Scientific Computation HW5

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Exercise 5.11

Determine the characteristic polynomials $\rho(\zeta)$ and $\sigma(\zeta)$ for the following linear multistep methods. Verify that (5.48) holds in each case.

(a) The 3-step Adams-Bashforth method,
The 3-step Adams-Bashforth method is given by the following:

$$U^{n+3} = U^{n+2} + \frac{k}{12}(5f(U^n) - 16f(U^{n+1}) + 23f(U^{n+2}))$$

Rewriting, we find

$$-U^{n+2} + U^{n+3} = k\left(\frac{5}{12}f(U^n) - \frac{16}{12}f(U^{n+1}) + \frac{23}{12}f(U^{n+2})\right)$$

Then we can see our characteristic polynomials for the 3-step Adams-Bashforth method are

$$\rho(\zeta) = \zeta^3 - \zeta^2$$
$$\sigma(\zeta) = \frac{5}{12} - \frac{16}{12}\zeta + \frac{23}{12}\zeta^2$$

Now we must verify that (5.48) holds:

$$\sum_{j=0}^{r} \alpha_j = 1 - 1 = 0$$
$$\sum_{j=0}^{r} j\alpha_j = 3 - 2 = 1$$
$$\sum_{j=0}^{r} \beta_j = \frac{5}{12} - \frac{16}{12} + \frac{23}{12} = 1 = \sum_{j=0}^{r} j\alpha_j$$

(b) The 3-step Adams-Moulton method,
The 3-step Adams-Moulton method is given by the following:

$$U^{n+3} = U^{n+2} + \frac{k}{24}(f(U^n) - 5f(U^{n+1}) + 19f(U^{n+2}) + 9f(U^{n+3}))$$

Rewriting, we find

$$-U^{n+2} + U^{n+3} = k\left(\frac{1}{24}f(U^n) - \frac{5}{24}f(U^{n+1}) + \frac{19}{24}f(U^{n+2}) + \frac{9}{24}f(U^{n+2})\right)$$

Then our characteristic polynomials are:

$$\rho(\zeta) = \zeta^3 - \zeta^2$$
$$\sigma(\zeta) = \frac{1}{24} - \frac{5}{24}\zeta + \frac{19}{24}\zeta^2 + \frac{9}{24}\zeta^3$$

Verifying (5.48):

$$\sum_{j=0}^{r} \alpha_j = -1 + 1 = 0$$
$$\sum_{j=0}^{r} j\alpha_j = 3 - 2 = 1$$
$$\sum_{j=0}^{r} \beta_j = \frac{1}{24} - \frac{5}{24} + \frac{19}{24} + \frac{9}{24} = 1 = \sum_{j=0}^{r} j\alpha_j$$

(c) The 2-step Simpson's method of Example 5.16.
The 2-step Simpson's method is given by the following:

$$U^{n+2} = U^n + \frac{2k}{6}(f(U^n) + 4f(U^{n+1}) + f(U^{n+2})$$

which we may rewrite as

$$-U^n + U^{n+2} = k\left(\frac{2}{6}f(U^n) + \frac{8}{6}f(U^{n+1}) + \frac{2}{6}f(U^{n+2})\right)$$

Then our characteristic polynomials are

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

Verifying (5.48):

$$\sum_{j=0}^{r} \alpha_j = 1 - 1 = 0$$
$$\sum_{j=0}^{r} j\alpha_j = 2$$
$$\sum_{j=0}^{r} \beta_j = \frac{1}{3} + \frac{4}{3} + \frac{1}{3} = 2 = \sum_{j=0}^{r} j\alpha_j$$

Exercise 5.12

(a) Verify that the predictor-corrector method (5.53) is second order accurate.
Recall the predictor-corrector method:

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

Rewriting, we have

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

Taylor expanding $f(U^n + kf(U^n))$, we find

$$f(U^n + kf(U^n)) = f(U^n) + kf(U^n)f'(U^n) + \frac{1}{2}(kf(U^n))^2 f''(U^n) + \mathcal{O}(k^3)$$

Now, to show this method is second order accurate, let us inspect the local truncation error:

$$\tau_n = \frac{u(t_{n+1}) - u(t_n)}{k} - \left(\frac{1}{2}(2f(u^n) + kf(u^n)f'(u^n) + \frac{1}{2}(kf(u^n))^2 f''(u^n) + \mathcal{O}(k^3)\right)$$

