Linear Multistep Methods

Linear Multistep Methods (LMM)

A LMM has the form

$$\sum_{j=0}^{k} \alpha_j x_{i+j} = h \sum_{j=0}^{k} \beta_j f_{i+j}, \quad \alpha_k = 1 \quad i \geq 0$$

for the approximate solution of the

$$\text{IVP} \quad x' = f(t,x), \quad x(a) = x_a \ .$$

We approximate $x(t)$ on $a \leq t \leq b$ at $t_i = a + ih$, $0 \leq i \leq \frac{b-a}{h}$.

Here $x_i \approx x(t_i)$, with $f_{i+j} = f(t_{i+j}, x_{i+j})$.

LMM is called a *k-step LMM* if at least one of the coefficients α_0 and β_0 is non-zero.

LMM is similar to a difference equation in that one is solving for x_{i+k} from $x_i, x_{i+1}, \ldots, x_{i+k-1}$. We assume as usual that IVP is well-posed, i.e. f is continuous in (t,x) and uniformly Lipschitz in x.

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For simplicity of notation, we will assume that $x(t)$ is real and scalar; the analysis that follows applies to $x(t) \in \mathbb{R}^n$ or $x(t) \in \mathbb{C}^n$ (viewed as $\mathbb{R}^{2n}$ for differentiability) with minor adjustments.

LMM Examples

Midpoint Rule (explicit)

$$x(t_{i+2}) - x(t_i) = \int_{t_i}^{t_{i+2}} x'(s)ds \approx 2hx'(t_{i+1}) = 2hf(t_{i+1}, x(t_{i+1})).$$

This approximate relationship suggests the LMM

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$$\textit{Midpoint rule}: \qquad x_{i+2} - x_i = 2hf_{i+1} \ .$$

Trapezoid Rule (implicit)

The approximation

$$x(t_{i+1}) - x(t_i) = \int_{t_i}^{t_{i+1}} x'(s)ds \approx \frac{h}{2}(x'(t_{i+1}) + x'(t_i))$$

suggests the LMM

$$\textit{Trapezoid rule}: \qquad x_{i+1} - x_i = \frac{h}{2}(f_{i+1} + f_i) \ .$$

Explicit vs Implicit

If $\beta_k = 0$, the LMM is called *explicit*: once we know $x_i, x_{i+1}, \ldots, x_{i+k-1}$, we compute immediately

$$x_{i+k} = \sum_{j=0}^{k-1} (h\beta_j f_{i+j} - \alpha_j x_{i+j}) \ .$$

On the other hand, if $\beta_k \neq 0$, the LMM is called *implicit*: knowing $x_i, x_{i+1}, \ldots, x_{i+k-1}$, we need to solve

$$x_{i+k} = h\beta_k f(t_{i+k}, x_{i+k}) - \sum_{j=0}^{k-1} (\alpha_j x_{i+j} - h\beta_j f_{i+j})$$

for x_{i+k}.

Existence of Implicit Solutions: Contraction Mapping Theorem

If h is sufficiently small, implicit LMM methods also have unique solutions given h and $x_0, x_1, \ldots, x_{k-1}$. To see this, let L be the Lipschitz constant for f. Given $x_i, \ldots, x_{i+k-1}$, the value for x_{i+k} is obtained by solving the equation

$$x_{i+k} = h\beta_k f(t_{i+k}, x_{i+k}) + g_i,$$

where

$$g_i = \sum_{j=0}^{k-1} (h\beta_j f_{i+j} - \alpha_j x_{i+j}) \quad \text{(constant)}$$

That is, we are looking for a fixed point of

$$\Phi(x) = h\beta_k f(t_{i+k}, x) + g_i \ .$$

Existence of Implicit Solutions: Contraction Mapping Theorem

$$\Phi(x) = h\beta_k f(t_{i+k}, x) + g_i$$

Note that if $h|\beta_k|L < 1$, then Φ is a contraction:

$$|\Phi(x) - \Phi(y)| \leq h|\beta_k|\,|f(t_{i+k}, x) - f(t_{i+k}, y)| \leq h|\beta_k|L|x - y|.$$

So by the Contraction Mapping Fixed Point Theorem, Φ has a unique fixed point. Any initial guess $x_{i+k}^{(0)}$ yields a convergent fixed point iteration:

$$\text{FPI} \qquad x_{i+k}^{(l+1)} = h\beta_k f(t_{i+k}, x_{i+k}^{(l)}) + g_i$$

which is initiated at some initial point $x_{i+k}^{(0)}$ (from an explicit method). In practice, one chooses either
(1) iterate to convergence, or (2) a fixed number of iterations.
A pairing of an explicit initialization $x_{i+k}^{(0)}$ with an implicit FPI is called a Predictor-Corrector Method.

