

# 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:

$$(0, 0), (1, 2), (2, 1), (3, 6)$$

with point weights:

$$2/10, 3/10, 3/10, 2/10.$$

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:

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

Using the weighted least squares formula:

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

Substituting the values:

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

After solving this system, we obtain:

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} -0.2571 \\ 1.5714 \end{bmatrix}$$

Thus, the equation of the line is:

$$\boxed{y = -0.2571 + 1.5714x}$$

```

a =
    1    0
    1    1
    1    2
    1    3

>> c

c =
    0.2000    0    0    0
         0    0.3000    0    0
         0    0    0.3000    0
         0    0    0    0.2000

>> b

b =
    0
    2
    1
    6

>> inv((a'*c*a))*a'*c*b

ans =
   -0.2571
    1.5714

```

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  $f'(x) = 0$ :

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

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

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

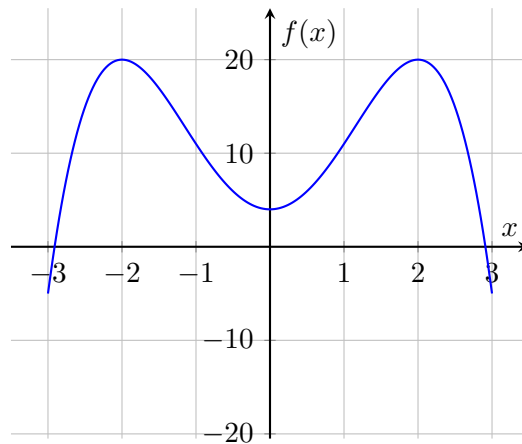
Now check the second derivative at these points: - At  $x = 0$ :

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

- At  $x = \pm 2$ :

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

3. Sketch the Graph and Determine Symmetry



$$\text{--- } f(x) = 4 + 8x^2 - x^4$$

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++ {
        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  $f'(x) = 0$ :

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

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  $x = 1$ :

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

- At  $x = -1$ :

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

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

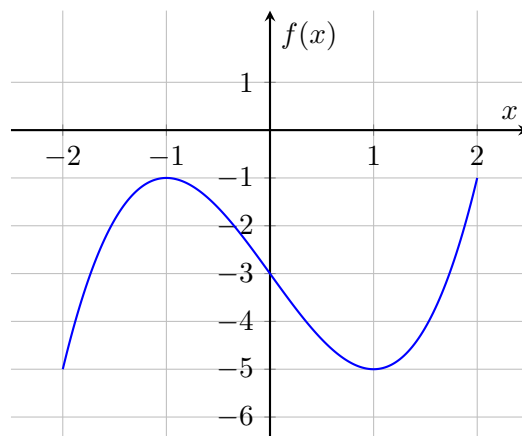
To check if the function is odd, we test the property  $f(-x) = -f(x)$ . For  $x = 1$ :

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

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



$$\text{— } f(x) = x^3 - 3x - 3$$



#### 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++ {
        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 {  
            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

```