Explicit Adams Methods

We now derive, following Adams, the first explicit multistep formulas. We introduce the notation $x_i = x_0 + ih$ for the grid points and suppose we know the numerical approximations $y_n, y_{n-1}, \ldots, y_{n-k+1}$ to the exact solution $y(x_n), \ldots, y(x_{n-k+1})$ of the differential equation

$$y' = f(x,y), \quad y(x_0) = y_0. \tag{1.1}$$

Adams considers (1.1) in integrated form,

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f\big(t, y(t)\big)\, dt. \tag{1.2}$$

On the right hand side of (1.2) there appears the unknown solution $y(x)$. But since the approximations $y_{n-k+1}, \ldots, y_n$ are known, the values

$$f_i = f(x_i, y_i) \qquad \text{for} \quad i = n-k+1, \ldots, n \tag{1.3}$$

are also available and it is natural to replace the function $f(t, y(t))$ in (1.2) by the interpolation polynomial through the points $\{(x_i, f_i) \mid i = n-k+1, \ldots, n\}$ (see Fig. 1.1).

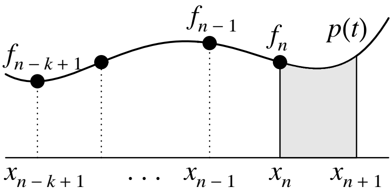

Fig. 1.1. Explicit Adams methods

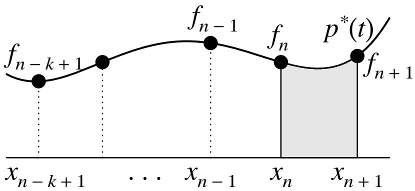

Fig. 1.2. Implicit Adams methods

This polynomial can be expressed in terms of backward differences

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

as follows:

$$p(t) = p(x_n + sh) = \sum_{j=0}^{k-1} (-1)^j \binom{-s}{j} \nabla^j f_n \tag{1.4}$$

(Newton's interpolation formula of 1676, published in Newton (1711), see e.g. Henrici (1962), p. 190). The numerical analogue to (1.2) is then given by

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} p(t)\, dt$$

or after insertion of (1.4) by

$$y_{n+1} = y_n + h \sum_{j=0}^{k-1} \gamma_j \nabla^j f_n \tag{1.5}$$

where the coefficients γ_j satisfy

$$\gamma_j = (-1)^j \int_0^1 \binom{-s}{j}\, ds \tag{1.6}$$

(see Table 1.1 for their numerical values). A simple recurrence relation for these coefficients will be derived below (formula (1.7)).

Table 1.1. Coefficients for the explicit Adams methods

j	0	1	2	3	4	5	6	7	8
γ_j	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\frac{19087}{60480}$	$\frac{5257}{17280}$	$\frac{1070017}{3628800}$

Special cases of (1.5). For $k=1,2,3,4$, after expressing the backward differences in terms of f_{n-j}, one obtains the formulas

$$\begin{aligned}
k=1: &\qquad y_{n+1} = y_n + hf_n \qquad\qquad \text{(explicit Euler method)}\\
k=2: &\qquad y_{n+1} = y_n + h\Big(\frac{3}{2}f_n - \frac{1}{2}f_{n-1}\Big)\\
k=3: &\qquad y_{n+1} = y_n + h\Big(\frac{23}{12}f_n - \frac{16}{12}f_{n-1} + \frac{5}{12}f_{n-2}\Big)\\
k=4: &\qquad y_{n+1} = y_n + h\Big(\frac{55}{24}f_n - \frac{59}{24}f_{n-1} + \frac{37}{24}f_{n-2} - \frac{9}{24}f_{n-3}\Big).
\end{aligned} \tag{1.5'}$$

Recurrence relation for the coefficients. Using Euler's method of *generating functions* we can deduce a simple recurrence relation for γ_i (see e.g. Henrici 1962). Denote by $G(t)$ the series

$$G(t) = \sum_{j=0}^{\infty} \gamma_j t^j .$$

With the definition of γ_j and the binomial theorem one obtains

$$\begin{aligned}
G(t) &= \sum_{j=0}^{\infty} (-t)^j \int_0^1 \binom{-s}{j}\, ds = \int_0^1 \sum_{j=0}^{\infty} (-t)^j \binom{-s}{j}\, ds\\
&= \int_0^1 (1-t)^{-s}\, ds = -\frac{t}{(1-t)\log(1-t)}.
\end{aligned}$$

This can be written as

$$-\frac{\log(1-t)}{t}\, G(t) = \frac{1}{1-t}$$

or as

$$\Big(1+\frac{1}{2}t+\frac{1}{3}t^2+\ldots\Big)\Big(\gamma_0+\gamma_1 t+\gamma_2 t^2+\ldots\Big) = \Big(1+t+t^2+\ldots\Big).$$

