

1 Solving Nonlinear Equations

”solve $f(x) = 0$ ” where $f(x)$ is a function of x . The values of x that make $f(x) = 0$ are called the roots of the equation. They are also called the zeros of $f(x)$.

The following non-linear equation can compute the friction factor, f :

$$\frac{1}{\sqrt{f}} = \left(\frac{1}{k}\right) \ln(RE\sqrt{f}) + \left(14 - \frac{5.6}{k}\right)$$

where the parameter k is known and RE, the so-called Reynold’s number. The equation for f is not solvable except by the numerical procedures of this chapter.

- **Interval Halving (Bisection).** Describes a method that is very simple and foolproof but is not very efficient. We examine how the error decreases as the method continues.
- **Linear Interpolation Methods.** Tells how approximating the function in the vicinity of the root with a straight line can find a root more efficiently. It has a better ”rate of convergence”.
- **Newton’s Method.** Explains a still more efficient method that is very widely used but there are pitfalls that you should know about. Complex roots can be found if complex arithmetic is employed.
- **Muller’s Method.** Approximates the function with a quadratic polynomial that fits to the function better than a straight line. This significantly improves the rate of convergence over linear interpolation.
- **Fixed-Point Iteration: $x = g(x)$ Method.** Uses a different approach: The function $f(x)$ is rearranged to an equivalent form, $x = g(x)$. A starting value, x_0 , is substituted into $g(x)$ to give a new x-value, x_1 . This in turn is used to get another x-value. If the function $g(x)$ is properly chosen, the successive values converge.

1.1 Interval Halving (Bisection)

- Interval halving (bisection), an ancient but effective method for finding a zero of $f(x)$.
- It begins with two values for x that bracket a root.
- The function $f(x)$ changes signs at these two x-values and, if $f(x)$ is continuous, there must be at least one root between the values.

- A plot of $f(x)$ is useful to know where to start.
- The bisection method then successively divides the initial interval in half, finds in which half the root(s) must lie, and repeats with the endpoints of the smaller interval.
- The test to see that $f(x)$ does change sign between points a and b is to see if $f(a) * f(b) < 0$.

$$f(x) = 3x + \sin(x) - e^x$$

Look at to the plot of the function (see Fig. 1) to learn where the function crosses the x-axis. MATLAB can do it for us:

```
>> f = inline ( ' 3 *x + sin ( x) - exp ( x) ' )
>> fplot ( f, [ 0 2 ] ) ; grid on
```

And we see from the figure that indicates there are zeros at about $x = 0.35$ and 1.9.

An algorithm for Halving the Interval (Bisection):

To determine a root of $f(x) = 0$ that is accurate within a specified tolerance value, given values x_1 and x_2 , such that $f(x_1) * f(x_2) < 0$,
 Repeat
 Set $x_3 = (x_1 + x_2)/2$
 If $f(x_3) * f(x_1) < 0$ Then
 Set $x_2 = x_3$
 Else Set $x_1 = x_3$ End If
 Until $(|x_1 - x_2|) < 2 * tolerance\ value$

- Think about the multiplication factor, 2
- The final Value of x_3 approximates the root, and it is in error by not more than $|x_1 - x_2|/2$.
- The method may produce a false root if $f(x)$ is discontinuous on $[x_1, x_2]$.

To obtain the true value for the root, which is needed to compute the actual error. MATLAB surely used a more advanced method than bisection.

```
>> solve('3*x + sin(x) - exp(x)')
ans=
.36042170296032440136932951583028
```

