第六章 常微分方程数值解

本章主要内容

- Euler公式, 后退的Euler公式, 梯形公式, 改进的Euler公式, 局部截断误差和阶数
- Runge－Kutta方法
- 单步法的收敛性和稳定性
- 线性多步法(Admas显式和隐式公式, 基于Taylor展开的线性多步法的构造)

本章讨论一阶常微分方程初值问题的数值解

$$\begin{cases} y' = f(x,y), \quad a \le x \le b, \\ y(a) = \eta. \end{cases} \tag{1}$$

假设

1) $f(x,y), \dfrac{\partial f(x,y)}{\partial y}$连续.

2) (1)存在唯一解$y(x)$且在$[a,b]$上充分光滑.

将$[a,b]$作n等分, 记$h=(b-a)/n$, $x_i = a + ih$, $(i=0,1,\cdots,n)$. 称h为步长. 所谓(1)的数值解, 是求初值问题(1)的解$y(x)$在离散点$x_i(i=0,1,\cdots)$处的近似值y_i.

在计算y_{i+1}时, 如果只用到前一步的值y_i, 称这类方法为单步法. 如果计算y_{i+1}时需用到前r步的值$y_i, y_{i-1}, \cdots, y_{i-r+1}$, 称这类方法是$r$步方法.

1 Euler公式

1.1 Euler公式

将方程(1)两边在$[x_i, x_{i+1}]$积分

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

得到

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))dx. \tag{2}$$

应用左矩形公式近似右端积分得

$$y(x_{i+1}) = y(x_i) + hf(x_i, y(x_i)) + R_{i+1}^{(1)},$$

其中

$$R_{i+1}^{(1)} = \frac{1}{2}\frac{df(x, y(x))}{dx}\Big|_{x=\xi_i} h^2 = \frac{1}{2}y''(\xi_i)h^2, \quad \xi_i \in (x_i, x_{i+1}),$$

上式中忽略$R_{i+1}^{(1)}$有

$$y(x_{i+1}) \approx y(x_i) + hf(x_i, y(x_i)), \quad 0 \le i \le n-1. \tag{3}$$

由初值条件有

$$y(x_0)=\eta\equiv y_0.$$

代入(3) 可得

$$y(x_1)\approx y(x_0)+hf(x_0,y(x_0))=y_0+hf(x_0,y_0). \tag{4}$$

一般地，若已知$y(x_i)$的近似值y_i,由(3)可得

$$y(x_{i+1})\quad\approx y(x_i)+hf(x_i,y(x_i))\approx y_i+hf(x_i,y_i)\equiv y_{i+1}. \tag{5}$$

综合(4)-(5)，得到

$$y_{i+1}=y_i+hf(x_i,y_i),\quad i=0,1,\cdots,n-1. \tag{6}$$

称(6)为Euler公式.由上式可依次得到

$$y_i,\quad 0\le i\le n.$$

将y_i作为$y(x_i)$的近似值.
Euler公式是一个单步显式公式.

一般的单步显式公式为

$$y_{i+1} = y_i + h\varphi(x_i, y_i, h), \tag{7}$$
$$y_0 = \eta. \tag{8}$$

$\varphi(x, y, h)$称为增量函数.

定义 1 *称*

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), h)]$$

为单步显式公式(7)在点x_{i+1}处的局部截断误差.

由上述定义, Euler公式(6)的局部截断误差为

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + hf(x_i, y(x_i))] = \frac{1}{2}h^2 y''(\xi_i),$$
$$\xi_i \in (x_i, x_{i+1}).$$

1.2 后退的Euler公式

(2)中的积分用右矩形公式近似得

$$y(x_{i+1}) = y(x_i) + hf(x_{i+1}, y(x_{i+1})) + R_{i+1}^{(2)},$$

其中

$$R_{i+1}^{(2)} = -\frac{h^2}{2}\frac{df(x, y(x))}{dx}\Big|_{x=\xi_i} = -\frac{h^2}{2}y''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}).$$

从而有

$$y(x_{i+1}) \approx y(x_i) + hf(x_{i+1}, y(x_{i+1})) \approx y_i + hf(x_{i+1}, y_{i+1}),$$

得后退的Euler公式为

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}), \quad , i = 0, 1, \cdots, n-1. \tag{9}$$

后退的Euler公式是单步隐式公式.

