Roots of nonlinear equations

Consider solving a nonlinear equation in one variable x

$$f(x) = 0$$

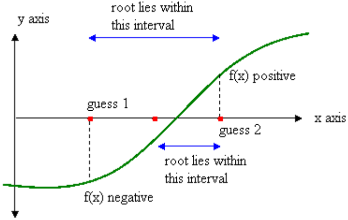
Assume $f(x)$ smoothly varying, continuous over the range $[a, b]$.

A few typical examples of $f(x)$ are,

$$f(x) = \cos x - x^3, \quad 3x + \sin x - e^x, \quad xe^x - 2, \quad x^3 + 3x - 5 \text{ etc.}$$

If x_0 in the interval $[a_0, b_0]$ satisfies equation $f(x_0) = 0$, then x_0 is a *root* or *zero* of the function and is **one** of the solutions in that interval.

Since $f(x)$ is continuous and $[a_0, b_0]$ so chosen such that $f(a_0)$ and $f(b_0)$ are of opposite signs, then according to *intermediate value theorem*, $f(x)$ has at least one root in the interval $[a_0, b_0]$.



Finding root numerically starts with guess $[a_0, b_0]$ – informed or trial-and-error – at which $f(x)$ has opposite signs.

$[a_0, b_0]$ are said to *bracket* the root.

Iterations proceed by producing a sequence of shrinking intervals $[a_0, b_0] \rightarrow [a_i, b_i]$ – shrunk intervals always contain one root of $f(x)$.

For convergence, necessary to have a good initial guess – *(i)* plotting $f(x)$ vs x or *(ii)* informed expectation.

Algorithms for finding roots of nonlinear equations :

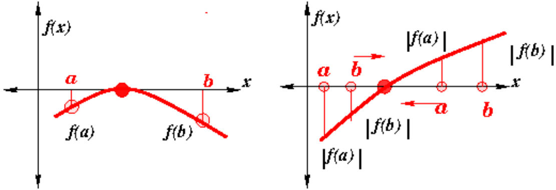
1. Bisection method
2. False position (Regula falsi) method
3. Newton-Raphson method
4. Fixed-point method
5. Laguerre's method (for roots of polynomials)

As is evident, the first four methods are iterative and, therefore, call for user specific precision ϵ, typically 10^{-4}.

Bisection method

Simplest, relatively slower but guaranteed to converge provided the bracketing is done carefully : $f(a)$ and $f(b)$ have opposite signs at the interval boundary $[a, b]$ and $f(x)$ is continuous.

Things can go wrong – *(i)* when $f(x) = 0$ is an extrema *i.e.* both $f(a)$, $f(b)$ are always of same sign, or *(ii)* multiple roots in the interval.



Steps involve in achieving **bracketing** :

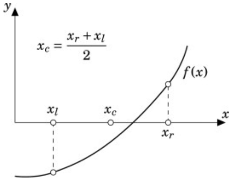
1. Choose $[a, b]$, calculate $f(a)$, $f(b)$. If $f(a) \star f(b) < 0$, bracketing done.
2. If $f(a) * f(b) > 0$ *i.e.* same sign, check for $|f(a)| \lessgtr |f(b)|$.
   2.1 If $|f(a)| < |f(b)|$, shift a further left by $a' = a - \beta(b - a)$
   2.2 If $|f(a)| > |f(b)|$, shift b further right by $b' = b + \beta(b - a)$

Steps involve in bisection method :

1. Choose bracket $[a, b]$, where $a < b$ and $f(a) * f(b) < 0$. If $|b - a| < \epsilon$, done! Check also $f(a)$ and/or $f(b) < \delta$.
2. Else bisect the interval $c = (a + b)/2$. Choose new interval
   - $\star$ $[a, c] \equiv [a_1, b_1]$ if $f(c) \star f(a) < 0$
   - $\star$ $[c, b] \equiv [a_1, b_1]$ if $f(c) \star f(b) < 0$.

