Homework 3

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Problem 1 (Theoretical)

Part 1: Derive the stability function $\phi(z)$ for each of the two RK methods below

- Predictor-corrector method (Heun's method)
- Classic 4-th order Runge-Kutta method (RK4)

Hint: Check your expression of $\phi(z)$ with the theorem we studied.

Theorem: If an RK method is p-th order accurate, then it must satisfies

$\phi(z) = e^z + O(|z|^{p+1})$ for any complex z with small $|z|$

Part 2: Study the zero-stability for each of the two LMMs below

- $u_{n+2} - 2u_{n+1} + u_n = hf(u_{n+1}, t_{n+1}) - hf(u_n, t_n)$
- $u_{n+2} - u_n = h\left[\frac{1}{3}f(u_{n+2}, t_{n+2}) + \frac{4}{3}f(u_{n+1}, t_{n+1}) + \frac{1}{3}f(u_n, t_n)\right]$

Part 1

To find a stability function we apply $u' = \gamma u$ to Heun's method and RK4

$U_{n+1} = \phi(z) U_n$ where $z = h\gamma$

B-T for Heun's method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \longrightarrow \text{RK form} \begin{cases} k_1 = hf(U_n, t_n) \\ k_2 = hf(U_n + k_1, t_n + h) \\ U_{n+1} = U_n + \frac{1}{2}k_1 + \frac{1}{2}k_2 \end{cases}$$

$f(U) = \gamma u$

Plugging into R-K form

$$k_1 = h\gamma u_n = zU_n$$

$$k_2 = hf(U_n + zU_n) = h\gamma(U_n + zU_n) = zU_n + z^2 U_n$$

$$U_{n+1} = U_n + \frac{1}{2}zU_n + \left(\frac{1}{2}z + \frac{1}{2}z^2\right)U_n$$

$$U_{n+1} = \left(1 + z + \frac{1}{2}z^2\right)U_n$$

$$\boxed{\phi(z) = 1 + z + \frac{1}{2}z^2}$$

Next for RK4

BT

$f(U) = \gamma u$

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \longleftrightarrow \text{R-K form} \left\{ \begin{array}{l} k_1 = hf(U_n) \\ k_2 = hf(U_n + \frac{1}{2}k_1) \\ k_3 = hf(U_n + \frac{1}{2}k_2) \\ k_4 = hf(U_n + k_3) \\ U_{n+1} = U_n + \frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4 \end{array} \right.$$

$$K_1 = h\gamma U_n = zU_n$$

$$K_2 = h\gamma\left(U_n + \frac{zU_n}{2}\right) = zU_n + \frac{1}{2}z^2U_n = \left(z + \frac{z^2}{2}\right)U_n$$

$$K_3 = h\gamma\left(U_n + \frac{(z + \frac{1}{2}z^2)U_n}{2}\right) = zU_n + \left(\frac{z^2}{2} + \frac{z^3}{4}\right)U_n = \left(z + \frac{z^2}{2} + \frac{z^3}{4}\right)U_n$$

$$K_4 = h\gamma\left(U_n + \left(z + \frac{z^2}{2} + \frac{z^3}{4}\right)U_n\right) = \left(z + z^2 + \frac{z^3}{2} + \frac{z^4}{4}\right)U_n$$

$$U_{n+1} = U_n + \left(\frac{z}{6} + \frac{z}{3} + \frac{z^2}{6} + \frac{z}{3} + \frac{z^2}{6} + \frac{z^3}{12} + \frac{z}{6} + \frac{z^2}{6} + \frac{z^3}{12} + \frac{z^4}{24}\right)U_n$$

$$U_{n+1} = \left(1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \frac{z^4}{24}\right)U_n$$

