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Identification of nonlinear dynamical system equations using dynamic mode decomposition under invariant quantity constraints

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ABSTRACT

In this paper, an algorithm for identifying equations representing a continuous nonlinear dynamical system from a noise-free state and time-derivative state measurements is proposed. It is based on a variant of the extended dynamic mode decomposition. A particular attention is paid to guarantee that the physical invariant quantities stay constant along the integral curves. The numerical methodology is validated on a two-dimensional Lotka–Volterra system. For this case, the differential equations are perfectly retrieved from data measurements. Perspectives of extension to more complex systems are discussed.

1. Introduction

In the context of today's facilitated access to data in terms of quality, cost and quantity, the machine learning discipline appears to be a promising complementary solution for the derivation of mathematical models in the science and engineering domain. We can have different situations or conditions.

1. For a given physical system, we have neither information on the system nor any available model. Then standard data analysis, knowledge/feature extraction or machine learning algorithms can be used in this case.
2. We still do not know any model, but we have partial knowledge of the system from physical considerations. For example, it is known that the system has an invariant quantity, or a decaying one during time (Lyapunov function). We then would like to derive a model from data that satisfies the invariance/decay property.
3. A model with a certain accuracy has already been derived from finer physical considerations or assumptions. In this case, one can try to improve the accuracy or reliability of the current model by adding some correction terms. These correction terms can be identified and calibrated from data/measurements (see [1] for example).

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This paper focuses more on the second intermediate situation. We try to identify the equations of a continuous autonomous dynamical system from data/measurements and it is supposed that the system preserves a known invariant quantity, denoted by η later on. As a starting work in this field, we will only consider the case of noise-free data in this paper. Beyond this restriction, for wide applicability reasons, we would like to get a global model (meaning that it is valid even in regions that have not been explored by the data) from only little data.

This paper is organized as follows. Section 2 is devoted to the setting of the problem. Then section 3 will introduce dynamic mode decomposition (DMD) and deal with DMD under skew-symmetry constraints on the searched matrix. The following step is the search of both coefficients matrix and nonlinear functions; this will the object of section 4. Then section 5 presents the whole greedy algorithm. The section 6 is dedicated to the numerical experiments and validation. We will end up with additional comments in section 7 and concluding remarks.

Notations We will use the Frobenius matrix inner products $\langle .,.\rangle_F$. Given two real-valued $m \times n$ matrices A and B, the Frobenius inner product is defined by the following summation:

$$\langle A, B\rangle_{F,m,n} = \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}B_{ij} = \mathrm{tr}(AB^{\mathsf{T}})$$

The corresponding Frobenius norm $\|.\|_{F,m,n}$ is defined by $\|A\|_{F,m,n} = \sqrt{\langle A, A\rangle_{F,m,n}}$. The usual vector Euclidean norm in $\mathbb{R}^d$ will be simply denoted by $\|.\|_{2,d}$.

2. Setting of the problem

Consider a physical time-continuous autonomous dynamical system governed by the system of nonlinear differential equations

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t)), \quad t > 0 \tag{1}$$

where $\boldsymbol{f} : \mathbb{R}^d \to \mathbb{R}^d$ is a locally Lipschitz continuous mapping. Added to this differential system, an initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$ is given. It is assumed that, starting from any initial condition in an open set $\mathcal{X} \subset \mathbb{R}^d$, maximal solutions are defined on the whole time domain $[0, +\infty)$, with all states $\boldsymbol{x}(t)$ in the admissible set $\mathcal{X}$.

Data generation From the physical system, it is assumed that one can measure the full states $\boldsymbol{x}^k$ (without noise in a first time) at N discrete times $\{t^k\}_{k=1,\dots,N}$, i.e. $\boldsymbol{x}^k = \boldsymbol{x}(t^k)$ but also the time derivatives $\boldsymbol{y}^k = \dfrac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}(t^k)$, $k = 1, \dots, N$. From the data matrices

$$X = [\boldsymbol{x}^1, \boldsymbol{x}^2, \dots, \boldsymbol{x}^N] \in \mathcal{M}_{dN}(\mathbb{R}), \quad Y = [\boldsymbol{y}^1, \boldsymbol{y}^2, \dots, \boldsymbol{y}^N] \in \mathcal{M}_{dN}(\mathbb{R}) \tag{2}$$

we would like to identify the equations (1) of the dynamical system. If this is not possible, at least we would like to find an accurate approximate differential model of (1) with some stability properties (large time stability, ...). In the sequel, we will assume that $N \geq d$.

