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Solution of equations by iteration

1.1 Introduction

Equations of various kinds arise in a range of physical applications and a substantial body of mathematical research is devoted to their study. Some equations are rather simple: in the early days of our mathematical education we all encountered the single *linear* equation $ax+b=0$, where a and b are real numbers and $a \neq 0$, whose solution is given by the formula $x = -b/a$. Many equations, however, are *nonlinear:* a simple example is $ax^2 + bx + c = 0$, involving a quadratic polynomial with real coefficients a, b, c, and $a \neq 0$. The two solutions to this equation, labelled x_1 and x_2, are found in terms of the coefficients of the polynomial from the familiar formulae

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}\,, \qquad x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}\,. \tag{1.1}$$

It is less likely that you have seen the more intricate formulae for the solution of cubic and quartic polynomial equations due to the sixteenth century Italian mathematicians Niccolo Fontana Tartaglia (1499–1557) and Lodovico Ferrari (1522–1565), respectively, which were published by Girolamo Cardano (1501–1576) in 1545 in his *Artis magnae sive de regulis algebraicis liber unus.* In any case, if you have been led to believe that similar expressions involving radicals (roots of sums of products of coefficients) will supply the solution to any polynomial equation, then you should brace yourself for a surprise: no such closed formula exists for a general polynomial equation of degree n when $n \geq 5$. It transpires that for each $n \geq 5$ there exists a polynomial equation of degree n with integer coefficients which cannot be solved in terms of radicals;[1] such is, for example, $x^5 - 4x - 2 = 0$.

Since there is no general formula for the solution of polynomial equations, no general formula will exist for the solution of an arbitrary nonlinear equation of the form $f(x) = 0$ where f is a continuous real-valued function. How can we then decide whether or not such an equation possesses a solution in the set of real numbers, and how can we find a solution?

The present chapter is devoted to the study of these questions. Our goal is to develop simple numerical methods for the approximate solution of the equation $f(x) = 0$ where f is a real-valued function, defined and continuous on a bounded and closed interval of the real line. Methods of the kind discussed here are iterative in nature and produce sequences of real numbers which, in favourable circumstances, converge to the required solution.

1.2 Simple iteration

Suppose that f is a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line. It will be tacitly assumed throughout the chapter that $a < b$, so that the interval is nonempty. We wish to find a *real number* $\xi \in [a, b]$ such that $f(\xi) = 0$. If such ξ exists, it is called a **solution** to the equation $f(x) = 0$.

Even some relatively simple equations may fail to have a solution in the set of real numbers. Consider, for example,

$$f\colon\ x \mapsto x^2 + 1\,.$$

Clearly $f(x) = 0$ has no solution in any interval $[a, b]$ of the real line. Indeed, according to (1.1), the quadratic polynomial x^2+1 has two roots: $x_1 = \sqrt{-1} = \imath$ and $x_2 = -\sqrt{-1} = -\imath$. However, these belong to the set of imaginary numbers and are therefore excluded by our definition of solution which only admits *real* numbers. In order to avoid difficulties of this kind, we begin by exploring the existence of solutions to the equation $f(x) = 0$ in the set of real numbers. Our first result in this direction is rather simple.

[1] This result was proved in 1824 by the Norwegian mathematician Niels Henrik Abel (1802–1829), and was further refined in the work of Evariste Galois (1811–1832) who clarified the circumstances in which a closed formula may exist for the solution of a polynomial equation of degree n in terms of radicals.

Theorem 1.1 *Let f be a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line. Assume, further, that $f(a)f(b) \leq 0$; then, there exists ξ in $[a, b]$ such that $f(\xi) = 0$.*

Proof If $f(a) = 0$ or $f(b) = 0$, then $\xi = a$ or $\xi = b$, respectively, and the proof is complete. Now, suppose that $f(a)f(b) \neq 0$. Then, $f(a)f(b) < 0$; in other words, 0 belongs to the open interval whose endpoints are $f(a)$ and $f(b)$. By the Intermediate Value Theorem (Theorem A.1), there exists ξ in the open interval (a, b) such that $f(\xi) = 0$. □

To paraphrase Theorem 1.1, if a continuous function f has opposite signs at the endpoints of the interval $[a, b]$, then the equation $f(x) = 0$ has a solution in (a, b). The converse statement is, of course, false. Consider, for example, a continuous function defined on $[a, b]$ which changes sign in the open interval (a, b) an even number of times, with $f(a)f(b) \neq 0$; then, $f(a)f(b) > 0$ even though $f(x) = 0$ has solutions inside $[a, b]$. Of course, in the latter case, there exist an even number of subintervals of (a, b) at the endpoints of each of which f *does* have opposite signs. However, finding such subintervals may not always be easy.

To illustrate this last point, consider the rather pathological function

$$f\colon\ x \mapsto \frac{1}{2} - \frac{1}{1 + M|x - 1.05|}\,, \tag{1.2}$$

depicted in Figure 1.1 for x in the closed interval $[0.8, 1.8]$ and $M = 200$. The solutions $x_1 = 1.05 - (1/M)$ and $x_2 = 1.05 + (1/M)$ to the equation $f(x) = 0$ are only a distance $2/M$ apart and, for large and positive M, locating them computationally will be a challenging task.

Remark 1.1 *If you have access to the mathematical software package Maple, plot the function f by typing*

```
plot(1/2-1/(1+200*abs(x-1.05)), x=0.8..1.8, y=-0.5..0.6);
```

at the Maple command line, and then repeat this experiment by choosing $M = 2000$, 20000, 200000, 2000000, and 20000000 in place of the number 200. What do you observe? For the last two values of M, replot the function f for x in the subinterval $[1.04999, 1.05001]$. ◇

An alternative sufficient condition for the existence of a solution to the equation $f(x) = 0$ is arrived at by rewriting it in the equivalent form $x - g(x) = 0$ where g is a certain real-valued function, defined

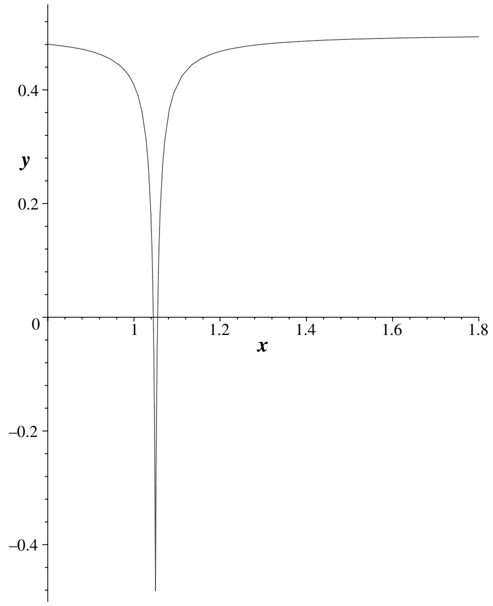


Fig. 1.1. Graph of the function $f\colon x \mapsto \frac{1}{2} - \frac{1}{1+200|x-1.05|}$ for $x \in [0.8, 1.8]$.

and continuous on $[a, b]$; the choice of g and its relationship with f will be clarified below through examples. Upon such a transformation the problem of solving the equation $f(x) = 0$ is converted into one of finding ξ such that $\xi - g(\xi) = 0$.

Theorem 1.2 (Brouwer's Fixed Point Theorem) *Suppose that g is a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line, and let $g(x) \in [a, b]$ for all $x \in [a, b]$. Then, there exists ξ in $[a, b]$ such that $\xi = g(\xi)$; the real number ξ is called a* **fixed point of the function** *g.*

Proof Let $f(x) = x - g(x)$. Then, $f(a) = a - g(a) \le 0$ since $g(a) \in [a, b]$ and $f(b) = b - g(b) \ge 0$ since $g(b) \in [a, b]$. Consequently, $f(a)f(b) \le 0$, with f defined and continuous on the closed interval $[a, b]$. By Theorem 1.1 there exists $\xi \in [a, b]$ such that $0 = f(\xi) = \xi - g(\xi)$. □

Figure 1.2 depicts the graph of a function $x \mapsto g(x)$, defined and continuous on a closed interval $[a, b]$ of the real line, such that $g(x)$ belongs to $[a, b]$ for all x in $[a, b]$. The function g has three fixed points in the interval $[a, b]$: the x-coordinates of the three points of intersection of the graph of g with the straight line $y = x$.

Of course, any equation of the form $f(x) = 0$ can be rewritten in the

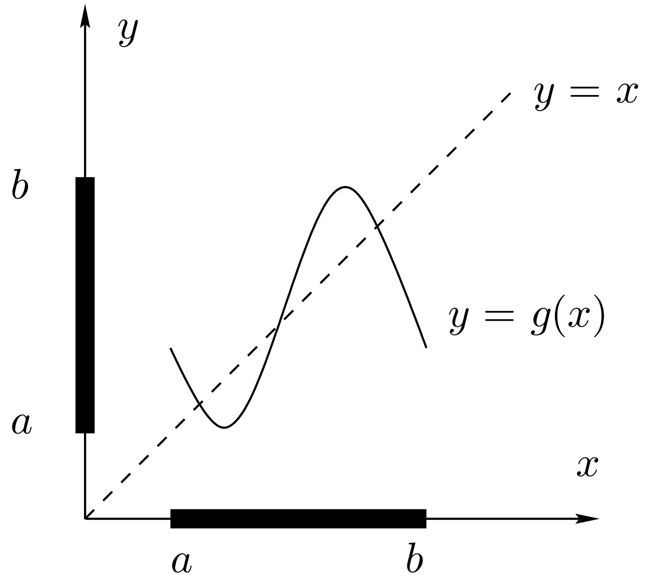


Fig. 1.2. Graph of a function g, defined and continuous on the interval $[a, b]$, which maps $[a, b]$ into itself; g has three fixed points in $[a, b]$: the x-coordinates of the three points of intersection of the graph of g with $y = x$.

equivalent form of $x = g(x)$ by letting $g(x) = x + f(x)$. While there is no guarantee that the function g, so defined, will satisfy the conditions of Theorem 1.2, there are many alternative ways of transforming $f(x) = 0$ into $x = g(x)$, and we only have to find one such rearrangement with g continuous on $[a, b]$ and such that $g(x) \in [a, b]$ for all $x \in [a, b]$. Sounds simple? Fine. Take a look at the following example.

Example 1.1 *Consider the function f defined by $f(x) = \mathrm{e}^x - 2x - 1$ for $x \in [1, 2]$. Clearly, $f(1) < 0$ and $f(2) > 0$. Thus we deduce from Theorem 1.1 the existence of ξ in $[1, 2]$ such that $f(\xi) = 0$.*

In order to relate this example to Theorem 1.2, let us rewrite the equation $f(x) = 0$ in the equivalent form $x - g(x) = 0$, where the function g is defined on the interval $[1, 2]$ by $g(x) = \ln(2x + 1)$; here (and throughout the book) ln means $\log_{\mathrm{e}}$. As $g(1) \in [1, 2]$, $g(2) \in [1, 2]$ and g is monotonic increasing, it follows that $g(x) \in [1, 2]$ for all $x \in [1, 2]$, showing that g satisfies the conditions of Theorem 1.2. Thus, again, we deduce the existence of $\xi \in [1, 2]$ such that $\xi - g(\xi) = 0$ or, equivalently, $f(\xi) = 0$.

We could have also rewritten our equation as $x = (\mathrm{e}^x - 1)/2$. However, the associated function $g\colon x \mapsto (\mathrm{e}^x - 1)/2$ does not map the interval $[1, 2]$ into itself, so Theorem 1.2 cannot then be applied. $\diamond$

Although the ability to verify the existence of a solution to the equation $f(x) = 0$ is important, none of what has been said so far provides a *method* for solving this equation. The following definition is a first step in this direction: it will lead to the construction of an algorithm for computing an approximation to the fixed point ξ of the function g, and will thereby supply an approximate solution to the equivalent equation $f(x) = 0$.

