POLITECNICO MILANO 1863

SCUOLA DI INGEGNERIA INDUSTRIALE E DELL'INFORMAZIONE

Root Finding.
Part 1

Calcoli di Processo dell' Ingegneria Chimica

Timoteo Dinelli, Marco Mehl

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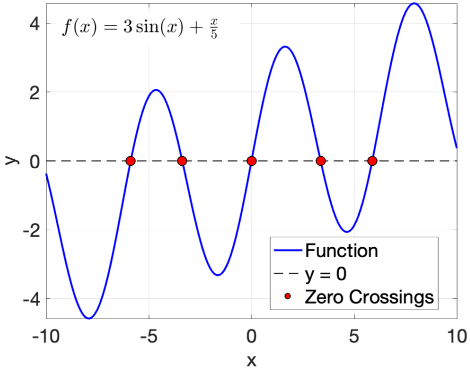
Department of Chemistry, Materials and Chemical Enginering, G. Natta. Politecnico di Milano.
email: timoteo.dinelli@polimi.it
email: marco.mehl@polimi.it

Root Finding

We will discuss different general algorithms that seek to find the solution x of the following canonical equation:

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



General strategy

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

1. Make a (reasonable) first guess (x_0) or first guesses (x_0, x_1).
2. Test the value of $f(x_0)$.
3. Then make a new INTELLIGENT guess, based on x_0 and $f(x_0)$.
4. Repeat this process, as long as, the required precision on the function value is close to selected tolerance ϵ_f:

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

and the solution was found to be convergent.

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

Bisection method

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

Starting with an interval $[a,\ b]$, $f(x)$ and a tolerance ϵ such that $\|c - \hat{c}\| < \epsilon$. Where $\hat{c}$ is the zero of our function.

1. Compute $c = \frac{a+b}{2}$.
2. If $b - c \leq \epsilon$ then c is the solution and stop otherwise go to the next point.
3. If $sign\left(f(b)\right) \times sign\left(f(a)\right) \leq 0$ then $a = c$, else $b = c$, then go back to point 1 and repeat.

Newton method

1. Make a reasonable first guess x_0.
2. Compute the next guess according to the following iterative formula:

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

3. Repeat the loop till the required precision is reached.

Problem

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

Newton method

1. Make a reasonable first guess x_0.
2. Compute the next guess according to the following iterative formula:

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

3. Repeat the loop till the required precision is reached.

Problem

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

Derivatives

Classical analysis:

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

Numerical analysis: pick a small value for h (e.g. $1 * 10^{-7}$):

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

Secant method

The newton method tries to simplify the solution of the base problem $f(x) = 0$ using the tangent as an approximation of the function we are trying to zero. Assuming to know the value of the function $f(x)$ for two distinct values of x (x_0 and x_1) close enough to the solution α:

1. Make a reasonable first guess x_0 and x_1.
2. Compute the values $f(x_0)$ and $f(x_1)$ then given the secant equation compute the value of x_2.

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

   Then loop until convergence.

Generalizing we get the secant method based on the following iterative formula:

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

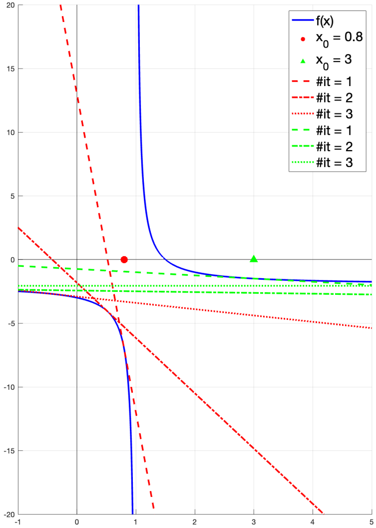
Regula falsi method

The *regula falsi* method is similar to the secant method and to the bisection method. This method uses secants and a succession of points as the secant method, but throws in in the mix the uncertainty interval represented by two extremes where the function to be zeroed (which is assumed to be continuous) has opposite signs. Along the iterations, the two points determine the boundaries of the uncertainty interval.

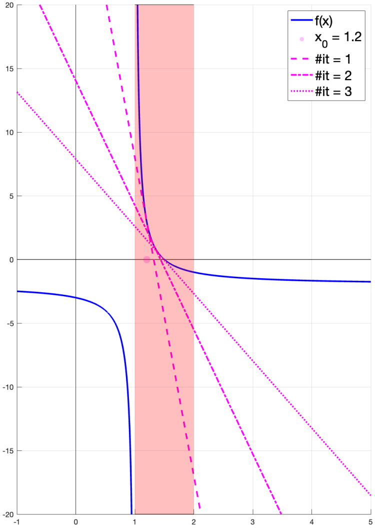
Exercises

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



f(x)
x0 = 1.2
#it = 1
#it = 2
#it = 3

- 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 the attention!