Machine Learning Approaches in Computational Fluid Mechanics

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Motivation

- Current turbulence models perform poorly in separated flows.
- Machine learning provides potential framework for improvement.
- Predicting anisotropy tensor in barycentric coordinates can help enforce realizability in data-driven turbulence modeling.
- What mean flow features are most useful in predicting anisotropy tensor?

Turbulence Anisotropy

- Non-dimensional anisotropy tensor, b_{ij},

$$b_{ij} = \frac{\tau_{ij}}{2k} - \frac{1}{3}\delta_{ij}$$

- Use eigendecomposition to represent in barycentric coordinates,

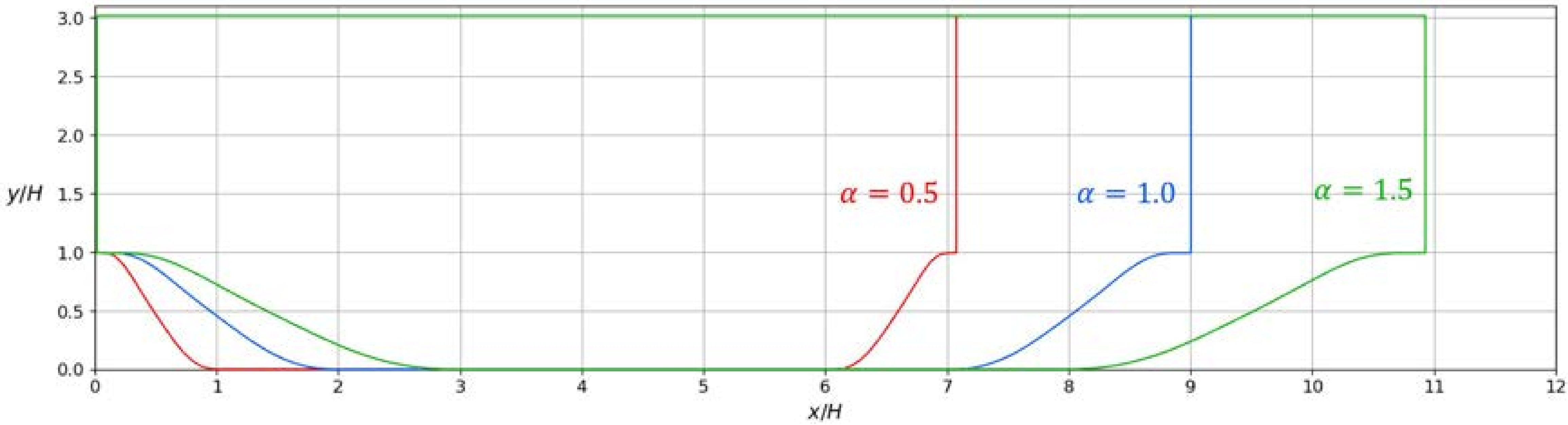
$$C_1 = \lambda_1 - \lambda_2, \qquad C_2 = 2(\lambda_2 - \lambda_3), \qquad C_3 = 3\lambda_3 + 1$$

$$\lambda_1 \geq \lambda_2 \geq \lambda_3, \qquad C_1 + C_2 + C_3 = 1, \qquad 0 \leq C_i \leq 1$$

- Corners represent limiting states of turbulence; barycentric coordinates represent strength of component:
  - Corner 1, $C_1 \rightarrow$ One-component
  - Corner 2, $C_2 \rightarrow$ Two-component, axisymmetric
  - Corner 3, $C_3 \rightarrow$ Isotropic