Definition 1.1 *Suppose that g is a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line, and assume that $g(x) \in [a, b]$ for all $x \in [a, b]$. Given that $x_0 \in [a, b]$, the recursion defined by*

$$\boxed{x_{k+1} = g(x_k)\,, \qquad k = 0, 1, 2, \ldots\,, \qquad (1.3)}$$

is called a **simple iteration***; the numbers x_k, $k \geq 0$, are referred to as* **iterates***.*

If the sequence (x_k) defined by (1.3) converges, the limit must be a fixed point of the function g, since g is continuous on a closed interval. Indeed, writing $\xi = \lim_{k\to\infty} x_k$, we have that

$$\xi = \lim_{k\to\infty} x_{k+1} = \lim_{k\to\infty} g(x_k) = g\left(\lim_{k\to\infty} x_k\right) = g(\xi)\,, \qquad (1.4)$$

where the second equality follows from (1.3) and the third equality is a consequence of the continuity of g.

A sufficient condition for the convergence of the sequence (x_k) is provided by our next result which represents a refinement of Brouwer's Fixed Point Theorem, under the additional assumption that the mapping g is a contraction.

Definition 1.2 (Contraction) *Suppose that g is a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line. Then, g is said to be a* **contraction** *on $[a, b]$ if there exists a constant L such that $0 < L < 1$ and*

$$|g(x) - g(y)| \leq L|x - y| \quad \forall\, x, y \in [a, b]\,. \qquad (1.5)$$

Remark 1.2 *The terminology 'contraction' stems from the fact that when (1.5) holds with $0 < L < 1$, the distance $|\,g(x) - g(y)\,|$ between the images of the points x, y is (at least $1/L$ times)* smaller *than the distance*

$|\, x - y \,|$ *between* x *and* y. *More generally, when* L *is any positive real number, (1.5) is referred to as a* **Lipschitz condition**.[1]

Armed with Definition 1.2, we are now ready to state the main result of this section.

Theorem 1.3 (Contraction Mapping Theorem) *Let* g *be a real-valued function, defined and continuous on a bounded closed interval* $[a, b]$ *of the real line, and assume that* $g(x) \in [a, b]$ *for all* $x \in [a, b]$. *Suppose, further, that* g *is a contraction on* $[a, b]$. *Then,* g *has a unique fixed point* ξ *in the interval* $[a, b]$. *Moreover, the sequence* (x_k) *defined by (1.3) converges to* ξ *as* $k \to \infty$ *for any starting value* x_0 *in* $[a, b]$.

Proof The existence of a fixed point ξ for g is a consequence of Theorem 1.2. The uniqueness of this fixed point follows from (1.5) by contradiction: for suppose that g has a second fixed point, η, in $[a, b]$. Then,

$$|\, \xi - \eta \,| = |\, g(\xi) - g(\eta) \,| \leq L |\, \xi - \eta \,| \,,$$

i.e., $(1 - L)|\, \xi - \eta \,| \leq 0$. As $1 - L > 0$, we deduce that $\eta = \xi$.

Let x_0 be any element of $[a, b]$ and consider the sequence (x_k) defined by (1.3). We shall prove that (x_k) converges to the fixed point ξ. According to (1.5) we have that

$$|\, x_k - \xi \,| = |\, g(x_{k-1}) - g(\xi) \,| \leq L |\, x_{k-1} - \xi \,| \,, \qquad k \geq 1 \,,$$

from which we then deduce by induction that

$$|\, x_k - \xi \,| \leq L^k |\, x_0 - \xi \,| \,, \qquad k \geq 1 \,. \tag{1.6}$$

As $L \in (0, 1)$, it follows that $\lim_{k \to \infty} L^k = 0$, and hence we conclude that $\lim_{k \to \infty} |\, x_k - \xi \,| = 0$. □

Let us illustrate the Contraction Mapping Theorem by an example.

Example 1.2 *Consider the equation* $f(x) = 0$ *on the interval* $[1, 2]$ *with* $f(x) = \mathrm{e}^x - 2x - 1$, *as in Example 1.1. Recall from Example 1.1 that this equation has a solution,* ξ, *in the interval* $[1, 2]$, *and* ξ *is a fixed point of the function* g *defined on* $[1, 2]$ *by* $g(x) = \ln(2x + 1)$.

[1] Rudolf Otto Sigismund Lipschitz (14 May 1832, Königsberg, Prussia (now Kaliningrad, Russia) – 7 October 1903, Bonn, Germany) made important contributions to number theory, the theory of Bessel functions and Fourier series, the theory of ordinary and partial differential equations, and to analytical mechanics and potential theory.

Table 1.1. *The sequence (x_k) defined by (1.8).*

k	x_k
0	1.000000
1	1.098612
2	1.162283
3	1.201339
4	1.224563
5	1.238121
6	1.245952
7	1.250447
8	1.253018
9	1.254486
10	1.255323
11	1.255800

Now, the function g is defined and continuous on the interval $[1,2]$, and g is differentiable on $(1,2)$. Thus, by the Mean Value Theorem (Theorem A.3), for any x, y in $[1,2]$ we have that

$$|\, g(x) - g(y)\,| = |\, g'(\eta)(x-y)\,| = |g'(\eta)|\,|\,x-y\,| \tag{1.7}$$

for some η that lies between x and y and is therefore in the interval $[1,2]$. Further, $g'(x) = 2/(2x+1)$ and $g''(x) = -4/(2x+1)^2$. As $g''(x) < 0$ for all x in $[1,2]$, g' is monotonic decreasing on $[1,2]$. Hence $g'(1) \geq g'(\eta) \geq g'(2)$, *i.e.*, $g'(\eta) \in [2/5, 2/3]$. Thus we deduce from (1.7) that

$$|\, g(x) - g(y)\,| \leq L|\,x-y\,| \qquad \forall\, x, y \in [1,2]\,,$$

with $L = 2/3$. According to the Contraction Mapping Theorem, the sequence (x_k) defined by the simple iteration

$$x_{k+1} = \ln(2x_k + 1)\,, \qquad k = 0, 1, 2, \dots, \tag{1.8}$$

converges to ξ for any starting value x_0 in $[1,2]$. Let us choose $x_0 = 1$, for example, and compute the next 11 iterates, say. The results are shown in Table 1.1. Even though we have carried six decimal digits, after 11 iterations only the first two decimal digits of the iterates x_k appear to have settled; thus it seems likely that $\xi = 1.26$ to two decimal digits. ◇

You may now wonder how many iterations we should perform in (1.8) to ensure that all six decimals have converged to their correct values. In order to answer this question, we need to carry out some analysis.

Theorem 1.4 *Consider the simple iteration (1.3) where the function g satisfies the hypotheses of the Contraction Mapping Theorem on the bounded closed interval $[a,b]$. Given $x_0 \in [a,b]$ and a certain tolerance $\varepsilon > 0$, let $k_0(\varepsilon)$ denote the smallest positive integer such that x_k is no more than ε away from the (unknown) fixed point ξ, i.e., $|x_k - \xi| \le \varepsilon$, for all $k \ge k_0(\varepsilon)$. Then,*

$$k_0(\varepsilon) \le \left[\frac{\ln|\,x_1 - x_0\,| - \ln(\varepsilon(1-L))}{\ln(1/L)}\right] + 1\,, \tag{1.9}$$

where, for a real number x, $[x]$ signifies the largest integer less than or equal to x.

Proof From (1.6) in the proof of Theorem 1.3 we know that

$$|x_k - \xi| \le L^k\,|x_0 - \xi|\,, \quad k \ge 1\,.$$

Using this result with $k = 1$, we obtain

$$\begin{aligned} |x_0 - \xi| &= |x_0 - x_1 + x_1 - \xi| \\ &\le |x_0 - x_1| + |x_1 - \xi| \\ &\le |x_0 - x_1| + L|x_0 - \xi|\,. \end{aligned}$$

Hence

$$|x_0 - \xi| \le \frac{1}{1-L}|x_0 - x_1|\,.$$

By substituting this into (1.6) we get

$$|x_k - \xi| \le \frac{L^k}{1-L}|x_1 - x_0|\,. \tag{1.10}$$

Thus, in particular, $|x_k - \xi| \le \varepsilon$ provided that

$$L^k \frac{1}{1-L}\,|x_1 - x_0| \le \varepsilon\,.$$

On taking the (natural) logarithm of each side in the last inequality, we find that $|x_k - \xi| \le \varepsilon$ for all k such that

$$k \ge \frac{\ln|x_1 - x_0| - \ln(\varepsilon(1-L))}{\ln(1/L)}\,.$$

Therefore, the smallest integer $k_0(\varepsilon)$ such that $|x_k - \xi| \le \varepsilon$ for all

$k \geq k_0(\varepsilon)$ cannot exceed the expression on the right-hand side of the inequality (1.9). □

This result provides an upper bound on the maximum number of iterations required to ensure that the error between the kth iterate x_k and the (unknown) fixed point ξ is below the prescribed tolerance ε. Note, in particular, from (1.9), that if L is close to 1, then $k_0(\varepsilon)$ may be quite large for any fixed ε. We shall revisit this point later on in the chapter.

Example 1.3 *Now we can return to Example 1.2 to answer the question posed there about the maximum number of iterations required, with starting value $x_0 = 1$, to ensure that the last iterate computed is correct to six decimal digits.*

Letting $\varepsilon = 0.5 \times 10^{-6}$ and recalling from Example 1.2 that $L = 2/3$, the formula (1.9) yields $k_0(\varepsilon) \leq [32.778918] + 1$, so we have that $k_0(\varepsilon) \leq 33$. In fact, 33 is a somewhat pessimistic overestimate of the number of iterations required: computing the iterates x_k successively shows that already x_{25} is correct to six decimal digits, giving $\xi = 1.256431$. ◇

Condition (1.5) can be rewritten in the following equivalent form:

$$\left| \frac{g(x) - g(y)}{x - y} \right| \leq L \qquad \forall\, x, y \in [a, b]\,, \quad x \neq y\,,$$

with $L \in (0, 1)$, which can, in turn, be rephrased by saying that the absolute value of the slope of the function g does not exceed $L \in (0, 1)$. Assuming that g is a differentiable function on the open interval (a, b), the Mean Value Theorem (Theorem A.3) tells us that

$$\frac{g(x) - g(y)}{x - y} = g'(\eta)$$

for some η that lies between x and y and is therefore contained in the interval (a, b).

We shall therefore adopt the following assumption that is somewhat stronger than (1.5) but is easier to verify in practice:

$$\begin{aligned} &g \text{ is differentiable on } (a, b) \text{ and} \\ &\exists L \in (0, 1) \text{ such that } |g'(x)| \leq L \text{ for all } x \in (a, b)\,. \end{aligned} \tag{1.11}$$

Consequently, Theorem 1.3 still holds when (1.5) is replaced by (1.11).

We note that the requirement in (1.11) that g be differentiable is indeed more demanding than the Lipschitz condition (1.5): for example, $g(x) = |x|$ satisfies the Lipschitz condition on any closed interval of the real line, with $L = 1$, yet g is not differentiable at $x = 0$.[1]

Next we discuss a local version of the Contraction Mapping Theorem, where (1.11) is only assumed in a neighbourhood of the fixed point ξ rather than over the entire interval $[a, b]$.