一般的单步隐式公式为

$$y_{i+1} = y_i + h\psi(x_i, y_i, y_{i+1}, h), \quad i = 0, 1, \cdots, n-1 \tag{10}$$

$$y_0 = \eta. \tag{11}$$

其中$\psi(x_i, y_i, y_{i+1}, h)$称为增量函数.

定义 2 *称*

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\psi(x_i, y(x_i), y(x_{i+1}), h)]$$

为单步隐式公式(10)的局部截断误差.

由定义2, 后退的Euler公式的局部截断误差为

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

1.3 梯形公式

将(2)中积分用梯形公式近似得

$$y(x_{i+1}) = y(x_i) + \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] + R_{i+1}^{(3)},$$

其中

$$\begin{aligned} R_{i+1}^{(3)} &= -\frac{h^3}{12}\frac{d^2 f(x, y(x))}{dx^2}\Big|_{x=\xi_i} \\ &= -\frac{1}{12}y'''(\xi_i)h^3, \quad \xi_i \in (x_i, x_{i+1}). \end{aligned}$$

略去$R_{i+1}^{(3)}$得

$$\begin{aligned} y(x_{i+1}) &\approx y(x_i) + \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] \\ &\approx y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1})], \end{aligned}$$

所以得梯形公式

$$y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1})],\ i = 0, 1, \cdots, n-1. \quad (12)$$

它是一个单步隐式公式. 由单步隐式公式局部截断误差的定义得梯形公式的局部截断误差为

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

1.4 改进的Euler公式

预测校正公式

$$\begin{cases} y_{i+1}^{(p)} = y_i + hf(x_i, y_i) & \text{预测公式} \\ y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1}^{(p)})] & \text{校正公式} \end{cases}$$

称上式为改进的Euler公式. 它是单步显式公式. 也可将上式写为如下两种形式

$$\begin{cases} y_{i+1}^{(p)} = y_i + hf(x_i, y_i) \\ y_{i+1}^{(c)} = y_i + hf(x_{i+1}, y_{i+1}^{(p)}) \\ y_{i+1} = \frac{1}{2}(y_{i+1}^{(p)} + y_{i+1}^{(c)}) \end{cases}$$

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

其局部截断误差为

$$\begin{aligned} R_{i+1} &= y(x_{i+1}) \\ &\quad - \left\{ y(x_i) + \frac{h}{2}\Big[f(x_i, y(x_i)) + f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))\Big] \right\}. \end{aligned}$$

用两种方法求上面的局部截断误差.

法一

$$
\begin{aligned}
&R_{i+1}\\
&=y(x_{i+1})-y(x_i)-\frac{h}{2}[f(x_i,y(x_i))+f(x_{i+1},y(x_{i+1}))]\\
&+\frac{h}{2}[f(x_{i+1},y(x_{i+1}))-f(x_{i+1},y(x_i)+hf(x_i,y(x_i)))]\\
&=-\frac{1}{12}y'''(\xi_i)h^3+\frac{h}{2}\frac{\partial f(x_{i+1},\eta_{i+1})}{\partial y}[y(x_{i+1})-y(x_i)-hf(x_i,y(x_i))]\\
&=-\frac{1}{12}y'''(\xi_i)h^3+\frac{h}{2}\times\frac{1}{2}\frac{\partial f(x_{i+1},\eta_{i+1})}{\partial y}y''(\tilde{\xi}_i)h^2\\
&=\left[-\frac{1}{12}y'''(\xi_i)+\frac{1}{4}\frac{\partial f(x_{i+1},\eta_{i+1})}{\partial y}y''(\tilde{\xi}_i)\right]h^3,\quad \xi_i,\tilde{\eta}_i\in(x_i,x_{i+1}).
\end{aligned}
$$

