Introduction to the Numerical Solution of IVP for ODE

Consider the IVP: DE $x' = f(t,x)$, IC $x(a) = x_a$. For simplicity, we will assume here that $x(t) \in \mathbb{R}^n$ (so $\mathbb{F} = \mathbb{R}$), and that $f(t,x)$ is continuous in t, x and uniformly Lipschitz in x (with Lipschitz constant L) on $[a,b] \times \mathbb{R}^n$. So we have global existence and uniqueness for the IVP on $[a,b]$.

Moreover, the solution of the IVP $x' = f(t,x)$, $x(a) = x_a$ depends continuously on the initial values $x_a \in \mathbb{R}^n$. This IVP is an example of a *well-posed problem*: for each choice of the "data" (here, the initial values x_a), we have:

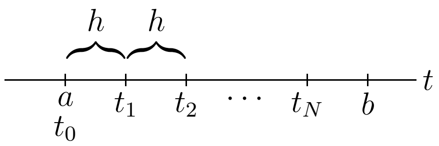
(1) **Existence.** There exists a solution of the IVP on $[a,b]$.

(2) **Uniqueness.** The solution, for each given x_a, is unique.

(3) **Continuous Dependence.** The solution depends continuously on the data.

Here, e.g., the map $x_a \mapsto x(t, x_a)$ is continuous from $\mathbb{R}^n$ into $(C([a,b]), \|\cdot\|_\infty)$. A well-posed problem is a reasonable problem to approximate numerically.

Grid Functions



Choose a mesh width h (with $0 < h \le b-a$), and let $N = \left[\frac{b-a}{h}\right]$ (greatest integer $\le (b-a)/h$). Let $t_i = a + ih$ $(i = 0, 1, \ldots, N)$ be the grid points in t (note: $t_0 = a$), and let x_i denote the approximation to $x(t_i)$. Note that t_i and x_i depend on h, but we will usually suppress this dependence in our notation.

Explicit One-Step Methods

Form of method: start with x_0 (presumably $x_0 \approx x_a$). Recursively compute $x_1, \ldots, x_N$ by

$$x_{i+1} = x_i + h\psi(h, t_i, x_i), \qquad i = 0, \ldots, N-1.$$

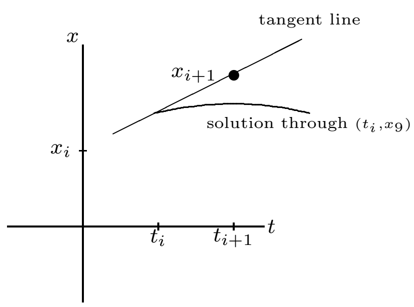
Here, $\psi(h,t,x)$ is a function defined for $0 \le h \le b-a$, $a \le t \le b$, $x \in \mathbb{R}^n$, and ψ is associated with the given function $f(t,x)$.

Examples.

Euler's Method.

$$x_{i+1} = x_i + hf(t_i, x_i)$$

Here, $\psi(h,t,x) = f(t,x)$.



Taylor Methods.

Let p be an integer ≥ 1. To see how the Taylor Method of order p is constructed, consider the Taylor expansion of a C^{p+1} solution $x(t)$ of $x' = f(t,x)$:

$$x(t+h) = x(t) + hx'(t) + \cdots + \frac{h^p}{p!}x^{(p)}(t) + \underbrace{O(h^{p+1})}_{\text{remainder term}}$$

where the remainder term is $O(h^{p+1})$ by Taylor's Theorem with remainder. In the approximation, we will neglect the remainder term, and use the DE $x' = f(t,x)$ to replace $x'(t), x''(t), \ldots$ by expressions involving f and its derivatives:

$$\begin{aligned} x'(t) &= f(t,x(t)) \\ x''(t) &= \frac{d}{dt}(f(t,x(t))) = \overset{(n\times 1)}{D_t f}\Big|_{(t,x(t))} + \overset{(n\times n)}{D_x f}\Big|_{(t,x(t))} \overset{(n\times 1)}{\frac{dx}{dt}} \\ &= (D_t f + (D_x f)f)\Big|_{(t,x(t))} \qquad \text{(for } n=1\text{, this is } f_t + f_x f\text{).} \end{aligned}$$

For higher derivatives, inductively differentiate the expression for the previous derivative, and replace any occurrence of $\frac{dx}{dt}$ by $f(t,x(t))$. These expansions lead us to define the Taylor methods of order p:

$$p = 1: \qquad x_{i+1} = x_i + hf(t_i, x_i) \qquad \text{(Euler's method, } \psi(h,t,x) = f(t,x)\text{)}$$

$$p = 2: \qquad x_{i+1} = x_i + hf(t_i, x_i) + \frac{h^2}{2}(D_t f + (D_x f)f)\Big|_{(t_i,x_i)}$$

For the case $p = 2$, we have

$$\psi(h,t,x) = T_2(h,t,x) \equiv \left(f + \frac{h}{2}(D_t f + (D_x f)f)\right)\Big|_{(t,x)}.$$

We will use the notation $T_p(h,t,x)$ to denote the $\psi(h,t,x)$ function for the Taylor method of order p.

