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Qualifying Training Datasets for Data-Driven Turbulence Closures

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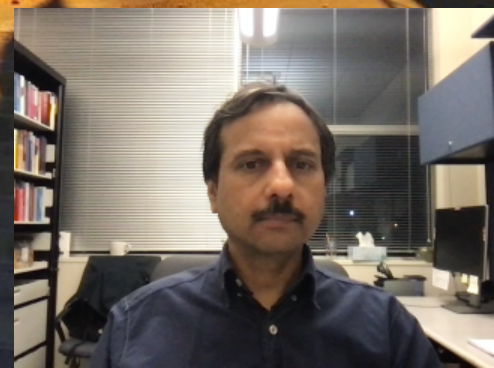

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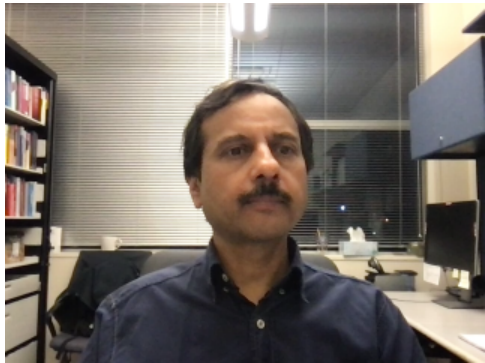
Introduction

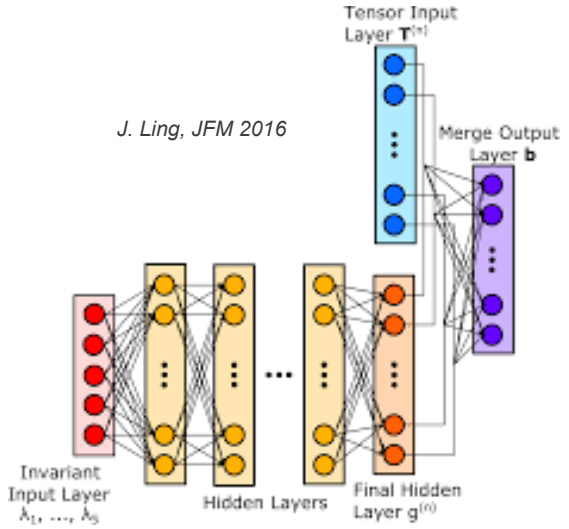
- Aim: Devise a way to qualify training datasets (TD) used for machine-learned (ML) turbulence closures
  - Also, a method to qualify the ML closure trained on the TD
- Datasets & ML models
  - Training data: DNS datasets – 5 channel flows, channel w/ wavy wall, flow around square cylinder
  - Test data: Impinging jet
  - Model: Tensor-basis neural net (TBNN) RANS closure
- Why does this matter? ML closures very inaccurate when extrapolating
  - Need to qualify it – identify when it can & cannot be used
    - Easier to qualify the TD data instead, and then explain the neural network

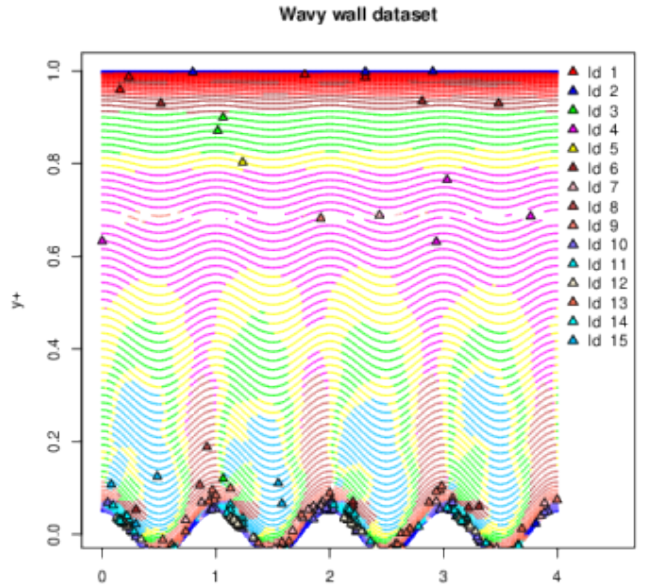
Takeaway: Need a way to assess quality of a ML closure and bound its use



