

Chapter 9

Numerical Ordinary Differential Equations - Initial Value Problems

The problem to be considered in this chapter is to solve the initial value problem (IVP):

$$\begin{aligned}\frac{dy}{dx} &= f(x, y) \\ y(x_0) &= y_0\end{aligned}\tag{9.1}$$

where $f : R \times R^n \rightarrow R^n$ satisfies the Lipschitz condition in y , i.e.,

$$\|f(x, y_1) - f(x, y_2)\| \leq L\|y_1 - y_2\|\tag{9.2}$$

for every $y_1, y_2 \in R^n$.

Remarks. (a) The Lipschitz condition is sufficient to prove that the IVP (9.1) has a unique solution near x_0 .

(b) Any higher-order ordinary differential equation

$$\frac{d^m y}{dx^m} = f\left(x, y, \frac{dy}{dx}, \dots, \frac{d^{m-1}y}{dx^{m-1}}\right)\tag{9.3}$$

can be reduced to a first-order system. This is done simply by letting

$$y_1 := y, y_2 := \frac{dy_1}{dx}, \dots, y_m := \frac{dy_{m-1}}{dx}\tag{9.4}$$

and by considering the differential equation associated with $(y_1, \dots, y_m)^T$.

Definition 9.0.1 Let $x_0 < x_1 \dots$ be a sequence of points at which the solution $y(x)$ of (9.1) is approximated by the values y_1, y_1, \dots . Any numerical method that computes y_{i+1} by using information at $x_i, x_{i-1}, \dots, x_{i-k+1}$ is called a k -step method.

Example. The simplest 1-step method for solving (9.1) is the so called Euler method

$$y_{n+1} = y_n + h_n f(x_n, y_n) \quad (9.5)$$

where $x_{n+1} = x_n + h_n$ and h_n is the step size. Several questions are typical topics in the numerical ODE theory — What is the global $e_n := y(x_n) - y_n$? How is it constituted? How does it propagated? How does the step size affect the error?

9.1 Linear Multi-step Methods

Definition 9.1.1 By a linear $(p + 1)$ -step method of step size h , we mean a numerical scheme of the form

$$y_{n+1} = \sum_{i=0}^p a_i y_{n-i} + h \sum_{i=-1}^p b_i f_{n-i} \quad (9.6)$$

where $x_k = x_0 + kh$, $f_{n-i} := f(x_{n-i}, y_{n-i})$, and $a_p^2 + b_p^2 \neq 0$. If $b_{-1} = 0$, then the method is said to be explicit; otherwise, it is implicit.

Remark. In order to obtain y_{n+1} from an implicit method, usually it is necessary to solve a nonlinear equation. Such a difficulty quite often is compensated by other more desirable properties which are missing from explicit methods. One such a desirable property is the stability.

Obviously, the choice of the coefficients a_i and b_i should not be arbitrary. The choice is made with at least two concerns in mind:

- (a) The truncation error made in each step should be as small as possible.
- (b) The propagation of errors in overall steps should be as slow as possible.

Definition 9.1.2 The difference operator L associated with the linear $(p + 1)$ -step method (9.6) is defined to be, with $a_{-1} = -1$,

$$L[y(x), h] := \sum_{i=-1}^p a_i y(x + (p - i)h) + h \sum_{i=-1}^p b_i y'(x + (p - i)h). \quad (9.7)$$

Definition 9.1.3 When applying the scheme (9.6) to an initial value problem (9.1), we say the local truncation error at x_{n+1} is $L[y(x_{n-p}), h]$.

Remark. Assume $y_{n-i} = y(x_{n-i})$ for $i = 0, \dots, p$. Then

$$\begin{aligned} L[y(x_{n-p}), h] &= hb_{-1}[f(x_{n+1}, y(x_{n+1})) - f(x_{n+1}, y_{n+1})] \\ &\quad + a_{-1}(y(x_{n+1}) - y_{n+1}). \end{aligned} \quad (9.8)$$