Notice

$$u(t_{n+1}) = u(t_n) + ku'(t_n) + \frac{k^2}{2}u''(t_n) + \frac{k^3}{6}u'''(t_n) + \mathcal{O}(k^4)$$

So

$$\tau_n = u'(t_n) + \frac{k}{2}u''(t_n) + \frac{k^2}{6}u'''(t_n) - f(u(t_n)) - \frac{k}{2}f(u(t_n))f'(u(t_n)) - \frac{1}{4}(kf(u(t_n)))^2 f''(u(t_n)) + \mathcal{O}(k^3)$$

Since $f(u) = u'$, we have $f'(u)u' = u''$, we have

$$\begin{aligned}
\tau_n &= u'(t_n) + \frac{k}{2}u''(t_n) + \frac{k^2}{6}u'''(t_n) - u'(t_n) - \frac{k}{2}u''(t_n) - \frac{1}{4}(kf(u(t_n)))^2 f''(u(t_n)) + \mathcal{O}(k^3) \\
&= \frac{k^2}{6}u'''(t_n) - \frac{1}{4}(kf(u(t_n)))^2 f''(u(t_n)) + \mathcal{O}(k^3) \\
&= \mathcal{O}(k^2)
\end{aligned}$$

So the predictor corrector method is second order accurate.

(b) Show that the predictor-corrector method obtained by predicting with the 2-step Adams-Bashforth method followed by correcting with the 2-step Adams Moulton method is third order accurate.
The predictor-corrector method described above is given by the following:

$$\begin{aligned}
\hat{U}^{n+2} &= U^{n+1} + \frac{k}{2}(-f(U^n) + 3f(U^{n+1})) \\
U^{n+2} &= U^{n+1} + \frac{k}{12}(-f(U^n) + 8f(U^{n+1}) + 5f(\hat{U}^{n+2})
\end{aligned}$$

Then the local truncation error is given by

$$\tau_n = 12\frac{u_{n+2} - u_{n+1}}{k} - (-f(u_n) + 8f(u_{n+1}) + 5f(\hat{u}_{n+2}))$$

Let us begin by expanding $(u_{n+2} - u_{n+1})/k$ and simplifying by means of Taylor series:

$$\begin{aligned}
\frac{u_{n+2} - u_{n+1}}{k} &= u_n' + \frac{3k}{2}u_n'' + \frac{7k^2}{6}u_n''' + \frac{15k^3}{24}u_n'''' + \mathcal{O}(k^4) \\
12\frac{u_{n+2} - u_{n+1}}{k} &= 12u_n' + 18ku_n'' + 14k^2u_n''' + \frac{15k^3}{2}u_n'''' + \mathcal{O}(k^4)
\end{aligned}$$

Now, we must expand $-f(u_n) + 8f(u_{n+1}) + 5f(\hat{u}_{n+2})$. Let us begin by expanding $f(\hat{u}_{n+2})$:

$$\begin{aligned}
f(\hat{u}_{n+2}) &= f\left(u_{n+1} + \frac{k}{2}(-f(u_n) + 3f(u_{n+1}))\right) \\
&= \lambda\left(u_{n+1} + \frac{k}{2}(-\lambda u_n + 3\lambda u_{n+1})\right) \\
&= \lambda\left(u_n + ku_n' + \frac{k^2}{2}u_n'' + frack^3 6u_n''' + \lambda k u_n + \frac{3k^2}{2}\lambda u_n' + \frac{3k^3}{4}\lambda u_n'' + \mathcal{O}(k^4)\right) \\
&= \lambda\left(u_n + 2ku_n' + 2k^2u_n'' + \frac{11k^3}{12}u_n''' + \mathcal{O}(k^4)\right) \\
&= u_n' + 2ku_n'' + 2k^2u_n''' + \frac{11k^3}{12}u_n'''' + \mathcal{O}(k^4)
\end{aligned}$$

Now $-f(u_n) + 8f(u_{n+1})$:

$$\begin{aligned}
-f(u_n) + 8f(u_{n+1}) &= -\lambda u_n + 8\lambda\left(u_n + ku_n' + \frac{k^2}{2}u_n'' + \frac{k^3}{6}u_n''' + \mathcal{O}(k^4)\right) \\
&= 7u_n' + 8ku_n'' + 4k^2u_n''' + \frac{4k^3}{3}u_n'''' + \mathcal{O}(k^4)
\end{aligned}$$

