2.1 Runge-Kutta 方法的构造思想

由

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))\, dx$$

可以得到

$$y(x_{i+1}) = y(x_i) + hf(x_i + \theta h, y(x_i + \theta h)),$$

称 $f(x_i + \theta h, y(x_i + \theta h))$ 为 $y(x)$ 在 $[x_i, x_{i+1}]$ 上的平均斜率, 记为 k^*.
记

$$k_1 = f(x_i, y_i), \quad k_2 = f(x_{i+1}, y_i + hk_1),$$

若用 k_1 近似 k^*, 则得一阶 Euler 公式, 若用 $\frac{k_1+k_2}{2}$ 近似 k^*, 则得 2 阶改进的 Euler 公式.

一般的 r 级 Runge-Kutta 方法为

$$\begin{cases} y_{i+1} = y_i + h\sum_{j=1}^{r}\alpha_j k_j, \\ k_1 = f(x_i, y_i), \\ k_j = f\left(x_i + \lambda_j h, y_i + h\sum_{l=1}^{j-1}\mu_{jl}k_l\right), \quad j = 2, 3, \cdots, r. \end{cases} \tag{2.1}$$

选择参数 $\alpha_j, \lambda_j, \mu_{jl}$ 使其具有一定的阶数. 具体将局部截断误差

$$R_{i+1} = y(x_{i+1}) - y(x_i) - h\sum_{j=1}^{r}\alpha_j K_j,$$

其中

$$K_1 = f(x_i, y(x_i)),$$
$$K_j = f\left(x_i + \lambda_j h, y(x_i) + h\sum_{l=1}^{j-1}\mu_{jl}K_l\right), \quad j = 2, 3, \cdots, r,$$

展开为 h 的幂级数

$$R_{i+1} = c_0 + c_1 h + \cdots + c_p h^p + c_{p+1} h^{p+1} + \cdots$$

选择参数 $\alpha_j, \lambda_j, \mu_{jl}$, 使得 $c_0 = c_1 = \cdots = c_p = 0$, 而 $c_{p+1} \neq 0$, 则公式 (2.1) 是 p 阶的.

2.2 2 阶 Runge-Kutta 公式

2 阶 Runge-Kutta 公式一般形式为

$$\begin{cases} y_{i+1} = y_i + h(\alpha_1 k_1 + \alpha_2 k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \lambda_2 h, y_i + h\mu_{21} k_1) \end{cases} . \tag{2.2}$$

其局部截断误差是

$$\begin{cases} R_{i+1} = y(x_{i+1}) - y(x_i) - h(\alpha_1 K_1 + \alpha_2 K_2) \\ K_1 = f(x_i, y(x_i)) \\ K_2 = f(x_i + \lambda_2 h, y(x_i) + h\mu_{21} K_1) \end{cases}$$

$$
\begin{aligned}
y(x_{i+1}) =& y(x_i) + hy'(x_i) + \frac{1}{2}h^2 y''(x_i) + \frac{1}{3!}h^3 y'''(x_i) + O(h^4) \\
=& y(x_i) + hy'(x_i) + \frac{1}{2}h^2 \left[\frac{\partial f}{\partial x}(x_i, y(x_i)) + y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i)) \right] + \frac{h^3}{6} y'''(x_i) + O(h^4) \\
K_1 =& y'(x_i), \\
K_2 =& f(x_i, y(x_i)) + \lambda_2 h \frac{\partial f}{\partial x}(x_i, y(x_i)) + h\mu_{21} y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i)) \\
& + \frac{1}{2}\left[(\lambda_2 h)^2 \frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) + 2\lambda_2\mu_{21} h^2 y'(x_i) \frac{\partial^2 f}{\partial y^2}(x_i, y(x_i)) \right. \\
& \left. + (\mu_{21} h y'(x_i))^2 \frac{\partial^2 f}{\partial y^2}(x_i, y(x_i)) \right] + O(h^3)
\end{aligned}
$$

