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16.3 Modified Midpoint Method

This section discusses the *modified midpoint method*, which advances a vector of dependent variables $y(x)$ from a point x to a point $x + H$ by a sequence of n substeps each of size h,

$$h = H/n \tag{16.3.1}$$

In principle, one could use the modified midpoint method in its own right as an ODE integrator. In practice, the method finds its most important application as a part of the more powerful Bulirsch-Stoer technique, treated in §16.4. You can therefore consider this section as a preamble to §16.4.

The number of right-hand side evaluations required by the modified midpoint method is $n + 1$. The formulas for the method are

$$\begin{aligned} z_0 &\equiv y(x) \\ z_1 &= z_0 + hf(x, z_0) \\ z_{m+1} &= z_{m-1} + 2hf(x + mh, z_m) \qquad \text{for} \quad m = 1, 2, \ldots, n-1 \\ y(x + H) \approx y_n &\equiv \frac{1}{2}[z_n + z_{n-1} + hf(x + H, z_n)] \end{aligned} \tag{16.3.2}$$

Here the z's are intermediate approximations which march along in steps of h, while y_n is the final approximation to $y(x + H)$. The method is basically a "centered difference" or "midpoint" method (compare equation 16.1.2), except at the first and last points. Those give the qualifier "modified."

The modified midpoint method is a second-order method, like (16.1.2), but with the advantage of requiring (asymptotically for large n) only one derivative evaluation per step h instead of the two required by second-order Runge-Kutta. Perhaps there are applications where the simplicity of (16.3.2), easily coded in-line in some other program, recommends it. In general, however, use of the modified midpoint method by itself will be dominated by the embedded Runge-Kutta method with adaptive stepsize control, as implemented in the preceding section.

The usefulness of the modified midpoint method to the Bulirsch-Stoer technique (§16.4) derives from a "deep" result about equations (16.3.2), due to Gragg. It turns

out that the error of (16.3.2), expressed as a power series in h, the stepsize, contains only *even* powers of h,

$$y_n - y(x+H) = \sum_{i=1}^{\infty} \alpha_i h^{2i} \tag{16.3.3}$$

where H is held constant, but h changes by varying n in (16.3.1). The importance of this even power series is that, if we play our usual tricks of combining steps to knock out higher-order error terms, we can gain *two* orders at a time!

For example, suppose n is even, and let $y_{n/2}$ denote the result of applying (16.3.1) and (16.3.2) with half as many steps, $n \to n/2$. Then the estimate

$$y(x+H) \approx \frac{4y_n - y_{n/2}}{3} \tag{16.3.4}$$

is *fourth-order* accurate, the same as fourth-order Runge-Kutta, but requires only about 1.5 derivative evaluations per step h instead of Runge-Kutta's 4 evaluations. Don't be too anxious to implement (16.3.4), since we will soon do even better.

Now would be a good time to look back at the routine `qsimp` in §4.2, and especially to compare equation (4.2.4) with equation (16.3.4) above. You will see that the transition in Chapter 4 to the idea of Richardson extrapolation, as embodied in Romberg integration of §4.3, is exactly analogous to the transition in going from this section to the next one.

Here is the routine that implements the modified midpoint method, which will be used below.

```
SUBROUTINE mmid(y,dydx,nvar,xs,htot,nstep,yout,derivs)
INTEGER nstep,nvar,NMAX
REAL htot,xs,dydx(nvar),y(nvar),yout(nvar)
EXTERNAL derivs
PARAMETER (NMAX=50)
    Modified midpoint step. Dependent variable vector y(1:nvar) and its derivative vector
    dydx(1:nvar) are input at xs. Also input is htot, the total step to be made, and nstep,
    the number of substeps to be used. The output is returned as yout(1:nvar), which need
    not be a distinct array from y; if it is distinct, however, then y and dydx are returned
    undamaged.
INTEGER i,n
REAL h,h2,swap,x,ym(NMAX),yn(NMAX)
h=htot/nstep                    Stepsize this trip.
do 11 i=1,nvar
    ym(i)=y(i)
    yn(i)=y(i)+h*dydx(i)        First step.
enddo 11
x=xs+h
call derivs(x,yn,yout)          Will use yout for temporary storage of derivatives.
h2=2.*h
do 13 n=2,nstep                 General step.
    do 12 i=1,nvar
        swap=ym(i)+h2*yout(i)
        ym(i)=yn(i)
        yn(i)=swap
    enddo 12
    x=x+h
    call derivs(x,yn,yout)
```

```
      enddo 13
      do 14 i=1,nvar                    Last step.
        yout(i)=0.5*(ym(i)+yn(i)+h*yout(i))
      enddo 14
      return
      END
```

CITED REFERENCES AND FURTHER READING:

Gear, C.W. 1971, *Numerical Initial Value Problems in Ordinary Differential Equations* (Englewood Cliffs, NJ: Prentice-Hall), §6.1.4.

Stoer, J., and Bulirsch, R. 1980, *Introduction to Numerical Analysis* (New York: Springer-Verlag), §7.2.12.

16.4 Richardson Extrapolation and the Bulirsch-Stoer Method

The techniques described in this section are not for differential equations containing nonsmooth functions. For example, you might have a differential equation whose right-hand side involves a function that is evaluated by table look-up and interpolation. If so, go back to Runge-Kutta with adaptive stepsize choice: That method does an excellent job of feeling its way through rocky or discontinuous terrain. It is also an excellent choice for quick-and-dirty, low-accuracy solution of a set of equations. A second warning is that the techniques in this section are not particularly good for differential equations that have singular points *inside* the interval of integration. A regular solution must tiptoe very carefully across such points. Runge-Kutta with adaptive stepsize can sometimes effect this; more generally, there are special techniques available for such problems, beyond our scope here.

Apart from those two caveats, we believe that the Bulirsch-Stoer method, discussed in this section, is the best known way to obtain high-accuracy solutions to ordinary differential equations with minimal computational effort. (A possible exception, infrequently encountered in practice, is discussed in §16.7.)

Three key ideas are involved. The first is *Richardson's deferred approach to the limit*, which we already met in §4.3 on Romberg integration. The idea is to consider the final answer of a numerical calculation as itself being an analytic function (if a complicated one) of an adjustable parameter like the stepsize h. That analytic function can be probed by performing the calculation with various values of h, *none* of them being necessarily small enough to yield the accuracy that we desire. When we know enough about the function, we *fit* it to some analytic form, and then *evaluate* it at that mythical and golden point $h = 0$ (see Figure 16.4.1). Richardson extrapolation is a method for turning straw into gold! (Lead into gold for alchemist readers.)

The second idea has to do with what kind of fitting function is used. Bulirsch and Stoer first recognized the strength of *rational function extrapolation* in Richardson-type applications. That strength is to break the shackles of the power series and its limited radius of convergence, out only to the distance of the first pole in the complex