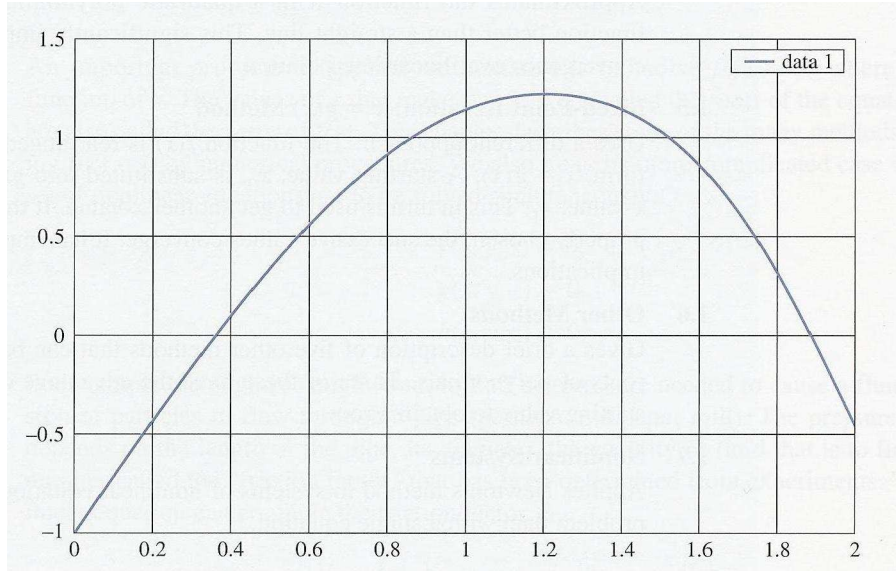


Figure 1: Plot of the function: $f(x) = 3x + \sin(x) - e^x$

Table 1: The bisection method for $f(x) = 3x + \sin(x) - e^x$, starting from $x_1 = 0, x_2 = 1$, using a tolerance value of $1E-4$.

Iteration	X_1	X_2	X_3	$F(X_3)$	Maximum error	Actual error
1	0.00000	1.00000	0.50000	0.33070	0.50000	0.13958
2	0.00000	0.50000	0.25000	-0.28662	0.25000	-0.11042
3	0.25000	0.50000	0.37500	0.03628	0.12500	0.01458
4	0.25000	0.37500	0.31250	-0.12190	0.06250	-0.04792
5	0.31250	0.37500	0.34375	-0.04196	0.03125	-0.01667
6	0.34375	0.37500	0.35938	-0.00262	0.01563	-0.00105
7	0.35938	0.37500	0.36719	0.01689	0.00781	0.00677
8	0.35938	0.36719	0.36328	0.00715	0.00391	0.00286
9	0.35938	0.36328	0.36133	0.00227	0.00195	0.00091
10	0.35938	0.36133	0.36035	-0.00018	0.00098	-0.00007
11	0.36035	0.36133	0.36084	0.00105	0.00049	0.00042
12	0.36035	0.36084	0.36060	0.00044	0.00024	0.00017
13	0.36035	0.36060	0.36047	0.00013	0.00012	0.00005

- The main advantage of interval halving is that it is guaranteed to work if $f(x)$ is continuous in $[a, b]$ and if the values $x = a$ and $x = b$ actually bracket a root (This guarantee can be avoided, if the function has a slope very near to zero at the root, the precision of the computations may be inadequate.)
- Another important advantage that few other root-finding methods share is that the number of iterations to achieve a specified accuracy is known in advance.
- Because the interval $[a, b]$ is halved each time, the last value of x_3 differs from the true root by less than $\frac{1}{2}$ the last interval. So we can say with surety that

$$\text{error after } n \text{ iterations} < \left| \frac{(b - a)}{2^n} \right|$$

- The major objection of interval halving has been that it is slow to converge.
- Observe in Table 1 that the estimate of the root may be better at an earlier iteration than at later (we are closer at iteration 6 than at iteration 7.)
- In spite of arguments that other methods find roots with fewer iterations, interval halving is an important tool. Bisection is generally recommended for finding an approximate value for the root, and then this value is refined by more efficient methods. The reason is that most other root-finding methods require a starting value near to a root (lacking this, they may fail completely).
- When there are multiple roots, interval halving may not be applicable, because the function may not change sign at points on either side of the roots.

1.2 Linear Interpolation Methods

Bisection is simple to understand but it is not the most efficient way to find where $f(x)$ is zero.

Most functions can be approximated by a straight line over a small interval.

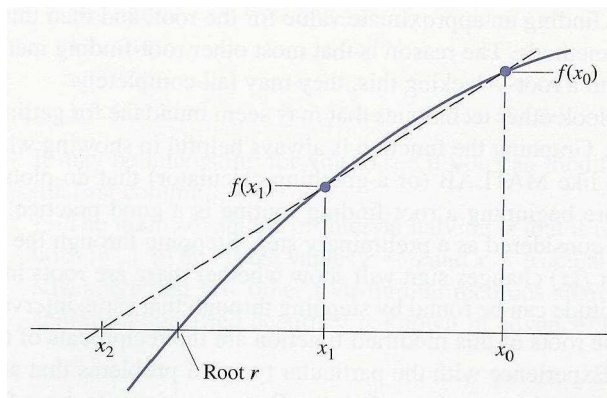


Figure 2: Graphical illustration of the Secant Method.

