```
        endif
        if(p.gt.0.) q=-q           Check whether in bounds.
        p=abs(p)
        if(2.*p .lt. min(3.*xm*q-abs(tol1*q),abs(e*q))) then
            e=d                    Accept interpolation.
            d=p/q
        else
            d=xm                   Interpolation failed, use bisection.
            e=d
        endif
    else                           Bounds decreasing too slowly, use bisection.
        d=xm
        e=d
    endif
    a=b                            Move last best guess to a.
    fa=fb
    if(abs(d) .gt. tol1) then      Evaluate new trial root.
        b=b+d
    else
        b=b+sign(tol1,xm)
    endif
    fb=func(b)
enddo 11
pause 'zbrent exceeding maximum iterations'
zbrent=b
return
END
```

CITED REFERENCES AND FURTHER READING:

Brent, R.P. 1973, *Algorithms for Minimization without Derivatives* (Englewood Cliffs, NJ: Prentice-Hall), Chapters 3, 4. [1]

Forsythe, G.E., Malcolm, M.A., and Moler, C.B. 1977, *Computer Methods for Mathematical Computations* (Englewood Cliffs, NJ: Prentice-Hall), §7.2.

9.4 Newton-Raphson Method Using Derivative

Perhaps the most celebrated of all one-dimensional root-finding routines is *Newton's method*, also called the *Newton-Raphson method*. This method is distinguished from the methods of previous sections by the fact that it requires the evaluation of both the function $f(x)$, *and* the derivative $f'(x)$, at arbitrary points x. The Newton-Raphson formula consists geometrically of extending the tangent line at a current point x_i until it crosses zero, then setting the next guess x_{i+1} to the abscissa of that zero-crossing (see Figure 9.4.1). Algebraically, the method derives from the familiar Taylor series expansion of a function in the neighborhood of a point,

$$f(x+\delta) \approx f(x) + f'(x)\delta + \frac{f''(x)}{2}\delta^2 + \dots. \tag{9.4.1}$$

For small enough values of δ, and for well-behaved functions, the terms beyond linear are unimportant, hence $f(x+\delta) = 0$ implies

$$\delta = -\frac{f(x)}{f'(x)}. \tag{9.4.2}$$

Newton-Raphson is not restricted to one dimension. The method readily generalizes to multiple dimensions, as we shall see in §9.6 and §9.7, below.

Far from a root, where the higher-order terms in the series *are* important, the Newton-Raphson formula can give grossly inaccurate, meaningless corrections. For instance, the initial guess for the root might be so far from the true root as to let the search interval include a local maximum or minimum of the function. This can be death to the method (see Figure 9.4.2). If an iteration places a trial guess near such a local extremum, so that the first derivative nearly vanishes, then Newton-Raphson sends its solution off to limbo, with vanishingly small hope of recovery. Like most powerful tools, Newton-Raphson can be destructive used in inappropriate circumstances. Figure 9.4.3 demonstrates another possible pathology.

Why do we call Newton-Raphson powerful? The answer lies in its rate of convergence: Within a small distance ϵ of x the function and its derivative are approximately:

$$\begin{aligned} f(x+\epsilon) &= f(x) + \epsilon f'(x) + \epsilon^2 \frac{f''(x)}{2} + \cdots, \\ f'(x+\epsilon) &= f'(x) + \epsilon f''(x) + \cdots \end{aligned} \tag{9.4.3}$$

By the Newton-Raphson formula,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}, \tag{9.4.4}$$

so that

$$\epsilon_{i+1} = \epsilon_i - \frac{f(x_i)}{f'(x_i)}. \tag{9.4.5}$$

When a trial solution x_i differs from the true root by ϵ_i, we can use (9.4.3) to express $f(x_i), f'(x_i)$ in (9.4.4) in terms of ϵ_i and derivatives at the root itself. The result is a recurrence relation for the deviations of the trial solutions

$$\epsilon_{i+1} = -\epsilon_i^2 \frac{f''(x)}{2f'(x)}. \tag{9.4.6}$$

Equation (9.4.6) says that Newton-Raphson converges *quadratically* (cf. equation 9.2.3). Near a root, the number of significant digits approximately *doubles* with each step. This very strong convergence property makes Newton-Raphson the method of choice for any function whose derivative can be evaluated efficiently, and whose derivative is continuous and nonzero in the neighborhood of a root.

