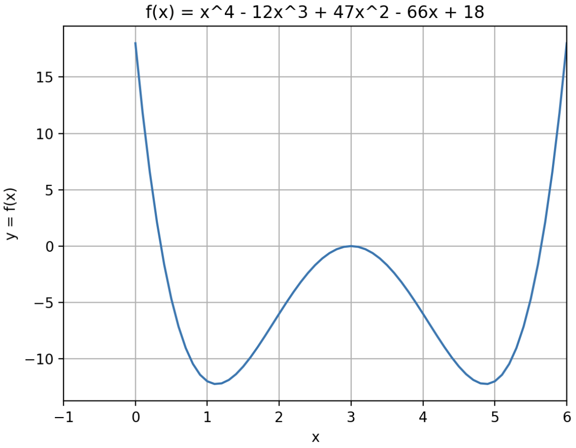

Figure 1. Plot y = f(x) vs x.

Part [2a] (4 pts). Show that the Newton Raphson update formula for equation 17 can be written:

$$x_{n+1} = x_n - \left[\frac{(x_n - a)h(x_n)}{mh(x_n) + (x_n - a)h^{'}(x_n)} \right]. \tag{19}$$

Solution: First, we differentiate equation 17:

$$f^{'}(x) = m(x-a)^{m-1}h(x) + (x-a)^m h^{'}(x). \tag{20}$$

Substituting equations 17 and 20 into the standard N-R update formula and cancelling common terms gives:

$$x_{n+1} = x_n - \left[\frac{f(x_n)}{f'(x_n)} \right] = x_n - \left[\frac{(x_n - a)h(x_n)}{mh(x_n) + (x_n - a)h'(x_n)} \right]. \tag{21}$$

Part [2b] (3 pts). Determine appropriate values of a, m and $h(x)$ for equation 18,

Solution: Equation 18 factors into:

$$f(x) = (x - 3)^2 \left(x^2 - 6x + 2 \right). \tag{22}$$

Hence, a = 3, m = 2, and $h(x)$ = $\left(x^2 - 6x + 2 \right)$.

Part [2c] (3 pts). Starting from an initial value, x_o = 0.0, compute no more than three iterations of approximation to the lowest root of equation 18. I suggest your organize your computations into a table that shows iteration no, x, $(x - a)^m$, $h(x)$ and $f(x)$.

Solution:

```
Iteration:        x:     (x-3)^2:       h(x):       f(x):
-------------------------------------------------------
        0     0.000        9.000       2.000      18.000
        1     0.273        7.438       0.438       3.258
        2     0.349        7.030       0.030       0.212
        3     0.354        7.000       0.000       0.001
-------------------------------------------------------
```

Question 3: 10 points

Problem Statement. This question covers function interpolation with the methods of divided differences and lagrange interpolation, and curve fitting with the method of least squares.

The whole question is motivated by the small dataset:

```
   x |  0.0 |   2.0 |   3.0 |   5.0
----------------------------------
f(x) |  0.0 |   8.0 |  27.0 | 125.0
```

Part [3a] (5 pts). Use the method of **divided differences** to find a polynomial of lowest order that will fit the dataset.

Solution: We seek a third order polynomial p(x):

$$p(x) = f[x_0]+f[x_o,x_1](x-x_o)+f[x_o,x_1,x_2](x-x_o)(x-x_1)+f[x_o,x_1,x_2,x_3](x-x_o)(x-x_1)(x-x_2). \tag{23}$$

where

x_i	$f[x_i] = f(x_i)$	$f[,]$	$f[,,]$	$f[,,,]$
0.0	0	$f[x_0,x_1]$	$f[x_0,x_1,x_2]$	$f[x_0,x_1,x_2,x_3]$
2.0	8	$f[x_1,x_2]$	$f[x_1,x_2,x_3]$	
3.0	27	$f[x_2,x_3]$		
5.0	125			

Elements in the divided difference table are as follows:

$$f[x_0,x_1] = \left[\frac{f(x_1)-f(x_0)}{x_1-x_0}\right] = \left[\frac{8-0}{2-0}\right] = 4. \tag{24}$$

$$f[x_1,x_2] = \left[\frac{f(x_2)-f(x_1)}{x_2-x_1}\right] = \left[\frac{27-8}{3-2}\right] = 19. \tag{25}$$

$$f[x_2,x_3] = \left[\frac{f(x_2)-f(x_1)}{x_2-x_1}\right] = \left[\frac{125-27}{5-3}\right] = 49. \tag{26}$$

The second column of computations:

$$f[x_0, x_1, x_2] = \left[\frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}\right] = \left[\frac{19 - 4}{3 - 0}\right] = 5.0. \tag{27}$$

$$f[x_1, x_2, x_3] = \left[\frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}\right] = \left[\frac{49 - 19}{5 - 2}\right] = 10.0. \tag{28}$$

The third column computations:

$$f[x_0, x_1, x_2, x_3] = \left[\frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_3]}{x_3 - x_0}\right] = \left[\frac{10 - 5}{5 - 0}\right] = 1.0 \tag{29}$$

Thus, the interpolated polynomial is:

$$\begin{aligned} f(x) &= f[x_0] + f[x_o, x_1](x - x_o) + f[x_0, x_1, x_2](x - x_o)(x - x_1) \\ &= 0 + 4(x - 0) + 5(x - 0)(x - 2) + 1(x - 0)(x - 2)(x - 3) \\ &= x^3 \end{aligned}$$

Part [3b] (5 pts). Check your answer in part 3a by computing the functional form via the method of **Lagrange Interpolation**.

