Hermite interpolation for the approximation of ordinary differential equations □

François Dubois ⋆

- **Dynamical system.**

Let n be an integer greater than the unity. We study an autonomous dynamical system in the finite dimensional space $\mathbb{R}^n$

$$(1) \qquad \frac{\mathrm{d}u}{\mathrm{d}t} \,=\, f\big(u(t)\big)\,, \qquad t > 0\,,$$

$$(2) \qquad u(0) \,=\, u_0\,,$$

where $\mathbb{R}^n \ni v \longmapsto f(v) \in \mathbb{R}^n$ is a sufficiently regular function. We discretize the time with a time step $h > 0$ and we search an approximation u_h of $u(h)$ with a one-step method, *id est* using **only** the knowledge of the initial vector u_0 and the **entire** function $f(\bullet)$.

- **One step numerical schemes.**

We integrate the equation (1) between 0 and h, we take into account the initial condition (2), divide by h and make an elementary change of variables inside the associated integral. It comes :

$$(3) \qquad \frac{u(h) - u_0}{h} \,=\, \int_0^1 f\big(u(\theta\, h)\big)\, \mathrm{d}\theta\,.$$

A good one-step method consists in approaching at best the right hand side of the relation (3). The choice of a constant interpolation conducts to the explicit Euler scheme when $\int_0^1 f\big(u(\theta\, h)\big)\,\mathrm{d}\theta \simeq f(u(0))$ and to the implicit Euler scheme if we choose $\int_0^1 f\big(u(\theta\, h)\big)\,\mathrm{d}\theta \simeq f(u(h))$. We refer *e.g.* to the book of Crouzeix and Mignot [CM84] for an introduction to the numerical analysis of ordinary differential equations. Nevertheless, a classical approach consists in making an **affine** interpolation $\varphi_1(\bullet)$ of the function $\varphi(\bullet)$ defined by

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⋆ Conservatoire National des Arts et Métiers, Paris, France.

(4) $\qquad [0,\, 1] \ni \theta \longmapsto \varphi(\theta) \equiv f\big(u(\theta\, h)\big) \in \mathbb{R}^n \,.$

Note that the function $\varphi_1(\bullet)$ is parameterized by $f(u_0)$ which is known and by $f(u(h))$ which is unknown and that we write $f(u_h)$ after having done the approximation :

(5) $\qquad \varphi_1(\theta) \equiv (1-\theta)\, f(u_0) + \theta\, f(u_h)\,.$

We obtain in that manner after integrating the function $\varphi_1(\bullet)$ on the interval $[0,\, 1]$ the so-called Crank-Nicolson scheme :

(6) $$\frac{u_h - u_0}{h} \;=\; \frac{1}{2}\,\big(\, f(u_h) \,+\, f(u_0)\,\big)\,.$$

- **Third order Hermite interpolation.**

We follow this interpolation idea with the following remark. If the state u_0 is known, then $\frac{{\rm d}u}{{\rm d}t}(0) = f(u_0)$ is known, but the second derivative $\frac{{\rm d}^2 u}{{\rm d}t^2}(0) = {\rm d}f(u_0) \bullet f(u_0)$ is also known. In a similar way, if the final state $u(h)$ is known, we have the same property for the first derivative $\frac{{\rm d}u}{{\rm d}t}(h) = f(u(h))$ **and** for the second derivative $\frac{{\rm d}^2 u}{{\rm d}t^2}(h) = {\rm d}f(u(h)) \bullet f(u(h))$. In that way, we have inside our hands **four** numerical values that characterize $\varphi(\bullet)$ introduced at the relation (4) at the two ends of the interval $[0,\, 1]$: $\varphi(0) = f(u_0)$, $\varphi'(0) = h\; {\rm d}f(u_0){\bullet}f(u_0)$, $\varphi(1) = f(u(h))$, $\varphi'(1) = h\; {\rm d}f(u(h)){\bullet}f(u(h))$. We use these four values and the classical Hermite basis for polynomials of degree at least three (see *e. g.* Hildebrand [Hil87]) to approximate the function $\varphi(\bullet)$ introduced at relation (4) by a polynomial function $\varphi_2(\bullet)$:

(7) $$\varphi(\theta) \;\simeq\; \varphi_2(\theta) \;\equiv\; \left\{ \begin{array}{l} (1+2\theta)\,(\theta-1)^2\,\varphi(0) \,+\, \theta\,(\theta-1)^2\,\varphi'(0) + \\ +\,\theta^2\,(3-2\theta)\,\varphi(1) \,+\, \theta^2\,(\theta-1)\,\varphi'(1)\,. \end{array} \right.$$