法二 将$y(x_{i+1})$在x_i点Taylor展开, 将$f(x_{i+1}, y(x_i)+hf(x_i, y(x_i)))$在$(x_i, y(x_i))$ 点Taylor展开

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{1}{2!}h^2y''(x_i) + \frac{1}{3!}h^3y'''(x_i) + O(h^4),$$

$$\begin{aligned}
& f(x_{i+1}, y(x_i) + hf(x_i, y(x_i))) = f(x_i + h, y(x_i) + hf(x_i, y(x_i))) \\
& = f(x_i, y(x_i)) + h\frac{\partial f}{\partial x}(x_i, y(x_i)) + hf(x_i, y(x_i))\frac{\partial f}{\partial y}(x_i, y(x_i)) \\
& + \frac{1}{2!}\Big[h^2\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) \\
& \quad + 2h^2 f(x_i, y(x_i))\frac{\partial^2 f}{\partial x \partial y}(x_i, y(x_i)) \\
& + h^2(f(x_i, y(x_i)))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))\Big] + O(h^3) \\
& = y'(x_i) + hy''(x_i) + \frac{1}{2}h^2\left(y'''(x_i) - y''(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))\right) + O(h^3).
\end{aligned}$$

将上面2式代入误差式并利用$y(x)$及其导数和$f(x, y(x))$的关系

$$\begin{aligned}
R_{i+1} &= y(x_i) + hy'(x_i) + \frac{1}{2!}h^2y''(x_i) + \frac{1}{3!}h^3y'''(x_i) + O(h^4) \\
&\quad -y(x_i) - \frac{1}{2}hy'(x_i) \\
&\quad -\frac{1}{2}h\left[y'(x_i) + hy''(x_i) + \frac{1}{2}h^2\left(y'''(x_i) - y''(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))\right) + O(h^3)\right] \\
&= \left[-\frac{1}{12}y'''(x_i) + \frac{1}{4}y''(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))\right]h^3 + O(h^4).
\end{aligned}$$

定义 3 *如果一个求解公式的局部截断误差为*$R_{i+1} = O(h^{p+1})$, *则称该公式是p阶的, 或具有p阶精度.*

根据这定义, Euler公式、后退的Euler公式是1阶的, 梯形公式和改进的Euler公式是2阶的.

2 Runge-Kutta方法

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

$$\begin{cases} y_{i+1} = y_i + h\sum\limits_{j=1}^{r} \alpha_j k_j \\ k_1 = f(x_i, y_i) \\ k_j = f\left(x_i + \lambda_j h, y_i + h\sum\limits_{l=1}^{j-1} \mu_{jl} k_l\right), \quad j = 2, 3, \cdots, r. \end{cases} \tag{13}$$

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(13)是$p$阶的.

2.2 2阶Runge-Kutta公式

2阶Runge-Kutta公式一般形式为

$$\begin{cases} y_{i+1} = y_i + h(\alpha_1 k_1 + \alpha_2 k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \lambda_2 h, y_i + h\mu_{21} k_1) \end{cases}. \tag{14}$$

其局部截断误差是

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

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{1}{2}h^2y''(x_i) + \frac{1}{3!}h^3y'''(x_i) + O(h^4)$$

$$= y(x_i) + hy'(x_i) + \frac{1}{2}h^2\left[\frac{\partial f}{\partial x}(x_i, y(x_i))\right.$$

$$\left.+y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))\right] + \frac{h^3}{6}y'''(x_i) + O(h^4)$$

$$K_1 = y'(x_i),$$

$$K_2 = f(x_i, y(x_i)) + \lambda_2 h\frac{\partial f}{\partial x}(x_i, y(x_i)) + h\mu_{21}y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))$$

$$+\frac{1}{2}\left[(\lambda_2 h)^2\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) + 2\lambda_2\mu_{21}h^2y'(x_i)\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))\right.$$

$$\left.+(\mu_{21}hy'(x_i))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))\right] + O(h^3)$$

将上面3式代入局部截断误差得

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

要使(14)具有2阶精度, 则

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

显然α_2不能为零.

