Computer Science/Mathematics 455
Lecture Notes
Lecture # 34

The Adams Methods

We are still considering the initial value problem (IVP)

$$\begin{aligned} \mathbf{x}'(t) &= \mathbf{f}(t, \mathbf{x}(t)) \\ \mathbf{x}(t_0) &= \mathbf{x}_0 \end{aligned}$$

where t is time, and $\mathbf{x}(t)$ is a vector valued function.

We construct an approximate solution

$$\begin{aligned} \mathbf{x}_n &\approx \mathbf{x}(t_n) \\ \mathbf{f}_n &= \mathbf{f}(t_n, \mathbf{x}_n) = \mathbf{x}'(t_n). \end{aligned}$$

Use the fact that

$$x(t_{n+1}) - x(t_n) = \int_{t_n}^{t_{n+1}} x'(t)dt.$$

Let $h = t_{n+1} - t_n$ and let $t = t_n + sh$. Then

$$\int_{t_n}^{t_{n+1}} x'(t)dt = h\int_0^1 x'(t_n + sh)ds \approx h\sum_{j=0}^{N} \beta_j f_{n+1-i}.$$

If $\beta_0 \neq 0$, we get the implicit Adams–Moulton methods. If $\beta_0 = 0$, we get the explicit Adams–Bashforth methods.

For the 3-step third order Adams–Bashforth method we create the exact matching integral formula for $F(t) = 1, t, t^2$ such that

$$\int_0^1 F(t)dt = \beta_1 F(0) + \beta_2 F(-1) + \beta_2 F(-2).$$

We solve the Vandermonde system

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & -2 \\ 0 & 1 & 4 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1/2 \\ 1/3 \end{pmatrix}.$$

The solution is

$$\beta_1 = 23/12, \quad \beta_2 = -4/3, \quad \beta_3 = 5/12,$$

so that we have

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \frac{h}{12}(23\mathbf{f}_n - 16\mathbf{f}_{n-1} + 5\mathbf{f}_{n-2}).$$

To get the implicit Adams–Moulton third order method, we fit

$$\int_0^1 F(t)dt = \hat{\beta}_0 F(1) + \hat{\beta}_1 F(0) + \hat{\beta}_2 F(-1)$$

and make it exact matching for $F(t) = 1, t, t^2$. (I derived this in the last lecture using numerical differentiation formulas and Taylor series).

We obtain the Vandermonde system

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1/2 \\ 1/3 \end{pmatrix}.$$

The solution is $\hat{\beta}_0 = 5/12$,$\hat{\beta}_1 = 2/3$, and $\hat{\beta}_2 = -1/12$. This is the method

$$\begin{aligned} \mathbf{x}_{n+1} &= \mathbf{x}_n + \frac{h}{12}(5\mathbf{f}_{n+1} + 8\mathbf{f}_n - \mathbf{f}_{n-1}) \\ &= \mathbf{x}_n + \frac{h}{12}(5\mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}) + 8\mathbf{f}_n - \mathbf{f}_{n-1}) \qquad (1) \end{aligned}$$

Explicit methods are easy to evaluate, but implicit methods are necessary to produce stable solutions. So we pair them together to get a predictor–corrector method. The following is the Adams–Bashforth–Moulton third order pair.

The predictor step obtains an initial guess to the solution of (1) for the Adams–Bashforth explicit method.

$$\mathbf{x}_{n+1}^{(0)} = \mathbf{x}_n + \frac{h}{12}(23\mathbf{f}_n - 16\mathbf{f}_{n-1} + 5\mathbf{f}_{n-2}).$$

Subsequent guesses are obtained from the applying the Adams–Moulton method again and again.

$$\mathbf{x}_{n+1}^{(k+1)} = \mathbf{x}_n + \frac{h}{12}(5\mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}^{(k)}) + 8\mathbf{f}_n - \mathbf{f}_{n-1}) \qquad (2)$$

for $k = 0, 1, 2, \cdots$.

The question here is how many steps do we need to take. We would prefer as few as possible.

First, both the predictor (explicit Adams–Bashforth) and the corrector (implicit Adams–Moulton) are third order. If we use our local truncation error model (scalar version)

$$\begin{aligned} z_n'(t) &= f(t, z_n(t)) \\ z_n(t_n) &= x_n \end{aligned}$$

then

$$z_n(t_{n+1}) - x_{n+1}^{(0)} = \alpha_4 z_n^{(4)}(t_n) h^4 + O(h^5).$$

And the solution to the Adams–Moulton implicit equation satisfies

$$z_n(t_{n+1}) - x_{n+1} = \hat{\alpha}_4 z_n^{(4)}(t_n) h^4 + O(h^5)$$

where $|\hat{\alpha}_4| < |\alpha_4|$. We would like this equation to be satisfied as closely as possible.

We note that if we subtract (2) from (1) then

$$x_{n+1} - x_{n+1}^{(k+1)} = \frac{5h}{12}(f(t_{n+1}, x_{n+1}) - f(t_{n+1}, x_{n+1}^{(k)})).$$

From the Lipschitz condition in the existence theorem (yes, this really is useful!),

$$|f(t_{n+1}, x_{n+1}) - f(t_{n+1}, x_{n+1}^{(k)})| \leq L|x_{n+1} - x_{n+1}^{(k)}|$$

thus

$$|x_{n+1} - x_{n+1}^{(k+1)}| \leq \frac{5hL}{12}|x_{n+1} - x_{n+1}^{(k)}|. \tag{3}$$

Thus if $\frac{5hL}{12} < 1$, then

$$\lim_{k \to \infty} x_{n+1}^{(k)} = x_{n+1}.$$

However, in numerical analysis, more convergence is not enough, fast convergence is necessary!

We note that

$$x_{n+1} - x_{n+1}^{(0)} = (\alpha_4 - \hat{\alpha}_4) z_n^{(4)}(t_n) h^4 + O(h^5)$$

so from (3)

$$|x_{n+1} - x_{n+1}^{(1)}| \le \frac{5}{12}|\alpha_4 - \hat{\alpha}_4||z_n^{(4)}(t_n)|h^5 + O(h^6).$$

Thus

$$\begin{aligned}
|z_n(t_{n+1}) - x_{n+1}^{(1)}| &\le |z_n(t_{n+1}) - x_{n+1}| + |x_{n+1} - x_{n+1}^{(1)}| \\
&\le |z_n(t_{n+1}) - x_{n+1}| + \frac{5}{12}|\alpha_4 - \hat{\alpha}_4||z_n^{(4)}(t_n)|h^5 + O(h^6) \\
&= |z_n(t_{n+1}) - x_{n+1}| + O(h^5) = |\hat{\alpha}_4 z_n^{(4)}(t_n)|h^4 + O(h^5).
\end{aligned}$$

Thus $x_{n+1}^{(1)}$ has the same first order local error term as x_{n+1}. That means we can get away with just one iteration.

Thus we have the following simple third order method.

Predictor

$$\mathbf{x}_{n+1}^{(0)} = \mathbf{x}_n + \frac{h}{12}(23\mathbf{f}_n - 16\mathbf{f}_{n-1} + 5\mathbf{f}_{n-2}).$$

Corrector

$$\mathbf{x}_{n+1}^{(1)} = \mathbf{x}_n + \frac{h}{12}(5\mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}^{(0)}) + 8\mathbf{f}_n - \mathbf{f}_{n-1})$$

Do one function evaluation for future steps.

$$\mathbf{f}_{n+1} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}^{(1)}).$$

Next time, we compare and contrast Adams and Runge–Kutta methods.