Chapter 5 Initial-Value Problems for Ordinary Differential Equations

Baodong LIU
baodong@sdu.edu.cn

Initial-value problem of Ordinary Differential Equation

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y), \quad a \le t \le b. \tag{1}$$

subject to an initial condition:

$$y(a) = \alpha. \tag{2}$$

System of first order differential equations

$$\begin{cases} \dfrac{\mathrm{d}y_1}{\mathrm{d}t} = f_1(t, y_1, y_2, \cdots, y_n), \\ \dfrac{\mathrm{d}y_2}{\mathrm{d}t} = f_2(t, y_1, y_2, \cdots, y_n), \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ \dfrac{\mathrm{d}y_n}{\mathrm{d}t} = f_n(t, y_1, y_2, \cdots, y_n), \end{cases}$$

for $a \leq t \leq b$, subject to the initial conditions

$$y_1(a) = \alpha_1, y_2(a) = \alpha_2, \cdots, y_n(a) = \alpha_n.$$

The nth order initial value problem of ordinary differential equation:

$$y^{(n)} = f(t, y', y'', \cdots, y^{(n-1)}),$$

for $a \le t \le b$, subject to the initial conditions

$$y(a) = \alpha_1, y'(a) = \alpha_2, \cdots, y^{(n-1)}(a) = \alpha_n.$$

DEFINITION 5.1

- A function $f(t, y)$ is said to satisfy a **Lipschitz Condition（–李普希兹条件）** in the variable y on a set $D \subset \Re^2$, if a constant $L > 0$ exists with the property that

$$|f(t, y_1) - f(t, y_2)| \leq L|y_1 - y_2|$$

whenever $(t, y_1), (t, y_2) \in D$.

- The constant L is called a **Lipschitz Constant** for f.

DEFINITION 5.2 (Convex Set)

A set $D \subset \Re^2$ is said to be convex if whenever

$$(t_1, y_1), (t_2, y_2) \in D,$$

the point

$$((1-\lambda)t_1 + \lambda t_2, (1-\lambda)y_1 + \lambda y_2) \in D$$

for each $\lambda \in [0, 1]$.

THEOREM 5.3

- Suppose $f(t, y)$ is defined on a convex set $D \subset \Re^2$.
- If a constant L exists with

$$\left|\frac{\partial f}{\partial y}(t, y)\right| \leq L, \quad \text{for all} \qquad (t, y) \in D.$$

- Then f satisfies a Lipschitz condition on D in the variable y with Lipschitz constant L.

THEOREM5.4

- Suppose that

$$D = \{(t, y) | a \le t \le b, -\infty < y < \infty\}$$

and that $f(t, y)$ is continuous on D.

- If f satisfies a Lipschitz condition on D in the variable y, then the initial-value problem

$$\begin{cases} y'(t) = f(t, y), & a \le t \le b \\ y(a) = \alpha. \end{cases}$$

has a unique solution $y(t)$ for $a \le t \le b$.

DEFINITION 5.5

The initial problem

$$\begin{cases} \frac{dy}{dt} = f(t, y), a \leq t \leq b \\ y(a) = \alpha \end{cases} \tag{3}$$

is said to be **well-posed problem** if

1. A unique solution $y(t)$, to the problem exists;
2. For any $\epsilon > 0$, there exists a positive constant $k(\epsilon)$ with the property that, whenever $|\epsilon_0| < \epsilon$ and $\delta(t)$ is continuous with $|\delta(t)| < \epsilon$ on $[a, b]$, a unique solution, $z(t)$ to the problem

$$\begin{cases} \frac{\mathrm{d}z}{\mathrm{d}t} = f(t, z) + \delta(t), \quad a \leq t \leq b, \\ z(a) = \alpha + \epsilon_0, \end{cases} \tag{4}$$

exists with $|z(t) - y(t)| < k(\epsilon)\epsilon, \ a \leq t \leq b.$

- Problem specified by Eq. (4) is called a **perturbed problem** associated with the **original problem** Eq.(3).

THEOREM 5.6

Suppose that

$$D = \{(t, y) | a \leq t \leq b, -\infty < y < \infty\}.$$

If $f(t, y)$ is continuous and satisfies a Lipschitz condition on D in the variable y on the set D, then the initial-value problem

$$y'(t) = f(t, y), a \leq t \leq b, y(a) = \alpha,$$

is well-posed.

5.2 Euler's Method — 欧拉方法

- To solve a well-posed initial-value problem

$$\begin{cases} y'(t) = f(t, y), & a \le t \le b, \\ y(a) = \alpha. \end{cases}$$

- First, we construct the **mesh points** in the interval $[a, b]$ with equal space.

$$a = t_0 < t_1 < \cdots < t_N = b$$

with equal **step size**

$$h = (b - a)/N,$$

where

$$t_j = a + jh, \;\; j = 0, 1, 2, \cdots, N.$$

- If $y(t_j)$ is known, then by Taylor formula, we have:

$$y(t_{j+1}) = y(t_j) + (t_{j+1} - t_j)y'(t_j) + \frac{(t_{j+1} - t_j)^2}{2} y''(\xi_j)$$

where ξ_j lies in $[t_j, t_{j+1}]$.

- Since $y'(t)$ satisfies the equation $y'(t) = f(t, y)$, and $h = t_{j+1} - t_j$ implies that

$$y(t_{j+1}) = y(t_j) + hf(t_j, y(t_j)) + \frac{h^2}{2} y''(\xi_j)$$

数值计算格式设计: 泰勒方法

- If $y(t_j)$ is known, then by Taylor formula, we have:

$$y(t_{j+1}) = y(t_j) + (t_{j+1} - t_j)y'(t_j) + \frac{(t_{j+1} - t_j)^2}{2} y''(\xi_j)$$

  where ξ_j lies in $[t_j, t_{j+1}]$.

- Since $y'(t)$ satisfies the equation $y'(t) = f(t, y)$, and $h = t_{j+1} - t_j$ implies that

$$y(t_{j+1}) = y(t_j) + hf(t_j, y(t_j)) + \frac{h^2}{2} y''(\xi_j)$$

- Deleting the remainder term $\frac{h^2}{2}y''(\xi_j)$.
- Let $w_j \approx y(t_j)$ be the value of numerical approximation of $y(t_j)$ for each $j = 1, 2, \cdots, N$, then we get the known **Euler's Method**:

$$\begin{cases} w_0 = \alpha, \\ w_{j+1} = w_j + hf(t_j, w_j), \quad j = 0, 1, \cdots, N-1, \end{cases} \tag{5}$$

- Equation (5) is called the **difference equation** associated with **Euler's method** .
- **Questions: Geometrical means and well-posed implies what?**

ALGORITHM 5.1 Euler's Method

INPUT: endpoints a, b; integer N, and initial condition α.

OUTPUT: approximation w to y at $N+1$ points of t.

STEP 1 set $h = (b-a)/N; t = a; w = \alpha;$

- OUTPUT t, w.

STEP2 for $i = 1, 2, \cdots, N$, do STEP3,4.

STEP 3 set $w = w + h * f(t, w)$ (compute w_i)

- $t = a + ih$ (compute t_i)

STEP 4 OUTPUT (t, w).

STEP 5 STOP.

欧拉格式的误差估计理论

LEMMA 5.7

For all $x \geq -1$ and any positive m, we have

$$0 \leq (1+x)^m \leq e^{mx}.$$

Proof: Using the Taylor'S formula for e^x on $x_0 = 0$, and $n = 1$, gives

$$e^x = 1 + x + \frac{1}{2}x^2 e^{\xi}.$$

where ξ is between x and zero.

Since $x \geq -1$, thus,

$$0 \leq 1 + x \leq 1 + x + \frac{1}{2}x^2 e^{\xi} = e^x$$

so

$$0 \leq (1+x)^m \leq e^{mx}. \blacksquare\blacksquare\blacksquare$$

LEMMA 5.8

If s and t are positive real number, $\{a_j\}_{j=0}^{k}$ is a sequence satisfying $a_0 \geq -\frac{t}{s}$,and

$$a_{j+1} \leq (1+s)a_j + t, \quad \text{for each} \quad j = 0, 1, \cdots, k,$$

then

$$a_{j+1} \leq e^{(j+1)s}\left(a_0 + \frac{t}{s}\right) - \frac{t}{s}.$$

Proof: From known condition

$$a_{j+1} \leq (1+s)a_j + t, \text{for each} \quad j = 0, 1, \cdots, k,$$

we can drive that

$$\begin{aligned}
a_{j+1} &\leq (1+s)a_j + t \\
&\leq (1+s)[(1+s)a_{j-1} + t] + t \\
&\leq (1+s)\{(1+s)[(1+s)a_{j-2} + t] + t\} + t \\
&\vdots \\
&\leq (1+s)^{j+1}a_0 \\
&\quad +[1 + (1+s) + (1+s)^2 + \cdots + (1+s)^j]t.
\end{aligned}$$

Since

$$1 + (1+s) + (1+s)^2 + \cdots + (1+s)^j = \frac{1-(1+s)^{j+1}}{1-(1+s)}$$

$$a_{j+1} \quad \leq \quad (1+s)^{j+1}\left(a_0 + \frac{t}{s}\right) - \frac{t}{s}.$$

and by the LEMMA 5.7, we have

$$a_{j+1} \leq e^{(j+1)s}\left(a_0 + \frac{t}{s}\right) - \frac{t}{s}.\blacksquare\blacksquare\blacksquare.$$

THEOREM 5.9

- Suppose f is continuous and satisfies a Lipschitz Condition with Constant L on

$$D = \{(t, y) | a \leq t \leq b, -\infty < y < \infty\},$$

and that a constant M exists with the property that

$$|y''(t)| \leq M, \quad \text{for all} \quad t \in [a, b].$$

- Let $y(t)$ be the unique solution to the initial problem (1), and $w_j, j = 0, 1, \cdots, N$ be the approximations generated by Euler's method for some positive number N.
- Then for each $j = 0, 1, 2, \cdots, N$,

$$|y(t_j) - w_j| \leq \frac{hM}{2L}[e^{L(t_j - a)} - 1] \tag{6}$$

Proof.

