Exercise 2.1 Derive the three-step and four-step Adams–Moulton methods and the three-step Adams–Bashforth method.

Solution: For the three-step Adams–Moulton method set $\rho(w) = w^2(w-1)$ and look for the polynomial $\sigma(w)$ of degree 3 such that

$$\rho(w) - \sigma(w)\log w = \mathcal{O}\big(|w-1|^4\big).$$

Substituting $\xi = w - 1$ yields

$$\begin{aligned}\frac{\rho(w)}{\log w} = \frac{\rho(1+\xi)}{\log(1+\xi)} &= \frac{(1+\xi)^2\xi}{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \frac{1}{4}\xi^4 + \mathcal{O}(\xi^5)}\\ &= \frac{1+2\xi+\xi^2}{1 - \frac{1}{2}\xi + \frac{1}{3}\xi^2 - \frac{1}{4}\xi^3 + \mathcal{O}(\xi^4)}.\end{aligned}$$

Next, since

$$\frac{1}{1-\alpha} = 1 + \alpha + \alpha^2 + \alpha^3 + \frac{\alpha^4}{1-\alpha}$$

then setting

$$\begin{aligned}\alpha &= \tfrac{1}{2}\xi - \tfrac{1}{3}\xi^2 + \tfrac{1}{4}\xi^3 + \mathcal{O}(\xi^4)\\ \alpha^2 &= \tfrac{1}{4}\xi^2 - \tfrac{1}{3}\xi^3 + \mathcal{O}(\xi^4)\\ \alpha^3 &= \tfrac{1}{8}\xi^3 + \mathcal{O}(\xi^4)\end{aligned}$$

yields

$$\frac{\xi}{\log(1+\xi)} = 1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \tfrac{1}{24}\xi^3 + \mathcal{O}(\xi^4).$$

Consequently,

$$\begin{aligned}\frac{\rho(w)}{\log w} &= (1+2\xi+\xi^2)\big(1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \tfrac{1}{24}\xi^3 + \mathcal{O}(\xi^4)\big)\\ &= 1 + \tfrac{5}{2}\xi + \tfrac{23}{12}\xi^2 + \tfrac{3}{8}\xi^3 + \mathcal{O}(\xi^4)\end{aligned}$$

and we take

$$\begin{aligned}\sigma(w) &= 1 + \tfrac{5}{2}(w-1) + \tfrac{23}{12}(w-1)^2 + \tfrac{3}{8}(w-1)^3\\ &= 1 + \tfrac{5}{2}(w-1) + \tfrac{23}{12}(w^2-2w+1) + \tfrac{3}{8}(w^3-3w^2+3w-1)\\ &= \tfrac{3}{8}w^3 + \tfrac{19}{24}w^2 - \tfrac{5}{24}w + \tfrac{1}{24}.\end{aligned}$$

Therefore the 3-step Adams–Moulton method is

$$\begin{aligned} y_{n+3} = y_{n+2} + h\big[\tfrac{3}{8} f(t_{n+3}, y_{n+3}) &+ \tfrac{19}{24} f(t_{n+2}, y_{n+2}) \\ &- \tfrac{5}{24} f(t_{n+1}, y_{n+1}) + \tfrac{1}{24} f(t_n, y_n)\big]. \end{aligned}$$

The four-step Adams–Moulton method is similar. Set $\rho(w) = w^3(w-1)$ and look for the polynomial $\sigma(w)$ of degree 4 such that

$$\rho(w) - \sigma(w)\log w = \mathcal{O}\big(|w-1|^5\big).$$

Substituting $\xi = w - 1$ and taking all expansions one step further

$$\begin{aligned} \frac{\rho(w)}{\log w} = \frac{\rho(1+\xi)}{\log(1+\xi)} &= \frac{(1+\xi)^3\xi}{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \frac{1}{4}\xi^4 + \frac{1}{5}\xi^5 + \mathcal{O}(\xi^6)} \\ &= \frac{1 + 3\xi + 3\xi^2 + \xi^3}{1 - \frac{1}{2}\xi + \frac{1}{3}\xi^2 - \frac{1}{4}\xi^3 + \frac{1}{5}\xi^4 + \mathcal{O}(\xi^5)}. \end{aligned}$$

