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Model reduction, data-based and advanced discretization in computational mechanics

Model order reduction for dynamical systems: A geometric approach

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ABSTRACT

The aim of this paper is to ask the question as whether it is possible, for a given dynamical system defined by a vector field over a finite dimensional inner product space, to construct a reduced-order model over a finite dimensional manifold. In order to give a positive answer to this question, we prove that if the manifold under consideration is an immersed submanifold of the vector space, considered as ambient manifold, then it is possible to construct explicitly a reduced-order vector field over this submanifold. In particular, we found that the reduced-order vector field satisfies the variational principle of Dirac–Frenkel and that we can formulate the Proper Orthogonal Decomposition under this framework. Finally, we propose a local-point estimator of the time-dependent error between the original vector field and the reduced-order one.

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1. Introduction

Model reduction applied to a dynamical system (described by an ordinary differential equation) allows one to extract the most significant features of this system, representing them in a reduced system of coordinates. The goal of this approach is to construct a computational low-cost procedure that reproduces the dominant physical mechanisms of the original model. The interested reader is referred to the following review papers and books [1–4].

One of the more widely used model reduction technique is the Proper Orthogonal Decomposition (POD). Its main goal is to obtain a lower dimensional approximation of a given dynamical system, as follows. Let be an ordinary differential equation (ODE)

$$\frac{d\mathbf{u}}{dt} = X(t, \mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0 \quad (1)$$

for $t \in [0, t_f]$, with $\mathbf{u}, \mathbf{u}_0 \in \mathbb{R}^n$ and $X : [0, t_f] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$. Consider next the solutions to (1) at m -time points $\{\mathbf{u}(t_1), \dots, \mathbf{u}(t_m)\}$ collected in the $n \times m$ -matrix $A = [\mathbf{u}(t_1) - \bar{\mathbf{x}} \cdots \mathbf{u}(t_m) - \bar{\mathbf{x}}]$ and where $\bar{\mathbf{x}} = \frac{1}{r} \sum_{i=1}^m \mathbf{u}(t_i)$ is the mean of these observations. POD seeks a r -dimensional subspace S of \mathbb{R}^n ($r \leq n$) and the corresponding projection matrix $\Pi_S \in \mathbb{R}^{n \times n}$, so that $\|A - \Pi_S A\|$ is minimized over all k -dimensional subspaces. The projection matrix corresponding to the optimal subspace S is obtained as $\Pi_S = ZZ^T$, where the matrix $Z \in \mathbb{R}^{n \times r}$ consists of the columns of the singular vectors corresponding

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to the r largest singular values obtained from A . In a coordinate system embedded in S , the projection of a point \mathbf{u} onto S is represented by $\xi = Z^T(\mathbf{u} - \bar{\mathbf{x}}) \in \mathbb{R}^r$. In particular, if $\mathbf{x} \in \bar{\mathbf{x}} + S$ then $\mathbf{x} - \bar{\mathbf{x}} = Z\xi$ for some $\xi \in \mathbb{R}^r$. A POD-based reduced model that approximates the original problem (1) can then be constructed by the following rule. For any point $\mathbf{x} = Z\xi \in S$, compute the vector-field $X(t, \bar{\mathbf{x}} + Z\xi) \in \mathbb{R}^n$ and take the projection $Z^T X(t, \bar{\mathbf{x}} + Z\xi) \in \mathbb{R}^r$ onto the subspace S . Therefore, we obtain

$$\frac{d\xi}{dt} = Z^T X(t, \bar{\mathbf{x}} + Z\xi), \quad \xi(0) = Z^T \mathbf{u}_0 \quad (2)$$

The dynamical system (2) allows an efficient (typically low-dimensional) representation of the key system behaviour. This framework appears useful in a wide variety of applications.

The Dirac–Frenkel variational principle is a well-known tool in the numerical treatment of equations of quantum dynamics. It was originally proposed by Dirac and Frenkel in 1930 to approximately solve the time-dependent Schrödinger equation. It assumes the existence of a vector field over a configuration space represented by a Hilbert space. This configuration space contains an immersed submanifold, the so-called Hartree manifold, and the reduced-order model is then obtained by projecting the vector field at each point of the submanifold onto its tangent space (see [1,5]). It allows also one to introduce the so-called geometric numerical integration methods for differential equations (see VI.9 in [6]).

