ODEs with a structure worth preserving

While it is important to produce quantitatively accurate approximate solutions for ODEs, sometimes the differential equations we want to simulate have some underlined geometric or dynamic structure worth preserving.

- The **dynamic properties** relate to the behaviour at infinity, the periodicity of the solutions, the presence of chaos, or the presence of fixed points.
- The **geometric properties** instead relate to features which are invariant in time, for example the level sets of a conserved energy, the non linear manifold where the solution belongs, or some symmetry properties of the solutions.

In principle, there is no reason why a numerical method should preserve automatically these properties also in the discrete time setting, and this is why one needs to build specific discretisation strategies adapted to the structure of interest.

Before moving to the details behind some of these methods, we want to further motivate the need for geometric integrators by showing some examples of differential equations having some geometric structure worth preserving.

1 ODEs with a first integral

Definition 1 (First integral)**.** *A system of differential equations* $\dot{\mathbf{x}}(t) = \mathcal{F}(\mathbf{x}(t))$*,* $\mathcal{F} \in \mathfrak{X}(\mathbb{R}^d)$*, admits a first integral* $I : \mathbb{R}^d \to \mathbb{R}$ *if and only if the function* I *is constant along the solutions of the differential equation, i.e.,*

$$\frac{d}{dt} I(\mathbf{x}(t)) = \nabla I(\mathbf{x}(t)) \cdot \dot{\mathbf{x}}(t) = \nabla I(\mathbf{x}(t)) \cdot \mathcal{F}(\mathbf{x}(t)) = 0$$

for every $t \geq 0$*.*

There are several systems admitting a first integral and, at least for Morse functions, they can be written in the form

$$\dot{\mathbf{x}}(t) = (A(\mathbf{x}(t)) - A(\mathbf{x}(t))^\top) \nabla I(\mathbf{x}(t)), \tag{1}$$

since

$$\mathcal{F}(\mathbf{x}(t)) = \frac{\mathcal{F}(\mathbf{x}(t)) \nabla I(\mathbf{x}(t))^\top - \nabla I(\mathbf{x}(t)) \mathcal{F}(\mathbf{x}(t))^\top}{\|\nabla I(\mathbf{x}(t))\|_2^2} \nabla I(\mathbf{x}(t)).$$

For these systems, the level sets $\mathcal{I}_c = \{\mathbf{x} \in \mathbb{R}^d : \ I(\mathbf{x}) = c\}$ are invariant with respect to the flow map $\phi^t_{\mathcal{F}}$, and it is sometimes desirable to have the same property also at a discrete level. A reason why this could be interesting is for stability/boundedness purposes, since if the level sets of I are compact and they are numerically preserved, the discrete solution will also remain bounded.

2 Hamiltonian systems

Even though Hamiltonian systems can be formulated in a much more general and abstract way, we will focus only on systems on $\mathbb{R}^{2d}$, with the canonical symplectic structure.

By Hamiltonian system we refer to systems of differential equations of the form

$$\dot{\mathbf{x}}(t) = \mathbb{J}\nabla H(\mathbf{x}(t)) := X_H(\mathbf{x}(t)) \in \mathbb{R}^{2d}, \tag{2}$$

where $H : \mathbb{R}^{2d} \to \mathbb{R}$ is a smooth function of its inputs called Hamiltonian energy, and

$$\mathbb{J} = \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix} \in \mathbb{R}^{2d\times 2d}$$

is the so-called canonical symplectic matrix. We will see that a convenient setup for the numerical discretisation of the solutions of (2) is provided by the separable case, where H is of the form

$$H(\mathbf{q}, \mathbf{p}) = K(\mathbf{p}) + U(\mathbf{q})$$

for a kinetic energy $K : \mathbb{R}^d \to \mathbb{R}$ and a potential energy $U : \mathbb{R}^d \to \mathbb{R}$, where $\mathbf{x} = (\mathbf{q}, \mathbf{p})$ is a partitioning of the phase space variable.

