6.4 Adams-Bashforth-Moulton methods

The most famous linear multistep methods are constructed by the means of interpolation. For instance by the following strategy:

The solution of the ODE satisfy the integral equation

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} f(t, y(t))dt. \tag{48}$$

Assume that we have found $f_i = f(t_i, y_i)$ for $i = n-k+1, \cdots, n$, with $t_i = t_0 + ih$. Construct the polynomial of degree $k-1$, satisfying

$$p_{k-1}(t_i) = f(t_i, y_i), \qquad i = n-k+1, \ldots, n.$$

The interpolation points are equidistributed (constant stepsize), so Newton's backward difference formula can be used in this case (see Exercise 2), that is

$$p_{k-1}(t) = p_{k-1}(t_n + sh) = f_n + \sum_{j=1}^{k-1} (-1)^j \binom{-s}{j} \nabla^j f_n$$

where

$$(-1)^j \binom{-s}{j} = \frac{s(s+1)\cdots(s+j-1)}{j!}$$

and

$$\nabla^0 f_n = f_n, \qquad \nabla^j f_n = \nabla^{j-1} f_n - \nabla^{j-1} f_{n-1}.$$

Using $y_{n+1} \approx y(t_{n+1})$. $y_n \approx y(t_n)$ and $p_{k-1}(t) \approx f(t, y(t))$ in (48) gives

$$\begin{aligned} y_{n+1} - y_n \int_{t_n}^{t_{n+1}} p_{k-1}(t)dt &= h \int_0^1 p_{k-1}(t_n + sh)ds \\ &= hf_n + h \sum_{j=1}^{k-1} \left((-1)^j \int_0^1 \binom{-s}{1} ds \right) \nabla^j f_n. \end{aligned} \tag{49}$$

This gives the *Adams-Bashforth methods*

$$y_{n+1} - y_n = h \sum_{j=0}^{k-1} \gamma_j \nabla^j f_n, \qquad \gamma_0 = 1, \quad \gamma_j = (-1)^j \int_0^1 \binom{-s}{j} ds.$$

Example 6.6. *We get*

$$\gamma_0 = 1, \quad \gamma_1 = \int_0^1 sds = \frac{1}{2}, \quad \gamma_2 = \int_0^1 \frac{s(s+1)}{2} ds = \frac{5}{12}$$

and the first few methods becomes:

$$\begin{aligned} y_{n+1} - y_n &= hf_n \\ y_{n+1} - y_n &= h \left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1} \right) \\ y_{n+1} - y_n &= h \left(\frac{23}{12} f_n - \frac{4}{3} f_{n-1} + \frac{5}{12} f_{n-1} \right) \end{aligned}$$

A k-step Adams-Bashforth method is explicit, has order k (which is the optimal order for explicit methods) and it is zero-stable. In addition, the error constant $C_{p+1} = \gamma_k$. Implicit Adams methods are constructed similarly, but in this case we include the (unknown) point (t_{n+1}, f_{n+1}) into the set of interpolation points. So the polynomial

$$p_k^*(t) = p_k^*(t_n + sh) = f_{n+1} + \sum_{j=1}^{k} (-1)^j \binom{-s+1}{j} \nabla^j f_{n+1}$$

interpolates the points (t_i, f_i), $i = n-k+1, \ldots, n+1$. Using this, we get the *Adams-Moulton* methods

$$y_{n+1} - y_n = h \sum_{j=0}^{k} \gamma_j^* \nabla^j f_{n+1}, \qquad \gamma_0^* = 1, \quad \gamma_j^* = (-1)^j \int_0^1 \binom{-s+1}{j} ds.$$

Example 6.7. *We get*

$$\gamma_0^* = 1, \quad \gamma_1^* = \int_0^1 (s-1) ds = -\frac{1}{2}, \quad \gamma_2^* = \int_0^1 \frac{(s-1)s}{2} ds = -\frac{1}{12}$$

and the first methods becomes

$$\begin{aligned} y_{n+1} - y_n &= h f_{n+1} && \textit{(Backward Euler)} \\ y_{n+1} - y_n &= h \left(\frac{1}{2} f_{n+1} + \frac{1}{2} f_n \right) && \textit{(Trapezoidal method)} \\ y_{n+1} - y_n &= h \left(\frac{5}{12} f_{n+1} + \frac{2}{3} f_n - \frac{1}{12} f_{n-1} \right). \end{aligned}$$

A k-step Adams-Moulton method is implicit, of order $k+1$ and is zero-stable. The error constant $C_{p+1} = \gamma_{k+1}^*$. Despite the fact that the Adams-Moulton methods are implicit, they have some advantages compared to their explicit counterparts: They are of one order higher, the error constants are much smaller, and the linear stability properties (when the methods are applied to the linear test problem $y' = \lambda y$) are much better.

k	0	1	2	3	4	5	6
γ_k	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\frac{19087}{60480}$
γ_k^*	1	$-\frac{1}{2}$	$-\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{19}{720}$	$-\frac{3}{160}$	$-\frac{863}{60480}$

Table 1: The γ's for the Adams methods.

6.5 Predictor-corrector methods

A predictor-corrector (PC) pair is a pair of one explicit (predictor) and one implicit (corrector) methods. The nonlinear equations from the application of the implicit method are solved by a fixed number of fixed point iterations, using the solution by the explicit method as starting values for the iterations.

