POLITECNICO MILANO 1863
DEPARTMENT OF CHEMISTRY MATERIALS AND CHEMICAL ENGINEERING

Root Finding

Calcoli di Processo dell'Ingegneria Chimica

Timoteo Dinelli

October 30th, 2025

Department of Chemistry, Materials and Chemical Engineering, "Giulio Natta"
Politecnico di Milano
email: timoteo.dinelli@polimi.it

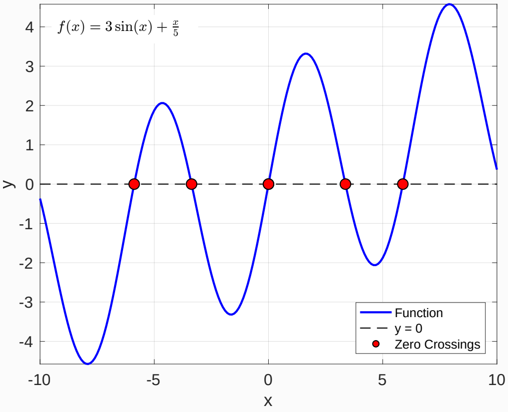
Root Finding

We will discuss different general algorithms that seek to find the solution $\mathbf{x}$ of the following canonical equation:

$$f(\mathbf{x}) = 0$$

Key concepts:

- Iterative approaches
- Convergence criteria
- Numerical precision



General Strategy

Given the equation:

$$f(\mathrm{x}) = 0$$

1. Make a reasonable first guess x_0 (or first guesses x_0, x_1)
2. Test the value of $f(x_0)$
3. Make a new intelligent guess based on x_0 and $f(x_0)$
4. Repeat until convergence criteria are met:

Function precision:

$$\|f(x_{i+1})\| < \epsilon_f$$

Solution convergence:

$$\|x_{i+1} - x_i\| < \epsilon_x$$

Bisection Method

Theoretical foundation:

Under Bolzano's theorem, if a function $f(x)$ is continuous in the interval $[a, b]$ and takes values of opposite sign at the boundaries, then it has a root in that interval.

Algorithm:

Starting with interval $[a, b]$, function $f(x)$, and tolerance ϵ such that $\|c - \hat{c}\| < \epsilon$, where $\hat{c}$ is the root:

1. Compute midpoint: $c = \dfrac{a+b}{2}$
2. If $b - c \leq \epsilon$, then c is the solution — stop; otherwise, continue
3. If $\text{sign}(f(b)) \times \text{sign}(f(c)) \leq 0$, then $a = c$; else $b = c$
4. Return to step 1 and repeat

Newton's Method

Algorithm:

1. Make a reasonable first guess x_0
2. Compute the next guess using:

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

3. Repeat until required precision is reached

Challenge: How do we compute $f'(x_i)$?

Computing Derivatives

Classical Analysis:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

Exact mathematical definition using limits

Numerical Analysis:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

Pick a small value for h (e.g., $h = 1 \times 10^{-7}$)

Finite difference approximation enables practical computation

Secant Method

The Newton method simplifies $f(x) = 0$ using the tangent as an approximation. The secant method uses a secant line instead, requiring two initial guesses.

Algorithm:

Assuming we know $f(x)$ for two distinct values x_0 and x_1 close to the solution α:

1. Make reasonable first guesses x_0 and x_1
2. Compute $f(x_0)$ and $f(x_1)$, then calculate:

$$x_2 = x_1 - \frac{f(x_1)(x_1 - x_0)}{f(x_1) - f(x_0)}$$

3. Loop until convergence

General iterative formula:

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

Regula Falsi Method

Hybrid approach: Combines features of bisection and secant methods

The *regula falsi* (false position) method:

- Uses secants like the secant method
- Maintains an uncertainty interval like bisection
- Requires function values of opposite signs at interval boundaries
- Guarantees convergence for continuous functions

Key difference from secant: The two points always bracket the root, ensuring the solution remains within the interval throughout iterations.

