

The average of the forward and backward difference operators is

$$(3.46) \quad \frac{1}{2}(\Delta_+ + \Delta_-) = 2 \sinh kD .$$

Note that the centered difference operator δ can be expressed as the average of the forward and backward operators for a half step size, so we obtain

$$(3.47) \quad \delta = 2 \sinh \frac{kD}{2} ,$$

from where

$$(3.48) \quad D = \frac{2}{k} \operatorname{arcsinh} \frac{\delta}{2} .$$

The Taylor series expansion of $\operatorname{arcsinh} x$ around $x = 0$ is

$$(3.49) \quad \operatorname{arcsinh} x = x - \frac{x^3}{6} + \frac{3x^5}{40} - \frac{5x^7}{112} + \frac{35x^9}{1152} -$$

so the first few terms from (3.48) are

$$(3.50) \quad D = \frac{1}{k} \left(\delta - \frac{1}{24} \delta^3 - \frac{3}{640} \delta^5 - \frac{5}{7168} \delta^7 + \frac{35}{294912} \delta^9 - \dots \right) .$$

Notice that the series only contains odd powers of δ . We can show by induction that truncation of the series at δ^{2n-1} gives a formula of $O(k^{2n})$ accuracy.

4. Common finite difference methods

Let us now consider how numerical algorithms may be built to solve the IVP (2.1) using finite differences.

4.1. Taylor series. The basic task of a finite difference method that solves (2.1) numerically is to furnish a value at the next time step $q(t+k)$ in terms of known values at previous time steps. An immediate way of doing this is by use of a Taylor series expansion

$$(4.1) \quad q(t+k) = q + kq' + \frac{k^2}{2!} q'' + \frac{k^3}{3!} q''' + \dots$$

To ease notation, function arguments not explicitly written out are considered to be t , i.e. q' means $q'(t)$. The ODE specifies that $q' = f(t, q)$. From this we can compute higher derivatives

$$(4.2) \quad q'' = \frac{d}{dt} f(t, q(t)) = f_t + f_q q' =$$

$$(4.3) \quad q''' = \frac{d}{dt} q'' = \frac{d}{dt} (f_t + f_q f) = f_{tt} + f_{tq} f + (f_{qt} + f_{qq} f) f + f_q (f_t + f_q f)$$

Truncation of the Taylor series to various orders leads to the algorithms:

(1) $O(k)$, Euler's method

$$(4.4) \quad Q^{n+1} = Q^n + kf(Q^n)$$

(2) $O(k^2)$

$$(4.5) \quad Q^{n+1} = Q^n + kf(Q^n) + \frac{k^2}{2} [f_t(Q^n) + f_q(Q^n)f(Q^n)]$$

$$(3) O(k^3)$$

$$(4.6) \quad Q^{n+1} = Q^n + kf + \frac{k^2}{2} [f_t + f_q f] + \frac{k^3}{6} [f_{tt} + f_{tq} f + (f_{qt} + f_{qq} f) f + f_q (f_t + f_q f)]$$

with f and its derivatives evaluated at Q^n .

Formulas of arbitrarily high order can be built up through this procedure but evaluation of all the derivatives of f is tedious. In recent years the symbolic computational capabilities of computers has led to renewed interest in the Taylor series method.

4.2. Runge-Kutta methods. The Runge-Kutta class of methods aims to achieve arbitrary accuracy not by evaluating the function f and its derivatives at t but just by evaluations of the function f at various points in the interval $[t, t+k]$. The general form of a Runge-Kutta method is

$$(4.7) \quad q(t+k) = q(t) + \sum_{l=0}^s \gamma_l f_l$$

where f_l denotes evaluation of the function f at

$$(4.8) \quad t^l = t + \alpha_l k$$

$$(4.9) \quad q^l = q(t) + k \sum_{m=0}^s \beta_{l,m} f_m$$

Essentially this amounts to replacing the Taylor series expansion (4.1) with a weighted average of the values of f along the integration step. Two common Runge-Kutta methods should be known to all practitioners of numerical methods.

(1) A common two-stage Runge-Kutta method

$$(4.10) \quad K_1 = k f(t^n, Q^n)$$

$$(4.11) \quad K_2 = k f(t^n + k/2, Q^n + K_1/2)$$

$$(4.12) \quad Q^{n+1} = Q^n + K_2$$

(2) A common four-stage Runge-Kutta method

$$(4.13) \quad K_1 = k f(t^n, Q^n)$$

$$(4.14) \quad K_2 = k f(t^n + k/2, Q^n + K_1/2)$$

$$(4.15) \quad K_3 = k f(t^n + k/2, Q^n + K_2/2)$$

$$(4.16) \quad K_4 = k f(t^n + k, Q^n + K_3)$$

$$(4.17) \quad Q^{n+1} = Q^n + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4)$$

4.3. Linear multi-step methods. Linear multi-step methods (LMM) carry out the weighted average idea one step further and postulate a relationship of the form

$$(4.18) \quad \sum_{j=0}^r a_j Q^{(n+j)} = k \sum_{j=0}^r b_j f(t^{(n+j)}, Q^{(n+j)})$$

so we not only have a weighted average of the f values but also of the function values Q . Note that r starting values $\{Q^{(0)}, Q^{(1)}, \dots, Q^{(r-1)}\}$ are needed to apply (4.18),

but only one initial condition $Q^{(0)} = q_0$ is apparent from the IVP. The additional starting values are determined by some other procedure, for example by applying a Runge-Kutta method to determine $\{Q^{(1)}, Q^{(2)}, \dots, Q^{(r-1)}\}$. It is convenient to define a LMM by the polynomials

$$(4.19) \quad \rho(\zeta) = \sum_{j=0}^r a_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^r b_j \zeta^j .$$

Some common LMM methods are:

- (1) r -step Adams-Bashforth methods

$$(4.20) \quad \rho(\zeta) = \zeta^r - \zeta^{r-1}, \quad \sigma(\zeta) =$$

5. Linear difference equations

Relations such as (4.18) arise frequently in both ODE and PDE methods and it is important to be able to analyze the induced behavior. Consider the finite difference equation

$$(5.1) \quad \sum_{j=0}^r a_j Q^{(n+j)} = 0 .$$

We wish to find solutions to this equation given r initial conditions $Q^{(0)}, Q^{(1)}, \dots, Q^{(r-1)}$, that is to find the sequence $\{Q^{(l)}\}_{l \geq r}$. Parentheses around superscripts are useful here in order to more easily distinguish between exponents and superscripts. We try to find solutions of the form

$$(5.2) \quad Q^{(l)} = \zeta^l$$

where ζ is some non-zero constant ($\zeta = 0$ leads to uninteresting, trivial solutions). We see that ζ must satisfy the polynomial equation

$$(5.3) \quad \rho(\zeta) = \sum_{j=0}^r a_j \zeta^j = 0 .$$

called the *characteristic equation* of the linear difference equation (5.1). Similarly $\rho(\zeta)$ is called the *characteristic polynomial*. Let $\zeta_1, \zeta_2, \dots, \zeta_r$ be the roots of the characteristic polynomial

$$(5.4) \quad \rho(\zeta_m) = 0, \quad m = 1, 2, \dots, r .$$

Since (5.1) is linear, a linear combination of the roots is also a solution. The general form of the solution is

$$(5.5) \quad Q^{(n)} = \sum_{j=0}^r c_j \zeta_j^n .$$

The constants c_j are determined from the initial conditions

$$(5.6) \quad \sum_{j=0}^r c_j \zeta_j^l = Q^{(l)}, \quad l = 0, 1, \dots, r-1$$

a linear system of r equations and r unknowns.