I. Prove that the one-step error of the classical fourth-order RK method is

$$\mathcal{L}u(t_n) = O(k^5)$$

Solution:

classical fourth-order RK

$$\begin{cases} y_1 = f(U^n, t_n) \\ y_2 = f(U^n + \frac{k}{2}y_1, t_n + \frac{k}{2}) \\ y_3 = f(U^n + \frac{k}{2}y_2, t_n + \frac{k}{2}) \\ y_4 = f(U^n + ky_3, t_n + k) \\ U^{n+1} = U^n + \frac{k}{6}(y_1 + 2y_2 + 2y_3 + y_4) \end{cases}$$

设

$$\begin{aligned} y_1(t_n) &= f(u(t_n), t_n) \\ y_2(t_n) &= f(u(t_n) + \frac{k}{2}y_1(t_n), t_n + \frac{k}{2}) \\ y_3(t_n) &= f(u(t_n) + \frac{k}{2}y_2(t_n), t_n + \frac{k}{2}) \\ y_4(t_n) &= f(u(t_n) + ky_3(t_n), t_n + k) \end{aligned}$$

那么 $\mathcal{L}u(t_n) = u(t_{n+1}) - u(t_n) - \frac{k}{6}(y_1(t_n) + 2y_2(t_n) + 2y_3(t_n) + y_4(t_n))$

将 $u(t_{n+1})$ 展开到 k^5 项，$y_1(t_n), y_2(t_n), y_3(t_n)$ 展开到 k^4 项

$f_{u^m t^n} := \frac{\partial^{m+n} f}{\partial u^m \partial t^n}$, 并用 f 表示 $f(u(t_n), t_n)$, 其他同理，得

$$\begin{aligned} u(t_{n+1}) =& u + ku' + \frac{k^2}{2}u'' + \frac{k^3}{6}u''' + \frac{k^4}{24}u^{(4)} + \frac{k^5}{120}u^{(5)} + O(k^6) \\ u' =& f \\ u'' =& f_u f + f_t \\ u''' =& f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + f_u^2 f + f_u f_t \\ u^{(4)} =& f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3} + 4f_u f_{u^2}f^2 + 5f_u f_{ut}f + f_u f_{t^2} + 3f_{u^2}f_t f + 3f_{ut}f_t + f_u^3 f + f_u^2 f_t \\ u^{(5)} =& \ldots(27\text{项}) \end{aligned}$$

$$\begin{aligned} y_1(t_n) =& f \\ y_2(t_n) =& f + \frac{k}{2}(f_u f + f_t) + \frac{k^2}{8}(f_{u^2}f^2 + 2f_{ut}f + f_{t^2}) \\ &+ \frac{k^3}{48}(f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3}) \\ &+ \frac{k^4}{384}(f_{u^4}f^4 + 4f_{u^3t}f^3 + 6f_{u^2t^2}f^2 + 4f_{ut^3}f + f_{t^4}) + O(k^5) \end{aligned}$$

$$
\begin{aligned}
y_3(t_n) =& f + \frac{k}{2}(f_u f + f_t) + \frac{k^2}{8}(f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + 2f_u^2 f + 2f_u f_t) \\
&+ \frac{k^3}{48}(f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3} + 9f_u f_{u^2}f^2 + 12f_u f_{ut}f + 3f_u f_{t^2} + 6f_{u^2}f_t f + 6f_{ut}f_t) \\
&+ \frac{k^4}{384}(f_{u^4}f^4 + 4f_{u^3t}f^3 + 6f_{u^2t^2}f^2 + 4f_{ut^3}f + f_{t^4} + 16f_u f_{u^3}f^3 + 36f_u f_{u^2t}f^2 + 24f_u f_{ut^2}f + 4f_u f_{t^3} \\
&+ 12f_{u^2}f_u^2 f^2 + 24f_{u^2}f_u f_t f + 12f_{u^2}f_t^2 + 12f_{u^2}f_{ut}f^2 + 24f_{ut}^2 f + 12f_{ut}f_{t^2} + 12f_{u^3}f_t f^2 + 24f_{u^2t}f_t f + 12f_{ut^2}f_t) \\
&+ O(k^5)
\end{aligned}
$$