Euler公式
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当$\alpha_2 \neq 0$可解得即

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

于是我们可以得到一类2阶Runge-Kutta公式

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

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

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

若$\alpha_2 = \frac{3}{4}$, 则得

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

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 单步法的收敛性和稳定性

3.1 收敛性

定义 4 *设$\{y(x_i)\}_{i=1}^n$是微分方程(1)的解, $\{y_i^{[h]}\}_{i=1}^n$是用某种数值方法得到的近似解. 则称*

$$E(h) = \max_{1 \le i \le n} \left| y(x_i) - y_i^{[h]} \right|$$

为该方法的整体截断误差. 如果

$$\lim_{h \to 0} E(h) = 0,$$

则称该方法收敛.

考虑单步显式公式

$$\begin{cases} y_{i+1} = y_i + h\varphi(x_i, y_i, h), & i = 0, 1, \cdots n-1, \\ y_0 = \eta. \end{cases} \tag{15}$$

定理 1 设$y(x)$是微分方程(1)的解, $\{y_i\}_{i=0}^{n}$为单步显式公式(15)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

$$\max_{\substack{(x,y)\in D_\delta \\ 0\le h\le h_0}} \left|\frac{\partial\varphi(x,y,h)}{\partial y}\right| \le L.$$

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 5 *对于初值问题(1), 设$\{y_i\}_{i=0}^n$是由单步法(15)得到的的近似解, $\{z_i\}_{i=0}^n$ 是(15)扰动后的解, 即满足*

$$\begin{cases} z_{i+1} = z_i + h[\varphi(x_i, y_i, h) + \delta_{i+1}], \quad i = 0, 1, \cdots n-1, \\ z_0 = \eta + \delta_0, \end{cases} \tag{16}$$

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(15)稳定.

定理 2 *在定理1的条件下, 单步公式(15)是稳定的.*

4 线性多步法

一般的线性k步方法为

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}). \tag{17}$$

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 6 *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(17)在点x_{i+1}处的局部截断误差. 当

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

时, 称(17)是p阶公式.

定义 7 *如果线性k步公式(17)至少是1阶的, 则称是相容的; 如果是p($p \geq 1$)阶的, 则称是p阶相容的.*

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

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

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 $L_r(x)$, 有

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

我们有

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

将上式代入(18)得

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

$$= \quad y(x_i) + \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=0\\ l\neq j}}^{r} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}} dx$$

$$+\frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)}(\eta_i) \prod_{j=0}^{r} (x - x_{i-j}) dx$$

$$= \quad y(x_i) + h \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{\substack{l=0\\ l\neq j}}^{r} \frac{l+t}{l-j} dt \quad (\text{令} x = x_i + th)$$

$$+h^{r+2} y^{(r+2)}(\xi_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^{r} (j+t) dt. \quad (\text{积分中值定理})$$

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

$$\begin{aligned} y(x_{i+1}) = \quad & y(x_i) + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) \\ & + \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i). \end{aligned} \tag{18}$$

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:

$$y_{i+1} = y_i + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y_{i-j}). \tag{19}$$

