Chapter 1. Computer Solution of Nonlinear Equations

Numerical methods

Finding the roots of the equation f(x)=0 by numerical method

Two basic methods for finding the roots (zeros of a constraint),

- 1. The Bisection method (Closed or Bracketing method) and
- 2. The Newton-Raphson method (Open method).

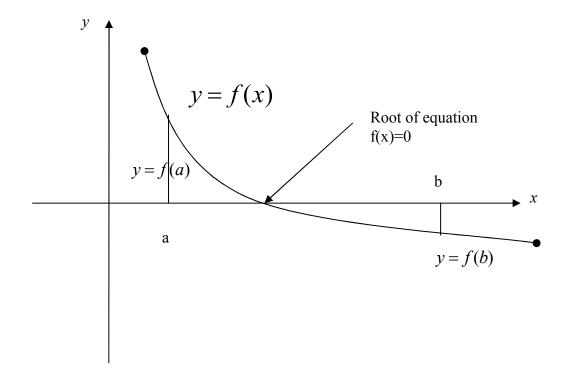
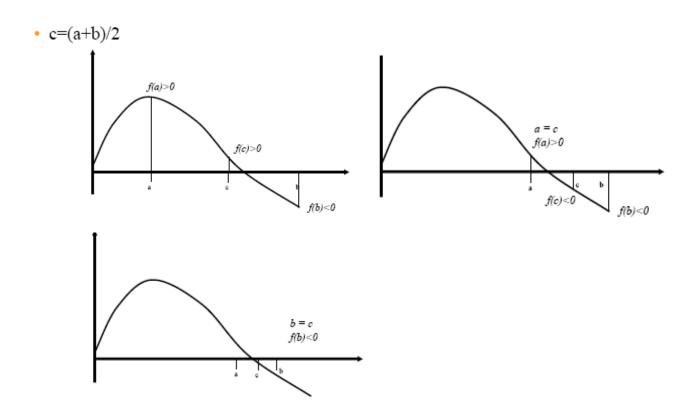


Fig. 1 Numerical method (Bisection method) in finding a root

1. Bracketing Method

HALF-INTERVAL SEARCH (binary search method or bisection method)

If f(a)*f(b)<0, then there is at least one real root between a and b. Using bisection method, the solution is c=(a+b)/2, and slowly converges to the root.



Let us solve the transcendental equation:

$$e^{-x} - \sin(\pi x/2) = 0$$

or
 $f(x) = e^{-x} - \sin(\pi x/2) = 0$

This equation has a single solution between 0 and 1. Using the bisection method, we should find f(x) at 0.5 and determine whether the root is between 0 - 0.5 or 0.5 -1.

By computing f(x) at the midpoint of the known interval x=c, the root can be found to within desired accuracy ε , said 0.01.

Iteration I	С	f(c)
1	0.5	-0.100576
2	0.25	0.396117
3	0.375	0.131719
4	0.4375	0.011255
5	0.46875	-0.04577495
6	0.45125	-0.0175341
7	0.4453125	-0.0032075

This method starts with a search interval [a,b] over which the function to be solved changes sign, or f(a)*f(b)<0, and continues to reduce the interval by $\frac{1}{2}$ until |b-a| is so small that all values of c in |a|< c< b| satisfy $|f(c)|< \varepsilon$.

Procedures:

Check if the mid point c = (a+b)/2 is close enough to satisfy $|f(c)| < \varepsilon$, if yes c is the solution,

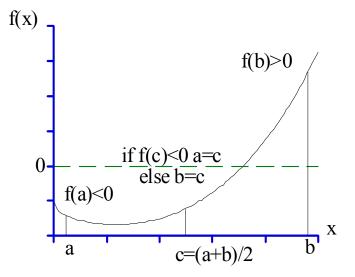
if not

set
$$a=c$$
 if $f(c)*f(a)>0$ else $b=c$.

Now the search interval is reduced by $\frac{1}{2}$, and the process can start again until the interval is so small that f(c) must be less than the tolerance ε .

Given an ε =0.01, we can be sure that no more than 7 iterations will

be needed for a root between [a,b].



Summary of Bisection Method Algorithms

Step 1: Choose lower **a** and upper **b** guesses for the root such that the function changes sign over the interval. f(a)f(b)<0.

Step 2: An estimate of the root c where c=(a+b)/2.

Step 3: Determine which interval the root lies by:

- (i) if f(a)f(c)<0, the root lies in the lower interval, set b=c.
- (ii) if f(a)f(c)>0, the root lies in the upper interval, set a=c.
- (iii) if f(a)f(c)=0, the root equal to c, terminate the computation.

Termination criteria

At the beginning of computation, the initial guess for the root is *a*. At the first iteration:

$$x_1^{new} - x_1^{old} = \frac{b-a}{2}$$

$$x_1^{new} = \frac{a+b}{2}$$

At the r-th iteration, a and b are changed. The above relations still apply.

Define the approximate percentage relative error

at the r - th iteration

$$\varepsilon_a = \left| \frac{x_r^{new} - x_r^{old}}{x_r^{new}} \right| \times 100\%$$

 ε_a tends to zero when iteration r increases and can be used as termination criteria. For example, if $\varepsilon_a < \varepsilon_s$, the tolerance of error (said 0.01), stop the computation. Otherwise repeat the process.

Example 1:

$$f(x) = 5x^3 - 5x^2 + 6x - 2 = 0$$
. Find the root between $(0, 1)$

Solution:

1st iteration:

Present new root is $c = \frac{a+b}{2} = \frac{0+1}{2} = 0.5$

$$\varepsilon_a = \left| \frac{b-a}{b+a} \right| \times 100\% = \left| \frac{1-0}{1+0} \right| \times 100\% = 100\%$$

$$f(a)f(c) = f(0)f(0.5) = -2(0.375) = -0.75$$

Therefore, the new bracket is a = 0 and b = 0.5.