Local Truncaton Error (LTE)

Initial Values. To start a k-step LMM, we need $x_0, x_1, \ldots, x_{k-1}$. We usually take $x_0 = x_a$, and approximate $x_1, \ldots, x_{k-1}$ using a one-step method (e.g., a Runge-Kutta method).

Local Truncation Error. For a true solution $x(t)$ to $x' = f(t, x)$, define the LTE to be

$$l(h, t) = \sum_{j=0}^{k} \alpha_j x(t + jh) - h \sum_{j=0}^{k} \beta_j x'(t + jh).$$

Local Truncaton Error (LTE)

$$l(h,t) = \sum_{j=0}^{k} \alpha_j x(t+jh) - h\sum_{j=0}^{k} \beta_j x'(t+jh)$$

$$\begin{aligned} x(t+jh) &= x(t) + jhx'(t) + \cdots + \frac{(jh)^p}{p!}x^{(p)}(t) + O(h^{p+1}) \quad \text{and} \\ hx'(t+jh) &= hx'(t) + jh^2x''(t) + \cdots + \frac{j^{p-1}h^p}{(p-1)!}x^{(p)}(t) + O(h^{p+1}) \end{aligned}$$

and so

$$l(h,t) = C_0 x(t) + C_1 hx'(t) + \cdots + C_p h^p x^{(p)}(t) + O(h^{p+1}),$$

where

$$\begin{aligned} C_0 &= \alpha_0 + \cdots + \alpha_k \\ C_1 &= (\alpha_1 + 2\alpha_2 + \cdots + k\alpha_k) - (\beta_0 + \cdots + \beta_k) \\ &\vdots \\ C_q &= \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + \cdots + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_1 + 2^{q-1}\beta_2 + \cdots + k^{q-1}\beta_k). \end{aligned}$$

Accuracy of Order p

A LMM is called *accurate of order p* if $l(h,t) = O(h^{p+1})$ for any solution of $x' = f(t,x)$ which is C^{p+1}.

Fact *Since*

$$l(h,t) = C_0 x(t) + C_1 h x'(t) + \cdots + C_p h^p x^{(p)}(t) + O(h^{p+1}),$$

an LMM is accurate of order at least p iff

$$C_0 = C_1 = \cdots = C_p = 0.$$

Note: It is called accurate of order **exactly** p if $C_{p+1} \neq 0$.

LMM Consistency

(i) For the LTE of a method to be $o(h)$ for all f's, we must have $C_0 = C_1 = 0$. Indeed, for any $f \in C^1$, all solutions $x(t)$ are C^2, so

$$l(h,t) = C_0 x(t) + C_1 h x'(t) + O(h^2) \;=\; o(h) \quad \text{iff} \quad C_0 = C_1 = 0\,.$$

(ii) Note that $C_0, C_1, \ldots$ depend only on $\alpha_0, \ldots, \alpha_k, \beta_0, \ldots, \beta_k$ and not on f. So here, “minimal accuracy” is first order.

Definition *A LMM is called consistent if $C_0 = C_1 = 0$ (i.e., at least first-order accurate).*

If an LMM is consistent, then any solution $x(t)$ has $l(h,t) = o(h)$.

LMM Convergence

A k-step LMM

$$\sum \alpha_j x_{i+j} = h \sum \beta_j f_{i+j}$$

is called *convergent* if for each

$$\text{IVP} \qquad x' = f(t,x),\ x(a) = x_a \ \text{ on } \ [a,b]$$

and for any choice of $x_0(h), \ldots, x_{k-1}(h)$ for which

$$\lim_{h\to 0} |x(t_i(h)) - x_i(h)| = 0 \quad \text{for} \quad i = 0, \ldots, k-1,$$

we have

$$\lim_{h\to 0} \max_{\{i: a \le t_i(h) \le b\}} |x(t_i(h)) - x_i(h)| = 0 \ .$$

Remarks

(i) Convergence asks for *uniform* decrease of the error on the grid as $h \to 0$.