A similar approach is used in the so-called *dynamical low-rank approximation* for time-dependent data matrices and tensors [7,8]. The reduced model is obtained by using the Dirac–Frenkel variational principle, over a manifold of matrices (respectively, tensors) of fixed rank (respectively, tensor rank).

To the authors' knowledge, there is no proof, in a general setting, that the reduced-order dynamical system is a vector field, that is, a differentiable map between the immersed submanifold and its tangent bundle. This fact implies that the existence and uniqueness of the solutions to the reduced dynamical system is not ensured. The main result of this paper is to give a positive answer to the above question. In particular, given a vector field defined over a finite dimensional inner product space, we will prove the following. Assume that the manifold chosen to construct the reduced-order dynamical system is an immersed submanifold of the vector space, considered as ambient manifold. Then we will show that it is possible to construct explicitly a reduced-order vector field over this submanifold.

The paper is organized as follows. In the next section, we give some preliminary definitions. In Section 3, we state and prove the main result of this paper. We also give some examples and we propose a point estimator of the time-dependent error between the original vector field and the reduced order one. Finally, in Section 4, some conclusions are given.

2. Preliminary definitions

A differentiable manifold can be seen as a configuration space used to describe a particular physical system. The most obvious examples are related to mechanical systems for the study of the movements of a pendulum or of a system of solids. It may equally well be used to model the evolution of a chemical system where the parameters are the temperature and the concentrations of various species. One of main characteristics of these abstract objects is the property to describe a neighbourhood on each point in the configuration space by using a set of (local) coordinates into an open set of a particular finite-dimensional normed space. This neighbourhood and its corresponding set of local coordinates are known as a chart, and the whole set of charts constitutes an atlas for the manifold. The atlas can be used to endow the manifold with a topology. Since we need to perform infinitesimal variations in our configuration space, a compatibility condition between two different coordinates systems is needed.

Along this paper, we will consider a manifold as a pair $(\mathbb{M}, \mathcal{A})$ where \mathbb{M} is a subset of some finite-dimensional vector space V and \mathcal{A} is an atlas representing the local coordinate system of \mathbb{M} . We recall the definition of an atlas associated with a set \mathbb{M} .

Definition 2.1. Let \mathbb{M} be a set. An atlas of class C^p ($p \geq 0$) or analytic on \mathbb{M} is a family of charts with some indexing set A , namely $\{(U_\alpha, \varphi_\alpha) : \alpha \in A\}$, having the following properties (see [9]):

AT1 $\{U_\alpha\}_{\alpha \in A}$ is a covering of \mathbb{M} , that is, $U_\alpha \subset \mathbb{M}$ for all $\alpha \in A$ and $\cup_{\alpha \in A} U_\alpha = \mathbb{M}$;

AT2 for each $\alpha \in A$, $(U_\alpha, \varphi_\alpha)$ stands for a bijection $\varphi_\alpha : U_\alpha \rightarrow W_\alpha$ of U_α onto an open set W_α of a finite-dimensional normed space $(X_\alpha, \|\cdot\|_\alpha)$, and for any α and β the set $\varphi_\alpha(U_\alpha \cap U_\beta)$ is open in X_α ;

AT3 finally, if we let $U_\alpha \cap U_\beta = U_{\alpha,\beta}$ and $\varphi_\alpha(U_{\alpha,\beta}) = U_{\alpha,\beta}$, the transition mapping $\varphi_\beta \circ \varphi_\alpha^{-1} : U_{\alpha,\beta} \rightarrow U_{\beta,\alpha}$ is a diffeomorphism of class C^p ($p \geq 0$) or is analytic.

Since different atlases can give the same manifold, we say that two atlases are *compatible* if each chart of one atlas is compatible with the charts of the other one in the sense of AT3. One verifies that the relation of compatibility between atlases is an equivalence relation.

Definition 2.2. An equivalence class of atlases of class C^p on \mathbb{M} , also denoted by \mathcal{A} , is said to define a structure of a C^p -manifold on \mathbb{M} , and hence we say that $(\mathbb{M}, \mathcal{A})$ is a finite-dimensional manifold. In a similar way, if an equivalence class of atlases is given by analytic maps, then we say that $(\mathbb{M}, \mathcal{A})$ is an analytic finite-dimensional manifold.

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