SCIENTIFIC MACHINE LEARNING

Lecture notes in Chinese:
http://faculty.bicmr.pku.edu.cn/~huangdz/teaching.html

Scientific Computing

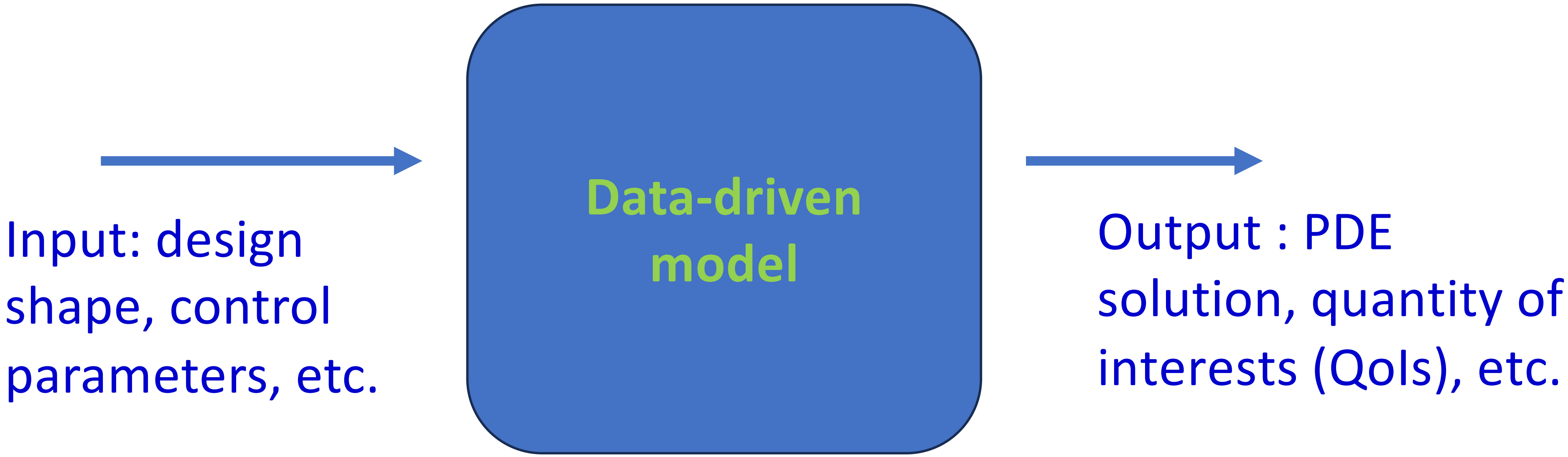
Applications: engineering design optimization, real-time control, uncertainty quantification, and so on

Input: design shape, control parameters, etc. → **Partial differential equation (PDE) based model** → Output : PDE solution, quantity of interests (QoIs), etc.

Challenges: high computational cost and many query problems

Surrogate Models

Applications: engineering design optimization, real-time control, uncertainty quantification, and so on



Challenges: high computational cost and many query problems

Surrogate Models

- Projection-Based Reduced Order Model

  - PDE-based model (high dimensional model)

$$r(u, \mu) = 0, \qquad u \in R^N$$

  - A low-dimensional model is constructed using target system knowledge to capture its main behavior

$$V \in R^{N\times k}, \qquad u = u_0 + V\Delta y, \qquad \Delta y \in R^k, \qquad k \ll N$$

basis matrix

$$r(u_0 + V\Delta y, \mu) = 0, \qquad \Delta y \in R^k$$

Surrogate Models

Literatures

Linear reduced-order model: Antoulas, Athanasios C. " Approximation of large-scale dynamical systems." Society for Industrial and Applied Mathematics, 2005.

Nonlinear reduced-order model: Chaturantabut, Saifon, and Danny C. Sorensen. "Nonlinear model reduction via discrete empirical interpolation." SIAM Journal on Scientific Computing 32, no. 5 (2010): 2737-2764.