Even where Newton-Raphson is rejected for the early stages of convergence (because of its poor global convergence properties), it is very common to "polish up" a root with one or two steps of Newton-Raphson, which can multiply by two or four its number of significant figures!

For an efficient realization of Newton-Raphson the user provides a routine that evaluates both $f(x)$ and its first derivative $f'(x)$ at the point x. The Newton-Raphson formula can also be applied using a numerical difference to approximate the true local derivative,

$$f'(x) \approx \frac{f(x+dx) - f(x)}{dx}. \tag{9.4.7}$$

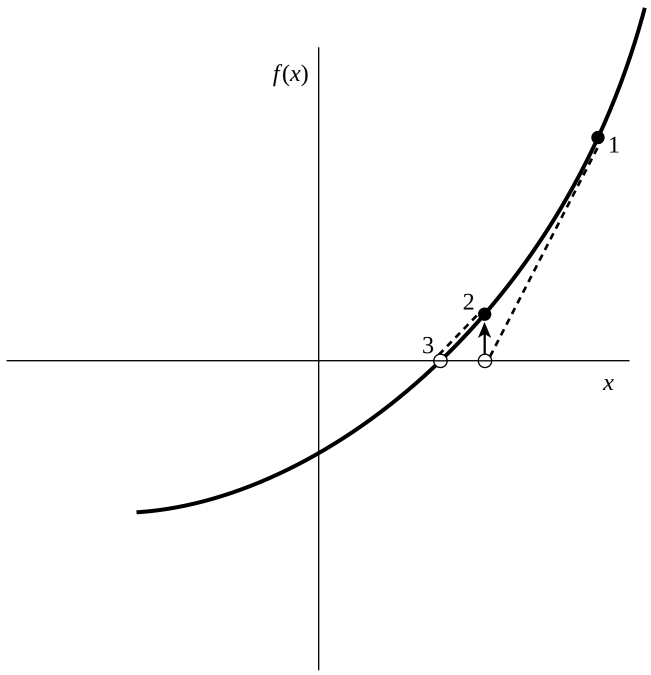

Figure 9.4.1. Newton's method extrapolates the local derivative to find the next estimate of the root. In this example it works well and converges quadratically.

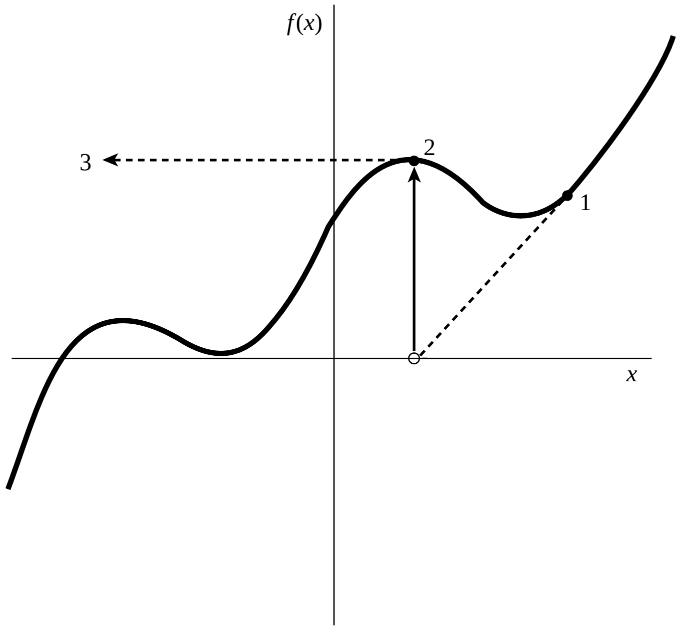

Figure 9.4.2. Unfortunate case where Newton's method encounters a local extremum and shoots off to outer space. Here bracketing bounds, as in `rtsafe`, would save the day.