$$
\begin{aligned}
y_4(t_n) =& f + k(f_u f + f_t) + \frac{k^2}{2}(f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + f_u^2 f + f_u f_t) \\
&+ \frac{k^3}{24}(4f_{u^3}f^3 + 12f_{u^2t}f^2 + 12f_{ut^2}f + 4f_{t^3} \\
&+ 15f_u f_{u^2}f^2 + 18f_u f_{ut}f + 3f_u f_{t^2} + 12f_{u^2}f_t f + 12f_{ut}f_t + 6f_u^3 f + 6f_u^2 f_t) \\
&+ \frac{k^4}{24}((f_{u^4}f^4 + 4f_{u^3t}f^3 + 6f_{u^2t^2}f^2 + 4f_{ut^3}f + f_{t^4}) \\
&+ \frac{1}{2}(f_u f_{u^3}f^3 + 3f_u f_{u^2t}f^2 + 3f_u f_{ut^2}f + f_u f_{t^3} + 9f_u^2 f_{u^2}f^2 + 12f_u^2 f_{ut}f + 3f_u^2 f_{t^2} + 6f_u f_{u^2}f_t f + 6f_u f_{ut}f_t) \\
&+ 3(f_u^2 f_{u^2}f^2 + 2f_u f_{u^2}f_t f + f_{u^2}f_t^2) + 3(f_{u^2}f_{ut}f^2 + 2f_{ut}^2 f + f_{ut}f_{t^2} + 2f_u^2 f_{ut}f + 2f_u f_{ut}f_t) \\
&+ 6(f_u f_{u^3}f^3 + f_{u^3}f_t f^2) + 12(f_u f_{u^2t}f^2 + f_{u^2t}f_t f) + 6(f_u f_{ut^2}f + f_{ut^2}f_t)) \\
&+ O(k^5)
\end{aligned}
$$

代回到 $\mathcal{L}u(t_n) = u(t_{n+1}) - u(t_n) - \frac{k}{6}(y_1(t_n) + 2y_2(t_n) + 2y_3(t_n) + y_4(t_n))$

- k: $u' - \frac{1}{6}(f + 2f + 2f + f) = u' - f = 0$
- k^2: $\frac{1}{2}u'' - \frac{1}{6}3(f_u f + f_t) = \frac{1}{2}(u' - f_u f - f_t) = 0$
- k^3: 因为

  $$f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + 2f_u^2 f + 2f_u f_t = 2(f_{u^2}f^2 + 2f_{ut}f + f_{t^2} + f_u^2 f + f_u f_t) = 2u'''$$

  所以 k^3 的系数为 $\frac{1}{6}u''' - \frac{1}{6}(2 \times (\frac{1}{8}2u''') + \frac{1}{2}u''') = 0$

- k^4:

  $$
  \begin{aligned}
  &(f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3}) \\
  &+(f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3} + 9f_u f_{u^2}f^2 + 12f_u f_{ut}f + 3f_u f_{t^2} + 6f_{u^2}f_t f + 6f_{ut}f_t) \\
  &+(4f_{u^3}f^3 + 12f_{u^2t}f^2 + 12f_{ut^2}f + 4f_{t^3} + 15f_u f_{u^2}f^2 + 18f_u f_{ut}f + 3f_u f_{t^2} + 12f_{u^2}f_t f + 12f_{ut}f_t + 6f_u^3 f + 6f_u^2 f_t) \\
  =&6(f_{u^3}f^3 + 3f_{u^2t}f^2 + 3f_{ut^2}f + f_{t^3} + 4f_u f_{u^2}f^2 + 5f_u f_{ut}f + f_u f_{t^2} + 3f_{u^2}f_t f + 3f_{ut}f_t + f_u^3 f + f_u^2 f_t) \\
  =&6u^{(4)}
  \end{aligned}
  $$