Next, since

$$\frac{1}{1-\alpha} = 1 + \alpha + \alpha^2 + \alpha^3 + \alpha^4 + \frac{\alpha^5}{1-\alpha}$$

then setting

$$\begin{aligned} \alpha &= \tfrac{1}{2}\xi - \tfrac{1}{3}\xi^2 + \tfrac{1}{4}\xi^3 - \tfrac{1}{5}\xi^4 + \mathcal{O}(\xi^5) \\ \alpha^2 &= \tfrac{1}{4}\xi^2 - \tfrac{1}{3}\xi^3 + \tfrac{13}{36}\xi^4 + \mathcal{O}(\xi^5) \\ \alpha^3 &= \tfrac{1}{8}\xi^3 - \tfrac{1}{4}\xi^4 + \mathcal{O}(\xi^5) \\ \alpha^4 &= \tfrac{1}{16}\xi^4 + \mathcal{O}(\xi^5) \end{aligned}$$

yields

$$\frac{\xi}{\log(1+\xi)} = 1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \tfrac{1}{24}\xi^3 - \tfrac{19}{720}\xi^4 + \mathcal{O}(\xi^5).$$

Consequently,

$$\begin{aligned} \frac{\rho(w)}{\log w} &= (1 + 3\xi + 3\xi^2 + \xi^3)\big(1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \tfrac{1}{24}\xi^3 - \tfrac{19}{720}\xi^4 + \mathcal{O}(\xi^5)\big) \\ &= 1 + \tfrac{7}{2}\xi + \tfrac{53}{12}\xi^2 + \tfrac{55}{24}\xi^3 + \tfrac{251}{720}\xi^4 + \mathcal{O}(\xi^5) \end{aligned}$$

and we take

$$\begin{aligned}\sigma(w) &= 1 + \tfrac{7}{2}(w-1) + \tfrac{53}{12}(w-1)^2 + \tfrac{55}{24}(w-1)^3 + \tfrac{251}{720}(w-1)^4 \\ &= \tfrac{251}{720}w^4 + \tfrac{323}{360}w^3 - \tfrac{11}{30}w^2 + \tfrac{53}{360}w - \tfrac{19}{720}.\end{aligned}$$

Therefore the 4-step Adams–Moulton method is

$$\begin{aligned}y_{n+4} = y_{n+3} + h\big[&\tfrac{251}{720}f(t_{n+4},y_{n+4}) + \tfrac{323}{360}f(t_{n+3},y_{n+3}) \\ &- \tfrac{11}{30}f(t_{n+2},y_{n+2}) + \tfrac{53}{360}f(t_{n+1},y_{n+1}) - \tfrac{19}{720}f(t_n,y_n)\big].\end{aligned}$$

The last is the three-step Adams–Bashforth method. In this case $\rho(w) = w^2(w-1)$ as for the three-step Adams–Moulton method but $\sigma(w)$ is now chosen to be the second degree polynomial such that

$$\rho(w) - \sigma(w)\log w = \mathcal{O}\big(|w-1|^3\big).$$

Therefore, everything can be computed using fewer terms. Substituting $\xi = w - 1$ yields

$$\begin{aligned}\frac{\rho(w)}{\log w} = \frac{\rho(1+\xi)}{\log(1+\xi)} &= \frac{(1+\xi)^2\xi}{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 + \mathcal{O}(\xi^4)} \\ &= \frac{1 + 2\xi + \xi^2}{1 - \frac{1}{2}\xi + \frac{1}{3}\xi^2 + \mathcal{O}(\xi^3)}.\end{aligned}$$

Next, since

$$\frac{1}{1-\alpha} = 1 + \alpha + \alpha^2 + \frac{\alpha^3}{1-\alpha}$$

then setting

$$\begin{aligned}\alpha &= \tfrac{1}{2}\xi - \tfrac{1}{3}\xi^2 + \mathcal{O}(\xi^3) \\ \alpha^2 &= \tfrac{1}{4}\xi^2 + \mathcal{O}(\xi^3)\end{aligned}$$

yields

$$\frac{\xi}{\log(1+\xi)} = 1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \mathcal{O}(\xi^3).$$

Consequently,

$$\begin{aligned}\frac{\rho(w)}{\log w} &= (1 + 2\xi + \xi^2)\big(1 + \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \mathcal{O}(\xi^3)\big) \\ &= 1 + \tfrac{5}{2}\xi + \tfrac{23}{12}\xi^2 + \mathcal{O}(\xi^3)\end{aligned}$$

and we take

$$\begin{aligned}\sigma(w) &= 1 + \tfrac{5}{2}(w-1) + \tfrac{23}{12}(w-1)^2\\ &= 1 + \tfrac{5}{2}(w-1) + \tfrac{23}{12}(w^2-2w+1)\\ &= \tfrac{23}{12}w^2 - \tfrac{4}{3}w + \tfrac{5}{12}.\end{aligned}$$

Therefore the 3-step Adams–Bashforth method is

$$y_{n+3} = y_{n+2} + h\big[\tfrac{23}{12}f(t_{n+2},y_{n+2}) - \tfrac{4}{3}f(t_{n+1},y_{n+1}) + \tfrac{5}{12}f(t_n,y_n)\big].$$

As a remark, it seems odd to me that this problem ends with the 3-step Adams–Bashforth method which is the easiest to derive scheme.