Remark. Taylor methods of order ≥ 2 are rarely used computationally. They require derivatives of f to be programmed and evaluated. They are, however, of theoretical interest in determining the order of a method.

Remark. A "one-step method" is actually an association of a function $\psi(h,t,x)$ (defined for $0 \leq h \leq b-a, a \leq t \leq b, x \in \mathbb{R}^n$) to each function $f(t,x)$ (which is continuous in t,x and Lipschitz in x on $[a,b]\times\mathbb{R}^n$). We study "methods" looking at one function f at a time. Many methods (e.g., Taylor methods of order $p \geq 2$) require more smoothness of f, either for their definition, or to guarantee that the solution $x(t)$ is sufficiently smooth. Recall that if $f \in C^p$ (in t and x), then the solution $x(t)$ of the IVP $x' = f(t,x)$, $x(a) = x_a$ is in $C^{p+1}([a,b])$. For "higher-order" methods, this smoothness is essential in getting the error to be higher order in h. We will assume from here on (usually tacitly) that f is sufficiently smooth when needed.

Examples.

Modified Euler's Method

$$\begin{aligned} x_{i+1} &= x_i + hf\left(t_i + \tfrac{h}{2}, x_i + \tfrac{h}{2} f(t_i, x_i)\right) \\ (\text{so } \psi(h,t,x) &= f\left(t + \tfrac{h}{2}, x + \tfrac{h}{2} f(t,x)\right)). \end{aligned}$$

Here $\psi(h,t,x)$ tries to approximate

$$x'\left(t + \tfrac{h}{2}\right) = f\left(t + \tfrac{h}{2}, x\left(t + \tfrac{h}{2}\right)\right),$$

using the Euler approximation to $x\left(t + \frac{h}{2}\right)$ $\left(\approx x(t) + \frac{h}{2} f(t, x(t))\right)$.

Improved Euler's Method (or Heun's Method)

$$\begin{aligned} x_{i+1} &= x_i + \tfrac{h}{2}\left(f(t_i, x_i) + f\left(t_{i+1}, x_i + hf(t_i, x_i)\right)\right) \\ (\text{so } \psi(h,t,x) &= \tfrac{1}{2}\left(f(t,x) + f\left(t+h, x + hf(t,x)\right)\right)). \end{aligned}$$

Here again $\psi(h,t,x)$ tries to approximate

$$x'\left(t + \tfrac{h}{2}\right) \approx \tfrac{1}{2}(x'(t) + x'(t+h)).$$

Or $\psi(h,t,x)$ can be viewed as an approximation to the trapezoid rule applied to

$$\frac{1}{h}\left(x(t+h) - x(t)\right) = \frac{1}{h}\int_t^{t+h} x' \approx \tfrac{1}{2}x'(t) + \tfrac{1}{2}x'(t+h).$$

Modified Euler and Improved Euler are examples of 2$^{\text{nd}}$ order two-stage Runge-Kutta methods. Notice that no derivatives of f need be evaluated, but f needs to be evaluated *twice* in each step (from x_i to x_{i+1}).

Before stating the convergence theorem, we introduce the concept of *accuracy*.

Local Truncation Error

Let $x_{i+1} = x_i + h\psi(h, t_i, x_i)$ be a one-step method, and let $x(t)$ be a solution of the DE $x' = f(t,x)$. The *local truncation error* (LTE) for $x(t)$ is defined to be

$$l(h,t) \equiv x(t+h) - (x(t) + h\psi(h,t,x(t))),$$

that is, the local truncation error is *the amount by which the true solution of the DE fails to satisfy the numerical scheme.* $l(h,t)$ is defined for those (h,t) for which $0 < h \leq b-a$ and $a \leq t \leq b-h$.

