Deep Learning-Boosted Reduced Order Modeling and Simulation of Spatiotemporal Systems

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I. Global Model Reduction

Many important tasks in engineering require us to efficiently model and predict the behavior of complex spatiotemporal systems like fluid flows. Modeling such systems is particularly challenging because of their high dimensionality and emergence of complex behavior including turbulence. Computational Fluid Dynamics (CFD) techniques are becoming more sophisticated and accurate, yet lack the speed needed to evaluate objective functions used for design optimization or reinforcement learning-based control of large-scale systems. Even though some modeling is used to reduce the cost of simulations including sub-grid scale models in LES and turbulence models in Reynolds Averaged Navier-Stokes, CFD relies on fine discretization to capture the behavior of governing equations. While CFD simulations can be thought of as dynamical systems, the state space is too high dimensional for modern control system design.

Luckily, fluid flows are not completely random and display a range of coherent structures which have recently been used to create low-dimensional models and obtain insights about the fundamental behavior [1]. Data-driven model reduction and system identification has become attractive due to availability of detailed simulations and experimental data. Some techniques which fall under this category include the Proper Orthogonal Decomposition (POD) and Galerkin projection method [1], Balanced Proper Orthogonal Decomposition (BPOD) [2], Dynamic Mode Decomposition (DMD) and its variants [3], [4], as well as Recurrent Neural Networks (RNNs) [5], [6]. In all of these methods, simulation or experimental data are taken from the complete system or subdomain under investigation and used to learn appropriate features for building reduced order models. We refer to the above approach as "global model reduction" since features and reduced order models of the whole system are being discovered.

My work so far relates to the Extended Dynamic Mode Decomposition (EDMD) [7] and its kernel method variant KDMD [8] which provide data-driven approximations of the Koopman operator on dictionaries of observables. In particular, I have been focusing on developing methods for discovering extremely low-dimensional subspaces of observables which contain rich information about the full high-dimensional state and its evolution. For this purpose I combined a deep contractive autoencoder with a linear dynamics model for the encoded observables to form an architecture I call a Linearly-Recurrent Autoencoder Network or LRAN. Using deep neural networks allows highly complex features to be extracted from the data and has recently been successfully used to learn dictionaries for EDMD [9].

Up to the present, all methods have relied on linear reconstruction of the full state from the feature space. This places a rather restrictive assumption on the observables used to form a reduced order model — namely that the full state can be recovered in their span. Instead, the LRAN incorporates a nonlinear decoder neural network which is trained simultaneously with the encoder and the state transition matrix. This forces the learned observables to be highly informative in order to nonlinearly reconstruct the full state while retaining the property of linear dynamics. Furthermore, nonlinear reconstruction using the deep decoder network allows for an extremely small subset of observables to be learned.

The LRAN can be unfolded for an arbitrary number of time steps allowing us to take advantage of long data sequences. This helps the encoder to learn low-amplitude features which have large influence on the future dynamics of non-normal systems. The LRAN has already achieved impressive results on a cylinder wake flow problem as well as artificial dynamical systems nonlinearly embedded in images. I am currently in the process of training an LRAN on data produced by simulating the Kuramoto-Sivashinsky equation. A paper intended for the SIADS Journal is forthcoming.

As it turns out, EDMD and KDMD can be made into a kind of shallow LRAN unfolded for a single time step. The method begins by constructing an over-specified linear model of the dynamics in a nonlinear feature space using EDMD or KDMD. Treating this as a state-space system together with output given by linearly reconstructing the full state, a balanced reduced order model can be found using BPOD. Finally, nonlinear regression can be used to reconstruct the full state from the resulting small set of observables.

Future work on LRANs will incorporate control inputs to the system as well as introducing generative stochastic networks and stochastic dynamics in order to quantify uncertainty [6]. Adversarial training [5] will be used to improve the plausibility of generative reconstructions including turbulent detail by training the LRAN to fool a classifier network with its predictions. An interesting aspect of this work is that neural networks are used to learn sophisticated features which have simple dynamics in time. I think this is powerful since it enables humans to interpret these complex features based on their simple behavior. The idea can be extended to learning low-dimensional nonlinear normal forms for high-dimensional systems by adding homogeneous polynomial nonlinearities in the encoded state dynamics.