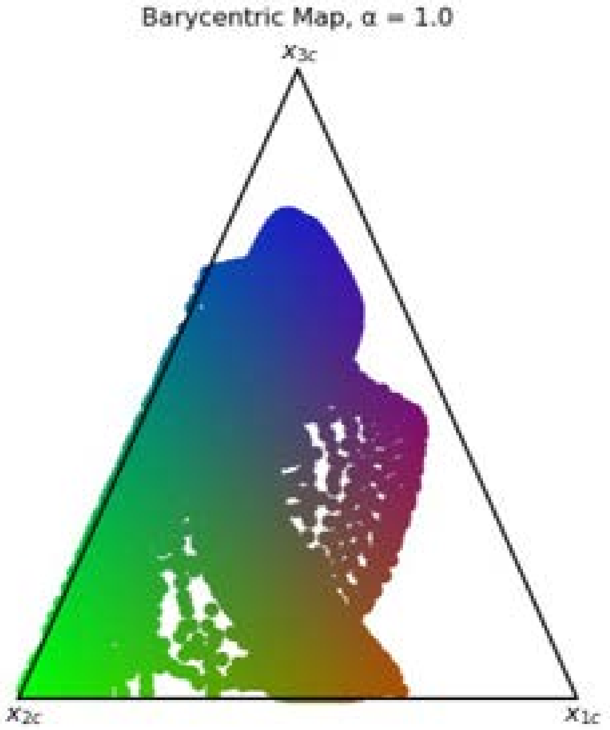
Periodic Hills Dataset

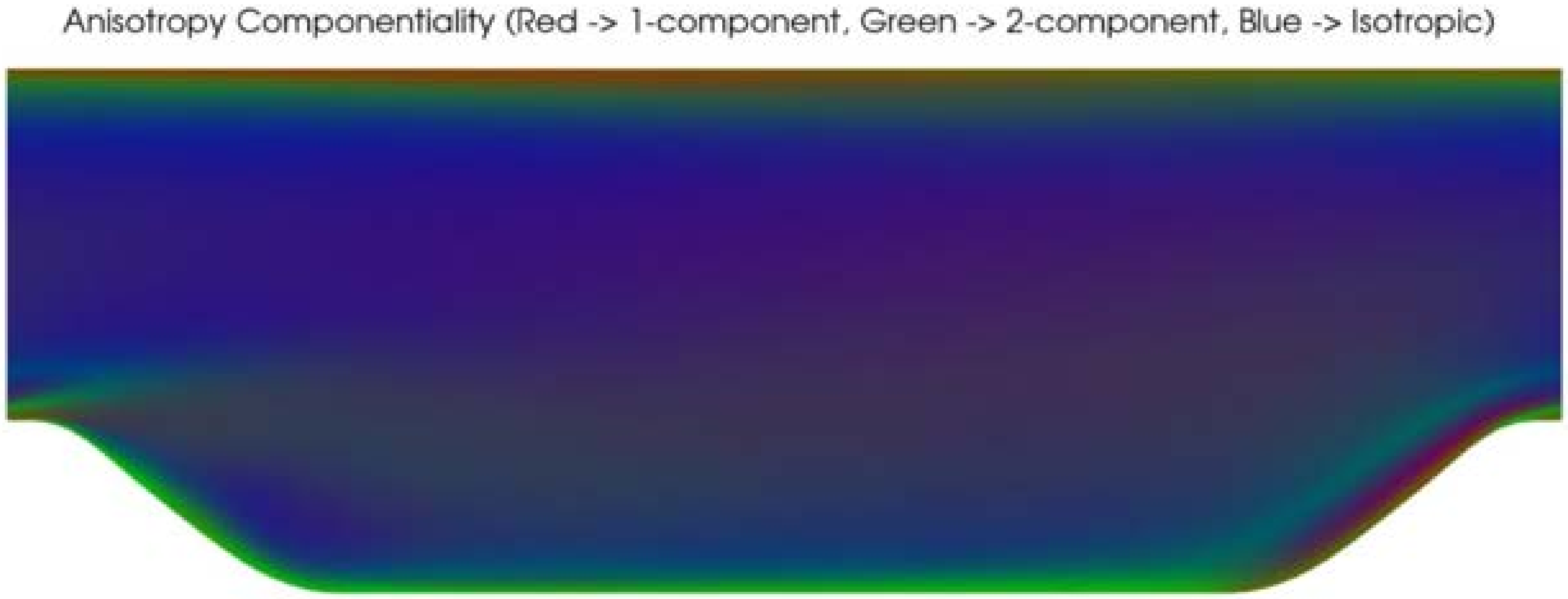
- DNS dataset generated by (Xiao et al. 2020). OpenFOAM case files provided. 29 combinations of hill width, domain height, and streamwise length.
- Flow ranges from attached to massively separated by left hill depending on hill slope parameter, α.
- Three cases used: baseline hill height and domain height, $\alpha = 0.5,\ 1.0,\ 1.5$.



