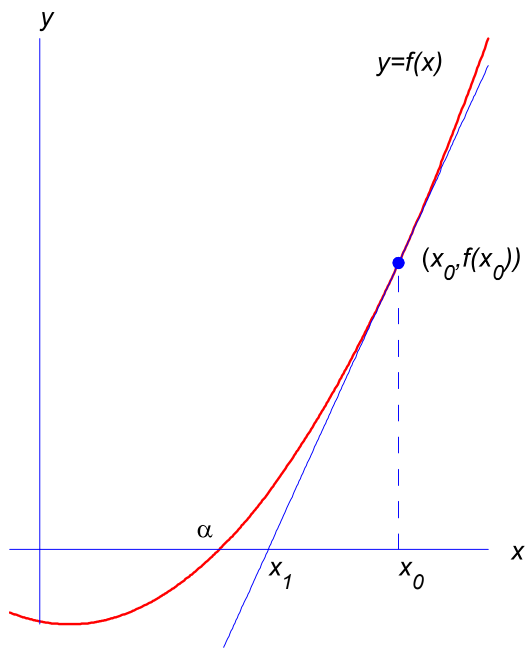
ROOTFINDING : A PRINCIPLE

We want to find the root α of a given function $f(x)$. Thus we want to find the point x at which the graph of $y = f(x)$ intersects the x-axis. One of the principles of numerical analysis is the following.

If you cannot solve the given problem, then solve a "nearby problem".

How do we obtain a nearby problem for $f(x) = 0$? Begin first by asking for types of problems which we can solve easily. At the top of the list should be that of finding where a straight line intersects the x-axis. Thus we seek to replace $f(x) = 0$ by that of solving $p(x) = 0$ for some linear polynomial $p(x)$ that approximates $f(x)$ in the vicinity of the root α.



Given an estimate of α, say $\alpha \approx x_0$, approximate $f(x)$ by its linear Taylor polynomial at $(x_0, f(x_0))$:

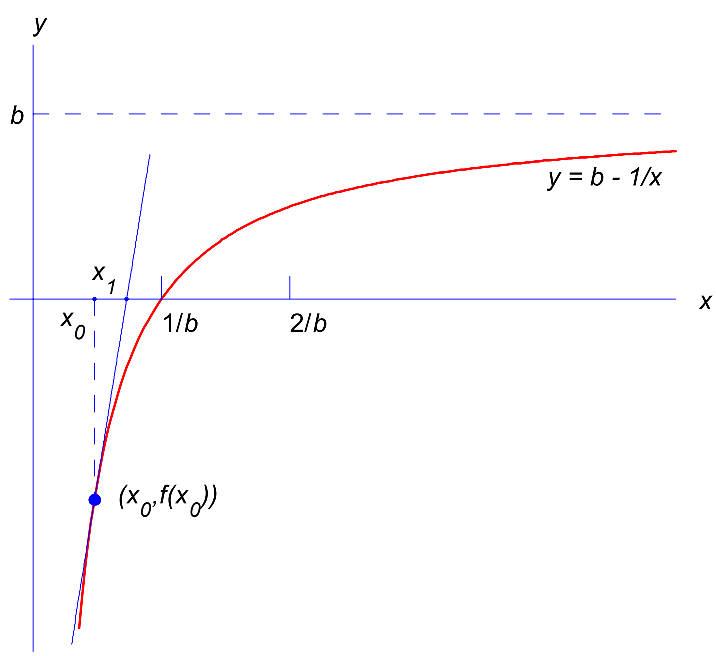
$$p(x) = f(x_0) + (x - x_0)\, f'(x_0)$$

If x_0 is very close to α, then the root of $p(x)$ should be close to α. Denote this approximating root by x_1; repeat the process to further improve our estimate of α.

To illustrate this procedure, we consider a well-known example. For a number $b > 0$, consider solving the equation

$$f(x) \equiv b - \frac{1}{x} = 0$$

The solution is, of course, $\alpha = 1/b$. Nonetheless, bear with the example as it has some practical application.