1.2.1 The Secant Method

- The secant method begins by finding two points on the curve of $f(x)$, hopefully near to the root we seek.
- As Figure 2 illustrates, we draw the line through these two points and find where it intersects the x-axis.
- If $f(x)$ were truly linear, the straight line would intersect the x-axis at the root.
- The intersection of the line with the x-axis is not at $x = r$ but it should be close to it. From the obvious similar triangles we can write

$$\frac{(x_1 - x_2)}{f(x_1)} = \frac{(x_0 - x_1)}{f(x_0) - f(x_1)} \implies x_2 = x_1 - f(x_1) \frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$$

- Because $f(x)$ is not exactly linear, x_2 is not equal to r , but it should be closer than either of the two points we began with. If we repeat this, we have:

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

- The net effect of this rule is to set $x_0 = x_1$ and $x_1 = x_2$, after each iteration.
- The technique we have described is known as, the secant method because the line through two points on the curve is called the secant line.

Table 2: The Secant method for $f(x) = 3x + \sin(x) - e^x$, starting from $x_0 = 1, x_1 = 0$, using a tolerance value of 1E-6.

Iteration	x_0	x_1	x_2	$f(x_2)$
1	1	0	0.4709896	0.2651588
2	0	0.4709896	0.3722771	2.953367E-02
3	0.4709896	0.3722771	0.3599043	-1.294787E-03
4	0.3722771	0.3599043	0.3604239	5.552969E-06
5	0.3599043	0.3604239	0.3604217	3.554221E-08

At $x = .3604217$, tolerance of .0000001 met!

An algorithm for the Secant Method:

To determine a root of $f(x) = 0$, given two values, x_0 and x_1 , that are near the root,
 If $|f(x_0)| < |f(x_1)|$ Then
 Swap x_0 with x_1
 Repeat
 Set $x_2 = x_1 - f(x_1) * \frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$
 Set $x_0 = x_1$
 Set $x_1 = x_2$
 Until $|f(x_2)| < tolerance\ value$

- If $f(x)$ is not continuous, the method may fail.
- An alternative stopping criterion for the secant method is when the pair of points being used are sufficiently close together.
- Table 2 shows the results from the secant method for the same function that was used to illustrate bisection.
- An objection is sometimes raised about the secant method. If the function is far from linear near the root, the successive iterates can fly off to points far from the root, as seen if Fig. 3.
- If the method is being carried out by a program that displays the successive iterates, the user can interrupt the program should such improvident behavior be observed. Also, if the function was plotted before starting the method, it is unlikely that the problem will be encountered, because a better starting value would be used.

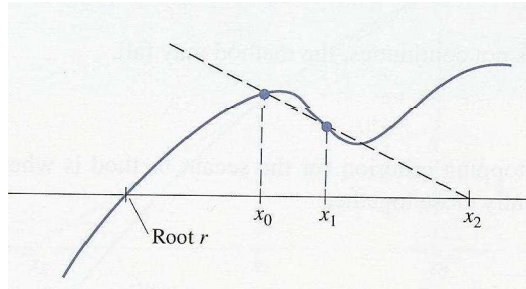


Figure 3: A pathological case for the secant method.

1.2.2 Linear Interpolation (False Position)

- A way to avoid such pathology is to ensure that the root is bracketed between the two starting values and remains between the successive pairs. When this is done, the method is known as linear interpolation
- This technique is similar to bisection except the next iterate is taken at the intersection of a line between the pair of x-values and the x-axis rather than at the midpoint.
- Doing so gives faster convergence than does bisection, but at the expense of a more complicated algorithm.

