I. Compute first five coefficients $C_j's$ of the trapezoidal rule and midpoint rule

Solution:

I-a. trapezoidal rule

$$s=1,\ \alpha_1=1,\ \alpha_0=-1,\ \beta_1=\beta_0=\frac{1}{2}$$

So

$$\begin{aligned}
C_0 &= \alpha_0+\alpha_1=0\\
C_1 &= \alpha_1-(\beta_0+\beta_1)=0\\
C_2 &= \frac{1}{2}\alpha_1-\beta_1=0\\
C_3 &= \frac{1}{6}\alpha_1-\frac{1}{2}\beta_1=-\frac{1}{12}\\
C_4 &= \frac{1}{24}\alpha_1-\frac{1}{6}\beta_1=-\frac{1}{24}
\end{aligned}$$

I-b. midpoint rule

$$s=2,\ \alpha_2=1,\ \alpha_1=0,\ \alpha_0=-1,\ \beta_1=2,\ \beta_0=\beta_2=0$$

So

$$\begin{aligned}
C_0 &= \alpha_0+\alpha_1+\alpha_2=0\\
C_1 &= 2\alpha_2-\beta_1=0\\
C_2 &= \frac{1}{2}2^2\alpha_2-\beta_1=0\\
C_3 &= \frac{1}{6}2^3\alpha_2-\frac{1}{2}\beta_1=\frac{1}{3}\\
C_4 &= \frac{1}{24}2^4\alpha_2-\frac{1}{6}\beta_1=\frac{1}{3}
\end{aligned}$$

II. Express conditions of $\|\mathcal{L}\mathbf{u}(t_n)\|=O(k^3)$using the characteristic polynomials

Solution:

由引理 10.94 可知 $\|\mathcal{L}\mathbf{u}(t_n)\|=O(k^3)$ 的条件是 $C_0=C_1=C_2=0$, 即

$$\begin{aligned}
&\rho(1)=\sum_{j=0}^{s}\alpha_j=0\\
&\rho'(1)=\sum_{j=1}^{s}j\alpha_j=\sum_{j=0}^{s}j\alpha_j=\sum_{j=0}^{s}\beta_j=\sigma(1)\\
&\sigma'(1)=\sum_{j=1}^{s}j\beta_j=\frac{1}{2}\sum_{j=0}j^2\alpha_j=\frac{1}{2}(\sum_{j=2}^{s}j(j-1)\alpha_j+\sum_{j=2}^{s}j\alpha_j+\alpha_1)=\frac{1}{2}(\rho''(1)+\rho'(1))
\end{aligned}$$

综上，条件为 $\rho(1)=1,\ \rho'(1)=\sigma(1),\ \sigma'(1)=\frac{1}{2}(\rho''(1)+\rho'(1))$

III. Derive coefficients of LMMs shown below by the method of undetermined coefficients and a programming language with symbolic computation

Solution:

本题使用 python 的 sympy 符号计算库实现, 代码见`coefficients.py`

安装 sympy(`pip install sympy`) 后运行`python3 coefficients.py`即可得到如下结果

```
Adams-Bashforth formulas
s = 1  p = 1  b1 = 0 {b0: 1}
s = 2  p = 2  b2 = 0 {b0: -1/2, b1: 3/2}
s = 3  p = 3  b3 = 0 {b0: 5/12, b1: -4/3, b2: 23/12}
s = 4  p = 4  b4 = 0 {b0: -3/8, b1: 37/24, b2: -59/24, b3: 55/24}

Adams-Moulton formulas
s = 1  p = 1 {b1: 1}
s = 1  p = 2 {b0: 1/2, b1: 1/2}
s = 2  p = 3 {b0: -1/12, b1: 2/3, b2: 5/12}
s = 3  p = 4 {b0: 1/24, b1: -5/24, b2: 19/24, b3: 3/8}
s = 4  p = 5 {b0: -19/720, b1: 53/360, b2: -11/30, b3: 323/360, b4: 251/720}

Backward differentiation formulas
s = 1  p = 1  a1 = 1 {a0: -1, b1: 1}
s = 2  p = 2  a2 = 1 {a0: 1/3, a1: -4/3, b2: 2/3}
s = 3  p = 3  a3 = 1 {a0: -2/11, a1: 9/11, a2: -18/11, b3: 6/11}
s = 4  p = 4  a4 = 1 {a0: 3/25, a1: -16/25, a2: 36/25, a3: -48/25, b4: 12/25}
```

与讲义中结果一致

其中 Adams-Moulton formulas 中 $s = 1, p = 1$ 的情况结果为 $\beta_1 = 1 - \beta_0$

程序中取 $\beta_0 = 0$ 得到如上结果，即后向欧拉折线

IV. For the third-order BDF, derive its characteristic polynomials and apply Theorem 10.105 to verify that the order of accuracy is indeed 3

Solution:

$$\rho(z) = \sum_{j=0}^{3} \alpha_j z^j = -\frac{2}{11} + \frac{9}{11}z - \frac{18}{11}z^2 + z^3 s,\ \sigma(z) = \sum_{j=0}^{3} \beta_j z^j = \frac{6}{11}z^3$$

将

$$g(z) := \frac{\rho(z)}{\sigma(z)} = \frac{11}{6} - 3\frac{1}{z} + \frac{3}{2}\frac{1}{z^3} - \frac{1}{3}\frac{1}{z^3}$$

