LECTURE 7

Numerical Methods for ODEs, III

1. Multistep Methods

We have been developing numerical methods for obtaining solutions to first order ODEs of the form

$$x'(t) = F(t, x) \quad .$$

The numerical methods we have developed thus far (i.e., the Euler method and Runge-Kutta methods) have been based on Taylor's formula

$$x(t+h) = x(t) + x'(t)h + \frac{1}{2!}x''(t)h^2 + \frac{1}{3!}x'''(t)h^3 + \cdots$$

In the Euler method one uses the first order approximation

$$x(t+h) \approx x(t) + x'(t)h + \mathcal{O}\left(h^2\right)$$

to establish the recursive formula

$$\begin{aligned} t_i &= t_{i-1} + \Delta t \\ x_i &= x_{i-1} + F(t_{i-1}, x_{i-1})\Delta t \end{aligned}$$

The Runge-Kutta method uses some tricks that push the error inherent to any Taylor approximation to higher order in h.

These methods described 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. The **multistep methods** we shall develop today are algorithms that utilize values at several preceding steps to determine successive values of the unknown function x.

Since multi-step methods will be allowed to 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

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

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

1.0.1. *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

$$x(t_{n+1}) - x(t_n) = \int_{t_n}^{t_{n+1}} F(t, x(t))\, dt \tag{1}$$

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 $x(t_{n+1})$.

2. Digression: Polynomial Interpolation

Let me give you a simple example of polynomial interpolation. Suppose you knew a function $f(x)$ actually had to be a polynomial of degree two; i.e., there exist constants a_0, a_1, a_2 such that

$$f(x) = a_0 + a_1 x + a_2 x^2 \qquad \forall\ x \tag{2}$$

Then you could figure out exactly what polynomial of degree two $f(x)$ is by simply sampling $f(x)$ at three points: say

$$f(0) = f_0 \quad , \quad f(1) = f_1 \quad , \quad f(2) = f_2$$

For the equations

$$\begin{aligned} f_0 &= a_0 + 0 + 0 \\ f_1 &= a_0 + a_1 + a_2 \\ f_2 &= a_0 + 2a_1 + 4a_2 \end{aligned}$$

will furnish you with three independent linear equations for the three unknowns a_0, a_1, a_2. And once you know a_0, a_1, a_2, you can then compute the value of $f(x)$ at any point x via (2).

Now suppose you know only that $f(x)$ is *approximately* equal to a polynomial of degree 2 near a point x_0. Then by sampling $f(x)$ at 3 different points close to x_0 you could still figure out (as in the preceding example) an appropriate quadratic polynomial with which to approximate $f(x)$.

More generally, one could sample a function $f(x)$ at $n+1$ points to obtain enough equations to determine the coefficients of a polynomial of degree n that approximates $f(x)$. This procedure is known as **polynomial interpolation.** (And naturally, the more sampling of $f(x)$ you carry out, the better the polynomial approximation so obtained.)

However, in practice, solving linear equations to get the coefficients of a polynomial interpolation of $f(x)$ is not the way to go. Let $\{x_0, x_1, \ldots, x_n\}$ be a set of sampling points, consider the polynomials

$$\ell_i(x) = \prod_{j \neq i} \frac{x - x_j}{x_i - x_j}$$

These polynomials will have the property that

$$\ell_i(x_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

and so the sum

$$P_f(x) = \sum_{i=0}^{n} f(x_i)\, \ell_i(x)$$

will be a polynomial of degree n such that

$$P_f(x) = f(x) \text{ at each sampling point } x_0, \ldots, x_n$$

By the uniqueness of the interpolation polynomial, $P_f(x)$ is our guy.

3. Back to Multistep Methods

Suppose then that we know a set of (perhaps approximate) points on the graph of the solution of (1)

$$(t_0, x(t_0)),\ (t_1, x(t_1)),\ (t_2, x_2(t_2)),\ \cdots,\ (t_n, x(t_n))$$

then we also have a corresponding sequence of values of $F(t,x)$

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

for $i = 0, 1, \ldots, n$. Regarding $F(t, x(t))$ as a function $\widetilde{F}(t)$ of t alone, we could then utilize these $(n+1)$ values of $\widetilde{F}(t)$ to obtain a polynomial of degree n that approximates $\widetilde{F}(t)$.

$$F(t, x(t))$$

In fact, we could use the j values $f_{n-j}, f_{n-j+1}, \ldots, f_n$ to interpolate the function $f(t, x(t))$ on the interval $[t_{n-j}, t_{n+1}]$

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

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

$$x_{n+1} \approx x_n + \int_{t_n}^{t_n+h} \left(\sum_{i=n-j}^{n} f_i \ell_i(t) \right) dt = x_n + \sum_{i=n-j}^{n} c_i f_i \tag{3}$$

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) calculated. Equations of the form (3) are known as **Adams-Bashforth formulae**. In the case where the number j of preceding values used to determine x_{n+1} is 4

$$x_{n+1} = x_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$$

and when $j = 5$ we have

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

3.1. Predictor-Corrector Method. Suppose we approximate the right hand side of (1) by interpolating the integrand $f(t, x(t))$ at the points $\{t_{n-j-2}, t_{n-j-3}, \ldots, t_{n+1}\}$. 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

$$x_{n+1} = x_n + \frac{h}{720}[251f_{n+1} + 646f_n - 264f_{n-1} + 106f_{n-2} - 19f_{n-3}] \tag{5}$$

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 ot 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 (4) to **predict** a value for x_{n+1} and hence f_{n+1}; and then use an Adams-Moulton formula like (5) 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 $f_0, f_1, \ldots, f_n$. 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.