STOCHASTIC SUBSPACE VIA PROBABILISTIC PCA TO CHARACTERIZE AND CORRECT MODEL ERROR

Ruda Zhang[1*]

[1]*University of Houston*

ABSTRACT

Complex engineering systems give rise to high-dimensional computational models that resolve multi-physics coupling and multi-scale processes, pushing the ever-expanding limit of computing power. Yet errors in system input, model parameters and model representation limit the predictive value of such models. Such model error shall be quantified and adjusted based on experimental measurement data, for predictive modeling and digital twinning. A seminal work [1] on this topic proposed a stochastic surrogate model that consists of projection-based reduced-order models (ROM) derived from a high-dimensional model, where the reduced-order bases are randomized. The use of ROM allows tractable uncertainty quantification, while learning a probabilistic model for the basis can improve model accuracy. We follow this strategy and design new probabilistic models for stochastic ROM.

Specifically, we propose a probabilistic model of subspaces based on the probabilistic principal component analysis (PCA). Given a sample of system state vectors, commonly known as a snapshot matrix, this method uses quantities derived from the PCA to construct distributions of the sample matrix as well as subspaces of all dimensions of the state space. It is applicable to projection-based reduced-order modeling methods, such as proper orthogonal decomposition and related model reduction methods. The stochastic subspace thus constructed can be used, for example, to characterize model error in computational mechanics. With experimental validation data, the stochastic subspace model can be adapted in a Bayesian approach to correct model error and improve accuracy.

The proposed method has multiple desirable properties: (1) it is naturally justified by a probabilistic interpretation of PCA, and in some cases has analytical forms for the induced probabilistic models on related matrix manifolds; (2) it satisfies linear constraints, such as boundary conditions of all kinds, by default; (3) it has only one hyper-parameter, which dramatically simplifies the training procedure; (4) its algorithm is very easy to implement. We compare the proposed method with existing approaches [1,2] visually in a low-dimensional example, and demonstrate its performance in modeling the dynamics of a space structure.

REFERENCES

[1] Soize, C. & Farhat, C. A nonparametric probabilistic approach for quantifying uncertainties in low-dimensional and high-dimensional nonlinear models. IJNME, 2017, 109, 837-888.

[2] Zhang, H. & Guilleminot, J. A Riemannian stochastic representation for quantifying model uncertainties in molecular dynamics simulations. CMAME, 2023, 403, 115702.

[3] Yadav, A. & Zhang, R. Stochastic Subspace via Probabilistic Principal Component Analysis. arXiv, 2024.