将上面 3 式代入局部截断误差得

$$
\begin{aligned}
R_{i+1} =& h(1-\alpha_1-\alpha_2)y'(x_i) \\
&+ h^2\left[\left(\frac{1}{2}-\alpha_2\lambda_2\right)\frac{\partial f}{\partial x}(x_i, y(x_i)) + \left(\frac{1}{2}-\alpha_2\mu_{21}\right)y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))\right] \\
&+ h^3\Bigg[\frac{1}{6}y'''(x_i) - \frac{1}{2}\alpha_2\Bigg((\lambda_2)^2\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) + 2\lambda_2\mu_{21}y'(x_i)\frac{\partial^2 f}{\partial x\partial y}(x_i, y(x_i)) \\
&+ (\mu_{21}y'(x_i))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))\Bigg)\Bigg] + O(h^4).
\end{aligned}
$$

要使 (2.2) 具有 2 阶精度, 则

$$\begin{cases} 1-\alpha_1-\alpha_2=0, \\ \frac{1}{2}-\alpha_2\lambda_2=0, \\ \frac{1}{2}-\alpha_2\mu_{21}=0. \end{cases}$$

显然 α_2 不能为零. 当 $\alpha_2 \neq 0$, 可得

$$\begin{cases} \alpha_1=1-\alpha_2, \\ \lambda_2=\dfrac{1}{2\alpha_2}, \\ \mu_{21}=\dfrac{1}{2\alpha_2}. \end{cases}$$

于是我们可以得到一类 2 阶 Runge-Kutta 公式

$$\begin{cases} y_{i+1} = y_i + h[(1-\alpha_2)k_1 + \alpha_2 k_2], \\ k_1 = f(x_i, y_i), \\ k_2 = f\left(x_i + \dfrac{1}{2\alpha_2}h, y_i + \dfrac{1}{2\alpha_2}hk_1\right). \end{cases}$$

当 $\alpha_2 = \frac{1}{2}$, 得改进的 Euler 公式. 当 $\alpha_2 = 1$, 得变形的 Euler 公式:

$$\begin{cases} y_{i+1} = y_i + hk_2, \\ k_1 = f(x_i, y_i), \\ k_2 = f\left(x_i + \dfrac{1}{2}h, y_i + \dfrac{1}{2}hk_1\right). \end{cases}$$

若 $\alpha_2 = \frac{3}{4}$, 则得

$$\begin{cases} y_{i+1} = y_i + \dfrac{h}{4}(k_1 + 3k_2), \\ k_1 = f(x_i, y_i), \\ k_2 = f\left(x_i + \dfrac{2}{3}h, y_i + \dfrac{2}{3}hk_1\right). \end{cases}$$

利用上述构造方法可以得到 3 阶或 4 阶等高阶 Runge-Kutta 公式.

3.1 收敛性

考虑单步显式公式

$$\begin{cases} y_{i+1} = y_i + h\varphi(x_i, y_i, h), \quad i = 0, 1, \cdots n-1, \\ y_0 = \eta. \end{cases} \tag{3.1}$$

定理 3.1

设 $y(x)$ 是微分方程 (0.1) 的解, $\{y_i\}_{i=0}^{n}$ 为单步显式公式 (3.1) 的解. 如果

1. 存在常数 $c_0 > 0$, 使得 $|R_{i+1}| \le c_0 h^{p+1}, \quad i = 0, 1, \cdots, n-1,$
2. 存在 $h_0 > 0$, $L > 0$, 使得 $\max\limits_{\substack{(x,y)\in D_\delta \\ 0\le h\le h_0}} \left|\frac{\partial\varphi(x,y,h)}{\partial y}\right| \le L.$

则当 $h \le \min\left\{h_0, \sqrt[p]{\frac{\delta}{c}}\right\}$ 时, 有

$$E(h) \le ch^p.$$

其中 $D_\delta = \{(x, y) \mid a \le x \le b, y(x) - \delta \le y \le y(x) + \delta\}$, $c = \frac{c_0}{L}\left[e^{L(b-a)} - 1\right]$.

3.2 稳定性

定义 3.1

对于初值问题 (0.1)，设 $\{y_i\}_{i=0}^n$ 是由单步法 (3.1) 得到的的近似解，$\{z_i\}_{i=0}^n$ 是 (3.1) 扰动后的解，即满足

$$\begin{cases} z_{i+1} = z_i + h[\varphi(x_i, y_i, h) + \delta_{i+1}], \quad i = 0, 1, \cdots n-1, \\ z_0 = \eta + \delta_0, \end{cases} \tag{3.2}$$

如果存在正常数 C, ε_0, h_0，使得对所有 $\varepsilon \in (0, \varepsilon_0]$，$h \in (0, h_0]$，当 $\max\limits_{0\le i\le n} |\delta_i| \le \varepsilon$ 时，有

$$\max_{0\le i\le n} |y_i - z_i| \le C\varepsilon,$$

则称单步法 (3.1) 稳定.

