## UW-Madison Math/CS 714

Methods of Computational Mathematics I

Initial value problems II

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As for boundary value problems, we would like to ensure that our numerical method will converge to the exact solution.

For a fixed time T > 0, we would like our numerical solution  $U^N$  to approach u(T). Define N = T/k. Then convergence means that

$$\lim_{k\to 0,\ Nk=T}U^N=u(T).$$

It is possible that a method may converge for one problem but not for another. For a mathematical definition, we would like to ensure that a method converges for all problems in a reasonably large class and for all reasonable starting values.

Let  $U^n(k)$  be the numerical solution with step size k. For reasonable starting values, we might require that  $U^{\nu}(k)$  should approximate  $u(\nu k)$  for  $\nu=0,1,\ldots,r-1$ .

Since  $k \to 0$ , a weaker condition that we could impose is

$$\lim_{k \to 0} U^{\nu}(k) = \eta \tag{1}$$

for  $\nu = 0, 1, \dots, r - 1$ , where  $u(0) = \eta$  is our initial condition.

Definition. An r-step method is convergent if applying the method to any ODE u'(t) = f(u(t), t) where f(u, t) is Lipschitz continuous in u, and with any set of starting values satisfying Eq. (1), we obtain convergence in the sense that

$$\lim_{k\to 0,\ Nk=T}U^N=u(T)$$

for any T > 0 where the ODE has a unique solution.

## Convergence for a test problem

Consider the linear ODE

$$u'(t) = \lambda u(t) + g(t)$$

where  $u(t_0) = \eta$ . This has general solution

$$u(t) = e^{\lambda(t-t_0)}\eta + \int_{t_0}^t e^{\lambda(t-\tau)}g(\tau)d au.$$

Applying Euler's method to the test problem gives

$$U^{n+1} = U^n + k(\lambda U^n + g(t_n)) = (1 + k\lambda)U^n + kg(t_n).$$

The local truncation error is

$$\tau^{n} = \left(\frac{u(t_{n+1}) - u(t_{n})}{k}\right) - (\lambda u(t_{n}) + g(t_{n})) = \frac{k}{2}u''(t_{n}) + O(k^{2}).$$

Since

$$u(t_{n+1}) = (1 + k\lambda)u(t_n) + kg(t_n) + k\tau^n,$$

then defining global error as  $E^n = U^n - u(t_n)$  gives

$$E^{n+1} = (1 + k\lambda)E^n - k\tau^n.$$

Applying this recursively shows that

$$E^{n} = (1 + k\lambda)E^{n-1} - k\tau^{n-1}$$
  
= (1 + k\lambda) \[ (1 + k\lambda)E^{n-2} - k\tau^{n-2} \] - k\tau^{n-1}

and

$$E^{n} = (1 + k\lambda)E^{0} - k\sum_{m=1}^{n} (1 + k\lambda)^{n-m}\tau^{m-1}.$$

Note that  $|1+k\lambda| \leq e^{k|\lambda|}$  and hence

$$(1+k\lambda)^{n-m} \le e^{(n-m)k|\lambda|} \le e^{nk|\lambda|} \le e^{|\lambda|T}$$

where  $t_n = nk \leq T$ .

Then

$$\begin{split} |E^n| &\leq e^{|\lambda|T} \left( |E_0| + k \sum_{m=1}^n |\tau^{m-1}| \right) \\ &\leq e^{|\lambda|T} \left( |E_0| + nk \max_{m \in \{1, \dots, n\}} |\tau^{m-1}| \right) \end{split}$$

Let N = T/k be the number of timesteps to reach T. Define

$$\|\tau\|_{\infty} = \max_{0 \le n \le N-1} |\tau^n|$$

where we expect from our previous analysis that

$$\|\tau\|_{\infty} pprox \frac{k}{2} \|u''\|_{\infty} = O(k)$$

where  $||u''||_{\infty}$  is the maximum of u'' over [0, T].

Then for 
$$t = nk \le T$$
, 
$$|E^n| < e^{|\lambda|T}(|E^0| + T||\tau||_{\infty}).$$

From the condition about starting values,  $|E^0| \to 0$  as  $k \to 0$ . Indeed, if  $U^0$  is chosen to be  $u(t_0)$ , then  $E^0 = 0$ . Hence

$$|E^n| \le e^{|\lambda|T} T \|\tau\|_{\infty} = O(k)$$

as  $k \to 0$ . Hence the method converges and is first order accurate.

## Euler's method for general problems

Suppose the same analysis is applied to u' = f(u, t) where f(u, t) is Lipschitz continuous with constant L. Then<sup>1</sup>

$$|E^n| \le e^{LT} T \|\tau\|_{\infty} = O(k).$$

The bound exponentially diverges, although in practice the numerical errors are much smaller than this.

For general one-step methods, if the local truncation error is  $O(k^p)$  then the global error will also be  $O(k^p)$ . Hence the method converges as  $k \to 0$ , which is referred to as zero-stability.

<sup>&</sup>lt;sup>1</sup>See the ODE workshop slides for more detail.