Exercise 2.4 Determine the order of the three-step method

$$\begin{aligned}y_{n+3} - y_n = h\big[&\tfrac{3}{8}f(t_{n+3}, y_{n+3}) + \tfrac{9}{8}f(t_{n+2}, y_{n+2}) + \tfrac{9}{8}f(t_{n+1}, y_{n+1}) \\ &+ \tfrac{3}{8}f(t_n, y_n)\big],\end{aligned}$$

the three-eights scheme. Is it convergent?

Solution: The truncation error is

$$\begin{aligned}\psi_n &= y(t_{n+3}) - y(t_n) - h\big[\tfrac{3}{8}f(t_{n+3}, y(t_{n+3})) + \tfrac{9}{8}f(t_{n+2}, y(t_{n+2})) \\ &\qquad + \tfrac{9}{8}f(t_{n+1}, y(t_{n+1})) + \tfrac{3}{8}f(t_n, y(t_n))\big] \\ &= y(t_{n+3}) - y(t_n) - h\big[\tfrac{3}{8}y'(t_{n+3}) + \tfrac{9}{8}y'(t_{n+2}) \\ &\qquad + \tfrac{9}{8}y'(t_{n+1}) + \tfrac{3}{8}y'(t_n)\big].\end{aligned}$$

Taylor series imply

$$\begin{aligned}&y(t_{n+3}) - y(t_n) \\ &\quad = 3hy'(t_n) + \frac{(3h)^2}{2}y''(t_n) + \frac{(3h)^3}{6}y^{(3)}(t_n) + \frac{(3h)^4}{24}y^{(4)}(t_n) + \mathcal{O}(h^5) \\ &\quad = 3hy'(t_n) + \tfrac{9h^2}{2}y''(t_n) + \tfrac{9h^3}{2}y^{(3)}(t_n) + \tfrac{9h^4}{8}y^{(4)}(t_n) + \mathcal{O}(h^5)\end{aligned}$$

and also

$$\begin{aligned}y'(t_{n+3}) &= y'(t_n) + 3hy''(t_n) + \frac{(3h)^2}{2}y^{(3)}(t_n) + \frac{(3h)^3}{6}y^{(4)}(t_n) + \mathcal{O}(h^4) \\ y'(t_{n+2}) &= y'(t_n) + 2hy''(t_n) + \frac{(2h)^2}{2}y^{(3)}(t_n) + \frac{(2h)^3}{6}y^{(4)}(t_n) + \mathcal{O}(h^4) \\ y'(t_{n+1}) &= y'(t_n) + hy''(t_n) + \frac{h^2}{2}y^{(3)}(t_n) + \frac{h^3}{6}y^{(4)}(t_n) + \mathcal{O}(h^4).\end{aligned}$$

Since

$$\begin{aligned}\tfrac{3}{8}y'(t_{n+3}) &= \tfrac{3}{8}y'(t_n) + \tfrac{9h}{8}y''(t_n) + \tfrac{27h^2}{16}y^{(3)}(t_n) + \tfrac{27h^3}{16}y^{(4)}(t_n) + \mathcal{O}(h^4) \\ \tfrac{9}{8}y'(t_{n+2}) &= \tfrac{9}{8}y'(t_n) + \tfrac{9h}{4}y''(t_n) + \tfrac{9h^2}{4}y^{(3)}(t_n) + \tfrac{3h^3}{2}y^{(4)}(t_n) + \mathcal{O}(h^4) \\ \tfrac{9}{8}y'(t_{n+1}) &= \tfrac{9}{8}y'(t_n) + \tfrac{9h}{8}y''(t_n) + \tfrac{9h^2}{16}y^{(3)}(t_n) + \tfrac{3h^3}{16}y^{(4)}(t_n) + \mathcal{O}(h^4)\end{aligned}$$

then

$$\begin{aligned}
&\tfrac{3}{8}y'(t_{n+3}) + \tfrac{9}{8}y'(t_{n+2}) + \tfrac{9}{8}y'(t_{n+1}) + \tfrac{3}{8}y'(t_n) \\
&\qquad\qquad = 3y'(t_n) + \tfrac{9h}{2}y''(t_n) + \tfrac{9h^2}{2}y^{(3)}(t_n) + \tfrac{27h^3}{8}y^{(4)}(t_n) + \mathcal{O}(h^4).
\end{aligned}$$