定理 3.2

在定理 3.1 的条件下，单步公式 (3.1) 是稳定的.

一般的线性 k 步方法为

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}). \tag{4.1}$$

其中 a_{k-1}, b_{k-1} 不同时为零. 当 $b_{-1} = 0$ 时为显式公式; 当 $b_{-1} \neq 0$ 时为隐式公式.

定义 4.1

称

$$R_{i+1} = y(x_{i+1}) - \left[\sum_{j=0}^{k-1} a_j y(x_{i-j}) + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y(x_{i-j})) \right]$$

为 k 步公式 (4.1) 在点 x_{i+1} 处的局部截断误差. 当

$$R_{i+1} = O(h^{p+1})$$

时, 称 (4.1) 是 p 阶公式.

定义 4.2

称

$$R_{i+1} = y(x_{i+1}) - \left[\sum_{j=0}^{k-1} a_j y(x_{i-j}) + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y(x_{i-j})) \right]$$

为 k 步公式 (4.1) 在点 x_{i+1} 处的局部截断误差. 当

$$R_{i+1} = O(h^{p+1})$$

时, 称 (4.1) 是 p 阶公式.

4.1 基于积分的构造方法 —-Adams 公式

将方程 $y'(x) = f(x, y(x))$ 在 $[x_i, x_{i+1}]$ 上积分，得

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))\,dx. \tag{4.2}$$

(1) Adams 显式公式

作 $f(x, y(x))$ 以 $x_i, x_{i-1}, \cdots, x_{i-r}$ 为插值节点的 r 次 Lagrange 插值多项式 $L_{i,r}(x)$，有

$$L_{i,r}(x) = \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j}))\,l_{i-j}(x) = \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=0\\ l\neq j}}^{r} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}.$$

我们有

$$\begin{aligned} f(x, y(x)) =& L_{i,r}(x) + R_{i,r}(x) = L_{i,r}(x) + \frac{1}{(r+1)!}\frac{d^{r+1} f(x, y(x))}{dx^{r+1}}\Big|_{x=\eta_i} \prod_{j=0}^{r}(x - x_{i-j}) \\ =& L_{i,r}(x) + \frac{1}{(r+1)!} y^{(r+2)}(\eta_i) \prod_{j=0}^{r}(x - x_{i-j}). \end{aligned}$$

将上式代入 (4.2) 得

$$\begin{aligned}
y(x_{i+1}) =& y(x_i) + \int_{x_i}^{x_{i+1}} L_{i,r}(x)\,dx + \int_{x_i}^{x_{i+1}} R_{i,r}(x)\,dx \\
=& y(x_i) + \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=0\\ l\neq j}}^{r} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}\,dx \\
&+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)}(\eta_i) \prod_{j=0}^{r} (x - x_{i-j})\,dx \\
=& y(x_i) + h\sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{\substack{l=0\\ l\neq j}}^{r} \frac{l+t}{l-j}\,dt \quad (\text{令} x = x_i + th) \\
&+ h^{r+2} y^{(r+2)}(\xi_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^{r} (j+t)\,dt. \quad (\text{积分中值定理})
\end{aligned}$$

其中 $\xi_i \in (x_{i-r}, x_{i+1})$.

记

$$\beta_{rj} = \int_0^1 \prod_{\substack{l=0 \\ l \neq j}}^{r} \frac{l+t}{l-j} dt, \quad j = 0, 1, \cdots, r,$$

$$\alpha_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^{r} (j+t)\, dt,$$

则

$$y(x_{i+1}) = y(x_i) + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) + \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i). \tag{4.3}$$

忽略 $\alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i)$, 并用 y_{i-j} 代替 $y(x_{i-j})$ 得 $(r+1)$ 步 Adams 显式公式:

$$y_{i+1} = y_i + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y_{i-j}). \tag{4.4}$$

(4.4) 的局部截断误差是

$$\begin{aligned} R_{i+1} &= y(x_{i+1}) - \left[y(x_i) + h\sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) \right] \\ &= \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i). \end{aligned}$$