(19)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(19)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

$$y_{i+1}=y_i+\frac{h}{12}[23f(x_i,y_i)-16f(x_{i-1},y_{i_1})+5f(x_{i-2},y_{i-2})],$$

$$R_{i+1}=\frac{3}{8}h^4y^{(4)}(\xi_i),\quad \xi_i\in(x_{i-2},x_{i+1}).$$

(d) $r=3$, 得

$$\begin{aligned}y_{i+1}=y_i+\frac{h}{24}[&55f(x_i,y_i)-59f(x_{i-1},y_{i-1})\\&+37f(x_{i-2},y_{i-2})-9f(x_{i-3},y_{i-3})],\end{aligned}$$

$$R_{i+1}=\frac{251}{720}h^5y^{(5)}(\xi_i),\quad \xi_i\in(x_{i-3},x_{i+1}).$$

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$L_r(x)$, 有

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

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(18)得

$$y(x_{i+1}) = y_{(}x_i) + \int_{x_i}^{x_{i+1}} L_{i,r}(x)dx + \int_{x_i}^{x_{i+1}} R_{i,r}(x)dx$$

$$= \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=-1\\ l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}} dx$$

$$+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)}(\bar{\eta}_i) \prod_{j=-1}^{r-1} (x - x_{i-j}) dx$$

$$= y(x_i) + h \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{\substack{l=-1\\ l\neq j}}^{r-1} \frac{l+t}{l-j} dt \quad (\text{令} x = x_i + th)$$

$$+ h^{r+2} y^{(r+2)}(\bar{\xi}_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{r-1} (j+t) dt. \quad (\text{积分中值定理})$$

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

$$\begin{aligned} y(x_{i+1}) &= y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) \\ &\quad + \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i). \end{aligned} \tag{20}$$

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:

$$y_{i+1} = y_i + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y_{i-j}). \tag{21}$$

(21)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(21)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

$$y_{i+1} = y_i + \frac{h}{12}[5f(x_{i+1}, y_{i+1}) + 8f(x_i, y_i) - f(x_{i-1}, y_{i-1})],$$

$$R_{i+1} = -\frac{1}{24}h^4 y^{(4)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1}).$$

(c) $r=3$, 得

$$R_{i+1} = -\frac{19}{720}h^5 y^{(5)}(\xi_i), \quad \xi_i \in (x_{i-2}, x_{i+1}).$$

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:

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

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:

$$\begin{aligned} y_{i+1}^{(p)} = y_i + \frac{h}{24}[&55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2}) \\ &-9f(x_{i-3}, y_{i-3})], \end{aligned}$$
$$\begin{aligned} y_{i+1} = y_i + \frac{h}{24}\Big[&9f(x_{i+1}, y_{i+1}^{(p)}) + 19f(x_i, y_i) \\ &-5f(x_{i-1}, y_{i_1}) + f(x_{i-2}, y_{i-2})\Big]. \end{aligned}$$

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

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}). \qquad (22)$$

求系数a_j, b_j, 使公式具有一定的阶数. 局部截断误差为:

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

利用方程(1)和Taylor展开得

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

要使公式(22)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 1 *给定微分方程初值问题*

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

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

$$\begin{aligned}R_{i+1}&=y(x_{i+1})-\alpha y(x_{i-1})-h[\beta_0 f(x_{i+1},y(x_{i+1}))\\&\quad+\beta_1 bf(x_i,y(x_i))+\beta_2 f(x_{i-1},y(x_{i-1}))]\\&=y(x_{i+1})-\alpha y(x_{i-1})-\beta_0 hy'(x_{i+1})-\beta_1 hy'(x_i)-\beta_2 hy'(x_{i-1})\end{aligned}$$