We intregrate the relation (7) over the interval $[0,\, 1]$, we replace the exact value $u(h)$ by an approximate one u_h and obtain in this way an approximate method for the ordinary differential equation (1). It an be written :

(8) $$\frac{u_h - u_0}{h} \;=\; \frac{1}{2}\,\big(f(u_h) \,+\, f(u_0)\big) \;-\; \frac{h}{12}\,\big[\,{\rm d}f(u_h){\bullet}f(u_h) - {\rm d}f(u_0){\bullet}f(u_0)\,\big]\,.$$

- **Proposition 1. Fourth order scheme.**

Let $u(\bullet)$ be the solution of the dynamical system (1)(2) and in particular let $u(h)$ be the solution of this system at time h. We define the truncation error $\mathcal{T}_h$ associated with the scheme (8) by the relation

(9) $$\mathcal{T}_h \;\equiv\; \left\{ \begin{array}{l} \dfrac{u(h) - u_0}{h} \;-\; \dfrac{1}{2}\,\big(f(u(h)) \,+\, f(u_0)\big) \\ \qquad\qquad\qquad\quad +\, \dfrac{h}{12}\,\big[\,{\rm d}f(u(h)){\bullet}f(u(h)) - {\rm d}f(u_0){\bullet}f(u_0)\,\big]\;. \end{array} \right.$$

Then we have

$$(10) \qquad \mid \mathcal{T}_h \mid \,\leq\, \frac{1}{720} \, \sup_{0 \leq t \leq h} \, || \, u^{(5)}(t) \, || \,\,\, h^4 \, .$$

- **A two-steps scheme based on Crank-Nicolson.**

The scheme (8) is implicit and the operator $\mathbb{R}^n \ni v \longmapsto \mathrm{d}f(v) \bullet f(v) \in \mathbb{R}^n$ can be complicated to manipulate algebraically. We propose to replace the nonlinear scheme (8) by a multistep procedure based on the Crank-Nicolson scheme (6). We first consider a predicted value u_h^1 evaluated with the Crank-Nicolson scheme :

$$(11) \qquad \frac{u_h^1 - u_0}{h} \,=\, \frac{1}{2} \big(\, f(u_h^1) \,+\, f(u_0) \, \big) \, .$$

Then we substitute this value u_h^1 in the second term of the right hand side of relation (8). We obtain in this way the following equation to deduce u_h^2 from the initial value u_0 and the predicted value u_h^1 :

$$(12) \qquad \frac{u_h^2 - u_0}{h} \,=\, \frac{1}{2} \big(f(u_h^2) + f(u_0) \big) - \frac{h}{12} \big[\, \mathrm{d}f(u_h^1) \bullet f(u_h^1) - \mathrm{d}f(u_0) \bullet f(u_0) \, \big] \, .$$

We remark that the resolution of both nonlinear equations (11) and (12) just needs to solve an equation of unknown w the form

$$(13) \qquad w \,-\, \frac{h}{2} \, f(w) \,=\, g \, ,$$

with the dynamics function $f(\bullet)$ in the operator to inverse at the left hand side of relation (13).

- **Proposition 2. Fourth order for two-step scheme.**

Let $u(h)$ be the solution of the dynamical system (1)(2) at time h. Let u_h^2 be computed according to the predictor-corrector scheme (11) (12). Then u_h^2 and $u(h)$ have the same Taylor expansion up to the order 4.

- **Hermite interpolation of higher order.**

We can generalize the previous schemes (8) and (11) (12) at an arbitrary order. We first observe that, according to the Faà di Bruno formula (see *e.g.* Hairer *et al* [HNW87]), we can express the j^o derivative of the solution $u(\bullet)$ of the dynamical system (1) with the function $f(\bullet)$ and its successive derivatives :

$$(14) \qquad \frac{\mathrm{d}^j \, u}{\mathrm{d}t^j}(t) \,\equiv\, \Phi_j \big(f, \, \mathrm{d}f, \, \cdots, \, \mathrm{d}^{j-1} f \, ; \, u(t) \, \big) \, .$$