Obviously, if the scheme is explicit, then

$$|L[y(x_{n-p+1}), h]| = |y(x_{n+1}) - y_{n+1}| \quad (9.9)$$

indeed represents the error introduced by the scheme at the present step when no errors occur in all previous steps. If the scheme is implicit, then, by the mean value theorem,

$$|L[y(x_{n-p+1}), h]| = |hb_{-1} \frac{\partial f}{\partial y}(x_{n+1}, \eta_{n+1}) + a_{-1}| |y(x_{n+1}) - y_{n+1}|. \quad (9.10)$$

Upon expanding the right hand side of (9.7) about x by the Taylor series and collecting the like powers of h , we have

$$L[y(x), h] = c_0 y(x) + c_1 h y^{(1)}(x) + \dots + c_q h^q y^{(q)}(x) + \dots \quad (9.11)$$

where

$$c_0 = \sum_{i=-1}^p a_i, \quad (9.12)$$

$$c_1 = \sum_{i=-1}^{p-1} (p-i)a_i + \sum_{i=-1}^p b_i, \quad (9.13)$$

$$c_q = \frac{1}{q!} \sum_{i=-1}^{p-1} (p-i)^q a_i + \frac{1}{(q-1)!} \sum_{i=-1}^{p-1} (p-i)^{q-1} b_i, \quad q \geq 2. \quad (9.14)$$

Definition 9.1.4 A linear multi-step method is said to be of order r if $c_0 = c_1 = \dots = c_r = 0$, but $c_{r+1} \neq 0$ in the corresponding difference operator, i.e., if $L[y(x), h] = c_{r+1} y^{(r+1)}(\eta) h^{r+1}$.

Definition 9.1.5 A linear multi-step method is said to be consistent if and only if its order $r \geq 1$.

By integrating both sides of (9.1) from x_n to x_{n+1} , we obtain

$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx. \quad (9.15)$$

Suppose we have already known $(x_n, y_n), (x_{n-1}, y_{n-1}), \dots, (x_{n-p}, y_{n-p})$. We may approximate $f(x, y(x))$ by a p -th degree interpolation polynomial $p_p(x)$. In this way, we obtain an explicit scheme

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} p_p(x) dx = y_n + \sum_{i=0}^p \beta_{pi} f_{n-i} \quad (9.16)$$

where b_i are the quadrature coefficients. Such a method is called an Adams-Bashforth method. Similarly, if we also include (x_{n+1}, y_{n+1}) in the data of interpolation, then we end up with an implicit scheme

$$y_{n+1} = y_n + \sum_{i=-1}^p \beta_{pi} f_{n-i} \quad (9.17)$$

which is called an Adams-Moulton method.

Examples. (a) Some Adams-Bashforth methods:

| | 0 | 1 | 2 | 3 | 4 |
|-----------------|------|-------|------|-------|-----|
| β_{0i} | 1 | | | | |
| $2\beta_{1i}$ | 3 | -1 | | | |
| $12\beta_{2i}$ | 23 | -16 | 5 | | |
| $24\beta_{3i}$ | 55 | -59 | 37 | -9 | |
| $720\beta_{4i}$ | 1901 | -2774 | 2616 | -1274 | 251 |

(b) Some Adams-Moulton methods:

| | -1 | 0 | 1 | 2 | 3 |
|-----------------|-----|-----|------|-----|-----|
| β_{0i} | 1 | | | | |
| $2\beta_{1i}$ | 1 | 1 | | | |
| $12\beta_{2i}$ | 5 | 8 | -1 | | |
| $24\beta_{3i}$ | 9 | 19 | -5 | 1 | |
| $720\beta_{4i}$ | 251 | 646 | -264 | 106 | -19 |

9.2 Stability Theory of Multi-step Methods

Example. Suppose we want to apply the midpoint rule

$$y_{n+1} = y_{n-1} + 2hf_n \quad (9.18)$$

to the initial value problem

$$y' = -y, y(0) = 1. \quad (9.19)$$

The exact solution is $y(x) = e^{-x}$. The numerical scheme will produce a finite difference equation

$$y_{n+1} = y_{n-1} - 2hy_n. \quad (9.20)$$

To solve (9.20) we try a solution of the form

$$y_n = r^n. \quad (9.21)$$

Then r is a zero of the polynomial $r^2 + 2hr - 1 = 0$. Therefore, the general solution of (9.20) is given by