It follows that

$$\begin{aligned}
\psi_n &= 3hy'(t_n) + \tfrac{9h^2}{2}y''(t_n) + \tfrac{9h^3}{2}y^{(3)}(t_n) + \tfrac{9h^4}{8}y^{(4)}(t_n) + \mathcal{O}(h^5) \\
&\quad - h\big[3y'(t_n) + \tfrac{9h}{2}y''(t_n) + \tfrac{9h^2}{2}y^{(3)}(t_n) + \tfrac{27h^3}{8}y^{(4)}(t_n) + \mathcal{O}(h^4)\big] \\
&= -\tfrac{9h^4}{4}y^{(4)}(t_n) + \mathcal{O}(h^5).
\end{aligned}$$

As $\psi_n = \mathcal{O}(h^4)$ and no more, then the three-eights method is order 3.

The fact that the three-eights method convergent follows from the Dahlquist equivalence by checking the root condition. In this case

$$\rho(w) = w^3 - 1 = (w-1)(w^2 + w + 1)$$

and setting $a = 1$, $b = 1$ and $c = 1$ in the quadratic formula yields

$$w = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-1 \pm i\sqrt{3}}{2}$$

which are the two complex cubic roots of unity.

As all roots are simple and on the boundary of the unit disk, the root condition is satisfied. This shows the method is convergent.

Exercise 2.7 Prove that the backward differentiation formulae

$$y_{n+2} - \tfrac{4}{3}y_{n+1} + \tfrac{1}{3}y_n = \tfrac{2}{3}hf(t_{n+2}, y_{n+2}) \tag{2.15}$$

$$y_{n+3} - \tfrac{18}{11}y_{n+2} + \tfrac{9}{11}y_{n+1} - \tfrac{2}{11}y_n = \tfrac{6}{11}hf(t_{n+3}, y_{n+3}) \tag{2.16}$$

are convergent.

Solution: By the Dahlquist equivalence theorem it is sufficient to show that the multistep method is of order $p \geq 1$ and the polynomial ρ obeys the root condition. From the derivations of (2.15) and (2.16) we already know the orders of these methods are $p = 2$ and $p = 3$ respectively. What's left is to check the root condition.

For (2.15) we have

$$\rho(w) = w^2 - \tfrac{4}{3}w + \tfrac{1}{3}$$

Since $\rho(1) = 0$ as it always will, we know that $w - 1$ is a factor. Dividing then yields that

$$\rho(w) = (w - 1)(w - \tfrac{1}{3})$$

and so the roots are $w = 1$ and $w = \frac{1}{3}$. The root $w = 1$ is on the boundary of the unit disk and simple (multiplicity 1) while the root $w = \frac{1}{3}$ is strictly inside. Therefore the root condition is satisfied and the method convergent.

For (2.16) we have

$$\rho(w) = w^3 - \tfrac{18}{11}w^2 + \tfrac{9}{11}w - \tfrac{2}{11}$$

In this case dividing by $w - 1$ yields

$$\rho(w) = (w - 1)(w^2 - \tfrac{7}{11}w + \tfrac{2}{11})$$

The roots of the quadratic term may be obtained setting $a = 1$, $b = -\frac{7}{11}$ and $c = \frac{2}{11}$ in the quadratic formula as

$$w = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{7/11 \pm \sqrt{(7/11)^2 - 4(2/11)}}{2} = \frac{7 \pm i\sqrt{39}}{22}.$$

Since

$$\Big|\frac{7 \pm i\sqrt{39}}{22}\Big| = \frac{\sqrt{7^2 + 39}}{22} = \frac{\sqrt{88}}{22} = \sqrt{\frac{2}{11}} < 1$$

the roots of the quadratic factor are strictly inside the unit disc. Therefore the method is convergent.

Exercise 2.9 An s-step method with $\sigma(w) = \beta w^{s-1}(w+1)$ and order s might be superior to a BDF in certain situations.

a Find a general formula for ρ and β as done for the BDF.