Define
$$\tau(h,t) = \frac{l(h,t)}{h}$$
and set $\tau_i(h) = \tau(h,t_i)$. Also, set
$$\tau(h) = \max_{a\leq t\leq b-h} |\tau(h,t)| \quad \text{for } 0 < h \leq b-a.$$
Note that
$$l(h,t_i) = x(t_{i+1}) - (x(t_i) + h\psi(h,t_i,x(t_i))),$$
explicitly showing the dependence of l on h, t_i, and $x(t)$.

Definition. A one-step method is called [formally] *accurate of order* p (for a positive integer p) if for any solution $x(t)$ of the DE $x' = f(t,x)$ which is C^{p+1}, we have $l(h,t) = O(h^{p+1})$.

Definition. A one-step method is called *consistent* if $\psi(0,t,x) = f(t,x)$. Consistency is essentially minimal accuracy:

Proposition. A one-step method
$$x_{i+1} = x_i + h\psi(h,t_i,x_i),$$
where $\psi(h,t,x)$ is continuous for $0 \leq h \leq h_0$, $a \leq t \leq b$, $x \in \mathbb{R}^n$ for some $h_0 \in (0, b-a]$, is consistent with the DE $x' = f(t,x)$ if and only if $\tau(h) \to 0$ as $h \to 0^+$.

Proof. Suppose the method is consistent. Fix a solution $x(t)$. For $0 < h \leq h_0$, let
$$Z(h) = \max_{a\leq s,t\leq b,\ |s-t|\leq h} |\psi(0,s,x(s)) - \psi(h,t,x(t))|.$$
By uniform continuity, $Z(h) \to 0$ as $h \to 0^+$. Now
$$\begin{aligned} l(h,t) &= x(t+h) - x(t) - h\psi(h,t,x(t)) \\ &= \int_t^{t+h} [x'(s) - \psi(h,t,x(t))]\, ds \\ &= \int_t^{t+h} [f(s,x(s)) - \psi(h,t,x(t))]\, ds \\ &= \int_t^{t+h} [\psi(0,s,x(s)) - \psi(h,t,x(t))]\, ds, \end{aligned}$$
so $|l(h,t)| \leq hZ(h)$. Therefore $\tau(h) \leq Z(h) \to 0$.

Conversely, suppose $\tau(h) \to 0$. For any $t \in [a,b)$ and any $h \in (0, b-t]$,
$$\frac{x(t+h) - x(t)}{h} = \psi(h,t,x(t)) + \tau(h,t).$$
Taking the limit as $h \downarrow 0$ gives $f(t,x(t)) = x'(t) = \psi(0,t,x(t))$. □

Convergence Theorem for One-Step Methods

Theorem. Suppose $f(t,x)$ is continuous in t,x and uniformly Lipschitz in x on $[a,b]\times\mathbb{R}^n$. Let $x(t)$ be the solution of the IVP $x' = f(t,x)$, $x(a) = x_a$ on $[a,b]$. Suppose that the function $\psi(h,t,x)$ in the one step method satisfies the following two conditions:

1. (*Stability*) $\psi(h,t,x)$ is continuous in h,t,x and uniformly Lipschitz in x (with Lipschitz constant K) on $0 \le h \le h_0$, $a \le t \le b$, $x \in \mathbb{R}^n$ for some $h_0 > 0$ with $h_0 \le b-a$, and
2. (*Consistency*) $\psi(0,t,x) = f(t,x)$.

Let $e_i(h) = x(t_i(h)) - x_i(h)$, where x_i is obtained from the one-step method $x_{i+1} = x_i + h\psi(h,t_i,x_i)$. (Note that $e_0(h) = x_a - x_0(h)$ is the error in the initial value $x_0(h)$.) Then

$$|e_i(h)| \le e^{K(t_i(h)-a)}|e_0(h)| + \tau(h)\left(\frac{e^{K(t_i(h)-a)}-1}{K}\right),$$

so

$$|e_i(h)| \le e^{K(b-a)}|e_0(h)| + \frac{e^{K(b-a)}-1}{K}\tau(h).$$

Moreover, $\tau(h) \to 0$ as $h \to 0$. Therefore, if $e_0(h) \to 0$ as $h \to 0$, then

$$\max_{0\le i\le \frac{b-a}{h}} |e_i(h)| \to 0 \quad \text{as} \quad h \to 0,$$

that is, the approximations converge uniformly on the grid to the solution.