$$y_n = \alpha_1 r_1^n + \alpha_2 r_2^n \quad (9.22)$$

with $r_i = -h \pm \sqrt{h^2 + 1}$. Initial condition implies $\alpha_1 + \alpha_2 = 1$. We need one more value y_1 to start the scheme (9.18). Expressing α_1 and α_2 in terms of y_1 ,

we have

$$\alpha_1 = \frac{r_2 - y_1}{r_2 - r_1} = \frac{\sqrt{h^2 + 1} + h + y_1}{\sqrt[2]{h^2 + 1}} \quad (9.23)$$

$$\alpha_2 = \frac{r_1 - y_1}{r_1 - r_2} = \frac{-h + \sqrt{h^2 + 1} - y_1}{\sqrt[2]{h^2 + 1}}. \quad (9.24)$$

We note that $|r_1| < 1$ and $|r_2| > 1$. Therefore, unless y_1 is chosen such that $\alpha_2 = 0$, y_n grows unboundedly and, hence, deviated from the exact solution regardless of the step size. Such a phenomenon is called numerical instability.

Consider a general finite difference equation

$$\sum_{i=-1}^p a_i y_{n-i} = \phi_n \quad (9.25)$$

where a_i are constants independent of n , $a_{-1} \neq 0$, $a_p \neq 0$, and $n \geq p + 1$. Given starting values y_0, \dots, y_p , a solution of the difference equation is a sequence of value $\{y_n\}_{p+1}^\infty$ that satisfies the equation (9.25) identically for all $n = p + 1, \dots$. The general solution of (9.25) can be written as $y_n = \hat{y}_n + \psi_n$ where \hat{y}_n is the general solution of the homogeneous equation

$$\sum_{i=-1}^p a_i y_{n-i} = 0 \quad (9.26)$$

and ψ_n is a particular solution of (9.25). To determine \hat{y}_n , we try $\hat{y}_n = r^n$ for some appropriate r . Then we find r must be a root of the polynomial

$$P(r) := \sum_{i=-1}^p a_i r^{p-i} = a_{-1} r^{p+1} + a_0 r^p + \dots + a_p. \quad (9.27)$$

Let the roots of $P(r)$ be denoted by r_0, r_1, \dots, r_p . Then

(a) Suppose all the roots of $P(r)$ are distinct. Then $r_j^n, j = 0, \dots, p$ are linearly independent in the sense that

$$\sum_{j=0}^p \alpha_j r_j^n = 0 \text{ for all } n \implies \alpha_j = 0 \text{ for all } j. \quad (9.28)$$

Hence, the general solution \hat{y}_n of (9.26) is given by

$$\hat{y}_n = \sum_{j=0}^p \alpha_j r_j^n \quad (9.29)$$

where α_j are arbitrary constants to be determined by the starting values.

(b) Suppose some or all the roots of $P(r)$ are repeated. For example, suppose $r_0 = r_1 = r_2$ and suppose the remaining roots are distance. Then it can be

proved that $r_0^n, nr_1^n, n(n-1)r_2^n, r_3^n, \dots, r_p^n$ are linearly independent. In this case, the general solution \hat{y}_n is given by

$$\hat{y}_n = \alpha_0 r_0^n + \alpha_1 n r_1^n + \alpha_2 n^2 r_2^n + \sum_{j=3}^p \alpha_j r_j^n. \quad (9.30)$$

Remark. We note that \hat{y}_n is bounded as $n \rightarrow \infty$ if and only if all roots of $P(r) = 0$ have modulus $|r_j| \leq 1$ and those with modulus 1 are simple.

Definition 9.2.1 *The first and the second characteristic polynomials associated with a linear multistep method*

$$\sum_{i=-1}^p a_i y_{n-i} + h \sum_{i=-1}^p b_i f_{n-i} = 0, \quad (9.31)$$

are defined, respectively, by

$$P_1(r) := \sum_{i=-1}^p a_i r^{p-i} \quad (9.32)$$

$$P_2(r) := \sum_{i=-1}^p b_i r^{p-i}. \quad (9.33)$$

We say the method is zero-stable if and only if all roots of $P_1(r)$ have modulus ≤ 1 and those with modulus 1 are simple.