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

Part 2

$$U_{n+2} - 2U_{n+1} + U_n = hf(U_{n+1}, t_{n+1}) - hf(U_n, t_n)$$

$$\rho(\xi) = \xi^2 - 2\xi + 1 \qquad \sigma(\xi) = \xi - 1$$

find roots of $\rho(\xi) = 0$

$$(\xi - 1)(\xi - 1) = 0 \qquad \xi = 1, \text{ with multiplicity } 2$$

Thus this LMM is not zero stable because the root condition is not satisfied
"all roots with multiplicity above 1 satisfy $|\xi| < 1$" ■

$$U_{n+2} - U_n = \frac{1}{3} h f(U_{n+2}, t_{n+2}) + \frac{4}{3} h f(U_{n+1}, t_{n+1}) + \frac{1}{3} f(U_n, t_n)$$

$$\rho(\xi) = \xi^2 - 1 \qquad \sigma(\xi) = \frac{1}{3}\xi^2 + \frac{4}{3}\xi + \frac{1}{3}$$

find roots of $\rho(\xi) = 0$

$\xi^2 - 1 = 0 \Rightarrow \xi_1 = 1 \quad \xi_2 = -1$ two simple root where $|\xi_i| \le 1$ thus this LMM is zero-stable. ■

Problem 2 (Theoretical)

Consider the Runge-Kutta method described by Butcher tableau

Butcher tableau:

$$\begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1-\alpha & \alpha \\ \hline & 1-\alpha & \alpha \end{array}$$

where $\alpha > 0$. This is called a 2s-DIRK (2-Stage Diagonally Implicit Runge-Kutta) method.

The matrix A of a DIRK method is lower triangular so $\{k_1, k_2, k_3, \ldots\}$ can be solved sequentially. The first row of A gives an equation on k_1 without involving $\{k_2, k_3, \ldots\}$. The second row of A gives an equation on k_2 without involving $\{k_3, \ldots\}$ where k_1 is already known. This is in contrast to a fully implicit Runge-Kutta where $\{k_1, k_2, k_3, \ldots\}$ has to be solved simultaneously in a joint system.

Part 1: Show that method is second order for $\alpha = 1 - 1/\sqrt{2}$.

Hint: check the internal consistency condition, the condition for first order and the additional condition for second order.

Part 2: Apply the 2s-DIRK to solving $u' = \gamma u$.

Derive the expressions for k_1, k_2 and the stability function $\phi(z)$.

Part 1 BT

$$\begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1-\alpha & \alpha \\ \hline & 1-\alpha & \alpha \end{array}$$

To show above method is second order for $\alpha = 1 - 1/\sqrt{2}$

check the internal condition, the first order order condition, and additional condition for second order

Internal condition

$$C_i = \sum_{j=1}^{2} a_{ij} \quad i=1,2$$

$$C_1 = \alpha \qquad \sum_{j=1}^{2} a_{1j} = \alpha \checkmark$$

$$C_2 = 1 \qquad \sum_{j=1}^{2} a_{2j} = 1 \checkmark$$

First order condition

$$\sum_{i=1}^{2} b_i = 1 \qquad b_1 = 1-\alpha$$

$$b_2 = \alpha$$

$$b_1 + b_2 = 1 - \alpha + \alpha = 1 \checkmark$$

Second order condition

$$\sum_{i=1}^{2} b_i C_i = \tfrac{1}{2} \qquad b_1 = 1-\alpha \quad C_1 = \alpha$$

$$b_2 = \alpha \quad C_2 = 1$$

$$\sum_{i=1}^{2} b_i C_i = \alpha - \alpha^2 + \alpha = 2\alpha - \alpha^2 \qquad \alpha = 1 - 1/\sqrt{2}$$

$$\Rightarrow \quad 2 - \frac{2}{\sqrt{2}} - \left(1 - \frac{2}{\sqrt{2}} + \frac{1}{2}\right)$$