2.1. Invariant quantity and structure hypotheses

Let us assume that there exists a differentiable function $\eta : \mathcal{X} \to \mathbb{R}$ being invariant along all integral curves, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta(\boldsymbol{x}(t)) = \nabla\eta(\boldsymbol{x}(t)) \cdot \dot{\boldsymbol{x}}(t) = \nabla\eta(\boldsymbol{x}(t)) \cdot \boldsymbol{f}(\boldsymbol{x}(t)) = 0 \tag{3}$$

Then, for integral curves of (1), we have the property

$$\nabla\eta(\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x}) = 0 \quad \forall \boldsymbol{x} \in \mathcal{X} \tag{4}$$

meaning that for any initial condition $\boldsymbol{x}_0 \in \mathcal{X}$, the quantity $\eta(\boldsymbol{x})$ is kept constant on trajectories of (1).

As a consequence, there exists a skew-symmetric matrix $A(\boldsymbol{x})$ such that

$$\boldsymbol{f}(\boldsymbol{x}) = A(\boldsymbol{x})\,\nabla\eta(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \mathcal{X} \tag{5}$$

This is a direct consequence of the following lemma.

Lemma 2.1. *For any $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^d$,*

$$(\boldsymbol{u} \perp \boldsymbol{v}) \iff (\forall A,\ \boldsymbol{v} = A\boldsymbol{u} \implies A \text{ is skew symmetric})$$

Remark 2.1. In (5), the mapping $\boldsymbol{x} \mapsto A(\boldsymbol{x})$ is continuous as soon as both $\boldsymbol{f}$ and $\nabla\eta$ are continuous too.

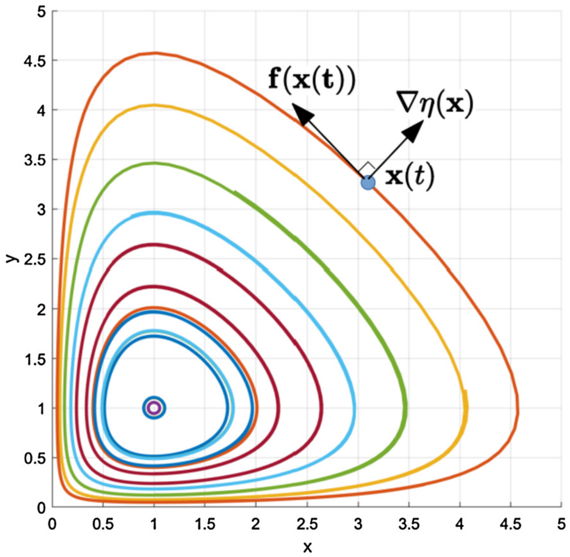

Fig. 1. Different orbits of the Lotka–Volterra system and orthogonality between $\nabla\eta(\boldsymbol{x}(t))$ and $\boldsymbol{f}(\boldsymbol{x}(t))$ for a point $\boldsymbol{x}(t)$ or the orbit.

Example Consider the time-continuous two-equation prey-predator Lotka–Volterra dynamical system (see [2]):

$$\dot{x} = (1-y)x \tag{6}$$

$$\dot{y} = (x-1)y \tag{7}$$

with initial condition $x(0) = x_0 > 0,\ y(0) = y_0 > 0$. For this two-equation system, it can be shown that maximal solutions stay in the positive orthant $\mathcal{X} = (0, +\infty)^2$. It is easy to check that the quantity

$$\eta(\boldsymbol{x}) = \log(xy) - x - y \tag{8}$$

is invariant along integral curves of the system. Each equation $\eta(\boldsymbol{x}) = \eta(\boldsymbol{x}_0)$ defines an orbit of the system. We have $\nabla\eta(\boldsymbol{x}) = (1/x - 1, 1/y - 1)^\mathsf{T}$. One can observe that $\boldsymbol{f}(\boldsymbol{x})$ can be written in the form

$$\boldsymbol{f}(\boldsymbol{x}) = A(\boldsymbol{x})\nabla\eta(\boldsymbol{x})$$

with $A(\boldsymbol{x}) = xy\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

Fig. 1 shows different orbits or the Lotka–Volterra system. Since orbits are also level sets of the function η, we can check that $\boldsymbol{f}(\boldsymbol{x}(t))$ is orthogonal to $\nabla\eta(\boldsymbol{x}(t))$. Remark that such kinds of systems may require specific time integration schemes like sympletic schemes for stability or long range time simulation purposes. The reference [3] for example gives details on geometric computational methods for prey-predator systems.

