Non-expansive numerical methods

The non-expansivity property of a numerical method is a property one can use to ensure the non-linear stability of the method. For this reason, we start recalling the concept of linear stability, or A-stability, of one-step methods. A one-step method $\varphi^h : \mathbb{R}^d \to \mathbb{R}^d$ is A-stable if when applied to the linear test equation $\dot{x} = \lambda x$, $\lambda \in \mathbb{C}$, if $\mathrm{Re}(\lambda) < 0$, then $\lim_{n\to\infty} \left(\varphi^h\right)^n (\mathbf{x}) = 0$ for every fixed step size $h > 0$. For Runge–Kutta methods, one has

$$\varphi^h(x) = R(h\lambda)x,$$

for a suitable stability function $R : \mathbb{R} \to \mathbb{R}$. Thus, Runge–Kutta methods are A-stable if

$$S := \{z \in \mathbb{C} : |R(z)| < 1\} \supseteq \mathbb{C}^-.$$

We recall that no explicit Runge–Kutta method is A-stable, since for those methods the function R is a polynomial, and hence the stability region S is bounded.

1 Unconditionally non-linearly stable methods

There have been several other notions of numerical stability introduced in the literature. The one that refers to non-expansive/contractive vector fields in a norm $\|\cdot\|$ generated by an inner product $\langle\cdot,\cdot\rangle$ is called B-stability.

Definition 1 (B-stable method)**.** *A numerical method $\varphi^h : \mathbb{R}^d \to \mathbb{R}^d$ is B-stable if when applied to any vector field $X \in \mathfrak{X}(\mathbb{R}^d)$ which satisfies*

$$\left\|\phi^t_X(\mathbf{y}) - \phi^t_X(\mathbf{x})\right\| \leq \|\mathbf{y} - \mathbf{x}\|, \ \forall t \geq 0, \tag{1}$$

for a norm $\|\cdot\|$ generated by an inner product $\langle\cdot,\cdot\rangle$, it is also true that

$$\left\|\varphi^h_X(\mathbf{y}) - \varphi^h_X(\mathbf{y})\right\| \leq \|\mathbf{y} - \mathbf{x}\|, \ \forall h > 0.$$

This definition tells us that a method φ^h is B-stable if it preserves the non-expansivity nature of the dynamics at a discrete level.

An equivalent characterisation of (1) is given by the one-sided Lipschitz inequality

$$\langle X(\mathbf{y}) - X(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \leq 0.$$

Restricting to inner product norms allows us to have no barriers on the order of th emethods we declare to be stable or non-expansive. If we were to include also norms like ℓ^1 or ℓ^∞, then there would be a maximal reachable order of 1, see [2].

The conditions we have used to define B-stability are not so practical. We now provide a very operative procedure to decide if a Runge–Kutta method is B-stable or not.

Proposition 1 (B-stable Runge–Kutta methods)**.** *A Runge–Kutta method with tablea u (A, b, c) is B-stable if and only if said $B = \text{diag}(b)$, and $M = BA + A^T B - bb^T$, one has $B \geq 0$ and $M \geq 0$.*

Proof. Let us consider $X \in \mathfrak{X}(\mathbb{R}^d)$ that satisfies

$$\langle X(\mathbf{y}) - X(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq 0$$

for a fixed inner product $\langle \cdot, \cdot \rangle : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. We consider two generic initial conditions $\mathbf{x}_0, \mathbf{y}_0 \in \mathbb{R}^d$, and compute one update with the Runge–Kutta method having tableau (A, b, c) and step $h > 0$:

$$\mathbf{x}_1 = \mathbf{x}_0 + h \sum_{i=1}^{s} b_i X(\mathbf{k}_i), \qquad \mathbf{y}_1 = \mathbf{y}_0 + h \sum_{i=1}^{s} b_i X(\mathbf{h}_i),$$
$$\mathbf{k}_i = \mathbf{x}_0 + h \sum_{j=1}^{s} a_{ij} X(\mathbf{k}_j), \qquad \mathbf{h}_i = \mathbf{y}_0 + h \sum_{j=1}^{s} a_{ij} X(\mathbf{h}_j).$$

