Bi-Fidelity Data-assisted Neural Networks in Nonintrusive Reduced Order Modeling

Chuan Lu

April 22, 2019

High-fidelity simulations

- Formalized as parameterized PDEs
- Indispensible in science and engineering
- Require great computational cost, especially for many-query and real-time situations

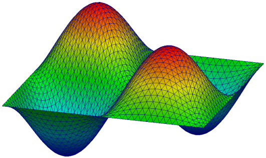

[1]

Figure: 2D Laplace equation

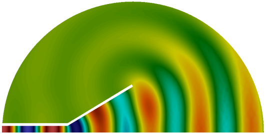

[1]

Figure: 2D Helmholtz equation

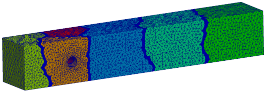

[1]

Figure: 3D Navier-Stokes equation

[1] A. Quarteroni, A. Manzoni and F. Negri. Reduced Basis Methods for Partial Differential Equations. An Introduction. Unitext, vol. 92. Springer, 2016. https://redbkit.github.io/redbKIT/

Problem setup

Parameterized PDE:

$$\begin{cases} \mathcal{L}u(x,z) = f, & \text{in } D, \\ u(x,z) = g, & \text{on } \partial D. \end{cases}$$

Many-query problem: solve the PDE for $z \in Z_{query} \subset I_z$.

Proper Orthogonal Decomposition (POD)

- Seek for a set of parameter-independent function basis for the full-order solution space
- Minimize the L_2 error

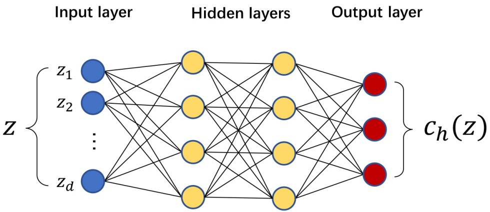
POD

1. Generate a full-order snapshot matrix $S = [u(x, z_1), \ldots, u(x, z_P)]$.
2. At dimension k, pick the first k left singular vectors of S to form the basis V of the reduced space.
3. Compute the reduced approximation by projection onto the reduced space: $c_{rb}(z) = V^\top u(x, z)$, $u_{rb}(x, z) = V c_{rb}$.

For nonintrusive methods, at the online stage, the coefficients $c_{rb}(z^*)$ are recovered without the projection of the full-order solution.

POD-NN

Use neural networks to learn the mapping $z \to c_{rb}(z)$[1].



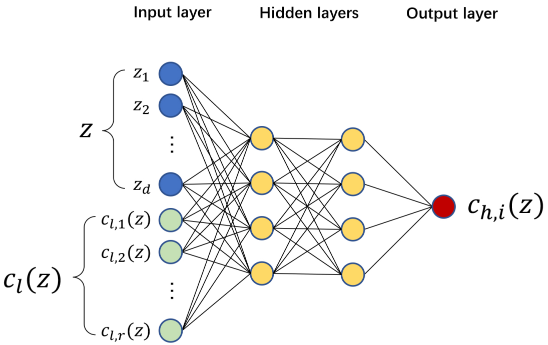
- For nonlinear problems, POD-NN has a good performance because of the nonlinear nature of neural networks.

Low-fidelity models

- Common in scientific and engineering applications
- Inaccurate, but can mimic important behaviours of the problem
- Much lower computational cost

BiFi-NN

- We incorporate additional features extracted from the low-fidelity model to the input of POD-NN[2].
- One possible choice is to use the low-fidelity POD coefficients.



BiFi-NN (cont.)

Two problems with BiFi-NN:

- In the offline stage, it needs a large collection of high-fidelity snapshots to generate the POD basis.
- In the online stage, it requires one additional low-fidelity simulation to extract the additional input feature.

BiFi-NN (cont.)

Two problems with BiFi-NN:

- In the offline stage, it needs a large collection of high-fidelity snapshots to generate the POD basis.
- In the online stage, it requires one additional low-fidelity simulation to extract the additional input feature.

