NSDE 1: LECTURE 7

TYRONE REES*

$$u' = f(t, u), \qquad u(t_0) = u_0.$$

For the last two weeks we've been looking at one-step methods. These use information (t_n, U_n) that is the most recent step to update the approximate solution U_{n+1} at $t_{n+1} = t_n + h$. To do this, we (in the case of Runge-Kutta methods) evaluate the function multiple times at points in between t_n and t_{n+1} to obtain a more accurate solution.

This can improve the accuracy, may not be the most efficient method, especially in the case where the function is expensive to evaluate.

Recall that the inpiration for one-step methods was re-writing the ODE over a time step as

$$u(t_{n+1}) - u(t_n) = \int_{t_n}^{t_{n+1}} u'(t)dt = \int_{t_n}^{t_{n+1}} f(t, u(t))dt.$$

Runge-Kutta methods evaluated the function at points in between t_n and t_{n+1} in order to better approximate the integral on the right hand side.

Instead, we could integrate over more than one time step, and get a more accurate numerical method by re-using function evaluations we already have. For example,

$$\int_{t_n}^{t_{n+2}} u'(t)dt = \int_{t_n}^{t_{n+2}} f(t, u(t))dt$$

Using, for example, Simpson's rule, we get

$$u(t_{n+2}) - u(t_n) \approx \frac{2h}{6}\left[f(t_{n+2}, u(t_{n+2})) + 4f(t_{n+1}, u(t_{n+1})) + f(t_n, u(t_n))\right],$$

which suggests the numerical method

$$U_{n+2} = U_n + \frac{h}{3}\left[f(t_{n+2}, U_{n+2}) + 4f(t_{n+1}, U_{n+1}) + f(t_n, U_n)\right],$$

We're given U_0, we can use a one-step method to find U_1, and then we can use this numerical scheme to approximate the solution at the other time steps.

General form The general form of a linear multistep method is

$$\sum_{j=0}^{k} \alpha_j U_{n+j} = h \sum_{j=0}^{k} \beta_j f(t_{n+j}, U_{n+j})$$

*Rutherford Appleton Laboratory, Chilton, Didcot, UK, tyrone.rees@stfc.ac.uk

As before, if $\beta_k = 0$ then the method is *explicit*, and if $\beta_k \neq 0$ then the method is *implicit*. (So Simpson's rule is an implicit 2-step method).

As before, we define:

The truncation error:

$$T_n = \frac{\sum_{j=0}^{k}[\alpha_j u(t_{n+j}) - h\beta_j u'(t_{n+j})]}{h\sum_{j=0}^{k}\beta_j}$$

consistency:

$$\lim_{h\to 0, n\to\infty, nh=t_n-t_0} T_n = 0$$

And a method is **pth order accurate** if:

$$|T_n| \leq Kh^p.$$

Note that

$$u(t_{n+j}) = u(t_n) + (jh)u'(t_n) + \frac{(jh)^2}{2!}u''(t_n) + \dots$$

and also

$$u'(t_{n+j}) = u'(t_n) + (jh)u''(t_n) + \frac{(jh)^2}{2!}u'''(t_n) + \dots$$

Subsituting this into T_n we get

$$T_n = \frac{1}{h\sum_{j=1}^{k}\beta_j}[C_0 u(t_n) + C_1 h u'(t_n) + C_2 h^2 u''(t_n) + \cdots]$$

where

$$C_0 = \sum_{j=0}^{k}\alpha_j,$$

$$C_1 = \sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k}\beta_j$$

$$\dots$$

$$C_q = \sum_{j=1}^{k}\frac{j^q}{q!}\alpha_j - \sum_{j=1}^{k}\frac{j^{q-1}}{(q-1)!}\beta_j$$

The method is *consistent* if $\lim T_n = 0$, which is equivalent to requiring that $C_0 = 0$ and $C_1 = 0$.

Furthermore, the method is pth order accurate if and only if

$$C_0 = C_1 = \cdots = C_p = 0 \text{ and } C_{p+1} \neq 0$$

and, in this case,

$$T_n = \frac{C_{p+1}}{\sum_{j=1}^{k} \beta_j} h^p u^{(p+1)}(t_n) + O(h^p)$$

C_{p+1} is called the *error constant.*

Adams methods

A particular class of methods, known as Adams methods, have the form

$$U^{n+k} = U^{n+k-1} + h \sum_{j=0}^{k} \beta_j f(t_{n+j}, U_{n+j})$$

i.e., $\alpha_k = 1, \alpha_{k-1} = -1, \alpha_j = 0, j < k-1$.

