Chapter 2: Roots of Algebraic Equations

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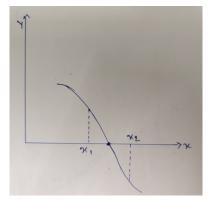
Course Name: Introduction to Numerical Analysis (PH 307)

Introduction

- Our aim in this chapter is to develop methods for finding the roots (or zeros) of an equation of the type f(x) = 0, where f(x) is a general real non-linear function of a real variable x.
- Note that when f(x) = ax+b, a linear function, the roots of the equation can be obtained trivially.

The Bisection Method

- It is a very robust method of finding the roots of an equation.
- The basic idea behind this method is very simple.
- The method starts out with an interval (x_1, x_2) in which the function changes sign.



• From the figure above it is obvious that at least one zero of the function is located in the interval.

Thus we start out with the function

$$f(x_1)f(x_2) \le 0 \tag{1}$$

• Then we bisect the interval and obtain

$$x_3 = \frac{x_1 + x_2}{2}$$

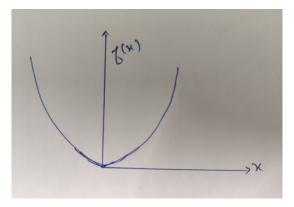
and check

$$f(x_1)f(x_3) \begin{cases} < 0 & \text{set } x_2 = x_3 \text{ and perform next iteration} \\ > 0 & \text{set } x_1 = x_3 \text{and perform iteration} \\ = 0 & \text{convergence achieved} \end{cases}$$
(2)

- This process of repeated bisections is continued until the interval is smaller than a specified criteria.
- As stated earlier, this method is very robust and is not affected by the presence of point of inflection or a local minimum, as the Newton's method is.

The main weaknesses of this method are:

 The method is not able to resolve multiple roots at which the function does not exhibit any sign change.



• Such a case can be handled by this method by looking for sign changes in the higher derivatives of the function.

- When there are many zeros in a given interval, this method may have trouble finding all the zeros if the search intervals are not properly chosen to handle this situation.
- To handle this situation, it is a good idea to compute the function on a grid and locate all the regions of sign change and then choose search intervals accordingly.

Newton's (or Newton-Raphson) Method

- Newton's method is an iterative method in which the function f(x) is approximated as a linear function
- This is done by Taylor expanding it near a initial guess of the root, x_k , and retaining only up to the first order terms

$$y(x) \approx f(x_k) + f'(x_k)(x - x_k) \tag{3}$$

• Clearly, the zero of this function, obtained by setting y(x) = 0, is located at

$$x = x_k - \frac{f(x_k)}{f'(x_k)}$$

• We take this value as the next guess for the root of f(x), i.e.,

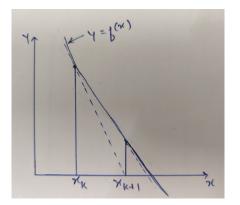
$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \tag{4}$$

- This procedure is continued iteratively until $f(x_{k+1}) \approx 0$, within a specified tolerance.
- Which means that $x = x_{k+1}$ is a root of the f(x) = 0.



Newton's (or Newton-Raphson) Method (contd.)

- Note that approximation 3 basically amounts to replacing the function f(x) by its tangent at $x = x_k$.
- Geometrically, the procedure can be represented as



• Clearly, in the method, the approach to the correct root is from one side.



Newton's (or Newton-Raphson) Method (contd.)

Convergence Properties:

- When the Newton's method converges, it does so very rapidly.
- We will prove next that the convergence of the Newton's method is quadratic.
- Let us suppose that the correct root of the equation f(x) = 0 is x = b.
- We know that in Newton's method

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

• If we define the error in the i-th step as

$$\varepsilon_i = x_i - b$$

we have,

$$\varepsilon_{i+1} = \varepsilon_i - \frac{f_i}{f_i'} \tag{5}$$

Newton's (or Newton-Raphson) Method (contd.)

• Let us expand $f(x_i)$ and $f'(x_i)$ about the root b

$$f(x_i) = f(b) + \varepsilon_i f'(b) + \frac{\varepsilon_i^2}{2} f''(b) + \dots$$

(where f(b) = 0)

$$f'(x_i) = f'(b) + \varepsilon_i f''(b) + \dots$$

With this we get in Eq. 5

$$\varepsilon_{i+1} = \varepsilon_i - \frac{\varepsilon_i f'(b) + \frac{\varepsilon_i^2}{2} f''(b) + \dots}{f'(b) + \varepsilon_i f''(b) + \dots}$$

or

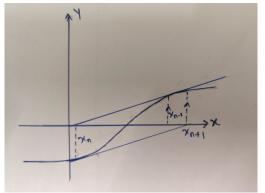
$$\varepsilon_{i+1} \approx \varepsilon_i^2 \frac{f''(b)}{f'(b)}$$
(6)

 Thus, clearly, near a root, the Newton's method has quadratic convergence which is very rapid.

Pathological Situations

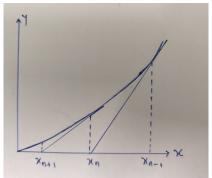
Following three situations lead to enormous convergence difficulties for the Newton's method.