Theorem 1.5 *Suppose that g is a real-valued function, defined and continuous on a bounded closed interval $[a, b]$ of the real line, and assume that $g(x) \in [a, b]$ for all $x \in [a, b]$. Let $\xi = g(\xi) \in [a, b]$ be a fixed point of g (whose existence is ensured by Theorem 1.2), and assume that g has a continuous derivative in some neighbourhood of ξ with $|g'(\xi)| < 1$. Then, the sequence (x_k) defined by $x_{k+1} = g(x_k)$, $k \geq 0$, converges to ξ as $k \to \infty$, provided that x_0 is sufficiently close to ξ.*

Proof By hypothesis, there exists $h > 0$ such that g' is continuous in the interval $[\xi - h, \xi + h]$. Since $|g'(\xi)| < 1$ we can find a smaller interval $I_\delta = [\xi - \delta, \xi + \delta]$, where $0 < \delta \leq h$, such that $|g'(x)| \leq L$ in this interval, with $L < 1$. To do so, take $L = \frac{1}{2}(1 + |g'(\xi)|)$ and then choose $\delta \leq h$ such that

$$|g'(x) - g'(\xi)| \leq \tfrac{1}{2}(1 - |g'(\xi)|)$$

for all x in I_δ; this is possible since g' is continuous at ξ. Hence,

$$|g'(x)| \leq |g'(x) - g'(\xi)| + |g'(\xi)| \leq \tfrac{1}{2}(1 - |g'(\xi)|) + |g'(\xi)| = L$$

for all $x \in I_\delta$. Now, suppose that x_k lies in the interval I_δ. Then,

$$x_{k+1} - \xi = g(x_k) - \xi = g(x_k) - g(\xi) = (x_k - \xi)g'(\eta_k)$$

by the Mean Value Theorem (Theorem A.3), where η_k lies between x_k and ξ, and therefore also belongs to I_δ. Hence $|g'(\eta_k)| \leq L$, and

$$|x_{k+1} - \xi| \leq L|x_k - \xi|\,. \tag{1.12}$$

This shows that x_{k+1} also lies in I_δ, and a simple argument by induction shows that if x_0 belongs to I_δ, then all x_k, $k \geq 0$, are in I_δ, and also

$$|x_k - \xi| \leq L^k|x_0 - \xi|\,, \qquad k \geq 0\,. \tag{1.13}$$

Since $0 < L < 1$ this implies that the sequence (x_k) converges to ξ. □

[1] If you are familiar with the concept of Lebesgue measure, you will find the following result, known as **Rademacher's Theorem**, revealing. *A function f satisfying the Lipschitz condition (1.5) on an interval $[a, b]$ is differentiable on $[a, b]$, except, perhaps, at the points of a subset of zero Lebesgue measure.*

If the conditions of Theorem 1.5 are satisfied in the vicinity of a fixed point ξ, then the sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k \geq 0$, will converge to ξ for any starting value x_0 that is sufficiently close to ξ. If, on the other hand, the conditions of Theorem 1.5 are violated, there is no guarantee that any sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k \geq 0$, will converge to the fixed point ξ for any starting value x_0 near ξ. In order to distinguish between these two cases, we introduce the following definition.

Definition 1.3 *Suppose that g is a real-valued function, defined and continuous on the bounded closed interval $[a, b]$, such that $g(x) \in [a, b]$ for all $x \in [a, b]$, and let ξ denote a fixed point of g. We say that ξ is a* **stable fixed point** *of g, if the sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k \geq 0$, converges to ξ whenever the starting value x_0 is sufficiently close to ξ. Conversely, if no sequence (x_k) defined by this iteration converges to ξ for any starting value x_0 close to ξ, except for $x_0 = \xi$, then we say that ξ is an* **unstable fixed point** *of g.*

We note that, with this definition, a fixed point may be neither stable nor unstable (see Exercise 2).

As will be demonstrated below in Example 1.5, even some very simple functions may possess both stable and unstable fixed points. Theorem 1.5 shows that if g' is continuous in a neighbourhood of ξ, then the condition $|g'(\xi)| < 1$ is sufficient to ensure that ξ is a stable fixed point. The case of an unstable fixed point will be considered later, in Theorem 1.6.

Now, assuming that ξ is a stable fixed point of g, we may also be interested in the speed at which the sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k \geq 0$, converges to ξ. Under the hypotheses of Theorem 1.5, it follows from the proof of that theorem that

$$\lim_{k\to\infty} \frac{|x_{k+1} - \xi|}{|x_k - \xi|} = \lim_{k\to\infty} \left| \frac{g(x_k) - g(\xi)}{x_k - \xi} \right| = |g'(\xi)| \,. \tag{1.14}$$

Consequently, we can regard $|g'(\xi)| \in (0, 1)$ as a measure of the speed of convergence of the sequence (x_k) to the fixed point ξ.

Definition 1.4 *Suppose that $\xi = \lim_{k\to\infty} x_k$. We say that the sequence (x_k) converges to ξ* **at least linearly** *if there exist a sequence (ε_k) of positive real numbers converging to 0, and $\mu \in (0, 1)$, such that*

$$|x_k - \xi| \leq \varepsilon_k \,, \quad k = 0, 1, 2, \ldots \,, \qquad \text{and} \qquad \lim_{k\to\infty} \frac{\varepsilon_{k+1}}{\varepsilon_k} = \mu \,. \tag{1.15}$$

If (1.15) holds with $\mu = 0$, then the sequence (x_k) is said to converge to ξ **superlinearly***.*

If (1.15) holds with $\mu \in (0,1)$ and $\varepsilon_k = |x_k - \xi|$, $k = 0, 1, 2, \ldots$, then (x_k) is said to converge to ξ **linearly***, and the number $\rho = -\log_{10} \mu$ is then called the* **asymptotic rate of convergence** *of the sequence. If (1.15) holds with $\mu = 1$ and $\varepsilon_k = |x_k - \xi|$, $k = 0, 1, 2, \ldots$, the rate of convergence is slower than linear and we say that the sequence converges to ξ* **sublinearly***.*

The words 'at least' in this definition refer to the fact that we only have inequality in $|x_k - \xi| \leq \varepsilon_k$, which may be all that can be ascertained in practice. Thus, it is really the sequence of bounds ε_k that converges linearly.

For a linearly convergent sequence the asymptotic rate of convergence ρ measures the number of correct decimal digits gained in one iteration; in particular, the number of iterations required in order to gain one more correct decimal digit is at most $[1/\rho] + 1$. Here $[1/\rho]$ denotes the largest integer that is less than or equal to $1/\rho$.

Under the hypotheses of Theorem 1.5, the equalities (1.14) will hold with $\mu = |g'(\xi)| \in [0, 1)$, and therefore the sequence (x_k) generated by the simple iteration will converge to the fixed point ξ linearly or superlinearly.

Example 1.4 *Given that α is a fixed positive real number, consider the function g defined on the interval $[0,1]$ by*

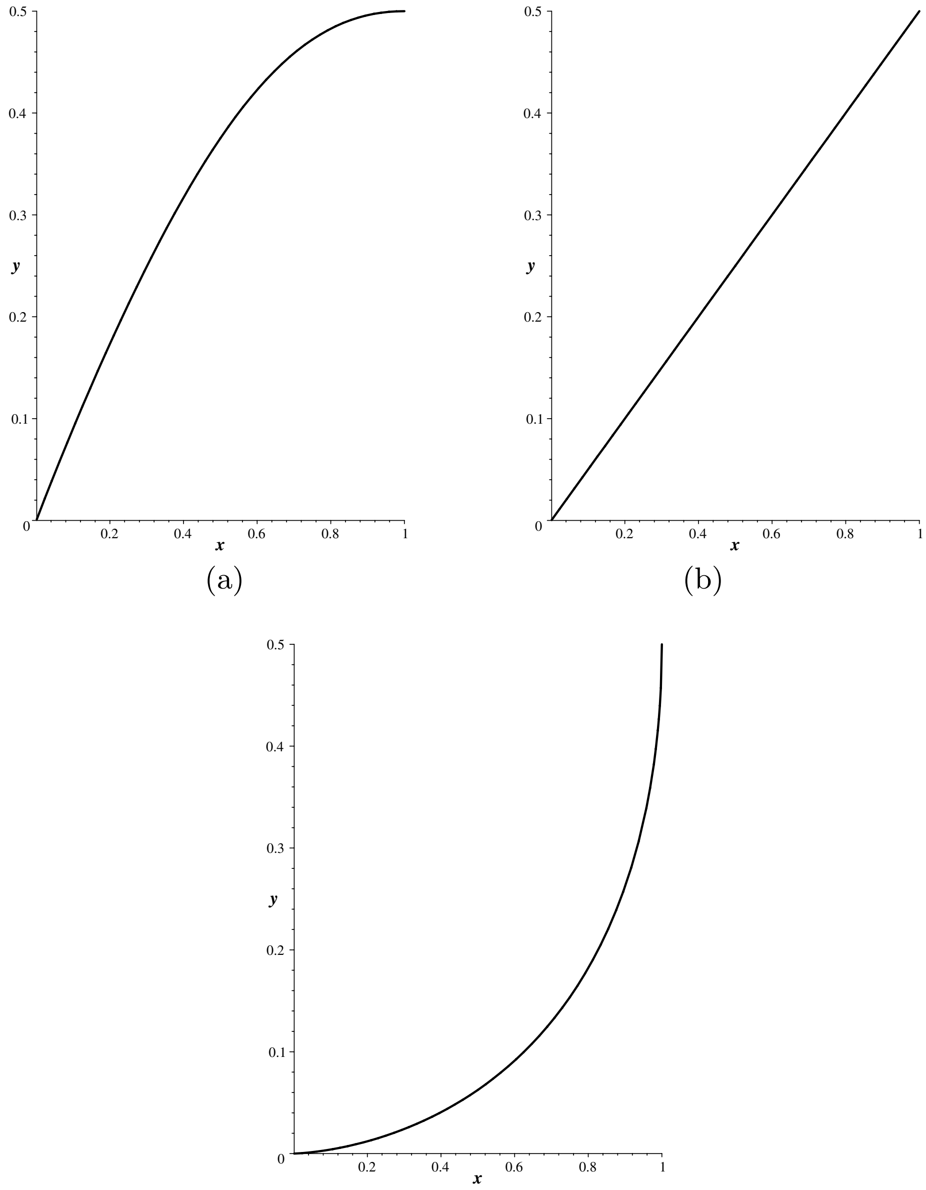
$$g(x) = \begin{cases} 2^{-\left\{1+(\log_2(1/x))^{1/\alpha}\right\}^{\alpha}} & \textit{for } 0 < x \leq 1\,, \\ 0 & \textit{for } x = 0\,. \end{cases}$$

As $\lim_{x \to 0+} g(x) = 0$, the function g is continuous on $[0,1]$. Moreover, g is strictly monotonic increasing on $[0,1]$ and $g(x) \in [0, 1/2] \subset [0,1]$ for all x in $[0,1]$. We note that $\xi = 0$ is a fixed point of g (cf. Figure 1.3).

Consider the sequence (x_k) defined by $x_{k+1} = g(x_k)$, $k \geq 0$, with $x_0 = 1$. It is a simple matter to show by induction that $x_k = 2^{-k^{\alpha}}$, $k \geq 0$. Thus we deduce that (x_k) converges to $\xi = 0$ as $k \to \infty$. Since

$$\lim_{k \to \infty} \left| \frac{x_{k+1}}{x_k} \right| = \mu = \begin{cases} 1 & \text{for } 0 < \alpha < 1\,, \\ \frac{1}{2} & \text{for } \alpha = 1\,, \\ 0 & \text{for } \alpha > 1\,, \end{cases}$$

we conclude that for $\alpha \in (0,1)$ the sequence (x_k) converges to $\xi = 0$ sublinearly. For $\alpha = 1$ it converges to $\xi = 0$ linearly with asymptotic rate



(a)

(b)

(c)

Fig. 1.3. Graph of the function g from Example 1.4 on the interval $x \in [0, 1]$ for (a) $\alpha = 1/2$, (b) $\alpha = 1$, (c) $\alpha = 2$.

$\rho = -\log_{10} \mu = \log_{10} 2$. When $\alpha > 1$, the sequence converges to the fixed point $\xi = 0$ superlinearly. The same conclusions could have been reached by showing (through tedious differentiation) that $\lim_{x \to 0+} g'(x) = \mu$, with μ as defined above for the various values of the parameter α. ◇

For a linearly convergent simple iteration $x_{k+1} = g(x_k)$, where g' is continuous in a neighbourhood of the fixed point ξ and $0 < |g'(\xi)| < 1$, Definition 1.4 and (1.14) imply that the asymptotic rate of convergence of the sequence (x_k) is $\rho = -\log_{10}|g'(\xi)|$. Evidently, a small value of $|g'(\xi)|$ corresponds to a large positive value of ρ and will result in more rapid convergence, while if $|g'(\xi)| < 1$ but $|g'(\xi)|$ is very close to 1, ρ will be a small positive number and the sequence will converge very slowly.[1]

Next, we discuss the behaviour of the iteration (1.3) in the vicinity of an *unstable fixed point* ξ. If $|g'(\xi)| > 1$, then the sequence (x_k) defined by (1.3) does not converge to ξ from any starting value x_0; the next theorem gives a rigorous proof of this fact.

