Probabilistic neural network-based reduced-order surrogate for fluid flows

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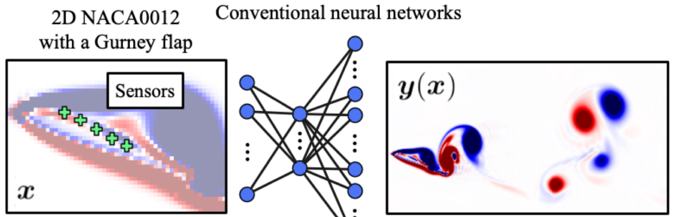
Introduction

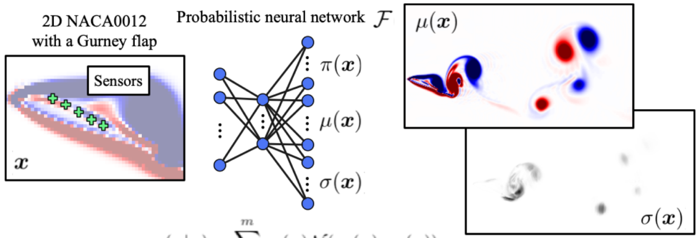


$$\boldsymbol{w} = \mathrm{argmin}_{\boldsymbol{w}}[E(\boldsymbol{y}, \mathcal{F}(\boldsymbol{x};\boldsymbol{w}))]$$

- Neural networks (NNs) have shown their great potential as an universal approximator in physical sciences
- NNs are usually handled as Black box
  - No feedback for us
  - L_2 error based deterministic regression: no notion of confidence intervals
- How is the probabilistic view?
  - Variational inference[1], Gaussian process approximation[2]
  - Enables us to not only assess model and data but also quantify uncertainty

[1] Blundell et al., arXiv preprint, 2015
[2] Damianou and Lawrence, Artificial Intelligence and Statistics, 2013

Probabilistic neural network (PNN)[3]



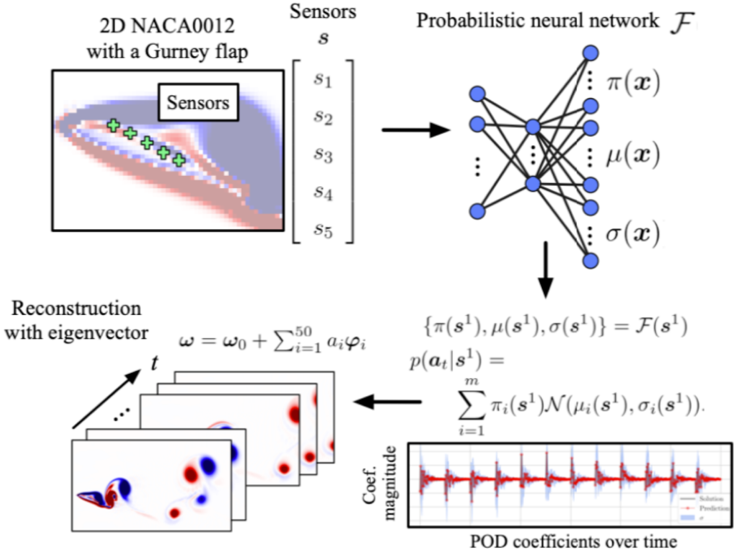
$$p(\boldsymbol{y}|\boldsymbol{x}) = \sum_{i=1}^{m} \pi_i(\boldsymbol{x})\mathcal{N}(\mu_i(\boldsymbol{x}), \sigma_i(\boldsymbol{x}))$$

$$\boldsymbol{w} = \mathrm{argmin}_{\boldsymbol{w}}[\mathcal{E}], \quad \text{where} \quad \mathcal{E} \equiv -\log\mathcal{L} = -\sum_{k=1}^{K} p(y_{k,p}|x_k)\log p(y_{k,t})$$

- Focus on probability distribution of estimation, which can be approximated as linear superposition
- Attempts to get the probability distribution of output directly
  - Loss function: Maximization of log-likelihood
  - Suitable to utilize the full distribution of estimation by PNN