  所以系数为 $\frac{1}{24}u^{(4)} - \frac{1}{6}\frac{1}{24}6u^{(4)} = 0$

- k^5: 因为 $u^{(5)}$ 有 27 项而 $k(y_1(t_n) + 2y_2(t_n) + 2y_3(t_n) + y_4(t_n))$ 展开式中 k^5 系数只有 21 项, 所以相减后不为 0

综上所述，可知对于 classical fourth-order RK

$$\mathcal{L}u(t_n) = O(k^5)$$

II. Show that the classical fourth-order RK method has its stability function as

$$R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4$$

Solution:

对于 classical fourth-order RK

$$\begin{aligned}
R(z) &= 1 + z\mathbf{b}^T(1 - zA)^{-1}\mathbf{1} \\
&= 1 + \frac{z}{6}\begin{pmatrix}1 & 2 & 2 & 1\end{pmatrix}\begin{pmatrix}1 & & & \\ -\frac{z}{2} & 1 & & \\ & -\frac{z}{2} & 1 & \\ & & -z & 1\end{pmatrix}^{-1}\begin{pmatrix}1\\1\\1\\1\end{pmatrix} \\
&= 1 + \frac{z}{6}\begin{pmatrix}1 & 2 & 2 & 1\end{pmatrix}\begin{pmatrix}1 & & & \\ \frac{z}{2} & 1 & & \\ \frac{z^2}{4} & \frac{z}{2} & 1 & \\ \frac{z^3}{4} & \frac{z^2}{2} & z & 1\end{pmatrix}\begin{pmatrix}1\\1\\1\\1\end{pmatrix} \\
&= 1 + \frac{z}{6}\begin{pmatrix}1 & 2 & 2 & 1\end{pmatrix}\begin{pmatrix}1 \\ \frac{z}{2}+1 \\ \frac{z^2}{4}+\frac{z}{2}+1 \\ \frac{z^3}{4}+\frac{z^2}{2}+z+1\end{pmatrix} \\
&= 1 + \frac{z}{6}(1 + 2(\frac{z}{2}+1) + 2(\frac{z^2}{4}+\frac{z}{2}+1) + \frac{z^3}{4} + \frac{z^2}{2} + z + 1) \\
&= 1 + \frac{z}{6}(6 + 3z + z^2 + \frac{z^3}{4}) \\
&= 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4
\end{aligned}$$

III. Define $S_s := \{z : |R_s(z)| \leq 1\}$ where $s = 1, 2, 3, 4$ and R_s is the stability function of the s-stage, sth-order ERK method. Show that

$$S_1 \subset S_2 \subset S_3$$

Does this hold for ERK methods with a higher stage? Why?

Solution:

$R_1(z) = 1 + z,\ R_2(z) = 1 + z + \frac{z^2}{2},\ R_3(z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{6}$

$\mathbf{S_1 \subset S_2}$

$\forall z^* \in S_1,\ |1 + z^*| \leq 1,\ |R_2(z^*)| = |1 + z^* + \frac{z^{*2}}{2}| = |\frac{1}{2}(z^*+1)^2 + \frac{1}{2}| \leq \frac{1}{2}|z^*+1|^2 + \frac{1}{2} \leq 1$

