The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences

EQUIPPING NEURAL NETWORK SURROGATES WITH UNCERTAINTY FOR PROPAGATION IN PHYSICAL SYSTEMS

GRAHAM PASH

Collaborators: Malik Hassanaly & Shashank Yellapantula

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DOE CSGF

NREL
Transforming ENERGY

Talk Outline

1. **Introduction**
2. Modeling uncertainty with BNNs
3. A Priori Results
4. Uncertainty Propagation
5. Concluding remarks

Motivating Example: Reacting Flows

- Large eddy simulation (LES) applies a **low-pass** filter to the. Navier-Stokes equations
  - Resolves largest length scales
  - Models small scales effects
    - Ex: Progress variable subfilter scale (SFS) dissipation rate
- Data-driven approach
  - Filter direct numerical simulation (DNS) data to generate training pairs
  - Flexible
  - Introduces new uncertainties

[1] Wimer, Nicholas T., et al. Examination of a Methane/Diesel RCCI Engine Using Pele. No. NREL/CP-2C00-84700. National Renewable Energy Lab.(NREL), Golden, CO (United States), 2023.

Dissipation Rate Model

- Physics-based algebraic models
- Gaussian processes
- Neural networks

$$\widetilde{\chi}_{C,sgs} = 2\widetilde{D_C|\nabla C|^2} - 2\widetilde{D_C}|\nabla \widetilde{C}|^2$$

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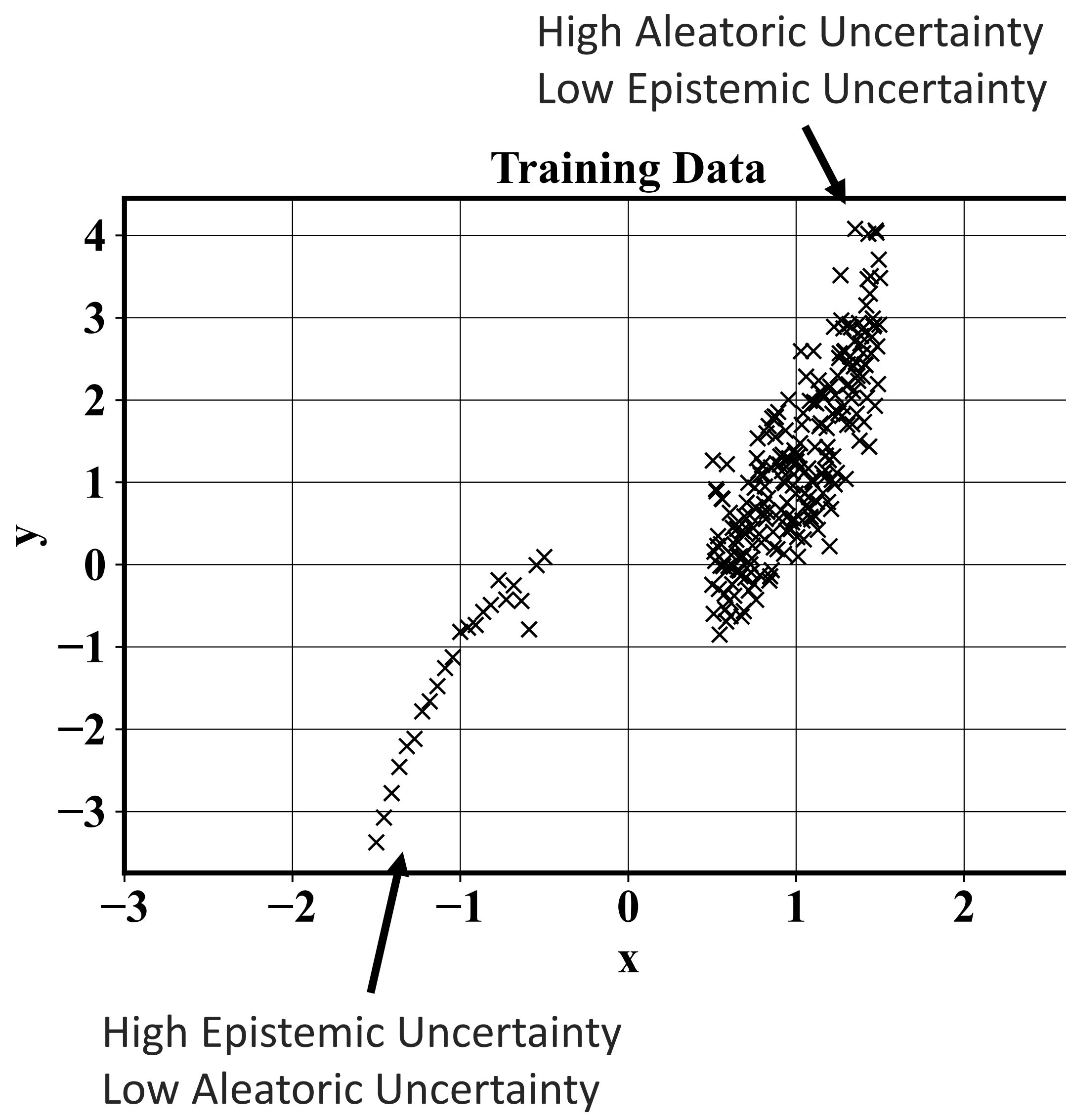
Forms of Uncertainty

Epistemic

- Reducible with additional data
- DNS data availability in phase space
- Extrapolatory uncertainty