$$
\begin{aligned}
&= y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \frac{h^3}{3!}y'''(x_i) + \frac{h^4}{4!}y^{(4)}(x_i)\\
&+\frac{h^5}{5!}y^{(5)}(x_i) + O(h^6)\\
&-\alpha\Big[y(x_i) - hy'(x_i) + \frac{h^2}{2}y''(x_i) - \frac{h^3}{3!}y'''(x_i) + \frac{h^4}{4!}y^{(4)}(x_i)\\
&-\frac{h^5}{5!}y^{(5)}(x_i) + O(h^6)\Big]\\
&-\beta_0 h\Big[y'(x_i) + hy''(x_i) + \frac{h^2}{2}y'''(x_i) + \frac{h^3}{3!}y^{(4)}(x_i)\\
&+\frac{h^4}{4!}y^{(5)}(x_i) + O(h^5)\Big] - \beta_1 hy'(x_i)\\
&-\beta_2 h\Big[y'(x_i) - hy''(x_i) + \frac{h^2}{2}y'''(x_i) - \frac{h^3}{3!}y^{(4)}(x_i)\\
&+\frac{h^4}{4!}y^{(5)}(x_i) + O(h^5)\Big]
\end{aligned}
$$

$$
\begin{aligned}
= \quad & (1-\alpha)y(x_i) + (1+\alpha-\beta_0-\beta_1-\beta_2)hy'(x_i) \\
& +\Big(\frac{1}{2}-\frac{\alpha}{2}-\beta_0+\beta_2\Big)h^2y''(x_i) \\
& +\Big(\frac{1}{6}+\frac{\alpha}{6}-\frac{\beta_0}{2}-\frac{\beta_2}{2}\Big)h^3y'''(x_i) + \left(\frac{1}{24}-\frac{\alpha}{24}-\frac{\beta_0}{6}+\frac{\beta_2}{6}\right)h^4y^{(4)}(x_i) \\
& +\left(\frac{1}{120}+\frac{\alpha}{120}-\frac{\beta_0}{24}-\frac{\beta_2}{24}\right)h^5y^{(5)}(x_i)+O(h^6).
\end{aligned}
$$

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.

5 习 题

p.305-307

§6.2　　1, 3, 4

§6.3　5(1), 6

§6.5　7, 8, 10, 11, 12.

上机题　23

数值积分公式

左矩形公式

$$\int_a^b g(x)dx = (b-a)g(a) + \frac{(b-a)^2}{2}g'(\xi), \quad \xi \in (a,b).$$

右矩形公式

$$\int_a^b g(x)dx = (b-a)g(b) - \frac{(b-a)^2}{2}g'(\xi), \quad \xi \in (a,b).$$

中矩形公式

$$\int_a^b g(x)dx = (b-a)g\left(\frac{a+b}{2}\right) - \frac{(b-a)^3}{24}g''(\xi), \quad \xi \in (a,b).$$

梯形公式

$$\int_a^b g(x)dx = \frac{b-a}{2}[g(a)+b(b)] - \frac{(b-a)^3}{12}g''(\xi), \quad \xi \in (a,b).$$

一元函数Taylor展开

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y'''(x) + \cdots$$

二元函数Taylor展开

$$f(x+\Delta x, y+\Delta y) = f(x,y) + \frac{\partial f(x,y)}{\partial x}\Delta x + \frac{\partial f(x,y)}{\partial y}\Delta y$$

$$+\frac{1}{2!}\left(\frac{\partial^2 f(x,y)}{\partial x^2}(\Delta x)^2 + 2\frac{\partial^2 f(x,y)}{\partial x \partial y}(\Delta x)(\Delta y) + \frac{\partial^2 f(x,y)}{\partial y^2}(\Delta y)^2\right) + \cdots$$

常用的几个公式

$$
\begin{aligned}
y'(x) &= f(x, y(x)) \\
y''(x) &= \frac{\partial f}{\partial x}(x, y(x)) + y'(x)\frac{\partial f}{\partial y}(x, y(x)) \\
y'''(x) &= \frac{\partial^2 f}{\partial x^2}(x, y(x)) + 2y'(x)\frac{\partial^2 f}{\partial x \partial y}(x, y(x)) \\
&\quad + (y'(x))^2\frac{\partial^2 f}{\partial y^2}(x, y(x)) + y''(x)\frac{\partial f}{\partial y}(x, y(x))
\end{aligned}
$$