Chapter 2

Numerical Solution of Nonlinear Equations

Many problems in engineering and science require the solution of nonlinear algebraic equations.

- In Thermodynamics: equations of state;

Redlich-Kwong $P = \frac{RT}{v-b} - \frac{a}{v(v+b)\sqrt{T}}$

Van der Waals $P = \frac{RT}{v-b} - \frac{a}{v^2}$

$$Pv^3 - (bP + RT)v^2 + av - ab = 0$$

- In calculation for multicomponent separation, it is often necessary to estimate the minimum reflux ratio of a multistage distillation column using the following equation

$$\sum_{j=1}^{n} \frac{\alpha_j Z_{jF} F}{\alpha_j - \phi} - F(1-q) = 0$$

F is the molar feed flow rate, *n* is the number of components in the feed, Z_{jF} is the mole fraction of each component in the feed, *q* is the quality of the feed, Φ_j is the relative volatility of each component at average column conditions and is the root of equation.

- The fanning friction factor *f* for turbulent flow of an incompressible fluid in a smooth pipe

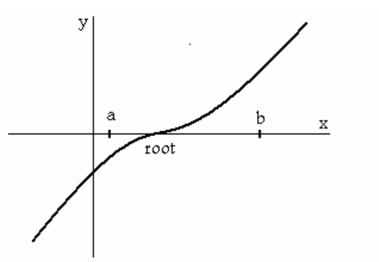
$$\sqrt{\frac{2}{f}} = \frac{1}{k}\ln\left(N_{\mathrm{Re}}\sqrt{\frac{f}{8}}\right) + B - A$$

where *A*, *B*, and *k* are constants and N_{Re} is the *Reynolds number*.

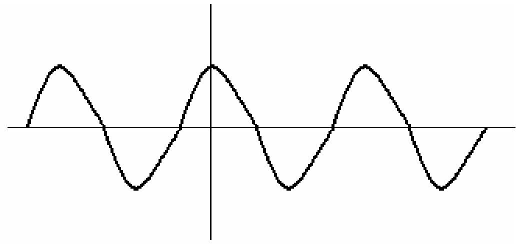
All the nonlinear equations presented above are all of the general form $f(x) = 0$
Where *x* is a single variable which can have multiple values (roots) that satisfy this equation.

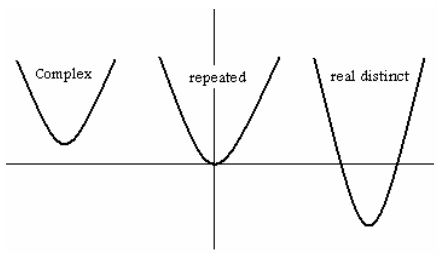
Type of Roots

- Real and distinct
- Real and repeated
- Complex conjugates
- A mixture of all of above.

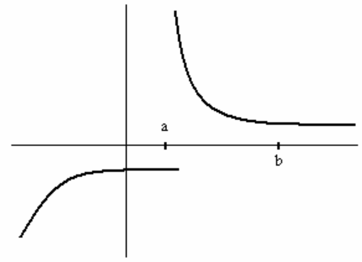


Isolated real root bracketed by two points a and b at which the function has opposite signs.


Pathologicak function with many roots



It is not necessarily a sign change in the function near a double root.



The function has opposite signs at points a and b, but the points bracket a singularity, not a root.

1) Method of Bisection

- For $f(x) = 0$, assume f is a real-valued function of a real variable x, with a number of roots in the interval I: $a<x<b$. If f is **continuous** the sign of $f(a)$ is opposite to that of $f(b)$.
- This method may give a **false** root if $f(x)$ is **discontinuous** on $[a, b]$.

Procedure

1. Specify bounds $\boldsymbol{x_0}$ and $\boldsymbol{x_1}$
2. Evaluate $f_0 = f(x_0)$ and $f_1 = f(x_1)$
3. Check that sign $f_0 \neq$ sign f_1. If they have same sign then change one of the initial guesses either x_0 or x_1.
4. Start iteration.
5. Let $x_2 = (x_0 + x_1)/2$
6. Evaluate $f_2 = f(x_2)$
7. If sign f_2 = sign f_0 then make $x_0 = x_2$ and $f_0 = f_2$
8. Else make $x_1 = x_2$ and $f_1 = f_2$
9. If $f_2 \approx 0$ or $|x_0 - x_1| \leq$ Tolerance then stop.
10. Repeat from step 4