More robust than secant method, faster than bisection

Method Comparison

Method	Initial Guesses	Convergence Rate	Derivative
Bisection	2 (bracketing)	Linear	Not required
Newton	1	Quadratic	Required
Secant	2 (any)	Superlinear	Not required
Regula Falsi	2 (bracketing)	Superlinear	Not required

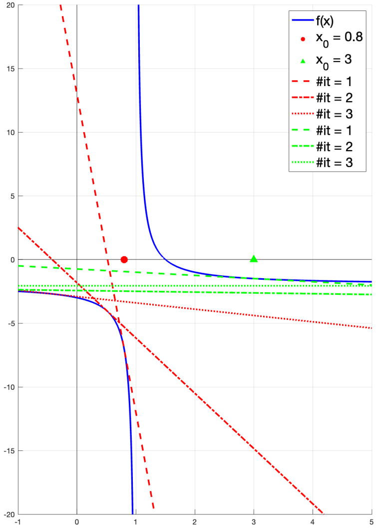
Selection criteria:

- **Newton:** Fastest when derivative is easily computed
- **Secant:** Good balance when derivative is costly
- **Bisection:** Most robust, guaranteed convergence
- **Regula Falsi:** Combines robustness with better speed

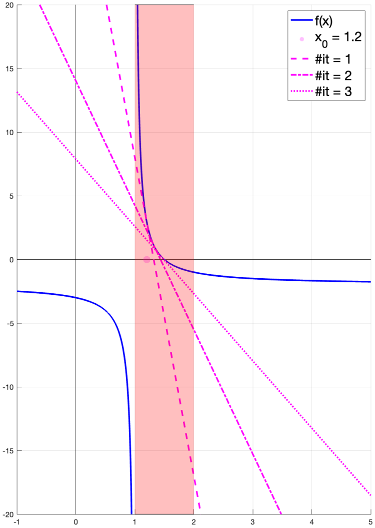
Exercises

Exercise

- Let's implement the Bisection and Newton method to find the zero of a function. Test them against $f(x) = 3e^x - 4cos(x)$.
- (Exam 05/02/19, Exercise 4): Find the root of the function $f(x) = \frac{1}{x-2} - 2$. After several attempts it can be noticed that the Newton method fails for first guesses as $x_0 = 1.8$ and $x_0 = 4$, while converge rapidly if the first guess is equal to $x_0 = 2.2$. Explain why this happens using also a graphical representation, determine the interval where is possible to identify a first guess that allows the method to converge. Compute the solution using Newton method and Bisection method with a precision of $1e^{-2}$. Then compare the results obtained with the Matlab's built-in method fzero and fsolve.



f(x)
x0 = 0.8
x0 = 3
#it = 1
#it = 2
#it = 3
#it = 1
#it = 2
#it = 3
20
15
10
5
0
-5
-10
-15
-20
-1
0
1
2
3
4
5



f(x)
x0 = 1.2
#it = 1
#it = 2
#it = 3
20
15
10
5
0
-5
-10
-15
-20
-1
0
1
2
3
4
5

- From the DIPPR® database we learn that, for WATER (H_2O), the Vapor Pressure can be calculated In the range 273.16 K to 647.13 K as follows:

$$P^0_{vap}(T) = exp\left(A + \frac{B}{T} + C \times ln(T) + D \times T^E\right) \quad [Pa]$$

Where: T is the temperature in Kelvin, $A = 7.3649e^{+01}$, $B = -7.2582e^{+03}$, $C = -7.3037e^{+00}$, $D = 4.1653e^{-06}$, $E = 2.0000e^{+00}$. Determine, using the newton method, for which temperature the vapor pressure is 0.5 atm

- Write a function that calculates the bubble temperture of a binary blend of NC6 and NC7 (70/30 molar) at atmospheric pressure using a solver you developed (the solver will be a function that takes the function to be solved, the interval or the first guess needed to start the iterative procedure and the desired precision of the solution and returns the zero of the function. Bubble Temperature of a mixture.

$$\sum_{i=1}^{NS} y_i = 1 \longrightarrow y_i = \frac{P_i^0(T)}{P} z_i$$

$$f(x) = 1 - \sum_{i=1}^{NS} \frac{P_i^0(T_{bubble})}{P} z_i = 0$$

Thank you for your attention!