$$2 - \sqrt{2} - 1 + \sqrt{2} - \frac{1}{2} = \frac{1}{2} \checkmark$$

We have shown that this method is 2^{nd} order when $\alpha = 1 - 1/\sqrt{2}$ ∎

Part 2

$\alpha = 1 - 1/\sqrt{2}$

$$\begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1-\alpha & \alpha \\ \hline & 1-\alpha & \alpha \end{array} \xrightarrow[\text{form}]{RK} \begin{cases} k_1 = hf(U_n + \alpha k_1, t_n + \alpha h) \\ k_2 = hf(U_n + (1-\alpha)k_1 + \alpha k_2, t_n + h) \\ U_{n+1} = U_n + (1-\alpha)k_1 + \alpha k_2 \end{cases}$$

Next we find stability function

$$f(U) = \gamma U$$

$$k_1 = h\gamma f(U_n + \alpha k_1) = z U_n + z\alpha k_1 \Rightarrow k_1 - z\alpha k_1 = zU_n$$

$$\boxed{k_1 = \frac{z}{1-z\alpha} U_n}$$

$$k_2 = h\gamma f(U_n + (1-\alpha)k_1 + \alpha k_2) = z\left(U_n + (1-\alpha)\frac{z}{1-z\alpha}U_n + \alpha k_2\right)$$

$$k_2 = \left(z + (1-\alpha)\frac{z^2}{1-z\alpha}\right)U_n + z\alpha k_2$$

$$k_2 = \frac{\left(z + (1-\alpha)\frac{z^2}{1-z\alpha}\right)}{1-z\alpha} U_n = \boxed{\frac{z(1-z\alpha) + (1-\alpha)z^2}{(1-z\alpha)^2} U_n}$$

$$U_{n+1} = U_n + (1-\alpha)\frac{z}{1-z\alpha}U_n + \frac{\alpha\left(z + (1-\alpha)\frac{z^2}{1-z\alpha}\right)}{1-z\alpha}U_n$$

$$U_{n+1} = \left(1 + \frac{z - z\cancel{\alpha}}{1-\cancel{z}\alpha} + \frac{z\cancel{\alpha}}{\cancel{1}-z\alpha}\frac{+(\alpha-\alpha^2)z^2}{(1-z\alpha)^2}\right)U_n$$

$$= \left(1 + \frac{z}{1-z\alpha} + \frac{z^2\alpha - z^2\alpha^2}{(1-z\alpha)^2}\right) u_n$$

$$\phi(z) = 1 + \frac{z}{1-z\alpha} + \frac{z^2\alpha - z^2\alpha^2}{(1-z\alpha)^2}$$

$$= \frac{1 - 2z\alpha + \cancel{z^2\alpha^2} + z - \cancel{z^2\alpha} + \cancel{z^2\alpha} - \cancel{z^2\alpha^2}}{(1-z\alpha)^2}$$

$$= \boxed{\frac{1 - 2z\alpha + z}{(1-z\alpha)^2}}$$

$$k_1 = \frac{z}{1-\alpha z} u_n, \quad k_2 = \frac{(1-\alpha z)z + (1-\alpha)z^2}{(1-\alpha z)^2} u_n$$

$$\phi(z) = \frac{1+(1-2\alpha)z}{(1-\alpha z)^2}$$

Part 3: Suppose the 2s-DIRK is A-stable for $\alpha = 1 - 1/\sqrt{2}$ (see Problem 4 below). Show that it satisfies the second condition of L-stability.

Part 3

Suppose 2s-DIRK is A-stable for $\alpha = 1 - \frac{1}{\sqrt{2}}$

$$\lim_{z \to \infty} \frac{1 + (1-2\alpha)z}{(1-\alpha z)^2} = 0$$

By definition if an RK method is A-Stable and $\phi(z) \to 0$ as $z \to \infty$ Then the method is L-Stable.