Let x_0 be an estimate of the root $\alpha = 1/b$. Then the line tangent to the graph of $y = f(x)$ at $(x_0, f(x_0))$ is given by

$$p(x) = f(x_0) + (x - x_0)\, f'(x_0)$$

with

$$f'(x) = \frac{1}{x^2}$$

Denoting the root of $p(x) = 0$ by x_1, we solve for x_1 in

$$f(x_0) + (x_1 - x_0)\, f'(x_0) = 0$$

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

For our particular case, this yields

$$x_1 = x_0 - \frac{b - \frac{1}{x_0}}{\frac{1}{x_0^2}} = x_0 - bx_0^2 + x_0$$

$$x_1 = x_0\,(2 - bx_0)$$

$$x_1 = x_0 (2 - b x_0)$$

Note that no division is used in our final formula.

If we repeat the process, now using x_1 as our initial estimate of α, then we obtain a sequence of numbers $x_1, x_2, ...$

$$x_{n+1} = x_n (2 - b x_n), \qquad n = 0, 1, 2, ...$$

Do these numbers x_n converge to the root α? We return to this after a bit.

This algorithm has been used in a practical way in a number of circumstances.

The general Newton's method for solving $f(x) = 0$ is derived exactly as above. The result is a sequence of numbers $x_0, x_1, x_2, \ldots$ defined by

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

Again, we want to know whether these numbers converge to the desired root α; and we would also like to know something about the speed of convergence (which says something about how many such iterates must actually be computed).

Return to the iteration

$$x_{n+1} = x_n \left(2 - b x_n\right), \qquad n = 0, 1, 2, \ldots$$

for solving

$$f(x) \equiv b - \frac{1}{x} = 0$$

We use a method of analysis which works for only this example, and later we use another approach to the general Newton's method.

Write

$$x_{n+1} = x_n (1 + r_n), \qquad r_n = 1 - bx_n$$

Note that the error and relative error in x_n are given by

$$e_n = \frac{1}{b} - x_n = \frac{r_n}{b}$$

$$\text{rel}(x_n) = \frac{e_n}{\alpha} = \frac{r_n}{b} \cdot b = r_n$$

Thus r_n is the relative error in x_n, and we have x_n converges to α if and only if r_n tends to zero.

We find a recursion formula for r_n, recalling that $r_n = 1 - bx_n$ for all n. Then

$$\begin{aligned} r_{n+1} &= 1 - bx_{n+1} \\ &= 1 - bx_n (1 + r_n) \\ &= 1 - (1 - r_n)(1 + r_n) \\ &= 1 - \left(1 - r_n^2\right) = r_n^2 \end{aligned}$$

Thus

$$r_{n+1} = r_n^2$$

for every integer $n \geq 0$. Thus

$$r_1 = r_0^2, \quad r_2 = r_1^2 = r_0^4, \quad r_3 = r_2^2 = r_0^8$$

By induction, we obtain

$$r_n = r_0^{2^n}, \qquad n = 0, 1, 2, 3, \ldots$$

We can use this to analyze the convergence of

$$x_{n+1} = x_n \left(1 + r_n\right), \qquad r_n = 1 - bx_n$$

In particular, we have $r_n \longrightarrow 0$ if and only if

$$|r_0| < 1$$

This is equivalent to saying

$$-1 < 1 - bx_0 < 1$$

$$0 < x_0 < \frac{2}{b}$$

A look at a graph of $f(x) \equiv b - \frac{1}{x}$ will show the reason for this condition. If x_0 is chosen greater than $\frac{2}{b}$, then x_1 will be negative, which is unacceptable. The interval

$$0 < x_0 < \frac{2}{b}$$

is called the 'interval of convergence'. With most equations, we cannot find this exactly, but rather only some smaller subinterval which guarantees convergence.

Using $r_{n+1} = r_n^2$ and $r_n = be_n$, we have

$$be_{n+1} = (be_n)^2$$

$$e_{n+1} = be_n^2$$

$$\alpha - x_{n+1} = b\,(\alpha - x_n)^2$$

Methods with this type of error behaviour are said to be quadratically convergent; and this is an especially desirable behaviour.

To see why, consider the relative errors in the above. Assume the initial guess x_0 has been so chosen that $r_0 = .1$. Then

$$r_1 = 10^{-2}, \quad r_2 = 10^{-4}, \quad r_3 = 10^{-8}, \quad r_4 = 10^{-16}$$

Thus very few iterates need be computed.

The iteration

$$x_{n+1} = x_n \left(1 + r_n\right), \qquad r_n = 1 - b x_n$$

has been used on a number of machines as a means of doing division, of calculating $1/b$.