We then introduce the notation

$$\begin{aligned} &\delta\mathbf{x}_r := \mathbf{y}_r - \mathbf{x}_r, \ r \in \{0, 1\}, \\ &\delta X_i := X(\mathbf{k}_i) - X(\mathbf{h}_i), \ i = 1, ..., s, \\ &\delta\mathbf{k}_i . = \mathbf{k}_i - \mathbf{h}_i, \ i = 1, ..., s. \end{aligned}$$

We now expand the norm of the difference after the first update to compare it to the initial norm:

$$\begin{aligned} \|\delta\mathbf{x}_1\|^2 = \langle \delta\mathbf{x}_1, \delta\mathbf{x}_1 \rangle = \|\delta\mathbf{x}_0\|^2 + h^2 \sum_{i,j=1}^{s} b_i b_j \langle \delta X_i, \delta X_j \rangle \\ + 2h \sum_{i=1}^{s} b_i \langle \delta\mathbf{x}_0, \delta X_i \rangle. \end{aligned} \tag{2}$$

As in the proof for Runge–Kutta methods preserving quadratic first integrals, we compute δx_0 in s different ways as

$$\delta x_0 = \delta\mathbf{k}_i - h \sum_{j=1}^{s} a_{ij} \delta X_j, \ i = 1, ..., s. \tag{3}$$

Replacing (3) into (3), we get

$$\|\delta\mathbf{x}_1\|^2 = \langle\delta\mathbf{x}_1, \delta\mathbf{x}_1\rangle = \|\delta\mathbf{x}_0\|^2 + h^2 \sum_{i,j=1}^{s} b_i b_j \langle\delta X_i, \delta X_j\rangle + \underbrace{2h \sum_{i=1}^{s} b_i \langle\delta\mathbf{k}_i, \delta X_i\rangle}_{\leq 0,\ \text{using } b_i \geq 0} - 2h^2 \sum_{i,j=1}^{s} b_i a_{ij} \langle\delta X_i, \delta X_j\rangle.$$

Similarly to the proof for quadratic first integrals, we can rewrite the last term in the previous equation by simmetry of inner products, and end up with

$$\|\delta\mathbf{x}_1\|^2 - \|\delta\mathbf{x}_0\|^2 = -h^2 \sum_{i,j=1}^{s} m_{ij} \langle\delta X_i, \delta X_j\rangle, \tag{4}$$

where m_{ij} is an entry of $M \in \mathbb{R}^{s\times s}$. From this relation we can conclude by using th positive semi-definiteness of M. A way to formalise this is to define

$$\delta X := \begin{bmatrix} \delta X_1 \\ \delta X_2 \\ \vdots \\ \delta X_s \end{bmatrix},\ \widetilde{M} = M \otimes I_d,$$

and rewrite the right-hand side of (4) as

$$-h^2 \delta X^T \widetilde{M} \delta X,$$

which is non-positive since if $M \geq 0$, so is $\widetilde{M}$. □

Remark 1. *B-stability implies A-stability since one can consider the system*

$$\dot{\mathbf{x}} = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix} \mathbf{x},$$

equivalent to $\dot{x} = \lambda x$, $\lambda = \alpha + i\beta$, *where if* $\alpha = \mathrm{Re}(\lambda) < 0$ *we have a non-expansive vector field. Thus, if a method* φ^h *is non-expansive, or non-linearly stable, it is also A-stable, or linearly stable. So explicit methods can not be B-stable too.*

2 Conditionally non-linearly stable methods

There are some applications where having to use implicit methods can be prohibitive. An example comes from the use of numerical integrators in the context of neural networks for high-dimensional problems, where solving non-linear equations iteratively can be too expensive.

We thus look for classes of explicit methods that still allow to have some stable behaviour when applied to non-expansive vector fields. A theory that allows us to do so, is the one of $r-$circle contractive methods. This section heavily relies on the results in [1]. Most of the results are reported without a proof, but they can all be found in the cited paper.