Hamiltonian systems have several interesting geometric and dynamic properties. First of all they are in the skew-gradient form (1), hence they conserve the energy function H. But even more importantly, they preserve a skew-symmetric bilinear form called the canonical symplectic form $\Omega : \mathbb{R}^{2d} \times \mathbb{R}^{2d} \to \mathbb{R}$ defined as

$$\Omega(\mathbf{v}, \mathbf{w}) := \mathbf{v}^\top \mathbb{J}\mathbf{w}.$$

A map preserving Ω is said to be symplectic. A matrix $A \in \mathbb{R}^{2d\times 2d}$ is symplectic if and only if it satisfies $A^\top \mathbb{J} A = \mathbb{J}$ and similarly we say the linear map $L(x) = Ax$ symplectic. Instead, we say a non-linear differentiable map $F : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ to be symplectic if for every $\mathbf{x} \in \mathbb{R}^{2d}$ it holds

$$F'(\mathbf{x})^\top \mathbb{J} F'(\mathbf{x}) = \mathbb{J}, \tag{3}$$

where $F'(\mathbf{x}) \in \mathbb{R}^{2d\times 2d}$ is the Jacobian matrix of F evaluated at $\mathbf{x}$. Equivalently, F is symplectic if it infinitesimally preserves Ω since (3) is equivalent to say

$$\Omega(F'(\mathbf{x})\mathbf{v}, F'(\mathbf{x})\mathbf{w}) = \Omega(\mathbf{v}, \mathbf{w}), \ \forall \mathbf{x}, \mathbf{v}, \mathbf{w} \in \mathbb{R}^{2d}.$$

Proposition 1. *The flow of a Hamiltonian system is symplectic.*

We could prove this quickly using the more abstract formulation based on differential forms and the Cartan's magic formula, but we now see the typical proof provided in numerical analysis books.

Proof. We recall that the flow map $\phi^t_{X_H} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ satisfies

$$\frac{d}{dt}\phi^t_{X_H}(\mathbf{x}_0) = X_H\left(\phi^t_{X_H}(\mathbf{x}_0)\right)$$

for every $t \geq 0$. Differentiating both sides with respect to $\mathbf{x}_0$, we get

$$\partial_{\mathbf{x}_0}\frac{d}{dt}\phi^t_{X_H}(\mathbf{x}_0) = \mathbb{J}\nabla^2 H(\phi^t_{X_H}(\mathbf{x}_0))\,\partial_{\mathbf{x}_0}\phi^t_{X_H}(\mathbf{x}_0),$$

where $\nabla^2 H$ is the Hessian matrix of H. Changing the differentiation order on the left, and calling $S_{\mathbf{x}_0}(t) = \partial_{\mathbf{x}_0}\phi^t_{X_H}(\mathbf{x}_0)$, we see that

$$\frac{d}{dt}S_{\mathbf{x}_0}(t) = \mathbb{J}\nabla^2 H(\phi^t_{X_H}(\mathbf{x}_0))S_{\mathbf{x}_0}(t), \tag{4}$$

which is the variational equation for the Hamiltonian system of ODEs. We can then compute

$$\begin{aligned}\frac{d}{dt}\left(S_{\mathbf{x}_0}(t)^\top \mathbb{J} S_{\mathbf{x}_0}(t)\right) &= \left(\frac{d}{dt}S_{\mathbf{x}_0}(t)\right)^\top \mathbb{J}S_{\mathbf{x}_0}(t) + S_{\mathbf{x}_0}(t)^\top\mathbb{J}\left(\frac{d}{dt}S_{\mathbf{x}_0}(t)\right)\\ &\overset{(4)}{=} \left(S_{\mathbf{x}_0}(t)^\top\nabla^2 H(\phi^t_{X_H}(\mathbf{x}_0))\mathbb{J}^\top\right)\mathbb{J}S_{\mathbf{x}_0}(t) + S_{x_0}(t)^\top\mathbb{J}\left(\mathbb{J}\nabla^2 H(\phi^t_{X_H}(\mathbf{x}_0))S_{x_0}(t)\right).\end{aligned}$$

Since $\mathbb{J}^\top\mathbb{J} = I_{2d}$ and $\mathbb{J}^2 = -I_{2d}$ we conclude that the quantity above is 0 and hence $S_{\mathbf{x}_0}(t)^\top\mathbb{J}S_{\mathbf{x}_0}(t) = S_{\mathbf{x}_0}(0)^\top\mathbb{J}S_{\mathbf{x}_0}(0)$. At time 0, we recall that

$$S_{\mathbf{x}_0}(0) = \partial_{\mathbf{x}_0}\phi^0_{X_H}(\mathbf{x}_0) = \partial_{\mathbf{x}_0}\mathbf{x}_0 = I_{2d}$$

which allows to conclude $S_{\mathbf{x}_0}(t)^\top\mathbb{J}S_{\mathbf{x}_0}(t) = \mathbb{J}$ for every $t \geq 0$ as desired. □

3 Differential equations with a contractive behaviour

Another interesting class of differential equations is the one showing a contractive behaviour. The study of contractive systems is of high interest in several fields, like in control theory, and the interested reader can see [1]. The notion of contractivity inherently depends on the choice of a metric over $\mathbb{R}^d$. We focus on the ℓ^2 metric, but similar arguments could be done for inner product-generated metrics.