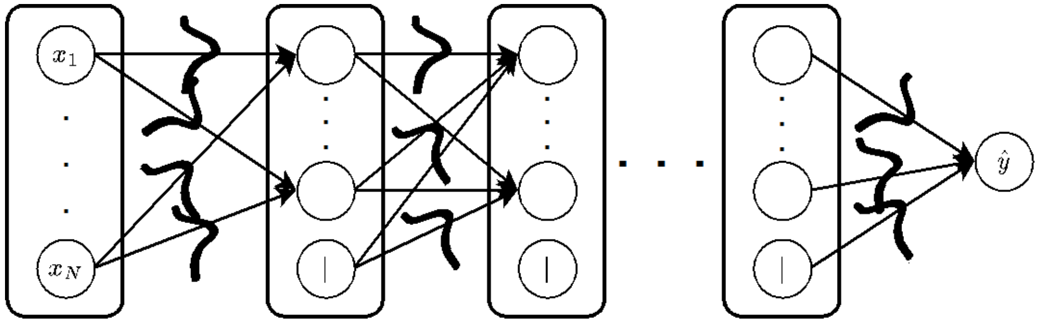
Aleatoric

- Irreducible with additional data
- Model features that we include
- Coarse-graining / filtering

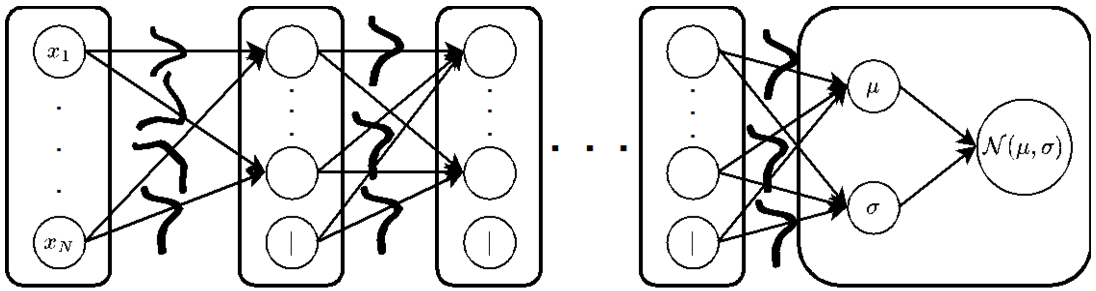


Modeling Uncertainty with BNNs

- Gaussian processes are a natural choice
  - Non-parametric and interpretable
  - Intractable training $\mathcal{O}(n^3)$
  - Expensive prediction $\mathcal{O}(n^2)$
- Bayesian neural networks (BNNs) are an attractive alternative
  - Flexible model form
  - Training amenable to big data regime
  - Quick to evaluate on-line
- BNNs gaining popularity with widespread adoption of variational inference



BNN modeling epistemic uncertainty



BNN modeling epistemic *and* aleatoric uncertainty

What's so Bayesian about BNNs?

- BNN trained with the Evidence LOwer Bound (ELBO)

$$\theta^* = \arg\min_\theta \mathrm{KL}\left[q(w|\theta)||p(w|\mathcal{D})\right]$$
$$= \arg\min_\theta \underbrace{\mathrm{KL}\left[q(w|\theta))||p(w)\right]}_{\text{Prior}} \underbrace{-\mathbb{E}_{q(w|\theta)}\left[\log p(\mathcal{D}|w)\right]}_{\text{Data Misfit}}$$

- How should we specify a prior?
  - Parametric view: *What distribution should weights come from?*
  - Functional view: *What is the functional form of the model?*
- How do we expect this model to extrapolate?

