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Efficient Sampling Methods for Machine Learning Error Models with application to Surrogates of Steady Hypersonic Flows

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Goal: Develop Error Models of Surrogates Faster

QOI Error

$$\boxed{\delta_s(\mu) \coloneqq s(\boldsymbol{\mu}) - \tilde{s}(\boldsymbol{\mu})}$$

$$\delta_s(\mu) \coloneqq s(\mu) - \tilde{s}(\mu)$$

Reducing Sampling Size

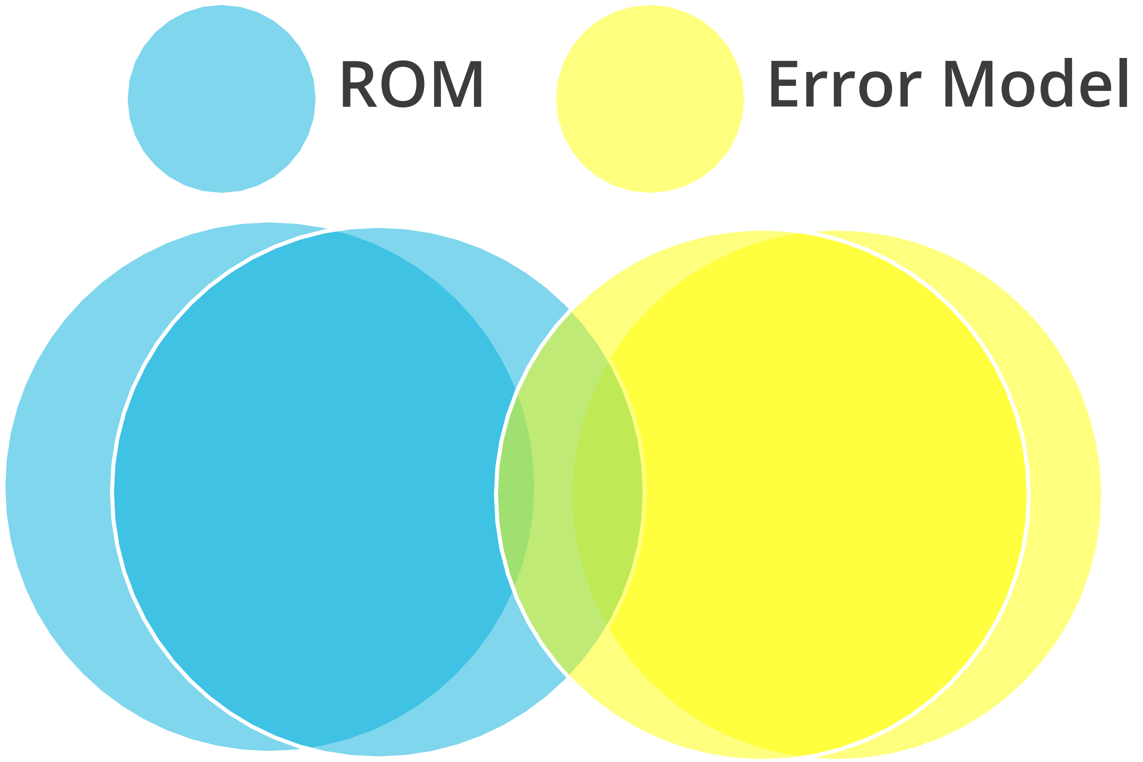
- Problem: FOM is computationally expensive
  - Necessary FOM training points for ROM and error model
- Solution:
  1. Sampling types
  2. Sampling strategies

Sampling Types

1. Latin Hypercube Sampling (LHS)
2. LHS with maximin criterion
   - Adds constraint on distance between sampling points
3. D-Optimal design
   - Maximizes determinant of information matrix
     - Reduces variance in results
   - Contains replicates not useful for computational experiments
     - Replace replicates with random LHS points
     - End result may not be a true D-Optimal design