故 (4.4) 是 $(r+1)$ 步、$(r+1)$ 阶显式的 Adams 公式.
(a) $r=0$, 得 Euler 公式

$$\begin{aligned} y_{i+1} &= y_i + hf(x_i, y_i), \\ R_{i+1} &= \frac{1}{2} h^2 y''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}). \end{aligned}$$

(b) $r=1$, 得

$$\begin{aligned} y_{i+1} &= y_i + \frac{h}{2}[3f(x_i, y_i) - f(x_{i-1}, y_{i-1})], \\ R_{i+1} &= \frac{5}{12} h^3 y^{(3)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1}). \end{aligned}$$

(c) $r = 2$, 得

$$y_{i+1} = y_i + \frac{h}{12}[23f(x_i, y_i) - 16f(x_{i-1}, y_{i_1}) + 5f(x_{i-2}, y_{i-2})],$$
$$R_{i+1} = \frac{3}{8}h^4 y^{(4)}(\xi_i), \quad \xi_i \in (x_{i-2}, x_{i+1}).$$

(d) $r = 3$, 得

$$y_{i+1} = y_i + \frac{h}{24}[55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2}) - 9f(x_{i-3}, y_{i-3})],$$
$$R_{i+1} = \frac{251}{720}h^5 y^{(5)}(\xi_i), \quad \xi_i \in (x_{i-3}, x_{i+1}).$$

(2) Admas 隐式公式

作 $f(x, y(x))$ 以 $x_{i+1}, x_i, x_{i-1}, \cdots, x_{i-r+1}$ 为插值节点的 r 次 Lagrange 插值多项式 $L_{i,r}(x)$，有

$$L_{i,r}(x) = \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j}))l_{i-j}(x) = \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=-1 \\ l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}.$$

我们有

$$\begin{aligned} f(x, y(x)) =& L_{i,r}(x) + R_{i,r}(x) \\ =& L_{i,r}(x) + \frac{1}{(r+1)!} \frac{d^{r+1} f(x, y(x))}{dx^{r+1}}\Big|_{x=\eta_i} \prod_{j=-1}^{r-1} (x - x_{i-j}) \\ =& L_{i,r}(x) + \frac{1}{(r+1)!} y^{(r+2)}(\bar{\eta}_i) \prod_{j=-1}^{r-1} (x - x_{i-j}). \end{aligned}$$

将上式代入 (4.2) 得

$$
\begin{aligned}
y(x_{i+1}) =& y_(x_i) + \int_{x_i}^{x_{i+1}} L_{i,r}(x)\,dx + \int_{x_i}^{x_{i+1}} R_{i,r}(x)\,dx \\
=& \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=-1 \\ l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}\,dx \\
&+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)}(\bar{\eta}_i) \prod_{j=-1}^{r-1} (x - x_{i-j})\,dx \\
=& y(x_i) + h \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{\substack{l=-1 \\ l\neq j}}^{r-1} \frac{l+t}{l-j}\,dt \quad (\text{令} x = x_i + th) \\
&+ h^{r+2} y^{(r+2)}(\bar{\xi}_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{r-1} (j+t)\,dt. \quad (\text{积分中值定理})
\end{aligned}
$$

其中 $\bar{\xi}_i \in (x_{i-r+1}, x_{i+1})$.

$$\bar{\beta}_{rj} = \int_0^1 \prod_{\substack{l=-1 \\ l\neq j}}^{r-1} \frac{l+t}{l-j} dt, \quad j = 0, 1, \cdots, r,$$

$$\bar{\alpha}_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{r-1} (j+t) dt,$$

则

$$y(x_{i+1}) = y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) + \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i). \tag{4.5}$$

忽略 $\bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\xi_i)$, 并用 y_{i-j} 代替 $y(x_{i-j})$ 得 r 步 Adams 隐式公式:

$$y_{i+1} = y_i + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y_{i-j}). \tag{4.6}$$

(4.6) 的局部截断误差是

$$
\begin{aligned}
R_{i+1} &= y(x_{i+1}) - \left[y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) \right] \\
&= \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i).
\end{aligned}
$$

故 (4.6) 是 r 步、$(r+1)$ 阶隐式的 Adams 公式.
(a) $r=1$, 得梯形公式

$$
y_{i+1} = y_i + \frac{h}{2}[f(x_{i+1}, y_{i+1}) + f(x_i, y_i)],
$$

$$
R_{i+1} = -\frac{1}{12} h^3 y'''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}).
$$