2.2. Truncated decomposition of skew-symmetric matrix-valued mappings

In this subsection, we give a particular expansion of skew-symmetric matrix-valued mappings. This will be useful for the structure of a search of equations in the identification procedure. Let us denote by E_{ij}, $1 \le i < j \le d$ the matrices that form the canonical basis of the vector space of skew-symmetric matrices, i.e. $E_{ij} = \boldsymbol{e}_i\,\boldsymbol{e}_j^\mathsf{T}$, where $\boldsymbol{e}_i$ denotes the i-th vector of the canonical basis in $\mathbb{R}^d$. For any $\boldsymbol{x} \in \mathcal{X}$, we can write the decomposition into this canonical basis

$$A(\boldsymbol{x}) = \sum_{1\le i<j\le d} a_{ij}(\boldsymbol{x})\,E_{ij}$$

with scalar coefficients $a_{ij}(\boldsymbol{x}) \in \mathbb{R}$. Each function $a_{ij} : \mathcal{X} \to \mathbb{R}$ is assumed to have reasonable regularity, say at least of regularity $L^2_\omega(\mathcal{X})$ (the weight function ω may be chosen fast-decaying at infinity in the case of unbounded domains). Then we consider a total orthonormal family $\{\varphi_k\}_k$ of $L^2_\omega(\mathcal{X})$. For each function a_{ij}, we have the decomposition

$$a_{ij}(\boldsymbol{x}) = \sum_{k\ge 0} a^k_{ij}\,\varphi_k(\boldsymbol{x})$$

giving the decomposition for $A(\boldsymbol{x})$:

$$A(\boldsymbol{x}) = \sum_{1\le i<j\le d} \sum_{k\ge 0} a_{ij}^k \, E_{ij} \, \varphi_k(\boldsymbol{x}) \tag{9}$$

which can also be written

$$A(\boldsymbol{x}) = \sum_{k\ge 0} A_k \, \varphi_k(\boldsymbol{x}) \tag{10}$$

(assuming that we can permute the two summation operators, see the Remark 2.2 below) where the skew-symmetric matrices A_k, $k \ge 0$ are defined by

$$A_k = \sum_{1\le i<j\le d} a_{ij}^k \, E_{ij}$$

By truncating the expansion in (10) up to a rank (say K), we define an approximation of the matrix $A(\boldsymbol{x})$. One can define a projection operator Π^K acting on $A(.)$ with projection on the K first functions φ_k:

$$\Pi^K A(\boldsymbol{x}) = \sum_{k=1}^{K} A_k \, \varphi_k(\boldsymbol{x}) \tag{11}$$

The projection error $(A - \Pi^K A)$ will decay fast with K as soon as the coefficient functions $a_{ik}^k(\boldsymbol{x})$ are smooth functions.

Remark 2.2. One can always choose a family $\{\varphi_k\}_{k\ge 0}$ such that the convergence when $K \to +\infty$ is uniform w.r.t. $\boldsymbol{x}$. The uniform convergence justifies the permutation of the two summations in (9).

Expression (11) gives us a way to build an algorithm to identify $A(\boldsymbol{x})$ in (5) from the data within a greedy procedure. As a preliminary step, in section 3 we introduce the DMD method for identifying a first approximate skew-symmetric matrix A. In section 4, we define the first step of the greedy algorithm, which involves both functions $\varphi_1(\boldsymbol{x})$ and matrix A_1. In section 5, we define the main iteration and the whole greedy algorithm.

