Exercise 4.4 Determine all value of θ such that the theta method

$$y_{n+1} = y_n + h[\theta f(t_n, y_n) + (1-\theta) f(t_{n+1}, y_{n+1})] \tag{1.13}$$

for $n = 0, 1, \ldots$ is A-stable.

Solution: Given the ordinary differential equation

$$y' = \lambda y \qquad \text{such that} \qquad y(0) = 1$$

the theta method yields

$$y_{n+1} = y_n + h[\theta\lambda y_n + (1-\theta)\lambda y_{n+1}].$$

Therefore

$$(1 - h(1-\theta)\lambda)y_{n+1} = (1 + h\theta\lambda)y_n$$

and consequently

$$y_{n+1} = r(h\lambda)y_n \qquad \text{where} \qquad r(z) = \frac{1+\theta z}{1-(1-\theta)z}.$$

Now apply Lemma 4.3 from the text which reads as

Lemma 4.3 *Let r be an arbitrary rational function that is not a constant. Then $|r(z)| < 1$ for all $z \in \mathbf{C}^-$ if and only if all the poles of r have positive real parts and $|r(it)| \le 1$ for all $t \in \mathbf{R}$.*

When $\theta = 1$ there are no poles; otherwise, $\theta \in [0, 1)$ in which case there is a pole is at $1/(1-\theta)$ which is real and clearly positive. It remains to check whether $|r(it)| \le 1$ for all $t \in \mathbf{R}$. Since

$$|1 + i\theta t|^2 = 1 + \theta^2 t^2$$
$$|1 - i(1-\theta)t|^2 = 1 + (1-\theta)^2 t^2,$$

we obtain that

$$|r(it)|^2 = \frac{1+\theta^2 t^2}{1+(1-\theta)^2 t^2}.$$

The numerator is smaller or equal the denominator only when when $\theta \le 1/2$. It follows that the theta method is A-stable for $\theta \le 1/2$.

Note that it's possible to explicitly calculate the linear stability domain of the theta method. For example, the boundary of $\mathcal{D} = \{\, z : |r(z)| < 1 \,\}$ may be determined by inverting r as a function of z and then letting r trace out all values on the unit circle. Since

$$\begin{aligned} 1+\theta z &= r(1-(1-\theta)z) \\ 1+\theta z &= r - r(1-\theta)z \\ r(1-\theta)z + \theta z &= r-1 \end{aligned}$$

implies

$$z = \frac{r-1}{(1-\theta)r+\theta}.$$

Substituting $r = e^{i\alpha}$ then yields

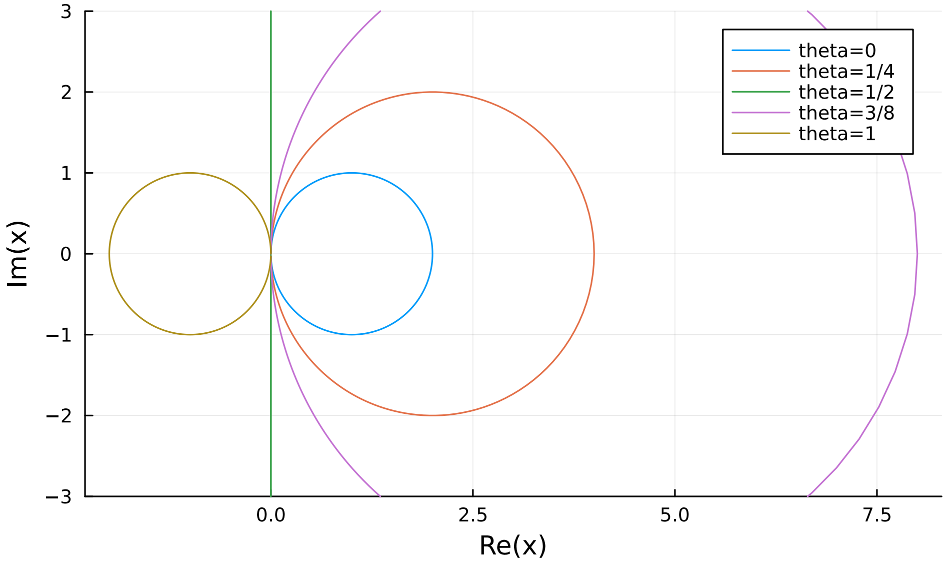
$$\partial\mathcal{D} = \left\{ \frac{e^{i\alpha}-1}{(1-\theta)e^{i\alpha}+\theta} : \alpha \in [0, 2\pi] \right\}.$$