(b) $r=2$, 得

$$
\begin{aligned}
y_{i+1} &= y_i + \frac{h}{12}[5f(x_{i+1}, y_{i+1}) + 8f(x_i, y_i) - f(x_{i-1}, y_{i-1})], \\
R_{i+1} &= -\frac{1}{24}h^4 y^{(4)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1}).
\end{aligned}
$$

(c) $r=3$, 得

$$
\begin{aligned}
y_{i+1} &= y_i + \frac{h}{24}[9f(x_{i+1}, y_{i+1}) + 19f(x_i, y_i) - f(x_{i-1}, y_{i-1}) + f(x_{i-2}, y_{i-2})], \\
R_{i+1} &= -\frac{19}{720}h^5 y^{(5)}(\xi_i), \quad \xi_i \in (x_{i-2}, x_{i+1}).
\end{aligned}
$$

(3) Admas 预测校正方法

将同阶的显式 Admas 公式和隐式 Admas 公式结合起来，组成预测校正公式. 如将 2 阶显式 Admas 公式和 2 阶隐式 Asmas 公式结合起来，得下面的预测校正公式:

$$\begin{cases} y_{i+1}^{(p)} = y_i + \dfrac{h}{2}[3f(x_i, y_i) - f(x_{i-1}, y_{i-1})], \\ y_{i+1} = y_i + \dfrac{h}{2}[f(x_{i+1}, y_{i+1}^{(p)}) + f(x_i, y_i)]. \end{cases}$$

又如将 4 阶显式 Admas 公式和 4 阶隐式 Admas 公式组成下面的预测校正公式:

$$\begin{cases} y_{i+1}^{(p)} = y_i + \dfrac{h}{24}[55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2}) - 9f(x_{i-3}, y_{i-3})], \\ y_{i+1} = y_i + \dfrac{h}{24}\left[9f(x_{i+1}, y_{i+1}^{(p)}) + 19f(x_i, y_i) - 5f(x_{i-1}, y_{i-1}) + f(x_{i-2}, y_{i-2})\right]. \end{cases}$$

4.2 基于 Taylor 展开的待定系数法

要构造下面的线性 k 步方法

$$y_{i+1}=\sum_{j=0}^{k-1}a_jy_{i-j}+h\sum_{j=-1}^{k-1}b_jf(x_{i-j},y_{i-j}). \tag{4.7}$$

求系数 a_j, b_j, 使公式具有一定的阶数. 局部截断误差为:

$$R_{i+1}=y(x_{i+1})-\left[\sum_{j=0}^{k-1}a_jy(x_{i-j})+h\sum_{j=-1}^{k-1}b_jf(x_{i-j},y(x_{i-j}))\right]$$

利用方程 (0.1) 和 Taylor 展开得

$$
\begin{aligned}
R_{i+1} =& y(x_{i+1}) - \sum_{j=0}^{k-1} a_j y(x_{i-j}) - h \sum_{j=-1}^{k-1} b_j y'(x_{i-j}) \\
=& \sum_{l=0}^{p+1} \frac{1}{l!} y^{(l)}(x_i) h^l + O(h^{p+2}) - \sum_{j=0}^{k-1} a_j \left[\sum_{l=0}^{p+1} \frac{1}{l!} y^{(l)}(x_i)(-jh)^l + O(h^{p+2}) \right] \\
& - h \sum_{j=-1}^{k-1} \left[b_j \sum_{l=0}^{p} \frac{1}{l!} y^{(l+1)}(x_i)(-jh)^l + O(h^{p+1}) \right] \\
=& \Big(1 - \sum_{j=0}^{k-1} a_j\Big) y(x_i) + \sum_{l=1}^{p+1} \frac{1}{l!} \left[1 - \sum_{j=0}^{k-1} (-j)^l a_j - l \sum_{j=-1}^{k-1} (-j)^{l-1} b_j \right] h^l y^{(l)}(x_i) + O(h^{p+2}).
\end{aligned}
$$

要使公式 (4.7) 为 p 阶，则

$$1-\sum_{j=0}^{k-1} a_j = 0$$

$$1-\sum_{j=0}^{k-1}(-j)^l a_j - l\sum_{j=-1}^{k-1}(-j)^{l-1} b_j = 0, \quad l = 1, 2\cdots, p.$$

