CS 4600/5600 Numerical Computing
Homework 1

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Problem 2: Roots - Open Methods

(b) Newton-Raphson Method

Given the function:

$$f(x) = x^3 - 6x^2 + 11x - 6.1$$

We need to determine the largest positive root using the Newton-Raphson method, starting with $x_0 = 3.5$.

The Newton-Raphson iteration formula is:

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

First, we find the derivative of $f(x)$:

$$f'(x) = 3x^2 - 12x + 11$$

Starting with $x_0 = 3.5$:

$$f(3.5) = (3.5)^3 - 6(3.5)^2 + 11(3.5) - 6.1 = 0.775$$

$$f'(3.5) = 3(3.5)^2 - 12(3.5) + 11 = 1.75$$

First iteration:

$$x_1 = 3.5 - \frac{0.775}{1.75} \approx 3.0571$$

Second iteration:

$$f(3.0571) = (3.0571)^3 - 6(3.0571)^2 + 11(3.0571) - 6.1 \approx 0.1123$$

$$f'(3.0571) = 3(3.0571)^2 - 12(3.0571) + 11 \approx 1.1714$$

$$x_2 = 3.0571 - \frac{0.1123}{1.1714} \approx 2.9612$$

Third iteration:

$$f(2.9612) = (2.9612)^3 - 6(2.9612)^2 + 11(2.9612) - 6.1 \approx 0.0053$$

$$f'(2.9612) = 3(2.9612)^2 - 12(2.9612) + 11 \approx 1.0783$$

$$x_3 = 2.9612 - \frac{0.0053}{1.0783} \approx 2.9563$$

The largest positive root after three iterations is approximately $x \approx 2.9563$.

(c) Modified Secant Method

Using the same function $f(x) = x^3 - 6x^2 + 11x - 6.1$, we apply the modified secant method with $x_0 = 3.5$ and $\delta = 0.01$.

The modified secant method iteration formula is:

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

First iteration:

$$f(3.5) = 0.775$$

$$f(3.5 + 0.01 \cdot 3.5) = f(3.535) = 0.771925$$

$$x_1 = 3.5 - \frac{0.01 \cdot 3.5 \cdot 0.775}{0.771925 - 0.775} \approx 3.0357$$

Second iteration:

$$f(3.0357) = 0.1087$$

$$f(3.0357 + 0.01 \cdot 3.0357) = f(3.0661) = 0.107092$$

$$x_2 = 3.0357 - \frac{0.01 \cdot 3.0357 \cdot 0.1087}{0.107092 - 0.1087} \approx 2.9634$$

Third iteration:

$$f(2.9634) = 0.0074$$

$$f(2.9634 + 0.01 \cdot 2.9634) = f(2.9930) = 0.0068$$

$$x_3 = 2.9634 - \frac{0.01 \cdot 2.9634 \cdot 0.0074}{0.0068 - 0.0074} \approx 2.9567$$

Fourth iteration:

$$f(2.9567) = 0.0027$$

$$f(2.9567 + 0.01 \cdot 2.9567) = f(2.9862) = 0.0026$$

$$x_4 = 2.9567 - \frac{0.01 \cdot 2.9567 \cdot 0.0027}{0.0026 - 0.0027} \approx 2.9559$$

Fifth iteration:

$$f(2.9559) = 0.0009$$

$$f(2.9559 + 0.01 \cdot 2.9559) = f(2.9855) = 0.0008$$

$$x_5 = 2.9559 - \frac{0.01 \cdot 2.9559 \cdot 0.0009}{0.0008 - 0.0009} \approx 2.9556$$

The largest positive root after five iterations is approximately $x \approx 2.9556$.

Problem 4: Optimization

Given the function:

$$f(x) = 4x - 1.8x^2 + 1.2x^3 - 0.3x^4$$

(b) Prove the function is concave for all values of x

A function is concave if its second derivative is negative for all values of x.

First, we find the first derivative of $f(x)$:

$$f'(x) = 4 - 3.6x + 3.6x^2 - 1.2x^3$$

Now, we find the second derivative:

$$f''(x) = -3.6 + 7.2x - 3.6x^2$$

For $f''(x)$ to be negative for all values of x, we need to check its sign:

$$f''(x) = -3.6 + 7.2x - 3.6x^2$$

Let's analyze the roots of $f''(x)$:

$$-3.6 + 7.2x - 3.6x^2 = 0$$

$$3.6x^2 - 7.2x + 3.6 = 0$$

$$x^2 - 2x + 1 = 0$$

$$(x-1)^2 = 0$$

$$x = 1$$

At $x = 1$:

$$f''(1) = -3.6 + 7.2(1) - 3.6(1)^2 = -3.6 + 7.2 - 3.6 = 0$$

The second derivative is zero at $x = 1$, so we need to analyze the behavior around $x = 1$: For $x < 1$, $f''(x)$ is positive. For $x > 1$, $f''(x)$ is negative.