2) False Position Method

- This method uses the linear interpolation technique to determine the root.
- To find a root of $f(x) = 0$ using the false position method the following procedure is used:

Procedure

1. Specify bounds x_0 and x_1
2. Evaluate $f_0 = f(x_0)$ and $f_1 = f(x_1)$

3. Check that sign $f_0 \neq$ sign f_1. If they have same sign then change one of the initial guesses either x_0 or x_1.
4. Start iteration.
5. Let $x_2 = x_0 - f_0 * \frac{(x_0 - x_1)}{(f_0 - f_1)}$
6. Evaluate $f_2 = f(x_2)$
7. If sign f_2 = sign f_0 then make $x_0 = x_2$ and $f_0 = f_2$
8. Else make $x_1 = x_2$ and $f_1 = f_2$
9. If $f_2 \approx 0$ or $|x_0 - x_1| \leq$ Tolerance then stop.
10. Repeat from step 4

3) Secant Method

- Secant method uses the linear interpolation technique to get better estimates of the root.
- The secant method does not bracket zero at each iteration, so the secant method is not guaranteed to converge.
- When secant method converges the convergence is usually more rapid than bisection method.

To find a root of $f(x) = 0$, given two values, x_0 and x_1, that are near the root use the following procedure:

1. Specify bounds x_0 and x_1
2. Evaluate $f_0 = f(x_0)$ and $f_1 = f(x_1)$
3. If $|f_0| > |f_1|$ Go to step 4, otherwise:
   Swap x_0 with x_1 [$x_0 = x_1$ and $x_1 = x_0$] Go to step 4
4. Start iteration.
5. Let $x_2 = x_0 - f_0 * \frac{(x_0 - x_1)}{(f_0 - f_1)}$ or $x_2 = x_1 - f_1 * \frac{(x_1 - x_0)}{(f_1 - f_0)}$
6. Evaluate $f_2 = f(x_2)$; if $|f_2| \leq$ Tolerance then stop, otherwise
7. Let $x_0 = x_1$ and $x_1 = x_2$
8. Repeat from step 5

4) Newton Raphson Method

- This method uses a straight line approximation to the function whose zero wish to find, but in this case the line is the tangent to the curve.
- The derivative of the function is required in the algorithm.
- The next approximation to the zero is the value where the tangent crosses the x-axis.
- Newton Raphson method is more rapidly convergent than any of the methods discussed above.
- The method may converge to a root different from the expected one.
- The method may diverge if the starting value is not close enough to the root.
- Newton's method works with complex roots if we give it a complex value for the starting value.

To find a root of $f(x) = 0$, given a value x_0 reasonably close to the root, use the following procedure:

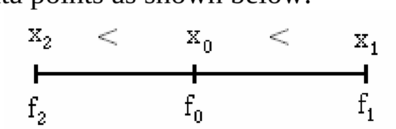
1. Calculate $f_0 = f(x_0)$
2. Calculate $f_0' = f'(x_0)$
3. If $f_0 \neq 0$ and $f' \neq 0$ then
4. Up-date the estimate using $x_k = x_{k-1} - \dfrac{f_{k-1}}{f_{k-1}'}$.
5. Evaluate $f_k = f(x_k)$; if $|f_k| \leq$ Tolerance then stop, otherwise
6. Let $x_0 = x_k$
7. Repeat from step 1

5) Muller's Method

- It is similar to the false position method but uses quadratic rather than linear interpolation to locate the root.
- This method requires 3 data points to start iteration and if you are given 2 data points only get the 3rd point as the mean value between the given points, i.e. $x_2 = (x_0 + x_1)/2$

To find a root of $f(x) = 0$, given values x_0, x_1, x_2, use the following procedure:

1. Calculate $f_0 = f(x_0)$, $f_1 = f(x_1)$, $f_2 = f(x_2)$
2. Arrange the given data points as shown below:



3. Calculate the following constants:

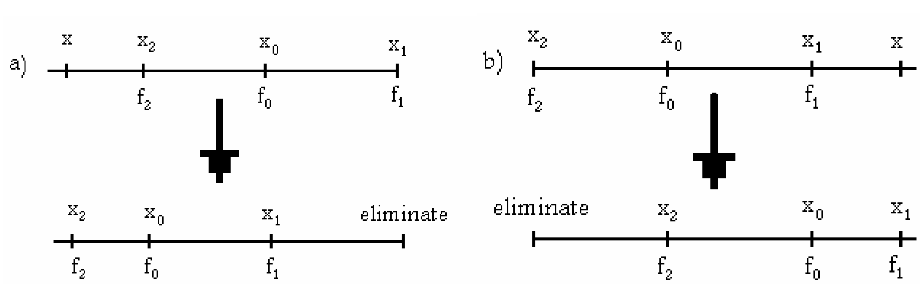
$$c_1 = \frac{f_1 - f_2}{x_1 - x_2}$$

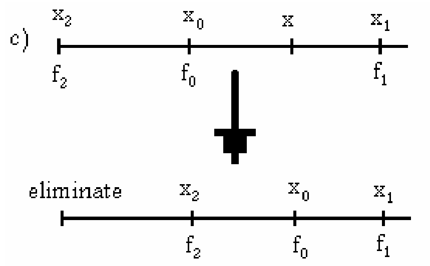
$$c_2 = \frac{f_0 - f_1}{x_0 - x_1}$$

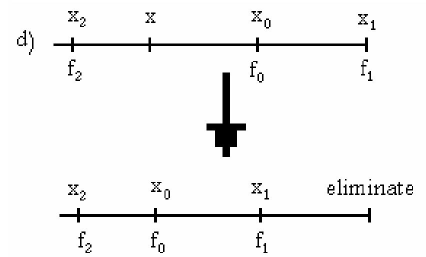
$$d_1 = \frac{c_2 - c_1}{x_0 - x_2}$$

$$s = c_2 + d_1(x_0 - x_1)$$

4. Calculate the expected root using $x = x_0 - \dfrac{2 f_0}{s + (sign \text{ of } s) * \sqrt{s^2 - 4 f_0 d_1}}$
5. If $|f_x| \leq$ Tolerance then stop, otherwise go to step 6.
6. Rearrange the data points as one of the following figures







7. Repeat iteration until you get the desired tolerance, i.e. go to step 3.

6) Fixed-Point Iteration

- Rearrange the function $f(x) = 0$ so that x is the left hand side of the equation, i.e. $x = g(x)$
- This transformation can be accomplished either by algebraic manipulation or by simply adding x to both sides of the original equation.
- Given an initial guess at the root x_i, the above equation can be used to compute a new estimate x_{i+1}

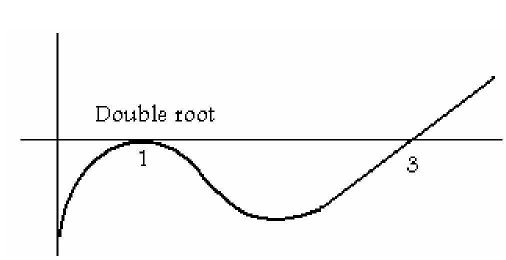
$$x_{i+1} = g(x_i)$$

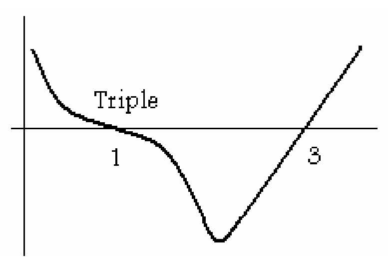
- Repeat until desired tolerance.
- The method may converge to a root different from the expected one, or may diverge.
- Different rearrangements will converge at different rates.
- This technique is used practically if $|g'(x_0)| < 1$

How does the technique work?

- The fixed point of $x = g(x)$ is the intersection of the line $y = x$ and the curve $y = g(x)$ and can be plotted:
- Start on the x-axis at the initial x_0.
- Go vertically to the curve, then horizontally to the line $y = x$, then vertically to the curve, and again horizontally to the line.
- Repeat this process until the points on the curve converge to a fixed point or else diverge.

Multiple Roots





- For even number of repeated roots the function does not cross the x-axis and slope of the function changes its sign as it touches the x-axis.
- For odd number of repeated roots the function crosses the x-axis and the function change its concavity as it crosses the axis.

Problems:

- For even number of repeated roots the function does not change sign. So we are limited to the open methods (un bracketing) that may diverge.
- Another possible problem is related to the fact that not only *f(x)* but also *f′*(x) goes to zero at the root. This poses problems for both the Newton's and secant methods. This could results in division by zero when the solution converges very close to the root.
- Modified Newton-Raphson method could be used to overcome this problem using the following equation to update the estimation:

$$x_k = x_{k-1} - \frac{f(x_{k-1})f'(x_{k-1})}{[f'(x_{k-1})]^2 - f(x_{k-1})f''(x_{k-1})}$$