Proof. Hold $h > 0$ fixed, and ignore rounding error. Subtracting

$$x_{i+1} = x_i + h\psi(h,t_i,x_i)$$

from

$$x(t_{i+1}) = x(t_i) + h\psi(h,t_i,x(t_i)) + h\tau_i,$$

gives

$$\begin{aligned} |e_{i+1}| &\le |e_i| + h|\psi(h,t_i,x(t_i)) - \psi(h,t_i,x_i)| + h|\tau_i| \\ &\le |e_i| + hK|e_i| + h\tau(h) \\ &= (1+hK)|e_i| + h\tau(h). \end{aligned}$$

So

$$\begin{aligned} |e_1| &\le (1+hK)|e_0| + h\tau(h), \quad \text{and} \\ |e_2| &\le (1+hK)|e_1| + h\tau(h) \\ &\le (1+hK)^2|e_0| + h\tau(h)(1+(1+hK)). \end{aligned}$$

By induction,

$$\begin{aligned} |e_i| &\le (1+hK)^i|e_0| + h\tau(h)(1+(1+hK)+(1+hK)^2+\cdots+(1+hK)^{i-1}) \\ &= (1+hK)^i|e_0| + h\tau(h)\frac{(1+hK)^i-1}{(1+hK)-1} \\ &= (1+hK)^i|e_0| + \tau(h)\frac{(1+hK)^i-1}{K} \end{aligned}$$

Since $(1+hK)^{\frac{1}{h}} \uparrow e^K$ as $h \to 0^+$ (for $K > 0$), and $i = \frac{t_i - a}{h}$, we have

$$(1+hK)^i = (1+hK)^{\frac{t_i-a}{h}} \le e^{K(t_i-a)}.$$

Thus

$$|e_i| \le e^{K(t_i-a)}|e_0| + \tau(h)\frac{e^{K(t_i-a)}-1}{K}.$$

The preceding proposition shows $\tau(h) \to 0$, and the theorem follows. $\square$

If f is sufficiently smooth, then we know that $x(t) \in C^{p+1}$. The theorem thus implies that if a one-step method is accurate of order p and stable [i.e. ψ is Lipschitz in x], then for sufficiently smooth f,

$$l(h,t) = O(h^{p+1}) \quad \text{and thus} \quad \tau(h) = O(h^p).$$

If, in addition, $e_0(h) = O(h^p)$, then

$$\max_i |e_i(h)| = O(h^p),$$

i.e. we have p^{th} order convergence of the numerical approximations to the solution.

Example. The "Taylor method of order p" is accurate of order p. If $f \in C^p$, then $x \in C^{p+1}$, and

$$l(h,t) = x(t+h) - \left(x(t) + hx'(t) + \cdots + \frac{h^p}{p!}x^{(p)}(t)\right) = \frac{1}{p!}\int_t^{t+h}(t+h-s)^p x^{(p+1)}(s)ds.$$

So

$$|l(h,t)| \le M_{p+1}\frac{h^{p+1}}{(p+1)!} \quad \text{where} \quad M_{p+1} = \max_{a\le t\le b}|x^{(p+1)}(t)|.$$

Fact. A one-step method $x_{i+1} = x_i + h\psi(h,t_i,x_i)$ is accurate of order p if and only if

$$\psi(h,t,x) = T_p(h,t,x) + O(h^p),$$

where T_p is the "ψ" for the Taylor method of order p.

Proof. Since

$$x(t+h) - x(t) = hT_p(h,t,x(t)) + O(h^{p+1}),$$

we have for any given one-step method that

$$\begin{aligned} l(h,t) &= x(t+h) - x(t) - h\psi(h,t,x(t)) \\ &= hT_p(h,t,x(t)) + O(h^{p+1}) - h\psi(h,t,x(t)) \\ &= h(T_p(h,t,x(t)) - \psi(h,t,x(t))) + O(h^{p+1}). \end{aligned}$$

So $l(h,t) = O(h^{p+1})$ iff $h(T_p - \psi) = O(h^{p+1})$ iff $\psi = T_p + O(h^p)$. $\square$

Remark. The controlled growth of the effect of the local truncation error (LTE) from previous steps in the proof of the convergence theorem (a consequence of the Lipschitz continuity of ψ in x) is called *stability*. The theorem states:

Stability + Consistency (minimal accuracy) $\Rightarrow$ Convergence.

In fact, here, the converse is also true.