Since $f''(x)$ changes sign, the function is not concave for all values of x.

(c) Differentiate the function and use a root-location method to solve for the maximum $f(x)$ and the corresponding value of x

First, we find the critical points by setting the first derivative to zero:

$$f'(x) = 4 - 3.6x + 3.6x^2 - 1.2x^3 = 0$$

We can use the Newton-Raphson method to find the root: Starting with $x_0 = 1$:

$$f'(1) = 4 - 3.6(1) + 3.6(1)^2 - 1.2(1)^3 = 0$$

$$f''(1) = -3.6 + 7.2(1) - 3.6(1)^2 = 0$$

Since $f''(1) = 0$, we use the modified Newton-Raphson method:

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

Second iteration:

$$f''(0.5) = -3.6 + 7.2(0.5) - 3.6(0.5)^2 = -3.6 + 3.6 - 0.9 = -0.9$$

$$x_1 = 0.5 - \frac{f'(0.5)}{f''(0.5)} \approx 0.5$$

The maximum $f(x)$ is at $x = 1$.

Problem 5: Optimization

Given the function:

$$f(x_1, x_2) = \frac{1}{2}(x_1^2 - x_2)^2 + \frac{1}{2}(1 - x_1)^2$$

(a) Minimum point

To find the minimum point, we need to find the gradient and set it to zero:

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right) = 0$$

First, we find the partial derivatives:

$$\frac{\partial f}{\partial x_1} = 2x_1(x_1^2 - x_2) - (1 - x_1)$$

$$\frac{\partial f}{\partial x_2} = -(x_1^2 - x_2)$$

Setting the gradient to zero:

$$2x_1(x_1^2 - x_2) - (1 - x_1) = 0$$

$$-(x_1^2 - x_2) = 0$$

Solving the system of equations, we get:

$$x_1^2 = x_2$$

$$2x_1(x_1^2 - x_2) - (1 - x_1) = 0$$

Simplifying, we find the minimum point is:

$$(x_1, x_2) = (1, 1)$$

(b) Newton's Method Iteration

Using the starting point $\begin{pmatrix} 2 \\ 2 \end{pmatrix}$, we perform one iteration of Newton's method for minimizing f.

The Hessian matrix is:

$$H = \begin{pmatrix} 6x_1^2 - 2x_2 + 1 & -2x_1 \\ -2x_1 & 1 \end{pmatrix}$$

The gradient at $\begin{pmatrix} 2 \\ 2 \end{pmatrix}$ is:

$$\nabla f = \begin{pmatrix} 2x_1(x_1^2 - x_2) - (1 - x_1) \\ -(x_1^2 - x_2) \end{pmatrix} = \begin{pmatrix} 2(2)(4-2) - (1-2) \\ -(4-2) \end{pmatrix} = \begin{pmatrix} 6 \\ -2 \end{pmatrix}$$

The Hessian at $\begin{pmatrix} 2 \\ 2 \end{pmatrix}$ is:

$$H = \begin{pmatrix} 6(2)^2 - 2(2) + 1 & -2(2) \\ -2(2) & 1 \end{pmatrix} = \begin{pmatrix} 17 & -4 \\ -4 & 1 \end{pmatrix}$$

The Newton step is:

$$\Delta x = -H^{-1} \nabla f$$

We need to invert the Hessian:

$$H^{-1} = \frac{1}{17 \cdot 1 - (-4)^2} \begin{pmatrix} 1 & 4 \\ 4 & 17 \end{pmatrix} = \frac{1}{1} \begin{pmatrix} 1 & 4 \\ 4 & 17 \end{pmatrix} = \begin{pmatrix} 1 & 4 \\ 4 & 17 \end{pmatrix}$$

The Newton step is:

$$\Delta x = -\begin{pmatrix} 1 & 4 \\ 4 & 17 \end{pmatrix} \begin{pmatrix} 6 \\ -2 \end{pmatrix} = -\begin{pmatrix} 1 \cdot 6 + 4 \cdot (-2) \\ 4 \cdot 6 + 17 \cdot (-2) \end{pmatrix} = -\begin{pmatrix} 6 - 8 \\ 24 - 34 \end{pmatrix} = -\begin{pmatrix} -2 \\ -10 \end{pmatrix} = \begin{pmatrix} 2 \\ 10 \end{pmatrix}$$

The new point after one iteration is:

$$\begin{pmatrix} 2 \\ 2 \end{pmatrix} + \begin{pmatrix} 2 \\ 10 \end{pmatrix} = \begin{pmatrix} 4 \\ 12 \end{pmatrix}$$