3. Dynamic mode decomposition approach under skew-symmetry constraints

First, we try to identify the dynamics of the system according to the (approximate) model

$$\tilde{\boldsymbol{f}}(\boldsymbol{x}) = A \, \nabla\eta(\boldsymbol{x}) \tag{12}$$

where A is a *constant* skew-symmetric matrix to be determined from the data. For the sake of simplicity, in all the sequel we will denote $\boldsymbol{g}(\boldsymbol{x}) := \nabla\eta(\boldsymbol{x})$. From the data $\boldsymbol{x}^k$ stored in the matrix X, one can compute a new matrix with column vectors $\boldsymbol{g}^k = \boldsymbol{g}(\boldsymbol{x}^k)$, $k = 1, ..., N$:

$$G = [\boldsymbol{g}^1, \boldsymbol{g}^2, ..., \boldsymbol{g}^N] \in \mathscr{M}_{dN}(\mathbb{R})$$

In the sequel, we will assume that $\operatorname{rank}(G) = d$. Then, following the same ideas from Dynamic Mode Decomposition (DMD, [4]), we look for a matrix that minimizes the constraint least squares problem:

$$\min_{A\in\mathscr{M}_d(\mathbb{R})} \quad J(A) = \frac{1}{2}\sum_{k=1}^{N} \|A\boldsymbol{g}^k - \boldsymbol{y}^k\|_{2,d}^2 \tag{13}$$

subject to A skew-symmetric matrix

The cost function J can be rewritten in matrix form

$$J(A) = \frac{1}{2}\|AG - Y\|_{F,d,N}^2$$

using the Frobenius norm.

Solution to the problem (13) The originality in problem (13) in the skew-symmetry constraint on A. Remark that, if the matrix A is skew-symmetric, then

$$\|AG - Y\|_{F,d,N} = \|A^\mathsf{T} G + Y\||_{F,d,N} = \|G^\mathsf{T} A + Y^\mathsf{T}\|_{F,N,d}$$

The minimal argument of (13) is the same as the minimal argument of

$$\min_{A\in\mathscr{M}_d(\mathbb{R})} \quad \frac{1}{2}\|AG-Y\|^2_{F,d,N} + \frac{1}{2}\|G^\top A + Y^\top\|^2_{F,N,d} \tag{14}$$

subject to A skew-symmetric matrix

Let us show that the unconstrained minimization problem

$$\min_{A\in\mathscr{M}_d(\mathbb{R})} \quad J(A) := \frac{1}{2}\|AG-Y\|^2_{F,d,N} + \frac{1}{2}\|G^\top A + Y^\top\|^2_{F,N,d}$$

has a unique solution A, which is skew-symmetric intrinsically, thus A will be also the solution to problem (13). An elementary differential calculus gives, for any $H \in \mathscr{M}_d(\mathbb{R})$,

$$\begin{aligned}\langle \nabla J(A), H\rangle_{F,d,d} &= \langle AG-Y, HG\rangle_{F,d,N} + \langle G^\top A + Y^\top, G^\top H\rangle_{F,N,d}\\ &= \langle AGG^\top - YG^\top, H\rangle_{F,d,d} + \langle GG^\top A + GY^\top, H\rangle_{F,d,d}\end{aligned}$$

The first-order optimality conditions give

$$A\,(GG^\top) + (GG^\top)\,A = YG^\top - GY^\top$$

in the form

$$AS + SA = Q \tag{15}$$

with $S = GG^\top$ and $Q = YG^\top - GY^\top$. We get a Lyapunov equation [5]. We observe that the matrix S is symmetric and the right-hand-side matrix Q is skew-symmetric. As soon as $\text{rank}(G) = d$ (meaning that we have d linearly independent vectors among the data), the matrix S is symmetric positive definite. Let us recall the following well-known result of existence and uniqueness of solutions to Sylvester equations.

Proposition 3.1. *Given complex $n \times n$ matrices A and B, Sylvester's equation $AX + XB = C$ has a unique solution X for all C if and only if A and $-B$ have no common eigenvalues.*

In the case of the Lyapunov equation (15), since S is symmetric positive definite, matrices S and $-S$ have no common eigenvalues and the Lyapunov equation has a unique solution A for all Q. Finally, let us show that A is skew-symmetric: since $Q^\top = -Q$, we have

$$SA^\top + A^\top S = -Q$$

Summing up with equation (15), we get

$$(A + A^\top)S + S(A + A^\top) = 0$$

showing that by uniqueness $A + A^\top = 0$ and then A is skew-symmetric.

