Hermite interpolation for the approximation of ordinary differential equations

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

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

$$u(0) \; = \; u_0 \,, \tag{2}$$

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 :

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

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

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 :

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

- **Third order Hermite interpolation.**

We follow this interpolation idea with the following remark. If the state u_0 is known, then $\frac{\mathrm{d}u}{\mathrm{d}t}(0) = f(u_0)$ is known, but the second derivative $\frac{\mathrm{d}^2u}{\mathrm{d}t^2}(0) = \mathrm{d}f(u_0) \bullet f(u_0)$ is also known. In a similar way, if the final state $u(h)$ is known, we have the same property for the first derivative $\frac{\mathrm{d}u}{\mathrm{d}t}(h) = f(u(h))$ **and** for the second derivative $\frac{\mathrm{d}^2u}{\mathrm{d}t^2}(h) = \mathrm{d}f(u(h)) \bullet f(u(h))$. 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 $[0,\,1]$: $\varphi(0) = f(u_0)$, $\varphi'(0) = h\;\mathrm{d}f(u_0)\bullet f(u_0)$, $\varphi(1) = f(u(h))$, $\varphi'(1) = h\;\mathrm{d}f(u(h))\bullet f(u(h))$. 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 $\varphi_2(\bullet)$:

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

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 :

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

- **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

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

Then we have

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

- **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 :

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

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

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

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 :

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

- **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

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

Then we have

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

for some constant $C > 0$.

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