Uncertainty in a Toy Model

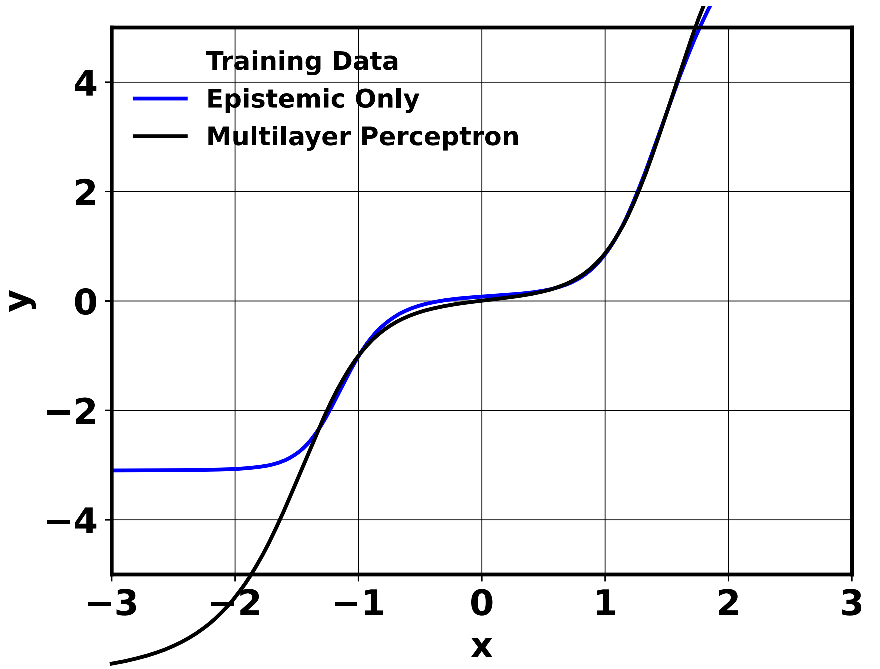
- Underlying data generating function

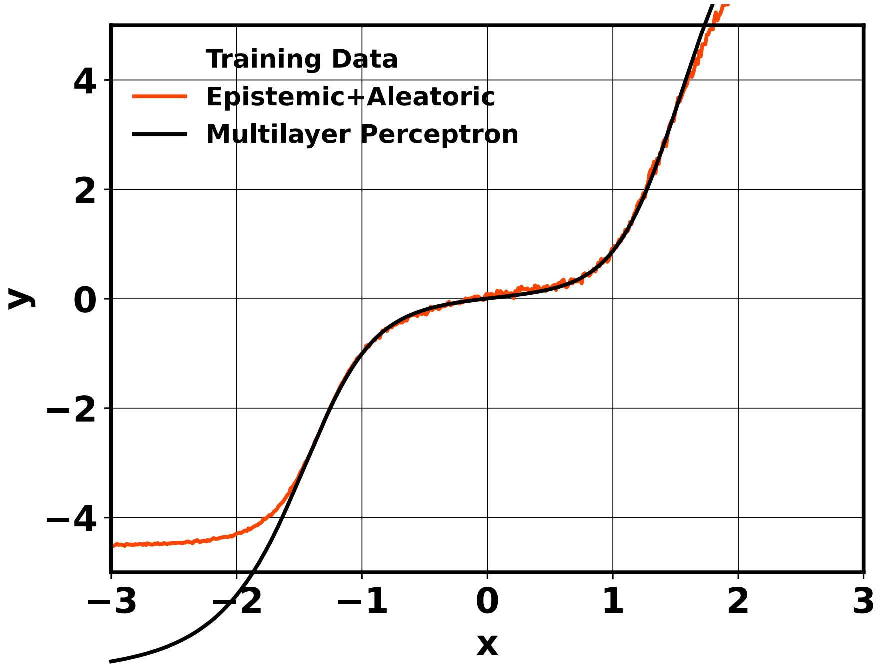
$$f(x) = x^3 + 0.1(1.5 + x)\varepsilon$$

$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

- Epistemic model captures model form better with increasing data
- Epistemic + aleatoric model captures heteroskedastic noise

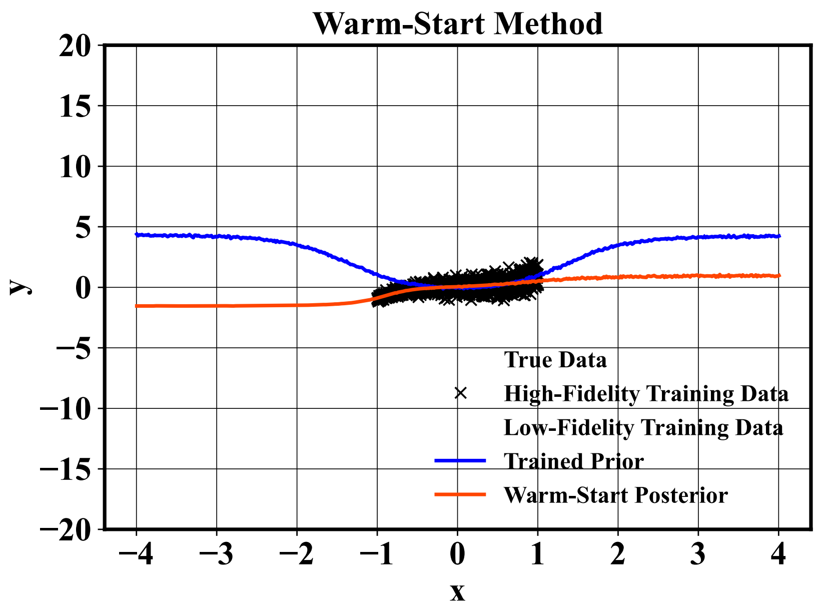
$$\mathrm{Var}(\mathbf{y}) = \underbrace{\mathbb{E}_{q(\mathbf{w}|\theta)}\left[\mathrm{Var}(\mathbf{y}|\mathbf{x}, \mathcal{D})\right]}_{\text{aleatoric}} + \underbrace{\mathrm{Var}\left(\mathbb{E}_{q(\mathbf{w}|\theta)}\left[\mathbf{y}|\mathbf{x}, \mathcal{D}\right]\right)}_{\text{epistemic}}$$

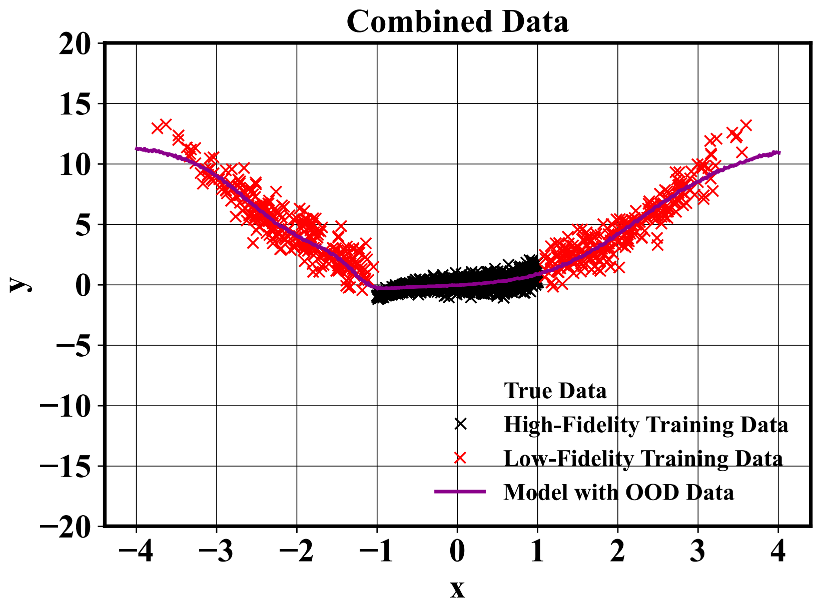




How to Handle Extrapolation?