Solution: For the given dataset,

$$f(x) = f(x_o)p_o(x) + f(x_1)p_1(x) + f(x_2)p_2(x) + f(x_3)p_3(x) \tag{30}$$

where

$$p_o(x) = \frac{(x - 2)(x - 3)(x - 5)}{(0 - 2)(0 - 3)(0 - 5)} = \left[\frac{-x^3 + 10x^2 - 31x + 30}{30}\right]. \tag{31}$$

$$p_1(x) = \frac{(x - 0)(x - 3)(x - 5)}{(2 - 0)(2 - 3)(2 - 5)} = \left[\frac{x^3 - 8x^2 + 15x}{6}\right]. \tag{32}$$

$$p_2(x) = \frac{x(x-2)(x-5)}{3(3-2)(3-5)} = \left[\frac{-x^3+7x^2-10x}{6}\right]. \tag{33}$$

$$p_3(x) = \frac{x(x-2)(x-3)}{5(5-2)(5-3)} = \left[\frac{x^3-5x^2+6x}{30}\right]. \tag{34}$$

Also note: f(x_o) = 0, f(x_1) = 8, f(x_2) = 27 and f(x_3) = 125.

Substitute equations 31 through 34 into equation 30. Notice that the constant term in equation 31 is one, and the linear and quadratic terms cancel out completely. This leaves:

$$f(x) = x^3. \tag{35}$$

Question 4: 10 points

Problem Statement. Figure 2 is a graph of $f(x) = \big[(x-2)^2 - 16\big]$ over the interval $[-2, 8]$.

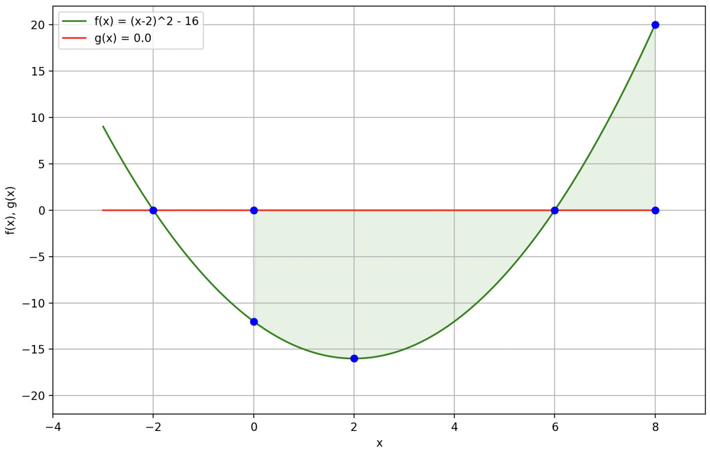

Figure 2. Graph of quadratic curve.

In this question we are interested in numerical approximations to the area of the green shaded region, i.e.,

$$I = \int_0^8 f(x) dx. \tag{36}$$

with the Trapezoid and Simpson's Integration Rules.

Part [4a] (7 pts). Suppose that equation 36 is estimated by one step of the Trapezoid Rule. Develop an expression for the actual error. Compute the error estimate (which we have covered in class). Is the latter less than the actual error?

Solution: The analytic solution to equation 36 is:

$$I = \int_0^8 (x^2 - 4x - 12) dx = \left[\frac{x^3}{3} - 2x^2 - 12x \right]_0^8 = -53.33. \tag{37}$$

With one step of Trapezoid:

$$T_1 = \frac{8}{2} \left[f(0) + f(8) \right] = \frac{8}{2} \left[-12 + 20 \right] = 32. \tag{38}$$

Thus, the actual error is 32 + 53.33 = 85.33. (terrible!) Our general formula for the trapezoid rule is:

$$I = \int_a^b f(x)dx = T_n - \frac{|f^2(\xi)|}{12} h^2(b-a). \tag{39}$$

where $[a \leq \xi \leq b]$. For our test problem, h = 8, $b - a$ = 8, and $|f^2(\xi)|$ = 2. Hence, the error estimate is:

$$\frac{|f^2(\xi)|}{12} h^2(b-a) = \frac{2}{12} \cdot 8^2 \cdot 8 = 85.33, \tag{40}$$

which matches the actual error exactly.

Part [4b] (3 pts). Show that one step of Simpson's Rule integrates the quadratic equation exactly.