Theorem 1.6 *Suppose that $\xi = g(\xi)$, where the function g has a continuous derivative in some neighbourhood of ξ, and let $|g'(\xi)| > 1$. Then, the sequence (x_k) defined by $x_{k+1} = g(x_k)$, $k \geq 0$, does not converge to ξ from any starting value x_0, $x_0 \neq \xi$.*

Proof Suppose that $x_0 \neq \xi$. As in the proof of Theorem 1.5, we can see that there is an interval $I_\delta = [\xi-\delta, \xi+\delta]$, $\delta > 0$, in which $|g'(x)| \geq L > 1$ for some constant L. If x_k lies in this interval, then

$$|x_{k+1} - \xi| = |g(x_k) - g(\xi)| = |(x_k - \xi)\, g'(\eta_k)| \geq L|x_k - \xi|\,,$$

for some η_k between x_k and ξ. If x_{k+1} lies in I_δ the same argument shows that

$$|x_{k+2} - \xi| \geq L|x_{k+1} - \xi| \geq L^2|x_k - \xi|\,,$$

and so on. Evidently, after a finite number of steps some member of the sequence $x_{k+1}, x_{k+2}, x_{k+3}, \ldots$ must be outside the interval I_δ, since $L > 1$. Hence there can be no value of $k_0 = k_0(\delta)$ such that $|x_k - \xi| \leq \delta$ for all $k \geq k_0$, and the sequence therefore does not converge to ξ. □

Example 1.5 *In this example we explore the simple iteration (1.3) for g defined by*

$$g(x) = \tfrac{1}{2}(x^2 + c)$$

where $c \in \mathbb{R}$ is a fixed constant.

The fixed points of the function g are the solutions of the quadratic equation $x^2 - 2x + c = 0$, which are $1 \pm \sqrt{(1-c)}$. If $c > 1$ there are no solutions (in the set $\mathbb{R}$ of real numbers, that is!), if $c = 1$ there is one solution in $\mathbb{R}$, and if $c < 1$ there are two.

[1] Thus $0 < \rho \ll 1$ corresponds to slow linear convergence and $\rho \gg 1$ to fast linear convergence. It is for this reason that we defined the asymptotic rate of convergence ρ, for a linearly convergent sequence, as $-\log_{10}\mu$ (or $-\log_{10}|g'(\xi)|$) rather than μ (or $|g'(\xi)|$).

Suppose now that $c < 1$; we denote the solutions by $\xi_1 = 1 - \surd(1-c)$ and $\xi_2 = 1 + \surd(1-c)$, so that $\xi_1 < 1 < \xi_2$. We see at once that $g'(x) = x$, so the fixed point ξ_2 is unstable, but that the fixed point ξ_1 is stable provided that $-3 < c < 1$. In fact, it is easy to see that the sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k \geq 0$, will converge to ξ_1 if the starting value x_0 satisfies $-\xi_2 < x_0 < \xi_2$. (See Exercise 1.) If c is close to 1, $g'(\xi_1)$ will also be close to 1 and convergence will be slow. When $c = 0$, $\xi_1 = 0$ so that convergence is superlinear. This is an example of quadratic convergence which we shall meet later. ◇

The purpose of our next example is to illustrate the concept of asymptotic rate of convergence. According to Definition 1.4, the asymptotic rate of convergence of a sequence describes the relative closeness of successive terms in the sequence to the limit ξ as $k \to \infty$. Of course, for small values of k the sequence may behave in quite a different way, and since in practical computation we are interested in approximating the limit of the sequence by using just a small number of terms, the asymptotic rate of convergence may sometimes give a misleading impression.

Example 1.6 *In this example we study the convergence of the sequences* (u_k) *and* (v_k) *defined by*

$$\begin{aligned} u_{k+1} &= g_1(u_k), \qquad k = 0, 1, 2, \ldots, \qquad u_0 = 1\,, \\ v_{k+1} &= g_2(v_k), \qquad k = 0, 1, 2, \ldots, \qquad v_0 = 1\,, \end{aligned}$$

where

$$g_1(x) = 0.99x \qquad \textit{and} \qquad g_2(x) = \frac{x}{(1 + x^{1/10})^{10}}\,.$$

Each of the two functions has a fixed point at $\xi = 0$, and we easily find that $g_1'(0) = 0.99$, $g_2'(0) = 1$. Hence the sequence (u_k) is linearly convergent to zero with asymptotic rate of convergence $\rho = -\log_{10} 0.99 \approx 0.004$, while Theorem 1.5 does not apply to the sequence (v_k). It is quite easy to show by induction that $v_k = (k+1)^{-10}$, so the sequence (v_k) also converges to zero, but since $\lim_{k\to\infty}(v_{k+1}/v_k) = 1$ the convergence is sublinear. This means that, in the limit, (u_k) will converge faster than (v_k). However, this is not what happens for small k, as Table 1.2 shows very clearly.

The sequence (v_k) has converged to zero correct to 6 decimal digits when $k = 4$, and to 10 decimal digits when $k = 10$, at which stage u_k

Table 1.2. *The sequences (u_k) and (v_k) in Example 1.6.*

k	u_k	v_k
0	1.000000	1.000000
1	0.990000	0.000977
2	0.980100	0.000017
3	0.970299	0.000001
4	0.960596	0.000000
5	0.950990	0.000000
6	0.941480	0.000000
7	0.932065	0.000000
8	0.922745	0.000000
9	0.913517	0.000000
10	0.904382	0.000000

is still larger than 0.9. Although (u_k) eventually converges faster than v_k, we find that $u_k = (0.99)^k$ becomes smaller than $v_k = (k+1)^{-10}$ when

$$k > \frac{10}{\ln(1/0.99)} \ln(k+1)\,.$$

This first happens when $k = 9067$, at which point u_k and v_k are both roughly 10^{-40}. In this rather extreme example the concept of asymptotic rate of convergence is not useful, since for any practical purposes (v_k) converges faster than (u_k). ◇

1.3 Iterative solution of equations

In this section we apply the idea of simple iteration to the solution of equations. Given a real-valued continuous function f, we wish to construct a sequence (x_k), using iteration, which converges to a solution of $f(x) = 0$. We begin with an example where it is easy to derive various such sequences; in the next section we shall describe a more general approach.

Example 1.7 *Consider the problem of determining the solutions of the equation $f(x) = 0$, where $f\colon x \mapsto \mathrm{e}^x - x - 2$.*

Since $f'(x) = \mathrm{e}^x - 1$ the function f is monotonic increasing for positive x and monotonic decreasing for negative values of x. Moreover,

$$\left.\begin{aligned} f(1) &= \mathrm{e} - 3 < 0\,, \\ f(2) &= \mathrm{e}^2 - 4 > 0\,, \\ f(-1) &= \mathrm{e}^{-1} - 1 < 0\,, \\ f(-2) &= \mathrm{e}^{-2} > 0\,. \end{aligned}\right\} \tag{1.16}$$

Hence the equation $f(x) = 0$ has exactly one positive solution, which lies in the interval $(1, 2)$, and exactly one negative solution, which lies in the interval $(-2, -1)$. This is illustrated in Figure 1.4, which shows the graphs of the functions $x \mapsto \mathrm{e}^x$ and $x \mapsto x + 2$ on the same axes. We shall write ξ_1 for the positive solution and ξ_2 for the negative solution.

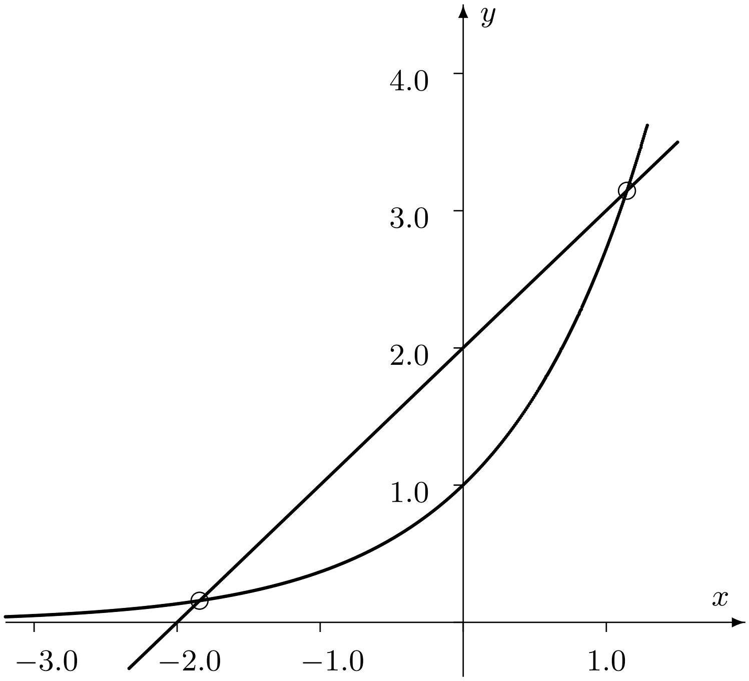


Fig. 1.4. Graphs of $y = \mathrm{e}^x$ and $y = x + 2$.

The equation $f(x) = 0$ may be written in the equivalent form

$$x = \ln(x + 2)\,,$$

which suggests a simple iteration defined by $g(x) = \ln(x + 2)$. We shall show that the positive solution ξ_1 is a stable fixed point of g, while ξ_2 is an unstable fixed point of g.

Clearly, $g'(x) = 1/(x + 2)$, so $0 < g'(\xi_1) < 1$, since ξ_1 is the positive solution. Therefore, by Theorem 1.5, the sequence (x_k) defined by the iteration

$$x_{k+1} = \ln(x_k + 2)\,, \qquad k = 0, 1, 2, \dots\,, \tag{1.17}$$

will converge to the positive solution, ξ_1, provided that the starting value x_0 is sufficiently close to it.[1] As $0 < g'(\xi_1) < 1/3$, the asymptotic rate of convergence of (x_k) to ξ_1 is certainly greater than $\log_{10} 3$.

On the other hand, $g'(\xi_2) > 1$ since $-2 < \xi_2 < -1$, so the sequence (x_k) defined by (1.17) cannot converge to the solution ξ_2. It is not difficult to prove that for $x_0 > \xi_2$ the sequence (x_k) converges to ξ_1 while if $x_0 < \xi_2$ the sequence will decrease monotonically until $x_k \leq -2$ for some k, and then the iteration breaks down as $g(x_k)$ becomes undefined.

The equation $f(x) = 0$ may also be written in the form $x = \mathrm{e}^x - 2$, suggesting the sequence (x_k) defined by the iteration

$$x_{k+1} = \mathrm{e}^{x_k} - 2\,, \qquad k = 0, 1, 2, \dots\,.$$

In this case $g(x) = \mathrm{e}^x - 2$ and $g'(x) = \mathrm{e}^x$. Hence $g'(\xi_1) > 1$, $g'(\xi_2) < \mathrm{e}^{-1}$, showing that the sequence (x_k) may converge to ξ_2, but cannot converge to ξ_1. It is quite straightforward to show that the sequence converges to ξ_2 for any $x_0 < \xi_1$, but diverges to $+\infty$ when $x_0 > \xi_1$.

As a third alternative, consider rewriting the equation $f(x) = 0$ as $x = g(x)$ where the function g is defined by $g(x) = x(\mathrm{e}^x - x)/2$; the fixed points of the associated iteration $x_{k+1} = g(x_k)$ are the solutions ξ_1 and ξ_2 of $f(x) = 0$, and also the point 0. For this iteration neither of the fixed points, ξ_1 or ξ_2, is stable, and the sequence (x_k) either converges to 0 or diverges to $\pm\infty$.

Evidently the given equation may be written in many different forms, leading to iterations with different properties. ◇

1.4 Relaxation and Newton's method

In the previous section we saw how various ingenious devices lead to iterations which may or may not converge to the desired solutions of a given equation $f(x) = 0$. We would obviously benefit from a more generally applicable iterative method which would, except possibly in special cases, produce a sequence (x_k) that always converges to a required solution. One way of constructing such a sequence is by relaxation.

[1] In fact, by applying the Contraction Mapping Theorem on an arbitrary bounded closed interval $[0, M]$ where $M > \xi_1$, we conclude that the sequence (x_k) defined by the iteration (1.17) will converge to ξ_1 from any positive starting value x_0.

Definition 1.5 *Suppose that f is a real-valued function, defined and continuous in a neighbourhood of a real number ξ.* **Relaxation** *uses the sequence (x_k) defined by*

$$\boxed{x_{k+1} = x_k - \lambda f(x_k)\,, \qquad k = 0, 1, 2, \dots\,, \qquad (1.18)}$$

where $\lambda \neq 0$ is a fixed real number whose choice will be made clear below, and x_0 is a given starting value near ξ.

