Advanced Scientific Engineering Homework 4

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1 QR Factorization of Matrix A

Given matrix A:

$$A = \begin{bmatrix} 3 & 0 \\ 0 & 2 \\ 1 & 0 \end{bmatrix}$$

We want to perform the QR factorization A = QR, where: - Q is an orthogonal matrix. - R is an upper triangular matrix.

Step 1: Construct the orthonormal set (columns of Q)

1. First, take the first column of A, $\mathbf{a_1} = \begin{bmatrix} 3 \\ 0 \\ 1 \end{bmatrix}$, and normalize it:

$$\|\mathbf{a_1}\| = \sqrt{3^2 + 0^2 + 1^2} = \sqrt{10}$$

So, the first column of Q is:

$$\mathbf{q_1} = \frac{1}{\sqrt{10}} \begin{bmatrix} 3\\0\\1 \end{bmatrix} = \begin{bmatrix} \frac{3}{\sqrt{10}}\\0\\\frac{1}{\sqrt{10}} \end{bmatrix}$$

2. For the second column, take $\mathbf{a_2} = \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix}$, and normalize it:

$$\|\mathbf{a_2}\| = \sqrt{0^2 + 2^2 + 0^2} = 2$$

So, the second column of Q is:

$$\mathbf{q_2} = \frac{1}{2} \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

Thus, the matrix Q is:

$$Q = \begin{bmatrix} \frac{3}{\sqrt{10}} & 0\\ 0 & 1\\ \frac{1}{\sqrt{10}} & 0 \end{bmatrix}$$

Step 2: Compute R

Using the relation $R = Q^T A$, we calculate R:

$$Q^T = \begin{bmatrix} \frac{3}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} \\ 0 & 1 & 0 \end{bmatrix}$$

Now, multiply Q^T by A:

$$R = Q^T A = \begin{bmatrix} \frac{3}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 2 \\ 1 & 0 \end{bmatrix}$$

Carrying out the matrix multiplication:

$$R = \begin{bmatrix} \frac{3}{\sqrt{10}} \cdot 3 + \frac{1}{\sqrt{10}} \cdot 1 & 0\\ 0 \cdot 3 + 1 \cdot 2 & 2 \end{bmatrix} = \begin{bmatrix} \frac{9}{\sqrt{10}} + \frac{1}{\sqrt{10}} & 0\\ 0 & 2 \end{bmatrix} = \begin{bmatrix} \sqrt{10} & 0\\ 0 & 2 \end{bmatrix}$$

Thus, $R = \begin{bmatrix} \sqrt{10} & 0 \\ 0 & 2 \end{bmatrix}$.

Final QR Factorization

$$A = QR = \begin{bmatrix} \frac{3}{\sqrt{10}} & 0\\ 0 & 1\\ \frac{1}{\sqrt{10}} & 0 \end{bmatrix} \begin{bmatrix} \sqrt{10} & 0\\ 0 & 2 \end{bmatrix}$$

2 Weighted Least Squares for Closest Line

By hand, find the closest line in a weighted least squares sense that approximates the following data points:

with point weights:

Hint: The inverse of a 2x2 matrix is as follows:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

We begin by defining the system:

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}, \quad \hat{\mathbf{u}} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \hat{\mathbf{b}} = \begin{bmatrix} 0 \\ 2 \\ 1 \\ 6 \end{bmatrix}$$

The transpose of matrix A is:

$$A^T = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix}$$

The weight matrix is:

$$C = \operatorname{diag}\left(\frac{1}{\sigma_n^2}\right)$$

Using the weighted least squares formula:

$$\hat{\mathbf{u}}^* = (A^T C A)^{-1} A^T C \hat{\mathbf{b}}$$

Substituting the values:

$$\hat{\mathbf{u}}^* = \left(\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} \frac{1}{.2^2} & 0 & 0 & 0 \\ 0 & \frac{1}{.3^2} & 0 & 0 \\ 0 & 0 & \frac{1}{.3^2} & 0 \\ 0 & 0 & 0 & \frac{1}{.2^2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} \frac{1}{.2^2} & 0 & 0 & 0 \\ 0 & \frac{1}{.3^2} & 0 & 0 \\ 0 & 0 & \frac{1}{.3^2} & 0 \\ 0 & 0 & 0 & \frac{1}{.2^2} \end{bmatrix} \begin{bmatrix} 0 \\ 2 \\ 1 \\ 6 \end{bmatrix}$$

After solving this system, we obtain:

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} -0.24977 \\ 1.85882 \end{bmatrix}$$

Thus, the equation of the line is:

$$y = -0.24977x + 1.85882$$

```
>> a = [1 0; 1 1; 1 2; 1 3]
a =
      1
             0
      1
             1
      1
             2
      1
             3
>> b = [0;2;1;6]
b =
      0
      2
      1
      6
>> c = [(1/.2^2) \ 0 \ 0 \ 0; \ 0 \ (1/.3^2) \ 0 \ 0; \ 0 \ 0 \ (1/.3^2) \ 0; \ 0 \ 0 \ (1/.2^2)]
c =
   25.0000
                                  0
               11.1111
                                  0
                                              0
           0
                      0
                           11.1111
          0
                      0
                                  0
                                       25.0000
>> (a'*c*a)^-1*a'*c*b
ans =
   -0.2498
    1.8588
```

Figure 1: MatLab Code For Solution

3 Deriving the Growth Term G for the Heat Equation

Given the heat equation:

$$u_t = Du_{xx}$$

where D is the diffusion coefficient, we are asked to use the backward Euler method for the time derivative and centered differences for the spatial derivative.