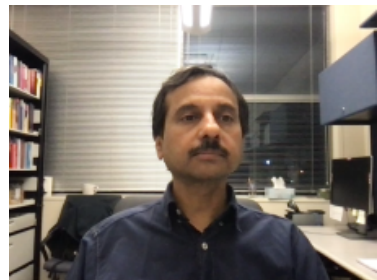
Background

- ML turbulence closures for RANS
  - Predict Reynolds stress or anisotropy, given features / local flow state
  - Random forests & various neural net architectures
- Characterizing training datasets (DOI:10.2514/1.J060919)
  - Physically meaningful partitions: Greedy algorithm to assemble a feature-space for Gaussian Mixture Model clustering of TD
    - Accommodates correlated features from an over-complete dictionary
  - Summarization of TD: Prototype placement, summarizing the TD
    - Supervised learning, with cluster IDs serving as labels
    - Illustrate distribution of TD in feature-space



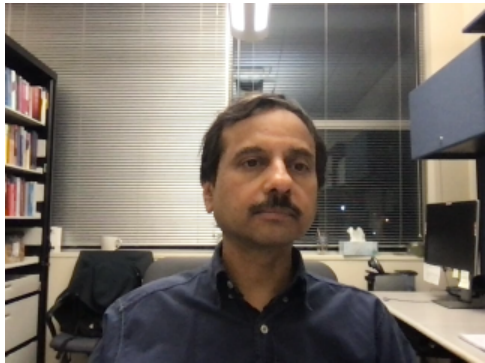


Takeaway: Unsupervised partitioning of TD into homogeneous clusters of turbulent processes

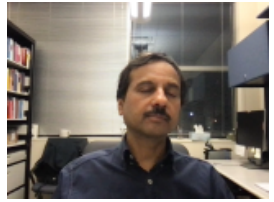


Outstanding questions

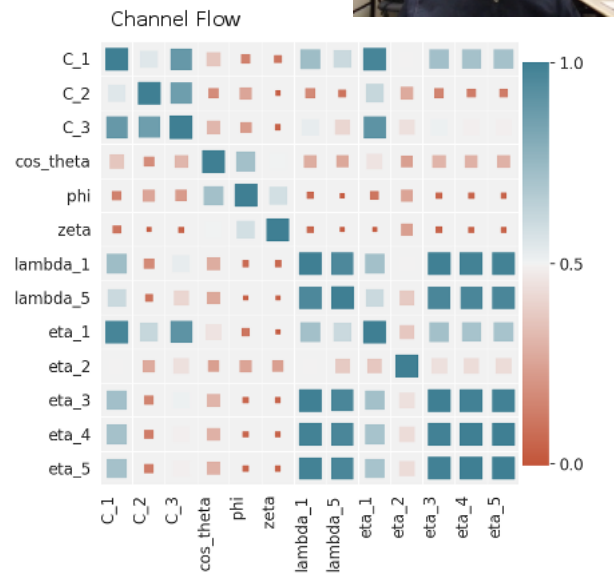
- Qualifying a TD: There exists a feature-space where clustering delivers physically-meaningful clusters
  - Is this feature-space unique?
  - Is it dependent on Gaussian Mixture Model clusters?
  - Can the clusters be used to create a one-class classifier?
    - Can the classifier be used to detect processes (in a ”test” dataset) not in the TD?
- Qualifying a ML closure: Does the closure adhere to turbulence theory?
  - Imbalance in TD will cause ML closure to be biased. Can we detect it from theory?
  - Insufficient TD will lead to a poorly trained NN. Can theory help with detection?

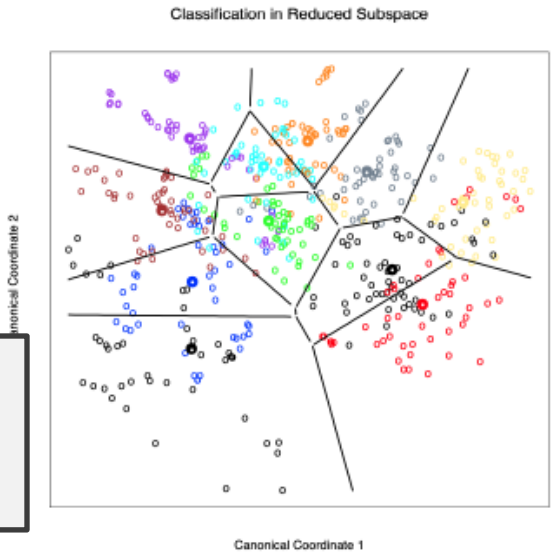


Finding # 1 – Feature-space not unique



- Alternative feature space:
  - Correlation analysis of features' dictionary yields new feature-space
    - Note: Still need a turbulence-informed dictionary of features
  - Classifiers in alternative feature-space are equally predictive of class labels
  - Mapping from class labels to features is rather simple
    - LDA and Random Forest classifiers have similar classification performance
- Alternative clustering methods: In alternative feature-space
  - Spectral clustering in alternative feature-space yields new clusters
    - But they overlap with original clusters 78% - 98% - so not really different