Explicit Runge-Kutta methods

One of the problems with Taylor methods is the need to evaluate higher derivatives of f. Runge-Kutta (RK) methods replace this with the much more reasonable need to evaluate f more than once to go from x_i to x_{i+1}. An m-stage (explicit) RK method is of the form

$$x_{i+1} = x_i + h\psi(h, t_i, x_i),$$

with

$$\psi(h, t, x) = \sum_{j=1}^{m} a_j k_j(h, t, x),$$

where $a_1, \ldots, a_m$ are given constants,

$$k_1(h, t, x) = f(t, x)$$

and for $2 \leq j \leq m$,

$$k_j(h, t, x) = f(t + \alpha_j h, x + h \sum_{r=1}^{j-1} \beta_{jr} k_r(h, t, x))$$

with $\alpha_2, \ldots, \alpha_m$ and β_{jr} $(1 \leq r < j \leq m)$ given constants. We usually choose $0 < \alpha_j \leq 1$, and for accuracy reasons we choose

$$(*) \qquad \alpha_j = \sum_{r=1}^{j-1} \beta_{jr} \qquad (2 \leq j \leq m).$$

Example. $m = 2$

$$x_{i+1} = x_i + h(a_1 k_1(h, t_i, x_i) + a_2 k_2(h, t_i, x_i))$$

where

$$\begin{aligned} k_1(h, t_i, x_i) &= f(t_i, x_i) \\ k_2(h, t_i, x_i) &= f(t_i + \alpha_2 h, x_i + h\beta_{21} k_1(h, t_i, x_i)). \end{aligned}$$

For simplicity, write α for α_2 and β for β_2. Expanding in h,

$$\begin{aligned} k_2(h, t, x) &= f(t + \alpha h, x + h\beta f(t, x)) \\ &= f(t, x) + \alpha h D_t f(t, x) + (D_x f(t, x))(h\beta f(t, x)) + O(h^2) \\ &= \left[f + h(\alpha D_t f + \beta(D_x f) f)\right](t, x) + O(h^2). \end{aligned}$$

So

$$\psi(h, t, x) = (a_1 + a_2) f + h(a_2 \alpha D_t f + a_2 \beta (D_x f) f) + O(h^2).$$

Recalling that

$$T_2 = f + \frac{h}{2}(D_t f + (D_x f) f),$$

and that the method is accurate of order two if and only if

$$\psi = T_2 + O(h^2),$$

we obtain the following necessary and sufficient conditions on a two-stage (explicit) RK method to be accurate of order two:

$$a_1 + a_2 = 1, \quad a_2\alpha = \tfrac{1}{2}, \quad \text{and} \quad a_2\beta = \tfrac{1}{2}.$$

We require $\alpha = \beta$ as in (*) (we now see why this condition needs to be imposed), whereupon these conditions become:

$$\boxed{a_1 + a_2 = 1, \qquad a_2\alpha = \tfrac{1}{2}}.$$

Therefore, there is a one-parameter family (e.g., parameterized by α) of 2^{nd} order, two-stage ($m = 2$) explicit RK methods.

Examples.

(1) Setting $\alpha = \frac{1}{2}$ gives $a_2 = 1$, $a_1 = 0$, which is the Modified Euler method.

(2) Choosing $\alpha = 1$ gives $a_2 = \frac{1}{2}$, $a_1 = \frac{1}{2}$, which is the Improved Euler method, or Heun's method.

Remark. Note that an m-stage explicit RK method requires m function evaluations (i.e., evaluations of f) in each step (x_i to x_{i+1}).

Attainable Orders of Accuracy for Explicit RK methods

# of stages (m)	highest order attainable	
1	1	← Euler's method
2	2	
3	3	
4	4	
5	4	
6	5	
7	6	
8	7	

Explicit RK methods are *always* stable: ψ inherits its Lipschitz continuity from f.

Example.

Modified Euler. Let L be the Lipschitz constant for f, and suppose $h \le h_0$ (for some $h_0 \le b - a$).

$$\begin{aligned} x_{i+1} &= x_i + hf\left(t_i + \tfrac{h}{2}, x_i + \tfrac{h}{2} f(t_i, x_i)\right) \\ \psi(t, h, x) &= f\left(t + \tfrac{h}{2}, x + \tfrac{h}{2} f(t, x)\right) \end{aligned}$$

So

$$\begin{aligned}|\psi(h,t,x)-\psi(h,t,y)| &\leq L\left|\left(x+\tfrac{h}{2}f(t,x)\right)-\left(y+\tfrac{h}{2}f(t,y)\right)\right| \\ &\leq L|x-y|+\tfrac{h}{2}L|f(t,x)-f(t,y)| \\ &\leq L|x-y|+\tfrac{h}{2}L^2|x-y| \\ &\leq K|x-y|\end{aligned}$$

where $K = L + \frac{h_0}{2}L^2$ is thus the Lipschitz constant for ψ.