To tackle these challenges, we apply the following methods:

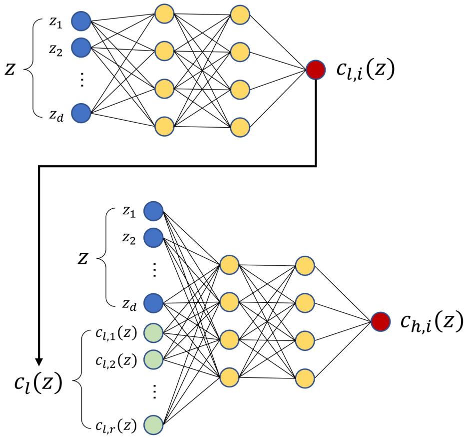
- Apply a point selection method to the low-fidelity snapshots to select a subset of parameters for generating the high-fidelity POD basis.
- Use a two-step prediction scheme, i.e., use another network to approximate the low-fidelity POD coefficients instead of the real ones.

Point selection

1. Simulate the low-fidelity model on a set of parameters $Z \subset I_z$.
2. Use point selection methods to select a subset $\tilde{Z} \subset Z$.
3. Simulate the high-fidelity model on $\tilde{Z}$ and compute the POD basis.

In this project, we use Cholesky selection method[3]. Alternative methods include rank-revealing QR (RRQR).

Two-step prediction



Online complexity: $O(S+F) \to O(2F)$.

2D Vorticity Equation

$$\begin{cases} \partial_t w = \mu \Delta w - (u \cdot \nabla) w, \ (x, y, \mu) \in [0, 2\pi] \times [0, 2\pi] \times [2 \times 10^{-3}, 5 \times 10^{-3}], \\ w|_{t=0} = \hat{w} + \epsilon(x, y), \end{cases}$$

where $w = \nabla \times u$,

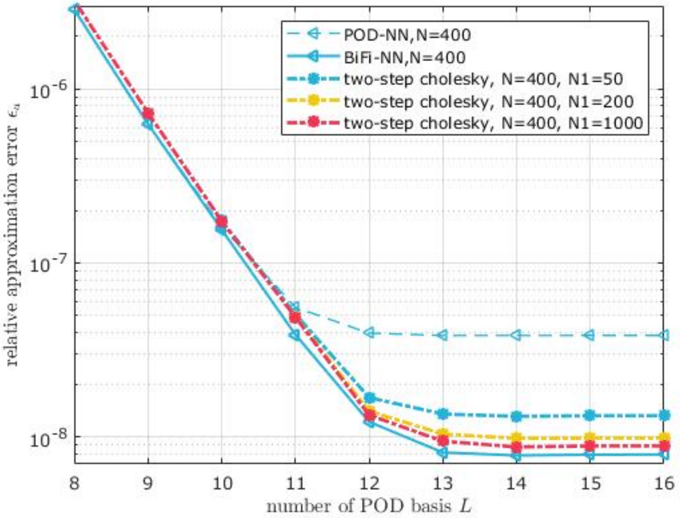
$$\begin{aligned} \hat{w}((x, y), 0) = \exp &\left(-\frac{(x - \pi + \pi/5)^2 + (y - \pi + \pi/5)^2}{0.3} \right) \\ &- \exp \left(-\frac{(x - \pi - \pi/5)^2 + (y - \pi + \pi/5)^2}{0.2} \right) \\ &+ \exp \left(-\frac{(x - \pi - \pi/5)^2 + (y - \pi - \pi/5)^2}{0.4} \right), \end{aligned}$$

and ϵ is a random noise uniformly distributed in [-1, 1]. We use Fourier spectral method to solve this problem until final time $T = 50$ with timestep $\Delta t = 0.1$.

2D Vorticity Equation (cont.)

- High-fidelity model: solved on a uniform grid of size 128×128 with average running time 7.73s.
- Low-fidelity model: solved on a uniform grid of size 16×16, with average running time 0.39s.
- For POD-NN and BiFi-NN, we use 300 independent snapshots to generate the high-fidelity POD basis; for BiFi-NN with Cholesky selection, only 26 values of the parameter are chosen from the low-fidelity snapshots. Thus, we reduced the number of high-fidelity snapshots for generating POD basis by 274.

2D Vorticity Equation (cont.)



References I

J. S. Hesthaven and S. Ubbiali.
Non-intrusive reduced order modeling of nonlinear problems using neural networks.
Journal of Computational Physics, 363:55–78, 2018.

C. Lu and X. Zhu.
Bifidelity data-assisted neural networks in nonintrusive reduced-order modeling.
arXiv preprint arXiv:1902.00148, 2019.

X. Zhu, A. Narayan, and D. Xiu.
Computational aspects of stochastic collocation with multifidelity models.
SIAM/ASA Journal on Uncertainty Quantification, 2(1):444–463, 2014.