   Check for $|b_1 - a_1| < \epsilon$ along with $f(a_1 \text{ or } b_1) < \delta$.
3. If not, keep on bisecting the interval and re-adjusting the interval till $|b_n - a_n| < \epsilon$ along with $f(a_n \text{ or } b_n) < \delta$ are satisfied.
4. Bisecting n times, we have a possible solution in the interval length

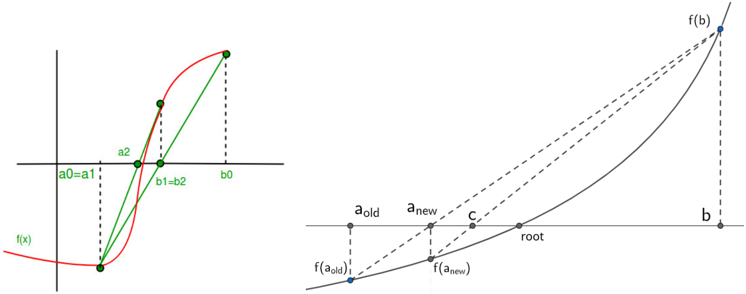
$$\frac{|b_n - a_n|}{2} = \frac{|b - a|}{2^n} \leq \epsilon$$



Regula falsi method

Interpolation to converge on a root faster than Bisection –

Find slope of the straight line joining $[a_0, b_0]$ that has bracketed the root. The point c_0 where this straight line crosses $x - axis$ is the new a or b depending on sign of $f(c_0)$.



Unlike Bisection, new interval boundary a_n or b_n directly given by $f(x)$.

Always converges and has improved speed of convergence. Here too, as (a, b) get close, can lose significant digits.

Steps involve in Regula falsi :

1. Choose bracket $[a_0, b_0]$, where $a_0 < b_0$ and $f(a) * f(b) < 0$. If $|b_0 - a_0| < \epsilon$, done! Check also $f(a_0)$ and/or $f(b_0) < \delta$.
2. Calculate slope of the line joining $f(a_0)$ and $f(b_0)$ and obtain c_0 where the line crosses abscissa $y(c_0) = 0$,

$$m = \frac{f(b_0) - f(a_0)}{b_0 - a_0} = \frac{f(b_0) - f(c_0)}{b_0 - c_0} \Rightarrow c_0 = b_0 - \frac{(b_0 - a_0) * f(b_0)}{f(b_0) - f(a_0)}$$

   Reference point can as well be $f(a_0)$. If $f(x)$ is convex or concave, then one of the points a, b is fixed and the other varies with iterations. After n-th step,

$$c_n = b_n - \frac{(b_n - a_n) * f(b_n)}{f(b_n) - f(a_n)}$$

3. If $f(a_n) * f(c_n) < 0$, then root lies to left of $c_n \Rightarrow b_{n+1} = c_n$ and $a_{n+1} = a_n$. If $|c_{n-1} - c_n| < \epsilon$ then c_n is the root $f(c_n) \approx 0$.
4. If $f(b_n) * f(c_n) < 0$, then root lies to right of $c_n \Rightarrow a_{n+1} = c_n$ and $b_{n+1} = b_n$. If $|c_{n-1} - c_n| < \epsilon$ then c_n is the root $f(c_n) \approx 0$.

Fixed Point method

Finding root of $f(x)$ amounts to finding x_0 where $f(x_0) = 0$.

⋆ Fixed point of a function $g(x)$ is $x = g(x)$.

In fixed point method, $f(x) = 0$ is replaced by $x = g(x)$.

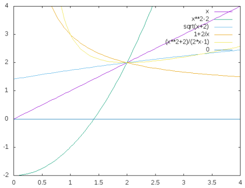
⋆ If x_n is a fixed point of $g(x)$, then x_n is a root of $f(x)$.

The iteration scheme is, starting from initial guess x_1, then $x_2, x_3, \ldots$

$$x_{n+1} = g(x_n) \quad \Rightarrow \quad x_{n+1} \approx g(x_n) \quad \textit{i.e.} \quad |x_{n+1} - x_n| < \epsilon$$

For a given $f(x) = 0$, there can be many equivalent fixed point problems with different choices for $g(x)$. For example,

$$f(x) = x^2 - x - 2 = 0 \;\; \Rightarrow \; x = g(x) = x^2 - 2, \; \sqrt{x+2}, \; 1 + \frac{2}{x}, \; \frac{x^2+2}{2x-1}, \; \ldots$$



Not all choices converge equally! Choices may introduce unwanted singularities!! Solution is not guaranteed!!!

Newton-Raphson method

Involves both $f(x)$ and $f'(x)$ but does not require bracketing. Method is based on Taylor's expansion.

Works for multivariate functions. Converges quadratically $\Rightarrow$ near root the number of significant digits approximately doubles with each step.