We now use Julia to plot $\partial\mathcal{D}$ for $\theta = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{8}$ and 1. This is accomplished by the script

```
1 using Plots
2
3 z(r,theta)=(r-1)/((1-theta)r+theta)
4 alphas=0:pi/100:2*pi
5 rs=exp.(1im*alphas)
6 plot(z.(rs,0),label="theta=0",aspect_ratio=1.0,yrange=[-3,3])
7 plot!(z.(rs,1/4),label="theta=1/4")
8 plot!(z.(rs,1/2),label="theta=1/2")
9 plot!(z.(rs,3/8),label="theta=3/8")
10 plot!(z.(rs,1),label="theta=1")
11 savefig("plot1.pdf")
```

Note that `yrange` is set in the first plot command on line 6 to prevent the vertical line which occurs when $\theta = \frac{1}{2}$ from stretching infinity. Also note that when `plot` is passed an vector of complex numbers it automatically plots them as real-imaginary pairs on the complex plane.

The resulting graph is



The previous stability analysis is confirmed because the boundaries lie in the right-half plane when $\theta \leq 1/2$.

Exercise 4.5 Prove that for every ν-stage explicit Runge–Kutta method

$$\begin{aligned}
\xi_1 &= y_n,\\
\xi_2 &= y_n + ha_{21}f(t_n,\xi_1),\\
\xi_3 &= y_n + ha_{31}f(t_n,\xi_1) + ha_{32}f(t_n+c_2h,\xi_2),\\
&\ \vdots\\
\xi_\nu &= y_n + h\sum_{i=1}^{\nu-1} a_{\nu i}f(t_n+c_ih,\xi_i),\\
y_{n+1} &= y_n + h\sum_{j=1}^{\nu} b_j f(t_n+c_jh,\xi_j),
\end{aligned}$$

of order ν it is true that

$$r(z) = \sum_{k=0}^{\nu} \frac{1}{k!}z^k \qquad \text{for} \qquad z\in\mathbf{C}.$$

Solution: Recall Lemma 4.4 in the text which states

Lemma 4.4 *Suppose the solution sequence y_n for $n = 0, 1, 2, \ldots$ which is produced by applying a method of order p to the linear equation $y' = \lambda y$ with $y(0) = 1$ with a constant step size obeys $y_n = [r(h\lambda)]^n$. Then necessarily*

$$r(z) = e^z + \mathcal{O}(z^{p+1}) \qquad \textit{as} \qquad z\to 0.$$

We know already for an explicit Runge–Kutta method that $y_n = [r(h\lambda)]^n$ for some polynomial r of degree ν. The above lemma implies that if the method is of order ν then

$$r(z) = e^z + \mathcal{O}(z^{\nu+1}) \qquad \text{as} \qquad z\to 0.$$

Uniqueness of the Taylor polynomial implies $r(z)$ must agree with the Taylor series for e^z up to degree ν which also happens to be the degree of r. The desired result then follows.

Exercise 4.6 Evaluate explicitly the function r for the following Runge–Kutta methods:

$$
\mathbf{a}\quad \begin{array}{c|cc} 0 & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}, \qquad
\mathbf{b}\quad \begin{array}{c|cc} \frac{1}{6} & \frac{1}{6} & 0 \\ \frac{5}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad
\mathbf{c}\quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ 1 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}.
$$

Are these methods A-stable?

Solution: For a Runge–Kutta method

$$r(z) = 1 + zb \cdot (I - zA)^{-1}\mathbf{1} \qquad \text{for} \qquad z \in \mathbf{C}$$

where $\mathbf{1} = (1, \ldots, 1)$ is the vector of length ν whose entries consist of ones.

