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Nonlinear Reduced DNN Models for State Estimation

Wolfgang Dahmen[1], Min Wang[2,*] and Zhu Wang[1]

[1] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA.*
[2] *Department of Mathematics, Duke University, Durham, NC 27708, USA.*

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Abstract. We propose in this paper a data driven state estimation scheme for generating nonlinear reduced models for parametric families of PDEs, directly providing *data-to-state maps*, represented in terms of Deep Neural Networks. A major constituent is a *sensor-induced* decomposition of a model-compliant Hilbert space warranting approximation in problem relevant metrics. It plays a similar role as in a Parametric Background Data Weak framework for state estimators based on Reduced Basis concepts. Extensive numerical tests shed light on several optimization strategies that are to improve robustness and performance of such estimators.

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1 Introduction

Understanding complex "physical systems" solely through observational data is an attractive but unrealistic objective if one insists on certifiable accuracy quantification. This, in turn, is an essential precondition for prediction capability. In fact, unlike application scenarios where an abundance of data are available, data acquisition for "Physics Informed Learning Task" typically relies on sophisticated sensor technology and is often expensive or even harmful. Therefore, a central task is to develop efficient ways for fusing the information provided by data with *background information* provided by physical laws governing the observed states of interest, typically represented by partial differential equations (PDEs). In principle, this falls into the framework of "Physics Informed Neural Networks" (PINN), however, with some noteworthy distinctions explained next.

*Corresponding author. *Email addresses:* `dahmen@math.sc.edu` (W. Dahmen), `wangmin@math.duke.edu` (M. Wang), `wangzhu@math.sc.edu` (Z. Wang)

The central objective of this note is to explore a machine learning approach to state estimation in the above sense. Our contributions concern two major aspects:

(i) In contrast to typical PINN formulations, we employ loss functions that are *equivalent* to the error of the estimator in a norm that is imposed by the continuous mathematical model. More precisely, this norm corresponds to a *stable variational formulation* of the PDE family. In other words, the generalization error for this loss function measures the accuracy of the estimator in a problem intrinsic norm without imposing any additional regularity properties.

(ii) When employing estimators, represented as Deep Neural Networks (DNNs), one has to accept a significant and unavoidable uncertainty about optimization success. Due to (i), one can at least measure the achieved accuracy at any stage of the optimization. We therefore take this fact as a starting point for a systematic *computational exploration* of a simple optimization strategy that seems to be particularly natural in combination with ResNet architectures.

Regarding (i), the proposed approach is, in principle, applicable to a much wider scope of problems than discussed below. Last but not least, in order to facilitate comparisons with other recovery schemes, specifically with methods that are based on *Reduced Basis* concepts, the numerical experiments focus on elliptic families of PDEs with *parameter dependent* diffusion fields. However, for this problem class we discuss in detail two rather different scenarios, namely diffusion coefficients with an *affine* parameter dependence, as well as *log-normal* parameter dependence. It is well known that the first scenario offers favorable conditions for Reduced Basis methods which have been well studied for this type of models and can therefore serve for comparisons. While in this case nonlinear schemes using neural networks do not seem to offer decisive advantages in terms of achievable certifiable estimation accuracy nor computational efficiency we see an advantage of the DNN approach in the second scenario because it seems that they can be better adapted to the challenges of this problem class.

It should be noted though that the present approach shares some conceptual constituents with so called One-Space methods or PBDW (Parametric Background Data Weak) methods (see [2, 4, 10]). We therefore briefly recollect some related basic ideas in Section 2.4. An important element is to represent the sensor functionals as elements of the trial space $\mathbb{U}$ for the underlying PDE. The $\mathbb{U}$-orthogonal projection to their span, termed "measurement space", provides a natural "zero-order approximation" to the observed state. To obtain an improved more accurate reconstruction, the data need to be "lifted" to the complement space. We view the construction of such a "lifting map" as "learning" the expected "label" associated with a given observation, see Section 2. This, in turn, is based on first projecting "synthetic data" in terms of parameter snapshots, to the $\mathbb{U}$-orthogonal complement of the measurement space. We then extract via SVD from these projected data a sufficiently accurate "effective" complement space that captures corresponding components of the solution manifold with high accuracy in $\mathbb{U}$. The lifting map is then expressed in terms of the coefficients of a $\mathbb{U}$-orthogonal basis of the effective complement space which, in turn, are represented by a neural network. The fact that