Roots of Non Linear Equation

Open End Methods:
The real root is within an interval specified as lower and upper limit for the bracketing methods. After that, through iteration the root becomes closer to the root's true value. It is said that these methods converge as they step closer to the truth as the calculation progresses. The open methods, on the other hand, are based on formulas that allow only one or more initial value of x that do not necessarily stop the root. Approximate root moves away or diverges from the true root at times in this situation. Generally they converge faster than bracketing methods when the open process converges.

Difference between Bracketing Methods and Open-end Methods:

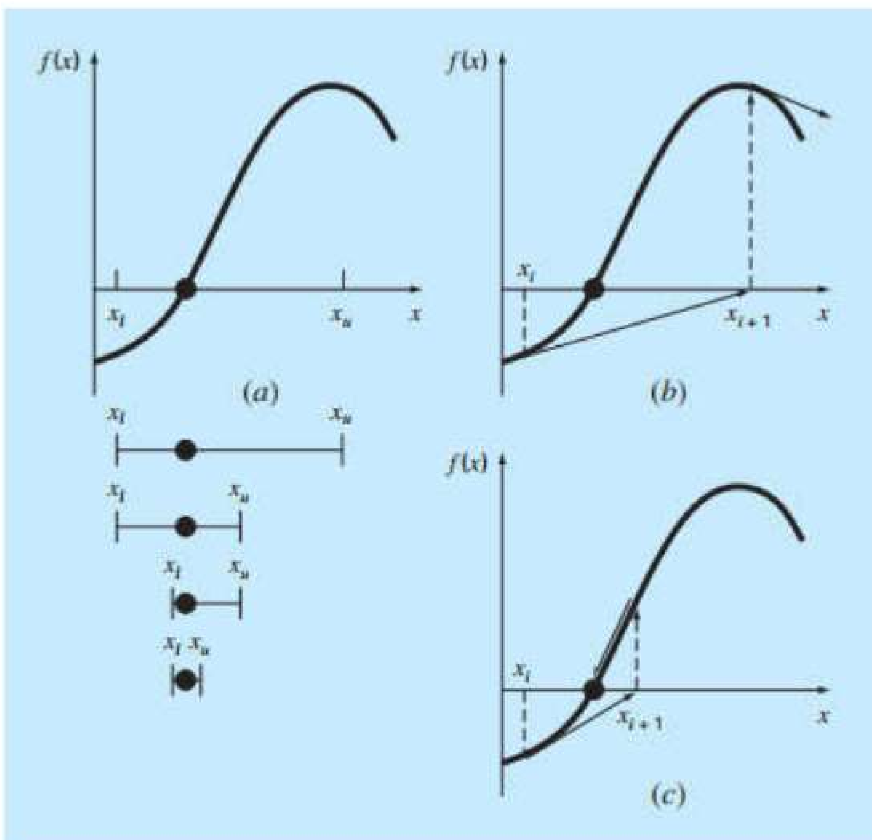

Figure 1: Graphical explanation of difference between Bracketing and Open-end Methods. [2]

- In figure 1 (a) which is bisection methods the real root lies within an interval x_i and x_{i+1} defined as lower and upper limit.
- In open-end methods depicted in figure 1(b) and (c) and projected from x_i to x_{i+1} in a iterative fashion the process may be diverge as in figure 1(b) or converge as in figure 1(c)

Newton-Raphson Method

Perhaps the most widely used of all root-locating formulas is the Newton-Raphson equation (Figure 2below). If the initial guess at the root is x_i, a tangent can be extended from the point [x_i, $f(xi)$]. The point where this tangent crosses the x axis usually represents an improved estimate of the root.

Graphical Representation:

Consider a graph f(x) as shown in the figure below. Let us assume that x1 is an approximate root of f(x) = 0. Draw a tangent at the curve f(x) at x = x1 as shown in the figure.