Example. A popular 4^{th} order four-stage RK method is

$$x_{i+1} = x_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

where

$$\begin{aligned}k_1 &= f(t_i, x_i) \\ k_2 &= f\left(t_i + \tfrac{h}{2}, x_i + \tfrac{h}{2}k_1\right) \\ k_3 &= f\left(t_i + \tfrac{h}{2}, x_i + \tfrac{h}{2}k_2\right) \\ k_4 &= f(t_i + h, x_i + hk_3).\end{aligned}$$

The same argument as above shows this method is stable.

Remark. RK methods require multiple function evaluations per step (going from x_i to x_{i+1}). One-step methods discard information from previous steps (e.g., x_{i-1} is not used to get x_{i+1} — except in its influence on x_i). We will next study a class of multi-step methods. But first, we consider linear difference equations.

Linear Difference Equations (Constant Coefficients)

In this discussion, x_i will be a (scalar) sequence defined for $i \geq 0$. Consider the linear difference equation (k-step)

$$\text{(LDE)} \qquad x_{i+k} + \alpha_{k-1}x_{i+k-1} + \cdots + \alpha_0 x_i = b_i \qquad (i \geq 0).$$

If $b_i \equiv 0$, the linear difference equation (LDE) is said to be homogeneous, in which case we will refer to it as (lh). If $b_i \neq 0$ for some $i \geq 0$, the linear difference equation (LDE) is said to be inhomogeneous , in which case we refer to it as (li).

Initial Value Problem (IVP): Given x_i for $i = 0, \ldots, k-1$, determine x_i satisfying (LDE) for $i \geq 0$.

Theorem. There exists a unique solution of (IVP) for (lh) or (li).

Proof. An obvious induction on i. The equation for $i = 0$ determines x_k, etc. □

Theorem. The solution set of (lh) is a k-dimensional vector space (a subspace of the set of all sequences $\{x_i\}_{i\geq 0}$).

Proof Sketch. Choosing

$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{k-1} \end{bmatrix} = e_j \in \mathbb{R}^k$$

for $j = 1, 2, \ldots k$ and then solving (lh) gives a basis of the solution space of (lh). □

Define the *characteristic polynomial* of (lh) to be

$$p(r) = r^k + \alpha_{k-1} r^{k-1} + \cdots + \alpha_0.$$

Let us assume that $\alpha_0 \neq 0$. (If $\alpha_0 = 0$, (LDE) isn't really a k-step difference equation since we can shift indices and treat it as a $\widetilde{k}$-step difference equation for a $\widetilde{k} < k$, namely $\widetilde{k} = k - \nu$, where ν is the smallest index with $\alpha_\nu \neq 0$.) Let $r_1, \ldots, r_s$ be the distinct zeroes of p, with multiplicities $m_1, \ldots, m_s$. Note that each $r_j \neq 0$ since $\alpha_0 \neq 0$, and $m_1 + \cdots + m_s = k$. Then a basis of solutions of (lh) is:

$$\left\{ \{i^l r_j^i\}_{i=0}^\infty \,:\, 1 \leq j \leq s,\ 0 \leq l \leq m_j - 1 \right\}.$$

Example. Fibonacci Sequence:

$$F_{i+2} - F_{i+1} - F_i = 0, \quad F_0 = 0, \quad F_1 = 1.$$

The associated characteristic polynomial $r^2 - r - 1 = 0$ has roots

$$r_\pm = \frac{1 \pm \sqrt{5}}{2} \qquad (r_+ \approx 1.6, r_- \approx -0.6).$$

The general solution of (lh) is

$$F_i = C_+ \left(\frac{1 + \sqrt{5}}{2} \right)^i + C_- \left(\frac{1 - \sqrt{5}}{2} \right)^i.$$

The initial conditions $F_0 = 0$ and $F_1 = 1$ imply that $C_+ = \frac{1}{\sqrt{5}}$ and $C_- = -\frac{1}{\sqrt{5}}$. Hence

$$F_i = \frac{1}{\sqrt{5}} \left(\left(\frac{1 + \sqrt{5}}{2} \right)^i - \left(\frac{1 - \sqrt{5}}{2} \right)^i \right).$$

Since $|r_-| < 1$, we have

$$\left(\frac{1 - \sqrt{5}}{2} \right)^i \to 0 \text{ as } i \to \infty.$$

Hence, the Fibonacci sequence behaves asymptotically like the sequence $\frac{1}{\sqrt{5}} \left(\frac{1+\sqrt{5}}{2} \right)^i$.