$\Rightarrow S_1 \subset S_2$

$\mathbf{S_2} \subset \mathbf{S_3}$

$\forall z^* \in S_2$, $|R_2(z^*)| \le 1$, 设 $z^* = x + y\mathbf{i}$, $x, y \in \mathbb{R}$
那么设

$$
\begin{aligned}
|R_3(z^*)|^2 &= \frac{x^6}{36} + \frac{x^5}{6} + \frac{x^4y^2}{12} + \frac{7x^4}{12} + \frac{x^3y^2}{3} + \frac{4x^3}{3} + \frac{x^2y^4}{12} + \frac{x^2y^2}{2} + 2x^2 + \frac{xy^4}{6} + 2x + \frac{y^6}{36} - \frac{y^4}{12} + 1 \\
&= f(x,y) + 1 \\
|R_2(z^*)|^2 &= \frac{x^4}{4} + x^3 + \frac{x^2y^2}{2} + 2x^2 + xy^2 + 2x + \frac{y^4}{4} + 1 \\
&= g(x,y) + 1
\end{aligned}
$$

由 $|R_2(z^*)| \le 1 \Longrightarrow g(x,y) \le 0$
那么求解最优化问题

$$
\begin{aligned}
&\min_{x,y} - f(x,y) \\
&\quad g(x,y) \le 0
\end{aligned}
$$

构造 Lagrange 函数 $L(x,y,\lambda,v) = -f(x,y) - \lambda(g(x,y) + v^2)$
那么就等价求解

$$
\begin{cases}
L_x(x,y,\lambda,v) = -f_x(x,y) - \lambda g_x(x,y) = 0 \\
L_x(x,y,\lambda,v) = -f_x(x,y) - \lambda g_x(x,y) = 0 \\
L_\lambda(x,y,\lambda,v) = g(x,y) + v^2 = 0 \\
L_v(x,y,\lambda,v) = -2\lambda v = 0
\end{cases}
$$

解得

- $(x,y) = (0,0)$, $f(x,y) = 0$
- $(x,y) = (-2,0)$, $f(x,y) = -\frac{8}{9}$
- $(x,y) = (-1,1)$, $f(x,y) = -\frac{7}{9}$
- $(x,y) = (-1,-1)$, $f(x,y) = -\frac{7}{9}$
- $(x,y) = (-1 - \frac{\sqrt[3]{27+27\sqrt{2}}}{3} + \frac{3}{\sqrt[3]{27+27\sqrt{2}}}, 0)$,
  $f(x,y) = -\frac{2\sqrt{2}}{\sqrt[3]{27+27\sqrt{2}}} - \frac{2}{\sqrt[3]{27+27\sqrt{2}}} - \frac{5}{12} - \frac{15\sqrt{2}}{27+27\sqrt{2}} - \frac{12}{27+27\sqrt{2}} - \frac{\sqrt{2}}{18} + \frac{81}{5832\sqrt{2}+8748} + \frac{2\left(27+27\sqrt{2}\right)^{\frac{2}{3}}}{27}$

所以 $f(x,y) \le 0 \Rightarrow |R_3(z^*)|^2 \le 1 \Rightarrow |R_3(z^*)| \le 1 \Rightarrow S_2 \subset S_3$
综上有

$$S_1 \subset S_2 \subset S_3$$

当 $s > 4$ 时不成立，因为 $s > 4$ 时不存在 s-stage s-order 的 ERK method

IV. Prove that an A-stable RK method with stability function as a rational polynomial $R(z) = \frac{P(z)}{Q(Z)}$ is L-stable if and only if deg $Q(z) >$ deg $P(z)$

Solution:

设

$$P(z) = \sum_{i=0}^{m} p_i z^i, \quad Q(z) = \sum_{i=0}^{n} q_i z^i \quad (p_m, q_n \neq 0)$$

必要性

由 RK method is L-stable, 可知

$$0 = \lim_{z\to\infty} |R(z)| = \lim_{z\to\infty} |\frac{\sum_{i=0}^{m} p_i z^i}{\sum_{i=0}^{n} q_i z^i}| = \lim_{z\to\infty} |\frac{p_m}{q_n} z^{m-n}|$$
$$\Rightarrow m - n < 0$$

