Scientific machine learning: methods to compute efficient surrogate models from small sets of observations

MARINE 2023

Francesco Di Fiore*, Pier Carlo Berri* and Laura Mainini*

* Department of Mechanical and Aerospace Engineering Politecnico di Torino Corso Duca degli Abruzzi 24, 10129 Torino, Italy e-mail: laura.mainini@polito.it

ABSTRACT

Design optimization, inverse problems and uncertainty quantification problems are commonly encountered across all the domains of transportation and industrial engineering. Main challenges relate to the complexity and the dimensionality of the simulation-based parametric studies associated with these problems, which frequently require to evaluate expensive numerical models many times (many-query). Within this context, statistical learning offers powerful methods to compute efficient surrogate representations of the expensive models which are commonly used in an offline-online fashion: offline the surrogate representations are computed from a set of evaluations of expensive models, online the surrogates are used for the many-query tasks to contain the costs of the individual model interrogations. An open research question relates to the reliability of the predictions obtained with these methods, in particular when the set of available parametric evaluations is small [1-3]. This work discusses scientific machine learning methods that build up on the synergies between model order reduction and statistical learning to obtain computationally efficient representations suitable for many-query and time-constrained engineering problems. In particular, projection based methods are used to constrain the learning process and make it amenable when only small sets of expensive evaluations (observations) can be collected. Different types of applications will be discussed with relevance to transportation and naval engineering: from simulation-based design problems to optimal data selection and allocation for system identification problems.

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