# 7 Linear multistep methods

A $k$-step linear multistep method (LMM) applied to the ODE

$$y' = f(t, y), \quad y(t_0) = y_0, \quad t_0 \le t \le t_{end}.$$

is given by

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = h \sum_{l=0}^{k} \beta_l f_{n+l}, \tag{26}$$

where $\alpha_l, \beta_l$ are the method coefficients, $f_j = f(t_j, y_j)$ and $t_j = t_0 + jh$, $h = (t_{end} - t_0)/Nstep$. Usually we require

$$\alpha_k = 1 \quad \text{and} \quad |\alpha_0| + |\beta_0| \neq 0.$$

To get started with a $k$-step method, we also need starting values $y_l \approx y(t_l)$, $l = 0, 1, \cdots, k-1$. A method is explicit if $\beta_k = 0$, otherwise implicit. The *leapfrog method*

$$y_{n+2} - y_n = 2hf(t_{n+1}, y_{n+1}) \tag{27}$$

and the method given by

$$y_{n+2} - y_{n+1} = h\left(\frac{3}{2} f_{n+1} - \frac{1}{2} f_n\right) \tag{28}$$

are both examples of explicit 2-step methods.

**Example 7.1.** *Given the problem*

$$y' = -2ty, \qquad y(0) = 1$$

*with exact solution* $y(t) = e^{-t^2}$. *Let* $h = 0.1$, *and* $y_1 = e^{-h^2}$. *This problem is solved by* (28), *and the numerical solution and the error is given by*

| $t_n$ | $y_n$ | $\|e_n\|$ |
|---|---|---|
| 0.0 | 1.000000 | 0.00 |
| 0.1 | 0.990050 | 0.00 |
| 0.2 | 0.960348 | $4.41 \cdot 10^{-4}$ |
| 0.3 | 0.912628 | $1.30 \cdot 10^{-3}$ |
| 0.4 | 0.849698 | $2.45 \cdot 10^{-3}$ |
| 0.5 | 0.775113 | $3.69 \cdot 10^{-3}$ |
| 0.6 | 0.692834 | $4.84 \cdot 10^{-3}$ |
| 0.7 | 0.606880 | $5.75 \cdot 10^{-3}$ |
| 0.8 | 0.521005 | $6.29 \cdot 10^{-3}$ |
| 0.9 | 0.438445 | $6.41 \cdot 10^{-3}$ |
| 1.0 | 0.361746 | $6.13 \cdot 10^{-3}$ |

*The corresponding MATLAB code is given in* `lmm.m`.

## 7.1 Consistency and order.

We define the *local discretization error* $\tau_{n+k}(h)$ by

$$h\tau_{n+k}(h) = \sum_{l=0}^{k} \left( \alpha_l y(t_{n+l}) - h\beta_l y'(t_{n+l}) \right). \tag{29}$$

You can think about the $h\tau_{n+k}$ as the defect obtained when plugging the exact solution into the difference equation (26). A method is *consistent* if $\tau_{n+k}(h) \underset{h\to 0}{\longrightarrow} 0$. The term $h\tau_{n+k}(h)$ can be written as a power series in $h$

$$h\tau_{n+k}(h) = C_0 y(t_n) + C_1 h y'(t_n) + C_2 h^2 y''(t_n) + \cdots + C_q h^q y^{(q)}(t_n) + \cdots,$$

by expanding $y(t_n + lh)$ and $y'(t_n + lh)$ into their Taylor series around $t_n$,

$$\begin{aligned} y(t_n + lh) &= y(t_n) + (lh)y'(t_n) + \frac{1}{2}(lh)^2 y''(t_n) + \cdots + \frac{(lh)^q}{q!} y^{(q)}(t_n) + \cdots \\ y'(t_n + lh) &= y'(t_n) + (lh)y''(t_n) + \frac{1}{2}(lh)^2 y'''(t_n) + \cdots + \frac{(lh)^{q-1}}{q-1!} y^{(q)}(t_n) + \cdots \end{aligned}$$

for sufficiently differentiable solutions $y(t)$. Insert this into (29), get the following expressions for $C_q$:

$$C_0 = \sum_{l=0}^{k} \alpha_l, \qquad C_q = \frac{1}{q!} \sum_{l=0}^{k} \left( l^q \alpha_l - q l^{q-1} \beta_l \right), \quad q = 1, 2, \cdots. \tag{30}$$