- Point of Inflection: When the zero happens to be a point of inflection, the Newton's method will never converge.
- As the iterations proceed, the successive guesses will oscillate around the correct root but will never converge to it.



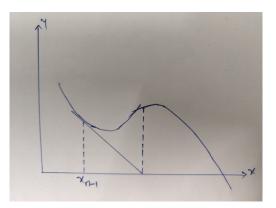
Pathological Situations (contd.)

- Multiple Zero's: When a zero of a function is a multiple zero of x_k then clearly near to zero the function, $f(x) \sim (x x_k)^n$ where n > 1 is the multiplicity of the root.
- Then clearly near x_k , $f'(x) \sim (x-x_k)^{n-1} o 0$
- Thus it is clear from Eq. 4 that as we approach the root, the convergence is slow and there will be trouble in the division step in order to get the next guess.
- Geometrically the situation is as below:



Pathological Situations (contd.)

• Local Minima: If a function has a local minimum near which of course f'(x) = 0, during the Newton iterations there is a clear cut risk that the next guess could be very far away. As illustrated below:



Improving Newton's Method

Following two modifications help resolve the troubles associated with the point of inflection and multiple roots:

- At every step we used |f(x)| as a measure of as to how close we are to the root.
- Thus, if $|f(x_{k+1})| \nleq |f(x)|$, we reject the step but instead we go back and halve the step

$$\Delta x_k = x_{k+1} - x_k = \frac{-f(x_k)}{f'(x_k)}$$

and use instead $\frac{\Delta x_k}{2}$

No new step is more then twice the previous step i.e.,

$$\Delta x_{k+1} \not\geq 2\Delta x_k$$

• This will help reduce tedious business of halving the steps.



Secant Method

- In the Newton's method we start out with a single initial guess, say, x_0 , and find the root iteratively
- However, in the iterative step we need to compute the derivative of the function f'(x)

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

- Suppose, we don't want to compute f'(x) because it may be computationally demanding
- ullet However, we do have two initial guesses x_1 and x_2
- Instead of approximating the f(x) as its tangent line at x_1 , we approximate it as its secant line y(x) connecting x_1 and x_2

$$y(x) - f(x_1) = \frac{f(x_2) - f(x_1)}{x_2 - x_1} (x - x_1)$$

$$\implies y(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1} (x - x_1)$$

Secant Method (contd.)

• The zero of y(x) is easily obtained by setting y(x) = 0

$$x = \frac{f(x_2)x_1 - f(x_1)x_2}{f(x_2) - f(x_1)}$$

• We interpret x above as the next guess x_3

$$x_3 = \frac{f(x_2)x_1 - f(x_1)x_2}{f(x_2) - f(x_1)},$$

which can be generalized to yield the iterative formula

$$x_{i+2} = \frac{f(x_{i+1})x_i - f(x_i)x_{i+1}}{f(x_{i+1}) - f(x_i)}$$
(7)

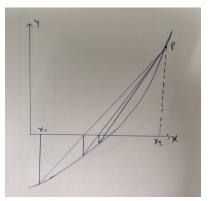
• The iterations are terminated when $f(x_{i+2}) \approx 0$, within a user-specified tolerance



Secant Method (contd.)

• Note that Eq. 7 is symmetric with respect to the interchange $(x_i, f(x_i)) \leftrightarrow (x_{i+1}, f(x_{i+1}))$

The convergence in secant method is also one sided, as is obvious from the graph below



False Position Method (Regula Falsi)

- This method is a combination of the bisection and secant methods
- It can be seen also as an attempt to increase the rate of convergence of the bisection method
- This method also starts out with an interval in which the function exhibits a sign change.
- That is the initial guesses x_1 and x_2 (or x_0 and x_1) are on the two sides of a root
- Our main goal, of course, is to decrease the interval.
- Now we approximate the function f(x) in this interval by the secant line connecting x_1 and x_2 just like in secant method, whose root is

$$x_3 = \frac{f(x_2)x_1 - f(x_1)x_2}{f(x_2) - f(x_1)}$$



Regula Falsi (contd.)

- After this the algorithm proceeds like the bisection method, i.e., as in Eq. 2
- This method will also not work for roots of even order where the sign flip doesn't occur

Modified False Position Method

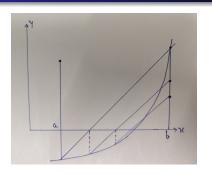
- This method is an attempt to improve the convergence of the false position method.
- One uses secant lines of varying slopes in this approach
- The modification is that one divides by two the value of the function at the end it is kept.
- Thus for a function f(x), if the starting values are a and b with $f(a)f(b) \le 0$ and $a \le x \le b$. Then the next value of x is

$$x = \frac{af(b) - bf(a)}{f(b) - f(a)}$$

• Calculate f(x)



Modified False Position Method (contd.)



Compute

$$f(x)f(a) \begin{cases} < 0 & \begin{cases} x \to b \\ f(x) \to f(b) \\ \frac{f(a)}{2} \to f(a) \end{cases} \\ = 0 & \text{done} \\ > 0 & \begin{cases} x \to a \\ f(x) \to f(a) \\ \frac{f(b)}{2} \to f(b) \end{cases} \end{cases}$$