Comparing the coefficients of t^m we get the desired recurrence relation

$$\gamma_m + \frac{1}{2}\gamma_{m-1} + \frac{1}{3}\gamma_{m-2} + \ldots + \frac{1}{m+1}\gamma_0 = 1. \tag{1.7}$$

Implicit Adams Methods

The formulas (1.5) are obtained by integrating the interpolation polynomial (1.4) from x_n to x_{n+1}, i.e., outside the interpolation interval (x_{n-k+1}, x_n). It is well known that an interpolation polynomial is usually a rather poor approximation outside this interval. Adams therefore also investigated methods where (1.4) is replaced by the interpolation polynomial which uses in addition the point (x_{n+1}, f_{n+1}), i.e.,

$$p^*(t) = p^*(x_n + sh) = \sum_{j=0}^{k} (-1)^j \binom{-s+1}{j} \nabla^j f_{n+1} \tag{1.8}$$

(see Fig. 1.2). Inserting this into (1.2) we obtain the following implicit method

$$y_{n+1} = y_n + h \sum_{j=0}^{k} \gamma_j^* \nabla^j f_{n+1} \tag{1.9}$$

where the coefficients γ_j^* satisfy

$$\gamma_j^* = (-1)^j \int_0^1 \binom{-s+1}{j} ds \tag{1.10}$$

and are given in Table 1.2 for $j \le 8$. Again, a simple recurrence relation can be derived for these coefficients (Exercise 3).

Table 1.2. Coefficients for the implicit Adams methods

j	0	1	2	3	4	5	6	7	8
γ_j^*	1	$-\frac{1}{2}$	$-\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{19}{720}$	$-\frac{3}{160}$	$-\frac{863}{60480}$	$-\frac{275}{24192}$	$-\frac{33953}{3628800}$

The formulas thus obtained are generally of the form

$$y_{n+1} = y_n + h\big(\beta_k f_{n+1} + \ldots + \beta_0 f_{n-k+1}\big). \tag{1.9'}$$

The first examples are as follows

$$\begin{aligned}
k=0:&\qquad y_{n+1}=y_n+hf_{n+1}=y_n+hf(x_{n+1},y_{n+1})\\
k=1:&\qquad y_{n+1}=y_n+h\Big(\frac{1}{2}f_{n+1}+\frac{1}{2}f_n\Big)\\
k=2:&\qquad y_{n+1}=y_n+h\Big(\frac{5}{12}f_{n+1}+\frac{8}{12}f_n-\frac{1}{12}f_{n-1}\Big)\\
k=3:&\qquad y_{n+1}=y_n+h\Big(\frac{9}{24}f_{n+1}+\frac{19}{24}f_n-\frac{5}{24}f_{n-1}+\frac{1}{24}f_{n-2}\Big).
\end{aligned}\tag{1.9"}$$

The special cases $k=0$ and $k=1$ are the implicit Euler method and the trapezoidal rule, respectively. They are actually one-step methods and have already been considered in Chapter II.7.

The methods (1.9) give in general more accurate approximations to the exact solution than (1.5). This will be discussed in detail when the concepts of order and error constant are introduced (Section III.2). The price for this higher accuracy is that y_{n+1} is only defined implicitly by formula (1.9). Therefore, in general a nonlinear equation has to be solved at each step.

Predictor-corrector methods. One possibility for solving this nonlinear equation is to apply fixed point iteration. In practice one proceeds as follows:

P: compute the predictor $\widehat{y}_{n+1}=y_n+h\sum_{j=0}^{k-1}\gamma_j\nabla^j f_n$ by the explicit Adams method (1.5); this already yields a reasonable approximation to $y(x_{n+1})$;

E: evaluate the function at this approximation: $\widehat{f}_{n+1}=f(x_{n+1},\widehat{y}_{n+1})$;

C: apply the corrector formula

$$y_{n+1}=y_n+h\big(\beta_k\widehat{f}_{n+1}+\beta_{k-1}f_n+\ldots+\beta_0 f_{n-k+1}\big)\tag{1.11}$$

to obtain y_{n+1}.

E: evaluate the function anew, i.e., compute $f_{n+1}=f(x_{n+1},y_{n+1})$.

This is the most common procedure, denoted by PECE. Other possibilities are: PECECE (two fixed point iterations per step) or PEC (one uses $\widehat{f}_{n+1}$ instead of f_{n+1} in the subsequent steps).

This predictor-corrector technique has been used by F.R. Moulton (1926) as well as by W.E. Milne (1926). J.C. Adams actually solved the implicit equation (1.9) by Newton's method, in the same way as is now usual for stiff equations (see Volume II).

Remark. Formula (1.5) is often attributed to Adams-Bashforth. Similarly, the multistep formula (1.9) is usually attributed to Adams-Moulton (Moulton 1926). In fact, both formulas are due to Adams.