If the sequence (x_k) defined by (1.18) converges to ξ, then ξ is a solution of the equation $f(x) = 0$, as we assume that f is continuous.

It is clear from (1.18) that relaxation is a simple iteration of the form $x_{k+1} = g(x_k)$, $k = 0, 1, 2, \dots$, with $g(x) = x - \lambda f(x)$. Suppose now, further, that f is differentiable in a neighbourhood of ξ. It then follows that $g'(x) = 1 - \lambda f'(x)$ for all x in this neighbourhood; hence, if $f(\xi) = 0$ and $f'(\xi) \neq 0$, the sequence (x_k) defined by the iteration $x_{k+1} = g(x_k)$, $k = 0, 1, 2, \dots$, will converge to ξ if we choose λ to have the same sign as $f'(\xi)$, to be not too large, and take x_0 sufficiently close to ξ. This idea is made more precise in the next theorem.

Theorem 1.7 *Suppose that f is a real-valued function, defined and continuous in a neighbourhood of a real number ξ, and let $f(\xi) = 0$. Suppose further that f' is defined and continuous in some neighbourhood of ξ, and let $f'(\xi) \neq 0$. Then, there exist positive real numbers λ and δ such that the sequence (x_k) defined by the relaxation iteration (1.18) converges to ξ for any x_0 in the interval $[\xi - \delta, \xi + \delta]$.*

Proof Suppose that $f'(\xi) = \alpha$, and that α is positive. If $f'(\xi)$ is negative, the proof is similar, with appropriate changes of sign. Since f' is continuous in some neighbourhood of ξ, we can find a positive real number δ such that $f'(x) \geq \frac{1}{2}\alpha$ in the interval $[\xi - \delta, \xi + \delta]$. Let M be an upper bound for $f'(x)$ in this interval. Hence $M \geq \frac{1}{2}\alpha$. In order to fix the value of the real number λ, we begin by noting that, for any $\lambda > 0$,

$$1 - \lambda M \leq 1 - \lambda f'(x) \leq 1 - \tfrac{1}{2}\lambda\alpha\,, \qquad x \in [\xi - \delta, \xi + \delta]\,.$$

We now choose λ so that these extreme values are equal and opposite, *i.e.*, $1 - \lambda M = -\vartheta$ and $1 - \frac{1}{2}\lambda\alpha = \vartheta$ for a suitable nonnegative real number ϑ. There is a unique value of ϑ for which this holds; it is given by the formula

$$\vartheta = \frac{2M - \alpha}{2M + \alpha}\,,$$

corresponding to

$$\lambda = \frac{4}{2M + \alpha}\,.$$

On defining $g(x) = x - \lambda f(x)$, we then deduce that

$$|g'(x)| \le \vartheta < 1\,, \quad x \in [\xi - \delta, \xi + \delta]\,. \tag{1.19}$$

Thus we can apply Theorem 1.5 to conclude that the sequence (x_k) defined by the relaxation iteration (1.18) converges to ξ, provided that x_0 is in the interval $[\xi - \delta, \xi + \delta]$. The asymptotic rate of convergence of the relaxation iteration (1.18) to ξ is at least $-\log_{10}\vartheta$. □

We can now extend the idea of relaxation by allowing λ to be a continuous function of x in a neighbourhood of ξ rather than just a constant. This suggests an iteration

$$x_{k+1} = x_k - \lambda(x_k)f(x_k)\,, \qquad k = 0, 1, 2, \dots\,,$$

corresponding to a simple iteration with $g(x) = x - \lambda(x)f(x)$. If the sequence (x_k) converges, the limit ξ will be a solution of $f(x) = 0$, except possibly when $\lambda(\xi) = 0$. Moreover, as we have seen, the ultimate rate of convergence is determined by $g'(\xi)$. Since $f(\xi) = 0$, it follows that $g'(\xi) = 1 - \lambda(\xi)f'(\xi)$, and (1.19) suggest using a function λ which makes $1 - \lambda(\xi)f'(\xi)$ small. The obvious choice is $\lambda(x) = 1/f'(x)$, and leads us to Newton's method.[1]

Definition 1.6 *Newton's method for the solution of $f(x) = 0$ is defined by*

$$\boxed{x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}\,, \qquad k = 0, 1, 2, \dots\,, \qquad (1.20)}$$

with prescribed starting value x_0. We implicitly assume in the defining formula (1.20) that $f'(x_k) \neq 0$ for all $k \ge 0$.

[1] Isaac Newton was born on 4 January 1643 in Woolsthorpe, Lincolnshire, England and died on 31 March 1727 in London, England. According to the calendar used in England at the time, Newton was born on Christmas day 1642, and died on 21 March 1727: the Gregorian calendar was not adopted in England until 1752. Newton made revolutionary advances in mathematics, physics, astronomy and optics; his contributions to the foundations of calculus were marred by priority disputes with Leibniz. Newton was appointed to the Lucasian chair at Cambridge at the age of 27. In 1705, two years after becoming president of the Royal Society (a position to which he was re-elected each year until his death), Newton was knighted by Queen Anne; he was the first scientist to be honoured in this way. Newton's *Philosophiae naturalis principia mathematica* is one of the most important scientific books ever written.

Newton's method is a simple iteration with $g(x) = x - f(x)/f'(x)$. Its geometric interpretation is illustrated in Figure 1.5: the tangent to the curve $y = f(x)$ at the point $(x_k, f(x_k))$ is the line with the equation $y - f(x_k) = f'(x_k)(x - x_k)$; it meets the x-axis at the point $(x_{k+1}, 0)$.

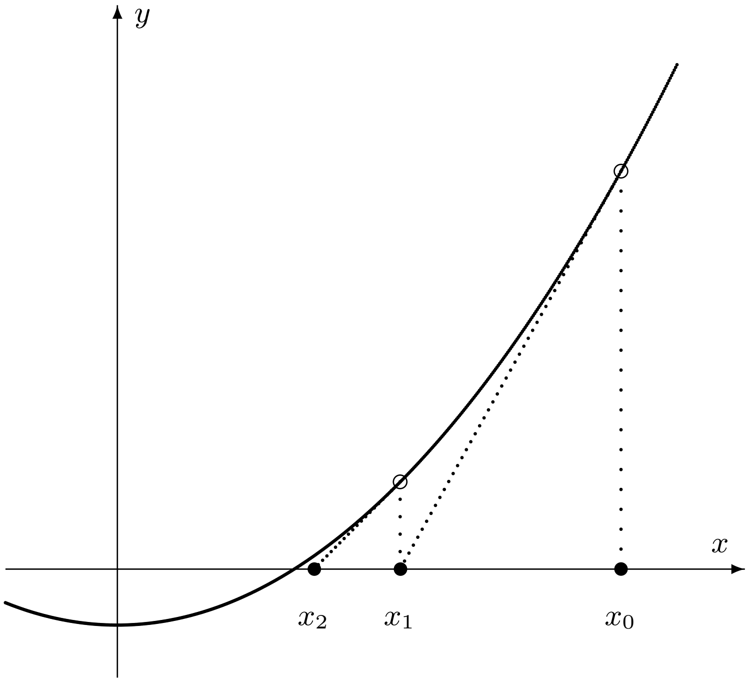


Fig. 1.5. Newton's method.

We could apply Theorem 1.5 to prove the convergence of this iteration, but since generally it converges much faster than ordinary relaxation it is better to apply a special form of proof. First, however, we give a formal definition of quadratic convergence.

Definition 1.7 *Suppose that $\xi = \lim_{k\to\infty} x_k$. We say that the sequence (x_k) converges to ξ* **with at least order** *$q > 1$, if there exist a sequence (ε_k) of positive real numbers converging to 0, and $\mu > 0$, such that*

$$|x_k - \xi| \le \varepsilon_k\,, \quad k = 0, 1, 2, \ldots, \qquad \text{and} \qquad \lim_{k\to\infty} \frac{\varepsilon_{k+1}}{\varepsilon_k^q} = \mu\,. \tag{1.21}$$

If (1.21) holds with $\varepsilon_k = |x_k - \xi|$ for $k = 0, 1, 2, \ldots$, then the sequence (x_k) is said to converge to ξ **with order** *q. In particular, if $q = 2$, then we say that the sequence (x_k) converges to ξ* **quadratically**.

We note that unlike the definition of linear convergence where μ was required to belong to the interval $(0, 1)$, all we demand here is that $\mu > 0$. The reason is simple: when $q > 1$, (1.21) implies suitably rapid decay of the sequence (ε_k) irrespective of the size of μ.

Example 1.8 *Let $c > 1$ and $q > 1$. The sequence (x_k) defined by $x_k = c^{-q^k}$, $k = 0, 1, 2, \ldots$, converges to 0 with order q.*

Theorem 1.8 (Convergence of Newton's method) *Suppose that f is a continuous real-valued function with continuous second derivative f'', defined on the closed interval $I_\delta = [\xi - \delta, \xi + \delta]$, $\delta > 0$, such that $f(\xi) = 0$ and $f''(\xi) \neq 0$. Suppose further that there exists a positive constant A such that*

$$\frac{|f''(x)|}{|f'(y)|} \leq A \qquad \forall\, x, y \in I_\delta\,.$$

If $|\xi - x_0| \leq h$, where h is the smaller of δ and $1/A$, then the sequence (x_k) defined by Newton's method (1.20) converges quadratically to ξ.

Proof Suppose that $|\xi - x_k| \leq h = \min\{\delta, 1/A\}$, so that $x_k \in I_\delta$. Then, by Taylor's Theorem (Theorem A.4), expanding about the point $x_k \in I_\delta$,

$$0 = f(\xi) = f(x_k) + (\xi - x_k)f'(x_k) + \frac{(\xi - x_k)^2}{2} f''(\eta_k)\,, \tag{1.22}$$

for some η_k between ξ and x_k, and therefore in the interval I_δ. Recalling (1.20), this shows that

$$\xi - x_{k+1} = -\frac{(\xi - x_k)^2 f''(\eta_k)}{2f'(x_k)}\,. \tag{1.23}$$

Since $|\xi - x_k| \leq \frac{1}{A}$, we have $|\xi - x_{k+1}| \leq \frac{1}{2}|\xi - x_k|$. As we are given that $|\xi - x_0| \leq h$ it follows by induction that $|\xi - x_k| \leq 2^{-k}h$ for all $k \geq 0$; hence (x_k) converges to ξ as $k \to \infty$.

Now, η_k lies between ξ and x_k, and therefore (η_k) also converges to ξ as $k \to \infty$. Since f' and f'' are continuous on I_δ, it follows from (1.23) that

$$\lim_{k\to\infty} \frac{|x_{k+1} - \xi|}{|x_k - \xi|^2} = \left|\frac{f''(\xi)}{2f'(\xi)}\right|\,, \tag{1.24}$$

which, according to Definition 1.7, implies quadratic convergence of the sequence (x_k) to ξ with $\mu = |f''(\xi)/2f'(\xi)|$, $\mu \in (0, A/2]$. □

The conditions of the theorem implicitly require that $f'(\xi) \neq 0$, for otherwise the quantity $f''(x)/f'(y)$ could not be bounded in a neighbourhood of ξ. (See Exercises 6 and 7 for what happens when $f'(\xi) = 0$.)

One can show that if $f''(\xi) = 0$ and we assume that $f(x)$ has a continuous third derivative, and require certain quantities to be bounded, then the convergence is *cubic* (*i.e.*, convergence with order $q = 3$).

It is possible to demonstrate that Newton's method converges over a wider interval, if we assume something about the signs of the derivatives.

Theorem 1.9 *Suppose that the function f satisfies the conditions of Theorem 1.8 and also that there exists a real number X, $X > \xi$, such that in the interval $J = [\xi, X]$ both f' and f'' are positive. Then, the sequence (x_k) defined by Newton's method (1.20) converges quadratically to ξ from any starting value x_0 in J.*

Proof It follows from (1.23) that if $x_k \in J$, then $x_{k+1} > \xi$. Moreover, since $f'(x) > 0$ on J, f is monotonic increasing on J. As $f(\xi) = 0$, it then follows that $f(x) > 0$ for $\xi < x \leq X$. Hence, $\xi < x_{k+1} < x_k$, $k \geq 0$. Since the sequence (x_k) is bounded and monotonic decreasing, it is convergent; let $\eta = \lim_{k\to\infty} x_k$. Clearly, $\eta \in J$. Further, passing to the limit $k \to \infty$ in (1.20) we have that $f(\eta) = 0$. However, ξ is the only solution of $f(x) = 0$ in J, so $\eta = \xi$, and the sequence converges to ξ.

