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Hamiltonian Reduction Using a Convolutional Auto-Encoder Coupled to a Hamiltonian Neural Network

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Abstract. The reduction of Hamiltonian systems aims to build smaller reduced models, valid over a certain range of time and parameters, in order to reduce computing time. By maintaining the Hamiltonian structure in the reduced model, certain long-term stability properties can be preserved. In this paper, we propose a non-linear reduction method for models coming from the spatial discretization of partial differential equations: it is based on convolutional auto-encoders and Hamiltonian neural networks. Their training is coupled in order to learn the encoder-decoder operators and the reduced dynamics simultaneously. Several test cases on non-linear wave dynamics show that the method has better reduction properties than standard linear Hamiltonian reduction methods.

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Key words: Hamiltonian dynamics, model order reduction, convolutional auto-encoder, Hamiltonian neural network, non-linear wave equations, shallow water equation.

1 Introduction

Hamiltonian reduced order modeling techniques have been successfully developed in order to perform accelerated numerical simulations of some parameterized Hamiltonian models of large dimension [16,25,30]. The spatial discretization of some wave-like partial differential equations gives rise to very large such Hamiltonian systems. Reduced order

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models can be essential for real-time simulations or when a large number of simulation instances are required as part of a control, optimisation or uncertainty quantification algorithm. Starting from the initial model, a large differential system, the methods consist into constructing a differential system of a smaller size that can produce valid approximate solutions for a predefined range of times and parameters. Many physical models have a Hamiltonian structure and this gives the system a certain number of geometrical properties like the conservation of energy and the symplecticity of the phase space flows. In particular, the preservation of this structure at the discrete level enables to ensure large-time stability of the numerical simulations [14]. In order to build consistent and robust reduced models, it is therefore interesting to preserve this Hamiltonian structure through the reduction. The construction of reduced models can be divided in two steps: (i) find a so-called pair of encoder and decoder operators that goes from the full to the reduced variables and inversely; (ii) identify the dynamics followed by the reduced variables. The construction of the encoder and decoder operators relies on a large number of data produced by numerical simulations in the range of time and parameters of interest.

The first approach to reduce a large Hamiltonian system relies on a linear approximation: the solutions manifold is approximated with a symplectic vector space of small dimension [25]. The encoder is here a linear mapping, which is also constructed to be symplectic so that the Hamiltonian structure is preserved into the reduced model. Such symplectic mapping can be constructed from data through greedy algorithms [1] or through a Singular Value Decomposition (SVD) methodology: this is the Proper Symplectic Decomposition (PSD) proposed in [25]. In this work, several algorithms have been proposed to define approximated optimal symplectic mappings: for instance, the cotangent-lift algorithm devise a symplectic mapping which is also orthogonal and have a block diagonal structure. Then the reduced model is obtained using the Galerkin projection method: the model is constructed by supposing that a symplectic projection of the residual vanishes, where the residual stands for the error obtained after replacing the original variables by the decoded reduced variables.

Such linear reductions, however, can hardly handle non-linear dynamics: this is the case for convection-dominated or non-linear wave like problems for which the solution manifold is badly approximated by hyperplanes. In order to build more expressive reduced models, one possibility is to consider time adaptive reduced methods [15,22]. Another widely investigated possibility is to consider non-linear reduction methods.

Regarding the construction of non-linear encoder-decoder operators, a first class of methods rely on manifold learning techniques [4,27]. Such methods are based on the geometrical analysis of the neighbors graph of the data thanks to the computation of geodesic distances (ISOMAP method, [28]), of eigenfunctions of the graph Laplacian (EigenMaps method [2]) or of diffusion processes (DiffusionMaps method [8]). This provides reduced variables for each data that can be further interpolated using the Nyström formula [3].

Since the explosion of deep learning in the early 2010s, new dimension reduction methods grounded on neural networks have been developed. The convolutional auto-