Ordinary Differential Equations

Single-step methods for ODEs

[Recall that we are solving $\dfrac{dy}{dx} = f(x,y)$, subject to an initial condition $y = y_0$ when $x = x_0$.]

The Euler and Modified Euler Methods for ODEs are the simplest examples of single-step methods. These have the pattern:

- Choose a step-length h.
- Starting out from $x = x_0$, $y = y_0$ at slope $f(x_0, y_0)$, 'explore' the interval $x_0 \leqslant x \leqslant x_1 = x_0 + h$ to find the estimated increment k in y over that interval.
- 'Shift camp' to a new 'base' at $x = x_1$, $y = y_1 = y_0 + k$.
- Repeat the whole process, until x reaches some desired value, to build up a table of values of y.

Pro: • No special starting procedure needed.
• Can 'adaptively' change h as required.
• Easy to program.

Con: • Typically not very efficient, as we are throwing away information when we shift camp.

The most usual single-step methods are known collectively as Runge–Kutta methods. In these, we obtain successive estimates k_1, k_2, ... of the expected increment in y by going out varying proportions of the way between x_0 and x_1, in directions that depend on the earlier parts of the exploration, and use these to estimate some average k. The [many] parameters in this process that are at our disposal are chosen so as to maximise the number of terms of agreement between our estimate and the Taylor series of y about $x = x_0$.

The Runge–Kutta method is:

$$k_1 = hf(x_0, y_0);$$

$$k_2 = hf(x_0 + \tfrac{1}{2}h, y_0 + \tfrac{1}{2}k_1);$$

$$k_3 = hf(x_0 + \tfrac{1}{2}h, y_0 + \tfrac{1}{2}k_2);$$

$$k_4 = hf(x_0 + h, y_0 + k_3);$$

$$k = \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

[Compare Simpson's Rule.] More generally, k_4, for example, would depend directly on k_1 and k_2 as well as on k_3, and how much we increment x would also vary more 'interestingly'.

There are many, many variants, especially with more or fewer evaluations of f per step [which is a measure of the work done]. Left for anyone interested to look up. Modified Euler is a particularly simple RK method. You will also see especially a variant called Kutta–Merson, and, as used in Maple, Runge–Kutta–Fehlberg, which trades off an extra evaluation of f for also getting an estimate of the error.

A different simple way to estimate the error is to repeat the calculation of two RK steps using one step but with h doubled. This uses therefore 11 evaluations per double step instead of 8, but it gives a chance for Richardson extrapolation, and if you find the error is getting too small or too large, then you can double or halve h, and some of the work is already done.

Multi-step methods

The basic idea here is that having built up a table of values of y and f for different values of x, we can interpolate to find f as a function of x between x_n and x_{n+1}, and integrate that to get the next y value.

Pro: • Makes efficient use of f, so is fast and accurate.

Con: • Needs several starting values, so we have to use some other method [such as RK] at first.
• Which is not *necessarily* that hard, for example if it is easy to get a Taylor series expansion of y from the differential equation near $x = x_0$.
• But it does make these methods somewhat harder to program up.
• Hard[er] to change h.

A typical example is the 3-point Adams–Bashforth formula, in which we use the most recent three values of f to estimate f as a quadratic function of x, and integrate that:

$$y_1 = y_0 + \frac{h}{12}(23f_0 - 16f_{-1} + 5f_{-2}).$$

[Details left as an exercise.]

Compare Simpson's Rule. In that we would be using the quadratic to integrate between x_{-2} and x_0, which is relatively nice. here we are using it to *extrapolate* to 'new' values of x and integrate between x_0 and x_1, which is relatively nasty.

So Adams−Bashforth is not usually used on its own, but as part of a *predictor-corrector* process. We use AB to produce an *estimate*, the prediction, y_1^*, of y_1, and use this estimate in a slightly different process, called Adams−Moulton. This uses the old values of f and the new estimated f_1^* to produce a better interpolated polynomial, which we integrate up to get a corrected value of y_1 and so of f_1. Specifically, the 4-point Adams−Moulton formula is

$$y_1 = y_0 + \frac{h}{24}(9f_1^* + 19f_0 - 5f_{-1} + f_{-2}).$$

where $f_1^* = f(x_1, y_1^*)$. [Details again left as an exercise.]

In principle, if AB and AM differ too much, we could use the first AM value as predictor in a second round of AM; but if this happens, it is usually a sign that h is too large. In AM, the discrepancy between predictor and corrector can be used to give an error estimate, or, as with RK, we can re-do the calculation with a different h.

As with RK methods, there are many variations. In principle, we should use difference table methods to determine what degree of polynomial [if any] should be used in the AB/AM interpolations, but it is more usual in practice to just choose a particular number of 'points', as above.

Also as with RK, Euler and Modified Euler are again just the simplest possible multi-step methods, the 1-point AB predictor with a 2-point AM corrector.

How well do these methods work in practice? The table shows RK and AB/AM as described above on our standard example, $f(x,y) = xy$, starting with $y = 1$ when $x = 0$, and using $h = 0.1$.

To start AB off, we use the ODE itself to give a Taylor series for f: As $f = xy$, $f' = xy' + y = xf + y$, so $f'' = xf' + f + y' = xf' + 2f$, and then $f''' = xf'' + 3f'$, $f^{(4)} = xf''' + 4f''$, $f^{(5)} = xf^{(4)} + 5f'''$, and so on. Substituting $x = 0$, $y = 1$, we find successively that $f = 0$, $f' = 1$, $f'' = 0$, $f''' = 3$, $f^{(4)} = 0$ and $f^{(5)} = 15$, so

$$f(x) = x + \tfrac{1}{2}x^3 + \tfrac{1}{8}x^5 + \ldots; \quad y(x) = 1 + \tfrac{1}{2}x^2 + \tfrac{1}{8}x^4 + \tfrac{1}{48}x^6 + \ldots.$$

Substituting $x = 0.1$, we estimate $f(\pm 0.1) \approx \pm 0.10050125$, $y(\pm 0.1) \approx 1.0050125$. This gives us three values of f and y to start us off.

x	RK	AB/AM
0.0	1.00000000	1.00000000
0.1	1.00501252	1.00501252
0.2	1.02020134	1.02020077
0.3	1.04602786	1.04602664
0.4	1.08328706	1.08328503
0.5	1.13314845	1.13314526
0.6	1.19721735	1.19721245
0.7	1.27762128	1.27761376
0.8	1.37712769	1.37711613
0.9	1.49930236	1.49928456
1.0	1.64872101	1.64869362

Again, the final values should be compared with $e^{\frac{1}{2}} \approx 1.64872127$. Runge–Kutta has done extremely well. [But note that it has done considerably more work, evaluating f four times per step.] Adams–Bashforth has not done quite so well, though much better than Modified Euler [for the same two evaluations of f per step], and note that we could move to a much more accurate 4- or 5-point formula at very little cost [and the same number of function evaluations].