Problem 3 (Theoretical)

Consider the implicit 2-step method below

$$u_{n+2}-u_n=h\left[\frac{1}{3}f(u_{n+2},t_{n+2})+\frac{4}{3}f(u_{n+1},t_{n+1})+\frac{1}{3}f(u_n,t_n)\right]$$

Part 1: Use Taylor expansion to show $e_n(h) = O(h^5)$.

Hint: Expand everything around t_{n+1}.

Part 2: The stability polynomial is

$$\pi(\xi,z)=(\xi^2-1)-z\left(\frac{1}{3}\xi^2+\frac{4}{3}\xi+\frac{1}{3}\right)$$

Consider $z = -\varepsilon$ with small $\varepsilon > 0$. We examine the two roots of $\pi(\xi, -\varepsilon)$.

Show that the two roots $\xi_1(\varepsilon)$ and $\xi_2(\varepsilon)$ have the expansions

$$\xi_1(\varepsilon)=1-\varepsilon+O(\varepsilon^2),\quad \xi_2(\varepsilon)=-\left(1+\frac{\varepsilon}{3}\right)+O(\varepsilon^2)$$

Therefore, $z = -\varepsilon$ is NOT in the region of absolute stability.

Remarks:

- This method demonstrates that the Dahlquist barrier on accuracy of implicit LMMs: $p \le r+2$ is actually attainable.
- Although this method has the 4th order, it is not practically useful. When applied to solving $u' = -u$, the numerical solution contains a decaying mode (corresponding to the exact solution), and an oscillating and exponentially growing mode (which will eventually ruin the numerical solution). This is similar to the situation with the 2-step midpoint method.

Part 1

$$U_{n+2}-U_n=h\left[\frac{1}{3}f(U_{n+2},t_{n+2})+\frac{4}{3}f(U_{n+1},t_{n+1})+\frac{1}{3}f(U_n,t_n)\right]$$

$$e_n(h) = U(t_{n+1}-h)-U(t_{n+1}+h)+\frac{h}{3}f(U(t_{n+1}+h),t_{n+1}+h)$$
$$+\frac{4}{3}hf(U(t_{n+1}),t_{n+1})+\frac{h}{3}f(U(t_{n+1}-h),t_{n+1}-h)$$

Since this is a LMM we know that

$f(u_n+jh)=u'(t_n+jh)\ \forall j$

$$e_n(h)=U(t_{n+1}-h)-U(t_{n+1}+h)+\frac{h}{3}U'(t_{n+1}+h)+\frac{4h}{3}U'(t_{n+1})+\frac{h}{3}U'(t_{n+1}-h)$$

Next we expand around t_{n+1}

$$U(t_{n+1}-h)=U(t_{n+1})-hU'(t_{n+1})+\frac{h^2}{2!}U''(t_{n+1})-\frac{h^3}{3!}U^{(3)}(t_{n+1})+\frac{h^4}{4!}U^{(4)}(t_{n+1})+O(h^5)$$

$$U(t_{n+1}+h)=U(t_{n+1})+hU'(t_{n+1})+\frac{h^2}{2!}U''(t_{n+1})+\frac{h^3}{3!}U^{(3)}(t_{n+1})+\frac{h^4}{4!}U^{(4)}(t_{n+1})+O(h^5)$$

$$U'(t_{n+1}+h) = U'(t_{n+1}) + hU''(t_{n+1}) + \frac{h^2}{2!}U'''(t_{n+1}) + \frac{h^3}{3!}U^{(4)} + O(h^4)$$

$$U'(t_{n+1}-h) = U'(t_{n+1}) - hU''(t_{n+1}) + \frac{h^2}{2!}U'''(t_{n+1}) - \frac{h^3}{3!}U^{(4)} + O(h^4)$$