Adding them up $(-f(u_n) + 8f(u_{n+1}) + 5f(\hat{u}_{n+2}))$:

$$\begin{aligned}
-f(u_n) + 8f(u_{n+1}) + 5f(\hat{u}_{n+2}) &= 7u_n' + 8ku_n'' + 4k^2u_n''' + \frac{4k^3}{3}u_n'''' + 5u_n' + 10ku_n'' + 10k^2u_n''' + \frac{55k^3}{12}u_n'''' + \mathcal{O}(k^4) \\
&= 12u_n' + 18ku_n'' + 14k^2u_n''' + \frac{59k^3}{12}u_n'''' + \mathcal{O}(k^4)
\end{aligned}$$

Finally,

$$\begin{aligned}
\tau_n &= 12u_n' + 18ku_n'' + 14k^2u_n''' + \frac{15k^3}{2}u_n'''' - 12u_n' - 18ku_n'' - 14k^2u_n''' - \frac{55k^3}{12}u_n'''' + \mathcal{O}(k^4) \\
&= \frac{35k^3}{12}u_n'''' + \mathcal{O}(k^4) \\
&= \mathcal{O}(k^3)
\end{aligned}$$

So this method is third order accurate (at least for the problem $u' = \lambda u$).

Exercise 5.13

Consider the Runge-Kutta methods defined by the tableaux below. In each case show that the method is third order accurate in two different ways: First by checking that the order conditions (5.35), (5.37), and (5.38) are satisfied, and then by applying one step of the method to $u' = \lambda u$ and verifying that the Taylor series expansion of $e^{k\lambda}$ is recovered to the expected order.

We must show the following conditions are satisfied for each method:

$$\sum_{j=1}^{r} a_{ij} = c_i, \quad i = 1, 2, \ldots, r,$$
$$\sum_{j=1}^{r} b_j = 1$$
$$\sum_{j=1}^{r} b_j c_j = \frac{1}{2}$$
$$\sum_{j=1}^{r} b_j c_j^2 = \frac{1}{3}$$
$$\sum_{i=1}^{r} \sum_{j=1}^{r} b_i a_{ij} c_j = \frac{1}{6}$$

(a) Runge's 3rd order method:

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1 & 0 & 1 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/3 & 0 & 1/6 \end{array}$$

By inspection, we can see that the first condition ($\sum_{j=1}^{r} a_{ij} = c_i$) is satisfied since each row in the tableaux clearly adds up to the leftmost column. Now, let us confirm the second condition:

$$\sum_{j=1}^{r} b_j = \frac{1}{6} + \frac{2}{3} + 0 + \frac{1}{6} = 1$$

Now the third condition:

$$\sum_{j=1}^{r} b_j c_j = 0\left(\frac{1}{6}\right) + \frac{1}{2}\left(\frac{2}{3}\right) + 1(0) + 1\left(\frac{1}{6}\right) = \frac{1}{3} + \frac{1}{6} = \frac{1}{2}$$

And the fourth condition:

$$\sum_{j=1}^{r} b_j c_j^2 = \left(\frac{1}{6}\right) 0^2 + \left(\frac{2}{3}\right)\left(\frac{1}{2}\right)^2 + 0(1)^2 + \left(\frac{1}{6}\right)(1)^2 = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$$

And finally, the fifth condition:

$$\begin{aligned} \sum_{i=1}^{r} \sum_{j=1}^{r} b_i a_{ij} c_j &= \sum_{i=1}^{r} b_i (a_{i1} c_1 + a_{i2} c_2 + a_{i3} c_3 + a_{i4} c_4) \\ &= c_1 \sum_{j=1}^{r} b_i a_{i1} + c_2 \sum_{j=1}^{r} b_i a_{i2} + c_3 \sum_{j=1}^{r} b_i a_{i3} + c_4 \sum_{j=1}^{r} b_i a_{i4} \\ &= 0\left(\frac{1}{3}\right) + \frac{1}{2}(0) + 1\left(\frac{1}{6}\right) + 1(0) \\ &= \frac{1}{6} \end{aligned}$$

So all the conditions are satisfied. So Runge's 3rd order method is indeed 3rd order method.