Remark. In a $(p+1)$ -step method (9.31), totally there are $2p+3$ undetermined coefficients ($a_{-1} = -1$). Thus, it appears that we may choose these numbers so that $c_0 = \dots = c_{2p+2} = 0$. Indeed, such a choice is always possible. Therefore, the maximal order for an implicit method is $2p+2$. However, the maximal order method is often useless because of the well known Dalquist barrier theorem:

Theorem 9.2.1 *Any $(p+1)$ -step method (9.31) of order $\geq p+3$ is unstable. More precisely, if p is odd, then the highest order of a stable method is $p+3$; if p is even, then the highest order of a stable method is of order $p+2$.*

Remark. The Simpson's rule is the best zero-stable 2-step method that attains the optimal order 4.

We now apply the multistep method (9.31) to the text problem

$$y' = \lambda y \quad (9.34)$$

where $\lambda \in R$ is a fixed constant. Recall that the local truncation error T_{n+1} at x_{n+1} is defined by

$$T_{n+1} := \sum_{i=-1}^p a_i y(x_{n-i}) + h \sum_{i=-1}^p b_i \lambda y(x_{n-i}). \quad (9.35)$$

Due to the floating-point arithmetic, we often will introduce round-off errors in applying the scheme (9.31). Suppose

$$R_{n+1} = \sum_{i=-1}^p a_i \tilde{y}_{n-i} + h \sum_{i=-1}^p b_i f(x_{n-i}, \tilde{y}_{n-i}). \quad (9.36)$$

Then the global errors $\tilde{e}_n := y(x_n) - \tilde{y}_{n-i}$ satisfy the difference equation

$$\sum_{i=-1}^p a_i \tilde{e}_{n-i} + \lambda h \sum_{i=-1}^p b_i \tilde{e}_{n-i} = T_{n+1} - R_{n+1}. \quad (9.37)$$

It is reasonable to assume that $T_{n+1} - R_{n+1} \approx \phi \equiv \text{constant}$. According to the theory we develop earlier, a general solution of (9.37) would be

$$\tilde{e}_n = \sum_{j=0}^p \alpha_j r_j^n + \frac{\phi}{\lambda h \sum_{i=-1}^p b_i}, \quad (9.38)$$

if we assume all roots r_0, \dots, r_p of the polynomial $\sum_{i=-1}^p (a_i + \lambda h b_i) r^{p-i}$ are distinct.

Definition 9.2.2 Let $\bar{h} := \lambda h$. The polynomial

$$\prod(r, \bar{h}) := P_1(r) + \bar{h} P_2(r) = \sum_{i=-1}^p (a_i + \bar{h} b_i) r^{p-i} \quad (9.39)$$

is called the stability polynomial of the multistep method (9.31).

Definition 9.2.3 The linear multistep method (9.31) is said to be absolutely stable for a given \bar{h} if all roots r_j of $\prod(r, \bar{h})$ satisfies $|r_j| < 1$. The interval S is called the interval of absolute stability if the method is absolutely stable for all $\bar{h} \in S$.

Remark. It can be proved that every consistent, zero-stable method is absolutely unstable for small positive \bar{h} .

Example. Consider the Simpson's rule. Then $P_1(r) = -r^2 + 1$, $P_2(r) = \frac{1}{3}(r^2 + 4r + 1)$, $\prod(r, \bar{h}) = \left(\frac{\bar{h}}{3} - 1\right)r^2 + \frac{4}{3}\bar{h}r + \left(1 + \frac{\bar{h}}{3}\right)$. The roots of $\prod(r, \bar{h})$ can be checked to be

$$r_1 = 1 + \bar{h} + 0(h^{-2}) \quad (9.40)$$

$$r_2 = -1 + \frac{1}{3}\bar{h} + 0(h^{-2}). \quad (9.41)$$

Hence, if $\bar{h} > 0$, then $r_1 > 0$ and $r_2 > -1$. If $\bar{h} < 0$, then $r_1 < 1$ and $r_2 < -1$. In other words, Simpson's rule is no where absolutely stable.