Part a When

$$A = \begin{bmatrix} 0 & 0 \\ \frac{1}{3} & \frac{1}{3} \end{bmatrix} \qquad \text{and} \qquad b = \begin{bmatrix} \frac{1}{4} \\ \frac{3}{4} \end{bmatrix}$$

we obtain that

$$(I - zA)^{-1} = \begin{bmatrix} 1 & 0 \\ -\frac{1}{3}z & 1 - \frac{1}{3}z \end{bmatrix}^{-1} = \frac{1}{1 - \frac{1}{3}z} \begin{bmatrix} 1 - \frac{1}{3}z & 0 \\ \frac{1}{3}z & 1 \end{bmatrix}.$$

Therefore

$$r(z) = 1 + z \begin{bmatrix} \frac{1}{4} \\ \frac{3}{4} \end{bmatrix} \cdot \frac{1}{1 - \frac{1}{3}z} \begin{bmatrix} 1 - \frac{1}{3}z \\ \frac{1}{3}z + 1 \end{bmatrix} = 1 + z\frac{1 + \frac{1}{6}z}{1 - \frac{1}{3}z} = \frac{1 + \frac{2}{3}z + \frac{1}{6}z^2}{1 - \frac{1}{3}z}.$$

To check if the method is A-stable first note there is a pole at 1/3 in the right half plane. However, since

$$\begin{aligned} |r(it)|^2 &= \frac{|1 + i\frac{2}{3}t - \frac{1}{6}t^2|^2}{|1 - i\frac{1}{3}t|^2} = \frac{(1 - \frac{1}{6}t^2)^2 + \frac{4}{9}t^2}{1 + \frac{1}{9}t^2} \\ &= \frac{1 + \frac{1}{9}t^2 + \frac{1}{36}t^4}{1 + \frac{1}{9}t^2} > 1 \qquad \text{for} \qquad t \neq 0, \end{aligned}$$

it follows that the method is not A-stable.

Part b When

$$A = \begin{bmatrix} \frac{1}{6} & 0 \\ \frac{2}{3} & \frac{1}{6} \end{bmatrix} \qquad \text{and} \qquad b = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$

we obtain that

$$(I - zA)^{-1} = \begin{bmatrix} 1 - \frac{1}{6}z & 0 \\ -\frac{2}{3}z & 1 - \frac{1}{6}z \end{bmatrix}^{-1} = \frac{1}{1 - \frac{1}{3}z + \frac{1}{36}z^2} \begin{bmatrix} 1 - \frac{1}{6}z & 0 \\ \frac{2}{3}z & 1 - \frac{1}{6}z \end{bmatrix}.$$

Therefore

$$\begin{aligned} r(z) &= 1 + z \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \cdot \frac{1}{1 - \frac{1}{3}z + \frac{1}{36}z^2} \begin{bmatrix} 1 - \frac{1}{6}z \\ 1 + \frac{1}{2}z \end{bmatrix} \\ &= 1 + z \frac{1 + \frac{1}{6}z}{1 - \frac{1}{3}z + \frac{1}{36}z^2} = \frac{1 + \frac{2}{3}z + \frac{7}{36}z^2}{1 - \frac{1}{3}z + \frac{1}{36}z^2}. \end{aligned}$$

To check if the method is A-stable first note there is a pole of multiplicity two at 1/6 in the right half plane. However, since

$$\begin{aligned} |r(it)|^2 &= \frac{|1 + i\frac{2}{3}t - \frac{7}{36}t^2|^2}{|1 - i\frac{1}{3}t - \frac{1}{36}t^2|^2} = \frac{(1 - \frac{7}{36}t^2)^2 + \frac{4}{9}t^2}{(1 - \frac{1}{36}t^2)^2 + \frac{1}{9}t^2} \\ &= \frac{1 + \frac{1}{18}t^2 + \frac{49}{1296}t^4}{1 + \frac{1}{18}t^2 + \frac{1}{1296}t^4} > 1 \qquad \text{for} \qquad t \neq 0, \end{aligned}$$

it again follows that the method is not A-stable.