## Zero-stability for multistep methods

For multistep methods, the previous results do not apply directly. Consider the following two-step example:

$$U^{n+2} - 3U^{n+1} + 2U^n = -kf(U^n).$$

The truncation error is

$$\tau^{n} = \frac{u(t_{n+2}) - 3u(t_{n+1}) + 2u(t_{n}) - ku'(t_{n})}{k}$$
$$= \frac{5k}{2}u''(t_{n}) + O(k^{2}).$$

so the method is consistent.

## Stability of a multistep scheme

Consider applying this method to u'=0 with u(0)=0. The solution is given by

$$U^{n+2} - 3U^{n+1} + 2U^n = 0.$$

Two starting values are needed. If  $U^0 = U^1 = 0$ , then  $U^n = 0$  for all n, and the numerical results match the exact solution.

But suppose that  $U^1 = \epsilon \neq 0$  due to some numerical error. Then we can show that

$$U^n = \epsilon(2^n - 1)$$

which blows up exponentially. Similar results would be seen when applying this to any ODE, showing that the method is not stable.

## Linear difference equations

The previous numerical example involves a linear difference equation which can be written generally as

$$\sum_{j=0}^{r} \alpha_j U^{n+j} = 0.$$

Consider looking for a solution of the form  $U^n = \zeta^n$  (where the n on the RHS is a power). Then

$$\sum_{j=0}^{r} \alpha_j \zeta^{n+j} = 0$$

and hence

$$\sum_{j=0}^{r} \alpha_j \zeta^j = \rho(\zeta) = 0,$$

where  $\rho(\zeta)$  is the first characteristic polynomial introduced previously.

## Linear difference equations

In general  $\rho$  can be factorized as

$$\rho(\zeta) = \alpha_r(\zeta - \zeta_1)(\zeta - \zeta_2) \dots (\zeta - \zeta_r)$$

where the roots  $\zeta_j$  may be complex. Since the difference equation is linear, any linear combination of solutions will satisfy it.

Assuming the roots are all distinct, the general solution is

$$U^n = c_1 \zeta_1^n + c_2 \zeta_2^n + \ldots + c_r \zeta_r^n.$$

Given initial data  $U^0, U^1, \ldots, U^{r-1}$ , the constants  $c_j$  can be determined.

## Linear difference equations

For the example difference equation  $U^{n+2} - 3U^{n+1} + 2U^n = 0$ , the characteristic polynomial factorizes as

$$\rho(\zeta) = 2 - 3\zeta + \zeta^2 = (\zeta - 1)(\zeta - 2),$$

so the roots are  $\zeta_1 = 1$  and  $\zeta_2 = 2$ . The general solution is therefore

$$U^n=c_1+c_22^n,$$

which matches is consistent with the solution presented previously.

In general, the presence of a root where  $|\zeta_j|>1$  will lead to an exponentially divergent solution.

## Repeated roots

More generally, it is possible that some roots may be repeated. Suppose that the distinct roots are  $\zeta_1, \ldots, \zeta_l$  where  $l \leq r$ , and let  $m_i$  be the multiplicity of  $\zeta_i$ . Hence

$$\sum_{j=1}^{l} m_j = r$$

The general solution of the difference equation is

$$U^n = \sum_{j=1}^l p_j(n) \zeta_j^n$$

where  $p_j$  is a polynomial of degree  $m_j - 1$ .

#### Repeated roots example

Consider the linear multistep method

$$U^{n+2}-2U^{n+1}+U^n=\frac{k(f(U^{n+2})+f(U^n))}{2}.$$

The characteristic polynomial is

$$\rho(\zeta) = \zeta^2 - 2\zeta + 1 = (\zeta - 1)^2$$

and so  $\zeta_1 = 1$  is a root with multiplicity 2. Therefore the general solution is

$$U^n = p_1(n)\zeta_1^n$$

where  $p_1(n)$  is a polynomial of degree 1, so

$$U^n=c_1+c_2n.$$

In general, a repeated root with  $|\zeta_i| = 1$  is enough to create an algebraic divergence.

#### The root condition

This leads to the follow theorem for determining zero-stability.

Theorem. An r-step linear multistep method is said to be zero-stable if the roots  $\zeta_i$  of the characteristic polynomial  $\rho(\zeta)$  satisfy:

- $ightharpoonup |\zeta_j| \le 1$  for all j,
- ▶ If  $\zeta_j$  is a repeated root, then  $|\zeta_j| < 1$ .

#### **Examples**

The program *z\_stabilty.py* integrates three different multistep schemes:

Stable:

$$24U^{n+3} - 24U^{n+2} = k(9f(U^{n+3}) + 19f(U^{n+2}) - 5f(U^{n+1}) + f(U^{n}))$$

Exponentially unstable:

$$11U^{n+3} + 27U^{n+2} - 27U^{n+1} - 11U^{n}$$

$$= 3k(f(U^{n+3}) + 9f(U^{n+2}) + 9f(U^{n+1}) + f(U^{n}))$$

► Algebraically unstable:

$$U^{n+3} + U^{n+2} - U^{n+1} - U^n = 2k(f(U^{n+2}) + f(U^{n+1}))$$

A theorem due to Dahlquist shows that for linear multistep methods

$$({\sf consistency}) \quad + \quad ({\sf zero\text{-}stability}) \quad \Longleftrightarrow \quad ({\sf convergence})$$

This is an asymptotic statement about the case when  $k \to 0$ . In practice, obtaining a convergence may also depend on the size of the timestep k.