The method is consistent if $C_0 = C_1 = 0$. It is *of order* $p$ if

$$C_0 = C_1 = \cdots = C_p = 0, \qquad C_{p+1} \neq 0.$$

The constant $C_{p+1}$ is called the *error constant.*

**Example 7.2.** *The LMM (28) is defined by*

$$\alpha_0 = 0,\ \alpha_1 = -1,\ \alpha_2 = 1,\ \beta_0 = -\frac{1}{2},\ \beta_1 = \frac{3}{2},\ \beta_2 = 0,$$

*thus*

$$\begin{aligned} C_0 &= \alpha_0 + \alpha_1 + \alpha_2 = 0. \\ C_1 &= \alpha_1 + 2\alpha_2 - (\beta_0 + \beta_1 + \beta_2) = 0 \\ C_2 &= \frac{1}{2!} \left( \alpha_1 + 2^2 \alpha_2 - 2(\beta_1 + 2\beta_2) \right) = 0 \\ C_3 &= \frac{1}{3!} \left( \alpha_1 + 2^3 \alpha_2 - 3(\beta_1 + 2^2 \beta_2) \right) = \frac{5}{12}. \end{aligned}$$

*The method is consistent and of order 2.*

**Example 7.3.** *Is it possible to construct an explicit 2-step method of order 3? There are 4 free coefficients $\alpha_0, \alpha_1, \beta_0, \beta_1$, and 4 order conditions to be solved ($C_0 = C_1 = C_2 = C_3 = 0$). The solution is*

$$\alpha_0 = -5,\ \alpha_1 = 4,\ \beta_0 = 2,\ \beta_1 = 4.$$

*Test this method on the ODE of Example 2.1. (Replace the method coefficients in* `lmm.m`*.) The result is nothing but disastrous. Taking smaller steps only increase the problem.*

To see why, you have to know a bit about how to solve difference equations.

## 7.2 Linear difference equations

A linear difference equation with constant coefficients is given by

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = \varphi_n, \qquad n = 0, 1, 2, \cdots . \tag{31}$$

The solution of this equation is a sequence $\{y_n\}$ of numbers (or vectors). Let $\{y_n\}$ be the general solution of the homogeneous problem

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = 0. \tag{32}$$

Let $\psi_n$ be one particular solution of (31). The general solution of (31) is then $\{y_n\}$ where $y_n = \tilde{y}_n + \psi_n$. To find a unique solution, we will need the starting values $y_0, y_1, \cdots, y_{k-1}$.

Let us try $\tilde{y}_n = r^n$ as a solution of the homogeneous equation (32). This is true if

$$\sum_{l=0}^{k} \alpha_l r^{n+l} = r^n \sum_{l=0}^{k} \alpha_l r^l = 0.$$

The polynomial $\rho(r) = \sum_{l=0}^{k} \alpha_l r^l$ is called *the characteristic polynomial*, and $\{r^n\}$ is a solution of (32) if $r$ is a root of $\rho(r)$. The $k$th degree polynomial $\rho(r)$ has $k$ roots altogether, $r_1, r_2, \cdots, r_k$, they can be distinct and real, they can be distinct and complex, in which case they appear in complex conjugate pairs, or they can be multiple. In the latter case, say $r_1 = r_2 = \cdots = r_\mu$ we get a set of linear independent solutions $\{r_1^n\}$, $\{nr_1^n\}$, $\cdots$, $\{n^{\mu-1}r_1^n\}$. Altogether we have found $k$ linear independent solutions $\{\tilde{y}_{n,l}\}$ of the homogeneous equation, and the general solution is given by

$$y_n = \sum_{l=1}^{k} \kappa_l \tilde{y}_{n,l} + \psi_n.$$

The coefficients $\kappa_l$ can be determined from the starting values.