- Warm-starting exhibits “catastrophic forgetting”
- A “low-fidelity” model can directly prescribe extrapolatory behavior
  - Need to balance separation and quantity to avoid spoiling desired extrapolation from tuned BNN
- Out-of-distribution (OOD) data can be generated





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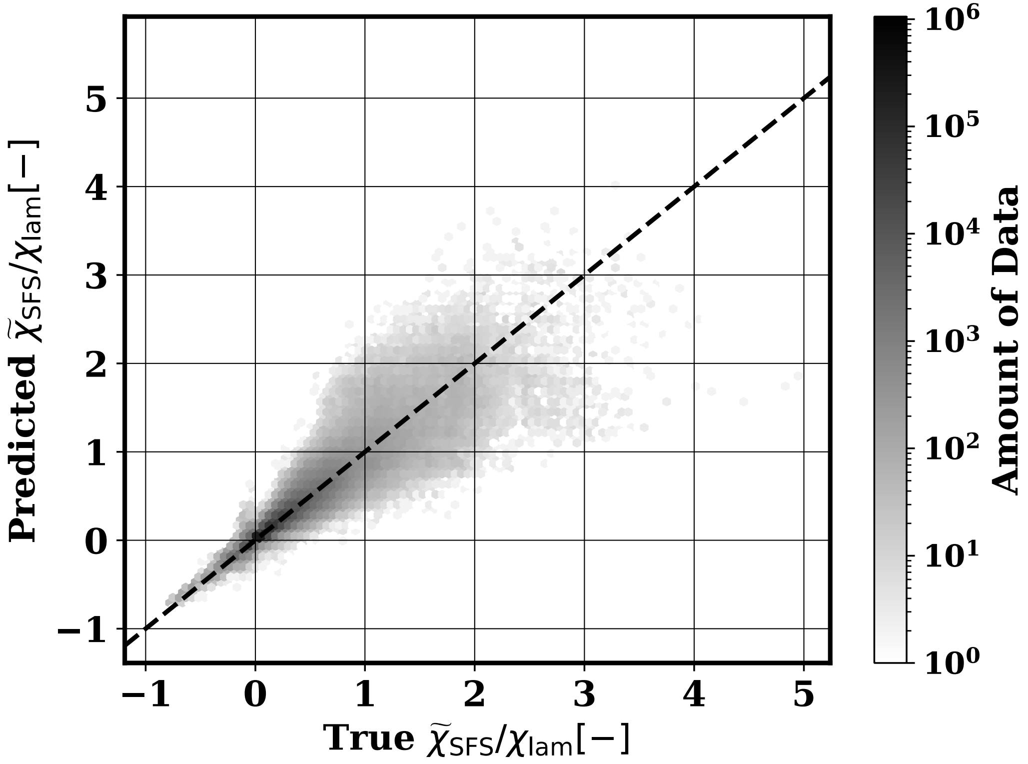
Performance on Test Dataset

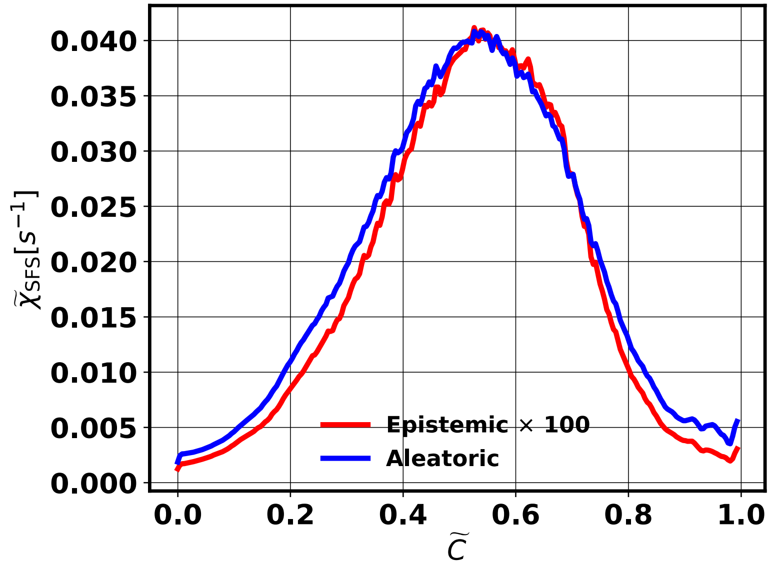
Symbol	Name	Value
n_h	Number of units in hidden layer	20
n_l	Number of hidden layers	4
M	Batch size	2048
η	Learning rate	1e−04
σ	Nonlinear activation function	Sigmoid