- When $j = 0$, since $w_0 = y(t_0) = \alpha.$, the result is true.
- When $j = 1, 2, \cdots, N$, by the Taylor's theorem, gives

$$y(t_{j+1}) = y(t_j) + hf(t_j, y(t_j)) + \frac{h^2}{2} y''(\xi_j)$$

and from the Euler difference equation,

$$w_{j+1} = w_j + hf(t_j, w_j)$$

- Thus

$$
\begin{aligned}
y(t_{j+1}) - w_{j+1} &= y(t_j) - w_j \\
&\quad + h[f(t_j, y(t_j)) - f(t_j, w_j)] \\
&\quad + \frac{h^2}{2} y''(\xi_j)
\end{aligned}
$$

and

$$
\begin{aligned}
|y(t_{j+1}) - w_{j+1}| &\leq |y(t_j) - w_j| \\
&\quad + h|f(t_j, y(t_j)) - f(t_j, w_j)| \\
&\quad + \frac{h^2}{2} |y''(\xi_j)|
\end{aligned}
$$

- Since f is continuous and satisfies a Lipchitz in y with constant L, and $|y''(t)| \leq M$, then we have

$$
|y(t_{j+1}) - w_{j+1}| \leq (1 + hL)|y(t_j) - w_j| + \frac{Mh^2}{2}
$$

- By the Lemma 5.8, and letting

$$a_j = |y(t_j) - w_j|$$

for each $j = 0, 1, 2, \cdots, N$, while $s = hL$ and $t = Mh^2/2$, we can see that

$$|y(t_{j+1}) - w_{j+1}| \leq e^{(j+1)hL}\left(|y(t_0) - w_0| + \frac{Mh^2}{2hL}\right) - \frac{Mh^2}{2hL}$$

- Since $|y(t_0) - w_0| = 0$ and $(j+1)h = t_{j+1} - t_0 = t_{j+1} - a$, we have

$$|y(t_{j+1}) - w_{j+1}| \leq \frac{Mh}{2L}[e^{(t_{j+1}-a)L} - 1],$$

for each $j = 0, 1, \cdots, N$.■■■

To consider the roundoff error(舍入误差) for each approximation, we use instead an equation of the form

$$\begin{aligned} u_0 &= a + \delta_0, \\ u_{j+1} &= u_j + hf(t_j, u_j) + \delta_{j+1} \end{aligned}$$

for each $j = 0, 1, \cdots, N-1$, where δ_j denotes the roundoff error associated with u_j.

THEOREM 5.10

Let $y(t)$ be the solution of initial-value problem

$$\begin{cases} y'(t) = f(t, y), \quad a \le t \le b, \\ y(a) = \alpha. \end{cases}$$

and $u_0, u_1, \cdots, u_N$ be the approximations obtained by using

$$\begin{cases} u_0 = a + \delta_0, \\ u_{j+1} = u_j + hf(t_j, u_j) + \delta_{j+1}. \end{cases}$$

If $|\delta_j| < \delta$ for each $j = 0, 1, \cdots, N$ and the hypotheses of Theorem 5.9 holds for original problem, then

$$|y(t_j) - u_j| \le \frac{1}{L}\left(\frac{hM}{2} + \frac{\delta}{h}\right)[e^{L(t_j - a)} - 1] + |\delta_0| e^{L(t_j - a)},$$

for each $j = 0, 1, \cdots, N$.

- To compare the error form of Theorem 5.10 with Theorem 5.9, we can find that the error bound of Theorem 5.10 is no longer linear in h.
- In fact, since

$$\lim_{h \to 0} \left(\frac{hM}{2} + \frac{\delta}{h} \right) = \infty,$$

  thus the error will be expected to become large for sufficient small value of h.

- Let
$$E(h) = \left(\frac{hM}{2} + \frac{\delta}{h}\right)$$
then
$$E'(h) = \left(\frac{M}{2} - \frac{\delta}{h^2}\right).$$
- If $h < \sqrt{2\delta/M}$ then $E'(h) < 0$, and $E(h)$is decreasing.
- If $h > \sqrt{2\delta/M}$ then $E'(h) > 0$, and $E(h)$is increasing.
- So the minimal value of $E(h)$ occurs when
$$h = \sqrt{\frac{2\delta}{M}}.$$

DEFINITION 5.11 (Local Truncation Error)

The difference method

$$\begin{aligned} w_0 &= \alpha \\ w_{i+1} &= w_i + h\phi(t_i, w_i), i = 0, 1, 2, \cdots, N-1, \end{aligned}$$

has **local truncation error** given by

$$\begin{aligned} \tau_{i+1}(h) &= \frac{y_{i+1} - (y_i + h\phi(t_i, y_i))}{h} \\ &= \frac{y_{i+1} - y_i}{h} - \phi(t_i, y_i), \end{aligned}$$

for each $i = 0, 1, 2, \cdots, N-1$.

The local truncation error for Euler's Method

- **To Consider Initial Value Problem of Ordinary Differential Equation**

$$\begin{cases} y'(t) = f(t, y), \quad a \le t \le b \\ y(a) = \alpha. \end{cases}$$

- By the Euler's method, we know

$$\begin{aligned} y_0 &= \alpha \\ y_{i+1} &= y_i + hf(t_i, y_i), i = 0, 1, 2, \cdots, N-1, \end{aligned}$$

- By the Taylor's theorem, gives

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2} y''(\xi_i)$$

- If $y_i = y(t_i)$ denotes the exact value of the solution at t_i, $i = 1, 2, \cdots, N$.
- So the local truncation error for Euler's Method is

$$\tau_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - f(t_i, y_i) = \frac{h}{2} y''(\xi_j),$$

- Further, if $|y''(\xi_i)| \leq M$ where $M > 0$ is a positive constant, thus, this implies

$$|\tau_{i+1}(h)| \leq \frac{h}{2} M.$$

- That is the **local truncation error for Euler's method** is $O(h)$.
- To improve the order of local truncation error, to get higher-order error, we construct Taylor Method of Order n

Taylor Method of Order n

- Suppose that the solution to the initial value problem of ordinary differential equation

$$\begin{cases} y'(t) = f(t, y), & a \leq t \leq b \\ y(a) = \alpha. \end{cases}$$

has $(n+1)$ continuous derivatives.

- By the nth Taylor Polynomial about t_i, we obtain

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + hy'(t_i) + \frac{h^2}{2} y''(t_i) + \cdots \\ &\quad + \frac{h^n}{n!} y^{(n)}(t_i) + \frac{h^{n+1}}{(n+1)!} y^{(n+1)}(\xi_i) \end{aligned} \tag{7}$$

for ξ_i in (t_i, t_{i+1}).

- Since for the solution $y(t)$ satisfies

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

thus we can get

$$\begin{aligned} y''(t) &= f'(t, y(t)), \\ y^{(3)}(t) &= f''(t, y(t)), \\ &\vdots \\ y^{(k)}(t) &= f^{(k-1)}(t, y(t)). \end{aligned}$$

- Substituting these results into Eq. (7), gives

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2} f'(t_i, y(t_i)) + \cdots \\ &+ \frac{h^n}{n!} f^{(n-1)}(t_i, y(t_i)) \\ &+ \frac{h^{n+1}}{(n+1)!} f^{(n)}(\xi_i, y(\xi_i)) \end{aligned} \tag{8}$$

- Based on the Eq. (8), we can construct the **Taylor Method of Order n:**

$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + hT^{(n)}(t_i, w_i), \quad i = 0, 1, 2, \cdots, N-1, \end{cases}$$

where

$$\begin{aligned} T^{(n)}(t_i, w_i) &= f(t_i, w_i) + \frac{h}{2} f'(t_i, w_i) + \cdots + \\ &\quad + \frac{h^{(n-1)}}{n!} f^{(n-1)}(t_i, w_i). \end{aligned}$$

- **Note that** the Euler's method is Taylor's method of order one.

- If $y_i = y(t_i)$ is the exact value of the solution at $t_i, i = 0, 1, 2, \cdots, n$
- Thus the local truncation error of the Taylor Method or Order n is

$$\begin{aligned}
\tau_{i+1}(h) &= \frac{y_{i+1} - y_i}{h} - T^{(n)}(t_i, y_i) \\
&= \frac{h^n}{(n+1)!} f^{(n)}(\xi_i, y(\xi_i)), \;\; i = 0, 1, , 2, \cdots, N-1
\end{aligned}$$

- Further if $y \in C^{n+1}[a, b]$, this implies that

$$y^{(n+1)}(t) = f^{(n)}(t, y(t))$$

is bounded on $[a, b]$ and that

$$\tau_i = O(h^n), \;\; i = 1, 2, \cdots, N.$$

THEOREM 5.12(Taylor Theorem—多元泰勒展开式)

- Suppose that $f(t, y)$ and its partial derivatives of order less than or equal to $n+1$ are continuous on
$$D = \{(t, y) | a \leq t \leq b, c \leq y \leq d\},$$
and let $(t_0, y_0) \in D$.
- For every $(t, y) \in D$, there exists ξ between t and t_0 and μ between y and y_0 with
$$f(t, y) = P_n(t, y) + R_n(t, y),$$

where

$$
\begin{aligned}
& P_n(t, y) \\
= \; & f(t_0, y_0) + \left[(t - t_0)\frac{\partial f}{\partial t}(t_0, y_0) + (y - y_0)\frac{\partial f}{\partial y}(t_0, y_0)\right] \\
& + \left[\frac{(t - t_0)^2}{2}\frac{\partial^2 f}{\partial t^2}(t_0, y_0) + (t - t_0)(y - y_0)\frac{\partial^2 f}{\partial t \partial y}(t_0, y_0)\right. \\
& \left. + (y - y_0)^2 \frac{\partial^2 f}{\partial y^2}(t_0, y_0)\right] + \cdots + \\
& + \left[\frac{1}{n!}\sum_{j=0}^{n} \left(\begin{array}{c} n \\ j \end{array} \right) (t - t_0)^{(n-j)} (y - y_0)^j \frac{\partial^n f}{\partial t^{n-j} \partial y^j}(t_0, y_0)\right].
\end{aligned}
$$

and

$$
\begin{aligned}
& R_n(t, y) \\
= \; & \frac{1}{(n+1)!}\sum_{j=0}^{n+1} \left(\begin{array}{c} n+1 \\ j \end{array} \right) (t - t_0)^{(n+1-j)} (y - y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j} \partial y^j}(\xi, \mu)
\end{aligned}
$$

- **Note that** the function $P_n(t,y)$ is called the n**th Taylor polynomial in two variables** for the function f about (t_0, y_0), and $R_n(t,y)$ is the **remainder term** associated with $P_n(t,y)$.
- The Runge-Kutta Method is new method with higher-order error, without repeated computing the higher-order derivatives of function $f(t,y)$, its general form is

$$y_{n+1} = y_n + \sum_{i=1}^{N} c_i K_i$$

where

$$\begin{aligned} K_1 &= hf(t_n, y_n) \\ K_i &= hf(t_n + \alpha_i h, y_n + \sum_{j=1}^{i-1} b_{ij} K_j), i = 2, 3, \cdots, N \end{aligned}$$

- For the case of $N = 2$, the Runge-Kutta method is

$$y_{n+1} = y_n + c_1 K_1 + c_2 K_2$$

where

$$\begin{aligned} K_1 &= hf(t_n, y_n) \\ K_2 &= hf(t_n + \alpha_2 h, y_n + b_{21} K_1), \end{aligned}$$

- **Question?** How to evaluate the coefficients $c_1, c_2, \alpha_2, b_{21}$?

