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Non-intrusive reduced order modeling of nonlinear problems using neural networks

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ABSTRACT

We develop a non-intrusive reduced basis (RB) method for parametrized steady-state partial differential equations (PDEs). The method extracts a reduced basis from a collection of high-fidelity solutions via a proper orthogonal decomposition (POD) and employs artificial neural networks (ANNs), particularly multi-layer perceptrons (MLPs), to accurately approximate the coefficients of the reduced model. The search for the optimal number of neurons and the minimum amount of training samples to avoid overfitting is carried out in the offline phase through an automatic routine, relying upon a joint use of the Latin hypercube sampling (LHS) and the Levenberg–Marquardt (LM) training algorithm. This guarantees a complete offline-online decoupling, leading to an efficient RB method – referred to as POD-NN – suitable also for general nonlinear problems with a non-affine parametric dependence. Numerical studies are presented for the nonlinear Poisson equation and for driven cavity viscous flows, modeled through the steady incompressible Navier–Stokes equations. Both physical and geometrical parametrizations are considered. Several results confirm the accuracy of the POD-NN method and show the substantial speed-up enabled at the online stage as compared to a traditional RB strategy.

1. Introduction

Many applications in engineering and the applied sciences involve mathematical models expressed as parametrized partial differential equations (PDEs), in which boundary conditions, material properties, source terms, loads or geometric features of the underlying physical problem are expressed by a parameter $\boldsymbol{\mu}$ [18,23,26]. A list of notable examples includes parameter estimation [6], topology optimization [5], optimal control [31] and uncertainty quantification [29]. In these examples, one is typically interested in a real-time evaluation of an *output of interest* (defined as a functional of the state variable [15]) for many parameter entries, i.e., for many configurations of the problem.

The increasing computational power and the simultaneous algorithmic improvements enable nowadays the *high-fidelity* numerical resolution of complex problems via standard discretization procedures, such as finite difference (FD), finite volume (FV), finite element (FE), or spectral methods [44]. However, these schemes remain prohibitively expensive in many-query and real-time contexts, both in terms of CPU time and memory demand, due to the large amount of degrees of freedom (DOFs) they need to accurately solve the PDE [1]. In light of this, *reduced order modeling* (ROM) methods have received

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a significant attention in the last decades. The objective of these methods is to replace the full-order system by one of significant smaller dimension, to decrease the computational burden while leading to a controlled loss of accuracy [11].

Reduced basis (RB) methods constitute a well-known and widely-used example of reduced order modeling techniques. They are generally implemented pursuing an offline-online paradigm [33]. Based upon an ensemble of *snapshots* (i.e., high-fidelity solutions to the parametrized differential problem), the goal of the *offline* step is to construct a solution-dependent basis, yielding a reduced space of globally approximating functions to represent the main dynamics of the full-order model [2,11]. For this, two major approaches have been proposed in the literature: proper orthogonal decomposition (POD) [32,49] and greedy algorithms [24]. The former relies on a deterministic or random sample in the parameter space to generate snapshots and then employs a singular value decomposition (SVD) to recover the reduced basis. In the second approach, the basis vectors coincide with the snapshots themselves, carefully selected according to some optimality criterion. As a result, a greedy strategy is typically more effective and efficient than POD, as it enables the exploration of a wider region of the parameter space while entailing the computation of many fewer high-fidelity solutions [23]. However, there exist problems for which a greedy approach is not feasible, simply because a natural criterion for the choice of the snapshots is not available [2].

Once a reduced order framework has been properly set up, an approximation to the *truth* solution for a new parameter value is sought *online* as a linear combination of the RB functions, with the expansion coefficients determined via a projection of the full-order system onto the reduced space [7]. To this end, a Galerkin procedure is the most popular choice.

Despite their established effectiveness, projection-based RB methods do not provide any computational gain with respect to a direct (expensive) approach for complex nonlinear problems with a non-affine dependence on the parameters. This is a result of the cost to compute the projection coefficients, which depends on the dimension of the full-order model. In fact, a full decoupling between the online stage and the high-fidelity scheme is the ultimate secret for the success of any RB procedure [44]. For this purpose, one may recover an affine expansion of the differential operator through the empirical interpolation method (EIM) [3] or its discrete variants [10,40]. However, for general nonlinear problems this is far from trivial.

A valuable alternative to address this concern is represented by *non-intrusive* RB methods, in which the high-fidelity model is used to generate the snapshots, but not in the projection process [11]. The projection coefficients are obtained via interpolation over the parameter domain of a database of reduced order information [9]. However, since reduced bases generally belong to nonlinear, matrix manifolds, standard interpolation techniques may fail, as they cannot enforce the constraints characterizing those manifolds, unless employing a large amount of samples [1,4].