Step 1: Centered Difference Approximation The centered difference approximation for the second spatial derivative u_{xx} is:

$$u_{xx}(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

Step 2: Backward Euler Method The backward Euler approximation for the time derivative is:

$$u^{n+1} = u^n + \Delta t \cdot f(u^{n+1}, u^n)$$

which simplifies to:

$$\frac{u^{n+1} - u^n}{\Delta t} = D \frac{u^{n+1}(x+h) - 2u^{n+1}(x) + u^{n+1}(x-h)}{h^2}$$

Step 3: Substituting $u = Ge^{ikx}$ We now substitute $u = Ge^{ikx}$ into the equation for both the time and spatial derivatives:

$$\frac{Ge^{ikx} - e^{ikx}}{\Delta t} = D\frac{e^{ik(x+h)} - 2e^{ikx} + e^{ik(x-h)}}{h^2}$$

Using the identity:

$$e^{ik\Delta x} + e^{-ik\Delta x} = 2\cos(k\Delta x)$$

the equation becomes:

$$\frac{G-1}{\Delta t} = D \frac{2(\cos(k\Delta x) - 1)}{h^2}$$

Step 4: Solving for G Rearranging the equation to solve for G:

$$G - 1 = D \cdot \frac{2(\cos(k\Delta x) - 1)}{h^2} \cdot \Delta t$$

$$G = 1 + \frac{2D(\cos(k\Delta x) - 1)}{h^2} \cdot \Delta t$$

Thus, the growth factor G is:

$$G = \frac{2D(\cos(k\Delta x) - 1)}{\Delta t} + 1$$

4 Analysis of the Function $f(x) = 4 + 8x^2 - x^4$

1. Find the first and second derivatives of f(x)

We are given the function:

$$f(x) = 4 + 8x^2 - x^4$$

The first derivative f'(x) is:

$$f'(x) = \frac{d}{dx}(4 + 8x^2 - x^4) = 16x - 4x^3$$

The second derivative f''(x) is:

$$f''(x) = \frac{d}{dx}(16x - 4x^3) = 16 - 12x^2$$

2. Find the y-intercept and determine any maxima or minima The y-intercept occurs when x = 0:

$$f(0) = 4 + 8(0)^2 - (0)^4 = 4$$

Thus, the y-intercept is at (0,4).

To find the critical points, set f'(x) = 0:

$$16x - 4x^3 = 0$$

$$4x(4-x^2) = 0$$

$$x = 0, \quad x = \pm 2$$

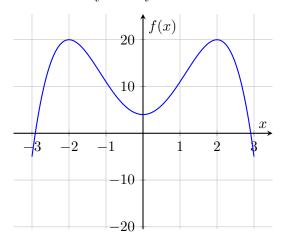
Now check the second derivative at these points: - At x = 0:

$$f''(0) = 16 > 0 \implies \text{local minimum at } (0,4)$$

- At $x = \pm 2$:

$$f''(2) = f''(-2) = 16 - 12(2)^2 = -32 < 0 \implies \text{local maximum at } (2,20) \text{ and } (-2,20)$$

3. Sketch the Graph and Determine Symmetry



$$--- f(x) = 4 + 8x^2 - x^4$$

Since f(x) only involves even powers of x, it is symmetric about the y-axis, indicating that the function is even.

4. Use Newton's Method to Approximate the x-intercept near x=3 We apply Newton's method with the following iteration formula:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Using the code provided:

```
// Function f(x) = 4 + 8x^2 - x^4
func f(x float64) float64 {
    return 4 + 8*x*x - math.Pow(x, 4)
}
// First derivative f'(x) = 16x - 4x^3
func f_prime(x float64) float64 {
    return 16*x - 4*math.Pow(x, 3)
}
// Newton's method for finding x-intercept
func newtonsMethod(x0 float64, iterations int) float64 {
    x := x0
    for i := 0; i < iterations; i++ {</pre>
        x = x - f(x)/f_prime(x)
        fmt.Printf("Iteration %d: x = \%.6f\n", i+1, x)
    return x
}
func main() {
    // Part 4: Newton's Method for x-intercept near x = 3
    fmt.Println("\nNewton's method to find x-intercept near x = 3:")
    initialGuess := 3.0
    iterations := 2
    xIntercept := newtonsMethod(initialGuess, iterations)
    fmt.Printf("Approximate x-intercept: %.6f\n", xIntercept)
}
   The output after two iterations approximates the x-intercept as:
```

