Computational Physics

Solving Nonlinear Equations

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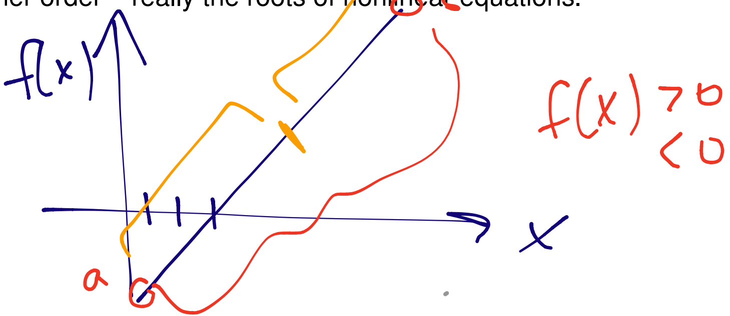
Solving nonlinear equations

Finding the zero of a function can be trivial

$$f(x) = x - 3 \text{ leading to } x - 3 = 0$$

closed form solutions exist for quadratic, cubit and quartic equations but not generally for polynomials of higher order. So we are looking for roots of higher order – really the roots of nonlinear equations.

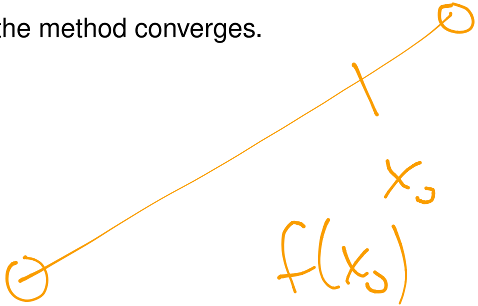
How?



Independently of the method under consideration, one needs to answer the following key points:

- Best choice for the initial guess x_0.
- Bracketing the root.
- Under which conditions the method converges.
- Speed of convergence.

error tolerance



Solving nonlinear equations

The classical root-finding problem consists of, given a function $f(x)$ with $x \in (a, b)$, finding the value(s) r such that

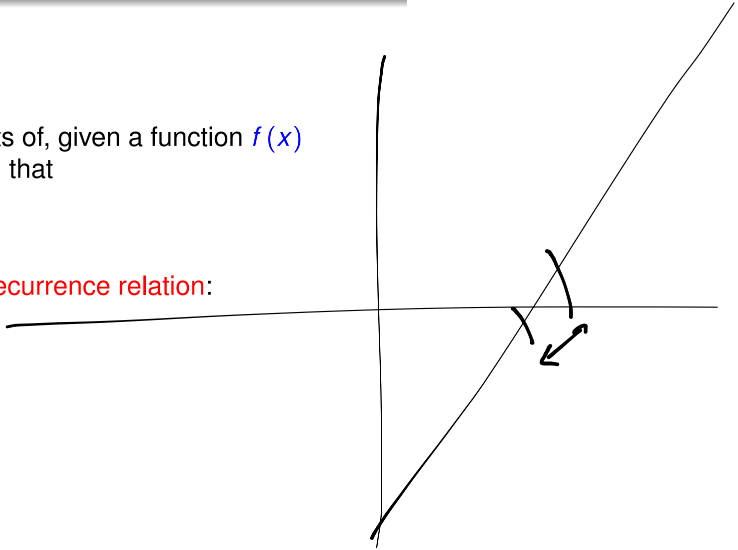
$$f(r) = 0$$

The most common approach involves a recurrence relation:

$$x_n = g(x_{n-1})$$

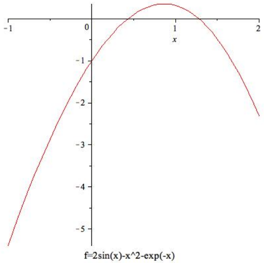
such that

$$\lim_{n \to \infty} x_n = r$$



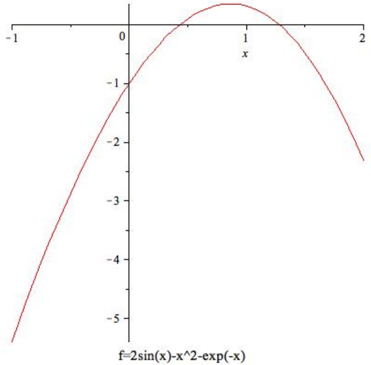
Consider the following function

$$f(x) = 2\sin(x) - x^2 - e^{-x}$$



- We are interested finding the root between $x_0 = 0$ and $x_1 = 1$.
- Notice that $f(0) = -1$ and $f(1) = 0.31506$
- Therefore, there must be at least one root since the function changes sign

We use then the following recurrence procedure



- $x_2 = (x_0 + x_1)/2 = 0.5$
  $\rightarrow f(0.5) = 0.1023$
- $x_3 = (x_0 + x_2)/2 = 0.25$
  $\rightarrow f(0.25) = -0.1732$
- $x_4 = (x_3 + x_2)/2 = 0.375$
  $\rightarrow f(0.375) = -0.0954$
- $x_5 = (x_4 + x_2)/2 = 0.4375$
  $\rightarrow f(0.4375) = 0.0103$
- $x_6 = (x_4 + x_5)/2 = 0.40625$
  $\rightarrow f(0.40625) = -0.0408$
- ...
- $x_n = r_1 \approx 0.4310378790$

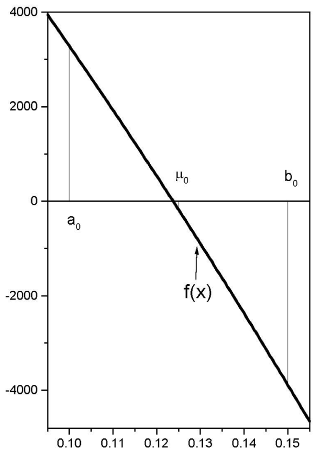
The other root is $r_2 = 1.279762546$.

Consider the interval $[a_0, b_0]$. If $f(a_0) \cdot f(b_0) < 0$, then there is at least one root within this interval. Next define, $\mu_0 = (a_0 + b_0)/2$. Then, either:

1. $f(\mu_0) \cdot f(a_0) < 0$
2. $f(\mu_0) \cdot f(b_0) < 0$
3. $f(\mu_0) = 0$

If (3), the root has been found, else we set a new interval

$$[a_1, b_1] = \begin{cases} [\mu_0, b_0] & \text{if} \quad (2) \\ [a_0, \mu_0] & \text{if} \quad (1) \end{cases}$$



Bisection Psuedocode

REPEAT
SET $x_3 = (x_1 + x_2)/2$
IF $f(x_3) \cdot f(x_1) < 0$
SET $x_2 = x_3$
ELSE
SET $x_1 = x_3$
ENDIF
UNTIL $|f(x_3)| < E$

findroot_class.