A classical algorithm for the numerical solution to the Sylvester/Lyapunov equations is the Bartels–Stewart algorithm [5], which consists in transforming the matrices into a Schur form using a QR algorithm, and then solving the resulting triangular system via back-substitution.

4. Dynamic mode decomposition with both matrix and function identification

As the next step, we now try to identify the dynamics of the system according to the more complex model

$$\tilde{\boldsymbol{f}}(\boldsymbol{x}) = \varphi(\boldsymbol{x}) A \nabla \eta(\boldsymbol{x})$$

where the real-valued function $\varphi(\boldsymbol{x})$ is searched as a linear combination of given functions (e.g., from a dictionary), i.e. in the form

$$\varphi(\boldsymbol{x}) = a_1\, b_1(\boldsymbol{x}) + a_2\, b_2(\boldsymbol{x}) + \ldots + a_M\, b_M(\boldsymbol{x})$$

Let us denote $\boldsymbol{a} = (a_1, a_2, \ldots, a_M)^\top$ the vector of coefficient a_i. Let us also write $\varphi(\boldsymbol{x})$ in the vector form

$$\varphi(\boldsymbol{x}) = \boldsymbol{a}^\top \boldsymbol{b}(\boldsymbol{x})$$

with $\boldsymbol{b}(\boldsymbol{x}) = (b_1(\boldsymbol{x}), b_2(\boldsymbol{x}), \ldots, b_M(\boldsymbol{x}))^\top$. So we want to find a pair $(A, \boldsymbol{a}) \in \mathscr{M}_d(\mathbb{R}) \times \mathbb{R}^M$, A skew-symmetric matrix, solution to the minimization problem

$$\min_{(A,\boldsymbol{a})} \quad J(A,\boldsymbol{a}) := \frac{1}{2}\sum_{k=1}^{N} \left\| \boldsymbol{y}^k - (\boldsymbol{a}\cdot\boldsymbol{b}(\boldsymbol{x}^k))\, A\boldsymbol{g}(\boldsymbol{x}^k) \right\|_{2,d}^2 \tag{16}$$

Without any constraints on $\boldsymbol{a}$, we can observe that if $(A,\boldsymbol{a})$ is a minimizer of (16), then $(\mu A, \frac{1}{\mu}\boldsymbol{a})$ for any $\mu \neq 0$ is also a minimizer of (16). To avoid nonuniqueness, one can add a constraint into the minimization problem, for example $\|A\|_\infty = 1$. So the minimization problem of interest is:

$$\min_{(A,\boldsymbol{a})} \quad J(A,\boldsymbol{a}) \tag{17}$$
$$\text{subject to } A \text{ skew-symmetric and } \|A\|_\infty = 1$$

Problem (17) becomes nonlinear and nonquadratic. A simple way to solve (17) is to apply an alternating direction relaxation minimization method that updates A and $\boldsymbol{a}$ sequentially within an iteration loop. When $\boldsymbol{a}$ is fixed, then the minimization problem in A (without the constraint $\|A\|_\infty = 1$) is essentially the same as the one seen in the previous section. Then the constraint $\|A\|_\infty = 1$ can be taken into account by means of a projection step. When A is fixed, the minimization problem in $\boldsymbol{a}$ is standard least squares s problem.

i) First consider the minimization problem

$$\min_{A \text{ skew symmetric}} \quad J(A,\boldsymbol{a})$$

at fixed vector $\boldsymbol{a}$. Let us first rewrite $J(A,\boldsymbol{a})$ in condensed matrix form. By denoting

$$D_m = \operatorname{diag}(b_m(\boldsymbol{x}^k),\ k=1,\dots,N), \quad G = [\boldsymbol{g}(\boldsymbol{x}^1), \boldsymbol{g}(\boldsymbol{x}^2), \dots, \boldsymbol{g}(\boldsymbol{x}^N)]$$

and Z_a the matrix

$$Z_a = G\,(a_1 D_1 + a_2 D_2 + \dots + a_M D_M)$$

it is easy to check that $J(A,\boldsymbol{a})$ can also be written as

$$J(A,\boldsymbol{a}) = \frac{1}{2}\|Y - AZ_a\|_{F,d,N}^2$$

Just like in the previous section, it is convenient to symmetrize the cost function, considering skew-symmetric matrices A:

$$J(A,\boldsymbol{a}) = \frac{1}{2}\|Y - AZ_a\|_{F,d,N}^2 + \frac{1}{2}\|[Z_a^\intercal A + Y^\intercal\|_{F,N,d}^2$$