An algorithm for the method of false position (regula falsi):

To determine a root of $f(x) = 0$, given two values of x_0 and x_1 that bracket a root: that is, $f(x_0)$ and $f(x_1)$ are of opposite sign,
 Repeat
 Set $x_2 = x_1 - f(x_1) * \frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$
 If $f(x_2)$ is of opposite sign to $f(x_0)$ Then
 Set $x_1 = x_2$,
 Else
 Set $x_0 = x_2$
 End If
 Until $|f(x_2)| < tolerance\ value.$

- If $f(x)$ is not continuous, the method may fail.
- Table 3 compares the results of three methods-interval halving (bisection), linear interpolation, and the secant method-on $f(x) = 3x + \sin(x) - e^x = 0$

Table 3: Comparison of methods, $f(x) = 3x + \sin(x) - e^x$, starting from $x_0 = 0, x_1 = 1$.

Iteration	Interval halving		False position		Secant method	
	x	$f(x)$	x	$f(x)$	x	$f(x)$
1	0.5	0.330704	0.470990	0.265160	0.470990	0.265160
2	0.25	-0.286621	0.372277	0.029533	0.372277	0.029533
3	0.375	0.036281	0.361598	$2.94 * 10^{-3}$	0.359904	$-1.29 * 10^{-3}$
4	0.3125	-0.121899	0.360538	$2.90 * 10^{-4}$	0.360424	$5.55 * 10^{-6}$
5	0.34375	-0.041956	0.360433	$2.93 * 10^{-5}$	0.360422	$3.55 * 10^{-7}$
Error after 5 iterations	0.01667		$-1.17 * 10^{-5}$		$< -1 * 10^{-7}$	
(Exact value of root is 0.360421703.)						

- Observe that the speed of convergence is best for the secant method, poorest for interval halving, and intermediate for false position.

1.3 Newton's Method

- One of the most widely used methods of solving equations is Newton's method (Newton did not publish an extensive discussion of this method, but he solved a cubic polynomial in *Principia* (1687). The version given here is considerably improved over his original example).
- Like the previous ones, this method is also based on a linear approximation of the function, but does so using a tangent to the curve. Figure 4 gives a graphical description
- Starting from a single initial estimate, x_0 , that is not too far from a root, we move along the tangent to its intersection with the x-axis, and take that as the next approximation.
- This is continued until either the successive x-values are sufficiently close or the value of the function is sufficiently near zero.
- The calculation scheme follows immediately from the right triangle shown in Fig. 4.

$$\tan\theta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1} \Rightarrow x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

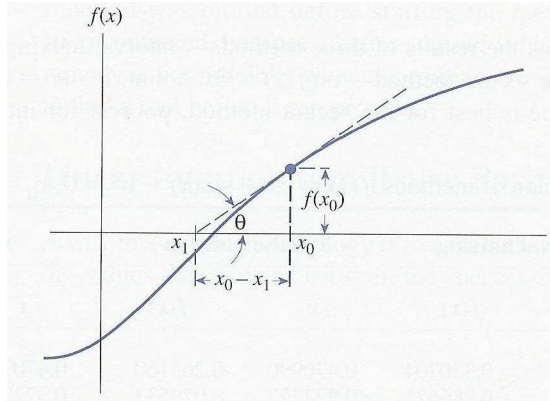


Figure 4: Graphical illustration of the Newton's Method.

and the general term is:

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

- Newton's algorithm is widely used because, it is more rapidly convergent than any of the methods discussed so far.
- The method is quadratically convergent, by which we mean that the error of each step approaches a constant K times the square of the error of the previous step.
- The net result of this is, that the number of decimal places of accuracy nearly doubles at each iteration.
- When Newton's method is applied to $f(x) = 3x + \sin x - e^x = 0$, if we begin with $x_0 = 0.0$:

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 0.0 - \frac{-1.0}{3.0} = 0.33333$$

$$x_2 = 0.36017$$

$$x_3 = 0.3604217$$

- After three iterations, the root is correct to seven digits; convergence is much more rapid than any previous method. In fact, the error after an iteration is about one-third of the square of the previous error.