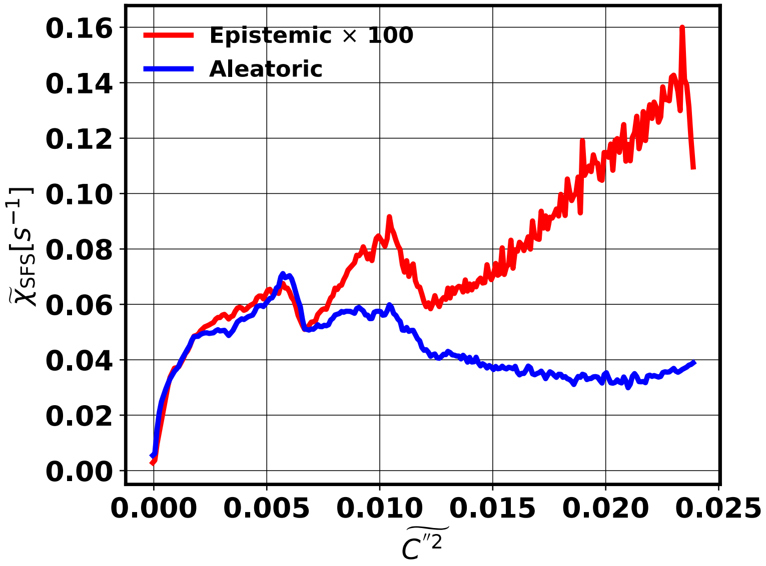
Input Feature	Description
$\widetilde{C}$	Filtered progress variable
$\widetilde{C''^2}$	Filtered progress variable variance
$2\widetilde{D}_C\lvert\nabla\widetilde{C}\rvert^2$	Resolved progress variable dissipation rate
$\widetilde{D}_C$	Filtered progress variable diffusivity
α, β, γ	First, second, and third principal rate of strain
$e_{\alpha,\beta,\gamma} \cdot \nabla\widetilde{C}/\lvert\nabla\widetilde{C}\rvert$	Alignment of local progress variable gradient with principal eigenvectors

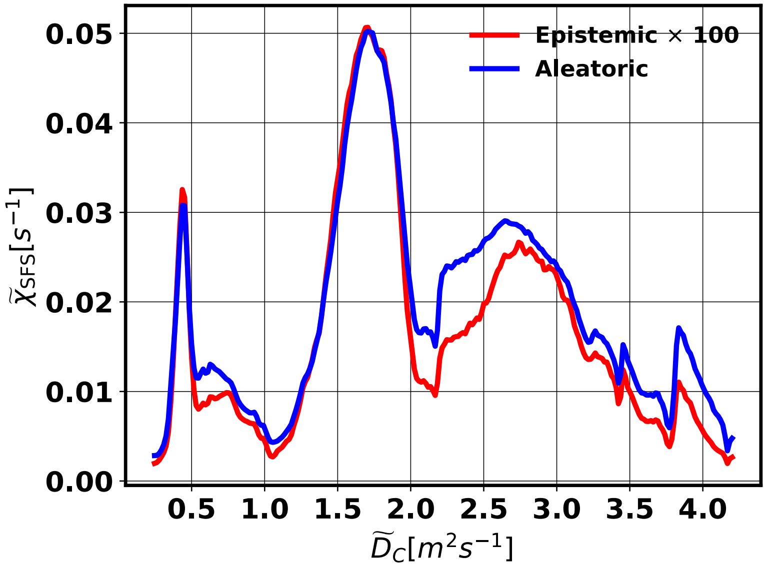


Epistemic Uncertainty

- Regions of high epistemic uncertainty show where additional data should be collected to better inform the closure model
- Aleatoric and epistemic uncertainties are similarly distributed due to uniform in phase space sampling
- Magnitudes differ by a few orders of magnitude