If we require an explicit method ($\beta_k = 0$), then we can pick the remaining k coefficients to eliminate as many terms as possible in the Taylor expansion. These methods are called **Adams-Bashforth** methods:

$U_{n+1} = U_n + hf(t_n, U_n)$ 1st order

$U_{n+2} = U_{n+1} + \dfrac{h}{2}(-f(t_n, U_n) + 3f(t_{n+1}, U_{n+1}))$ 2nd order

$U_{n+3} = U_{n+2} + \dfrac{h}{12}(5f(t_n, U_n) - 16f(t_{n+1}, U_{n+1}) + 23f(t_{n+2}, U_{n+2}))$ 3rd order

$U_{n+4} = U_{n+3} + \dfrac{h}{23}(-9f(t_n, U_n) + 37f(t_{n+1}, U_{n+1}) - 59f(t_{n+2}, U_{n+2}) + 55f(t_{n+3}, U_{n+3})$ 4th order

If we allow $\beta_k \neq 0$, then we have one more free parameter, and so can get a method of one order higher than the equivalent Adams-Bashforth method. These methods are called **Adams-Moulton** methods:

$U_{n+1} = U_n + \dfrac{h}{2}(f(t_n, U_n) + f(t_{n+1}, U_{n+1}))$ 2nd order

$U_{n+2} = U_{n+1} + \dfrac{h}{12}(-f(t_n, U_n) + 8f(t_{n+1}, U_{n+1}) + 5f(t_{n+3}, U_{n+3}))$

$U_{n+3} = U_{n+2} + \dfrac{h}{24}(f(t_n, U_n) - 5f(t_{n+1}, U_{n+1}) + 19f(t_{n+2}, U_{n+2}) + 9f(t_{n+3}, U_{n+3}))$

Zero-stability

Suppose we have a general $k-$step method

$$\sum_{j=0}^{k} \alpha_j U_{n+j} = h \sum_{j=0}^{k} \beta_j f(t_{n+j}, U_{n+j})$$

U_0 is given, $U_1, \ldots, U_{n-1}$ have to be computed. Question: how do the errors in $U_1, \ldots, U_{k-1}$ affect the later values?

Definintion A linear $k-$step method for

$$u' = f(t,u),\ u(t_0) = u_0,\ t \in [t_0, T_m]$$

is said to be zero-stable if there exists a constant K such that, for any two sequences $U_0, U_1, \ldots, U_{k-1}$, and $\hat{U}_0, \hat{U}_1, \ldots, \hat{U}_{k-1}$,

$$|U_n - \hat{U}_n| \leq K \max\{|U_0 - \hat{U}_0|, |U_1 - \hat{U}_1|, \ldots, |U_{k-1} - \hat{U}_{k-1}|\}$$

for $t_n \leq T_M$ and as $h \to 0$.

This isn't actually useful for checking zero stability – in practice we reformulate in terms of polynomials:

The first characteristic polynomial is given by

$$\rho(z) = \sum_{j=0}^{k} \alpha_j z^j$$

The second characteristic polynomial is given by

$$\sigma(z) = \sum_{j=0}^{k} \beta_j z^j$$

Theorem (Root condition)

A linear multistep method is zero stable for any ODE

$$u' = f(t,u)$$

where f obeys a Lipschitz condition if and only if all zeros of its first characteristic polynomial lie inside the closed unit disk, with any that lie on the unit circle being simple.

Example

Simpson rule method:

$$\begin{aligned} U_{n+2} - U_n &= \frac{h}{3}(f_{n+2} + 4f_{n+1} + f_n) \\ \rho(z) &= z^2 - 1 \\ z &= \pm 1 \end{aligned}$$

(where $f_n = f(t_n, U_n)$).

Simple roots on the unit circle, so the method is zero-stable.

Example

Adams-Bashforth method

$$U_{n+4} - U_{n+3} = \frac{h}{24}(-9f_n + 37f_{n+1} - 59f_{n+2} + 55f_{n+3})$$

$$\rho(z) = z^4 - z^3 = z^3(z-1)$$
$$z_1 = z_2 = z_3 = 0, z_4 = 1$$

Example A 3-step 6-th order accurate method:

$$11U_{n+3} + 27U_{n+2} - 27U_{n+1} - 11U_n = 3h(f_{n+3} + 9f_{n+2} + 9f_{n+1} + f_n)$$

$$\rho(z) = 11z^3 + 27z^2 - 27z - 11$$

$$z_1 = 1, z_2 \approx -0.3189, z_3 \approx -3.1356$$

since $|z_3| > 1$, the method is not zero stable.