To gain some understanding of what we aim to do, let us consider one of the simplest set ups. We consider the equation $\dot{\mathbf{x}} = -\mathbf{x} \in \mathbb{R}^d$, and the expliti Euler method applied to it, which writes $\varphi^h(\mathbf{x}) = \mathbf{x} - h\mathbf{x} = (1-h)\mathbf{x}$. The exact solution of the differential equation is $\phi^t(\mathbf{x}) = e^{-h}\mathbf{x}$, which is clearly a $1-$Lipschitz function in the ℓ^2 norm, hence defining a non-expansive dynamics. However, we notice that

$$\left\|\varphi^h(\mathbf{y}) - \varphi^h(\mathbf{x})\right\|_2 = |1-h| \left\|\mathbf{y} - \mathbf{x}\right\|_2,$$

which is not greater than $\|\mathbf{y}-\mathbf{x}\|_2$ only if $0 < h < 2$. This tells us that, although the explicit Euler method is not B-stable, we can get a non-expansive behaviour if we allow for a step size restriction, which might even be quite a mild restriction.

Sticking to the analysis of the explicit Euler method, we consider a vector field $X \in \mathfrak{X}(\mathbb{R}^d)$ which is $L-$Lipschitz and which satisfies

$$\langle X(\mathbf{y}) - X(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \leq -\mu \left\|\mathbf{y} - \mathbf{x}\right\|_2^2,\ \mu > 0.$$

The explicit Euler method $\varphi^h(\mathbf{x}) = \mathbf{x} + hX(\mathbf{x})$ applied to X leads to non-expansivity as long as

$$\begin{aligned}\left\|\varphi^h(\mathbf{y}) - \varphi^h(\mathbf{x})\right\|_2^2 &= \|\mathbf{y}-\mathbf{x}\|_2^2 + h^2 \|X(\mathbf{y}) - X(\mathbf{x})\|^2 \\ &\quad + 2h\langle \mathbf{y}-\mathbf{x}, X(\mathbf{y}) - X(\mathbf{x})\rangle \\ &\leq \left(1 + h^2L^2 - 2\mu h\right) \|\mathbf{y}-\mathbf{x}\|_2^2 \leq \|\mathbf{y}-\mathbf{x}\|_2^2,\end{aligned}$$

i.e., if $h < 2\mu/L^2$. This analysis can be generalised to more methods, also leading to milder conditions.

Definition 2 (r-circle Runge–Kutta methods)**.** *A Runge–Kutta method with tableau (A, b, c) is $r-$circle contractive if $\rho = -1/r$ is the largest scalar for which*

$$M \geq \rho B, \tag{5}$$

where $B = \mathrm{diag}(b)$ and $M = BA + A^TB - bb^T$.

We notice that if one could take r as large as desired while still having (5) satisfies, then we would recover the condition of B-stability.

Proposition 2. *Let us consider a vector field $X \in \mathfrak{X}(\mathbb{R}^d)$ that satisfies the monotonicity condition*

$$\langle X(\mathbf{y}) - X(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \leq -\nu \left\|X(\mathbf{y}) - X(\mathbf{x})\right\|^2,\ \nu > 0,$$

for a norm with $\|\cdot\|^2 = \langle\cdot,\cdot\rangle$. Then an $r-$circle contractive Runge–Kutta method φ^h is non-expansive when applied to solve $\dot{\mathbf{x}} = X(\mathbf{x})$ if $r = \infty$ or, if $r < \infty$, when $h/r < 2\nu$.

Going back to the explicit Euler method, which has tableau $A = 0$, $b = 1$, $c = 0$, we see that $M = -1$, and hence we see that the explicit Euler method is $1-$circle contractive.

References

[1] Germund G Dahlquist. Generalized disks of contractivity for explicit and implicit Runge-Kutta methods. Technical report, CM-P00069451, 1979.

[2] MN Spijker. Contractivity in the numerical solution of initial value problems. *Numerische Mathematik*, 42:271–290, 1983.