- Using the Taylor's Theorem, gives

$$\begin{aligned} K_2 &= h\left[f(t_n,y_n) + (\alpha_2 h\frac{\partial f}{\partial t}(t_n,y_n) + b_{21}hf(t_n,y_n)\frac{\partial f}{\partial y}(t_n,y_n))\right] \\ &\quad +hR_1(t_n,y_n). \end{aligned}$$

where

$$R_1(t_n,y_n) = \frac{\alpha_2^2 h^2}{2}\frac{\partial^2 f}{\partial t^2} + \alpha_2 b_{21}h^2 f\cdot\frac{\partial^2 f}{\partial t\partial y} + b_{21}^2 h^2 f^2\cdot\frac{\partial^2 f}{\partial y^2}|_{(\xi,\mu)}$$

- Substituting K_1, K_2 into $y_{n+1} = y_n + c_1K_1 + c_2K_2$, gives

$$\begin{aligned} y_{n+1} &= y_n + h(c_1+c_2)f(t_n,y_n) + c_2\alpha_2 h^2\frac{\partial f}{\partial t}(t_n,y_n) \\ &\quad +c_2 b_{21}h^2 f(t_n,y_n)\frac{\partial f}{\partial y}(t_n,y_n)) \\ &\quad +c_2h^3\left[\frac{\alpha_2^2}{2}\frac{\partial^2 f}{\partial t^2} + \alpha_2 b_{21}f\cdot\frac{\partial^2 f}{\partial t\partial y} + b_{21}^2 f^2\cdot\frac{\partial^2 f}{\partial y^2}\right]\Bigg|_{(\xi,\mu)} \end{aligned}$$

- Reconsidering the Taylor method of Order 2

$$y_{n+1} = y_n + hT^{(2)}(t_n, y_n),$$

where

$$\begin{aligned} T^{(2)}(t_n, y_n) &= f(t_n, y_n) + \frac{h}{2} f'(t_n, y_n) \\ &= f(t_n, y_n) + \frac{h}{2} \frac{\partial f}{\partial t}(t_n, y_n) \\ &\quad + \frac{h}{2} \frac{\partial f}{\partial y}(t_n, y_n) \cdot f(t_n, y_n) \end{aligned}$$

- **Note:**

$$f'(t, y) = \frac{\mathrm{d}f}{\mathrm{d}t}(t, y) = \frac{\partial f}{\partial t}(t, y) + \frac{\partial f}{\partial y}(t, y) \cdot y'(t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \cdot f.$$

- Thus

$$
\begin{aligned}
y_{n+1} &= y_n + hT^{(2)}(t_n, y_n) \\
&= y_n + hf(t_n, y_n) + \frac{h^2}{2}\frac{\partial f}{\partial t}(t_n, y_n) \\
&\quad + \frac{h^2}{2}\frac{\partial f}{\partial y}(t_n, y_n) \cdot f(t_n, y_n)
\end{aligned}
$$

- Comparing this equation with previous Runge-kutta method of the case $N = 2$

$$
\begin{aligned}
y_{n+1} &= y_n + h(c_1 + c_2)f(t_n, y_n) \\
&\quad + c_2\alpha_2 h^2 \frac{\partial f}{\partial t}(t_n, y_n) + c_2 b_{21} h^2 f(t_n, y_n)\frac{\partial f}{\partial y}(t_n, y_n)) \\
&\quad + c_2 h^3 \left[\frac{\alpha_2^2}{2}\frac{\partial^2 f}{\partial t^2} + \alpha_2 b_{21} f \cdot \frac{\partial^2 f}{\partial t \partial y} + b_{21}^2 f^2 \cdot \frac{\partial^2 f}{\partial y^2}\right]\Bigg|_{(\xi,\mu)}
\end{aligned}
$$

- If we choose

$$\begin{aligned} c_1 + c_2 &= 1, \\ c_2\alpha_2 &= 1/2, \\ c_2 b_{21} &= 1/2 \end{aligned}$$

- then the two equations have the same local truncation error of order $O(h^2)$, if we assume that all the second-order derivatives of f are bounded.
- Since the parameters $c_1, c_2, \alpha_2, b_{21}$ are determined not uniquely, then we can some specific Runge-Kutta Methods of Order 2.

Midpoint Method:

—$c_1 = 0, c_2 = 1, \alpha_2 = 1/2, b_{21} = 1/2$

$$\begin{aligned} y_0 &= \alpha \\ y_{i+1} &= y_i + hf(t_i + \frac{h}{2}, y_i + \frac{h}{2} f(t_i, y_i)), \end{aligned}$$

for each $i = 1, 2, \cdots, N-1$.

Modified Euler Method:

—$c_1 = 1/2, c_2 = 1/2, \alpha_2 = 1, b_{21} = 1$

$$\begin{aligned} y_0 &= \alpha \\ y_{i+1} &= y_i + \frac{h}{2}[f(t_i, y_i) + f(t_{i+1}, y_i + hf(t_i, y_i))], \end{aligned}$$

for each $i = 1, 2, \cdots, N-1$.

Heun's Method:

—$c_1 = 1/4, c_2 = 3/4, \alpha_2 = 2/3, b_{21} = 2/3$

$$\begin{aligned} y_0 &= \alpha \\ y_{i+1} &= y_i + \frac{h}{4}\Bigg[f(t_i, y_i) + \\ &\quad + f\left(t_i + \frac{2}{3}h, y_i + \frac{2h}{3} f(t_i + \frac{h}{3}, y_i + \frac{h}{3} f(t_i, y_i))\right)\Bigg], \end{aligned}$$

for each $i = 1, 2, \cdots, N-1$.

Runge-Kutta method of Order Four

$$
\begin{aligned}
y_0 &= \alpha, \\
K_1 &= hf(t_i, y_i), \\
K_2 &= hf(t_i + \frac{h}{2}, y_i + \frac{1}{2}K_1), \\
K_3 &= hf(t_i + \frac{h}{2}, y_i + \frac{1}{2}K_2), \\
K_4 &= hf(t_{i+1}, y_i + K_3), \\
y_{i+1} &= y_i + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)
\end{aligned}
$$

for each $i = 1, 2, \cdots, N-1$.

ALGORITHM Runge-Kutta (Order Four)

To approximate the solution of the initial-value problem

$$y' = f(t, y), a \le t \le b, y(a) = \alpha,$$

at

$$t_0 = a < t_1, < t_2 < \cdots < t_N = b$$

totally $(N+1)$ equally spaced numbers in the interval $[a, b]$:

INPUT endpoints a, b; integer N; initial condition α.

OUTPUT approximation w to y at the $(N+1)$ values of t.

Step 1 Set

$$h = (b-a)/N; t = a; w = \alpha;$$

OUTPUT (t, w)(output initial values at $t_0 = a$).

Step 2 For $i = 1, 2, \cdots, N$,do Steps 3-5.

Step 3 Set

$$\begin{aligned} K_1 &= hf(t, w), \\ K_2 &= hf(t + \frac{h}{2}, w + \frac{1}{2}K_1), \\ K_3 &= hf(t + \frac{h}{2}, w + \frac{1}{2}K_2), \\ K_4 &= hf(t + h, w + K_3), \end{aligned}$$

Step 4 Set

$$\begin{aligned} w &= w + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4), \\ &\quad (\text{Compute} w_i) \\ t &= a + ih. (\text{Compute} t_i) \end{aligned}$$

Step 5 OUTPUT (t, w).

Step 6 STOP.

5.5 Error Control and the Runge-Kutta-Fehlberg Method

- An ideal difference-equation method

$$y_{i+1} = y_i + h_i \phi(t_i, y_i, h_i), i = 0, 1, \cdots, N-1,$$

for approximating the solution, $y(t)$, to the initial-value problem

$$y'(t) = f(t, y), a \leq t \leq b, y(a) = \alpha$$

would have the property that:

- Given a tolerance $\varepsilon > 0$, the **minimal number of mesh points** would be used to ensure that the **global error**, $|y(t_i) - y_i|$, would not exceed ε for any $i = 0, 1, \cdots, N$.

- To illustrate the technique, suppose that we have two approximation techniques.
- The first is an nth-order method obtained from an nth-order Taylor method of the form

$$y(t_{i+1}) = y(t_i) + h\phi(t_i, y(t_i), h) + O(h^{n+1}),$$

  producing approximations

$$\begin{aligned} y_0 &= \alpha, \\ y(t_{i+1}) &= y_i + h\phi(t_i, y_i, h), \text{for} \quad i > 0 \end{aligned}$$

  with local truncation error $\tau_{i+1}(h) = O(h^n)$.
-

- The second method is similar but of higher order.
- For example, let us suppose it comes from an $(n+1)$st-order Taylor method of the form

$$y(t_{i+1}) = y(t_i) + h\tilde{\phi}(t_i, y(t_i), h) + O(h^{n+2}),$$

producing approximations

$$\begin{array}{rcl} \tilde{y}_0 & = & \alpha, \\ \tilde{y}(t_{i+1}) & = & \tilde{y}_i + h\tilde{\phi}(t_i, \tilde{y}_i, h), \text{for} \quad i > 0 \end{array}$$

with local truncation error$\tau_{i+1}(h) = O(h^{n+1})$.
- We first make the assumption that

$$y_i \approx y(t_i) \approx \tilde{y}_i$$

and choose a fixed step size h to generate the approximations y_{i+1} and $\tilde{y}_{i+1}$ to $y(t_{i+1})$.