In this work, we develop a non-intrusive RB method employing POD for the generation of the reduced basis and resort to (artificial) neural networks, in particular multi-layer perceptrons, in the interpolation step. Hence, in the following we refer to the proposed RB procedure as the POD-NN method. Being of non-intrusive nature, POD-NN is suitable for a fast and reliable resolution of complex nonlinear PDEs featuring a non-affine parametric dependence. To test this assertion, the POD-NN method is applied to the one- and two-dimensional nonlinear Poisson equation and to the steady incompressible Navier–Stokes equations. Both physical and geometrical parametrizations are considered.

The paper is organized as follows. Section 2 defines the (parametrized) functional and variational framework which is required to develop a finite element solver, briefly outlined in Subsection 2.2. The standard projection-based POD-Galerkin (POD-G) RB method is derived in Section 3. Section 4 discusses components, topology and learning process for artificial neural networks. This is preparatory for the subsequent Section 5, which details the non-intrusive POD-NN RB procedure; both theoretical and practical aspects are addressed. Several numerical results, aiming to show the reliability and efficiency of the proposed RB technique, are offered in Section 6 for the Poisson equation (Subsection 6.1) and the lid-driven cavity problem for the steady Navier–Stokes equations (Subsection 6.2). Finally, Section 7 gathers some relevant conclusions and suggests future developments.

2. Parametrized partial differential equations

Assume $\mathcal{P}_{ph} \subset \mathbb{R}^{P_{ph}}$ and $\mathcal{P}_g \subset \mathbb{R}^{P_g}$ are compact sets, and let $\boldsymbol{\mu}_{ph} \in \mathcal{P}_{ph}$ and $\boldsymbol{\mu}_g \in \mathcal{P}_g$ be respectively the *physical* and *geometrical* parameters characterizing the differential problem, so that $\boldsymbol{\mu} = (\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g) \in \mathcal{P} = \mathcal{P}_{ph} \times \mathcal{P}_g \subset \mathbb{R}^P$, with $P = P_{ph} + P_g$, represents the overall *input vector parameter*. While $\boldsymbol{\mu}_{ph}$ addresses material properties, source terms and boundary conditions, $\boldsymbol{\mu}_g$ defines the shape of the computational domain $\widetilde{\Omega} = \widetilde{\Omega}(\boldsymbol{\mu}_g) \subset \mathbb{R}^d$, $d = 1, 2$. We denote by $\widetilde{\Gamma}(\boldsymbol{\mu}_g) = \partial\widetilde{\Omega}(\boldsymbol{\mu}_g)$ the (Lipschitz) boundary of $\widetilde{\Omega}(\boldsymbol{\mu}_g)$, and by $\widetilde{\Gamma}_D(\boldsymbol{\mu}_g)$ and $\widetilde{\Gamma}_N(\boldsymbol{\mu}_g)$ the portions of $\widetilde{\Gamma}(\boldsymbol{\mu}_g)$ where Dirichlet and Neumann boundary conditions are enforced, respectively, with $\widetilde{\Gamma}_D \cup \widetilde{\Gamma}_N = \widetilde{\Gamma}$ and $\mathring{\widetilde{\Gamma}}_D \cap \mathring{\widetilde{\Gamma}}_N = \emptyset$.

Consider a Hilbert space $\widetilde{V} = \widetilde{V}(\boldsymbol{\mu}_g) = \widetilde{V}(\widetilde{\Omega}(\boldsymbol{\mu}_g))$ defined over the domain $\widetilde{\Omega}(\boldsymbol{\mu}_g)$, equipped with the scalar product $(\cdot,\cdot)_{\widetilde{V}}$ and the induced norm $\|\cdot\|_{\widetilde{V}} = \sqrt{(\cdot,\cdot)_{\widetilde{V}}}$. Furthermore, let $\widetilde{V}' = \widetilde{V}'(\boldsymbol{\mu}_g)$ be the dual space of $\widetilde{V}$. Denoting by $\widetilde{G} : \widetilde{V} \times \mathcal{P}_{ph} \to \widetilde{V}'$ the map representing a parametrized nonlinear second-order PDE, the differential (strong) form of the problem of interest reads: given $\boldsymbol{\mu} = (\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g) \in \mathcal{P}$, find $\widetilde{u}(\boldsymbol{\mu}) \in \widetilde{V}(\boldsymbol{\mu}_g)$ such that

$$\widetilde{G}(\widetilde{u}(\boldsymbol{\mu}); \boldsymbol{\mu}_{ph}) = 0 \quad \text{in } \widetilde{V}'(\boldsymbol{\mu}_g), \tag{2.1}$$

namely

$$\langle \widetilde{G}(\widetilde{u}(\boldsymbol{\mu}); \boldsymbol{\mu}_{ph}), v \rangle_{\widetilde{V}', \widetilde{V}} = 0 \quad \forall v \in \widetilde{V}(\boldsymbol{\mu}_g),$$