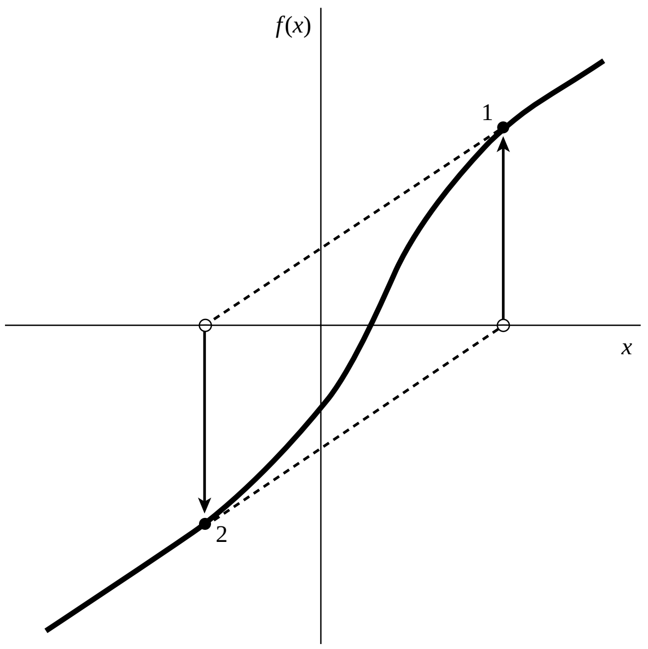

Figure 9.4.3. Unfortunate case where Newton's method enters a nonconvergent cycle. This behavior is often encountered when the function f is obtained, in whole or in part, by table interpolation. With a better initial guess, the method would have succeeded.

This is not, however, a recommended procedure for the following reasons: (i) You are doing two function evaluations per step, so *at best* the superlinear order of convergence will be only $\sqrt{2}$. (ii) If you take dx too small you will be wiped out by roundoff, while if you take it too large your order of convergence will be only linear, no better than using the *initial* evaluation $f'(x_0)$ for all subsequent steps. Therefore, Newton-Raphson with numerical derivatives is (in one dimension) always dominated by the secant method of §9.2. (In multidimensions, where there is a paucity of available methods, Newton-Raphson with numerical derivatives must be taken more seriously. See §§9.6–9.7.)

The following subroutine calls a user supplied subroutine `funcd(x,fn,df)` which returns the function value as `fn` and the derivative as `df`. We have included input bounds on the root simply to be consistent with previous root-finding routines: Newton does not adjust bounds, and works only on local information at the point `x`. The bounds are used only to pick the midpoint as the first guess, and to reject the solution if it wanders outside of the bounds.

```
FUNCTION rtnewt(funcd,x1,x2,xacc)
INTEGER JMAX
REAL rtnewt,x1,x2,xacc
EXTERNAL funcd
PARAMETER (JMAX=20)                  Set to maximum number of iterations.
   Using the Newton-Raphson method, find the root of a function known to lie in the interval
   [x1,x2]. The root rtnewt will be refined until its accuracy is known within ±xacc. funcd
   is a user-supplied subroutine that returns both the function value and the first derivative
   of the function at the point x.
INTEGER j
REAL df,dx,f
```

```
      rtnewt=.5*(x1+x2)                    Initial guess.
      do 11 j=1,JMAX
          call funcd(rtnewt,f,df)
          dx=f/df
          rtnewt=rtnewt-dx
          if((x1-rtnewt)*(rtnewt-x2).lt.0.)
     *         pause 'rtnewt jumped out of brackets'
          if(abs(dx).lt.xacc) return       Convergence.
      enddo 11
      pause 'rtnewt exceeded maximum iterations'
      END
```