- Then

$$\begin{aligned}
\tau_{i+1}(h) &= \frac{y(t_{i+1}) - y(t_i)}{h} - \phi(t_i, y(t_i), h) \\
&= \frac{y(t_{i+1}) - y_i}{h} - \phi(t_i, y_i, h) \\
&= \frac{y(t_{i+1}) - [y_i + h\phi(t_i, y_i, h)]}{h} \\
&= \frac{y(t_{i+1}) - y_{i+1}}{h}
\end{aligned}$$

- In a similar manner

$$\tilde{\tau}_{i+1}(h) = \frac{y(t_{i+1}) - \tilde{y}_{i+1}}{h}.$$

- As a consequence,

$$\begin{aligned}
\tau_{i+1}(h) &= \frac{y(t_{i+1}) - y_{i+1}}{h} \\
&= \frac{(y(t_{i+1}) - \tilde{y}_{i+1}) + (\tilde{y}_{i+1} - y_{i+1})}{h}
\end{aligned}$$

- Since $\tau_{i+1}(h)$ is $O(h^n)$ and $\tilde{\tau}_{i+1}(h)$ is $O(h^{n+1})$.
- So the significant portion of $\tau_{i+1}(h)$ must come from

$$\frac{\tilde{y}_{i+1} - y_{i+1}}{h}.$$

- This gives us an easily computed approximation for the local truncation error of the $O(h^n)$ method:

$$\tau_{i+1}(h) \approx \frac{\tilde{y}_{i+1} - y_{i+1}}{h}$$

- The object, however, is not simply to estimate the local truncation error but to adjust the step size to keep it within a specified bound.
- To do this, we now assume that since $\tau_{i+1}(h)$ is $O(h^n)$, a number K, independent of h, exists with

$$\tau_{i+1}(h) \approx Kh^n.$$

- Then the local truncation error produced by applying the nth-order method with a new step size qh can be estimated using the original approximations y_{i+1} and $\tilde{y}_{i+1}$:

- $$\begin{aligned}\tau_{i+1}(qh) &\approx K(qh)^n = q^n(Kh^n) \approx q^n \tau_{i+1}(h) \\ &\approx \frac{q^n}{h}(\tilde{y}_{i+1} - y_{i+1}).\end{aligned}$$
- To bound $\tau_{i+1}(qh)$ by ε, we choose q so that
$$\frac{q^n}{h}|\tilde{y}_{i+1} - y_{i+1}| \approx |\tau_{i+1}(qh)| \leq \varepsilon,$$
- that is, so that
$$q \leq \left(\frac{\varepsilon h}{|\tilde{y}_{i+1} - y_{i+1}|}\right)^{1/n}.$$

Runge- Kutta-Fehlberg method

- Using a Runge-Kutta method with local truncation error of order five:

$$\tilde{y}_{i+1} = y_i + \frac{16}{135}K_1 + \frac{6656}{12825}K_3 + \frac{28561}{56430}K_4 - \frac{9}{50}K_5 + \frac{2}{55}K_6,$$

to estimate the local error in a Runge- Kutta method of order four given by

$$y_{i+1} = y_i + \frac{25}{216}K_1 + \frac{1408}{2565}K_3 + \frac{2197}{4104}K_4 - \frac{1}{5}K_5,$$

where

$$
\begin{aligned}
K_1 &= hf(t_i, y_i), \\
K_2 &= hf(t_i + \frac{h}{4}, y_i + \frac{1}{4}K_1), \\
K_3 &= hf(t_i + \frac{3h}{8}, y_i + \frac{3}{32}K_1 + \frac{9}{32}K_2), \\
K_4 &= hf(t_i + \frac{12h}{13}, y_i + \frac{1932}{2197}K_1 - \frac{7200}{2197}K_2 + \frac{7296}{2197}K_3), \\
K_5 &= hf(t_i + h, y_i + \frac{439}{216}K_1 - 8K_2 + \frac{3680}{513}K_3 - \frac{845}{4104}K_4), \\
K_6 &= hf(t_i + \frac{h}{2}, y_i - \frac{8}{27}K_1 + 2K_2 - \frac{3544}{2565}K_3 + \frac{1859}{4104}K_4 - \frac{11}{40}K_5).
\end{aligned}
$$

Runge-Kutta-Fehlberg ALGORITHM

To approximate the solution of the initial-value problem

$$y' = f(t, y), a \leq t \leq b, y(a) = \alpha,$$

with local truncation error within a given tolerance:

INPUT endpoints a, b; initial condition α; tolerance TOL; maximum step size $hmax$; minimum step size $hmin$.

OUTPUT t, w, h where w approximates $y(t)$ and the step size h was used, or a message that the minimum step size was exceeded.

Step 1 Set $t = a; w = \alpha; h = hmax; FLAG = 1;$
OUTPUT (t, w).

Step 2 While $(FLAG = 1)$ do Steps 3-11.

Step 3 Set

$$
\begin{aligned}
K_1 &= hf(t, w); \\
K_2 &= hf(t + \frac{h}{4}, w + \frac{1}{4}K_1); \\
K_3 &= hf(t + \frac{3h}{8}, w + \frac{3}{32}K_1 + \frac{9}{32}K_2), \\
K_4 &= hf(t + \frac{12h}{13}, w + \frac{1932}{2197}K_1 - \frac{7200}{2197}K_2 + \frac{7296}{2197}K_3), \\
K_5 &= hf(t + h, w + \frac{439}{216}K_1 - 8K_2 + \frac{3680}{513}K_3 - \frac{845}{4104}K_4), \\
K_6 &= hf(t + \frac{h}{2}, w - \frac{8}{27}K_1 + 2K_2 - \frac{3544}{2565}K_3 + \frac{1859}{4104}K_4 - \frac{11}{40}K_5).
\end{aligned}
$$

Step 4 Set

$$R = \frac{1}{h}\left|\frac{1}{360}K_1 - \frac{128}{4275}K_3 - \frac{2197}{75240}K_4 + \frac{1}{50}K_5 + \frac{2}{55}K_6\right|.$$

(Note: $R = \frac{1}{h}|\tilde{y}_{i+1} - y_{i+1}|$.)

Step 5 If $R \leq TOL$ then do Steps 6 and 7.

- **Step 6** Set $t = t + h$; (Approximation accepted.)

$$w = w + \frac{25}{216}K_1 + \frac{1408}{2565}K_3 + \frac{2197}{4104}K_4 - \frac{1}{5}K_5.$$

- **Step 7** OUTPUT (t, w, h).

Step 8 Set $\delta = 0.84(TOL/R)^{1/4}$.

Step 9
- If $\delta \leq 0.1$ then set $h = 0.1h$
- else if $\delta \geq 4$ then set $h = 4h$
- else set $h = \delta h$. (Calculate new h.)

Step 10 If $h > hmax$, then set $h = hmax$.

Step 11
- If $t \geq b$ then set $FLAG = 0$
- else if $t + h > b$ then set $h = b - t$
- else if $h < hmin$ then set $FLAG = 0$;
- OUTPUT ('minimum h exceeded').
  (Procedure completed unsuccessfully.)

Step 12 (The procedure is complete.) STOP.

5.7 Multistep Methods

Review on Previous Sections:

- **Euler's Methods**
- **Higher-Order Taylor's Method**
- **Runge-Kutta's Method**
- **Definitions of Local Truncation Error, Global Error**
- **Error Control**

Basic idea:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y) \Rightarrow \mathrm{d}y = f(t, y)\mathrm{d}t$$

$$\int_{x_{i-k}}^{x_{i+1}} \mathrm{d}y = \int_{x_{i-k}}^{x_{i+1}} f(t, y)\mathrm{d}t$$

Definition 5.13 An m-step multistep method

For the initial-value problem

$$\begin{cases} y' = f(t, y), \quad a \le t \le b \\ y(a) = \alpha. \end{cases} \tag{9}$$

is one whose difference equation for finding the approximation y_{i+1} at the mesh point t_{i+1} can be represented by the following equation, where m is an integer greater than 1:

$$\begin{aligned} y_{i+1} \quad = \quad & a_{m-1} y_i + a_{m-2} y_{i-1} + a_{m-3} y_{i-2} + \cdots \\ & + a_0 y_{i-(m-1)} \\ & + h[b_m f(t_{i+1}, y_{i+1}) + b_{m-1} f(t_i, y_i) + \cdots \\ & + b_0 f(t_{i-(m-1)}, y_{i-(m-1)})], \end{aligned} \tag{10}$$

for $i = m-1, m, \cdots, N-1$, where $h = (b-a)/N$, the $a_0, a_1, \cdots, a_{m-1}$ and $b_0, b_1, \cdots, b_m$ are constants, and the starting values

$$y_0 = \alpha, y_1 = \alpha_1, y_2 = \alpha_2, \cdots, y_{m-1} = \alpha_{m-1}$$

are specified.

Notes:

- When $b_m = 0$, the method is called **explicit–显式格式**, or **open**, since Eq. (10) gives y_{i+1} explicitly in terms of previously determined values.
- When $b_m \neq 0$, the method is called **implicit–隐式格式**, or **closed**, since y_{i+1} occurs on both sides of Eq. (10) and is specified only implicitly
-
-

Fourth-order Adams-Bashforth method:

$$
\begin{aligned}
y_0 &= \alpha, y_1 = \alpha_1, y_2 = \alpha_2, y_3 = \alpha_3 \\
y_{i+1} &= y_i + \frac{h}{24}[55f(t_i, y_i) - 59f(t_{i-1}, y_{i-1}) \\
&\quad +37f(t_{i-2}, y_{i-2}) - 9f(t_{i-3}, y_{i-3})] \qquad (11)
\end{aligned}
$$

for each $i = 3, 4, \cdots, N-1$, define an **explicit four-step method**.