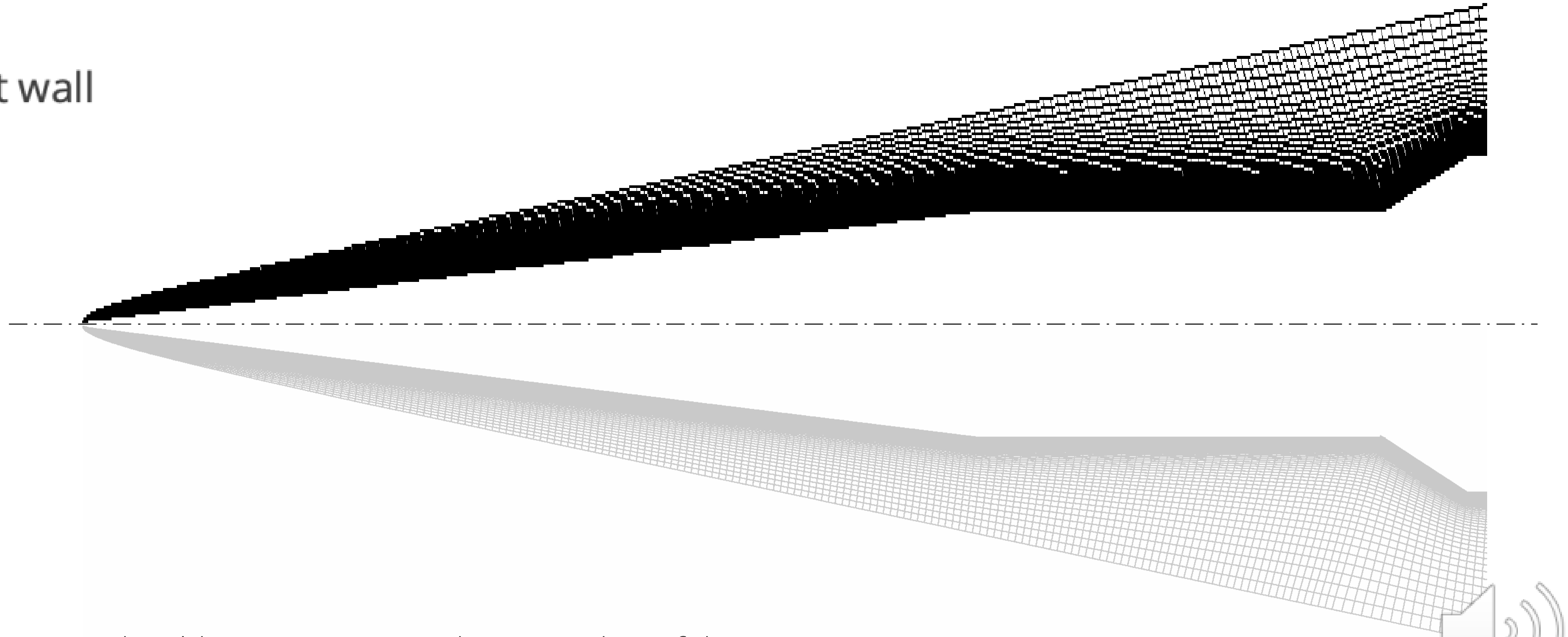
Sampling Strategies

- Distinct training set
- Augmented training set
- Single training set



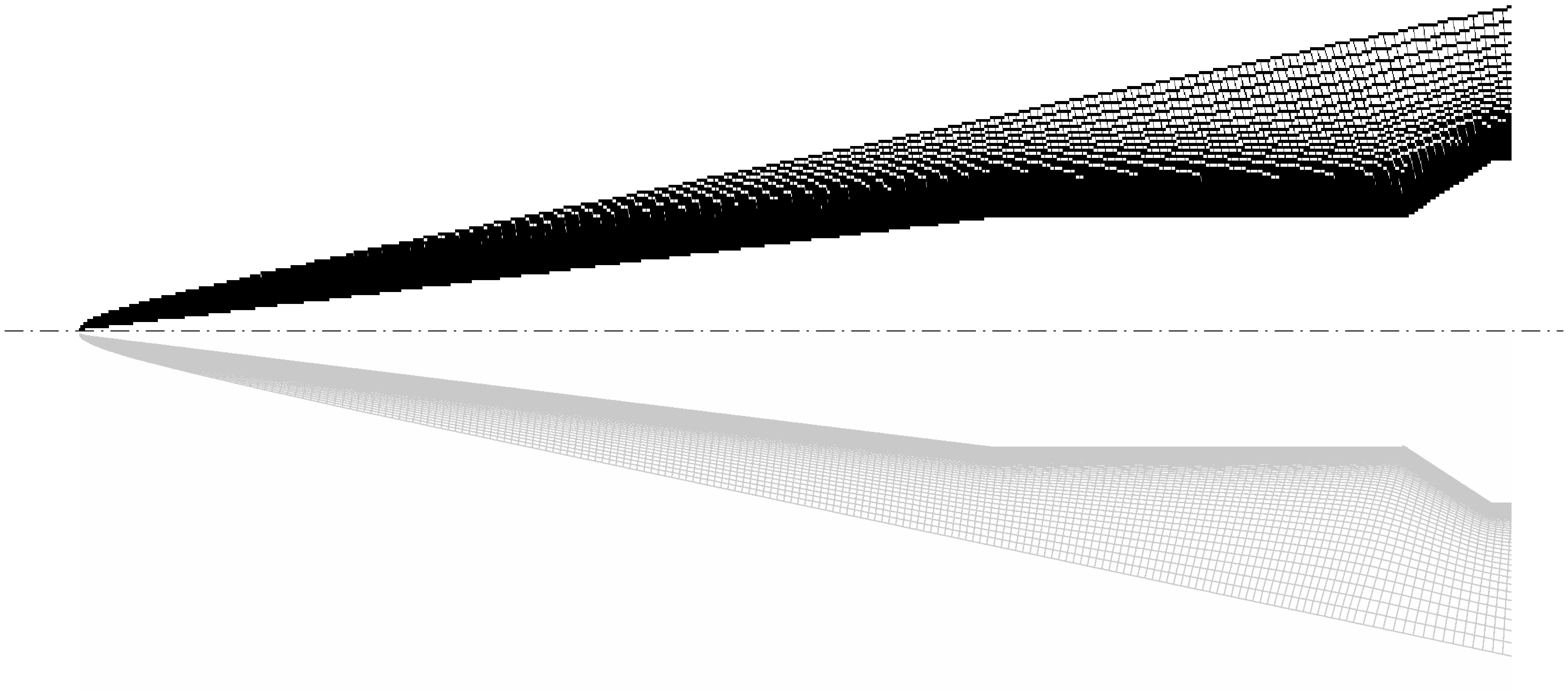
HIFiRE-1

- Run 30 of CALSPAN University of Buffalo HIFiRE-1 wind tunnel tests [1]
- $N = 32{,}768$ cells
- Boundary conditions:
  - Supersonic inlet
  - Supersonic outlet
  - No-slip enforced at wall
  - Fixed temperature



[1] Wadhams, T. P., Mundy, E., MacLean, M. G., and Holden, M. S., "Ground Test Studies of the HIFiRE-1 Transition Experiment Part 1: Experimental Results," *Journal of Spacecraft and Rockets*, Vol. 45, No. 6, 2008, pp. 1134–1148. https://doi.org/10.2514/1.38338.

Modeling HIFiRE-1



Full-Order Model → Reduced-Order Model → Error Model

Modeling HIFiRE-1

Full-Order Model → Reduced-Order Model → Error Model

Full-Order Model

- Compressible RANS Equations
- Turbulence modeled using SA
- CFD Solver: SPARC
  - Developed for transonic and hypersonic flows

Reduced-Order Model

- Reduced-order model developed using POD with LSPG
- ROM solver: Pressio*
  - Open source framework for ROMs
  - Solves large-scale nonlinear dynamical systems
  - Uses generic programming