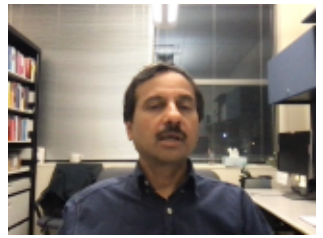




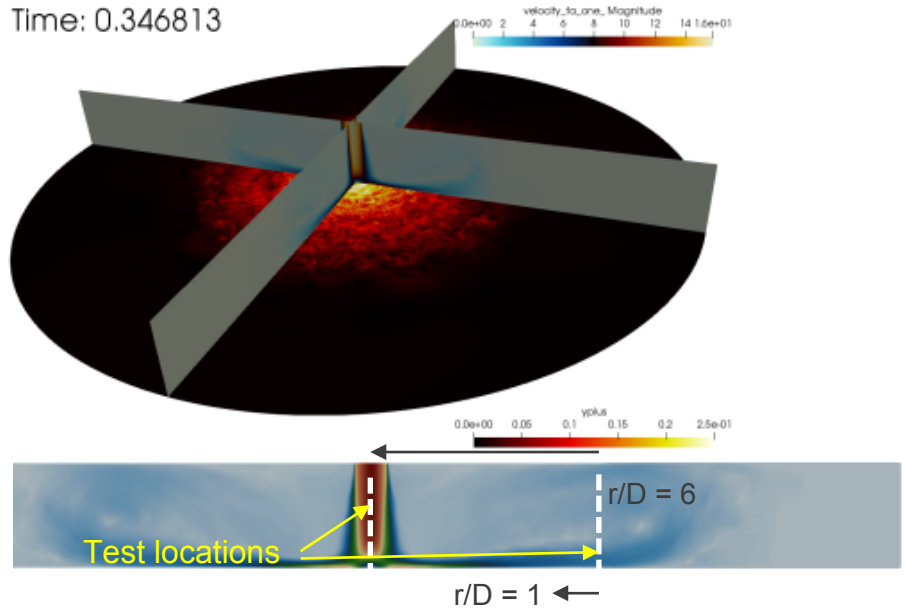
Takeaways:

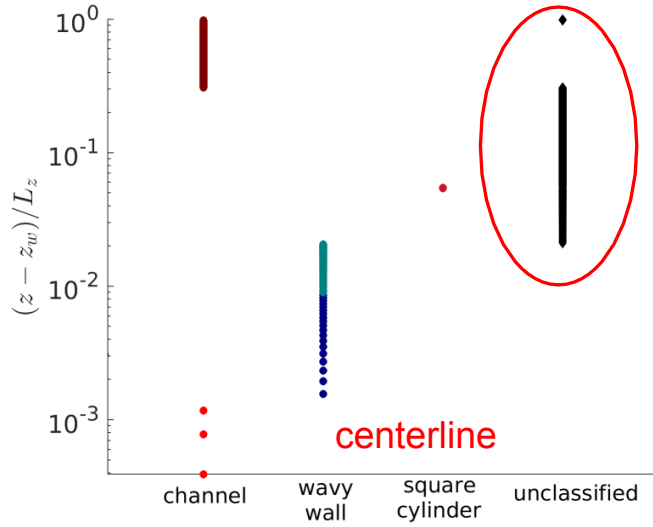
- Feature-space for clustering is not unique
- Clusters are independent of clustering method and feature-space

Finding # 2 – TD qualified with 1-class classifier



- Rationale: Clustering identifies partitions with homogeneous turbulent processes in TD
  - Implication: Given a “test” dataset, intersect with TD and find processes absent from it
    - Qualifies the TD!
- Procedure: Make a 1-class classifier to recognize known turbulent processes /clusters
  - Soft Independent Modeling of Class Analogs (SIMCA) & test
  - Test dataset: Impinging jet
- Outcome: Reliably finds processes absent in TD
  - Manually verified