(ii) By the continuity of $x(t)$, the condition on the initial values is equivalent to $x_i(h) \to x_a$ for $i = 0, 1, \ldots, k-1$.

The Dahlquist Root Condition

Fact *If an LMM is convergent, then the zeroes of the (first) characteristic polynomial of the method*

$$p(r) = \alpha_k r^k + \cdots + \alpha_0$$

satisfy the Dahlquist root condition:

(a) *all zeroes r satisfy* $|r| \leq 1$*, and*

(b) *multiple zeroes r satisfy* $|r| < 1$*.*

LMM Convergence: Example

Consider the IVP $x' = 0$, $a \leq t \leq b$, $x(a) = 0$. So $f \equiv 0$. Consider the LMM:

$$\sum \alpha_j x_{i+j} = 0 \ .$$

(1) Let r be any zero of $p(r)$. Then the solution with initial conditions

$$x_i = hr^i \quad \text{for} \quad 0 \leq i \leq k-1$$

is

$$x_i = hr^i \quad \text{for} \quad 0 \leq i \leq \frac{b-a}{h} \ .$$

Suppose $h = \frac{b-a}{m}$ for some $m \in \mathbb{Z}$. If the LMM is convergent, then $x_m(h) \to x(b) = 0$ as $m \to \infty$. But

$$x_m(h) = hr^m = \frac{b-a}{m} r^m.$$

So

$$|x_m(h) - x(b)| = \frac{b-a}{m} |r^m| \to 0 \quad \text{as} \quad m \to \infty$$

iff $|r| \leq 1$.

LMM Convergence: Examples

Again consider the LMM $\sum \alpha_j x_{i+j} = 0$.

(2) If r is a multiple zero of $p(r)$, taking $x_i(h) = hir^i$ for $0 \leq i \leq k-1$ gives

$$x_i(h) = hir^i, \quad 0 \leq i \leq \frac{b-a}{h} \ .$$

So if $h = \frac{b-a}{m}$, then

$$x_m(h) = \frac{b-a}{m} mr^m = (b-a)r^m,$$

so $x_m(h) \to 0$ as $h \to 0$ iff $|r| < 1$.

Zero-Stable LLMs

Definition *A LMM is called zero-stable if it satisfies the Dahlquist root condition.*

Recall from our discussion of linear difference equations that zero-stability is equivalent to requiring that all solutions of

$$(lh) \quad \sum_{j=0}^{k} \alpha_j x_{i+j} = 0 \quad \text{for} \quad i \geq 0$$

stay bounded as $i \to \infty$.

A consistent *one-step* LMM (i.e., $k = 1$) is always zero-stable. Indeed, consistency implies that $C_0 = C_1 = 0$, which in turn implies that $p(1) = \alpha_0 + \alpha_1 = C_0 = 0$ and so $r = 1$ is *the* zero of $p(r)$. Therefore $\alpha_1 = 1, \alpha_0 = -1$, so the characteristic polynomial is $p(r) = r - 1$, and the LMM is zero-stable.

The Key Convergence Theorem for LLMs

An LMM is convergent if and only if it is zero-stable and consistent.

Moreover, for zero-stable methods, we get an error estimate of the form

$$\max_{a \le t_i(h) \le b} |x(t_i(h)) - x_i(h)| \le$$

$$K_1 \underbrace{\max_{0 \le i \le k-1} |x(t_i(h)) - x_i(h)|}_{\text{initial error}} + K_2 \underbrace{\frac{\max_i |l(h, t_i(h))|}{h}}_{\substack{\text{“growth of error”} \\ \text{controlled by} \\ \text{zero-stability}}}$$

Dahlquist Condition implies Boundedness of (Ii)

Consider

$$(Ii) \qquad \sum_{j=0}^{k} \alpha_j x_{i+j} = b_i \quad \text{for} \quad i \geq 0 \qquad (\text{where } \alpha_k = 1),$$

with the initial values $x_0, \ldots, x_{k-1}$ given, and suppose that the characteristic polynomial $p(r) = \sum_{j=0}^{k} \alpha_j r^j$ satisfies the Dahlquist root condition. Then there is an $M > 0$ such that for $i \geq 0$,

$$|x_{i+k}| \leq M \left(\max\{|x_0|, \ldots, |x_{k-1}|\} + \sum_{\nu=0}^{i} |b_\nu| \right).$$

Proof

Let

$$A = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -\alpha_0 & & \cdots & -\alpha_{k-1} \end{bmatrix}.$$

The Dahlquist condition implies that there is an $M > 0$ such that $\|A^i\|_\infty < M$ for all i.