Fourth-order Adams-Moulton method:

$$\begin{aligned} y_0 &= \alpha, y_1 = \alpha_1, y_2 = \alpha_2, \\ y_{i+1} &= y_i + \frac{h}{24}[9f(t_{i+1}, y_{i+1}) + 19f(t_i, y_i) \\ &\quad -5f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})] \end{aligned} \tag{12}$$

for each $i = 2, 3, \cdots, N-1$, define an **implicit three-step method**

- For the initial- value problem (9), if integrated over the interval $[t_i, t_{i+1}]$, has the property that

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} y'(t)\mathrm{d}t = \int_{t_i}^{t_{i+1}} f(t, y(t))\mathrm{d}t$$

- Consequently

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))\mathrm{d}t \tag{13}$$

- Using an interpolating polynomial $P(t)$ instead of $f(t, y(t))$, which is determined by

$$(t_0, y_0), (t_1, y_1), \cdots, (t_i, y_i).$$

- Assume that $y(t_i) \approx y_i$, Eq. (13) becomes

$$y(t_{i+1}) \approx y_i + \int_{t_i}^{t_{i+1}} P(t)\mathrm{d}t \tag{14}$$

Newton backward-difference formula

- To derive an Adams-Bashforth explicit m-step technique, we form the backward-difference polynomial $P_{m-1}(t)$ through

$$(t_i, f(t_i, y(t_i))), (t_{i-1}, f(t_{i-1}, y(t_{i-1}))), \cdots,$$

$$(t_{i-(m-1)}, f(t_{i-(m-1)}, y(t_{i-(m-1)}))).$$

- Since $P_{m-1}(t)$ is an interpolatory polynomial of degree $m-1$, some number ξ_i in $(t_{i-(m-1)}, t_i)$ exists with

$$f(t, y(t)) = P_{m-1}(t) + \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}(t-t_i)(t-t_{i-1})\cdots(t-t_{i-(m-1)}).$$

-

Introducing the variable substitution $t = t_i + sh$, with $\mathrm{d}t = h\mathrm{d}s$ into $P_{m-1}(t)$ and the error term implies that

$$
\begin{aligned}
& \int_{t_i}^{t_{i+1}} f(t, y(t))\,dt \\
= \; & \int_{t_i}^{t_{i+1}} \sum_{k=0}^{m-1} (-1)^k \begin{pmatrix} -s \\ k \end{pmatrix} \nabla^k f(t_i, y(t_i))\,dt \\
& + \int_{t_i}^{t_{i+1}} \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!} (t - t_i)(t - t_{i-1}) \cdots (t - t_{i-(m-1)})\,dt \\
= \; & \sum_{k=0}^{m-1} (-1)^k \nabla^k f(t_i, y(t_i)) h \int_0^1 \begin{pmatrix} -s \\ k \end{pmatrix} ds \\
& + \frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_i, y(\xi_i))\,ds
\end{aligned}
$$

- The integrals $(-1)^k \int_0^1 \binom{-s}{k} ds$ for various values of k are easily evaluated and are listed in following Table.

k	0	1	2	3	4	5	$\cdots$
$(-1)^k \int_0^1 \binom{-s}{k} ds$	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\cdots$

- As a consequence,

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt = h\Big[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) \tag{15}$$

$$+\frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\Big]$$

$$+\frac{h^{m+1}}{m!}\int_0^1 s(s+1)(s+2)\cdots(s+m-1)f^{(m)}(\xi_i, y(\xi_i))ds. \tag{16}$$

Since $s(s+1)(s+2)\cdots(s+m-1)$ does not change sign on $[0,1]$, the weighted mean value theorem for the integrals can be used to reduce that for some number μ_i, where $t_{i-(m-1)} < \mu_i < t_{i+1}$, the error term in Eq. (15) becomes

$$\begin{aligned}
&\frac{h^{m+1}}{m!}\int_0^1 s(s+1)(s+2)\cdots(s+m-1)f^{(m)}(\xi_i, y(\xi_i))\mathrm{d}s \\
&= \frac{h^{m+1}f^{(m)}(\mu_i, y(\mu_i))}{m!}\int_0^1 s(s+1)(s+2)\cdots(s+m-1)\mathrm{d}s
\end{aligned}$$

or

$$h^{m+1}f^{(m)}(\mu_i, y(\mu_i))(-1)^m\int_0^1 \left(\begin{array}{c} -s \\ k \end{array}\right)\mathrm{d}s. \tag{17}$$

Since

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} f(t, y(t))\mathrm{d}t,$$

Eq. (15) can be written as

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + h\Big[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) \\ &\quad + \frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\Big] \\ &\quad + h^{m+1} f^{(m)}(\mu_i, y(\mu_i))(-1)^m \int_0^1 \begin{pmatrix} -s \\ m \end{pmatrix} \mathrm{d}s \end{aligned} \quad (18)$$

three-step Adams-Bashforth method

Consider Eq. (18) with $m = 3$:

$$
\begin{aligned}
y(t_{i+1}) &\approx y(t_i) + h\Big[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) \\
&\quad + \frac{5}{12}\nabla^2 f(t_i, y(t_i))\Big] \\
&= y(t_i) + h\Big\{f(t_i, y(t_i)) + \frac{1}{2}[f(t_i, y(t_i)) \\
&\quad - f(t_{i-1}, y(t_{i-1}))] \\
&\quad + \frac{5}{12}[f(t_i, y(t_i)) - 2f(t_{i-1}, y(t_{i-1})) \\
&\quad + f(t_{i-2}, y(t_{i-2}))]\Big\} \\
&= y(t_i) + \frac{h}{12}[23f(t_i, y(t_i)) \\
&\quad - 16f(t_{i-1}, y(t_{i-1})) + 5f(t_{i-2}, y(t_{i-2}))].
\end{aligned}
$$

Three-step Adams-Bashforth method

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, y_2 = \alpha_2, \\ y_{i+1} = y_i + \frac{h}{12}[23f(t_i, y_i) - 16f(t_{i-1}, y_{i-1}) + 5f(t_{i-2}, y_{i-2})] \end{cases}$$

for $i = 2, 3, \cdots, N-1$.

Note: Multistep methods can also be derived by using Taylor series.

Definition 5.14

- If $y(t)$ is the solution to the initial-value problem $y' = f(t, y), a \le t \le b, y(a) = \alpha$, and

$$\begin{aligned} y_{i+1} &= a_{m-1}y_i + a_{m-2}y_{i-1} + \cdots + a_0 y_{i+1-m} \\ &\quad + h[b_m f(t_{i+1}, y_{i+1}) + b_{m-1} f(t_i, y_i) + \cdots \\ &\quad + b_0 f(t_{i+1-m}, y_{i+1-m})] \end{aligned}$$

  is the $(i+1)$st step in a multistep method
- the local truncation error at this step is

$$\begin{aligned} \tau_{i+1}(h) &= \frac{y(t_{i+1}) - a_{m-1}y(t_i) + \cdots + a_0 y(t_{i+1-m})}{h} \\ &\quad - [b_m f(t_{i+1}, y(t_{i+1})) + b_{m-1} f(t_i, y(t_i)) + \cdots \\ &\quad + b_0 f(t_{i+1-m}, y(t_{i+1-m}))] \end{aligned} \tag{19}$$

  for each $i = m-1, m, \cdots, N-1$.

The local truncation error for the three-step Adams-Bashforth method:

- Consider the form of the error term in Eq.(17) with $m = 3$, we have

$$h^4 f^{(3)}(\mu_i, y(\mu_i))(-1)^3 \int_0^1 \left(\begin{array}{c} -s \\ 3 \end{array} \right) ds. = \frac{3h^4}{8} y^{(4)}(\mu_i),$$

  for some $\mu_i \in (t_{i-2}, t_{i+1})$.

- Using the fact that $f^{(3)}(\mu_i, y(\mu_i)) = y^{(4)}(\mu_i)$ and the difference equation derived in the three-step Adams-Bashforth method, we have

$$\begin{aligned} \tau_{i+1}(h) &= \frac{y(t_{i+1}) - y(t_i)}{h} - \frac{1}{12}[23f(t_i, y(t_i)) \\ &\quad -16f(t_{i-1}, y(t_{i-1})) + 5f(t_{i-2}, y(t_{i-2}))] \\ &= \frac{1}{h}\left[\frac{3h^4}{8} f^{(3)}(\mu_i, y(\mu_i))\right] \\ &= \frac{3h^3}{8} y^{(4)}(\mu_i), \text{for some} \mu_i \in (t_{i-2}, t_{i+1}). \end{aligned}$$

Some of the explicit multi-step methods together with their required starting values and local truncation errors are as follows.

- **Adams-Bashforth Two-Step Method:**

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, \\ y_{i+1} = y_i + \frac{h}{2}[3f(t_i, y_i) - f(t_{i-1}, y_{i-1}))] \end{cases} \tag{20}$$

  for $i = 1, 2, \cdots, N-1$.

- The local truncation error is

$$\tau_{i+1}(h) = \frac{5}{12} y'''(\mu_i) h^2,$$

  for some

$$\mu_i \in (t_{i-1}, t_{i+1}).$$

- **Adams-Bashforth Three-Step Method:**

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, y_2 = \alpha_2, \\ y_{i+1} = y_i + \frac{h}{12}[23f(t_i, y_i) - 16f(t_{i-1}, y_{i-1}) + 5f(t_{i-2}, y_{i-2})] \end{cases} \tag{21}$$

  for $i = 2, 3, \cdots, N-1$.

- The local truncation error is

$$\tau_{i+1}(h) = \frac{3}{8} y^{(4)}(\mu_i) h^3.$$

  for some

$$\mu_i \in (t_{i-2}, t_{i+1}).$$

- **Adams-Bashforth Four-Step Method:**

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, y_2 = \alpha_2, y_3 = \alpha_3, \\ y_{i+1} = y_i + \frac{h}{24}[55f(t_i, y_i) - 59f(t_{i-1}, y_{i-1})) \\ \qquad\qquad +37f(t_{i-2}, y_{i-2})) - 9f(t_{i-3}, y_{i-3}))] \end{cases} \tag{22}$$

for $i = 3, 4, \cdots, N-1$.

- The local truncation error is

$$\tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4$$

for some

$$\mu_i \in (t_{i-3}, t_{i+1}).$$

- **Adams-Bashforth Five-Step Method:**

$$
\begin{aligned}
y_0 &= \alpha, y_1 = \alpha_1, y_2 = \alpha_2, y_3 = \alpha_3, y_4 = \alpha_4 \\
y_{i+1} &= y_i + \frac{h}{720}[1901f(t_i, y_i) - 2774f(t_{i-1}, y_{i-1}) \\
&\quad +2616f(t_{i-2}, y_{i-2}) - 1274f(t_{i-3}, y_{i-3}) \\
&\quad +251f(t_{i-4}, y_{i-4})] \qquad (23)
\end{aligned}
$$

  for $i = 4, 5, \cdots, N-1$.

- The local truncation error is

$$
\tau_{i+1}(h) = \frac{95}{288} y^{(6)}(\mu_i) h^5,
$$

  for some $\mu_i \in (t_{i-4}, t_{i+1})$.

- Implicit methods are derived by using $(t_{i+1}, f(t_{i+1}, y(t_{i+1})))$ as an additional interpolation node in the approximation of the integral

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt.$$

- Some of the more common **implicit methods** are as follows.