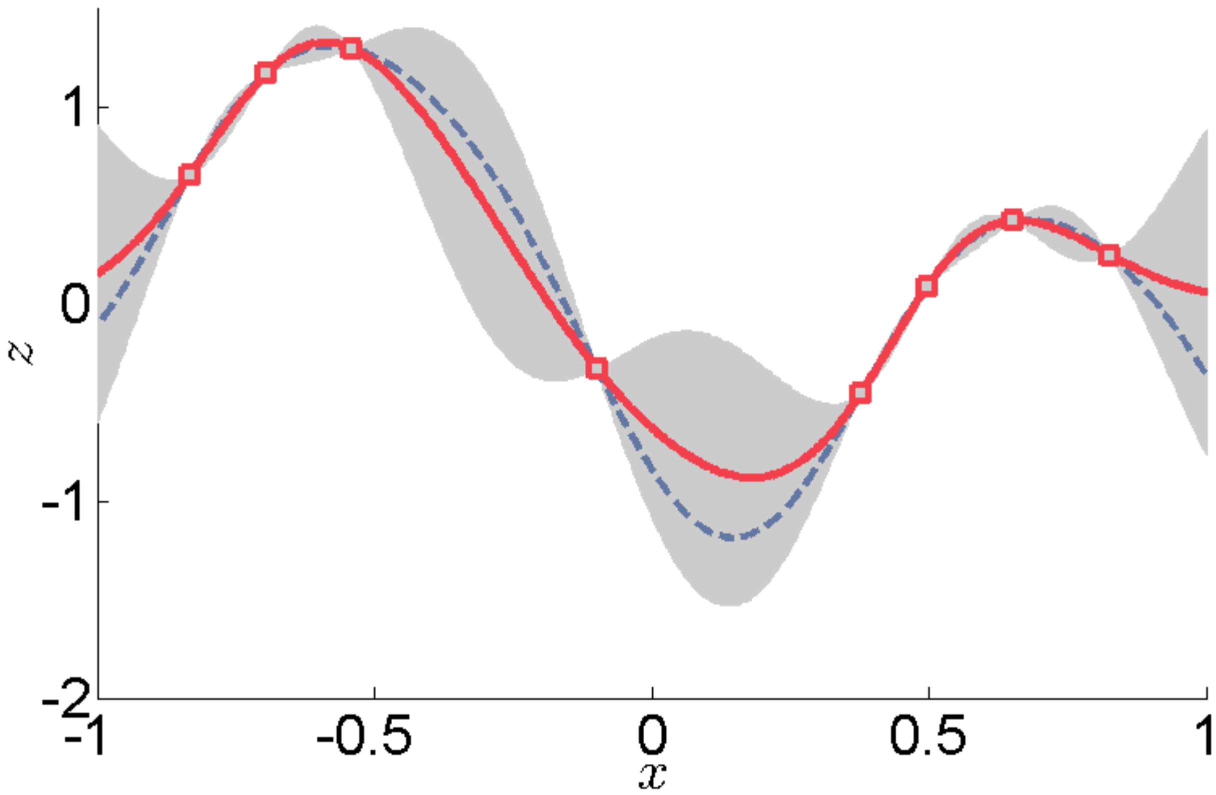
Nonlinear reduced-order model: Carlberg, Kevin, Charbel Bou-Mosleh, and Charbel Farhat. "Efficient nonlinear model reduction via a least-squares Petrov–Galerkin projection and compressive tensor approximations." International Journal for numerical methods in engineering 86, no. 2 (2011): 155-181.

Koopman operator: Mauroy, Alexandre, Yoshihiko Susuki, and Igor Mezić. "Introduction to the Koopman operator in dynamical systems and control theory." The koopman operator in systems and control (2020): 3-33.

Dynamic mode decomposition: Schmid, Peter J. "Dynamic mode decomposition of numerical and experimental data." Journal of fluid mechanics 656 (2010): 5-28.

Surrogate Models

- Gaussian Process Regression
  - Probabilistic Interpolation based on Gaussian processes with various kernels
  - Prediction and uncertainty quantification



Surrogate Models

- Literatures

Textbook: C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, Chapter 5.

Textbook: Wendland, Holger. Scattered data approximation. Vol. 17. Cambridge university press, 2004.

Random feature method: Rahimi, Ali, and Benjamin Recht. "Random features for large-scale kernel machines." Advances in neural information processing systems 20 (2007).

Learning PDE solution map: Nelsen, Nicholas H., and Andrew M. Stuart. "The random feature model for input-output maps between banach spaces." SIAM Journal on Scientific Computing 43, no. 5 (2021): A3212-A3243.

Solving PDE: Zhang, Xiong, Kang Zhu Song, Ming Wan Lu, and X. Liu. "Meshless methods based on collocation with radial basis functions." Computational mechanics 26 (2000): 333-343.

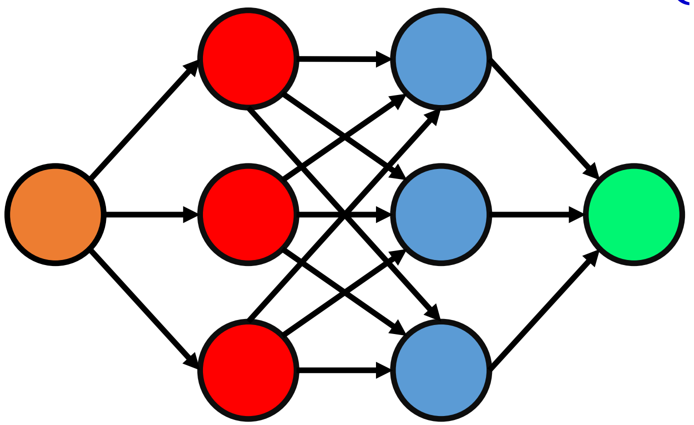
Learning PDE solution map: Batlle, Pau, Matthieu Darcy, Bamdad Hosseini, and Houman Owhadi. "Kernel methods are competitive for operator learning." Journal of Computational Physics 496 (2024): 112549.

Surrogate Models

- Neural Network/Operator
  - Effectively exploit high-dimensional and intricate relationships
  - Powerful software support and GPU acceleration

linear function: $x \mapsto Ax + b$

nonlinear activation function: $\sigma(x) \mapsto \begin{cases} x\ (x \geq 0) \\ 0\ (x < 0) \end{cases}$



Surrogate Models

- Literatures

CNN: Zhu, Yinhao, and Nicholas Zabaras. "Bayesian deep convolutional encoder–decoder networks for surrogate modeling and uncertainty quantification." Journal of Computational Physics 366 (2018): 415-447.

PCA-Net: Hesthaven, Jan S., and Stefano Ubbiali. "Non-intrusive reduced order modeling of nonlinear problems using neural networks." Journal of Computational Physics 363 (2018): 55-78.

FNO: Li, Zongyi, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Fourier neural operator for parametric partial differential equations." arXiv preprint arXiv:2010.08895 (2020).

DeepONet: Lu, Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. "Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators." Nature machine intelligence 3, no. 3 (2021): 218-229.