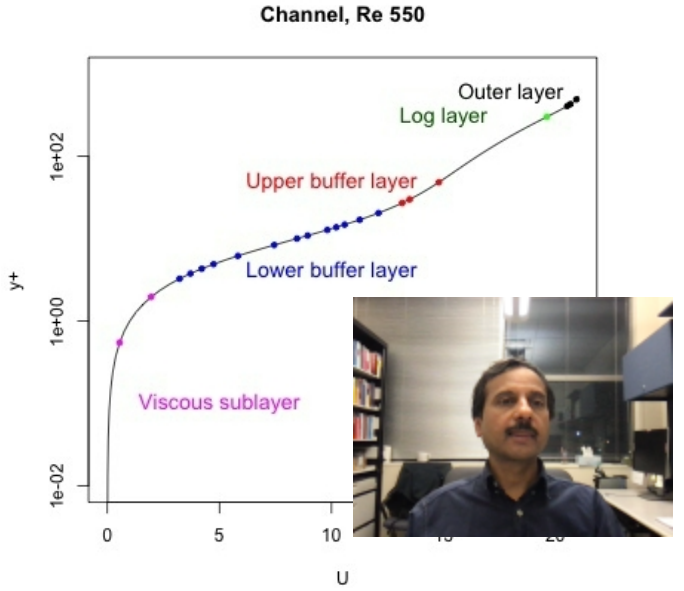


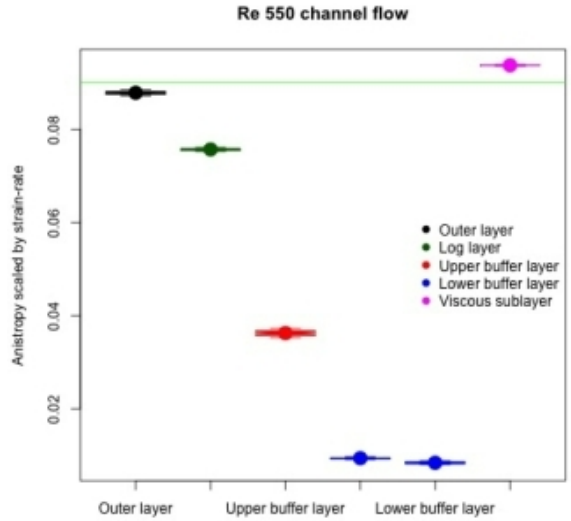
Takeaway: Physically meaningful clusters + 1-class classifier = Qualifiable Training Dataset

Finding # 3 – LIME explanations of ML closures

- A TBNN closure should resemble a linear eddy viscosity model
  - At least when trained on channel flow training data
- Use LIME to find the functional form of TBNN closure
  - At prototypes chosen from a turbulent boundary layer (TBL)
- Use TBNN evaluations near a prototype to fit a Generalized Linear Mixed-effects Model
  - Reveals the functional dependence on TBNN inputs
- Findings with 2 separate TDs:
  - TBL regions well represented in the TD resemble a LEVM
  - For insufficient TD, TBNN functional form is non-physical

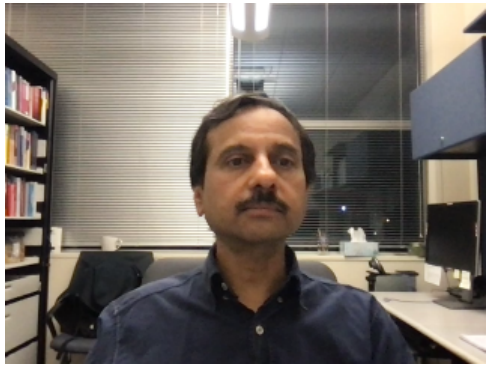
Takeaway: LIME can expose the functional form of a black-box closure for comparison with closed-form expressions





Summary

- A training dataset can be clustered into partitions with homogeneous turbulent process
  - The feature-space can be assembled from a theory-informed dictionary
  - The feature-space is not unique
  - Cluster IDs can become class labels
- A labeled TD can be used to identify absent processes and thus qualify it
  - and any model trained with it
  - Requires one to make a 1-class classifier (SIMCA, 1-class SVMs etc.)
- A black-box neural net closure can reduced to its functional form via LIME
  - Best done at prototypes taken from its TD
  - Allows comparison with closed-form expressions & identification of model shortcomings
- More info:
  - M. Barone et al, "Feature Selection, Clustering, and Prototype Placement for Turbulence Data Sets", *AIAA Journal,* 2022. DOI:10.2514/1.J060919
  - T. Banerjee et al, “Qualifying Training Datasets for Data-Driven Turbulence Closures”, *AIAA Aviation* 2022.



Acknowledgement

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