Proof

Let $\widetilde{x}_i = [x_i,\ x_{i+1},\ \ldots,\ x_{i+k-1}]^T$ and $\widetilde{b}_i = [0,\ \ldots,\ 0,\ b_i]^T$. Then $\widetilde{x}_{i+1} = A\widetilde{x}_i + \widetilde{b}_i$, so by induction

$$\widetilde{x}_{i+1} = A^{i+1}\widetilde{x}_0 + \sum_{\nu=0}^{i} A^{i-\nu}\widetilde{b}_\nu.$$

Thus

$$\begin{aligned}
|x_{i+k}| &\leq \|\widetilde{x}_{i+1}\|_\infty \\
&\leq \|A^{i+1}\|_\infty \|\widetilde{x}_0\|_\infty + \sum_{\nu=0}^{i} \|A^{i-\nu}\|_\infty \|\widetilde{b}_\nu\|_\infty \\
&\leq M(\|\widetilde{x}_0\|_\infty + \sum_{\nu=0}^{i} |b_\nu|).
\end{aligned}$$

Proof of LMM Convergence Theorem

The fact that convergence implies zero-stability and consistency is left as an exercise. Suppose a LMM is zero-stable and consistent. Let $x(t)$ be the true solution of the IVP $x' = f(t, x)$, $x(a) = x_a$ on $[a, b]$, let L be the Lipschitz constant for f, and set

$$\beta = \sum_{j=0}^{k} |\beta_j|.$$

Hold h fixed, and set

$$e_i(h) = x(t_i(h)) - x_i(h), \qquad E(h) = \max\{|e_0(h)|, \ldots, |e_{k-1}(h)|\},$$
$$l_i(h) = l(h, t_i(h)), \qquad \lambda(h) = \max_{i \in \mathcal{I}} |l_i(h)|,$$

where $\mathcal{I} = \{i \geq 0 : i + k \leq \frac{b-a}{h}\}$ (the remaining steps to b from k).

Proof: Step 1

The first step is to derive a “difference inequality” for $|e_i|$. This difference inequality is a discrete form of the integral inequality leading to Gronwall's inequality. For $i \in \mathcal{I}$, we have

$$
\begin{aligned}
\sum_{j=0}^{k} \alpha_j x(t_{i+j}) &= h \sum_{j=0}^{k} \beta_j f(t_{i+j}, x(t_{i+j})) + l_i \\
\sum_{j=0}^{k} \alpha_j x_{i+j} &= h \sum_{j=0}^{k} \beta_j f_{i+j}.
\end{aligned}
$$

Subtraction gives $\sum_{j=0}^{k} \alpha_j e_{i+j} = b_i$, where

$$
b_i \equiv h \sum_{j=0}^{k} \beta_j \left(f(t_{i+j}, x(t_{i+j})) - f(t_{i+j}, x_{i+j}) \right) + l_i .
$$

Then

$$
|b_i| \le h \sum_{j=0}^{k} |\beta_j| L |e_{i+j}| + |l_i|
$$

Proof: Step 1

By the preceeding Lemma with x_{i+k} replaced by e_{i+k}, we obtain for $i \in \mathcal{I}$

$$
\begin{aligned}
|e_{i+k}| &\le M\left[E + \sum_{\nu=0}^{i} |b_\nu|\right] \\
&\le M\left[E + hL\sum_{\nu=0}^{i}\sum_{j=0}^{k} |\beta_j||e_{\nu+j}| + \sum_{\nu=0}^{i} |l_\nu|\right] \\
&\le M\left[E + hL\sum_{j=0}^{k} |\beta_j|\sum_{\nu=0}^{i} |e_{\nu+j}| + \sum_{\nu=0}^{i} |l_\nu|\right] \\
&\le M\left[E + hL|\beta_k||e_{i+k}| + hL\sum_{j=0}^{k} |\beta_j|\sum_{\nu=0}^{i+k-1} |e_\nu| + \sum_{\nu=0}^{i} |l_\nu|\right]
\end{aligned}
$$