The process can be repeated until the approximate relative error falls below 10% and after 5 iterations yielding a root estimate of 0.40625.

iteration	а	b	C (root)	f(a)	f(c)	f(a)×f(c)	€a
1	0	1	0.5	-2	0.375	-0.75	
2	0	0.5	0.25	-2	-0.73438	1.46875	100.00%
3	0.25	0.5	0.375	-0.73438	-0.18945	0.13913	33.33%
4	0.375	0.5	0.4375	-0.18945	0.08667	-0.01642	14.29%
5	0.375	0.4375	0.40625	-0.18945	-0.05246	0.009939	7.69%

2. Newton-Raphson Method (Open Method)

Revision on Taylor's Expansion

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''}{3!}(x-a)^3 + \cdots + \frac{f'''}{m!}(x-a)^m$$

Taylor expansion on $f(x) = \sin(x)$ about x=0 gives:

$$\sin(x) = \sin(0) + (x - 0)\cos(0) - (x - 0)^{2} \frac{\sin(0)}{2!} + (x - 0)^{3} \frac{\cos(0)}{2!} + \dots + \dots$$

$$= x - \frac{x^{3}}{3!} + \frac{x^{5}}{5!} - \frac{x^{7}}{7!} + \dots + \dots$$

Similarly

$$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!} + \frac{x^{4}}{4!} + \dots + \dots$$

and

$$\ln(x+1) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots + \dots$$

Solving an equation f(x)=0

Based on Taylor expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \dots + R$$

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

Hence

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

Usually instead of exact differentiation f'(x), numerical approximation is used.

Therefore
$$f'(x) = \frac{f(x_{i+h}) - f(x_i)}{h}$$

is used to evaluate f'(x).

Graphically the Newton-Raphson method can be described as follows

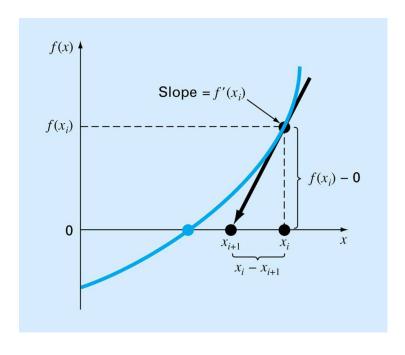


Fig. 2 Numerical method (Newton-Raphson method) in finding a root

If the initial guess x_0 is in the proximity of the root, the search could converge much faster than the bisection method.

Example 2:

Use Newton-Raphson Method to estimate the root of equation

$$f(x) = e^{-x} - x$$

By exact differentiating, we have $f'(x) = -e^{-x} - 1$

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

Starting an initial guess at $x_0=0$, we have $x_i=0.56714329$ after 4 iteration.

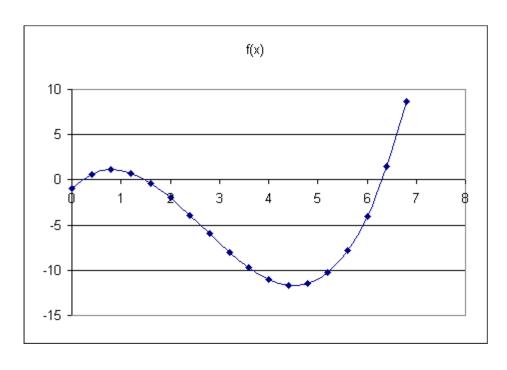
Example 3:

Use Newton-Raphson method to estimate the roots of equation

$$f(x) = -1 + 5.5x - 4x^2 + 0.5x^3$$

a) By graphical solution, 3 real roots at approximately 0.2, 1.5 and 6.3.

X	f(x)		
0	-1		
0.4	0.592		
0.8	1.096		
1.2	0.704		
1.6	-0.392		
2	-2		
2.4	-3.928		
2.8	-5.984		
3.2	-7.976		
3.6	-9.712		
4	-11		
4.4	-11.648		
4.8	-11.464		
5.2	-10.256		
5.6	-7.832		
6	-4		
6.4	1.432		
6.8	8.656		



b) The Newton-Raphson method can be set up as

$$x_{i+1} = x_i - \frac{-1 + 5.5x_i - 4x_i^2 + 0.5x_i^3}{5.5 - 8x_i + 1.5x_i^2}$$

The three roots as summarized in the following tables:

i	Xi	f(x)	f(x)	E a
0	0	-1	5.5	
1	0.181818	-0.12923	4.095041	100.00%
2	0.213375	-0.0037	3.861294	14.789%
3	0.214332	-3.4E-06	3.85425	0.4466%
4	0.214333	-2.8E-12	3.854244	0.000408%

i	Xi	f(x)	f(x)	Ea
0	2	-2	-4.5	
1	1.555556	-0.24143	-3.31481	28.57%
2	1.482723	-0.00903	-3.06408	4.912%
3	1.479775	-1.5E-05	-3.0536	0.199%
4	1.479769	-4.6E-11	-3.05358	0.00034%

i	Χį	f(x)	f(x)	E a
0	6	-4	11.5	
1	6.347826	0.625955	15.15974	5.479%
2	6.306535	0.009379	14.7063	0.6547%
3	6.305898	2.22E-06	14.69934	0.010114%
4	6.305898	1.42E-13	14.69934	0.000002%

Therefore, the roots are 0.214333, 1.479769, and 6.305898.