To solve $f(x) = 0$, Taylor expand $f(x)$ around initial guess x_0,

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{1}{2!}(x - x_0)^2 f''(x_0) + \cdots$$

If closer to root $(x - x_0)^2 \approx 0$, we stop at $f'(x)$ term,

$$f(x) = f(x_0) + (x - x_0)f'(x_0) = 0 \;\Rightarrow\; x = x_0 - \frac{f(x_0)}{f'(x_0)}$$

then x is better approximation of root than x_0 but involves taking derivative. Useful if derivative is cheaper to evaluate and hence to code.

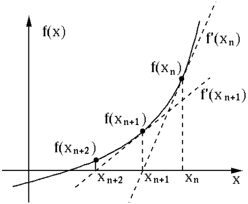
Approximation to the root can be improved iteratively to move from the x_0 towards the root,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n = 1, 2, \ldots$$

Alternatively, use finite difference to approximate derivative – a variant of Newton's method called Secant method,

$$f'(x) \approx \frac{1}{2h}\Big[f(x+h) - f(x-h)\Big] + \mathcal{O}(h^3)$$

Finite difference requires two initial guesses x_0, x_1 corresponding to $x \pm h$.



The steps of Newton-Raphson method are

1. Make a good guess of x_0.
2. Evaluate $f(x)$ and $f'(x)$ at $x = x_0$.
3. Use iterative updating $x_n \to x_{n+1}$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n = 1, 2, \ldots$$

4. Continue to improve the estimate of the root until $|x_{n+1} - x_n| < \epsilon$ and/or $f(x_n) \approx \delta$.

Multivariable system

Both Fixed point and Newton-Raphson can be employed for solving multivariable nonlinear system of equations.

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} f_1(x_1, x_2, \ldots, x_n) \\ f_2(x_1, x_2, \ldots, x_n) \\ \vdots \\ f_n(x_1, x_2, \ldots, x_n) \end{pmatrix} = 0 \quad \text{where} \quad \boldsymbol{x}^T = (x_1, x_2, \ldots, x_n)$$

No concept of bracketing in higher dimension $\Rightarrow$ guaranteed converging methods like Bisection does not exist!

The fixed point functions $\boldsymbol{g}(\boldsymbol{x})$ can be written as

$$\left.\begin{array}{lcl} x_1 & = & g_1(x_1, x_2, \ldots, x_n) \\ x_2 & = & g_2(x_1, x_2, \ldots, x_n) \\ \vdots & & \\ x_n & = & g_n(x_1, x_2, \ldots, x_n) \end{array}\right\} \quad \Rightarrow \quad \boldsymbol{x} = \boldsymbol{g}(\boldsymbol{x}) \quad \Rightarrow \quad \boldsymbol{x}_{k+1} = \boldsymbol{g}(\boldsymbol{x}_k)$$

The stopping criteria would be,

$$\frac{||\boldsymbol{x}_{k+1} - \boldsymbol{x}_k||}{||\boldsymbol{x}_{k+1}||} < \epsilon \quad \text{where,} \quad ||x_k||^2 = (x_1)_k^2 + (x_2)_k^2 + \cdots (x_n)_k^2$$

For example, try solving the following

$$x_1^2 + x_1 x_2 = 10 \quad \text{and} \quad x_2 + 3x_1 x_2^2 = 57$$

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \boldsymbol{g}(\boldsymbol{x}) = \begin{pmatrix} g_1(x_1, x_2) \\ g_2(x_1, x_2) \end{pmatrix} = \begin{pmatrix} \frac{10 - x_1^2}{x_2} \\ 57 - 3x_1 x_2^2 \end{pmatrix}$$

Using an initial guess of $x_1 = 1.5$, $x_2 = 3.5$ yields divergence!

$$x_1 = \frac{10 - (1.5)^2}{3.5} = 2.21429, \; x_2 = 57 - 3(2.21429)(3.5)^2 = -24.37516$$

$$x_1 = \frac{10 - (2.21429)^2}{-24.37516} = -0.20910, \; x_2 = 57 - 3(-0.20910)(-24.37516)^2 = 429.709$$

Continuing the iteration shows it is diverging in x_2. A different choice of $\boldsymbol{g}(\boldsymbol{x})$ works rather well,

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \sqrt{(10 - x_1 x_2} \\ \sqrt{(57 - x_2)/3x_1} \end{pmatrix}$$

x_1	x_2	x_1'	x_2'	ϵ
1.5000	3.5000	2.1794	2.8605	0.259459
2.1794	2.8605	1.9405	3.0496	0.084286
1.9405	3.0496	2.0205	2.9834	0.028792
⋮				
1.9999	3.0001	2.0000	3.0000	0.000046