Solution: One step of Simpson's Rule (h = 4) gives:

$$S_1 = \frac{h}{3}[f(0) + 4f(4) + f(8)] = \frac{4}{3}[-12 + 4(-12) + 20] = -53.33, \tag{41}$$

which matches the analytical solution.

Question 5: 10 points

Problem Statement. Theoretical considerations indicate that:

$$\int_1^5 x^4 dx = \frac{1}{5}\left[5^5 - 1^5\right] dx = 624.8. \tag{42}$$

Part [5a] (4 pts). Use the method of Romberg integration to obtain an $O(h^6)$ accurate estimate of equation 42. Be sure to show all steps in your working.

Solution: Apply Trapezoid Rule:

$$T_1 = \frac{5-1}{2}\left[1^4 + 5^4\right] = 1252.0 \tag{43}$$

$$T_2 = \frac{5-1}{4}\left[1^4 + 23^4 + 5^4\right] = 788.0 \tag{44}$$

$$T_4 = \frac{5-1}{8}\left[1^4 + 22^4 + 23^4 + 24^4 + 5^4\right] = 666.0 \tag{45}$$

Romberg Integration Table:

```
---   a =    1.0000 ...
---   b =    5.0000 ...
---   no intervals = 3 ...
---   Compute trapezoid rule for first column ...
---   Iterate over levels of refinement ...
---      Extrapolation for column  2 ...
---      Extrapolation for column  3 ...

Matrix: Romberg Integration Table (instantiated)
  1.25200000e+03   0.00000000e+00   0.00000000e+00
  7.88000000e+02   6.33333333e+02   0.00000000e+00
  6.66000000e+02   6.25333333e+02   6.24800000e+02
```

Column 2 elements O(h^4): R(1,1) = 633.3, R(2,1) = 625.3.

Column 3 elements O(h^6): R(2,2) = 624.8.

Part [5b] (3 pts). Evaluate equation 42 using 2-pt Gauss Quadrature. Be sure to show all steps in your working.

Solution: Two-point quadrature:

$$\int_a^b f(x)dx = w_o f(x_o) + w_1 f(x_1), \tag{46}$$

where: $w_o = 1$, $x_o = -1/\sqrt{3}$, $w_1 = 1$, $x_1 = 1/\sqrt{3}$.

Transforming integral onto the interval $[-1, 1]$:

$$x = \frac{b-a}{2}u + \frac{a+b}{2} = 2u + 3. \tag{47}$$

Hence,

$$dx = \frac{b-a}{2}du = 2dx. \tag{48}$$

Combining equations 46 – 48:

$$I = 2\int_{-1}^{1} (2u+3)^4 du = 2\left[\left(\frac{-2}{\sqrt{3}} + 3 \right)^4 + \left(\frac{2}{\sqrt{3}} + 3 \right)^4 \right] = 619.11. \tag{49}$$

Implementation in Python:

```
---   w0 =   1.000000e+00, u0 =  -5.773503e-01, x0 =   1.845299e+00 ...
---   w1 =   1.000000e+00, u1 =   5.773503e-01, x1 =   4.154701e+00 ...

---   f1(x0) =   1.159491e+01 ...
---   f1(x1) =   2.979606e+02 ...

---   Integral I = 6.19111111e+02 ...
```

Part [5c] (3 pts). Evaluate equation 42 using 3-pt Gauss Quadrature. Be sure to show all steps in your working.

Solution: As above,

$$I = \int_{1}^{5} x^4 dx = 2\int_{-1}^{1} (2u+3)^4 du = w_o f(x_o) + w_1 f(x_1) + w_2 f(x_2). \tag{50}$$

where: $w_o = \frac{5}{9}$, $x_o = -\sqrt{\frac{3}{5}}$, $w_1 = \frac{8}{9}$, $x_1 = 0$, $w_2 = \frac{5}{9}$, $x_2 = \sqrt{\frac{3}{5}}$.

Hence,

$$I = 2\int_{-1}^{1} (2u+3)^4 du = 2\left[\frac{5}{9}\left(-2\sqrt{\frac{3}{5}}+3\right)^4 + \frac{8}{9}(3)^4 + \frac{5}{9}\left(2\sqrt{\frac{3}{5}}+3\right)^4 +\right] = 624.8. \tag{51}$$

Implementation in Python:

```
---   w0 =   5.555556e-01, u0 =  -7.745967e-01, x0 =   1.450807e+00 ...
---   w1 =   8.888889e-01, u1 =   0.000000e+00, x1 =   3.000000e+00 ...
---   w2 =   5.555556e-01, u2 =   7.745967e-01, x2 =   4.549193e+00 ...

---   f1(x0) =   4.430351e+00 ...
---   f1(x1) =   8.100000e+01 ...
---   f1(x2) =   4.282896e+02 ...

---   Integral I = 6.24800000e+02 ...
```

Three-point Gauss Quadrature gives an exact answer.