A vector field $\mathcal{F} \in \mathfrak{X}(\mathbb{R}^d)$ is non-expansive in the ℓ^2 sense if for every time $t \geq 0$ and pair of initial conditions $\mathbf{x}_0, \mathbf{y}_0 \in \mathbb{R}^d$ one has

$$\left\|\phi^t_{\mathcal{F}}(\mathbf{y}_0) - \phi^t_{\mathcal{F}}(\mathbf{x}_0)\right\|_2 \leq \left\|\mathbf{y}_0 - \mathbf{x}_0\right\|_2. \tag{5}$$

Contractivity corresponds to the strict inequality in (5). We can see that there is a much more practical condition one can check for contractivity, and this is found by Taylor expanding the solutions as

$$\phi_{\mathcal{F}}^{t+h}(\mathbf{x}_0) = \phi_{\mathcal{F}}^{t}(\mathbf{x}_0)+h\mathcal{F}(\phi_{\mathcal{F}}^{t}(\mathbf{x}_0))+\mathcal{O}(h^2), \quad \phi_{\mathcal{F}}^{t+h}(\mathbf{y}_0) = \phi_{\mathcal{F}}^{t}(\mathbf{y}_0)+h\mathcal{F}(\phi_{\mathcal{F}}^{t}(\mathbf{y}_0))+\mathcal{O}(h^2),$$

under sufficient smoothness assumptions, and for $h \ll 1$. Thus, one gets

$$\begin{aligned}&\left\|\phi_{\mathcal{F}}^{t+h}(\mathbf{y}_0) - \phi_{\mathcal{F}}^{t+h}(\mathbf{x}_0)\right\|_2^2 - \left\|\phi_{\mathcal{F}}^{t}(\mathbf{y}_0) - \phi_{\mathcal{F}}^{t}(\mathbf{x}_0)\right\|_2^2 \\ &= 2h\langle \mathcal{F}(\phi_{\mathcal{F}}^{t}(\mathbf{y}_0)) - \mathcal{F}(\phi_{\mathcal{F}}^{t}(\mathbf{x}_0)), \phi_{\mathcal{F}}^{t}(\mathbf{y}_0) - \phi_{\mathcal{F}}^{t}(\mathbf{x}_0)\rangle + \mathcal{O}(h^2).\end{aligned}$$

For small enough h, we hence conclude that the flow of $\mathcal{F}$ does not expand distances if $\langle \mathcal{F}(\mathbf{y}) - \mathcal{F}(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \leq 0$ for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, and again contracts them in case of strict inequality.

Definition 2 (One-sided Lipschitz continuity)**.** *A vector field $\mathcal{F} \in \mathfrak{X}(\mathbb{R}^d)$ is one-sided Lipschitz continuous with respect to the ℓ^2 metric if there is a constant $\nu \in \mathbb{R}$ such that*

$$\langle \mathcal{F}(\mathbf{y}) - \mathcal{F}(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \leq \nu \|\mathbf{y} - \mathbf{x}\|_2^2$$

for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

Definition 3 (Non-expansive and contractive vector field)**.** *A vector field $\mathcal{F} \in \mathfrak{X}(\mathbb{R}^d)$ is non-expansive (resp. contractive) if it is one-sided Lipschitz continuous with constant $\nu \leq 0$ (resp. $\nu < 0$).*

Contractivity and non-expansivity are relatively common properties in dynamical systems. For example the family of negative gradient flows of convex potentials, that characterise gradient descent methods for optimisation problems, belong to this class since if $V : \mathbb{R}^d \to \mathbb{R}$ is convex

$$\langle \nabla V(\mathbf{y}) - \nabla V(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \geq 0$$

for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, and hence $\mathcal{F}(\mathbf{x}) = -\nabla V(\mathbf{x})$ is a non-expansive system. Contractivity could be obtained working with $\mu-$strongly convex potentials for which one also has

$$\langle \nabla V(\mathbf{y}) - \nabla V(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle \geq \mu \|\mathbf{y} - \mathbf{x}\|_2^2.$$

We will see how to get contractivity also with numerical methods both without having to restrict the step size of the method, and also with methods that need a restriction.

References

[1] F. Bullo. *Contraction Theory for Dynamical Systems*. Kindle Direct Publishing, 1.2 edition, 2024.