We have to solve the Euler equations $\nabla_A J(A,\boldsymbol{a}) = 0$ that lead to the following Lyapunov equations

$$AS_a + S_a A = Q_a \tag{18}$$

with $S_a = Z_a Z_a^\intercal$ and $Q_a = YZ_a^\intercal - Z_a Y^\intercal$.

ii) Let us now solve the minimization problem

$$\min_{\boldsymbol{a}} \quad J_A(\boldsymbol{a}) := \frac{1}{2}\sum_{k=1}^{N} \left\| \boldsymbol{y}^k - (\boldsymbol{a}\cdot\boldsymbol{b}(\boldsymbol{x}^k))\, A\boldsymbol{g}(\boldsymbol{x}^k) \right\|_{2,d}^2 \tag{19}$$

at fixed matrix A. Using the notations $\boldsymbol{b}^k = \boldsymbol{b}(\boldsymbol{x}^k)$ and $\boldsymbol{g}^k = \boldsymbol{g}(\boldsymbol{x}^k)$, we have

$$J_A(\boldsymbol{a}) = \frac{1}{2}\sum_{k=1}^{N} \|\boldsymbol{y}^k - A\boldsymbol{g}^k\,(\boldsymbol{b}^k)^\intercal\,\boldsymbol{a}\|_{2,d}^2$$

We get a standard least squares function to minimize. As soon as the rank of the matrix

$$C = \sum_{k=1}^{N} A\boldsymbol{g}^k\,(\boldsymbol{b}^k)^\intercal$$

is M, we get a unique solution. Otherwise, the least squares problem should be regularized by a Tykhonov regularization term or proximal term to get a well-posed problem.

4.1. Summary of the minimization algorithm

Finally, the alternating direction minimization algorithm is as follows.

1. Choose an initial guess $\boldsymbol{a}^0 \neq 0,\ p = 0$.
2. Loop on integer p
   - $p \leftarrow p + 1$;
   - compute the skew-symmetric matrix

     $$A^{(p)} = \arg\min_{A} J(A, \boldsymbol{a}^{(p)})$$

     by solving the Lyapunov equations (18) using $\boldsymbol{a} = \boldsymbol{a}^{(p)}$;
   - normalize the matrix $A^{(p)}$:

     $$A^{(p)} \leftarrow \frac{A^{(p)}}{\|A^{(p)}\|_\infty}$$

   - then compute the solution $\boldsymbol{a}^{(p+1)}$ to

     $$\boldsymbol{a}^{(p+1)} = \arg\min_{\boldsymbol{a}} J(A^{(p)}, \boldsymbol{a})$$

     by solving the (possibly regularized) least squares problem (19) using $A = A^{(p)}$.
3. Test the convergence stop criterion.

5. Greedy iterative procedure

The algorithm presented in the previous section can be advantageously used for the construction of a greedy enriching procedure. Assume that at the last iterate $(k-1)$, we get a differential model $\dot{\boldsymbol{x}} = \tilde{\boldsymbol{f}}^{(k-1)}(\boldsymbol{x})$. Then one can add a correction term in the form $\varphi_k(\boldsymbol{x}) A_k \nabla\eta(\boldsymbol{x})$, the function $\varphi_k(\boldsymbol{x})$, and the matrix A_k to determine to get the enriched model:

$$\tilde{\boldsymbol{f}}^{(k)}(\boldsymbol{x}) = \tilde{\boldsymbol{f}}^{(k-1)}(\boldsymbol{x}) + \varphi_k(\boldsymbol{x}) A_k \nabla\eta(\boldsymbol{x})$$

The identification of both matrix A_k and function $\varphi_k(\boldsymbol{x})$ can be achieved following the same methodology as before. We need a stopping criterion to break the iterative loop. From a given accuracy threshold ε_{tol}, one can use, for example the natural accuracy estimate:

$$\frac{\displaystyle\sum_{k=1}^{N} \|\boldsymbol{y}^k - \boldsymbol{f}^{(k)}(\boldsymbol{x}^k)\|_{2,d}^2}{\displaystyle\sum_{k=1}^{N} \|\boldsymbol{y}^k\|_{2,d}^2} \leq \varepsilon_{\text{tol}}$$