充分性

由 $m < n$ 可知

$$\lim_{z\to\infty} |R(z)| = \lim_{z\to\infty} |\frac{\sum_{i=0}^{m} p_i z^i}{\sum_{i=0}^{n} q_i z^i}| = \lim_{z\to\infty} |\frac{p_m}{q_n} z^{m-n}| = 0$$

所以该 RK method is L-stable

V. Show that if an A-stable RK method with a nonsingular RK matrix A satisfies

$$a_{i,1} = b_1, \quad i = 1, 2, \cdots, s,$$

then it is L-stable

Solution:

$$\begin{aligned}\lim_{z\to\infty} R(z) &= \lim_{z\to\infty} (1 + z\mathbf{b}^T (I - zA)^{-1} \mathbf{1}) \\ &= 1 + \lim_{z\to\infty} \mathbf{b}^T (\frac{1}{z} I - A)^{-1} \mathbf{1} \\ &= 1 - \mathbf{b}^T A^{-1} \mathbf{1}\end{aligned}$$

设 $\mathbf{b}^T A^{-1} = (x_1, x_2, \cdots, x_s) \Leftrightarrow (x_1, x_2, \cdots, x_s) A = \mathbf{b}^T$

可得 $\sum_{i=1}^{s} x_i a_{i,1} = b_1 \sum_{i=1}^{s} x_i = b_1 \Rightarrow \sum_{i=1}^{s} x_i = 1$

所以

$$\begin{aligned}\lim_{z\to\infty} R(z) &= 1 - \mathbf{b}^T A^{-1} \mathbf{1} \\ &= 1 - (x_1, x_2, \cdots, x_s) \mathbf{1} \\ &= 1 - \sum_{i=1}^{s} x_i \\ &= 0\end{aligned}$$

VI. Show that the collocation method

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\
\frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\
1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
$$

Solution:

取 $l = 1,2,3,4,5,6$ 可得

$$\sum_{j=1}^{s} b_j c_j^0 = 1$$
$$\sum_{j=1}^{s} b_j c_j^1 = \frac{1}{2}$$
$$\sum_{j=1}^{s} b_j c_j^2 = \frac{1}{3}$$
$$\sum_{j=1}^{s} b_j c_j^3 = \frac{1}{4}$$
$$\sum_{j=1}^{s} b_j c_j^4 = \frac{1}{5}$$
$$\sum_{j=1}^{s} b_j c_j^5 = \frac{101}{600} \neq \frac{1}{6}$$

可知该方法是 $B(5)$ 但是不是 $B(6)$ 的
由 RK order conditions 可知，若 RK method 是 p 阶精度的，那么一定是 $B(p)$ 的（取 $m = 0$）
所以该方法最多为 5 阶精度
下面将验证该方法是 $C(3)$ 的，取 $m = 1,2,3$

- $m = 1$ 时，$\sum_{j=1}^{s} a_{i,j} = c_i$ 成立
- $m = 2$ 时，

$$i = 1,\ a_{1,1}c_1 + a_{1,2}c_2 + a_{1,3}c_3 = \frac{11-4\sqrt{6}}{100} = \frac{c_1^2}{2}$$
$$i = 2,\ a_{2,1}c_1 + a_{2,2}c_2 + a_{2,3}c_3 = \frac{11-4\sqrt{6}}{100} = \frac{c_2^2}{2}$$
$$i = 3,\ a_{3,1}c_1 + a_{3,2}c_2 + a_{3,3}c_3 = \frac{1}{2} = \frac{c_3^2}{2}$$

- $m = 3$ 时，

$$i = 1,\ a_{1,1}c_1^2 + a_{1,2}c_2^2 + a_{1,3}c_3^2 = \frac{17}{375} - \frac{9}{500}\sqrt{6} = \frac{c_1^3}{3}$$
$$i = 2,\ a_{2,1}c_1^2 + a_{2,2}c_2^2 + a_{2,3}c_3^2 = \frac{17}{375} + \frac{9}{500}\sqrt{6} = \frac{c_2^3}{3}$$
$$i = 3,\ a_{3,1}c_1^3 + a_{3,2}c_2^2 + a_{3,3}c_3^2 = \frac{1}{3} = \frac{c_3^3}{3}$$