- **Adams-Multon Two-Step Method:**

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, \\ y_{i+1} = y_i + \frac{h}{12}[5f(t_{i+1}, y_{i+1}) + 8f(t_i, y_i)) - f(t_{i-1}, y(t_{i-1}))] \end{cases} \tag{24}$$

  for $i = 1, 2, \cdots, N-1$.

- The local truncation error is

$$\tau_{i+1}(h) = -\frac{1}{24} y^{(4)}(\mu_i) h^3$$

  for some

$$\mu_i \in (t_{i-1}, t_{i+1}).$$

- **Adams-Moulton Three-Step Method:**

$$\begin{cases} y_0 = \alpha, y_1 = \alpha_1, y_2 = \alpha_2, \\ y_{i+1} = y_i + \frac{h}{24}[9f(t_{i+1}, y_{i+1}) + 19f(t_i, y_i) \\ \qquad -5f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})] \end{cases} \tag{25}$$

  for $i = 2, 3, \cdots, N-1$.

- The local truncation error is

$$\tau_{i+1}(h) = -\frac{19}{720} y^{(5)}(\mu_i) h^4$$

  for some

$$\mu_i \in (t_{i-2}, t_{i+1}).$$

Adams-Moulton Four-Step Method:

$$\begin{aligned} y_0 &= \alpha, y_1 = \alpha_1, y_2 = \alpha_2, y_3 = \alpha_3, \\ y_{i+1} &= y_i + \frac{h}{720}[251f(t_{i+1}, y_{i+1})) + 646f(t_i, y_i) \\ &\quad -264f(t_{i-1}, y_{i-1})) + 106f(t_{i-2}, y_{i-2})) \\ &\quad -19f(t_{i-3}, y_{i-3}))] \end{aligned} \tag{26}$$

for $i = 3, 4, \cdots, N-1$.

The local truncation error is $\tau_{i+1}(h) = -\frac{3}{160}y^{(6)}(\mu_i)h^5$, for some $\mu_i \in (t_{i-3}, t_{i+1})$.

predictor-corrector method

- The combination of an explicit and implicit technique is called a **predictor-corrector method**.
- The explicit method predicts an approximation, and the implicit method corrects this prediction.

Example

- Consider the following fourth-order method for solving an initial-value problem.
- The first step is to calculate the starting values y_0, y_1, y_2, and y_3 using Runge-Kutta method of order four.
- The next step is to calculate an approximation, $y_4^{(0)}$, to $y(t_4)$ using the four-step Adams- Bashforth method as **predictor**:

$$\begin{aligned} y_4^{(0)} &= y_3 + \frac{h}{24}[55f(t_3, y_3) - 59f(t_2, y_2)) + \\ &\quad +37f(t_1, y_1)) - 9f(t_0, y_0))] \end{aligned}$$

- This approximation is improved by inserting $y_4^{(0)}$ in the right side of the three-step Adams- Moulton method and using that method as a **corrector**:

$$\begin{aligned} y_{i+1}^{(k+1)} &= y_i + \frac{h}{24}[9f(t_{i+1}, y_{i+1}^{(k)}) + 19f(t_i, y_i) \\ &\quad -5f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})], k = 0, 1, 2, \cdots \end{aligned}$$

ALGORITHM:Adams Fourth-Order Predictor-Corrector

To approximate the solution of the initial-value problem

$$y'(t) = f(t, y), a \le t \le b, y(a) = \alpha$$

at $(N+1)$ equally spaced numbers in the interval $[a, b]$:

INPUT: endpoints a, b; integer N; initial condition α.

OUTPUT approximation w to $y(t)$ at the $(N+1)$ values of t.

Step 1 Set $h = (b-a)/N$; $t_0 = a$; $w_0 = \alpha$; OUTPUT (t_0, w_0).

Step 2 For $i = 1, 2, 3$, do Steps 3-5. (Compute starting values using Runge-Kutta method.)

Step 3 Set

$$\begin{aligned} K_1 &= hf(t_{i-1}, w_{i-1}); \\ K_2 &= hf(t_{i-1} + h/2, w_i + K_1/2); \\ K_3 &= hf(t_{i-1} + h/2, w_i + K_2/2) \\ K_4 &= hf(t_{i-1} + h, w_i + K_3). \end{aligned}$$

Step 4 Set

$$w_i = w_{i-1} + (K_1 + 2K_2 + 2K_3 + K_4)/6;$$

$$t_i = a + ih.$$

Step 5 OUTPUT (t_i, w_i).

Step 6 For $i = 4, \cdots, N$ do Steps 7-10.

Step 7 Set $t = a + ih$;

$$\begin{aligned} w &= w_3 + h[55f(t_3, w_3) - 59f(t_2, w_2) + 37f(t_1, w_1) \\ &\quad -9f(t_0, w_0); (\text{Predict}\, w_i) \\ w &= w_3 + h[9f(t, w) + 19f(t_3, w_3) - 5f(t_2, w_2) \\ &\quad +f(t_1, w_1)]/24; (\text{Correct}\, w_i) \end{aligned}$$

Step 8 OUTPUT (t, w).

Step 9 For $j = 0, 1, 2$
set $t_j = t_{j+1}$; (Prepare for next iteration.)
$w_j = w_{j+1}$.

Step 10 Set $t_3 = t$;
$w_3 = w$.

Step 11 STOP.

Milne's method

- Other multistep methods can be derived using integration of interpolating polynomials over intervals of the form $[t_j, t_{i+1}]$, for $j \leq i-1$, to obtain an approximation to $y(t_{i+1})$.
- When an interpolating polynomial is integrated over $[t_{i-3}, t_{i+1}]$, the result is an explicit technique known as Milne's method

$$y_{i+1} = y_{i-3} + \frac{4h}{3}[2f(t_i, y_i) - f(t_{i-1}, y_{i-1}) + 2f(t_{i-2}, y_{i-2})],$$

which has local truncation error $\frac{14}{45}h^4 y^{(5)}(\xi_i)$, for some $\xi_i \in (t_{i-3}, t_{i+1})$.

- This method is occasionally used as a **predictor** for the **implicit Simpson's method**,

$$y_{i+1} = y_{i-1} + \frac{h}{3}[f(t_{i+1}, y_{i+1})4f(t_i, y_i) + f(t_{i-1}, y_{i-1})],$$

  which has local truncation error $-\frac{1}{90}h^4 y^{(5)}(\xi_i)$, for some $\xi_i \in (t_{i-1}, t_{i+1})$, and is obtained by integrating an interpolating polynomial over $[t_{i-1}, t_{i+1}]$.
- The local truncation error involved with a predictor-corrector method of the Milne- Simpson type is generally smaller than that of the Adams-Bashforth-Moulton method. But the technique has limited use because of problems of stability, which do not occur with the Adams procedure.

Reviews on Error Control Methods

1 **The Runge- Kutta- Fehlberg method is used for error control because at each step it provides, at little additional cost, two approximations that can be compared and related to the local error.**

2 **Predictor-corrector techniques always generate two approximations at each step, so they are natural candidates for error-control adaptation.**

To demonstrate the error-control procedure, we will construct a variable step-size predictor-corrector method using the **four-step Adams-Bashforth method as predictor and the three-step Adams-Moulton method as corrector**.

Adams-Bashforth four-step method comes from the relation

$$
\begin{aligned}
y(t_{i+1}) \;=\; & y(t_i) + \frac{h}{24}[55f(t_i, y(t_i)) \\
& -59f(t_{i-1}, y(t_{i-1})) + 37f(t_{i-2}, y(t_{i-2})) \\
& -9f(t_{i-3}, y(t_{i-3}))] + \frac{251}{720} y^{(5)}(\hat{\mu}_i) h^5,
\end{aligned}
$$

for some $\hat{\mu}_i \in (t_{i-3}, t_{i+1})$.

The assumption that the approximations $y_0, y_1, y_2, \cdots, y_i$ are all exact implies that the Adams- Bashforth truncation error is

$$\frac{y(t_{i+1}) - y_{i+1}^{(0)}}{h} = \frac{251}{720} y^{(5)}(\hat{\mu}_i) h^4. \tag{27}$$

A similar analysis of the **Adams-Moulton three-step method**, which comes'from

$$\begin{aligned} y(t_{i+1}) \quad &= \quad y(t_i) + \frac{h}{24}[9f(t_{i+1}, y(t_{i+1})) + 19f(t_i, y(t_i)) \\ &\quad -5f(t_{i-1}, y(t_{i-1})) + f(t_{i-2}, y(t_{i-2}))] \\ &\quad -\frac{19}{720} y^{(5)}(\tilde{\mu}_i) h^4, \end{aligned}$$

for some $\tilde{\mu}_i \in (t_{i-2}, t_{i+1})$ leads to the local truncation error

$$\frac{y(t_{i+1}) - y_{i+1}}{h} = -\frac{19}{720} y^{(5)}(\tilde{\mu}_i) h^4. \tag{28}$$

To proceed further, we must make the assumption that for small values of h,

$$y^{(5)}(\hat{\mu}_i) = y^{(5)}(\tilde{\mu}_i).$$

The effectiveness of the error-control technique depends directly on this assumption. If we subtract Eq. (28) from Eq. (27), we have

$$\begin{aligned}\frac{y_{i+1} - y_{i+1}^{(0)}}{h} &= -\frac{h^4}{720}[251 y^{(5)}(\hat{\mu}_i) + 19 y^{(5)}(\tilde{\mu}_i)] \\ &\approx \frac{3}{8} h^4 y^{(5)}(\tilde{\mu}_i),\end{aligned}$$

so

$$y^{(5)}(\tilde{\mu}_i) \approx \frac{8}{3h^5}(y_{i+1} - y_{i+1}^{(0)}) \tag{29}$$

Using this result to eliminate the term involving $y^{(5)}(\tilde{\mu}_i)h^4$ from (28) gives the approximation to the error

$$\begin{aligned}|\tau_{i+1}(h)| &= \frac{|y(t_{i+1}) - y_{i+1}|}{h} \\ &\approx \frac{19h^4}{720} \cdot \frac{8}{3h^5}|y_{i+1} - y_{i+1}^{(0)}| \\ &= \frac{19|y_{i+1} - y_{i+1}^{(0)}|}{270h}.\end{aligned}$$

Suppose we now reconsider (28) with a new step size qh generating new approximations $\hat{y}_{i+1}^{(0)}$ and $\hat{y}_{i+1}$. The object is to choose q so that the local truncation error given in (28) is bounded by a prescribed tolerance ε.