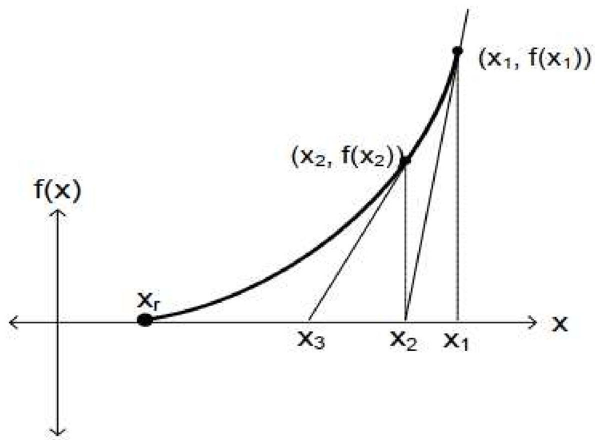

Figure 2: Newton Raphson Methods [1]

The point of intersection of this tangent with the x-axis gives the second approximation to the root. Let, the point of intersection be x2. The slope of the tangent is given by:

$$\tan(\alpha) = \frac{f(x_1)}{x_1 - x_2} = f'(x_1)$$

Where; $f'(x_1)$) is the slope of f(x) at x = x1.
Solving for x2, we get:

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

This is called Newton Raphson Formula for first iteration. Then the next approximation will be:

$$x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}$$

In general;

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

Derivation of Newton Raphson Formula by Taylor's Series Expansion:
Assume that: x_n is an estimate root of the function $f(x) = 0$ and consider a small interval 'h' such that:

$$h = x_{n+1} - x_n$$

Using Taylor's Series Expansion for $f(x_{n+1})$, we have:
$f(x_{n+1}) = f(x_n) + h f'(x_n) + h^2/2!\ f''(x_n) + \ldots.. = 0$

Neglecting the second and higher order derivatives, we have
$f(x_{n+1}) = f(x_n) + h f'(x_n) = 0;$
If x_{n+1} is the root of f(x), then: $f(x_{n+1}) = 0$
$0 = f(x_n) + h f'(x_n)$

which gives
$h = -f(x_n) / f'(x_n)$
$x_{n+1} - x_n = -f(x_n) / f'(x_n)$;
$x_{n+1} = x_n - f(x_n) / f'(x_n)$; ………………………………………………..(1)

Equation (1) is called Newton Raphson Method

The process will be continued till the absolute difference between two successive approximations is less than the specified error E i,e, $| x_{n+1} - x_n | < E$.

Algorithm: Newton-Raphson Method
1. Assign an initial value for x, say x_0 and stopping criterion E.
2. Compute $f(x_0)$ and $f'(x_0)$.
3. Find the improved estimate of x_0
   $x_1 = x_0 - f(x_0) / f'(x_0)$
4. Check for accuracy of the latest estimate.
   If $| (x_1 - x_0)/x_1 | < E$ then stop; otherwise continue.
5. Replace x_0 by x_1 and repeat steps 3 and 4.

- Newton-Raphson method is said to have *quadratic convergence*.

Example: Find the root of the equation $f(x) = x^2 - 3x + 2$ using Newton-Raphson method.
Solution: Here, $f'(x) = 2x - 3$
Let $x_1 = 0$ (First approximation)
$x_2 = x_1 - f(x_1) / f'(x_1) = 0 - 2 / (-3) = 2/3 = 0.6667$
Similarly,
$x_3 = 0.6667 - 0.4444/-1.6667 = 0.9333$
$x_4 = 0.9333 - 0.071/-1.334= 0.9959$
$x_5 = 0.6667 - 0.0041/-1.0082 = 0.9999$
$x_6 = 0.6667 - 0.0001/-1.0002 = 1.0000$
Since $f(1.0) = 0$, The root closer to the point x = 0 is 1.0000.

Convergence of Newton Raphson Method:
Let x_n be the estimate to the root of the function $f(x) = 0$. If x_n and x_{n+1} are close to each other, then using Taylor's Series Expansion:

$$f(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n) + f''(x_n)\frac{(x_{n+1} - x_n)^2}{2} \text{ …………(2)}$$

Let us assume that, the exact root of f(x) be x_r, then: $x_{n+1} = x_r$, then: $f(x_{n+1})=0$. So, equation (2) becomes:

$$0 = f(x_n) + f'(x_n)(x_r - x_n) + f''(x_n)\frac{(x_r - x_n)^2}{2} \text{…………..(3)}$$

As we have:

$x_{n+1} = x_n - f(x_n) / f'(x_n)$
$\Rightarrow f(x_n) = (x_{n+1} - x_n) f'(x_n)$

Putting the value of $f(x_n)$into equation (3), we get:

$$0 = (x_{n+1} - x_n) f'(x_n) + f'(x_n)(x_r - x_n) + f''(x_n)\frac{(x_r - x_n)^2}{2}$$

$$0 = f'(x_n)(x_r - x_{n+1}) + f''(x_n)\frac{(x_r - x_n)^2}{2} \text{……………………(4)}$$

We know that, the error in the estimate x_{n+1} is:

$$e_{n+1} = x_r - x_{n+1}$$

Similarly,

$$e_n = x_r - x_n$$

Now, neglecting the higher power terms and expressing equation (iii) in terms of error:

$$0 = f'(x_n)e_{n+1} + f''(x_n)\frac{(e_n)^2}{2}$$

Rearranging the term, we get:

$$e_{n+1} = -\frac{f''(x_n)}{2f'(x_n)}(e_n)^2$$

This shows that error is roughly proportional to the square of the error at previous iteration. Therefore, Newton Raphson method has quadratic convergence.

Limitations of Newton-Raphson method
The Newton-Raphson method has certain limitations and pitfalls. The method will fail in the following situations.

1. Division by zero may occur if $f'(x_i)$ is zero or very close to zero.
2. If the initial guess is too far away from the required root, the process may converge to some other root.
3. A particular value in the iteration sequence may repeat, resulting in an infinite loop. This occurs when the tangent to the curve f (x) at $x = x_{i+1}$ cuts the x-axis again at $x = x_i$.

Class Problem:
Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0= 0$.

Secant method

The calculation of the derivative is a potential problem in applying the Newton-Raphson process. While for polynomials and many other functions this is not inconvenient, there are certain functions whose derivatives can be extremely difficult or inconvenient to evaluate. For these cases, a backward finite divided difference will approximate the derivative.

Secant method uses two initial estimates, but they don't need to bracket the root. As shown in the figure 3 below, it can use two points x_1 and x_2 as starting values, although they do not support the root.

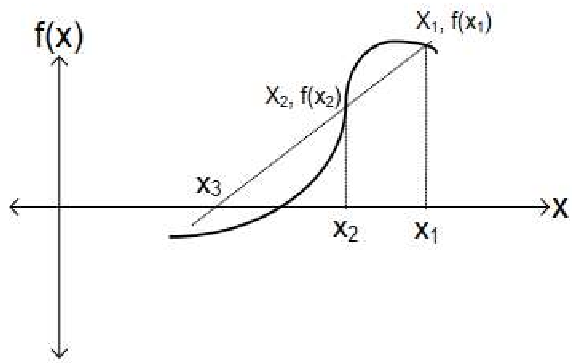

Figure 3: Secant Method [1]

Let us consider two points x_1 and x_2 in Figure above as starting values. Slope of the secant line passing through x_1 and x_2 is given by,

$$\frac{f(x_1)}{x_1 - x_3} = \frac{f(x_2)}{x_2 - x_3}$$

$$f(x_1)(x_2 - x_3) = f(x_2)(x_1 - x_3)$$

$$x_3[f(x_2) - f(x_1)] = f(x_2).x_1 - f(x_1).x_2$$

$$\therefore x_3 = \frac{f(x_2).x_1 - f(x_1).x_2}{f(x_2) - f(x_1)}$$

By adding and subtracting $f(x_2)\, x_2$ to the numerator and remaining the terms we have,

$$x_3 = x_2 - \frac{f(x_2)(x_2 - x_1)}{f(x_2) - f(x_1)}$$

which is called the *secant formula*.