Remark. If $\alpha_0 = \alpha_1 = \cdots = \alpha_{\nu-1} = 0$ and $\alpha_\nu \neq 0$ (i.e., 0 is a root of multiplicity ν), then $x_0, x_1, \ldots, x_{\nu-1}$ are completely independent of x_i for $i \geq \nu$. So $x_{i+k} + \cdots + \alpha_\nu x_{i+\nu} = b_i$ for $i \geq 0$ with x_i given for $i \geq \nu$ behaves like a $(k-\nu)$-step difference equation.

Remark. Define $\widetilde{x}_i = \begin{bmatrix} x_i \\ x_{i+1} \\ \vdots \\ x_{i+k-1} \end{bmatrix}$. Then $\widetilde{x}_{i+1} = A\widetilde{x}_i$ for $i \geq 0$, where

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

and $\widetilde{x}_0 = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{k-1} \end{bmatrix}$ is given by the I.C. So (lh) is equivalent to the one-step vector difference equation

$$\widetilde{x}_{i+1} = A\widetilde{x}_i, \quad i \geq 0,$$

whose solution is $\widetilde{x}_i = A^i \widetilde{x}_0$. The characteristic polynomial of (lh) is the characteristic polynomial of A. Because A is a companion matrix, each distinct eigenvalue has only one Jordan block. If $A = PJP^{-1}$ is the Jordan decomposition of A (J in Jordan form, P invertible), then

$$\widetilde{x}_i = PJ^iP^{-1}\widetilde{x}_0.$$

Let J_j be the $m_j \times m_j$ block corresponding to r_j (for $1 \leq j \leq s$), so $J_j = r_j I + Z_j$, where Z_j denotes the $m_j \times m_j$ shift matrix:

$$Z_j = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{bmatrix}.$$

Then

$$J_j^i = (r_j I + Z_j)^i = \sum_{l=0}^{i} \binom{i}{l} r_j^{i-l} Z_j^l.$$

Since $\binom{i}{l}$ is a polynomial in i of degree l and $Z_j^{m_j} = 0$, we see entries in $\widetilde{x}_i$ of the form (constant) $i^l r_j^i$ for $0 \leq l \leq m_j - 1$.

Remark. (li) becomes

$$\widetilde{x}_{i+1} = A\widetilde{x}_i + \widetilde{b}_i, \quad i \geq 0,$$

where $\widetilde{b}_i = [0, \ldots, 0, b_i]^T$. This leads to a discrete version of Duhamel's principle (exercise).

Remark. All solutions $\{x_i\}_{i\geq 0}$ of (lh) stay bounded (i.e. are elements of l^∞)

$\Leftrightarrow$ the matrix A is power bounded (i.e., $\exists\, M$ so that $\|A^i\| \leq M$ for all $i \geq 0$)

$\Leftrightarrow$ the Jordan blocks $J_1, \ldots, J_s$ are all power bounded

$$\Leftrightarrow \left\{ \begin{array}{lll} & \text{(a)} \quad \text{each } |r_j| \leq 1 & (\text{for } 1 \leq j \leq s) \\ \text{and} & \text{(b)} \quad \text{for any } j \text{ with } m_j > 1 \text{ (multiple roots)}, & |r_j| < 1 \end{array} \right. .$$

If (a) and (b) are satisfied, then the map $\widetilde{x}_0 \mapsto \{x_i\}_{i\geq 0}$ is a bounded linear operator from $\mathbb{R}^k$ (or $\mathbb{C}^k$) into l^∞ (exercise).

Linear Multistep Methods (LMM)

A LMM is a method of the form

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

for the approximate solution of an ODE IVP

$$x' = f(t, x), \quad x(a) = x_a \ .$$

Here we want to approximate the solution $x(t)$ of this IVP for $a \leq t \leq b$ at the points $t_i = a + ih$ (where h is the time step), $0 \leq i \leq \frac{b-a}{h}$. The term x_i denotes the approximation to $x(t_i)$. We have set $f_{i+j} = f(t_{i+j}, x_{i+j})$. We normalize the coefficients so that $\alpha_k = 1$. The above is called a *k-step LMM* (if at least one of the coefficients α_0 and β_0 is non-zero). The above equation 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 f is continuous in (t, x) and uniformly Lipschitz in x. 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.