If we assume that the value $y^{(5)}(\mu)$ in (28) associated with qh is also approximated using (29), then

$$\begin{aligned}\frac{|y(t_i+qh)-\hat{y}_{i+1}|}{qh} &= \frac{19}{720}|y^{(5)}(\mu)|q^4h^4 \\ &\approx \frac{19}{720}\left[\frac{8}{3h^5}|y_{i+1}-y_{i+1}^{(0)}|\right]q^4h^4,\end{aligned}$$

and we need to choose q so that

$$\frac{|y(t_i+qh)-\hat{y}_{i+1}|}{qh} \approx \frac{19}{720}\frac{|y_{i+1}-y_{i+1}^{(0)}|}{h}q^4 < \varepsilon,$$

That is, we choose q so that

$$q < \left(\frac{270}{19} \frac{h\varepsilon}{|y_{i+1} - y_{i+1}^{(0)}|} \right)^{1/4} \approx 2 \left(\frac{h\varepsilon}{|y_{i+1} - y_{i+1}^{(0)}|} \right)^{1/4}.$$

A number of approximation assumptions have been made in this development, so in practice q is chosen conservatively, usually as

$$q = 1.5 \left(\frac{h\varepsilon}{|y_{i+1} - y_{i+1}^{(0)}|} \right)^{1/4}.$$

A change in step size for a multistep method is more costly in terms of function evaluations than for a one-step method since new, equally-spaced starting values must be computed. As a consequence, it is common practice to ignore the step-size change whenever the local truncation error is between $\varepsilon/10$ and ε, that is, when

$$
\begin{aligned}
\frac{\varepsilon}{10} &< |\tau_{i+1}(h)| = \frac{|y(t_{i+1}) - y_{i+1}|}{h} \\
&\approx \frac{19|y_{i+1} - y_{i+1}^{(0)}|}{270h} < \varepsilon.
\end{aligned}
$$

Adams Variable Step-Size Predictor-Corrector
To approximate the solution of the initial-value problem

$$y' = f(t, y), a \leq t \leq b, y(a) = \alpha$$

with local truncation error within a given tolerance :

INPUT endpoints a, b; initial condition a; tolerance TOL; maximum step size $hmax$; minimum step size $hmin$.

OUTPUT i, t_i, y_i, h where at the ith step w_i approximates $y(t_i)$ and the step size h was used, or a message that the minimum step size was exceeded.

The steps of this algorithm are omitted.

Definition 5.17

A one-step difference-equation method with local truncation error $\tau_i(h)$ at the ith step is said to be **consistent** with the differential equation it approximates, if

$$\lim_{h\to 0} \max_{1\le i\le N} |\tau_i(h)| = 0.$$

Note: this definition is a *local* definition , since , for each of the values $\tau_i(h)$, we are assuming that the approximation y_{i-1} and the exact solution $y(t_{i-1})$ are the same.

- A more realistic means of analyzing the effects of making h small is to determine the **global** effect of the method.
- This is the maximum error of the method over the entire range of the approximation, assuming only that the method gives the exact result at the initial value.

Definition 5.18

A **one step difference equation** method is said to be **convergent** with respect to the differential equation it approximates if

$$\lim_{h \to 0} \max_{1 \leq i \leq N} |w_i - y(t_i)| = 0$$

where $y_i = y(t_i)$ denotes the exact value of the solution of the differential equation and w_i is the approximation obtained form the difference method at the ith step.

EXAMPLE: Consider the Euler's method.

- By the hypotheses of Theorem 5.9, we have

$$\max_{1\le i\le N} |w_i - y(t_i)| \le \frac{Mh}{2L}|e^{L(b-a)} - 1|.$$

  so the Euler's method is convergent with respect to a differential equation satisfying the conditions of this theorem , and the rate of convergence is $O(h)$.
- A one-step method is consistent precisely when the difference equation for the method approaches the differential equation when the step size goes to zero; that is , the local truncation error approaches zero as the step size approaches zero.
- The definition of convergence has a similar connotation.
- A method is **convergent** precisely when the solution to the difference equation approaches the solution to the differential equation as the step size goes to zero.

Stability

Definition 5.19

- A numerical method for initial value problems of Ordinary Differential Equations is **stable**, if in the sense that small changes or perturbations in the initial conditions, produce correspondingly small changes in the subsequent approximation.
- That is, a stable method is the one whose results depend continuously on the initial data.

THEOREM 5.20

- Suppose the initial-value problem

$$y' = f(t, y), a \leq t \leq b, y(a) = \alpha$$

is approximated by a **one-step difference method** in the form

$$w_o = \alpha$$

$$w_{i+1} = w_i + h\phi(t_i, w_i, h)$$

- Suppose also that a number $h_0 > 0$ exists and that $\phi(t, w, h)$ is **continuous** and satisfies a **Lipschitz condition** in the variable w with Lipschitz constant L on the set

$$D = (t, w, h)|a \leq t \leq b, -\infty < w < \infty, 0 \leq h \leq h_0$$

- Then
  1. The method is **stable**;
  2. the difference method is **convergent** if and only if it is consistent–that is ,if and only if

  $$\phi(t, y, 0) = f(t, y), \texttt{for all } a \leq t \leq b$$

  3. If a function τ exists, and for each $i = 1, 2, \cdots, N$, the local truncation error$\tau_i(h)$ satisfies $|\tau_i(h)| \leq \tau(h)$ whenever $0 \leq h \leq h_0$ then

  $$|y(t_i) - w_i| \leq \frac{\tau(h)}{L} d^{L(t_i - a)}$$

- **As an example,** we prove the **Modified Euler's method**, given by

$$\begin{aligned} w_0 &= \alpha \\ w_{i+1} &= w_i + \frac{h}{2}[f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))] \end{aligned}$$

  for $i = 0, 1, 2, \cdots, N-1$, satisfies the hypothesis of THEOREM 5.20.

- For this method,

$$\phi(t, w, h) = \frac{1}{2}f(t, w) + \frac{1}{2}f(t+h, w+hf(t, w)).$$

- f satisfies a Lipschitz condition on $\{(t, w) | a \leq t \leq b, -\infty < w < \infty\}$ in the variable w with constant L, then, since

$$
\begin{aligned}
&\phi(t, w, h) - \phi(t, \bar{w}, h) \\
&= \frac{1}{2} f(t, w) + \frac{1}{2} f(t + h, w + hf(t, w)) \\
&- \frac{1}{2} f(t, \bar{w}) - \frac{1}{2} f(t + h, \bar{w} + hf(t, \bar{w}))
\end{aligned}
$$

- the Lipschitz condition on f leads to

$$
\begin{aligned}
&|\phi(t, w, h) - \phi(t, \bar{w}, h)| \\
&= \frac{1}{2} L|w - \bar{w}| + \frac{1}{2} L|w + hf(t, w) - \bar{w} - hf(t, \bar{w})| \\
&\leq L|w - \bar{w}| + \frac{1}{2} L|hf(t, w) - hf(t, \bar{w})| \\
&\leq L|w - \bar{w}| + \frac{1}{2} hL^2 |w - \bar{w}| \\
&= \left(L + \frac{1}{2} hL^2 \right) |w - \bar{w}|.
\end{aligned}
$$

- Therefore, ϕ satisfies a Lipschitz condition in w on the set

$$\{(t, w, h) | a \leq t \leq b, -\infty < w < \infty, 0 \leq h \leq h_0\}.$$

for any $h_0 > 0$ with constant

$$L' = L + \frac{1}{2} h_0 L^2$$

- Finally, if f is continuous on the set

$$\{(t, w) | a \leq t \leq b, -\infty < w < \infty\},$$

then ϕ is also continuous on the set

$$\{(t, w, h) | a \leq t \leq b, -\infty < w < \infty, 0 < h < h_0\}.$$

- So the Modified Euler's method is stable, that means part (i) holds.
- Letting $h = 0$, we have

$$\phi(t, w, 0) = \frac{1}{2} f(t, w) + \frac{1}{2} f(t + 0, w + 0 \cdot f(t, w)) = f(t, w).$$

- So the consistency condition expressed in Theorem 5.20, part (ii), holds.Thus, the method is convergent.Moreover, we have seen that for this method the local truncation error is $O(h^2)$, so the convergence of the Modified Euler method also has rate $O(h^2)$$\blacksquare\blacksquare$.

The **general multistep method** for approximating the solution to the initial-value problem

$$y' = f(t, y), a \leq t \leq b, y(a) = \alpha \tag{30}$$

can be written in the form

$$\begin{aligned} w_0 &= \alpha, w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}, \\ w_{i+1} &= a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + hF(t_i, h, w_{i+1}, w_i, \cdots, w_{i+1-m},) \end{aligned} \tag{31}$$

for each $i = m-1, m, \cdots, N-1$, where a_0, a_1, $\cdots$, a_{m-1} are constants and , as usual, $h = (b-a)/N$ and $t_i = a + ih$.

The local truncation error for a multistep method expressed in this form is

$$\tau_{i+1}(h) = \frac{y(t_{i+1}) - a_{m-1}y(t_i) - \cdots - a_0 y(t_{i+1-m})}{h} - F(t_i, h, y(t_{i+1}), y(t_i), \cdots, y(t_{i+1-m})),$$

for each $i = m-1, m, ..., N-1$.

As in the one-step methods,the local truncation error measures how the solution $y(t)$ to the differential equation fails to satisfy the difference equation.