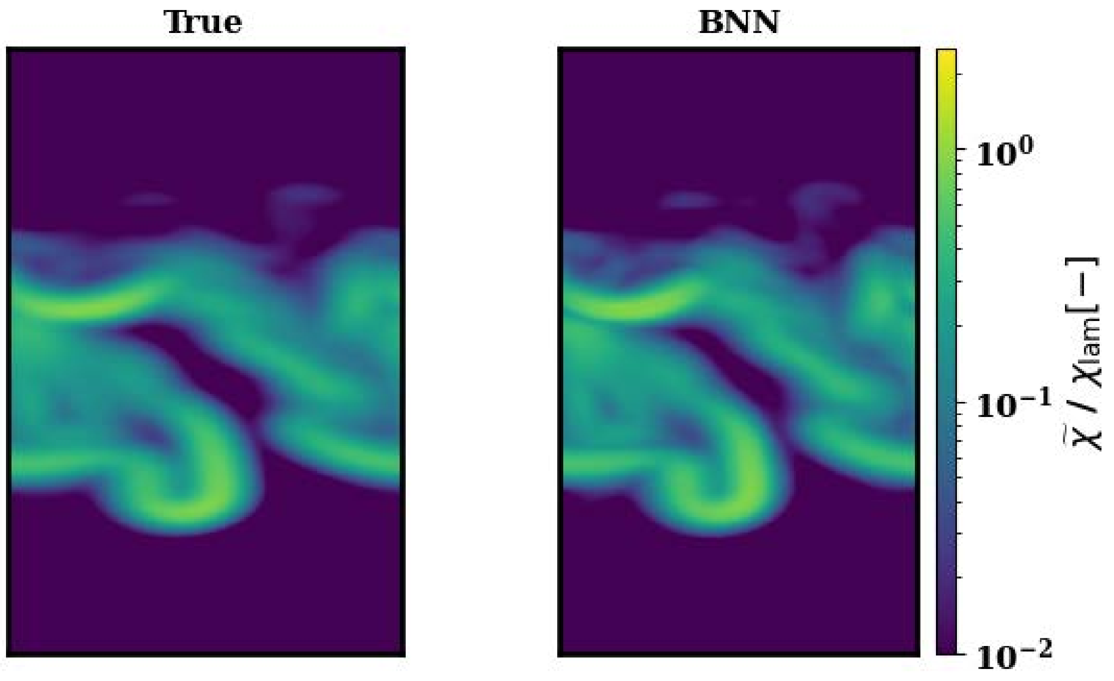




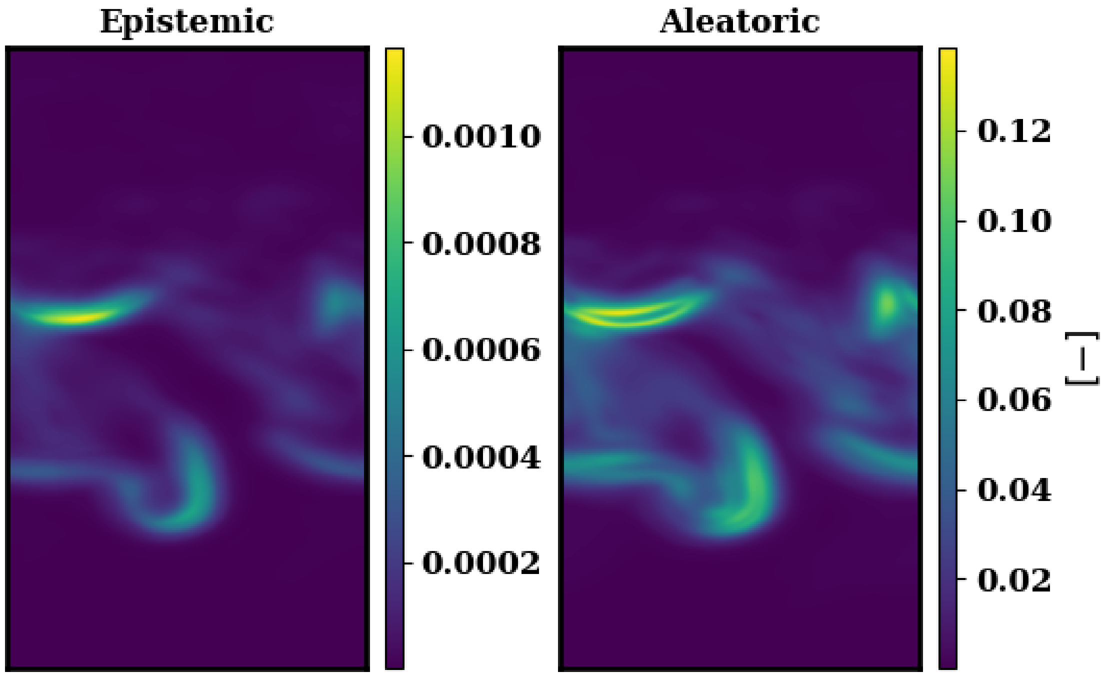


Flame Uncertainty Contours

- Mid-plane slice of a test flame (not included in training dataset)
- BNN mean prediction across different filter widths
- Can be used to predict the pointwise uncertainties



Filter Width: 16



Uncertainties

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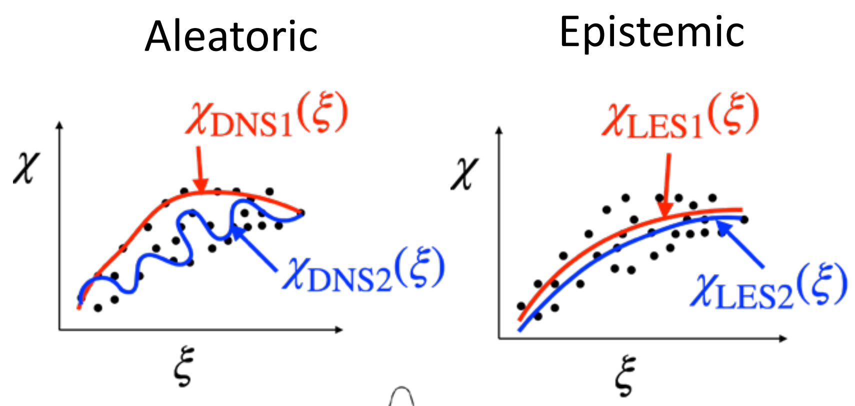
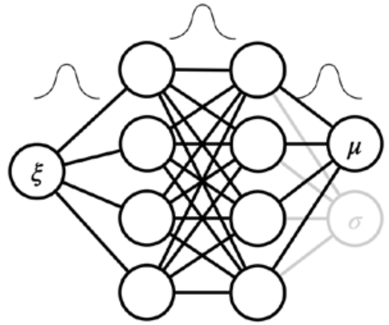
What Uncertainties Should we Propagate?