9.3 Predictor and Corrector Methods

A predictor-corrector (PC) method consists of an explicit method which is used to make an initial guess of the solution and an implicit method which is used to improve the accuracy of the solution. Generally, there are two ways to proceed a PC method: One is to repeat the correction until a preassigned tolerance $\|y_{n+1}^{(s+1)} - y_{n+1}^{(s)}\| < \epsilon$ is achieved. But more often, the PECE method is preferred.

Definition 9.3.1 Let P stand for the predictor

$$\sum_{i=-1}^{p^*} a_i^* y_{n-i} + h \sum_{i=0}^{p^*} b_i^* f_{n-i} = 0. \quad (9.42)$$

Let C stand for the corrector

$$\sum_{i=-1}^p a_i y_{n-i} + h \sum_{i=-1}^p b_i f_{n-i} = 0. \quad (9.43)$$

Let m be a fixed integer. Then by a $P(EC)^mE$ method we mean the following scheme:

$$y_{n+1}^{(0)} = \sum_{i=0}^{p^*} a_i^* y_{n-i}^{(m)} + h \sum_{i=0}^{p^*} b_i^* f_{n-i}^{(m)}, \quad (9.44)$$

$$\text{For } s = 0, \dots, m-1, \text{ do} \quad (9.45)$$

$$f_{n+1}^{(s)} = f(x_{n+1}, y_{n+1}^{(s)}) \quad (9.46)$$

$$y_{n+1}^{(s+1)} = \sum_{i=-1}^p a_i y_{n-i}^{(m)} + h \sum_{i=0}^p b_i f_{n-i}^{(m)} + hb_{-1} f_{n+1}^{(s)} \quad (9.47)$$

$$f_{n+1}^{(m)} = f(x_{n+1}, y_{n+1}^{(m)}). \quad (9.48)$$

The selection of the pair of the predictor and the corrector should not be arbitrary. Rather

Theorem 9.3.1 Let r^* and r be the order of the predictor and the corrector, respectively.

(1) If the correction to convergence is used and if $r^* \geq r$, then the principal local truncation error of the PC method is that of the corrector alone. The properties of the predictor is immaterial.

(2) If $P(EC)^m$ method is used and if $r^* = r - q, 0 \leq q < r$, then the local truncation of the PC method is

(a) that of the corrector alone if $m \geq q + 1$; or

(b) of the same order as the corrector (but the error constant is larger) is $m = q$; or

(c) of the form $O(h^{r-q+m+1})$ if $m \leq q - 1$.

Remark. From the above theorem, we conclude that the predictor should not be any better than the corrector. In practice, it is believed that the choice $r^* = r$ with $m = 1$ is the best combination.

An important advantage of the PC method is the ease of estimating local truncation errors. Suppose $r^* = r$. Then under the local assumption, we know

$$y(x_{n+1}) - y_{n+1}^{(0)} = c_{r+1}^* h^{r+1} y^{(r+1)} + O(h^{r+2}) \quad (9.49)$$

$$y(x_{n+1}) - y_{n+1}^{(m)} = c_{r+1} h^{r+1} y^{(r+1)} + O(h^{r+2}). \quad (9.50)$$

It follows that

$$y_{n+1}^{(m)} - y_{n+1}^{(0)} = (c_{r+1}^* - c_{r+1}) h^{r+1} y^{(r+1)} + O(h^{r+2}). \quad (9.51)$$

Therefore, the global error $y(x_{n+1}) - y_{n+1}^{(m)}$ is estimated by

$$y(x_{n+1}) - y_{n+1}^{(m)} \approx \frac{c_{r+1}}{c_{r+1}^* - c_{r+1}} \left(y_{n+1}^{(m)} - y_{n+1}^{(0)} \right). \quad (9.52)$$

Such an estimate of error is called the Milne's device. Note the right hand side of (9.52) does not involve any high order derivative calculation. Note also the local assumption is not realistic in practice. Thus the estimate should be used with conservation.