这时局部截断误差为

$$R_{i+1} = \frac{1}{(p+1)!}\left[1-\sum_{j=0}^{k-1}(-j)^{p+1} a_j - (p+1)\sum_{j=-1}^{k-1}(-j)^p b_j\right] h^{p+1} y^{(p+1)}(x_i) + O(h^{p+2}).$$

例 4.1

给定微分方程初值问题

$$\begin{cases} y'(x) = f(x, y(x)), \quad a \le x \le b, \\ y(a) = \eta, \end{cases}$$

取正整数 n, 并记 $h = (b-a)/n$, $x_i = a + ih$, $0 \le i \le n$. 试确定两步公式

$$y_{i+1} = \alpha y_{i-1} + h\Big[\beta_0 f(x_{i+1}, y_{i+1}) + \beta_1 f(x_i, y_i) + \beta_2 f(x_{i-1}, y_{i-1})\Big]$$

中的参数 $\alpha, \beta_0, \beta_1, \beta_2$, 使其具有尽可能高的精度, 并指出能达到的阶数.

解 局部截断误差为

$$
\begin{aligned}
R_{i+1} =& y(x_{i+1}) - \alpha y(x_{i-1}) - h[\beta_0 f(x_{i+1}, y(x_{i+1})) + \beta_1 bf(x_i, y(x_i)) + \beta_2 f(x_{i-1}, y(x_{i-1}))] \\
=& y(x_{i+1}) - \alpha y(x_{i-1}) - \beta_0 hy'(x_{i+1}) - \beta_1 hy'(x_i) - \beta_2 hy'(x_{i-1}) \\
=& y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \frac{h^3}{3!}y'''(x_i) + \frac{h^4}{4!}y^{(4)}(x_i) + \frac{h^5}{5!}y^{(5)}(x_i) + O(h^6) \\
&- \alpha\Big[y(x_i) - hy'(x_i) + \frac{h^2}{2}y''(x_i) - \frac{h^3}{3!}y'''(x_i) + \frac{h^4}{4!}y^{(4)}(x_i) - \frac{h^5}{5!}y^{(5)}(x_i) + O(h^6)\Big] \\
&- \beta_0 h\Big[y'(x_i) + hy''(x_i) + \frac{h^2}{2}y'''(x_i) + \frac{h^3}{3!}y^{(4)}(x_i) + \frac{h^4}{4!}y^{(5)}(x_i) + O(h^5)\Big] - \beta_1 hy'(x_i) \\
&- \beta_2 h\Big[y'(x_i) - hy''(x_i) + \frac{h^2}{2}y'''(x_i) - \frac{h^3}{3!}y^{(4)}(x_i) + \frac{h^4}{4!}y^{(5)}(x_i) + O(h^5)\Big] \\
=& (1-\alpha)y(x_i) + (1+\alpha-\beta_0-\beta_1-\beta_2)hy'(x_i) + \left(\frac{1}{2} - \frac{\alpha}{2} - \beta_0 + \beta_2\right)h^2y''(x_i) \\
&+ \left(\frac{1}{6} + \frac{\alpha}{6} - \frac{\beta_0}{2} - \frac{\beta_2}{2}\right)h^3y'''(x_i) + \left(\frac{1}{24} - \frac{\alpha}{24} - \frac{\beta_0}{6} + \frac{\beta_2}{6}\right)h^4y^{(4)}(x_i) \\
&+ \left(\frac{1}{120} + \frac{\alpha}{120} - \frac{\beta_0}{24} - \frac{\beta_2}{24}\right)h^5y^{(5)}(x_i) + O(h^6).
\end{aligned}
$$

要使公式精度尽量高，则

$$
\begin{aligned}
&1-\alpha=0\\
&1+\alpha-\beta_0-\beta_1-\beta_2=0\\
&\frac{1}{2}-\frac{\alpha}{2}-\beta_0+\beta_2=0\\
&\frac{1}{6}+\frac{\alpha}{6}-\frac{\beta_0}{2}-\frac{\beta_2}{2}=0
\end{aligned}
$$

解得 $\alpha=1,\beta_0=\frac{1}{3},\beta_1=\frac{4}{3},\beta_2=\frac{1}{3}$. 此时局部截断误差为

$$
R_{i+1}=-\frac{1}{90}h^5y^{(5)}(x_i)+O(h^6).
$$

所以该公式是 4 阶公式.