NEWTON'S METHOD

For a general equation $f(x) = 0$, we assume we are given an initial estimate x_0 of the root α. The iterates are generated by the formula

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

EXAMPLE Consider solving

$$f(x) \equiv x^6 - x - 1 = 0$$

for its positive root α. An initial guess x_0 can be generated from a graph of $y = f(x)$. The iteration is given by

$$x_{n+1} = x_n - \frac{x_n^6 - x_n - 1}{6x_n^5 - 1}, \qquad n \geq 0$$

We use an initial guess of $x_0 = 1.5$.

The column "$x_n - x_{n-1}$" is an estimate of the error $\alpha - x_{n-1}$; justification is given later.

n	x_n	$f(x_n)$	$x_n - x_{n-1}$	$\alpha - x_{n-1}$
0	1.5	8.89E + 1		
1	1.30049088	2.54E + 1	−2.00E − 1	−3.65E − 1
2	1.18148042	5.38E − 1	−1.19E − 1	−1.66E − 1
3	1.13945559	4.92E − 2	−4.20E − 2	−4.68E − 2
4	1.13477763	5.50E − 4	−4.68E − 3	−4.73E − 3
5	1.13472415	7.11E − 8	−5.35E − 5	−5.35E − 5
6	1.13472414	1.55E − 15	−6.91E − 9	−6.91E − 9

As seen from the output, the convergence is very rapid. The iterate x_6 is accurate to the machine precision of around 16 decimal digits. This is the typical behaviour seen with Newton's method for most problems, but not all.

We could also have considered the problem of solving the annuity equation

$$f(x) \equiv 1000\left[\left(1+\frac{x}{12}\right)^{480}-1\right]$$
$$-5000\left[1-\left(1+\frac{x}{12}\right)^{-240}\right]=0$$

However, it turns out that you have to be very close to the root in this case in order to get good convergence. This phenomena is discussed further at a later time; and the bisection method is preferable in this instance.

AN ERROR FORMULA

Suppose we use Taylor's formula to expand $f(\alpha)$ about $x = x_n$. Then we have

$$f(\alpha) = f(x_n) + (\alpha - x_n) f'(x_n) + \frac{1}{2} (\alpha - x_n)^2 f''(c_n)$$

for some c_n between α and x_n. Note that $f(\alpha) = 0$. Then divide both sides of this equation by $f'(x_n)$, yielding

$$0 = \frac{f(x_n)}{f'(x_n)} + \alpha - x_n + (\alpha - x_n)^2 \frac{f''(c_n)}{2f'(x_n)}$$

Note that

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

and thus

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

For x_n close to α, and therefore c_n also close to α, we have

$$\alpha - x_{n+1} \approx -\frac{f''(\alpha)}{2f'(\alpha)} (\alpha - x_n)^2$$

Thus Newton's method is quadratically convergent, provided $f'(\alpha) \neq 0$ and $f(x)$ is twice differentiable in the vicinity of the root α.

We can also use this to explore the 'interval of convergence' of Newton's method. Write the above as

$$\alpha - x_{n+1} \approx M (\alpha - x_n)^2, \qquad M = -\frac{f''(\alpha)}{2f'(\alpha)}$$

Multiply both sides by M to get

$$M (\alpha - x_{n+1}) \approx [M (\alpha - x_n)]^2$$

$$M(\alpha - x_{n+1}) \approx [M(\alpha - x_n)]^2$$

Then we want these quantities to decrease; and this suggests choosing x_0 so that

$$|M(\alpha - x_0)| < 1$$

$$|\alpha - x_0| < \frac{1}{|M|} = \left|\frac{2f'(\alpha)}{f''(\alpha)}\right|$$

If $|M|$ is very large, then we may need to have a very good initial guess in order to have the iterates x_n converge to α.

ADVANTAGES & DISADVANTAGES

Advantages: 1. It is rapidly convergent in most cases.
2. It is simple in its formulation, and therefore relatively easy to apply and program.
3. It is intuitive in its construction. This means it is easier to understand its behaviour, when it is likely to behave well and when it may behave poorly.

Disadvantages: 1. It may not converge.
2. It is likely to have difficulty if $f'(\alpha) = 0$. This condition means the x-axis is tangent to the graph of $y = f(x)$ at $x = \alpha$.
3. It needs to know both $f(x)$ and $f'(x)$. Contrast this with the bisection method which requires only $f(x)$.