(b) Heun's 3rd order method:

$$\begin{array}{c|ccc} 0 & & & \\ 1/3 & 1/3 & & \\ 2/3 & 0 & 2/3 & \\ \hline & 1/4 & 0 & 3/4 \end{array}$$

To begin, notice that each c_j is equal to the sum of the rows of the a_{ij}s, so the first condition is satisfied. Now, let us inspect the sum of the b_j:

$$\sum_{j=1}^{r} b_j = \frac{1}{4} + 0 + \frac{3}{4} = 1$$

So the second condition is satisfied. Now let us inspect the sum of $b_j c_j$:

$$\sum_{j=1}^{j} b_j c_j = 0\left(\frac{1}{4}\right) + \left(\frac{1}{3}\right)0 + \left(\frac{2}{3}\right)\left(\frac{3}{4}\right) = \frac{1}{2}$$

So the third condition is satisfied. Now let us inspect the sum of $b_j c_j^2$:

$$\sum_{j=1}^{r} b_j c_j^2 = \left(\frac{1}{4}\right)0^2 + 0\left(\frac{1}{3}\right)^2 + \left(\frac{3}{4}\right)\left(\frac{2}{3}\right)^2 = \frac{1}{3}$$

So the fourth condition is satisfied. Finally, let us inspect the sum of $b_j a_{ij} c_i$:

$$\begin{aligned} \sum_{i=1}^{r}\sum_{j=1}^{r} b_i a_{ij} c_j &= \sum_{i=1}^{r} b_i(a_{i1}c_1 + a_{i2}c_2 + a_{i3}c_3) \\ &= \frac{1}{3}\sum_{i=1}^{r} b_i a_{i2} + \frac{2}{3}\sum_{i=1}^{r} b_i a_{i3} \\ &= \frac{1}{3}\left(\frac{1}{2}\right) = \frac{1}{6} \end{aligned}$$

So all conditions for third order accuracy are satisfied. Thus, Heun's third order method is indeed third order accurate.

Exercise 17

(a) Apply the trapezoidal rule to the equation $u' = \lambda u$ and show

$$U^{n+1} = \frac{1 + z/2}{1 - z/2} U^n$$

where $z = \lambda k$.
Recall the trapezoidal rule:

$$\frac{U^{n+1} - U^n}{k} = \frac{1}{2}(f(U^n) + f(U^{n+1}))$$

Applying this to $u' = \lambda u$, we see $f(u) = \lambda u$ and so the trapezoidal rule in this case becomes

$$\begin{aligned} U^{n+1} &= U^n + \frac{\lambda k}{2} U^n + \frac{\lambda k}{2} U^{n+1} \\ \left(1 - \frac{\lambda k}{2}\right) U^{n+1} &= \left(1 + \frac{\lambda k}{2}\right) U^n \\ U^{n+1} &= \frac{1 + z/2}{1 - z/2} U^n \end{aligned}$$

where $z = \lambda k$.

(b) Let

$$R(z) = \frac{1 + z/2}{1 - z/2}$$

Show that $R(z) = e^z + \mathcal{O}(k^3)$ and conclude that the one step error of the trapezoidal method on this problem is $\mathcal{O}(k^3)$.
Notice that we may expand $\frac{1}{1-z/2}$ as

$$\frac{1}{1 - z/2} = 1 + \left(\frac{z}{2}\right) + \left(\frac{z}{2}\right)^2 + \left(\frac{z}{2}\right)^3 + \cdots$$

Multiplying by $1 + z/2$, we find

$$\begin{aligned} \frac{1 + z/2}{1 - z/2} &= 1 + \left(\frac{z}{2}\right) + \left(\frac{z}{2}\right)^2 + \left(\frac{z}{2}\right)^3 + \cdots + \frac{z}{2} + \left(\frac{z}{2}\right)^2 + \left(\frac{z}{2}\right)^3 + \left(\frac{z}{2}\right)^4 + \cdots \\ &= 1 + z + \frac{z}{2} + \frac{z^3}{6} + \frac{z^3}{12} + \frac{z^4}{6} + \cdots \\ &= e^z + \mathcal{O}(z^3) \end{aligned}$$

So this method is third order accurate for $u' = \lambda u$.