While Newton-Raphson's global convergence properties are poor, it is fairly easy to design a fail-safe routine that utilizes a combination of bisection and Newton-Raphson. The hybrid algorithm takes a bisection step whenever Newton-Raphson would take the solution out of bounds, or whenever Newton-Raphson is not reducing the size of the brackets rapidly enough.

```
      FUNCTION rtsafe(funcd,x1,x2,xacc)
      INTEGER MAXIT
      REAL rtsafe,x1,x2,xacc
      EXTERNAL funcd
      PARAMETER (MAXIT=100)                Maximum allowed number of iterations.
          Using a combination of Newton-Raphson and bisection, find the root of a function bracketed
          between x1 and x2. The root, returned as the function value rtsafe, will be refined until
          its accuracy is known within ±xacc. funcd is a user-supplied subroutine which returns
          both the function value and the first derivative of the function.
      INTEGER j
      REAL df,dx,dxold,f,fh,fl,temp,xh,xl
      call funcd(x1,fl,df)
      call funcd(x2,fh,df)
      if((fl.gt.0..and.fh.gt.0.).or.(fl.lt.0..and.fh.lt.0.))
     *     pause 'root must be bracketed in rtsafe'
      if(fl.eq.0.)then
          rtsafe=x1
          return
      else if(fh.eq.0.)then
          rtsafe=x2
          return
      else if(fl.lt.0.)then                Orient the search so that f(xl) < 0.
          xl=x1
          xh=x2
      else
          xh=x1
          xl=x2
      endif
      rtsafe=.5*(x1+x2)                    Initialize the guess for root,
      dxold=abs(x2-x1)                     the "stepsize before last,"
      dx=dxold                             and the last step.
      call funcd(rtsafe,f,df)
      do 11 j=1,MAXIT                      Loop over allowed iterations.
          if(((rtsafe-xh)*df-f)*((rtsafe-xl)*df-f).gt.0.   Bisect if Newton out of range,
     *         .or. abs(2.*f).gt.abs(dxold*df) ) then      or not decreasing fast enough.
              dxold=dx
              dx=0.5*(xh-xl)
              rtsafe=xl+dx
              if(xl.eq.rtsafe)return       Change in root is negligible.
          else                             Newton step acceptable. Take it.
              dxold=dx
              dx=f/df
              temp=rtsafe
          rtsafe=rtsafe-dx
          if(temp.eq.rtsafe)return
      endif
      if(abs(dx).lt.xacc) return      Convergence criterion.
      call funcd(rtsafe,f,df)         The one new function evaluation per iteration.
      if(f.lt.0.) then                Maintain the bracket on the root.
          xl=rtsafe
      else
          xh=rtsafe
      endif
enddo 11
pause 'rtsafe exceeding maximum iterations'
return
END
```

For many functions the derivative $f'(x)$ often converges to machine accuracy before the function $f(x)$ itself does. When that is the case one need not subsequently update $f'(x)$. This shortcut is recommended only when you confidently understand the generic behavior of your function, but it speeds computations when the derivative calculation is laborious. (Formally this makes the convergence only linear, but if the derivative isn't changing anyway, you can do no better.)

Newton-Raphson and Fractals

An interesting sidelight to our repeated warnings about Newton-Raphson's unpredictable global convergence properties — its very rapid local convergence notwithstanding — is to investigate, for some particular equation, the set of starting values from which the method does, or doesn't converge to a root.

Consider the simple equation

$$z^3 - 1 = 0 \tag{9.4.8}$$

whose single real root is $z = 1$, but which also has complex roots at the other two cube roots of unity, $\exp(\pm 2\pi i/3)$. Newton's method gives the iteration

$$z_{j+1} = z_j - \frac{z_j^3 - 1}{3z_j^2} \tag{9.4.9}$$

Up to now, we have applied an iteration like equation (9.4.9) only for real starting values z_0, but in fact all of the equations in this section also apply in the complex plane. We can therefore map out the complex plane into regions from which a starting value z_0, iterated in equation (9.4.9), will, or won't, converge to $z = 1$. Naively, we might expect to find a "basin of convergence" somehow surrounding the root $z = 1$. We surely do not expect the basin of convergence to fill the whole plane, because the plane must also contain regions that converge to each of the two complex roots. In fact, by symmetry, the three regions must have identical shapes. Perhaps they will be three symmetric 120° wedges, with one root centered in each?