Turbulence Componentiality

- Barycentric coordinates can be treated as pixel values. Used to create contour maps of anisotropy.
- Anisotropy componentiality of case, $\alpha = 1.0$.





Mean Flow Variables Considered

Raw Variable	Normalization Factor	Interpretation
$S_{kk}^2 = S_{ij}S_{ji}$	$\|\|\nabla\mathbf{U}\|\|^2$	Strain rate as fraction of total deformation rate.
$\mathrm{W}_{kk}^2 = W_{ij}W_{ji}$	$\|\|\nabla\mathbf{U}\|\|^2$	Rotation rate as fraction of total deformation rate.
$Q_{criterion} = \left(\|\|\boldsymbol{W}\|\|^2 - \|\|\boldsymbol{S}\|\|^2\right)/2$	$\|\|\nabla\mathbf{U}\|\|^2/2$	Excess vorticity as fraction of total deformation rate.
$\|\|\nabla \times \boldsymbol{U}\|\| = \sqrt{2W_{ij}W_{ij}}$	$\sqrt{2} * \|\|\nabla\mathbf{U}\|\|$	Ratio of vorticity magnitude to total deformation rate.
$u_j\left(\partial p/\partial x_j\right)$	$\|\|\boldsymbol{U}\|\| \cdot \|\|\nabla p\|\|$	Orthogonality of velocity and pressure gradient.
$u_j\left(\partial u/\partial x_j\right)$	$\|\|\boldsymbol{U}\|\| \cdot \|\|\nabla u\|\|$	Orthogonality of velocity and x-velocity gradient.
$u_j\left(\partial v/\partial x_j\right)$	$\|\|\boldsymbol{U}\|\| \cdot \|\|\nabla v\|\|$	Orthogonality of velocity and y-velocity gradient.
$Re_D = \sqrt{k}d/\nu$	N/A	Wall distance Reynolds number.

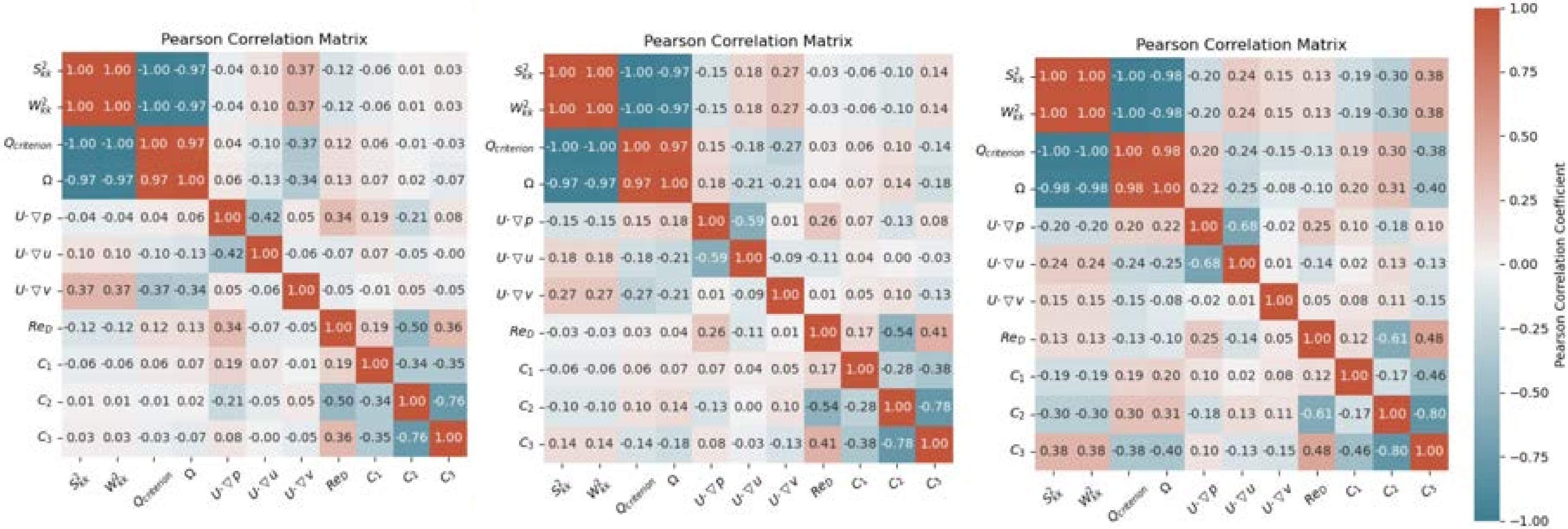
- All variables are normalized to range [-1,1]