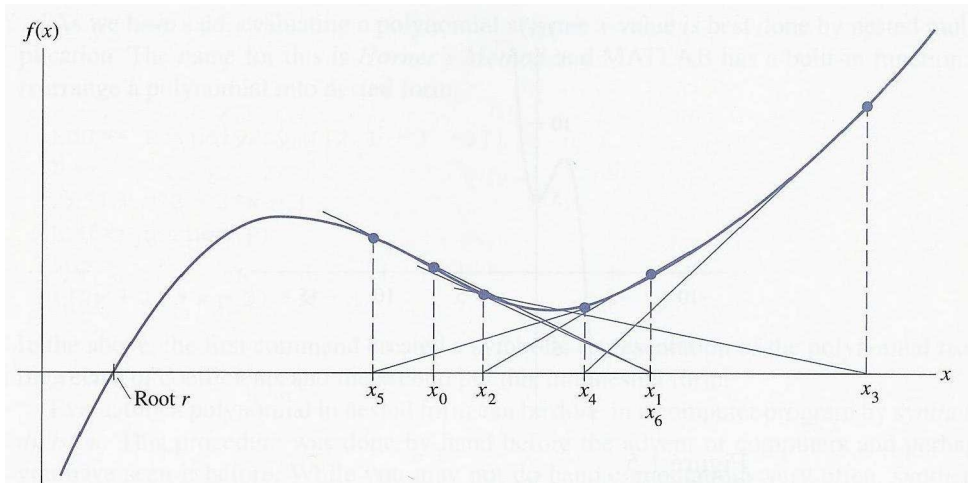


Figure 5: Graphical illustration of the case that Newton's Method will not converge.

- If a difficult problem requires many iterations to converge, the number of function evaluations with Newton's method may be many more than with linear iteration methods because Newton always uses two per iteration whereas the others take only one (after the first step that takes two).

An algorithm for the Newton's method :

To determine a root of $f(x) = 0$, given x_0 reasonably close to the root,
 Compute $f(x_0), f'(x_0)$
 If $(f(x_0) \neq 0)$ And $(f'(x_0) \neq 0)$ Then
 Repeat
 Set $x_1 = x_0$
 Set $x_0 = x_0 - \frac{f(x_0)}{f'(x_0)}$
 Until $(|x_1 - x_0| < tolerance\ value1)$ Or If $|f(x_0)| < tolerance\ value2)$
 End If.

- The method may converge to a root different from the expected one or diverge if the starting value is not close enough to the root.
- In some cases Newton's method will not converge. Figure 5 illustrates this situation.

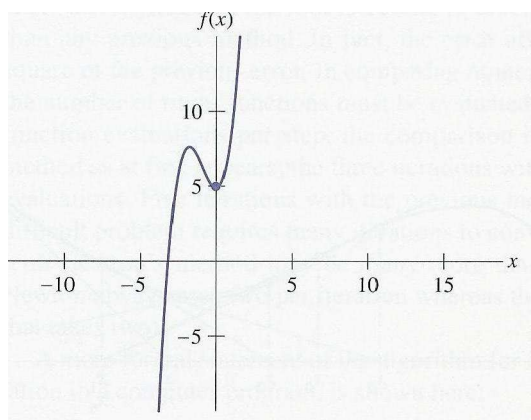


Figure 6: Plot of $f(x) = x^3 + 2x^2 - x + 5$.

- Starting with x_0 , one never reaches the root r because $x_6 = x_1$ and we are in an endless loop.
- Observe also that if we should ever reach the minimum or maximum of the curve, we will fly off to infinity.

1.3.1 Complex Roots

- Newton's method works with complex roots if we give it a complex value for the starting value.
- Use Newton's method on $f(x) = x^3 + 2x^2 - x + 5$. Figure 6 shows the graph of $f(x)$. It has, a real root at about $x = -3$, whereas the other two roots are complex because the x-axis is not crossed again.
- If we begin Newton's method with $x_0 = 1 + i$ (we used this in the lack of knowledge about the complex root), we get these successive iterates;

1. $0.486238 + 1.04587i$
2. $0.448139 + 1.23665i$
3. $0.462720 + 1.22242i$
4. $0.462925 + 1.22253i$
5. $0.462925 + 1.22253i$

- Because the fourth and fifth iterates agree to six significant figures, we are sure that we have an estimate good to at least that many figures.
- The second complex root is the conjugate of this: $0.462925 - 1.22253i$.

- If we begin with $x_0 = 1 - i$, the method converges to the conjugate.
- If we begin with a real starting value-say, $x_0 = -3$ -we get convergence to the root at $x = -2.92585$.