II. Local Multi-scale Modeling

The model reduction techniques described so far are applicable only when data coming from the complete system of interest is available. This limits their flexibility since they are unable to be applied to new problems with different spatial domains and boundary conditions. The aim of the proposed research is to create reduced-order models which can generalize to new configurations without needing to run expensive simulations or experiments of the full system.

Previous work in this direction utilizes an equation-free framework to simulate macroscopic behavior using pocket-sized microscopic simulators [10]. Macro-scale coarse-grained states are lifted to the micro-scale and simulated in small patches. A gap-tooth scheme is used to evolve these small patches and interpolate the results. The solution is then restricted to the set of coarsened features and advanced in time with projective integration. In theory, the method can be implemented recursively on a hierarchy of scales in order to efficiently simulate large domains and times. The primary challenge comes in identifying coarse-grained features which are informative enough about the small-scales to enable lifting and prediction.

I plan to further this work by utilizing deep feature learning as in the LRAN to perform the restriction step and identify a recursive hierarchy of renormalized coarse models. The lifting process will be aided by the recent developments in generative stochastic networks [5] which may enable plausible and detailed reconstruction of microscopic states as well as their probability distributions.

The proposed framework at each level of the model hierarchy can be used to learn discrete or continuous coarsened models. Continuous models are of particular interest since problem-dependent physics can be imposed by constraining the structure of the coarsened dynamics equations. Furthermore, learning a hierarchy of renormalized spatiotemporal PDEs might be used together with unstructured or meshfree solvers to speed up costly large-scale simulations. Analogies with the Koopman operator can be drawn in the case that linear renormalized PDEs are learned. Due to the local formulation, the models can be re-assembled in new spatial domains in order to make predictions and form low-order models of the large-scale dynamics.

Recursive coarse-graining using the proposed deep learning approach may also enable online identification of coarse equations from fewer fine-scale examples then would be required to simulate an entire large domain. A few small patches can be lifted and simulated in order to provide training data for coarser models. The process can be iterated by cycling over models at all scales until they converge. In this way, an online multi-scale renormalization process might be used to accelerate and perform simulations that are presently beyond our capability.

References

[1] P. Holmes, J. L. Lumley, G. Berkooz, and C. W. Rowley, *Turbulence, Coherent Structures, Dynamical Systems and Symmetry*. Cambridge University Press, 2012.

[2] C. W. Rowley, "Model reduction for fluids, using balanced proper orthogonal decomposition," *International Journal of Bifurcation and Chaos*, vol. 15, no. 03, pp. 997–1013, 2005.

[3] M. R. Jovanović, P. J. Schmid, and J. W. Nichols, "Sparsity-promoting dynamic mode decomposition," *Physics of Fluids*, vol. 26, no. 2, p. 024103, feb 2014. [Online]. Available: http://aip.scitation.org/doi/10.1063/1.4863670

[4] C. W. Rowley and S. T. Dawson, "Model reduction for flow analysis and control," *Annual Review of Fluid Mechanics*, vol. 49, no. 1, pp. 387–417, jan 2017. [Online]. Available: http://www.annualreviews.org/doi/10.1146/annurev-fluid-010816-060042

[5] I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning*. MIT Press, 2016.

[6] R. G. Krishnan, U. Shalit, and D. Sontag, "Structured inference networks for nonlinear state space models," in *Proc. 31st AAAI Conference on Artificial Intelligence (AAAI-17)*, 2017.

[7] M. O. Williams, I. G. Kevrekidis, and C. W. Rowley, "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," *Journal of Nonlinear Science*, vol. 25, no. 6, pp. 1307–1346, dec 2015. [Online]. Available: http://link.springer.com/10.1007/s00332-015-9258-5

[8] I. G. Kevrekidis, C. W. Rowley, and M. O. Williams, "A kernel-based method for data-driven Koopman spectral analysis," *Journal of Computational Dynamics*, vol. 2, no. 2, pp. 247–265, may 2016.

[9] Q. Li, F. Dietrich, E. M. Bollt, and I. G. Kevrekidis, "Extended dynamic mode decomposition with dictionary learning: a data-driven adaptive spectral decomposition of the Koopman operator," jul 2017.

[10] I. G. Kevrekidis, C. Gear, J. Hyman, P. G. Kevrekidid, O. Runborg, and C. Theodoropoulos, "Equation-free, coarse-grained multiscale computation: Enabling mocroscopic simulators to perform system-level analysis," *Communications in Mathematical Sciences*, vol. 1, jan 2003.