Part c It's possible to do this one using the same linear algebra framework as before, but for variety we work from first principles. By definition

$$\begin{aligned} \xi_1 &= y_n \\ \xi_2 &= y_n + \tfrac{1}{4}h\lambda\xi_1 + \tfrac{1}{4}h\lambda\xi_2 \\ \xi_3 &= y_n + h\lambda\xi_2. \end{aligned}$$

Substituting $z = h\lambda$ and solving yields

$$\xi_2 = y_n + \tfrac{1}{4}zy_n + \tfrac{1}{4}z\xi_2 \qquad \text{and therefore} \qquad \xi_2 = \frac{1 + \frac{1}{4}z}{1 - \frac{1}{4}z}y_n.$$

Also

$$\xi_3 = y_n + z\frac{1+\frac{1}{4}z}{1-\frac{1}{4}z}y_n = \frac{1+\frac{3}{4}z+\frac{1}{4}z^2}{1-\frac{1}{4}z}y_n.$$

Finally

$$y_{n+1} = y_n + \tfrac{1}{6}zy_n + \tfrac{2}{3}z\frac{1+\frac{1}{4}z}{1-\frac{1}{4}z}y_n + \tfrac{1}{6}z\frac{1+\frac{3}{4}z+\frac{1}{4}z^2}{1-\frac{1}{4}z}y_n = r(z)y_n$$

where

$$r(z) = 1 + \tfrac{1}{6}z + \tfrac{2}{3}z\frac{1+\frac{1}{4}z}{1-\frac{1}{4}z} + \tfrac{1}{6}z\frac{1+\frac{3}{4}z+\frac{1}{4}z^2}{1-\frac{1}{4}z} = \frac{1+\frac{3}{4}z+\frac{1}{4}z^2+\frac{1}{24}z^3}{1-\frac{1}{4}z}.$$

Since

$$|r(-6)| = \left|\frac{1-\frac{9}{2}+9-9}{1+\frac{3}{2}}\right| = \tfrac{7}{5} > 1,$$

it follows that the method is not A-stable.

Exercise 4.7 Prove that the Padé approximation $\hat{r}_{0/3}$ is not A-acceptable.

Solution: By definition the $\hat{r}_{0/3}$ Padé approximation is the rational function with constant numerator and denominator a polynomial of degree 3 that best approximates the exponential function. Formula for the numerator and denominator are given in Theorem 4.5 in the text which reads

Theorem 4.5 *Given any integers $\alpha, \beta \geq 0$, there exists a unique function*

$$\hat{r}_{\alpha/\beta}(z) = \frac{\hat{p}_{\alpha/\beta}(z)}{\hat{q}_{\alpha/\beta}(z)} \qquad \textit{with} \qquad \hat{q}_{\alpha/\beta}(0) = 1$$

of order $\alpha + \beta$. Here $\hat{p}_{\alpha/\beta}$ is a polynomial of degree at most α and $\hat{q}_{\alpha/\beta}$ is a polynomial of degree at most β. The explicit forms of the numerator and the denominator are respectively

$$\hat{p}_{\alpha/\beta}(z) = \sum_{k=0}^{\alpha} \binom{\alpha}{k} \frac{(\alpha+\beta-k)!}{(\alpha+\beta)!} z^k$$

and

$$\hat{q}_{\alpha/\beta}(z) = \sum_{k=0}^{\beta} \binom{\beta}{k} \frac{(\alpha+\beta-k)!}{(\alpha+\beta)!} (-z)^k.$$

Using these formula we compute

$$\hat{p}_{0/3} = \sum_{k=0}^{0} \binom{0}{k} \frac{(3-k)!}{3!} z^k = 1$$

and further that

$$\hat{q}_{0/3}(z) = \sum_{k=0}^{3} \binom{3}{k} \frac{(3-k)!}{3!} (-z)^k = 1 - z + \tfrac{1}{2}z^2 - \tfrac{1}{6}z^3.$$

Therefore

$$\hat{r}_{0/3}(z) = \frac{1}{1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3}.$$

To see that $\hat{r}_{0/3}$ is not A-acceptable note that

$$|r(i)|^2 = \frac{1}{|1 - i - \frac{1}{2} + \frac{1}{6}i|^2} = \frac{1}{\frac{1}{4} + \frac{25}{36}} = \tfrac{18}{17} > 1.$$