The approximate value of the root can be refined by repeating this procedure by replacing $x_1$and x_2 by x_2 and x_3, respectively. That is, the next approximate value is given by,

$$x_4 = x_3 - \frac{f(x_3)(x_3 - x_2)}{f(x_3) - f(x_2)};$$

Where,

$using\ back\ ward\ divide\ difference\ formula\ 1st\ derivatives\ of\ f'(x_3)$

$$f'(x_3) = \frac{f(x_3) - f(x_2)}{(x_3 - x_2)}$$

This procedure is continued till the desired level of accuracy is obtained.
We can express the Secant formula as follows:

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

Difference between Method of False Position and Secant Method:

The formula for the method of false position and the method of secant is similar and both use two initial estimates. Nonetheless, there is a significant difference in their implementation algorithms. The last approximation substitutes one of the end points of the interval in the false position method so that the root is bracketed by new interval. Nevertheless, the values are prefaced in strict sequence in secant system, i.e. x_{i-1} is replaced by xi and xi by x_{i+1}. The root may not be blocked by the points.

Algorithm: **Secant Method**

1. Decide two initial points x_1 and x_2 and required accuracy level E.
2. Compute $f_1 = f(x_1)$ and $f_2 = f(x_2)$
3. Compute $x_3 = (f_2 x_1 - f_1 x_2) / (f_2 - f_1)$
4. If $|(x_3 - x_2)/ x_3| > E$, then
   set $x_1 = x_2$ and $f_1 = f_2$
   set $x_2 = x_3$ and $f_2 = f(x_3)$
   go to step 3

   Else
   set root $= x_3$
   print results
5. Stop.

Comparison between the secant formula and the Newton-Raphson formula for estimating a root

Newton-Raphson formula: $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$

Secant formula: $x_{n+1} = x_n - \dfrac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$

This shows that the derivative of the function in the Newton formula $f'(x_n)$, has been replaced by the term $\dfrac{f(x_n) - f(x_{n-1})}{(x_n - x_{n-1})}$ in the secant formula.

This is a major advantage because there is no need for the evaluation of derivatives. There are many functions whose derivatives may be extremely difficult to evaluate.
However, one drawback of the secant formula is that the previous two iterates are required for estimating the new one. Another drawback of the secant method is its slower rate of convergence. It is proved that the rate of convergence of secant method is 1.618 while that of the Newton method is 2.

- The convergence of secant method is referred as *super linear convergence.*

Example: Use the secant method to estimate the root of the equation $f(x) = x^2 - 4x - 10 = 0$ with the initial estimates of $x_1 = 4$ and $x_2 = 2$.
Solution: Given $x_1 = 4$ and $x_2 = 2$ and E = 0.05

$f(x_1) = f(4) = -10 \qquad f(x_2) = f(2) = -14$
$x_3 = x_2 - ((f(x_2) * (x_2 - x_1)) / (f(x_2) - f(x_1)))$
$= 2 - (-14) * (2 - 4)/((-14) - (-10))$
$= 9$

For second iteration,
$x_1 = x_2 = 2 \qquad x_2 = x_3 = 9$
$f(x_1) = f(2) = -14$
$f(x_2) = f(9) = 95$
$x_3 = 9 - 35 * (9 - 2) / (35 + 14) = 4$

For third iteration,
$x_1 = x_2 = 9 \qquad x_2 = x_3 = 4$
$f(x_1) = f(9) = 95$
$f(x_2) = f(4) = -10$
$x_3 = 4 - (-10) * (4 - 9) / ((-10) - (-35)) = 5.1111$

For fourth iteration,
$x_1 = x_2 = 4 \qquad x_2 = x_3 = 5.1111$
$f(x_1) = f(4) = -10$
$f(x_2) = f(5.1111) = - 4.3207$
$x_3 = 5.1111 - (-4.3207) * (5.1111 - 4) / ((- 4.3207) - (-10)) = 5.9563$

For fifth iteration,
$x_1 = x_2 = 5.1111 \qquad x_2 = x_3 = 5.9563$
$f(x_1) = f(5.1111) = - 4.3207$
$f(x_2) = f(5.9563) = 5.0331$
$x_3 = 5.9563 - 5.0331 * (5.9563 - 5.1111)/(5.0331 + 4.3207) = 5.5014$

For sixth iteration,
$x_1 = x_2 = 5.9563 \qquad x_2 = x_3 = 5.5014$
$f(x_1) = f(5.9563) = 5.0331$
$f(x_2) = f(5.5014) = -1.7392$
$x_3 = 5.5014 - (-1.7392) * (5.5014 - 5.9563) / (-1.7392 - 5.0331) = 5.6182$

Hence, the root is: 5.6182, which is less than EPS = 0.05.