We have for example for the two first derivatives $\Phi_1 \big(f \, ; \, u \, \big) \,\equiv\, f(u)$ and $\Phi_2 \big(f, \, \mathrm{d}f \, ; \, u \, \big) \equiv \mathrm{d}f(u) \bullet f(u)$. Then for a given integer k and $0 \leq \theta \leq 1$, we interpolate the function $\varphi(\theta) = \frac{\mathrm{d}u}{\mathrm{d}t}(\theta\, h)$ introduced at the relation (4) with the Hermite interpolation polynomial $\varphi_k(\bullet)$ of degree lower or equal than $(2k-1)$ based on the degrees of freedom $u'(0),\ h\, u''(0),\ \cdots,\ h^{k-1}\, u^{(k)}(0)$ and $u'(h),\ h\, u''(h),\ \cdots,\ h^{k-1}\, u^{(k)}(h)$. Then we integrate the polynomial $\varphi_k(\bullet)$ on the interval $[0,\, 1]$. We obtain by doing this a variant of the Euler-Mac Laurin summation formula

$$(15)\qquad \left\{ \begin{aligned} & \int_0^1 \varphi(\theta)\,\mathrm{d}\theta \,\simeq\, \int_0^1 \varphi_k(\theta)\,\mathrm{d}\theta \,=\, \frac{1}{2}\big(\varphi(0)+\varphi(1)\big) \\ & \qquad -\frac{1}{12}\big(\varphi'(1)-\varphi'(0)\big) \,-\, \cdots \,-\, \frac{B_{2\,k}}{(2k)!}\,\big(\varphi^{(k-1)}(1) \,-\, \varphi^{(k-1)}(0)\big)\,, \end{aligned} \right.$$

where B_{2k} are the Bernoulli numbers (see *e.g.* [Hil87]). We have due to the relation (14)

$$(16)\qquad \varphi^{(j)}(\theta) \;=\; h^{j-1}\,\frac{\mathrm{d}^j\, u}{\mathrm{d}t^j}(\theta\, h) \;=\; h^{j-1}\,\Phi_j\big(f,\,\mathrm{d}f,\,\cdots,\,\mathrm{d}^{j-1}f\,;\,u(\theta\, t)\big)\,.$$

When we replace the previous expression inside the relation (15), the associated numerical scheme takes the form :

$$(17)\qquad \left\{ \begin{aligned} & \frac{u_h-u_0}{h} \;=\; \frac{1}{2}\,\big(f(u_h)+f(u_0)\big) \,-\, \frac{h}{12}\,\big[\mathrm{d}f(u_h){\bullet}f(u_h)-\mathrm{d}f(u_0){\bullet}f(u_0)\big] \\ & \qquad\qquad - \sum_{j=3}^{k} \frac{B_{2\,j}}{(2j)!}\,h^{j-1}\,\Big(\Phi_j\big(f,\,\mathrm{d}f,\,\cdots,\,\mathrm{d}^{j-1}f\,;\,u_h\big) \\ & \qquad\qquad\qquad\qquad - \Phi_j\big(f,\,\mathrm{d}f,\,\cdots,\,\mathrm{d}^{j-1}f\,;\,u_0\big)\Big)\,. \end{aligned} \right.$$

• **Proposition 3. Numerical scheme of order 2k.**

Let $u(\bullet)$ be the solution of the dynamical system (1)(2) and in particular let $u(h)$ be the solution of this system at time h. We define the truncation error $\mathcal{T}_h$ associated with the scheme (17) by the relation

$$(18)\qquad \left\{ \begin{aligned} & \mathcal{T}_h \;\equiv\; \frac{u(h)-u_0}{h} \,-\, \frac{1}{2}\,\big(f(u(h)) \,+\, f(u_0)\big) \\ & \qquad\qquad + \sum_{j=2}^{k} \frac{B_{2\,j}}{(2j)!}\,h^{j-1}\,\Big(\Phi_j\big(f,\,\mathrm{d}f,\,\cdots,\,\mathrm{d}^{j-1}f\,;\,u(h)\big) \\ & \qquad\qquad\qquad\qquad - \Phi_j\big(f,\,\mathrm{d}f,\,\cdots,\,\mathrm{d}^{j-1}f\,;\,u_0\big)\Big)\,. \end{aligned} \right.$$

Then we have

$$(19)\qquad \mid \mathcal{T}_h \mid \,\leq\, C \sup_{0\leq t\leq h} \,||\, u^{(2k+1)}(t)\,||\;\; h^{2k}\,.$$

for some constant $C>0$.

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