Taylor expansion in Newton-Raphson for multivariable function, say $f_1(x_1, x_2, \ldots, x_n)$ of $\boldsymbol{f}(\boldsymbol{x})$ in terms of solutions after i-th iteration

$$f_1\left(x_1^{(i+1)}, x_2^{(i+1)}, \ldots, x_n^{(i+1)}\right) \approx f_1\left(x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)}\right) + \left.\frac{\partial f_1}{\partial x_1}\right|_{x^{(i)}} \left(x_1^{(i+1)} - x_1^{(i)}\right) + \left.\frac{\partial f_1}{\partial x_2}\right|_{x^{(i)}} \left(x_2^{(i+1)} - x_2^{(i)}\right) + \cdots + \left.\frac{\partial f_1}{\partial x_n}\right|_{x^{(i)}} \left(x_n^{(i+1)} - x_n^{(i)}\right)$$

Similar Taylor expansion for $f_2,\ f_3, \ldots, f_n$ yields,

$$\boldsymbol{f}(\boldsymbol{x}^{(i+1)}) = \boldsymbol{f}(\boldsymbol{x}^{(i)}) + \boldsymbol{J}(\boldsymbol{x}^{(i)}) \left(\boldsymbol{x}^{(i+1)} - \boldsymbol{x}^{(i)}\right) = 0 \quad \Rightarrow \quad \boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} - \boldsymbol{J}^{-1}(\boldsymbol{x}^{(i)})\boldsymbol{f}(\boldsymbol{x}^{(i)})$$

where $\boldsymbol{J}(\boldsymbol{x}^{(i)})$ is the Jacobian matrix

$$\left[\boldsymbol{J}(\boldsymbol{x}^{(i)})\right]_{pq} = \left.\frac{\partial f_p(\boldsymbol{x})}{\partial x_q}\right|_{\boldsymbol{x}^{(i)}} = \begin{bmatrix} \frac{\partial f_1(\boldsymbol{x}^{(i)})}{\partial x_1} & \frac{\partial f_1(\boldsymbol{x}^{(i)})}{\partial x_2} & \cdots & \frac{f_1(\boldsymbol{x}^{(i)})}{\partial x_n} \\ & & \vdots & \\ \frac{\partial f_n(\boldsymbol{x}^{(i)})}{\partial x_1} & \frac{\partial f_n(\boldsymbol{x}^{(i)})}{\partial x_2} & \cdots & \frac{f_n(\boldsymbol{x}^{(i)})}{\partial x_n} \end{bmatrix}$$

Compare multivariable and single-variable Newton-Raphson,

$$x^{(i+1)} = x^{(i)} - \left(f'(x^{(i)})\right)^{-1} f(x^{(i)}) \ \text{ and } \boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} - \boldsymbol{J}^{-1}(\boldsymbol{x}^{(i)})\, \boldsymbol{f}(\boldsymbol{x}^{(i)})$$

Consider the previous example

$$\left.\begin{array}{rcl} x_1^2 + x_1x_2 - 10 & = & 0 \\ x_2 + 3x_1x_2^2 - 57 & = & 0 \end{array}\right\} \; \boldsymbol{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 + x_2 & x_1 \\ 3x_2^2 & 1 + 6x_1x_2 \end{bmatrix}$$

For initial guess, say $x_1^{(0)} = 1,\ x_2^{(0)} = 1$,

$$\boldsymbol{f}(\boldsymbol{x}^{(0)}) = \begin{pmatrix} f_1(x_1^{(0)}, x_2^{(0)}) \\ f_2(x_1^{(0)}, x_2^{(0)}) \end{pmatrix} = \begin{pmatrix} -8 \\ -53 \end{pmatrix} \;\Rightarrow\; \boldsymbol{J} = \begin{bmatrix} 3 & 1 \\ 3 & 7 \end{bmatrix} \rightarrow \boldsymbol{J}^{-1} = \frac{1}{18}\begin{bmatrix} 7 & -1 \\ -3 & 3 \end{bmatrix}$$

Hence the solution after first iteration is,

$$\begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{1}{18}\begin{bmatrix} 7 & -1 \\ -3 & 3 \end{bmatrix}\begin{pmatrix} -8 \\ -53 \end{pmatrix} = \begin{pmatrix} 1.1667 \\ 8.5000 \end{pmatrix}$$

n	x_1	x_2
1	1.1667	8.5000
2	1.5670	3.6878
3	2.0108	2.8824
4	1.9992	3.0023
5	2.0000	3.0000

Converges quadratically but cost of computing Jacobian is N^2 for function evaluations and N^3 for solving linear equations.