For the four-step Adams-Bashforth method, we have seen that

$$\tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4, \texttt{for some} \mu_i \in (t_{i-3}, t_{i+1})$$

whereas the three-step Adams-Moulton method has

$$\tau_{i+1}(h) = -\frac{19}{720} y^{(5)}(\mu_i) h^4, \texttt{for some} \mu_i \in (t_{i-2}, t_{i+1})$$

provided,of course ,that $y \in C^5[a, b]$

Throughout the analysis,two assumptions will be made concerning the function F:

1. If $f \equiv 0$ (that is,if the differential equation is homogeneous),then $F = 0$ also.

2. F satisfies a Lipschitz condition with respect to $\{w_j\}$,in the sense that a constant L exists and,for every pair of sequences $\{v_j\}_{j=0}^{N}$ and $\{\tilde{v}_j\}_{j=0}^{N}$ and for $i = m-1, m, \cdots, N-1$,we have

$$\begin{aligned} &|F(t_i, h, v_{i+1}, \cdots, v_{i+1-m}) \\ &-F(t_i, h, \tilde{v}_{i+1}, \cdots, \tilde{v}_{i+1-m})| \\ &\leq L \sum_{j=0}^{m} |v_{i+1-j} - \tilde{v}_{i+1-j}| \end{aligned}$$

The concept of **convergence for multistep methods** is the same as that for one-step methods:a multistep method is **convergent** if the solution to the difference equation approaches the solution to the differential **as the step size approaches zero.** This means that

$$\lim_{h \to 0} \max_{1 \leq i \leq N} |w_i - y(t_i)| = 0$$

For **consistency,** however ,a slightly different situation occurs. Again, we want a multistep method to be consistent provided that the difference equation approaches the differential equation as the step size approaches zero;that is, the local truncation error must approach zero at each step as the step size approaches zero. The additional condition occurs because of the number of starting values required for multistep methods. Since usually only the first starting value, $w_0 = \alpha$, is exact, we need to require that the errors in all the starting values $\{\alpha_i\}$ approaches zero.

So,both

$$\lim_{h\to 0} |\tau_i(h)| = 0, \texttt{for all } i = m, m+1, , \cdots, N, \tag{32}$$

and

$$\lim_{h\to 0} |\alpha_i - y(t_i)| = 0, \texttt{for all} i = 1, 2, \cdots, m-1 \tag{33}$$

must be true for a multistep method in the form (31)to be **consistent**.

Note that (33)implies that a multistep method will not be consistent unless the one-step method generating the starting values is also consistent.

The following theorem for multistep methods is similar to Theorem 5.20,part(iii) and gives a relationship between the local truncation error and global error of a multistep method.It provides the theoretical justification for attempting to control global error by controlling local truncation error .

Theorem 5.21 suppose the initial-value problem

$$y' = f(t, y), a \leq t \leq b, y(a) = \alpha$$

is approximated by an **Adams predictor-corrector method** with an **m-step Adams-Bashforth predictor** equation

$$\begin{aligned} w_{i+1} = w_i \quad + \quad & h[b_{m-1}f(t_i, w_i) + \cdots \\ & + b_0 f(t_{i+1-m}, w_{i+1-m})] \end{aligned}$$

with local truncation error $\tau_{i+1}(h)$.

And an **(m-1)-step Adams-Moulton corrector equation**

$$\begin{aligned} w_{i+1} = w_i \quad &+ \quad h[\tilde{b}_{m-1} f(t_i, w_{i+1}) + \cdots \\ & \quad\; + \tilde{b}_0 f(t_{i+2-m}, w_{i+2-m})] \end{aligned}$$

with local truncation error $\tilde{\tau}_{i+1}(h)$.

In addition ,suppose that $f(t, y)$ and $f_y(t, y)$ are continuous on $D = \{(t, y) | a \leq t \leq b \text{ and} - \infty < y < \infty\}$ and that f_y is bounded .Then the local truncation error $\sigma_{i+1}(h)$ of the predictor-corrector method is

$$\sigma_{i+1}(h) = \tilde{\tau}_{i+1}(h) + h\tau_{i+1}(h)\tilde{b}_{m-1}\frac{\partial f}{\partial y}(t_{i+1}, \theta_{i+1})$$

where θ_{i+1} is a number between zero and $h\tau_{i+1}(h)$.

Moreover there exist constants k_1 and k_2 such that

$$|w_i - y(t_i)| \leq \left[\max_{0 \leq j \leq m-1} |w_j - y(t_j)| + k_1 \sigma(h) \right] e^{k_2 (ti - a)}$$

where $\sigma(h) = \max_{m \leq j \leq N} |\sigma_j(h)| \blacksquare\blacksquare$.

Before discussing connections between **consistency ,convergence ,and stability** for mulitstep methods ,we need to consider in more detail the **difference equation** for a multistep method.

Consider the difference equation given at the beginning of this discussion

$$\begin{aligned} w_0 &= \alpha, w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}, \\ w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + hF(t_i, h, w_{i+1}, w_i, \cdots, w_{i+1-m}) \end{aligned}$$

Then the **characteristic equation** of this difference equation, is given by

$$\lambda^m - a_{m-1}\lambda^{m-1} - a_{m-2}\lambda^{m-2} - \cdots - a_1\lambda - a_0 = 0. \quad (34)$$

Let

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - a_{m-2}\lambda^{m-2} - \cdots - a_1\lambda - a_0.$$

is a polynomial, and called the **Characteristic Polynomial**.

The magnitudes of the roots of the characteristic equation of a multi-step method are associated with the stability of the method with respect to the roundoff error.

To see this, consider the trivial initial-value problem

$$y' \equiv 0, y(a) = \alpha, \texttt{where} \alpha \neq 0 \tag{35}$$

This problem has the exact solution $y(t) \equiv \alpha$, thus we can see that any multi-step methods will, in theory, produce the exact solution $w_n = \alpha$ for all n.

The only deviation from the exact solution is due to the inherent roundoff error associated with the calculations involved in the method.

The right side of the differential equation in (35) has $f(t, y) \equiv 0$,so by assumption (1),we have $F(t_i, h, w_{i+1}, w_i, \cdots, w_{i+1-m}) = 0$ in the difference equation (31).

As a consequence, the standard form of the difference equation becomes

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \tag{36}$$

Suppose λ is one of the roots of the characteristic equation associated with (31). since

$$\begin{aligned}
&\lambda^{i+1} - a_{m-1}\lambda^{i} - a_{m-2}\lambda^{i-1} - \cdots - a_0\lambda^{i+1-m} \\
&= \lambda^{i+1-m}[\lambda^{m} - a_{m-1}\lambda^{m-1} - \cdots - a_1\lambda - a_0] \\
&= 0,
\end{aligned}$$

then $w_n = \lambda^n$ for each n is a solution to (36)

If $\lambda_1, \lambda_2, \cdots, \lambda_m$ are distinct roots of the characteristic equation for (31), it can be shown that every solution to (36) can be expressed in the form

$$w_n = \Sigma_{i=1}^{m} c_i \lambda_i^n. \tag{37}$$

for some unique collection of constants $c_1, c_2, \cdots, c_m$.

Since the exact solution to

$$y' \equiv 0, y(a) = \alpha, \texttt{where} \alpha \neq 0$$

is

$$y(t) = \alpha, .$$

Then choose $w_n = \alpha$, for all n, it is obvious that $w_n = \alpha$ is a solution to

$$w_{i+1} = a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m}$$

and it gives

$$\begin{aligned} 0 &= \alpha - \alpha a_{m-1} - \alpha a_{m-2} - \cdots - \alpha a_0 \\ &= \alpha[1 - a_{m-1} - a_{m-2} - \cdots - a_0] \end{aligned}$$

This implies that $\lambda \equiv 1$ is one of the solutions of characteristic equation (34).

We assume that in the representation (37), this solution is described by $\lambda_1 = 1$ and $c_1 = \alpha$, so all solutions to (36) are expressed as

$$w_n = \alpha + \sum_{i=2}^{m} c_i \lambda_i^n \tag{38}$$

If all the calculations were exact, the constants $c_2, c_3, \cdots, c_m$ would all be zero .

In practice, the constants $c_2, c_3, \cdots, c_m$ are not zero due to roundoff error grows exponentially unless $|\lambda_i| \leq 1$ for each of the roots $\lambda_2, \lambda_3, \cdots, \lambda_m$.

The smaller the magnitude of these roots, the more stable the method will be with respect to the growth of roundoff error.

For the case that multiple roots occur. For example if $\lambda_1, \lambda_2, \cdots, \lambda_t$ are all distinct roots, with multiplicity $m_1, m_2, \cdots, m_t$, thus $m_1 + m_2 + \cdots, m_t = m$, then the solution to

$$w_{i+1} = a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m}$$

can be modified as

$$w_n = \sum_{j=1}^{m_1} c_{1j} n^{j-1} \lambda_1^n + \sum_{j=1}^{m_2} c_{2j} n^{j-1} \lambda_2^n + \cdots + \sum_{j=1}^{m_t} c_{tj} n^{j-1} \lambda_t^n$$

Although the form of the solution is modified , the roundoff effect if $|\lambda_k| > 1$ will grows exponentially.

Definition 5.22

Let $\lambda_1, \lambda_2, \lambda_3, \cdots, \lambda_m$ denote the(not necessarily distinct) roots of the characteristic equation

$$\lambda^m - a_{m-1}\lambda^{m-1} - a_{m-2}\lambda^{m-2} - \cdots - a_1\lambda - a_0 = 0$$

associated with the multistep difference method

$$w_0 = \alpha, w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}$$

and

$$\begin{aligned} w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + hF(t_i, h, w_{i+1}, w_i, \cdots, w_{i+1-m}) \end{aligned}$$

If $|\lambda_i| \leq 1$ for each $i = 1, 2, \cdots, m$ and all roots with absolute value 1 are simple roots,then the difference method is said to satisfy the **root condition**.■■

Definition 5.23

(i) Methods that satisfy the root condition and have $\lambda = 1$ as the only root of the characteristic equation of magnitude one are called **strongly stable**.

(ii) Methods that satisfy the root condition and have more than one distinct root with magnitude one are called **weakly stable**.

(iii) Methods that do not satisfy the root condition are called **unstable**.■■

Theorem 5.24 A multistep method of the form

$$w_0 = \alpha, w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}$$

where

$$\begin{aligned} w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + hF(t_i, h, w_{i+1}, w_i, \cdots, w_{i+1-m}) \end{aligned}$$

is stable if and only if it satisfies the root condition .

Moreover, if the difference method is consistent with the differential equation,then the method is stable if and only if it is convergent.■■

Example: Considering the fourth-order Adams-Bashforth method:

$$w_{i+1} = w_i + hF(t_i, h, w_{i+1}, w_i, \cdots, w_{i-3})$$

where

$$\begin{aligned}
&F(t_i, h, w_{i+1}, w_i, \cdots, w_{i-3}) \\
&= \frac{1}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) \\
&\quad +37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]
\end{aligned}$$

So $m = 4$, $a_0 = 0$, $a_1 = 0$, $a_2 = 0$, $a_3 = 1$.

The characteristic equation for this method is

$$\lambda^4 - \lambda^3 = \lambda^3(\lambda - 1) = 0.$$

which has roots $\lambda_1 = 1, \lambda_2 = \lambda_3 = \lambda_4 = 0$, it satisfy the root condition and is strongly stable.