$$
\begin{aligned}
|e_{i+k}| &\le M\left[E + hL|\beta_k||e_{i+k}| + hL\beta\sum_{\nu=0}^{i+k-1}|e_\nu| + \sum_{\nu=0}^{i}|l_\nu|\right] \\
&\le M\left[E + hL\beta|e_{i+k}| + hL\beta\sum_{\nu=0}^{k+i-1}|e_\nu| + \frac{b-a}{h}\lambda\right],
\end{aligned}
$$

From here on, assume h is small enough that

$$
MhL|\beta_k| \le \frac{1}{2}.
$$

Since $\left\{h \le b-a : MhL|\beta_k| \ge \frac{1}{2}\right\}$ is a compact subset of $(0, b-a]$, the estimate in the Key Theorem is clearly true for those values of h.

Proof: Step 1

$$
\begin{aligned}
|e_{i+k}| &\leq M\left[E + hL|\beta_k||e_{i+k}| + hL\beta \sum_{\nu=0}^{i+k-1} |e_\nu| + \frac{b-a}{h}\lambda\right] \\
&\leq \frac{1}{2}|e_{i+k}| + ME + MhL\beta \sum_{\nu=0}^{i+k-1} |e_\nu| + M\frac{b-a}{h}\lambda
\end{aligned}
$$

since $MhL|\beta_k| \leq \frac{1}{2}$.

Moving $\frac{1}{2}|e_{i+k}|$ to the LHS gives

$$
|e_{i+k}| \leq hM_1 \sum_{\nu=0}^{i+k-1} |e_\nu| + M_2 E + M_3 \lambda / h
$$

for $i \in \mathcal{I}$, where $M_1 = 2ML\beta$, $M_2 = 2M$, and $M_3 = 2M(b-a)$.

(Note: For explicit methods, $\beta_k = 0$, so the restriction $MhL|\beta_k| \leq \frac{1}{2}$ is unnecessary, and the factors of 2 in M_1, M_2, M_3 can be dropped.)

Proof: Step 2

$$|e_{i+k}| \leq hM_1 \sum_{\nu=0}^{i+k-1} |e_\nu| + M_2 E + M_3 \lambda/h$$

We now use a discrete "comparison" argument to bound $|e_i|$. Let y_i be the solution of

$$y_{i+k} = hM_1 \sum_{\nu=0}^{i+k-1} y_\nu + (M_2 E + M_3 \lambda/h) \quad \text{for } i \in \mathcal{I}, \qquad (*)$$

with initial values $y_j = |e_j|$ for $0 \leq j \leq k-1$. Then clearly by induction $|e_{i+k}| \leq y_{i+k}$ for $i \in \mathcal{I}$. Now

$$y_k \leq hM_1 kE + (M_2 E + M_3\ \lambda/h) \leq M_4 E + M_3 \lambda/h,$$

where $M_4 = (b-a)M_1 k + M_2$. Subtracting $(*)$ for i from $(*)$ for $i+1$ gives

$$y_{i+k+1} - y_{i+k} = hM_1 y_{i+k}, \quad \text{and so} \quad y_{i+k+1} = (1 + hM_1) y_{i+k}.$$

Proof: Step 2

Therefore, by induction we obtain for $i \in \mathcal{I}$:

$$\begin{aligned} y_{i+k} &= (1+hM_1)^i y_k \\ &\leq (1+hM_1)^{(b-a)/h} y_k \\ &\leq e^{M_1(b-a)} y_k \\ &\leq K_1 E + K_2 \lambda / h, \end{aligned}$$

where $K_1 = e^{M_1(b-a)} M_4$ and $K_2 = e^{M_1(b-a)} M_3$. Thus, for $i \in \mathcal{I}$,

$$|e_{i+k}| \leq K_1 E + K_2 \lambda / h;$$

since $K_1 \geq M_4 \geq M_2 \geq M \geq 1$, also $|e_j| \leq E \leq K_1 E + K_2 \lambda / h$ for $0 \leq j \leq k-1$. Since consistency implies $\lambda = o(h)$, we are done.