Feature Importance

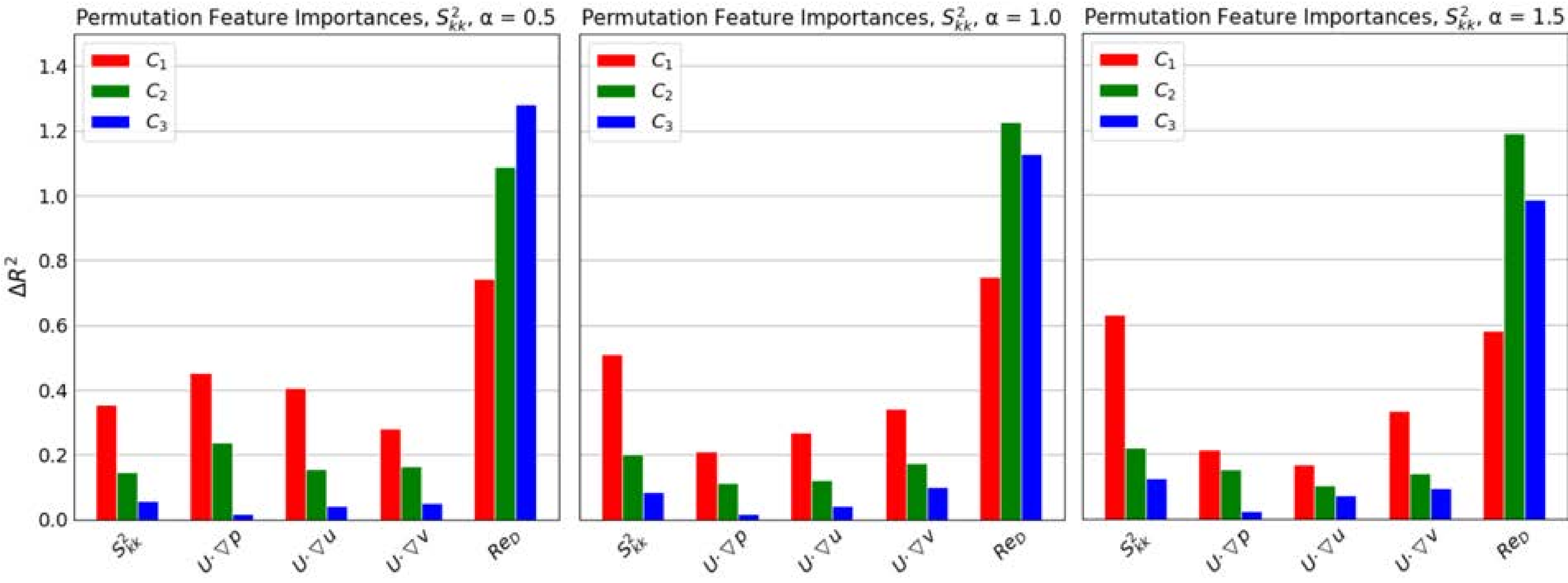
- Can be investigated using random forest model. Implemented in SciKit-Learn:
  - Max Depth: 10
  - Number of Estimators: 100
  - Random State: 0
  - 80/20 training/validation data split
  - Random seed: 12345 for training/validation split
- Permutation Importance…Calculated by permuting features in the validation set one by one and measuring reduction in accuracy.
  - Biased against highly correlated features.
- Check feature correlation using Pearson correlation coefficient.
  - Tests for linear relationship between variables.

Correlation Matrices

- S^2_{kk}, W^2_{kk}, $Q_{criterion}$, and Ω are highly correlated. Use only one from each group.



Permutation Feature Importances



Conclusions and Future Plans

- Re_D is most informative feature, especially for C_2 and C_3.
- C_1 shows significant dependence on all selected features. Dependence on S_{kk}^2 increases with α.
- Results can help inform selection of input features and approach to selecting from larger feature sets.
- In progress and future plans:
    - Developing new invariant map for use in ML turbulence modeling.
    - Designing modified tensor basis neural network architecture to ensure output realizability.
    - Implement proof of concept model using DNS and LES datasets.