

Multi-Step Methods

The methods described thus far (i.e., the Euler and Runge-Kutta methods) are referred to as one-step methods because to calculate the value of the unknown function x at step i the information required to next value of x depends only on the values of t and x at step i . Multistep methods are algorithm that utilize values at several preceding steps to determine successive values of the unknown function x .

Since multi-step methods utilize more information than single step methods, it is natural to expect multi-step methods to be more accurate than single step methods. We won't quantify this expectation here, but hopefully the following analogy makes this expectation a bit more convincing. Recall that we had several methods for computing derivatives numerically using Richardson extrapolations

$$\begin{aligned} x'(t) &= \frac{x(t+h) - x(t-h)}{2h} + \mathcal{O}(h^2) \\ x'(t) &= \frac{4}{3} \left(\frac{x(t+h/2) - x(t-h/2)}{h} \right) - \frac{1}{3} \left(\frac{x(t+h) - x(t-h)}{2h} \right) + \mathcal{O}(h^4) \\ x'(t) &= \frac{128}{45} \left(\frac{x(t+\frac{h}{4}) - x(t-\frac{h}{4})}{h} \right) - \frac{4}{9} \left(\frac{x(t+\frac{h}{2}) - x(t-\frac{h}{2})}{h} \right) + \frac{1}{90} \left(\frac{x(t+h) - x(t-h)}{2h} \right) + \mathcal{O}(h^6) \\ &\vdots \end{aligned}$$

Note how the accuracy of the derivatives increased as we take more and more data points.

0.0.1. *Adams-Bashforth Formulae*. Suppose we have a differential equation of the form

$$\frac{dx}{dt} = f(t, x)$$

We can use the Fundamental Theorem of Calculus to obtain from this equation an equivalent integral equation

$$(22.1) \quad x(t_{n+1}) - x(t_n) = \int_{t_n}^{t_{n+1}} f(t, x(t)) dt$$

Now of course this doesn't lead us any closer to an analytic solution, because before we can carry out the integration on the right hand side, we have to know exactly how $x(t)$ depends on t . However, if we have an approximate expression for $f(t, x(t))$, e.g. a polynomial interpolation of $f(t, x(t))$ then we could arrive at an approximate value for $x(t_{n+1})$.

Suppose then that we know values for

$$f_i \equiv f(t_i, x(t_i))$$

for $i = 0, 1, \dots, n$. Then we could use the j values $f_{n-j}, f_{n-j+1}, \dots, f_n$ to interpolate the function $f(t, x(t))$ on the interval $[t_{n-j}, t_{n+1}]$

$$f(t, x(t)) \approx f_{n-j} \ell_{n-j}(t) + f_{n-j+1} \ell_{n-j+1}(t) + \dots + f_n \ell_n(t)$$

where the ℓ_i are the cardinal functions associated with the nodes $t_i = ih$. We can thus write

$$(22.2) \quad x_{n+1} \approx x_n + \int_{t_n}^{t_n+h} \left(\sum_{i=n-j}^n f_i \ell_i(t) \right) dt = x_n + \sum_{i=n-j}^n c_i f_i$$

where of course

$$\begin{aligned} x_i &\equiv x(t_i) \\ c_i &\equiv \int_{t_n}^{t_n+h} \ell_i(t) dt \end{aligned}$$

The constants c_i are independent of f and can be readily (albeit strenuously) calculate. Equations of the form (22.2) are known as **Adams-Bashforth formulae**. In the case where the number j of preceding values used to determine x_{n+1} is 5 we have

$$(22.3) \quad x_{n+1} = x_n + \frac{h}{720} [1901f_n - 2774f_{n-1} + 2616f_{n-2} - 1274f_{n-3} - 251f_{n-4}]$$

0.1. Predictor-Corrector Method. Suppose we approximate the right hand side of (22.1) by interpolating the integrand $f(t, x(t))$ at the points $\{t_{n-j-2}, t_{n-j-3}, \dots, t_{n+1}\}$. We then arrive at a formula of the form

$$x_{n+1} = x_n + \sum_{i=n-j-2}^{n+1} C_i f_i$$

Formulae of this type are known as **Adams-Moulton formulae**. For the case where $j = 5$, an explicit calculation of the constants

$$C_i = \int_{t_n}^{t_{n+1}} \ell_i(t) dt$$

yields the following fifth order Adams-Moulton formula

$$(22.4) \quad x_{n+1} = x_n + \frac{h}{720} [251f_{n+1} + 646f_n - 264f_{n-1} + 106f_{n-2} - 19f_{n-3}]$$

Note, however, that in order to compute x_{n+1} we first need to compute

$$f_{n+1} = f(t_{n+1}, x_{n+1})$$

which depends on x_{n+1} . Clearly, any attempt to use an Adams-Moulton formula by itself will just cause us to run around in circles.

However, if we know j previous values of x_i , we can use an j^{th} -order Adams-Bashform formula to obtain an approximate value for x_{n+1} . We can then use this value to compute f_{n+1} and then use a j^{th} -order Adams-Moulton formula to refine our estimate of x_{n+1} . In other words we use an Adams-Bashforth formula like (22.3) to **predict** a value for x_{n+1} and hence f_{n+1} ; and then use an Adams-Moulton formula like (22.4) to **correct** (or at least refine) our approximate value for x_{n+1} . Such a method is known as a **predictor-corrector method**.

However, there is still one crucial step missing. In order to use a n^{th} -order Adams-Moulton formula we must first have the first n values of x so that we can compute f_0, f_1, \dots, f_n . These values are typically obtained by carrying out an n -step Runge-Kutta approximation to obtain the n data points need to initialize the Adams-Moulton method.