Example 6.8. *We may construct a PC method from a second order Adams-Bashforth scheme and the trapezoidal rule as follows:*

$$\begin{aligned}
&y_{n+1}^{[0]} = y_n + \frac{h}{2}(3f_n - f_{n-1}) && \textit{(P : Predictor)} \\
&\textit{for } l = 0, 1, \ldots, m \\
&\qquad f_{n+1}^{[l]} = f(t_{n+1}, y_{n+1}^{[l]}) && \textit{(E : Evaluation)} \\
&\qquad y_{n+1}^{[l+1]} = y_n + \frac{h}{2}(f_{n+1}^{[l]} + f_n) && \textit{(C : Corrector)} \\
&\textit{end} \\
&y_{n+1} = y_{n+1}^{[m]} \\
&f_{n+1} = f(t_{n+1}, y_{n+1}). && \textit{(E : Evaluation)}
\end{aligned}$$

Such schemes are commonly referred as P(EC)^{m}E schemes.

The predictor and the corrector is often by the same order, in which case only one or two iterations are needed.

Error estimation in predictor-corrector methods.

The local discretization error of some LMM is given by

$$h\tau_{n+1} = \sum_{l=0}^{k}(\alpha_l y(t_{n-k+1+l} - h\beta_l y'(t_{n-k+1+l})) = h^{p+1}C_{p+1}y^{(p+1)}(t_{n-k+1}) + \mathcal{O}(h^{p+2}).$$

But we can do the Taylor expansions of y and y' around t_n rather than t_{n-k+1}. This will not alter the principal error term, but the terms hidden in the expression $\mathcal{O}(h^{p+2})$ will change. As a consequence, we get

$$h\tau_{n+1} = h^{p+1}C_{p+1}y^{(p+1)}(t_n) + \mathcal{O}(h^{p+2}).$$

Assume that $y_i = y(t_i)$ for $i = n-k+1, \ldots, n$, and $\alpha_k = 1$. Then

$$h\tau_{n+1} = y(t_{n+1}) - y_{n+1} + \mathcal{O}(h^{p+2}) = h^{p+1}C_{p+1}y^{(p+1)}(t_n) + \mathcal{O}(h^{p+2}).$$

Assume that we have chosen a predictor-corrector pair, using methods of the same order p. Then

$$\begin{aligned}
&(P) \qquad && y(t_{n+1}) - y_{n+1}^{[0]} \approx h^{p+1}C_{p+1}^{[0]}y^{(p+1)}(t_n), \\
&(C) \qquad && y(t_{n+1}) - y_{n+1} \approx h^{p+1}C_{p+1}y^{(p+1)}(t_n),
\end{aligned}$$

and

$$y_{n+1} - y_{n+1}^{[0]} \approx h^{p+1}(C_{p+1}^{[0]} - C_{p+1})y^{(p+1)}(t_n).$$

From this we get the following local error estimate for the corrector, called *Milne's device*:

$$y(t_{n+1}) - y_{n+1} \approx \frac{C_{p+1}}{C^{[0]}_{p+1]} - C_{p+1}}(y_{n+1} - y^{[0]}_{n+1}).$$

Example 6.9. *Consider the PC-scheme of Example 6.8. In this case*

$$C^{[0]}_{p+1} = \frac{5}{12}, \qquad C_{p+1} = -\frac{1}{12}, \qquad \textit{so} \qquad \frac{C_{p+1}}{C^{[0]}_{p+1]} - C_{p+1}} = -\frac{1}{6}.$$

Apply the scheme to the linear test problem

$$y' = -y, \qquad y(0) = 1,$$

using $y_0 = 1$, $y_1 = e^{-h}$ *and* $h = 0.1$. *One step of the PC-method gives*

l	$y_2^{[l]}$	$\lvert y_2 - y_2^{[l]}\rvert$	$\lvert y(0.2) - y_2^{[l]}\rvert$	$\frac{1}{6}\lvert y_2^{[l]} - y_2^{[0]}\rvert$
0	0.819112	$4.49 \cdot 10^{-4}$	$3.81 \cdot 10^{-4}$	
1	0.818640	$2.25 \cdot 10^{-5}$	$9.08 \cdot 10^{-5}$	$7.86 \cdot 10^{-5}$
2	0.818664	$1.12 \cdot 10^{-6}$	$6.72 \cdot 10^{-5}$	$7.47 \cdot 10^{-5}$
3	0.818662	$5.62 \cdot 10^{-8}$	$6.84 \cdot 10^{-5}$	$7.49 \cdot 10^{-5}$

After 1-2 iterations, the iteration error is much smaller than the local error, and we also observe that Milne's device gives a reasonable approximation to the error.

Remark Predictor-corrector methods are not suited for stiff problems. You can see this by e.g. using the trapezoidal rule on $y' = \lambda y$. The trapezoidal rule has excellent stability properties. But the iteration scheme

$$y^{[l+1]}_{n+1} = y_n + \frac{h}{2}\lambda(y^{[l]}_{n+1} + y_n)$$

will only converge if $|h\lambda/2| < 1$.

For stiff system, the *Backward differentiation formulas* (BDF) is to be preferred. Those are derived in exercise 5.

References

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