Laguerre's method

A polynomial of degree n has exactly n roots α_i $(i = 1, 2, \ldots, n)$

$$P(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_n x^n = (x - \alpha_1)(x - \alpha_2) \cdots (x - \alpha_n)$$

Polynomials with real a_i, roots can be real or complex conjugate pair. We will restrict ourselves to only real roots.

A two step method –
(i) Laguerre's method followed by *(ii)* deflating the polynomial.

Using Laguerre's method determine the root α_1 of $P(x)$, then obtain a reduced polynomial $Q(x)$ of degree one less than $P(x)$.

$$\begin{aligned} P(x) &= (x - \alpha_1)\, Q(x) \\ Q(x) &= (x - \alpha_2)\, R(x) \quad \Rightarrow \quad P(x) = (x - \alpha_1)(x - \alpha_2)\, R(x) \ \text{ etc.} \end{aligned}$$

where the roots of $Q(x)$ are the remaining roots of $P(x)$. In each of n steps, the Laguerre determines the roots α_i while deflation determines the remainder polynomial.

Method used for deflation is synthetic division method (learnt in class IX).

Laguerre algorithm proceeds as

1. Begin with an initial guess β_0.
2. If β_0 is bang on one of the roots, *i.e.* $P(\beta_0) \approx 0$, go for deflation.
3. Else calculate the following

$$G = \frac{P'(\beta_k)}{P(\beta_k)}, \quad H = G^2 - \frac{P''(\beta_k)}{P(\beta_k)}$$
$$\Rightarrow \quad a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}}$$

   Choose the sign in the denominator of a such as to give the denominator the larger absolute value.

4. Set $\beta_{k+1} = \beta_k - a$ as new trial.
5. Iterate till $|\beta_{k+1} - \beta_k| < \epsilon$ and set $\alpha_1 = \beta_k$. Check $P(\alpha_1) \approx 0$.
6. Go for deflation to reduce the degree of the polynomial and do the above iteration all over again to find α_2 and so on.

Next deflation : divide $P(x)$ by $(x - \alpha_1)$ to get $Q(x)$

$$\frac{P(x)}{x - \alpha_1} = Q(x), \quad \text{followed by} \quad \frac{Q(x)}{x - \alpha_2} = R(x) \; etc.$$

Deflation by Synthetic division method :

★ Arrange terms in $P(x)$, the dividend, in descending order of power, 0 (zero) for missing power. Consider polynomial $-x^3 + 3x^2 - 4$

$$\frac{P(x)}{x - \alpha_1} = \frac{-x^3 + 3x^2 - 4}{x - 2} \Rightarrow \text{divisor} = 2, \ \text{coeffs} = [-1,\, 3,\, 0,\, -4]$$

★ Write the divisor and coefficients in the manner given below. Bring down the first or leading coefficient *i.e.* -1 below the horizontal line.

★ Multiply the coefficient of leading power -1 with the divisor $2 \times -1 = -2$ and add it to the coefficient of the next lower power $3 + (-2) = 1$ and bring it down below the horizontal line again.

★ Multiply it again with divisor and continue this process till the end.

$$\begin{array}{c|cccc} & -1 & 3 & 0 & -4 \\ 2 & + & -2 & 2 & 4 \\ \hline & -1 & 1 & 2 & 0 \end{array}$$

★ If $\alpha_1 = 2$ is a root then the last sum *i.e.* the last entry below the horizontal line, which gives the remainder, must be zero.

★ The reduced lower degree polynomial $Q(x)$ has the numbers below the horizontal line as its coefficients

$$\frac{P(x)}{x-\alpha_1} = \frac{-x^3+3x^2-4}{x-2} = -x^2+x+2 = Q(x)$$

★ Repeat the above process with $Q(x)$ and keep doing for successive roots till you get the final monomial $(x-\alpha_n)$.

$$\begin{array}{c|ccc} & -1 & 1 & 2 \\ 2 & + & -2 & -2 \\ \hline & -1 & -1 & 0 \end{array} \quad \Rightarrow \quad R(x) = -x-1$$

The polynomial in the example is thus factorized in terms of its roots as

$$P(x) = -x^3+3x^2-4 = (x-2)(x-2)(-x-1)$$

Find all the roots of the following polynomial

$$P(x) = 6x^3-11x^2-26x+15 \quad \text{answer}: \quad x = 3, -5/3, 1/2$$
$$P(x) = x^4-x^3-7x^2+x+6 \quad \text{answer}: \quad x = 1, -2, 3, -1$$