Example. The following is a 4-th order Adams-Bashforth-Moulton pair;

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{24} (55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}), T_{n+1} \approx \frac{251}{720} h^5 y^{(5)} \\ y_{n+1} &= y_n + \frac{h}{24} (9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}), T_{n+1} \approx -\frac{19}{720} h^5 y^{(5)}. \end{aligned}$$

It can be shown, analogous to the preceding section, that the stability polynomial for a $P(EC)^m E$ method is given by

$$\prod_{P(EC)^m E} \left(r, \bar{h} \right) - P_1(r) + \bar{h} \bar{P}_2(r) + M_m(\bar{h}) (P_1^*(r) + \bar{h} \bar{P}_2^*(r)) \quad (9.53)$$

where

$$M_m(\bar{h}) = \frac{(\bar{h} \bar{b}_{-1})^m (1 - \bar{h} \bar{b}_{-1})}{1 - (\bar{h} \bar{b}_{-1})^m}. \quad (9.54)$$

With somewhat more complicated analysis, one can show that the PC method is absolutely unstable for small $\bar{h} > 0$.

9.4 Runge-Kutta Methods

We have seen that higher order of accuracy can be attained by appropriately selected coefficients in a multistep methods. But the disadvantage is that a multistep methods requires additional starting values. Runge-Kutta methods, in contrast, preserves the one-step nature but sacrifices the linearity.

Definition 9.4.1 An R -stage Runge-Kutta method generally is defined by

$$y_{n+1} = y_n + h\phi(x_n, y_n, h) \quad (9.55)$$

where

$$\phi(x, y, h) = \sum_{r=1}^R c_r k_r, \quad (9.56)$$

$$k_r = f\left(x + ha_r, y + h \sum_{s=1}^R b_{rs} k_s\right), r = 1, \dots, R, \quad (9.57)$$

$$a_r = \sum_{s=1}^R b_{rs}. \quad (9.58)$$

Such a method usually is represented by an array

$$\begin{array}{c|c} a & B \\ \hline & c^T \end{array} \quad (9.59)$$

where $B = (b_{rs}), c^T = [c_1, \dots, c_R], a = [a_1, \dots, a_R]^T$. If B is strictly lower triangular, then the method is said to be explicit; otherwise, it is implicit.

Remark. Note an R -stage Runge-Kutta method involves R function evaluations per step. Each of the functions $k_r, r = 1, \dots, R$, may be interpreted as approximation to the derivative $y'(x)$ and the function ϕ as a weighted mean of these approximations.

Remark. An important application of Runge-Kutta methods is to provide additional starting values for a multistep predictor-corrector algorithm. If an error estimator is available, then a Runge-Kutta method is easier to change the step size than a multistep method.

Remark. Recall the initial value problem

$$y' = f(x, y), y(x_n) = y(x_n). \quad (9.60)$$

We can calculate the Taylor series

$$y(x_{n+1}) = y(x_n) + hy^{(1)}(x_n) + \frac{h^2}{2!}y^{(2)}(x_n) + \dots \quad (9.61)$$

Thus by defining

$$\phi_T(x, y, h) := f(x, y) + \frac{h}{2!} \frac{df}{dx}(x, y) + \dots \quad (9.62)$$

we see that the Taylor algorithm of order p falls within the class (9.55).

If we choose values for the constants c_r, a_r, b_{rs} such that the expansion of the function ϕ defined by (9.56) in powers of h differs from the expansion for $\phi_T(x, y)$

defined in (9.62) only in the p -th and higher powers of h , then the method clearly has order p . Although there is a great deal of tedious manipulation involved in deriving Runge-Kutta methods of higher order, some well known methods have already been developed. It is quite often that given a specific order, there are a 2-parameter family of Runge-Kutta methods all of which have the same order of accuracy.

Examples. Two fourth-order 4-stage explicit Runge-Kutta methods

$$\begin{array}{c|cccc}
 0 & 0 & & & \\
 1/2 & 1/2 & 0 & & \\
 1/2 & 0 & 1/2 & 0 & \\
 1 & 0 & 0 & 1 & 0 \\
 \hline
 & 1/6 & 2/6 & 2/6 & 1/6
 \end{array} \tag{9.63}$$

$$\begin{array}{c|cccc}
 0 & 0 & & & \\
 1/3 & 1/3 & 0 & & \\
 2/3 & -1/3 & 1 & 0 & \\
 1 & 1 & -1 & 1 & 0 \\
 \hline
 & 1/8 & 3/8 & 3/8 & 1/8
 \end{array} \tag{9.64}$$