在 $z=1$ 处泰勒展开得

$$\begin{aligned}
g(z) &= g(1)+g'(1)(z-1)+\frac{1}{2}g''(1)(z-1)^2-\frac{1}{6}g'''(1)(z-1)^3+\frac{1}{24}g^{(4)}(1)(z-1)^4-\cdots \\
&= (z-1)-\frac{1}{2}(z-1)^2+\frac{1}{3}(z-1)^3-\frac{1}{2}(z-1)^4+\cdots \\
&= \left[(z-1)-\frac{1}{2}(z-1)^2+\frac{1}{3}(z-1)^3-\cdots\right]+\Theta(-\frac{1}{4}(z-1)^4)
\end{aligned}$$

所以 third-order BDF 为 3 阶精度，error constant 为 $-\frac{1}{2}-(-\frac{1}{4})=-\frac{1}{4}$

V. Prove that an s-step LMM has order of accuracy p if and only if, when applied on an ODE $u_t = q(t)$, it gives exact results whenever q is a polynomial of degree < p, but not whenever q is a polynomial of degree p. Assume arbitrary continuous initial condition u_0 and exact numerical initial data $v^0, \cdots, s-1$

Solution:

由引理 10.94 知该问题一步误差为

$$\mathcal{L}\mathbf{u}(t_n) = C_0\mathbf{u}(t_n)+C_1\mathbf{u}_t(t_n)+C_2\mathbf{u}_{tt}(t_n)+\cdots$$

必要性

LMM 具有 p 阶精度，那么

$$\forall j=0,1,2,\cdots,p,\ C_j=0,\ C_{p+1}\neq 0$$

若 $q(t)$ 为任意阶数小于 p 的多项式，有

$$\forall k=p,p+1,\cdots,\ q^{(k)}(t)=0$$

又有 $\mathbf{u}_t = q(t)$, 所以 $\forall k=p,p+1,\cdots,\ \frac{\partial^{k+1}}{\partial t^{k+1}}\mathbf{u}(t)=q^{(k)}(t)=0$

所以此时问题的一步误差 $\mathcal{L}\mathbf{u}(t_n)=0$, 而给定初始条件和数据是准确的，所以解也是准确的

但是若 $q(t)$ 是 p 阶多项式，那么有 $\frac{\partial^{p+1}}{\partial t^{p+1}}\mathbf{u}(t)=q^{(p)}(t)\neq 0$ 且 $C_{p+1}\neq 0$

一步误差不为 0, 那么此时解就不是完全精确的

充分性

设 $q(t)$ 是 $\hat{p}$ 阶多项式，那么

$$\mathcal{L}\mathbf{u}(t_n) = C_0\mathbf{u}(t_n)+\sum_{k=1}^{\hat{p}}C_k\frac{\partial^k}{\partial t^k}\mathbf{u}(t)_n = C_0\mathbf{u}(t_n)+\sum_{k=1}^{\hat{p}}C_k q^{(k-1)}(t_n)$$

因为对任意的 $\hat{p}<p$ 都成立 $\mathcal{L}\mathbf{u}(t_n)=0$

取 $q(t)=0 \Rightarrow C_0=0$

取 $q(t)=1 \Rightarrow C_1=0$

以此类推直到取到 $\hat{p}=p-1$, 就有 $C_0=C_1=C_2=\cdots=C_p=0$

而当 $\hat{p}=p$ 时，$q^{(p)}(t)\neq 0$，又有 $\mathcal{L}\mathbf{u}(t_n)\neq 0 \Rightarrow C_{p+1}\neq 0$

所以此时 s-step LMM 是 p 阶精度

VI. Show that

$$p_M(z) = z^s + \sum_{j=0}^{s-1} \alpha_j z^j$$

is the characteristic polynomial of

$$M = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ -\alpha_0 & -\alpha_1 & \cdots & -\alpha_{s-2} & -\alpha_{s-1} \end{bmatrix} \in \mathbb{C}^{s\times s}$$

Solution:

设

$$p_M(z) = det(zI - M) = z^s + \sum_{j=0}^{s-1} a_j z^j$$

设 D_k 为 M 的 k 阶主子式之和，那么 $a_j = (-1)^{s-j} D_{s-j}$

设

$$M_k = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ -\alpha_{s-k} & -\alpha_{s-k+1} & \cdots & -\alpha_{s-2} & -\alpha_{s-1} \end{bmatrix} \in \mathbb{C}^{k\times k},\ k = 2, \cdots, s,\ M_1 = \begin{bmatrix} -\alpha_{s-1} \end{bmatrix}$$

有

$$\det(M_k) = (-1)^{k-1} \det\left(\begin{bmatrix} -\alpha_{s-k} & -\alpha_{s-k+1} & \cdots & -\alpha_{s-2} & -\alpha_{s-1} \\ 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \end{bmatrix} \right) = (-1)^k \alpha_{s-k}$$

那么对于 M 的 k 阶主子式，若选取下标连续但不包含 s，那么主子式为 $\det\left(\begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix} \right) = 0$

若选取下标包含 s 但不连续，那么会有一行中间会有一行元素全为 0, 矩阵不满秩，行列式为 0

所以 $D_k = \det(M_k) = (-1)^k \alpha_{s-k} \Rightarrow a_j = (-1)^{s-j} D_{s-j} = \alpha_j$

即 M 的特征多项式为

$$p_M(z) = det(zI - M) = z^s + \sum_{j=0}^{s-1} \alpha_j z^j$$