Having shown that the sequence (x_k) converges, the fact that it converges quadratically follows as in the proof of Theorem 1.8. □

We remark that the same result holds for other possible signs of f' and f'' in a suitable interval J. (See Exercise 8.) The interval J does not have to be bounded; considering, for instance, $f(x) = \mathrm{e}^x - x - 2$ from Example 1.7, it is clear that $f'(x)$ and $f''(x)$ are both positive in the unbounded interval $(0, \infty)$, and the Newton iteration converges to the positive solution of the equation $f(x) = 0$ from any positive starting value x_0.

Note that the definition of quadratic convergence only refers to the behaviour of the sequence for sufficiently large k. In the same example we find that the convergence of the Newton iteration from a large positive value of x_0 is initially very slow. (See Exercise 3.) The possibility of this early behaviour is often emphasised by saying that the convergence of Newton's method is *ultimately* quadratic.

1.5 The secant method

So far we have considered iterations which can be written in the form $x_{k+1} = g(x_k)$, $k \geq 0$, so that the new value is expressed in terms of the old one. It is also possible to define an iteration of the form $x_{k+1} = g(x_k, x_{k-1})$, $k \geq 1$, where the new value is expressed in terms of two previous values. In particular, we shall consider two applications of this idea, leading to the secant method and the method of bisection, respectively.

Remark 1.3 *We note in passing that one can consider more general iterative methods of the form*

$$x_{k+1} = g(x_k, x_{k-1}, \ldots, x_{k-\ell}), \qquad k = \ell, \ell+1, \ldots,$$

with $\ell \geq 1$ fixed; here, we shall confine ourselves to the simplest case when $\ell = 1$ as this is already sufficiently illuminating.

Using Newton's method to solve a nonlinear equation $f(x) = 0$ requires explicit knowledge of the first derivative f' of the function f. Unfortunately, in many practical situations f' is not explicitly available or it can only be obtained at high computational cost. In such cases, the value $f'(x_k)$ in (1.20) can be approximated by a difference quotient; that is,

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

Replacing $f'(x_k)$ in (1.20) by this difference quotient leads us to the following definition.

Definition 1.8 *The* **secant method** *is defined by*

$$\boxed{x_{k+1} = x_k - f(x_k)\left(\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}\right), \qquad k = 1, 2, 3, \ldots, \qquad (1.25)}$$

where x_0 and x_1 are given starting values. It is implicitly assumed here that $f(x_k) - f(x_{k-1}) \neq 0$ for all $k \geq 1$.

The method is illustrated in Figure 1.6. The new iterate x_{k+1} is obtained from x_{k-1} and x_k by drawing the chord joining the points $P(x_{k-1}, f(x_{k-1}))$ and $Q(x_k, f(x_k))$, and using as x_{k+1} the point at which this chord intersects the x-axis. If x_{k-1} and x_k are close together and f

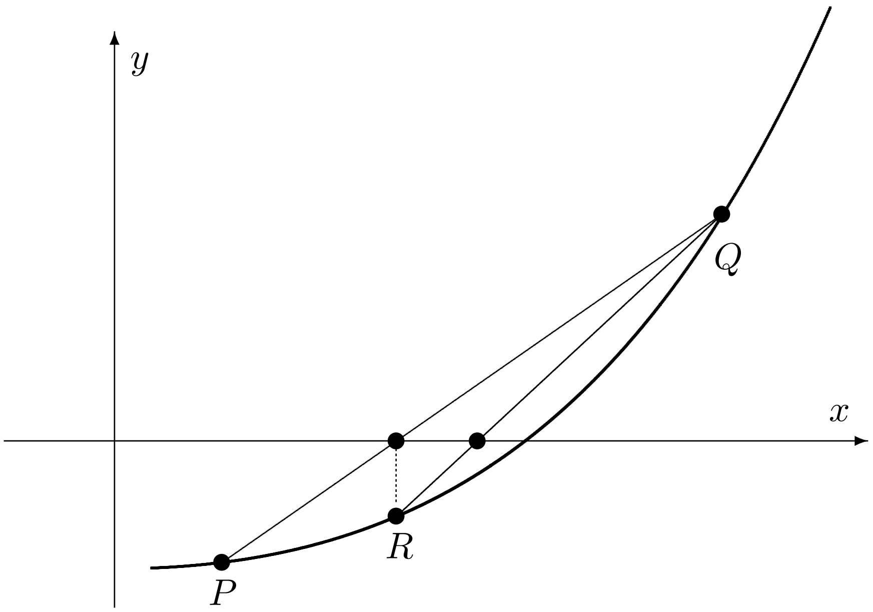


Fig. 1.6. Secant method.

is differentiable, x_{k+1} is approximately the same as the value supplied by Newton's method, which uses the tangent at the point Q.

Theorem 1.10 *Suppose that f is a real-valued function, defined and continuously differentiable on an interval $I = [\xi - h, \xi + h]$, $h > 0$, with centre point ξ. Suppose further that $f(\xi) = 0$, $f'(\xi) \neq 0$. Then, the sequence (x_k) defined by the secant method (1.25) converges at least linearly to ξ provided that x_0 and x_1 are sufficiently close to ξ.*

Proof Since $f'(\xi) \neq 0$, we may suppose that $f'(\xi) = \alpha > 0$; only minor changes are needed in the proof when $f'(\xi)$ is negative. Since f' is continuous on I, corresponding to any $\varepsilon > 0$ we can choose an interval $I_\delta = [\xi - \delta, \xi + \delta]$, with $0 < \delta \leq h$, such that

$$|f'(x) - \alpha| < \varepsilon\,, \qquad x \in I_\delta\,. \tag{1.26}$$

Choosing $\varepsilon = \frac{1}{4}\alpha$ we see that

$$0 < \tfrac{3}{4}\alpha < f'(x) < \tfrac{5}{4}\alpha\,, \qquad x \in I_\delta\,. \tag{1.27}$$

From (1.25) and using the Mean Value Theorem (Theorem A.3) together with the fact that $f(\xi) = 0$, we obtain

$$\xi - x_{k+1} = \xi - x_k + \frac{(x_k - \xi)f'(\vartheta_k)}{f'(\varphi_k)}\,, \tag{1.28}$$

Table 1.3. *Comparison of the secant method and Newton's method for the solution of* $\mathrm{e}^x - x - 2 = 0$.

	Secant method	Newton's method
0	1.000000	1.000000
1	3.000000	1.163953
2	1.036665	1.146421
3	1.064489	1.146193
4	1.153299	1.146193
5	1.145745	
6	1.146191	
7	1.146193	

where ϑ_k is between x_k and ξ, and φ_k lies between x_k and x_{k-1}. Hence, if $x_{k-1} \in I_\delta$ and $x_k \in I_\delta$, then also $\vartheta_k \in I_\delta$ and $\varphi_k \in I_\delta$. Therefore,

$$|\xi - x_{k+1}| \leq |\xi - x_k| \left|1 - \frac{5\alpha/4}{3\alpha/4}\right| = \tfrac{2}{3}|\xi - x_k|\,. \tag{1.29}$$

Thus, $x_{k+1} \in I_\delta$ and the sequence (x_k) converges to ξ at least linearly, with rate at least $\log_{10}(3/2)$, provided that $x_0 \in I_\delta$ and $x_1 \in I_\delta$. □

In fact, it can be shown that

$$\lim_{k\to\infty} \frac{|x_{k+1} - \xi|}{|x_k - \xi|^q} = \mu \tag{1.30}$$

where μ is a positive constant and $q = \frac{1}{2}(1 + \sqrt{5}) \approx 1.6$, so that the convergence of the sequence (x_k) to ξ is faster than linear, but not as fast as quadratic. (See Exercise 10.)

This is illustrated in Table 1.3, which compares two iterative methods for the solution of $f(x) = 0$ with $f\colon x \mapsto \mathrm{e}^x - x - 2$; the first is the secant method, starting from $x_0 = 1$, $x_1 = 3$, while the second is Newton's method starting from $x_0 = 1$.

This experiment shows the faster convergence of Newton's method, but it must be remembered that each iteration of Newton's method requires the calculation of both $f(x_k)$ and $f'(x_k)$, while each iteration of the secant method requires the calculation of $f(x_k)$ only (as $f(x_{k-1})$ has already been computed). In our examples the computations are quite trivial, but in a practical situation the calculation of each value of $f(x_k)$ and $f'(x_k)$ may demand a substantial amount of work, and then each iteration of Newton's method is likely to involve at least twice as much work as one iteration of the secant method.

1.6 The bisection method

Suppose that f is a real-valued function defined and continuous on a bounded closed interval $[a, b]$ of the real line and such that $f(\xi) = 0$ for some $\xi \in [a, b]$. A very simple iterative method for the solution of the nonlinear equation $f(x) = 0$ can be constructed by beginning with an interval $[a_0, b_0]$ which is known to contain the required solution ξ (*e.g.*, one may choose $[a_0, b_0]$ as the interval $[a, b]$ itself, with $a_0 = a$ and $b_0 = b$), and successively halving its size.

More precisely, we proceed as follows. Let $k \geq 0$, and suppose that it is known that $f(a_k)$ and $f(b_k)$ have opposite signs; we then conclude from Theorem 1.1 that the interval (a_k, b_k) contains a solution of $f(x) = 0$. Consider the midpoint c_k of the interval (a_k, b_k) defined by

$$c_k = \tfrac{1}{2}(a_k + b_k)\,, \tag{1.31}$$

and evaluate $f(c_k)$. If $f(c_k)$ is zero, then we have located a solution ξ of $f(x) = 0$, and the iteration stops. Else, we define the new interval (a_{k+1}, b_{k+1}) by

$$(a_{k+1}, b_{k+1}) = \begin{cases} (a_k, c_k) & \text{if } f(c_k)f(b_k) > 0\,, \\ (c_k, b_k) & \text{if } f(c_k)f(b_k) < 0\,, \end{cases} \tag{1.32}$$

and repeat this procedure.

This may at first seem to be a very crude method, but it has some important advantages. The analysis of convergence is trivial; the size of the interval containing ξ is halved at each iteration, so the sequence (c_k) defined by the bisection method converges linearly, with rate $\rho = \log_{10} 2$. Even Newton's method may often converge more slowly than this in the early stages, when the starting value is far from the desired solution. Moreover, the convergence analysis assumes only that the function f is continuous, and requires no bounds on the derivatives, nor even their existence.[1] Once we can find an interval $[a_0, b_0]$ such that $f(a_0)$ and $f(b_0)$ have opposite signs, we can guarantee convergence to a solution, and that after k iterations the solution ξ will lie in an interval of length

[1] Consider, for example, solving the equation $f(x) = 0$, where the function f is defined by (1.2). Even though f is not differentiable at the point $x = 1.05$, the bisection method is applicable. It has to be noted, however, that for functions of this kind it is not always easy to find an interval $[a_0, b_0]$ in which f changes sign.

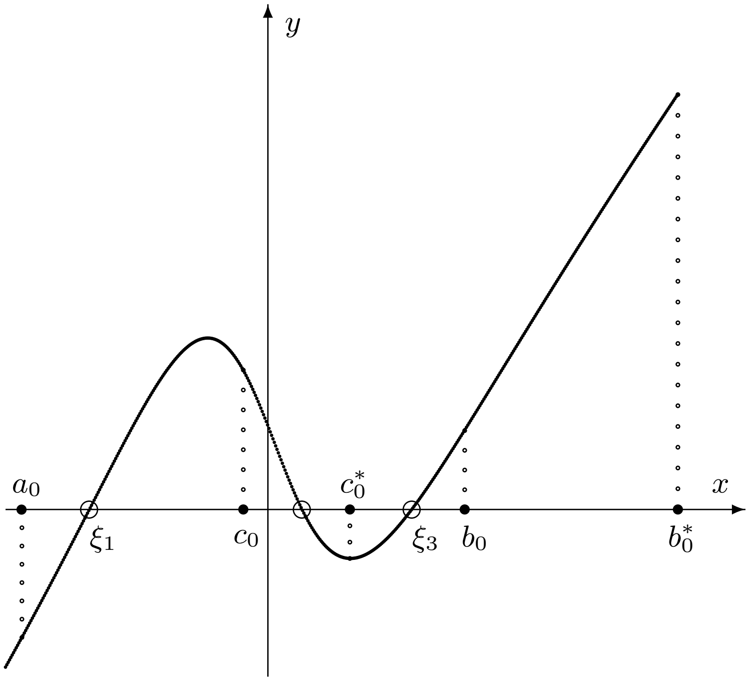


Fig. 1.7. Bisection; from the initial interval $[a_0, b_0]$ the next interval is $[a_0, c_0]$, but starting from $[a_0, b_0^*]$ the next interval is $[c_0^*, b_0^*]$.