 $x \approx 2.910723$

Thus, the approximate x-intercept near x = 3 is 2.910723.

```
Newton's method to find x-intercept near x = 3: Iteration 1: x = 2.916667 Iteration 2: x = 2.910723 Approximate x-intercept: 2.910723
```

5 Analysis of the Function $f(x) = x^3 - 3x - 3$

1. Find all extrema and points of inflection

Given the function $f(x) = x^3 - 3x - 3$, we first compute the first and second derivatives:

$$f'(x) = 3x^2 - 3$$
$$f''(x) = 6x$$

To find the critical points, set f'(x) = 0:

$$3x^2 - 3 = 0 \implies x^2 = 1 \implies x = \pm 1$$

Now, calculate the function values at these critical points:

$$f(1) = (1)^3 - 3(1) - 3 = -5$$

$$f(-1) = (-1)^3 - 3(-1) - 3 = -1$$

Now, check the second derivative at these points to determine whether they are maxima or minima: - At x = 1:

$$f''(1) = 6(1) = 6 > 0 \implies \text{absolute minimum at } (1, -5)$$

- At x = -1:

$$f''(-1) = 6(-1) = -6 < 0 \implies \text{absolute maximum at } (-1, -1)$$

2. Is the function odd, even, or neither?

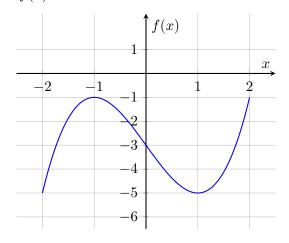
To check if the function is odd, we test the property f(-x) = -f(x). For x = 1:

$$f(1) = -5, \quad f(-1) = -1$$

Since $f(-1) \neq -f(1)$, the function is not odd.

To check if the function is even, we would test for symmetry across the y-axis, but there is no symmetry. Therefore, the function is neither odd nor even.

3. Sketch of the function $f(x) = x^3 - 3x - 3$



$$---f(x) = x^3 - 3x - 3$$

4. Newton's Method for Approximating the x-Intercept We apply Newton's method to approximate the x-intercept near $x_0 = 2$, using the formula:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

The function and its derivative are:

$$f(x) = x^3 - 3x - 3, \quad f'(x) = 3x^2 - 3$$

Using an initial guess $x_0 = 2$ and performing two iterations:

```
// Function f(x) = x^3 - 3x - 3
func f(x float64) float64 {
    return math.Pow(x, 3) - 3*x - 3
}
// First derivative f'(x) = 3x^2 - 3
func f_prime(x float64) float64 {
    return 3*math.Pow(x, 2) - 3
}
// Newton's method for finding x-intercept
func newtonsMethod(x0 float64, iterations int) float64 {
    x := x0
    for i := 0; i < iterations; i++ {</pre>
        x = x - f(x)/f_{prime}(x)
        fmt.Printf("Iteration %d: x = \%.6f\n", i+1, x)
    }
    return x
}
func main() {
    // Part 4: Newton's Method for x-intercept near x = 2
    initialGuess := 2.0
    iterations := 2
    xIntercept := newtonsMethod(initialGuess, iterations)
    fmt.Printf("Approximate x-intercept: %.6f\n", xIntercept)
}
```

The output after two iterations is approximately:

 $x \approx 2.103836$

Thus, the approximate x-intercept is $x \approx 2.103836$.

```
Newton's method to find x-intercept near x = 2:

Iteration 1: x = 2.111111

Iteration 2: x = 2.103836

Approximate x-intercept: 2.103836
```

6 Go Code for Bisection Method

Below is the Go code that calculates the root using the Bisection Method for $f(x) = x^2 - 3 = 0$ in the interval [1, 2].

```
package main
import (
 "fmt"
 "math"
// Function f(x) = x^2 - 3 = 0
func f(x float64) float64 {
return math. Pow(x, 2) - 3
}
func main() {
 // Initialize variables as float64
var lower_bound float64 = 1
 var upper_bound float64 = 2
 var root float64
 var iteration_count int
 var tolerance float64 = 0.000001 // Tolerance to check how close the result is to zero
// Set up the bisection method
 for {
 middle := (lower_bound + upper_bound) / 2
 potential_root := f(middle)
 // checks the root tolerance
  if math.Abs(potential_root) <= tolerance {</pre>
  root = middle
  break
  }
  // Adjust the bounds
```

```
if potential_root > 0 { upper_bound = middle } else { lower_bound = middle } // Keep count of the iterations iteration_count++ } // Output the result fmt.Printf("The calculated root is: %.6f\n", root) fmt.Printf("The number of iterations it took: %d\n", iteration_count) } The approximate solution using the bisection method is: x \approx 1.732051 The amount of iterations taken: n = 19
```

PS C:\Users\jacob\Documents\school\Adv_Sci_Engr\hw\hw_4> go run problem_6_bisection.go
The calculated root is: 1.732051
The number of iterations it took: 19