6. Numerical applications

6.1. Lotka–Volterra system

Let us recall that the two-dimensional Lotka–Volterra system (6), (7) has an invariant quantity (8) being constant over each integral curve. The vector field $\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x} = (x, y)^{\mathsf{T}}$ can be exactly written as

$$\boldsymbol{f}(\boldsymbol{x}) = \varphi(\boldsymbol{x})\, E_{12} \nabla\eta(\boldsymbol{x}) \tag{20}$$

with $\varphi(\boldsymbol{x}) = xy$. This means that the use of the only observable $\varphi(\boldsymbol{x}) = xy$ is sufficient to perfectly retrieve the system, as soon as we only have two linearly independent data $(\boldsymbol{x}^1, \boldsymbol{g}^1)$ and $(\boldsymbol{x}^2, \boldsymbol{g}^2)$. For the numerical experiment, the function $\varphi(\boldsymbol{x})$ is searched in the linear space of polynomials of degree not greater than two:

$$\varphi(\boldsymbol{x}) = a_1 + a_2 x + a_3 y + a_4 x^2 + a_5 xy + a_6 y^2$$

The search vector $\boldsymbol{a} = (a_1, \ldots, a_6)^{\mathsf{T}}$ is initialized with a random vector $\boldsymbol{a}^{(0)} \neq 0$. We use the alternating variable method as presented before. After a few iterates, we get the expected pair $(\boldsymbol{a}, A)$ with

$$\boldsymbol{a} = (0, 0, 0, 0, 1, 0), \quad A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

(up to floating number round-off error precision) using 20 samples in the dataset.

7. Closing comments

7.1. Three-dimensional Lotka–Volterra system

Consider here the more complex three-dimensional Lotka–Volterra system

$$\dot{x} = (2 - y - z)x \tag{21}$$

$$\dot{y} = y(x - z) \tag{22}$$

$$\dot{z} = z(x + y - 2) \tag{23}$$

with initial data $\boldsymbol{x}_0 = (x_0, y_0, z_0)$ such that $x_0, y_0, z_0 > 0$. It is easy to check that the quantity

$$\eta(\boldsymbol{x}) = \log(xyz) - x - y - z$$

is an invariant of the dynamical system, and we have $\dot{\boldsymbol{x}} = A(\boldsymbol{x})\nabla\eta(\boldsymbol{x})$, with

$$A(\boldsymbol{x}) = \begin{pmatrix} 0 & xy & xz \\ -xy & 0 & yz \\ -xz & -yz & 0 \end{pmatrix}$$

The skew-symmetric matrix $A(\boldsymbol{x})$ has the exact decomposition

$$A(\boldsymbol{x}) = \varphi_1(\boldsymbol{x})E_{12} + \varphi_2(\boldsymbol{x})E_{13} + \varphi_3(\boldsymbol{x})E_{23}$$

with $\varphi_1(\boldsymbol{x}) = xy$, $\varphi_2(\boldsymbol{x}) = xz$ and $\varphi_3(\boldsymbol{x}) = yz$. We observe that the greedy procedure needs at least three iterations to identify the system. Using a search dictionary composed of the first monomials should allow for a perfect identification of this system.

7.2. Links with extended dynamic mode decomposition

The identification method presented in this paper has close connections with the extended dynamic mode decomposition approach (EDMD). Indeed the search model in the form

$$\tilde{\boldsymbol{f}}(\boldsymbol{x}) = \left(\sum_{k=1}^{M} \varphi_k(\boldsymbol{x})A_k\right) \nabla\eta(\boldsymbol{x})$$

can be written in stacked EDMD-like form

$$\tilde{\boldsymbol{f}}(\boldsymbol{x}) = T\,\boldsymbol{\Psi}(\boldsymbol{x})$$

where T is a constant matrix and $\boldsymbol{\Psi}(\boldsymbol{x})$ is a vector of stacked nonlinear observables. We observe that is our approach, elements of $\boldsymbol{\Psi}(\boldsymbol{x})$ are made of products $\varphi_k(\boldsymbol{x})\partial_\ell\eta(\boldsymbol{x})$ that appear to be suitable observables of the system from the identification point of view.