$(b_0 - a_0)/2^k$. The bisection method is therefore very robust, though Newton's method will always win once the current iterate is sufficiently close to ξ.

If the initial interval $[a_0, b_0]$ contains more than one solution, the limit of the bisection method will depend on the positions of these solutions. Figure 1.7 illustrates a possible situation, where $[a_0, b_0]$ contains three solutions. Since $f(c_0)$ has the same sign as $f(b_0)$ the second interval is $[a_0, c_0]$, and the sequence (c_k) of midpoints defined by (1.31) converges to the solution ξ_1. If however the initial interval is $[a_0, b_0^*]$ the sequence of midpoints converges to the solution ξ_3.

1.7 Global behaviour

We have already seen how an iteration will often converge to a limit if the starting value is sufficiently close to that limit. The behaviour of the iteration, when started from an arbitrary starting value, can be very complicated. In this section we shall consider two examples. No theorems will be stated: our aim is simply to illustrate various kinds of behaviour.

First consider the simple iteration defined by

$$x_{k+1} = g(x_k)\,, \quad k = 0, 1, 2, \dots\,, \qquad \text{where } g(x) = a\,x(1-x)\,, \quad (1.33)$$

which is often known as the **logistic equation**. We require the constant a to lie in the range $0 < a \le 4$, for then if the starting value x_0 is in the interval $[0,1]$, then all members of the sequence (x_k) also lie in $[0,1]$. The function g has two fixed points: $x = 0$ and $x = 1 - 1/a$. The fixed point at 0 is stable if $0 < a < 1$, and the fixed point at $1 - 1/a$ is stable if $1 < a < 3$. The behaviour of the iteration for these values of a is what might be expected from this information, but for larger values of the parameter a the behaviour of the sequence (x_k) becomes increasingly complicated.

For example, when $a = 3.4$ there is no stable fixed point, and from any starting point the sequence eventually oscillates between two values, which are 0.45 and 0.84 to two decimal digits. These are the two stable fixed points of the double iteration

$$x_{k+1} = g^*(x_k)\,, \qquad g^*(x) = g(g(x)) = a^2x(1-x)[1-ax(1-x)]\,. \quad (1.34)$$

When $3 < a < 1 + \sqrt{6}$, the fixed points of g^* are the two fixed points of g, that is 0 and $1 - 1/a$, and also

$$\frac{1}{2}\left(1 + \frac{1}{a} \pm \frac{1}{a}\left[a^2 - 2a - 3\right]^{1/2}\right). \quad (1.35)$$

This behaviour is known as a stable two-cycle (see Exercise 12).

When $a > 1 + \sqrt{6}$ all the fixed points of g^* are unstable. For example, when $a = 3.5$ all sequences (x_k) defined by (1.33) tend to a stable 4-cycle, taking successive values 0.50, 0.87, 0.38 and 0.83.

For larger values of the parameter a the sequences become chaotic. For example, when $a = 3.99$ there are no stable fixed points or limit-cycles, and the members of any sequence appear random. In fact it can be shown that for such values of a the members of the sequence are *dense* in a subinterval of $[0,1]$: there exist real numbers α and β, $\alpha < \beta$, such that any subinterval of (α, β), however small, contains an infinite subsequence of (x_k). For the value $a = 3.99$ the maximal interval (α, β) is $(0.00995, 0.99750)$ to five decimal digits. Starting from $x_0 = 0.75$ we find that the interval $(0.70, 0.71)$, for example, contains the subsequence

$$x_{16}, x_{164}, x_{454}, x_{801}, x_{812}, \dots\,. \quad (1.36)$$

The sequence does not show any apparent regular behaviour. The calculation is extremely sensitive: if we replace x_0 by $x_0 + \delta x_0$, and write

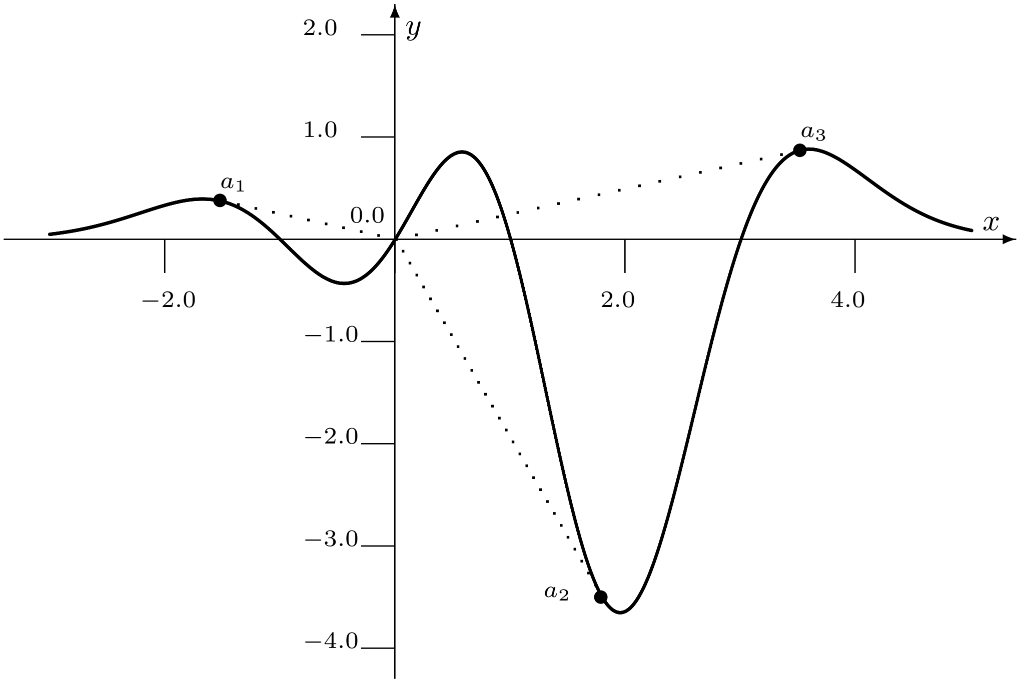


Fig. 1.8. Global behaviour of Newton's method.

$x_k + \delta x_k$ for the resulting perturbed value of x_k, it is easy to see that

$$\delta x_{k+1} = a(1 - 2x_k)\delta x_k\,,$$

provided that the changes δx_k are so small that $a(\delta x_k)^2$ can be ignored. With $x_0 = 0.75$ as above we find from the same calculation that $\delta x_{812}/\delta x_0$ is about 10^{231}, so that to determine x_{812} with reasonable accuracy it is necessary to carry through the whole calculation using 250 decimal digits.

Our second example, of more practical importance, is of Newton's method applied to a function f with several zeros. The example is

$$f(x) = x(x^2 - 1)(x - 3)\exp(-\tfrac{1}{2}(x - 1)^2)\,; \qquad (1.37)$$

the graph of the function is shown in Figure 1.8. The function has zeros at −1, 0, 1 and 3. The sequence generated by the Newton iteration will converge to one of these solutions if the starting value is fairly close to it. Moreover, the geometric interpretation of the iteration shows that if the starting point is sufficiently large in absolute value the iteration diverges rapidly to ∞; the iteration behaves as if the function had a zero at infinity, and the sequence can be loosely described as 'converging to ∞'. With this interpretation some numerical experimentation soon shows that from any starting value Newton's method eventually converges to a solution, which might be $\pm\infty$. However, it is certainly *not* true that the sequence converges to the solution closest to the starting point; indeed, if this were true, no sequence could converge to ∞. It is easy to see why the behaviour is much more complicated than this.

The Newton iteration converges to the solution at 0 from any point in the interval $(-0.327, 0.445)$. As we see from Figure 1.8, the iteration will converge exactly to 0 in one iteration if we start from the x-coordinate of any of the points a_1, a_2 and a_3; at each of these three points the tangent to the curve passes through the origin. Since f is continuous, this means that there is an open interval surrounding each of these points from which the Newton iteration will converge to 0. The maximal such intervals are $(-1.555, -1.487)$, $(1.735, 1.817)$ and $(3.514, 3.529)$ to three decimal digits. In the same way, there are several points at which the tangent to the curve passes through the point $(A_1, 0)$, where A_1 is the x-coordinate of the point a_1. Starting from one of these points, the Newton iteration will evidently converge exactly to the solution at 0 in two steps; surrounding each of these points there is an open interval from which the iteration will converge to 0.

Now suppose we define the sets S_m, $m = -1, 0, 1, 3, \infty, -\infty$, where S_m consists of those points from which the Newton iteration converges to the zero at m. Then, an extension of the above argument shows that each of the sets S_m is the union of an infinite number of disjoint open intervals. The remarkable property of these sets is that, if ξ is a boundary point of one of the sets S_m, then it is also a boundary point of all the other sets as well. This means that any neighbourhood of such a point ξ, however small, contains an infinite number of members of each of the sets S_m. For example, we have seen that the iteration starting from any point in the interval $(-0.327, 0.445)$ converges to 0. We find that the end of this interval lies between 0.4457855 and 0.4457860; Table 1.4 shows the limits of various Newton iterations starting from points near this boundary. Each of these points is, of course, itself surrounded by an open interval which gives the same limit.

1.8 Notes

Theorem 1.2 is a special case of Brouwer's Fixed Point Theorem. Luitzen Egbertus Jan Brouwer (1881–1966) was professor of set theory, function theory and axiomatics at the University of Amsterdam, and made major contributions to topology. Brouwer was a mathematical genius with

Table 1.4. *Limit of Newton's method near a boundary point.*

x_0	Limit
0.4457840	0
0.4457845	0
0.4457850	0
0.4457855	0
0.4457860	1
0.4457865	$-\infty$
0.4457870	-1
0.4457875	-1
0.4457880	$-\infty$
0.4457885	$-\infty$
0.4457890	$+\infty$
0.4457895	3
0.4457900	1

strong mystical and philosophical leanings. For an historical overview of Brouwer's life and work we refer to the recent book of Dirk Van Dalen, *Mystic, Geometer, and Intuitionist. The Life of L.E.J. Brouwer: the Dawning Revolution*, Clarendon Press, Oxford, 1999.

The Contraction Mapping Theorem, as stated here, is a simplified version of Banach's fixed point theorem. Stefan Banach[1] founded modern functional analysis and made outstanding contributions to the theory of topological vector spaces, measure theory, integration, the theory of sets, and orthogonal series. For an inspiring account of Banach's life and times, see R. Kaluza, *Through the Eyes of a Reporter: the Life of Stefan Banach*, Birkhäuser, Boston, MA, 1996.

In our definitions of linear convergence and convergence with order q, we followed Definitions 2.1 and 2.2 in Chapter 4 of

➧ Walter Gautschi, *Numerical Analysis: an Introduction*, Birkhäuser, Boston, MA, 1997.