- Aleatoric uncertainty
  - Captures all possible DNS realizations
  - Unclear how to formulate a model for each realization
- Epistemic Uncertainty
  - Captures all possible LES models given available data
  - Sample the BNN mean
- Monte Carlo sampling
  - Requires many forward evaluations of the LES model
  - Will work in high-dimensions
- Quadrature methods (Stochastic collocation, polynomial chaos, …)
  - Require fewer forward evaluations… if there is a low-dimensional space





Tractability Requires Dimension Reduction

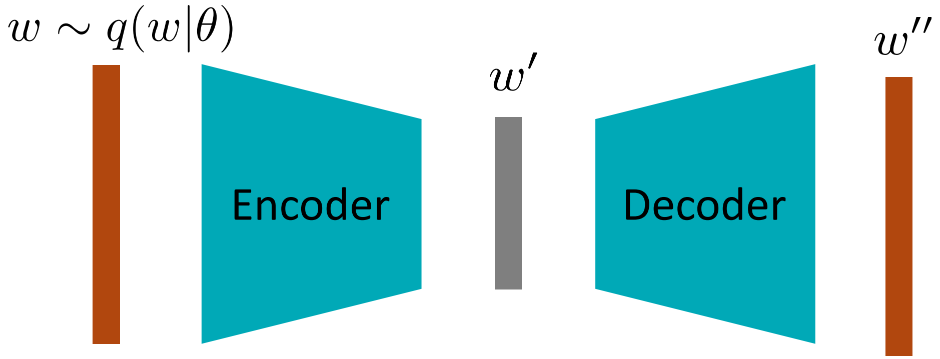
Mixed Variational Layers

Compose variational
and deterministic layers

Noise-to-Signal Ratio (N2S)

Compute ratio and truncate $\dfrac{\sigma_w}{|\mu_w|}$

Goal-Oriented Variational Autoencoder



$$\mathcal{L} = \underbrace{\frac{1}{N_\xi}\sum_{\xi_i}\left(\mathbb{E}_w\left[\chi\right] - \mathbb{E}_{w'}\left[\chi\right]\right)^2}_{\text{First Moment}} + \underbrace{\frac{1}{N_\xi}\sum_{\xi_i}\left(\mathrm{Var}_w\left[\chi\right] - \mathrm{Var}_{w'}\left[\chi\right]\right)^2}_{\text{Second Moment}}$$

Active Subspace Projection

Define objective function: $\mathcal{F}_\xi(w)$

Compute leading singular vectors of:

$$\mathbb{E}_\xi\left[\left(\nabla\mathcal{F}_\xi(w)\right)\left(\nabla\mathcal{F}_\xi(w)\right)^T\right]$$

Represent in the “active directions”

$$\mathcal{G}_\xi(w') \approx \mathcal{F}_\xi(w)$$

$$w' \approx \sum_j^r \alpha_j\phi_j\,, \quad \dim(w') = r \ll \dim(w)$$

Sampling from the Reduced Dimension

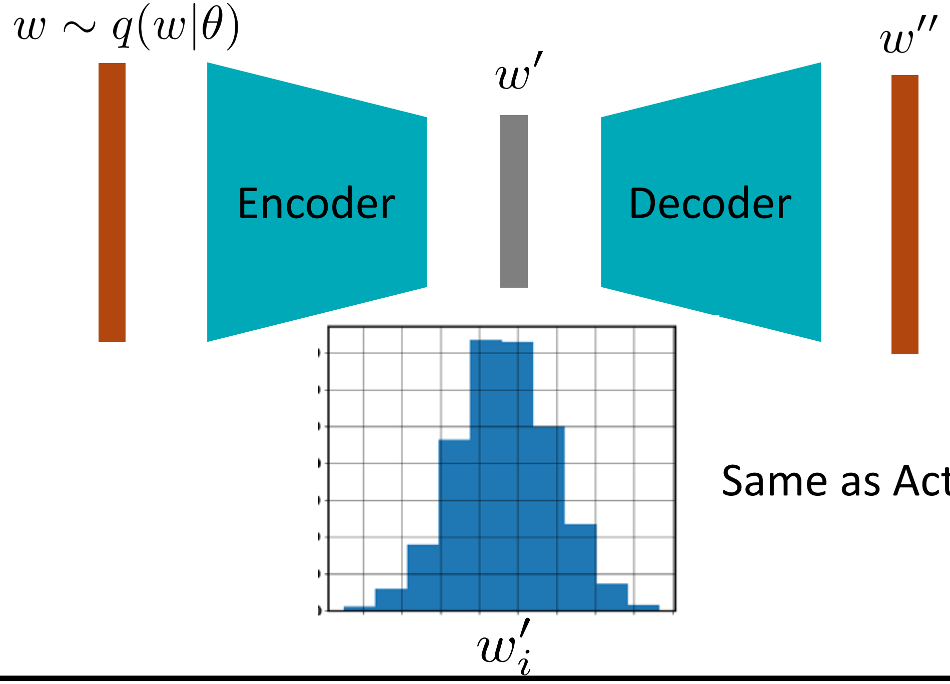
Mixed Variational Layers

Monte Carlo sampling of $q(w|\theta)$

Noise-to-Signal Ratio (N2S)

Monte Carlo sampling of $q(w'|\theta)$

Goal-Oriented Variational Autoencoder



Same as Active Subspace

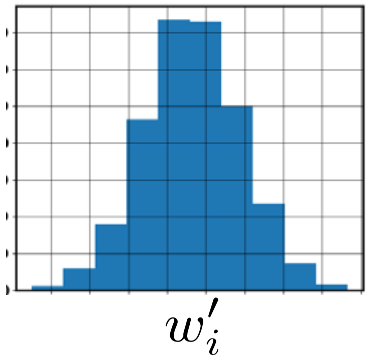
Active Subspace Projection

Monte Carlo sampling of $q(w|\theta)$

Projection onto active subspace

Fit distribution to active subspace representation of w'