Solution: As this is an implicit method, the goal is to find a monic polynomial $\rho(w)$ such that

$$\rho(w) - \sigma(w)\log w = \mathcal{O}\big(|w-1|^{s+1}\big).$$

In order to avoid multiplication of Taylor series we set $v = w^{-1}$, note that $\mathcal{O}(|w-1|^{s+1}) = \mathcal{O}(|v-1|^{s-1})$ as $w \to 1$ and write

$$v^s \rho(v^{-1}) = -\beta(1+v)\log v + \mathcal{O}\big(|v-1|^{s+1}\big).$$

Since

$$\log v = \log(1 + (v-1)) = \sum_{m=1}^{s} \frac{(-1)^{m-1}}{m}(v-1)^m + \mathcal{O}\big(|v-1|^{s+1}\big),$$

it follows that

$$\begin{aligned}
(1+v)\log v &= (2 + (v-1))\log v \\
&= 2\sum_{m=1}^{s} \frac{(-1)^{m-1}}{m}(v-1)^m + \sum_{m=1}^{s-1} \frac{(-1)^{m-1}}{m}(v-1)^{m+1} + \mathcal{O}\big(|v-1|^{s+1}\big) \\
&= 2(v-1) + \sum_{m=2}^{s} \left\{\frac{2(-1)^{m-1}}{m} + \frac{(-1)^m}{m-1}\right\}(v-1)^m + \mathcal{O}\big(|v-1|^{s+1}\big) \\
&= 2(v-1) + \sum_{m=2}^{s} \left\{\frac{(-1)^m}{m-1} - \frac{2(-1)^m}{m}\right\}(v-1)^m + \mathcal{O}\big(|v-1|^{s+1}\big) \\
&= 2(v-1) + \sum_{m=3}^{s} \frac{2-m}{m^2-m}(1-v)^m + \mathcal{O}\big(|v-1|^{s+1}\big).
\end{aligned}$$

We deduce that

$$v^s\rho(v^{-1}) = \beta\Big\{2(1-v) + \sum_{m=3}^{s} \frac{m-2}{m^2-m}(1-v)^m\Big\}$$

Therefore

$$\begin{aligned}\rho(w) &= \beta v^{-s}\Big\{2(1-v) + \sum_{m=3}^{s} \frac{m-2}{m^2-m}(1-v)^m\Big\}\\ &= \beta\Big\{2(w^s - w^{s-1}) + \sum_{m=3}^{s} \frac{m-2}{m^2-m} w^{s-m}(w-1)^m\Big\}\end{aligned}$$

To finish the problem we find the value of β so that $\rho(w)$ is a monic polynomial. Equating coefficients of w^s yields

$$\beta = \Big(2 + \sum_{m=3}^{s} \frac{m-2}{m^2-m}\Big)^{-1}.$$

b Derive explicitly such methods for $s = 2$ and $s = 3$.

Solution: If $s = 2$ then $\beta = 1/2$ and

$$\rho(w) = 2\beta(w^2 - w) = w^2 - w.$$

The resulting method is

$$y_{n+2} = y_{n+1} + \tfrac{h}{2}\big[f(t_{n+2}, y_{n+2}) + f(t_{n+1}, y_{n+1})\big]$$

which is actually a one-step method and the trapezoid method in disguise.

If $s = 3$ then $\beta = (2 + \frac{1}{6})^{-1} = \frac{6}{13}$ and

$$\begin{aligned}\rho(w) &= \tfrac{12}{13}(w^3 - w^2) + \tfrac{1}{13}(w-1)^3\\ &= \tfrac{12}{13}(w^3 - w^2) + \tfrac{1}{13}(w^3 - 3w^2 + 3w - 1)\\ &= w^3 - \tfrac{15}{13}w^2 + \tfrac{3}{13}w - \tfrac{1}{13}.\end{aligned}$$

The resulting method is

$$y_{n+3} = \tfrac{15}{13}y_{n+2} - \tfrac{3}{13}y_{n+1} - \tfrac{1}{13}y_n + \tfrac{6h}{13}\big[f(t_{n+3}, y_{n+3}) + f(t_{n+2}, y_{n+2})\big].$$

c Are the last two methods convergent?

Solution: When $s = 2$ the trapezoid method is convergent. When $s = 3$ we check the root condition. Factoring the root at $w = 1$ yields

$$\rho(w) = (w-1)(w^2 - \tfrac{2}{13}w + \tfrac{1}{13}).$$

The quadratic formula with $a = 1$, $b = -\frac{2}{13}$ and $c = \frac{1}{13}$ yields

$$w = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{2 \pm \sqrt{4 - 52}}{26} = \frac{1 \pm i\sqrt{12}}{13}.$$

Therefore

$$\left|\frac{1 \pm i\sqrt{12}}{13}\right| = \frac{\sqrt{13}}{13} = \frac{1}{\sqrt{13}} < 1$$

and the Dahlquist equivalence implies the $s = 3$ method is also convergent.