Exciting surveys of the history of Newton's method are available in T. Ypma, Historical development of the Newton–Raphson method, *SIAM Rev.* **37**, 531–551, 1995, H. Goldstine, *History of Numerical Analysis from the Sixteenth through the Nineteenth Century*, Springer, New York, 1977; and in Chapter 6 of Jean-Luc Chabert (Editor), *A History of Algorithms from the Pebble to the Microchip*, Springer, New York, 1999. As

[1] 30 March 1892, Kraków, Austria–Hungary (now in Poland) – 31 August 1945, Lvov, Ukraine, USSR (now independent).

is noted in these sources, Newton's *De analysi per aequationes numero terminorum infinitas*, probably dating from mid-1669, is sometimes regarded as the historical source of the method, despite the fact that, surprisingly, there is no trace in this tract of the familiar recurrence relation $x_{k+1} = x_k - f(x_k)/f'(x_k)$ bearing Newton's name, nor is there a mention of the idea of derivative. Instead, the paper contains an example of a cubic polynomial whose roots are found by purely algebraic and rather complicated substitutions. In 1690, Joseph Raphson (1648–1715) in the Preface to his *Analysis aequationum universalis* describes his version of Newton's method as 'not only, I believe, not of the same origin, but also, certainly, not with the same development' as Newton's method. Further improvements to the method, and its form as we know it today, were given by Thomas Simpson in his *Essays in Mathematicks* (1740). Simpson presents it as 'a new method for the solution of equations' using the 'method of fluxions', *i.e.*, derivatives. It is argued in Ypma's article that Simpson's contributions to this subject have been underestimated, and 'it would seem that the Newton–Raphson–Simpson method is a designation more nearly representing facts of history of this method which lurks inside millions of modern computer programs and is printed with Newton's name attached in so many textbooks'.

The convergence analysis of Newton's method was initiated in the first half of the twentieth century by L.V. Kantorovich.[1] More recently, Smale,[2] Dedieu and Shub,[3] and others have provided significant insight into the properties of Newton's method. A full discussion of the global behaviour of the logistic equation (1.33), and other examples, will be found in P.G. Drazin, *Nonlinear Systems*, Cambridge University Press, Cambridge, 1992, particularly Chapters 1 and 3.

The secant method is also due to Newton (cf. Section 3 of Ypma's paper cited above), and is found in a collection of unpublished notes termed 'Newton's Waste Book' written around 1665.

In this chapter, we have been concerned with the iterative solution of equations for a real-valued function of a single real variable. In Chapter 4, we shall discuss the iterative solution of nonlinear systems of equations

[1] L.V. Kantorovich, Functional analysis and applied mathematics, *Uspekhi Mat. Nauk* **3**, 89–185, 1948; English transl., Rep. 1509, National Bureau of Standards, Washington, DC, 1952.

[2] Steve Smale, Newton's method estimates from data at one point, in *The Merging of Disciplines: New Directions in Pure, Applied and Computational Mathematics*, R. Ewing, K. Gross, C. Martin, Eds., Springer, New York, 185–196, 1986.

[3] Jean-Pierre Dedieu and Michael Shub, Multihomogeneous Newton methods, *Math. Comput.* **69** (231), 1071–1098, 2000.

of the form $\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$ where $\boldsymbol{f}\colon \mathbb{R}^n \to \mathbb{R}^n$. There, corresponding to the case of $n = 2$, we shall say more about the solution of equations of the form $f(z) = 0$ where f is a complex-valued function of a single complex variable z.

This chapter has been confined to generally applicable iterative methods for the solution of a single nonlinear equation of the form $f(x) = 0$ for a real-valued function f of a single real variable. In particular, we have not discussed specialised methods for the solution of polynomial equations or the various techniques for locating the roots of polynomials in the complex plane and on the real line (by Budan and Fourier, Descartes, Hurwitz, Lobachevskii, Newton, Schur and others), although in Chapter 5 we shall briefly touch on one such polynomial root-finding method due to Sturm.[1] For a historical survey of the solution of polynomial equations and a review of recent advances in this field, we refer to the article of Victor Pan, Solving a polynomial equation: some history and recent progress, *SIAM Rev.* **39**, 187–220, 1997.

Exercises

1.1 The iteration defined by $x_{k+1} = \frac{1}{2}(x_k^2 + c)$, where $0 < c < 1$, has two fixed points ξ_1, ξ_2, where $0 < \xi_1 < 1 < \xi_2$. Show that

$$x_{k+1} - \xi_1 = \tfrac{1}{2}(x_k + \xi_1)(x_k - \xi_1)\,, \qquad k = 0, 1, 2, \dots\,,$$

and deduce that $\lim_{k\to\infty} x_k = \xi_1$ if $0 \le x_0 < \xi_2$. How does the iteration behave for other values of x_0?

1.2 Define the function g by $g(0) = 0$, $g(x) = -x\sin^2(1/x)$ for $0 < x \le 1$. Show that g is continuous, and that 0 is the only fixed point of g in the interval $[0, 1]$. By considering the iteration $x_{n+1} = g(x_n)$, $n = 0, 1, 2, \ldots$, starting, first from $x_0 = 1/(k\pi)$, and then from $x_0 = 2/((2k + 1)\pi)$, where k is an integer, show that according to Definition 1.3 the critical point is neither stable nor unstable.

1.3 Newton's method is applied to the solution of

$$\mathrm{e}^x - x - 2 = 0\,.$$

[1] For further details in this direction, we refer to M.A. Jenkins and J.F. Traub, A three-stage algorithm for real polynomials using quadratic iterations, *SIAM J. Numer. Anal.* **7**, 545–566, 1970, A.S. Householder, *The Numerical Treatment of a Single Nonlinear Equation,* McGraw–Hill, New York, 1970, and A. Ralston and P. Rabinowitz, *A First Course in Numerical Analysis*, Second Edition, McGraw–Hill, New York, 1978.

Show that if the starting value is positive, the iteration converges to the positive solution, and if the starting value is negative it converges to the negative solution. Obtain approximate expressions for x_1 if (i) $x_0 = 100$ and (ii) $x_0 = -100$, and describe the subsequent behaviour of the iteration. About how many iterations would be required to obtain the solution to six decimal digits in these two cases?

1.4 Consider the iteration

$$x_{k+1} = x_k - \frac{[f(x_k)]^2}{f(x_k + f(x_k)) - f(x_k)}\,, \qquad k = 0, 1, 2, \ldots\,,$$

for the solution of $f(x) = 0$. Explain the connection with Newton's method, and show that (x_k) converges quadratically if x_0 is sufficiently close to the solution. Apply this method to the same example as in Example 1.7, $f(x) = \mathrm{e}^x - x - 2$, and verify quadratic convergence beginning from $x_0 = 1$. Experiment with calculations beginning from $x_0 = 10$ and from $x_0 = -10$, and account for their behaviour.

1.5 It is sometimes said that Newton's method converges quadratically, and therefore in the successive approximations to the solution the number of correct digits doubles each time. Explain why this is not generally correct. Suppose that $f''(x)$ is defined and continuous in a neighbourhood of ξ and that x_k agrees with the solution ξ to m decimal digits; give an estimate of the number of correct decimal digits in x_{k+1}.

Illustrate your estimate by using Newton's method to determine the positive zero of $f(x) = \mathrm{e}^x - x - 1.000000005$, which is close to 0.0001; use $x_0 = 0.0005$.

1.6 Suppose that $f(\xi) = f'(\xi) = 0$, so that f has a double root at ξ, and that f'' is defined and continuous in a neighbourhood of ξ. If (x_k) is a sequence obtained by Newton's method, show that

$$\xi - x_{k+1} = -\tfrac{1}{2}\frac{(\xi - x_k)^2 f''(\eta_k)}{f'(x_k)} = \tfrac{1}{2}(\xi - x_k)\frac{f''(\eta_k)}{f''(\chi_k)}\,,$$

where η_k and χ_k both lie between ξ and x_k. Suppose, further, that $0 < m < |f''(x)| < M$ for all x in the interval $[\xi - \delta, \xi + \delta]$ for some $\delta > 0$, where $M < 2m$; show that if x_0 lies in this interval the iteration converges to ξ, and that convergence is linear, with rate $\log_{10} 2$. Verify this conclusion by finding the solution of $\mathrm{e}^x = 1 + x$, beginning from $x_0 = 1$.

1.7 Extend the result of the previous exercise to a case where f has a triple root at ξ, so that $f(\xi) = f'(\xi) = f''(\xi) = 0$.

1.8 Suppose that the function f has a continuous second derivative, that $f(\xi) = 0$, and that in the interval $[X, \xi]$, with $X < \xi$, $f'(x) > 0$ and $f''(x) < 0$. Show that the Newton iteration, starting from any x_0 in $[X, \xi]$, converges to ξ.

1.9 The secant method is used to determine solutions of the equation $x^2 - 1 = 0$. Starting from $x_0 = 1 + \varepsilon$, $x_1 = -1 + \varepsilon$, show that $x_2 = \frac{1}{2}\varepsilon + \mathcal{O}(\varepsilon^2)$, and determine x_3, x_4 and x_5, neglecting terms of order $\mathcal{O}(\varepsilon^2)$. Explain why, at least for sufficiently small values of ε, the sequence (x_k) converges to the solution -1.

Repeat the calculation with x_0 and x_1 interchanged, so that $x_0 = -1 + \varepsilon$ and $x_1 = 1 + \varepsilon$, and show that the sequence now converges to the solution 1.

1.10 Write the secant iteration in the form

$$x_{k+1} = \frac{x_k\, f(x_{k-1}) - x_{k-1}\, f(x_k)}{f(x_{k-1}) - f(x_k)}\,, \qquad k = 1, 2, 3, \dots\,.$$

Supposing that f has a continuous second derivative in a neighbourhood of the solution ξ of $f(x) = 0$, and that $f'(\xi) > 0$ and $f''(\xi) > 0$, define

$$\varphi(x_k, x_{k-1}) = \frac{x_{k+1} - \xi}{(x_k - \xi)(x_{k-1} - \xi)}\,,$$

where x_{k+1} has been expressed in terms of x_k and x_{k-1}. Find an expression for

$$\psi(x_{k-1}) = \lim_{x_k \to \xi} \varphi(x_k, x_{k-1})\,,$$

and then determine $\lim_{x_{k-1} \to \xi} \psi(x_{k-1})$. Deduce that

$$\lim_{x_k, x_{k-1} \to \xi} \varphi(x_k, x_{k-1}) = f''(\xi)/2f'(\xi)\,.$$

Now assume that

$$\lim_{k \to \infty} \frac{|x_{k+1} - \xi|}{|x_k - \xi|^q} = A\,.$$

Show that $q - 1 - 1/q = 0$, and hence that $q = \frac{1}{2}(1 + \sqrt{5})$.

Deduce finally that

$$\lim_{k\to\infty} \frac{|x_{k+1}-\xi|}{|x_k-\xi|^q} = \left(\frac{f''(\xi)}{2f'(\xi)}\right)^{q/(1+q)} .$$

1.11 A variant of the secant method defines two sequences u_k and v_k such that all the values $f(u_k),\ k = 0, 1, 2, \ldots,$ have one sign, and all the values $f(v_k),\ k = 0, 1, 2, \ldots$, have the opposite sign. From the numbers u_k and v_k the secant formula is used to define

$$w_k = \frac{u_k f(v_k) - v_k f(u_k)}{f(v_k) - f(u_k)} , \qquad k = 0, 1, 2, \ldots ;$$

we define $u_{k+1} = w_k,\ v_{k+1} = v_k$ if $f(w_k)$ has the same sign as $f(u_k)$, and otherwise $u_{k+1} = u_k,\ v_{k+1} = w_k$. Suppose that f'' is defined and continuous on the interval $[u_0, v_0]$, and that, for some K, f'' has constant sign in $[u_K, v_K]$. Explain, graphically or otherwise, why either $u_k = u_K$ for all $k \geq K$, or $v_k = v_K$ for all $k \geq K$. Deduce that the method converges linearly, and determine the asymptotic rate of convergence; explain clearly what you mean by convergence of this method. What advantages, if any, do you think this method has compared with the secant method of Definition 1.8?

1.12 A *two-cycle* of the iteration defined by the function g is a pair of distinct numbers a, b such that $b = g(a)$ and $a = g(b)$. Use the fact that a and b are fixed points of the iteration defined by the function $h(x) = g(g(x))$ to give a definition of *stability* for a two-cycle. Show that if $|g'(a)\,g'(b)| < 1$, then the two-cycle is stable, and that if $|g'(a)\,g'(b)| > 1$ the two-cycle is not stable.

Show that if a, b is a two-cycle for Newton's method for the function f, and if $|f(a)f(b)f''(a)f''(b)| < [f'(a)f'(b)]^2$, then the two-cycle is stable.

Show that Newton's method for the solution of $f(x) = 0$ with

$$f\colon x \mapsto x(x^2 - 1)$$

has a two-cycle of the form $a, -a$, and find the value of a; is this two-cycle stable?