**Example 7.4.** *Given*

$$y_{n+4} - 6y_{n+3} + 14y_{n+2} - 16y_{n+1} + 8y_n = n$$
$$y_0 = 1,\ y_1 = 2,\ y_2 = 3\ y_3 = 4.$$

*The characteristic polynomial is given by*

$$\rho(r) = r^4 - 6r^3 + 14r^2 - 16r + 8$$

*with roots* $r_1 = r_2 = 2$, $r_3 = 1 + i$, $r_4 = 1 - i$. *As a particular solution we try* $\psi_n = an + b$. *Inserted into the difference equation we find this to be a solution if* $a = 1$, $b = 2$. *The general solution has the form*

$$y_n = \kappa_1 2^n + \kappa_2 n 2^n + \kappa_3 (1+i)^n + \kappa_4 (1-i)^n + n + 2.$$

*From the starting values we find that $\kappa_1 = -1$, $\kappa_2 = \frac{1}{4}$, $\kappa_3 = -i/4$ and $\kappa_4 = i/4$. So, the solution of the problem is*

$$\begin{aligned} y_n &= 2^n\left(\frac{n}{4}-1\right) - \frac{i(1+i)^n}{4} + \frac{i(1-i)^n}{4} + n + 2 \\ &= 2^n\left(\frac{n}{4}-1\right) - 2^{\frac{n-2}{2}}\sin\left(\frac{n\pi}{4}\right) + n + 2. \end{aligned}$$

**Example 7.5.** *The homogeneous part of the difference equation of Example 5.2 is*

$$\rho(r) = r^2 + 4r - 5 = (r-1)(r+5).$$

*One root is 5. Thus, one solution component is multiplied by a factor -5 for each step, independent of the stepsize. Which explain why this method fails.*

## 7.3 Zero-stability and convergence

Let us start with the definition of convergence. As before, we consider the error at $t_{end}$, using $Nstep$ steps with constant stepsize $h = (t_{end} - t_0)/Nstep$.

**Definition 7.6.**

- *A linear multistep method* (26) *is* convergent *if, for all ODEs satisfying the conditions of Theorem 2.4 we get*

$$y_{Nstep} \underset{h\to 0}{\rightarrow} y(t_{end}), \qquad \textit{whenever} \qquad y_l \underset{h\to 0}{\rightarrow} y(t_0 + lh), \quad l = 0, 1, \cdots, k-1.$$

- *The method is* convergent of order $p$ *if, for all ODEs with $f$ sufficiently differentiable, there exists a positive $h_0$ such that for all $h < h_0$*

$$\|y(t_{end} - y_{Nstep}\| \le Kh^p \qquad \textit{whenever} \qquad \|y(t_0+lh) - y_l\| \le K_0 h^p, \quad l = 0, 1, \cdots, k-1.$$

The first characteristic polynomial of an LMM (26) is

$$\rho(r) = \sum_{l=0}^{k} \alpha_l r^l,$$

with roots $r_1, r_2, \cdots, r_k$. From the section on difference equation, it follows that for the boundedness of the solution $y_n$ we require:

1. $|r_i| \le 1$, for $i = 1, 2, \cdots, k$.
2. $|r_i| < 1$ if $r_i$ is a multiple root.

A method satisfying these two conditions is called *zero-stable.*

We can now state (without proof) the following important result:

**Theorem 7.7.** *(Dahlquist)*

$$\textit{Convergence} \qquad \Leftrightarrow \qquad \textit{Zero-stability + Consistency.}$$

For a consistent method, $C_0 = \sum_{l=0}^{k} \alpha_l = 0$ so the characteristic polynomial $\rho(r)$ will always have one root $r_1 = 1$.

The zero-stability requirement puts a severe restriction on the maximum order of a convergent $k$-step method:

**Theorem 7.8.** *(The first Dahlquist-barrier) The order $p$ of a zero-stable $k$-step method satisfies*

$$\begin{aligned} p &\le k+2 \quad \text{if } k \text{ is even,} \\ p &\le k+1 \quad \text{if } k \text{ is odd,} \\ p &\le k \qquad\;\; \text{if } \beta_k \le 0. \end{aligned}$$

Notice that the last line include all explicit LMMs.