7.3. Connections between invariants and Koopman theory

It is known that there are connections between EDMD and the Koopman theory of dynamical systems (see [6] and subsequent works). In this section, we would like to emphasize that is also a connection between invariant quantities like η and particular spectral properties of the Koopman operator. Let $\boldsymbol{x}_t(\boldsymbol{u})$ be the solution at time t to the initial value differential problem: $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}(t))$, $\boldsymbol{x}(0) = \boldsymbol{u}$. The Koopman operator (or compositional operator) $\mathscr{K}_t$ relative to the discrete mapping $\boldsymbol{x}_t(\boldsymbol{u})$ if defined as

$$(\mathscr{K}_t g)(\boldsymbol{u}) = g \circ \boldsymbol{x}_t(\boldsymbol{u})$$

The continuous Koopman operator is defined by

$$\mathscr{K}_0^c(g)(\boldsymbol{u}) = \lim_{t\to 0} \frac{(\mathscr{K}_t g)(\boldsymbol{u}) - g(\boldsymbol{u})}{t}$$

For differentiable functions g, we have $\mathscr{K}_0^c(g)(\boldsymbol{u}) = \nabla g(\boldsymbol{u}) \cdot \boldsymbol{f}(\boldsymbol{u})$. So we see that an invariant η of the system if an eigenfunction of the continuous Koopman operator with eigenvalue 0. It seems important to include these eigenfunctions as nonlinear observables to achieve a good identification of the system.

8. Concluding remarks and perspectives

In the paper, we have presented a computational approach for identifying equations of a continuous nonlinear dynamical system from data. The leading model is built in order to preserve a known invariant quantity of the system, thus providing large time stability behavior as well as reinforced accuracy. The numerical methodology is validated on a two-dimensional Lotka–Volterra system.

Perspectives of extension to more complex systems could be interesting to study. In 1997, Grmela and Öttinger [7] proposed a general framework to deal with thermodynamically-consistent dynamical models, the so-called GENERIC framework, standing for "General Equation for Non-Equilibrium Reversible-Irreversible Coupling". For a conservative thermodynamical system, the laws of dynamics are searched in the form

$$\dot{\boldsymbol{x}} = A(\boldsymbol{x})\,\nabla\mathscr{E}(\boldsymbol{x}) - S(\boldsymbol{x})\nabla\eta(\boldsymbol{x}) \tag{24}$$

where $\mathscr{E}$ denotes the total energy which is conserved and η is an entropy of the system. The entropy is supposed to decay during time, expressing the dissipative structure of the system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(\boldsymbol{x}(t)) = 0, \quad \frac{\mathrm{d}}{\mathrm{d}t}\eta(\boldsymbol{x}(t)) \le 0$$

For that, it is expected that matrices $A(\boldsymbol{x})$ and $S(\boldsymbol{x})$ in (24) are such that $A(\boldsymbol{x})$ is skew-symmetric, and $S(\boldsymbol{x})$ is symmetric, positive semi-definite with the additional constraints

$$A(\boldsymbol{x})\nabla\eta(\boldsymbol{x}) = 0, \quad S(\boldsymbol{x})\nabla\mathscr{E}(\boldsymbol{x}) = 0$$

It would be of interest to try to extend the work presented in this paper to the more complex case of GENERIC models.

Since the seminal work of 1997, the GENERIC formalism has been extensively used in the context of complex system modeling and simulation in Engineering Science. Recently, Moya et al. [8] and Gonzales et al. [9,1] have already used GENERIC in the data context for the derivation of consistent data-driven computational mechanics.

Another evident topic of interest is the more complex case of noisy data. Robust identification algorithms are required in this case. There are three options: i) either the model is seen deterministic, and the parameters are set as deterministic (real) quantities; ii) or the model is chosen deterministic, but the parameters are seen as random variables and we have to find the probabilistic laws; iii) or the model itself is seen as stochastic, involving for example stochastic differential equations, and parameters are seen either as deterministic or random variables. In the case of stochastic differential equations, we do not deal with invariant quantities, but with invariant measures. In the case of both deterministic models and parameters, one can adopt for example a "data assimilation" approach [10] where the problem is set under an optimization problem including Tykhonov-like regularization terms, with minimal a priori noise structure knowledge, for example a covariance matrix. This topic will be the object of future developments.

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