Sample the active subspace

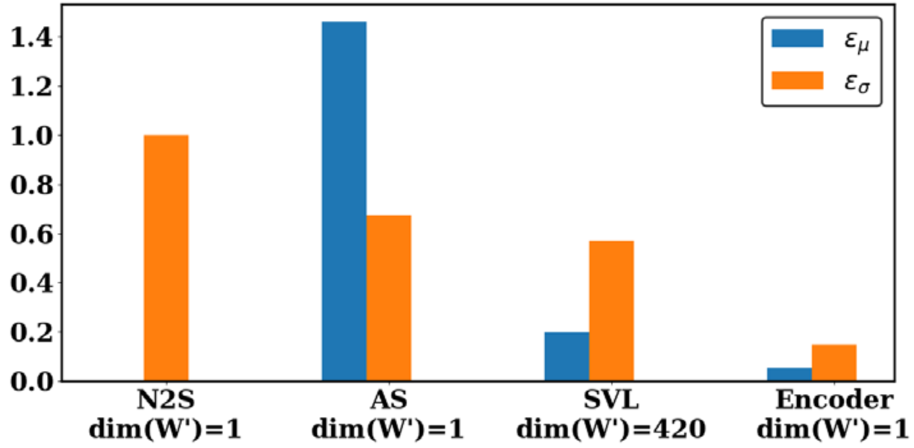


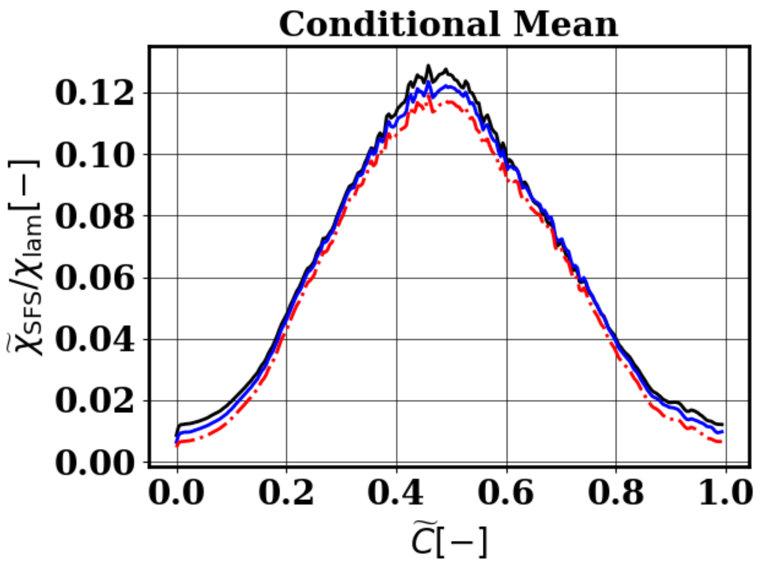
Preliminary Results

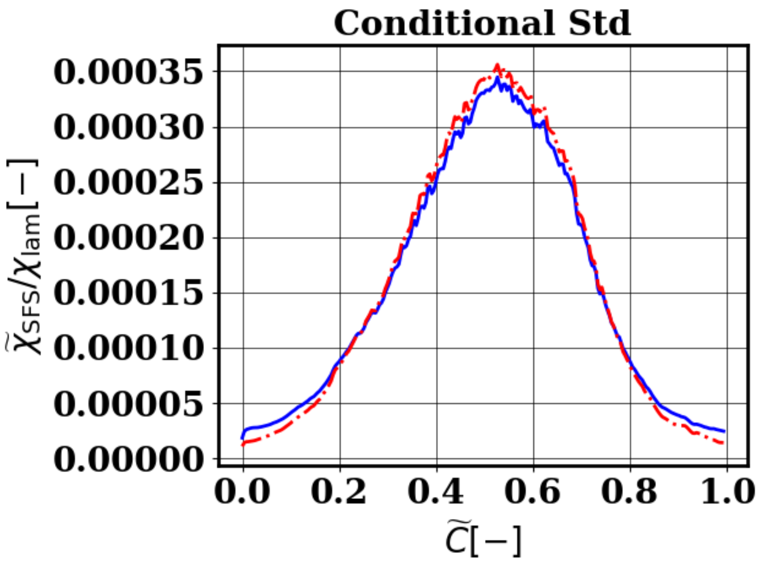
Use Relative error to compare reduced representations

$$\varepsilon_\mu = \frac{\|\mathbb{E}_w(\chi_\mu) - \mathbb{E}_{w'}(\chi_\mu)\|_2}{\|\mathbb{E}_w(\chi_\mu)\|_2}$$

$$\varepsilon_\sigma = \frac{\|\operatorname{Var}_w(\chi_\mu) - \operatorname{Var}_{w'}(\chi_\mu)\|_2}{\|\operatorname{Var}_w(\chi_\mu)\|_2}$$







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Conclusions and Future Work

- BNNs are a promising method to systematically model multiple forms of uncertainties arising in closure term modeling
- Low-fidelity data can be used to supplement high-fidelity training data to yield reasonable extrapolation uncertainty estimates
- Uncertainty propagation readily performed via Monte Carlo
  - More efficient representations are possible
- Future work / coming soon: propagation through LES codes
- Code availability: `github.com/nrel/mluq-prop`

[1] Graham Pash, Malik Hassanaly, Shashank Yellapantula. "*A Priori* Uncertainty Quantification of Reacting Turbulence Closure Models using Bayesian Neural Networks." 2024. Preprint. arxiv.org/abs/2402.18729

Thanks!

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