Title: Towards self-improving codes in computational fluid dynamics: an application to radial basis function approximation

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Abstract: The integration of machine learning methods within PDE numerical solvers to speed-up computation, to account for more detailed descriptions of systems or to improve the quality of the numerical solution has become a common practice. However, often the machine learning models considered are static in nature, they consist of a offline training phase, and once trained are deployed and remain static. This, in turn, places an extreme importance on the correct design of the training set and training procedure, and leads to models which might not be robust (e.g.: when unseen inputs are far away from the training set).

In this work, we present a hybrid computation framework in which the machine learning model continuously learns during run-time. In particular, using a novel procedure akin to *a posteriori limiting* [1], we obtain a more robust solver[6], by switching between a neural network, and a gold standard procedure (which is used to generate the original training data), which in turn will be used to re-train the neural network. In order to do this, we present two main directions of work:

1. Error estimators on the network's prediction, based on the uncertainty of the neural network's output through the use of Bayesian neural networks [2], as well as similarity of current input to training data input[3].

2. A batched online training strategy to improve the neural network.

To demonstrate the performance of this framework, we extend our previous work on selecting optimal parameters for radial basis functions approximations [4]. Namely, the choice of the shape parameter highly effects the behaviour of radial basis function (RBF) approximations, as it needs to be selected to balance between ill-condition of the interpolation matrix and high accuracy. Previously, we demonstrate how to use neural networks to determine the shape parameters in RBFs using an unsupervised learning strategy. In this new work, by using error estimators on the network's prediction, we can switch between the trained neural network, and an optimization procedure that can then be used to re-train the neural network.

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[6]Requirements for physical consistency and accuracy with the underlying PDE solver can also be included.

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