Example. The unique 2-stage implicit Runge-Kutta method of order 4:

$$\begin{array}{c|cc}
 1/2 + \sqrt{3}/6 & 1/4 & (1/4 + \sqrt{3}/6) \\
 1/2 - \sqrt{3}/6 & (1/4 - \sqrt{3}/6) & 1/4 \\
 \hline
 & 1/2 & 1/2
 \end{array} \tag{9.65}$$

Example. A 3-stage semi-explicit Runge-kutta method or order 4:

$$\begin{array}{c|ccc}
 0 & 0 & 0 & 0 \\
 1/2 & 1/4 & 1/4 & 0 \\
 1 & 0 & 1 & 0 \\
 \hline
 & 1/6 & 4/6 & 1/6
 \end{array} \tag{9.66}$$

Theorem 9.4.1 (*Butcher's attainable order theorem*)

(a) Let $P^*(R)$ be the highest order that can be attained by an R -stage explicit Runge-Kutta method. Then

$$\frac{R}{P^*(R)} \left| \begin{array}{c|c|c|c|c|c|c|c|c|c}
 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & \geq 10 \\
 \hline
 1 & 2 & 3 & 4 & 4 & 5 & 6 & 6 & 7 & \leq R-2
 \end{array} \right. \tag{9.67}$$

(b) For any $R \geq 2$, there exists an R -stage implicit Runge-Kutta method of order $2R$.

We now consider the absolute stability property of Runge-Kutta methods. We apply a Runge-Kutta method to the test problem $y' = \lambda y$. Define the global error $\tilde{e}_n := y(x_n) - \tilde{y}_n$, $\bar{h} := \lambda h$, $k = [k_1, \dots, k_R]^T$ and $E := [1, \dots, 1]^T$. We first observe that

$$k = \lambda e y_n + \bar{h} B k, \tag{9.68}$$

or equivalently,

$$k = \lambda(I - \overline{hB})^{-1}ey_n. \quad (9.69)$$

Thus, analogous to (9.37), we have

$$\tilde{e}_{n+1} = \tilde{e}_n + \overline{hc}^T (I - \overline{hB})^{-1}e\tilde{e}_n \quad (9.70)$$

$$+ \text{ (local error due to truncation and round-off) } \quad (9.71)$$

The Runge-Kutta method is said to be absolutely stable on the interval (α, β) if

$$r := 1 + \overline{hc}^T (I - \overline{hB})^{-1}e \quad (9.72)$$

satisfies $|r| < 1$ whenever $\overline{h} \in (\alpha, \beta)$. Note that, in contrast to the multistep method, the stability of a Runge-Kutta method is determined by only one root. In fact, it can be proved that

Theorem 9.4.2 For $R = 1, 2, 3, 4$, all R -stage explicit Runge-Kutta methods of order R have the same interval of absolute stability. In each of these cases,

$$r = 1 + \overline{h} + \frac{1}{2}\overline{h}^2 + \dots + \frac{1}{R!}\overline{h}^R. \quad (9.73)$$

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Examples.

| | Euler Rule | Midpoint Rule | Simpson's Rule | Trapezoidal Rule |
|----------|------------------------|-----------------------------|---|--|
| | $y_{n+1} = y_n + hf_n$ | $y_{n+1} = y_{n-1} + 2hf_n$ | $y_{n+1} = y_{n-1} + \frac{h}{3}(f_{n-1} + 4f_n + f_{n+1})$ | $y_{n+1} = y_n + \frac{h}{2}(f_n + f_{n+1})$ |
| a_{-1} | -1 | -1 | -1 | -1 |
| a_0 | 1 | 0 | 0 | 0 |
| a_1 | | 1 | 1 | 0 |
| b_{-1} | 0 | 0 | 1/3 | 1/2 |
| b_0 | 1 | 2 | 4/3 | 0 |
| b_1 | | 0 | 1/3 | 1/2 |
| r | 1 | 2 | 4 | 2 |
| $p+1$ | 1 | 2 | 2 | 1 |

Figure 9.1: Examples of Multi-step Methods.