Example. (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

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

Example. (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}.

Remark. 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

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

is a constant as far as x_{i+k} is concerned. That is, we are looking for a fixed point of

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

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 for x_{i+k} leads to a sequence converging to the fixed point using functional iteration

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

which is initiated at some initial point $x_{i+k}^{(0)}$. In practice, one chooses either

(1) iterate to convergence, or

(2) a fixed number of iterations, using an *explicit* method to get the initial guess $x_{i+k}^{(0)}$. This pairing is often called a Predictor-Corrector Method.

Function Evaluations. One FE means evaluating f once.

Explicit LMM: 1 FE per step (after initial start)
Implicit LMM: ? FEs per step if iterate to convergence
usually 2 FE per step for a Predictor-Corrector Method.

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

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

If $x \in C^{p+1}$, then

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

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

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

Definition. 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. A LMM is accurate of order at least p iff $C_0 = C_1 = \cdots = C_p = 0$. (It is called accurate of order exactly p if also $C_{p+1} \neq 0$.)

Remarks.

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

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

(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).

Remark. If a LMM is consistent, then any solution $x(t)$ for any f (continuous in (t, x), Lipschitz in x) has $l(h, t) = o(h)$. To see this, note that since $x \in C^1$,

$$x(t + jh) = x(t) + jhx'(t) + o(h) \quad \text{and} \quad hx'(t + jh) = hx'(t) + o(h),$$

so

$$l(h, t) = C_0 x(t) + C_1 hx'(t) + o(h).$$

Exercise: Verify that the $o(h)$ terms converge to 0 uniformly in t (after dividing by h) as $h \to 0$: use the uniform continuity of $x'(t)$ on $[a, b]$.

Definition. A k-step LMM

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

is called *convergent* if for each IVP $x' = f(t, x)$, $x(a) = x_a$ on $[a, b]$ ($f \in (C, \text{Lip})$) 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) This asks for *uniform* decrease of the error on the grid as $h \to 0$.

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

Fact. If a 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 $|r| \le 1$, and

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

Examples. Consider the IVP $x' = 0$, $a \le t \le b$, $x(a) = 0$. 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

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

is

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

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 $|r| \le 1$.

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

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

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 $|r| < 1$.

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) $\quad \sum_{j=0}^{k} \alpha_j x_{i+j} = 0$ for $i \ge 0$ stay bounded as $i \to \infty$.

Remark. 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.

Exercise: Show that if an LMM is convergent, then it is consistent.

Key Theorem. [LMM Convergence]

A 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

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

Remark. If $x \in C^{p+1}$ and the LMM is accurate of order p, then $|LTE|/h = O(h^p)$. To get p^{th}-order convergence (i.e., $LHS = O(h^p)$), we need

$$x_i(h) = x(t_i(h)) + O(h^p) \quad \text{for} \quad i = 0, \ldots, k-1.$$

This can be done using $k-1$ steps of a RK method of order $\geq p-1$.

Lemma. Consider

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

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 $i \geq 0$,

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

Remark. Recall that the Dahlquist root condition implies that there is an $M > 0$ for which $\|A^i\|_\infty \leq M$ for all $i \geq 0$, where

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

is the companion matrix for $p(r)$, and $\|\cdot\|_\infty$ is the operator norm induced by the vector norm $\|\cdot\|_\infty$. The M in the Lemma can be taken to be the same as this M bounding $\|A^i\|_\infty$.

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 the LMM Convergence Theorem. The fact that convergence implies zero-stability and consistency has already been discussed. 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

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

where $\mathcal{I} = \{i \geq 0 : i + k \leq \frac{b-a}{h}\}$.

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

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

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

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

From here on, assume h is small enough that

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

(Since $\left\{h \leq b-a : MhL|\beta_k| \geq \frac{1}{2}\right\}$ is a compact subset of $(0, b-a]$, the estimate in the Key Theorem is clearly true for those values of h.) Moving $MhL|\beta_k||e_{i+k}|$ 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.)

Step 2. We now use a discrete "comparison" argument to bound $|e_i|$. Let y_i be the solution of

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

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

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

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. □

Remarks.

(1) Note that K_1 and K_2 depend only on a, b, L, k, the α_j's and β_j's, and M.

(2) The estimate can be refined — we did not try to get the best constants K_1, K_2. For example, $e^{M_1(b-a)}$ could be replaced by $e^{M_1(t_i-a)}$ in both K_1 and K_2, yielding more precise estimates depending on i, similar to the estimate for one-step methods.