[3] Bishop, 1994

PNN-based reduced order model with proper orthogonal decomposition



1. Take POD for flow field and obtain temporal coefficients

$$\boldsymbol{q} = \boldsymbol{q}_0 + \sum_{i=1}^{M} a_i\boldsymbol{\varphi}_i$$

2. PNN attempts to predict a temporal evolution of POD coefficients over n time steps from local sensor information s at the first time step

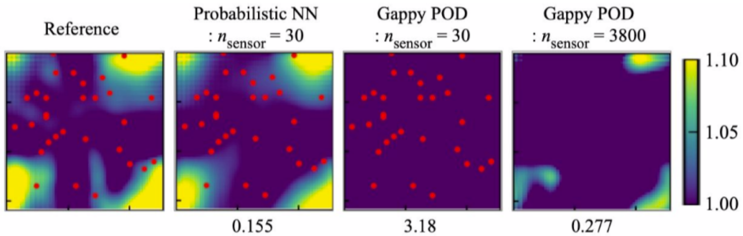
$$\{\pi(\boldsymbol{s}^1), \mu(\boldsymbol{s}^1), \sigma(\boldsymbol{s}^1)\} = \mathcal{F}(\boldsymbol{s}^1), \quad p(\boldsymbol{a}_t|\boldsymbol{s}^1) = \sum_{i=1}^{m} \pi_i(\boldsymbol{s}^1)\mathcal{N}(\mu_i(\boldsymbol{s}^1), \sigma_i(\boldsymbol{s}^1))$$

$$\boldsymbol{a}_t = [\boldsymbol{a}^1, \boldsymbol{a}^2, ..., \boldsymbol{a}^n], \text{ where } \boldsymbol{a}^t = [a_1^t, a_2^t, ..., a_M^t]$$

Results

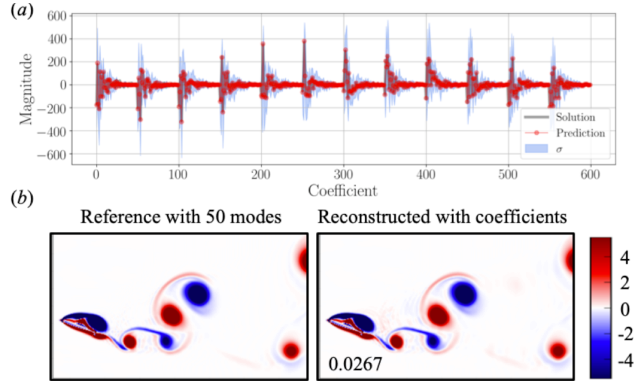
Comparison with benchmark linear method (Gappy POD)

Example: Two-dimensional inviscid shallow water equations



- PNN exhibits the significant advantage even at $n_{\mathrm{sensor}} = 3800$

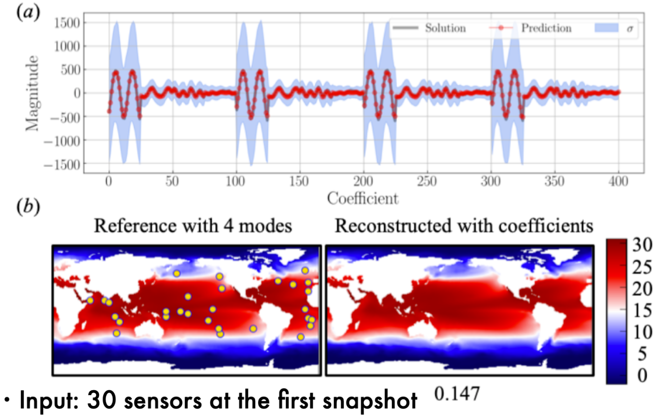
NACA0012 airfoil with a Gurney flap[4]



- Input: 5 sensors on surface of an airfoil at the first snapshot
- Output: 50 POD modes over 12 time steps
- PNN can accurately estimate the temporal evolution of POD while showing its confidence interval

[4] Gopalakrishnan Meena et al., AIAA J., 2018

NOAA sea surface temperature



- Input: 30 sensors at the first snapshot
- Output: 4 POD modes over 100 weeks
- PNN also performs well for real-world data set

Conclusions

- Introduced PNN to quantify uncertainties for fluid flow surrogate modeling and data reconstruction
- Provided confidence intervals can be useful for additional sensor placements in fluid flow data recovery tasks[5]

[5] Maulik et al., Phys. Rev. Fluids, 2020

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