Now take a look at Figure 9.4.4, which shows the result of a numerical exploration. The basin of convergence does indeed cover $1/3$ the area of the complex plane, but its boundary is highly irregular — in fact, *fractal*. (A fractal, so called, has self-similar structure that repeats on all scales of magnification.) How does this

Figure 9.4.4. The complex z plane with real and imaginary components in the range $(-2, 2)$. The black region is the set of points from which Newton's method converges to the root $z = 1$ of the equation $z^3 - 1 = 0$. Its shape is fractal.

fractal emerge from something as simple as Newton's method, and an equation as simple as (9.4.8)? The answer is already implicit in Figure 9.4.2, which showed how, on the real line, a local extremum causes Newton's method to shoot off to infinity. Suppose one is *slightly* removed from such a point. Then one might be shot off not to infinity, but — by luck — right into the basin of convergence of the desired root. But that means that in the neighborhood of an extremum there must be a tiny, perhaps distorted, copy of the basin of convergence — a kind of "one-bounce away" copy. Similar logic shows that there can be "two-bounce" copies, "three-bounce" copies, and so on. A fractal thus emerges.

Notice that, for equation (9.4.8), almost the whole real axis is in the domain of convergence for the root $z = 1$. We say "almost" because of the peculiar discrete points on the negative real axis whose convergence is indeterminate (see figure). What happens if you start Newton's method from one of these points? (Try it.)

CITED REFERENCES AND FURTHER READING:

Acton, F.S. 1970, *Numerical Methods That Work*; 1990, corrected edition (Washington: Mathematical Association of America), Chapter 2.

Ralston, A., and Rabinowitz, P. 1978, *A First Course in Numerical Analysis*, 2nd ed. (New York: McGraw-Hill), §8.4.

Ortega, J., and Rheinboldt, W. 1970, *Iterative Solution of Nonlinear Equations in Several Variables* (New York: Academic Press).

Mandelbrot, B.B. 1983, *The Fractal Geometry of Nature* (San Francisco: W.H. Freeman).

Peitgen, H.-O., and Saupe, D. (eds.) 1988, *The Science of Fractal Images* (New York: Springer-Verlag).

9.5 Roots of Polynomials

Here we present a few methods for finding roots of polynomials. These will serve for most practical problems involving polynomials of low-to-moderate degree or for well-conditioned polynomials of higher degree. Not as well appreciated as it ought to be is the fact that some polynomials are exceedingly ill-conditioned. The tiniest changes in a polynomial's coefficients can, in the worst case, send its roots sprawling all over the complex plane. (An infamous example due to Wilkinson is detailed by Acton [1].)

Recall that a polynomial of degree n will have n roots. The roots can be real or complex, and they might not be distinct. If the coefficients of the polynomial are real, then complex roots will occur in pairs that are conjugate, i.e., if $x_1 = a + bi$ is a root then $x_2 = a - bi$ will also be a root. When the coefficients are complex, the complex roots need not be related.

Multiple roots, or closely spaced roots, produce the most difficulty for numerical algorithms (see Figure 9.5.1). For example, $P(x) = (x - a)^2$ has a double real root at $x = a$. However, we cannot bracket the root by the usual technique of identifying neighborhoods where the function changes sign, nor will slope-following methods such as Newton-Raphson work well, because both the function and its derivative vanish at a multiple root. Newton-Raphson *may* work, but slowly, since large roundoff errors can occur. When a root is known in advance to be multiple, then special methods of attack are readily devised. Problems arise when (as is generally the case) we do not know in advance what pathology a root will display.

Deflation of Polynomials

When seeking several or all roots of a polynomial, the total effort can be significantly reduced by the use of *deflation*. As each root r is found, the polynomial is factored into a product involving the root and a reduced polynomial of degree one less than the original, i.e., $P(x) = (x - r)Q(x)$. Since the roots of Q are exactly the remaining roots of P, the effort of finding additional roots decreases, because we work with polynomials of lower and lower degree as we find successive roots. Even more important, with deflation we can avoid the blunder of having our iterative method converge twice to the same (nonmultiple) root instead of separately to two different roots.

Deflation, which amounts to synthetic division, is a simple operation that acts on the array of polynomial coefficients. The concise code for synthetic division by a monomial factor was given in §5.3 above. You can deflate complex roots either by converting that code to complex data type, or else — in the case of a polynomial with real coefficients but possibly complex roots — by deflating by a quadratic factor,

$$[x - (a + ib)]\,[x - (a - ib)] = x^2 - 2ax + (a^2 + b^2) \qquad (9.5.1)$$