Sub in expansions into $e_n(h)$

$$e_n(h) = -2hU'(t_{n+1}) - 2\frac{h^3}{3!}U^{(3)}(t_{n+1}) + \frac{h}{3}\left[2U'(t_{n+1}) + h^2U^{(3)}(t_{n+1}) + O(h^4)\right]$$

$$+ \frac{4h}{3}U'(t_{n+1}) + O(h^5)$$

$$= -2hU'(t_{n+1}) - \cancel{\frac{h^3}{3}U^{(3)}}(t_{n+1}) + \frac{2h}{3}U'(t_{n+1}) + \cancel{\frac{h^3}{3}U^{(3)}}(t_{n+1}) + \frac{4h}{3}U'(t_{n+1})$$
$$+ O(h^5)$$

$$= \cancel{-2hU'(t_{n+1})} + \cancel{\frac{6h}{3}U'(t_{n+1})} + O(h^5)$$

$$= O(h^5)$$ ■

Part 2

$$\Pi(\xi, z) = (\xi^2 - 1) - z\left(\frac{1}{3}\xi^2 + \frac{4}{3}\xi + \frac{1}{3}\right)$$

Small $\varepsilon > 0$

$$\Pi(\xi, -\varepsilon) = \xi^2 - 1 + \frac{\varepsilon}{3}\xi^2 + \frac{4\varepsilon}{3}\xi + \frac{\varepsilon}{3}$$

To find the roots of the above equation apply the quadratic equation

$$\xi = \frac{-4\varepsilon \pm \sqrt{12\varepsilon^2 + 36}}{6 + 2\varepsilon}$$

$$\xi_1 = \frac{-4\varepsilon + 2\sqrt{3(\varepsilon^2+3)}}{6(1+\frac{\varepsilon}{3})} = \frac{-4\varepsilon + 6\sqrt{\frac{\varepsilon^2}{3}+1}}{6(1+\frac{\varepsilon}{3})}$$

$$\xi_2 = \frac{-4\varepsilon - 2\sqrt{3(\varepsilon^2+3)}}{6(1+\frac{\varepsilon}{3})} = \frac{-4\varepsilon - 6\sqrt{\frac{\varepsilon^2}{3}+1}}{6(1+\frac{\varepsilon}{3})}$$

Want to expand around $\varepsilon = 0$
denominator first

$\alpha = -1$

$$\frac{1}{6}\left(1+\frac{\varepsilon}{3}\right)^{-1} = \frac{1}{6}\left[1 - \frac{\varepsilon}{3} + \frac{\varepsilon^2}{9} + O(\varepsilon^3)\right]$$

now numerator

$$6\left(1+\frac{\varepsilon^2}{3}\right)^{1/2} = 6\left[1 + \frac{\varepsilon^2}{6} + O(\varepsilon^4)\right]$$

Thus

$$\xi_1 = \left(-4\varepsilon + 6 + \frac{\varepsilon^2}{6}\right)\left(\frac{1}{6} - \frac{\varepsilon}{18} + \frac{\varepsilon^2}{54}\right)$$

$$= \frac{-4\varepsilon}{6} + O(\varepsilon^2) + O(\varepsilon^2) + 1 - \frac{6\varepsilon}{18} + O(\varepsilon^2)$$

$$= -\frac{2}{3}\varepsilon - \frac{1}{3}\varepsilon + 1 + O(\varepsilon^2)$$

$$= 1 - \varepsilon + O(\varepsilon^2) \quad \checkmark$$

$$\xi_2 = \left(-4\varepsilon - 6 - \frac{\varepsilon^2}{6}\right)\left(\frac{1}{6} - \frac{\varepsilon}{18} + \frac{\varepsilon^2}{54}\right)$$

$$= \frac{-4\varepsilon}{6} - 1 + \frac{6\varepsilon}{18} + O(\varepsilon^2)$$

$$= \frac{-2}{3}\varepsilon + \frac{1}{3}\varepsilon - 1 + O(\varepsilon^2)$$

$$= -1 - \frac{\varepsilon}{3} + O(\varepsilon^2) \checkmark \quad \blacksquare$$