所以该方法是 $C(3)$ 的，所以该方法是 $D(2)$ 的
又由 $5 \le 2*3+2$ 以及 $5 \le 2+3+1$ 可知该方法至少为 5 阶精度
综上所述，该方法是 5 阶精度的

由上表可知其 stability function 为

$$R(z) = 1 + z\mathbf{b}^T(I - zA)^{-1}\mathbf{1} = \frac{3z^2 + 24z + 60}{-z^3 + 9z^2 - 36z + 60}$$

1.

$$\begin{aligned}
&|R(y\mathbf{i})| \leq 1 \\
\iff& |-3y^2 + 24y\mathbf{i} + 60|^2 \leq |y^3\mathbf{i} - 9y^2 - 36y\mathbf{i} + 60|^2 \\
\iff& (-3y^2 + 60)^2 + (24y)^2 \leq (-9y^2 + 60)^2 + (y^3 - 36y)^2 \\
\iff& y^6 \geq 0
\end{aligned}$$

所以 $\forall y \in \mathbb{R}$，有 $|R(y\mathbf{i})| \leq 1$

2. $R(z)$ 的极点为

$$\begin{aligned}
&3 + \frac{3^{\frac{1}{3}}}{2} - \frac{3^{\frac{2}{3}}}{2} + (3^{\frac{2}{3}} - 3^{\frac{1}{3}})\frac{\sqrt{3}}{2}\mathbf{i} \\
&3 + \frac{3^{\frac{1}{3}}}{2} - \frac{3^{\frac{2}{3}}}{2} - (3^{\frac{2}{3}} - 3^{\frac{1}{3}})\frac{\sqrt{3}}{2}\mathbf{i} \\
&3 - 3^{\frac{1}{3}} + 3^{\frac{2}{3}}
\end{aligned}$$

都有正的实部

所以该方法是 A-stable
又有其 RK 矩阵 A 非奇异且 stiffly accurate
所以该 collocation method is L-stable

VII. Rewrite the implicit midpoint method

$$U^{n+1} = U^n + kf(\frac{U^n + U^{n+1}}{2}, t_n + \frac{k}{2})$$

in the standard form and derive its Butcher tableau. Show that it is B-stable

Solution:

$$\begin{cases} y_1 = f(U^n + \frac{k}{2}y_1, t_n + \frac{k}{2}) \\ U^{n+1} = U^n + ky_1 \end{cases}$$

Butcher tableau:

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

设 $e^n := U^n - V^n,\ U^* = U^n + \frac{k}{2}y_{u1},\ V^* = V^n + \frac{k}{2}y_{v1}$

$$\begin{aligned}
\|e^{n+1}\|^2 &= \langle e^{n+1}, e^{n+1} \rangle \\
&= \left\langle e^n + k(f(U^*, t_n + \frac{k}{2}) - f(V^*, t_n + \frac{k}{2})), e^n + k(f(U^*, t_n + \frac{k}{2}) - f(V^*, t_n + \frac{k}{2})) \right\rangle \\
&= \langle e^n, e^n \rangle + 2\left\langle e^n + \frac{k}{2}(f(U^*, t_n + \frac{k}{2}) - f(V^*, t_n + \frac{k}{2})), k(f(U^*, t_n + \frac{k}{2}) - f(V^*, t_n + \frac{k}{2})) \right\rangle \\
&= \|e^n\|^2 + 2\left\langle U^* - V^*, k(f(U^*, t_n + \frac{k}{2}) - f(V^*, t_n + \frac{k}{2})) \right\rangle \\
&\leq \|e^n\|^2
\end{aligned}$$

所以 implicit midpoint method is B-stable