Fixed Point method

It is also known as, direct substitution method or method of fixed point iteration or method of successive approximation. It is applicable if the equation $f(x) = 0$ can be expressed in terms of $x = g(x)$. If x_0 is the initial approximation to the root, then the next approximation will be: $x_1 = g(x_0)$ and the next again will be: $x_2 = g(x_1)$ and so on. In general:

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

Where, $x = g(x)$ is known as fixed point equation.
To find the root of the equation $f(x) = 0$, we rewrite this equation in this way $x = g(x)$
Let x_0 be an approximate value of the desire root. Substituting it for x as the right side of the equation, we obtain the first approximation $x_1 = g(x_0)$. Further approximation is given by

$x_2 = g(x_1)$.
This iteration process can be expressed in general form as

$$x_{i+1} = g(x_i) \qquad i = 0,1,2, \ldots..$$

which is called the *fixed point iteration formula*. The iteration process would be terminated when two successive approximations agree within some specified error.

- This method of solution is also known as the *method of successive approximations* or *method of direct substitution*.

Algorithm:

1. Read an initial guess: x_0 and E
2. Evaluate: $x_1 = g(x_0)$
3. Check for error: if $|x_1-x_0/x_1| < E$, x_1 is root, else continue.
4. Assign the value of x_1 to x_0, i.e. $x_0 = x_1$ and repeat steps 2 & 3.
5. Print x_1.
6. Stop

Example: Locate the root of the equation $f(x) = x^2 + x - 2 = 0$.
Solution: The given equation can be expressed as $x = 2 - x^2$.
Let us start with an initial value of $x_0 = 0$.

$x_1 = 2 - 0 = 2$
$x_2 = 2 - 4 = -2$
$x_3 = 2 - 4 = -2$

Since $x_3 - x_2 = 0$, -2 is one of the roots of the equation.

- The iteration function $g(x)$ can be formulated in different forms. But, not all forms result in convergence of solution. Convergence of the iteration process depends on the nature of g (x). The necessary condition for convergence is *$g'(x) < 1$*.

Convergence of Fixed Point Iteration:

$$x_{i+1} = g(x_i)\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4$$

Let x_f be a root of equation. Then,

$$x_f = g(x_f)\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Now, subtracting equation 5 with equation 4 and we get,

$$x_f - x_{i+1} = g\left(x_f\right) - g(x_i) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(6)$$

According to the mean value theorem there is at least one point between x_f *and* x_i, which is x =R and

$$g'(R) = \frac{g(x_f) - g(x_i)}{x_f - x_i}$$

$$\Rightarrow\ g(x_f) - g(x_i) = g'(R)x_f - x_i$$

$$error\ in\ ith\ iteration, e_i = x_f - x_i$$

$$error\ in\ i+1th\ iteration, e_{i+1} = x_f - x_{i+1}$$

$$so, e_{i+1} = g'(R)e_i\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

So, error will decrease with each iteration only if $g'(R) < 1$and the error is roughly proportional to error in previous step therefore fixed point is said to be early convergent.

Example: Evaluate the square root of 5 using the equation $x^2 - 5 = 0$ by applying the fixed-point method.
Solution: Let us organize the function as follows: $x = 5/x$ and assume $x_0 = 1$, Then

$x_1 = 5$
$x_2 = 1$
$x_3 = 5$
$x_4 = 1$

The process does not converge to the solution. This type of divergence is called ***oscillatory divergence*** and $g'(R)$ *is negative*.
Again, Let us organize the function as follows: $x = x^2 + x - 5$ and assume $x_0 = 0$, Then

$x_1 = -5$
$x_2 = 15$
$x_3 = 235$
$x_4 = 55455$

The process does not converge to the solution. This type of divergence is called ***monotone divergence*** and $g'(R)$ *is positive*.
Again, Let us organize the function as follows: $2x = 5/x + x$ *or* $x = \frac{x + 5/x}{2}$
and assume $x_0 = 1$, Then

$x_1 = 3$
$x_2 = 2.3333$
$x_3 = 2.2381$
$x_4 = 2.2361$
$x_5 = 2.2361$

The process converges rapidly to the solution. This square root of 5 is 2.2361.

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