Error Model

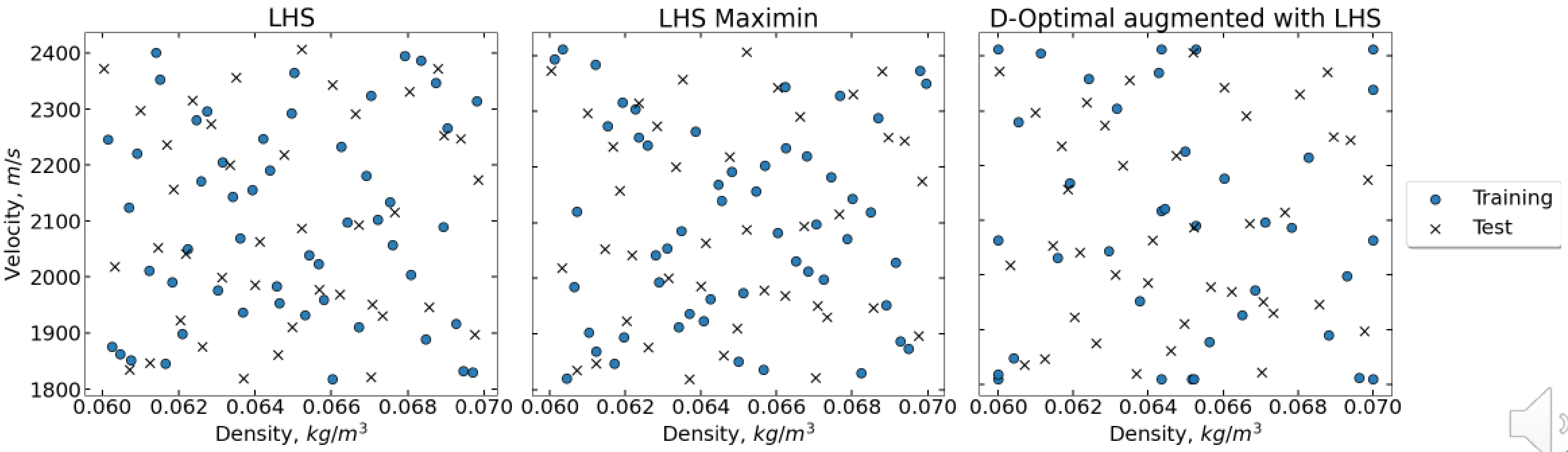
- Predict quantity of interest error
  $\delta_s(\mu) \coloneqq s(\boldsymbol{\mu}) - \tilde{s}(\boldsymbol{\mu})$
- Seven regression models
  - MLP, SVR with RBF, SVR with linear kernel, k-NN, linear OLS, quadratic OLS, RF

*https://github.com/Pressio

Distinct Training Sets

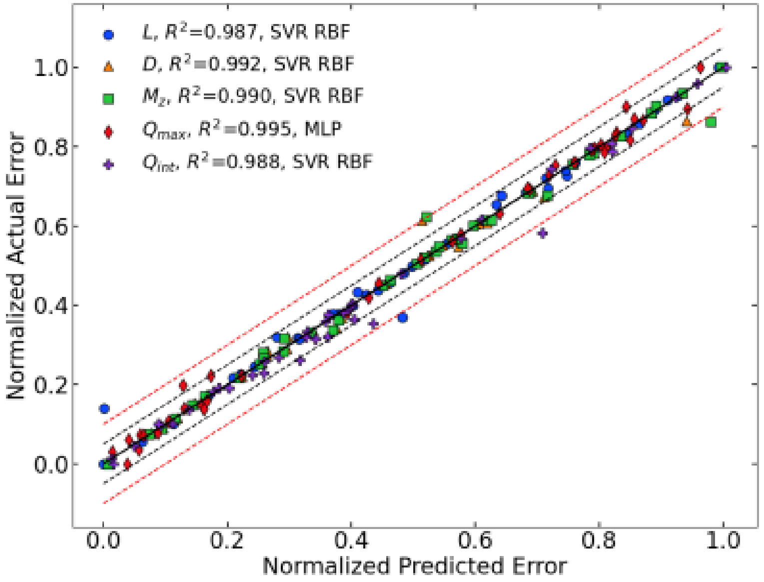
- Reduced-order model trained with 50 points
- Error model trained with 3 sampling types
  - Number of points determined by achieving statistical power of 80%

Sampling Type	
LHS	52
LHS Maximin	53
D-Optimal	37

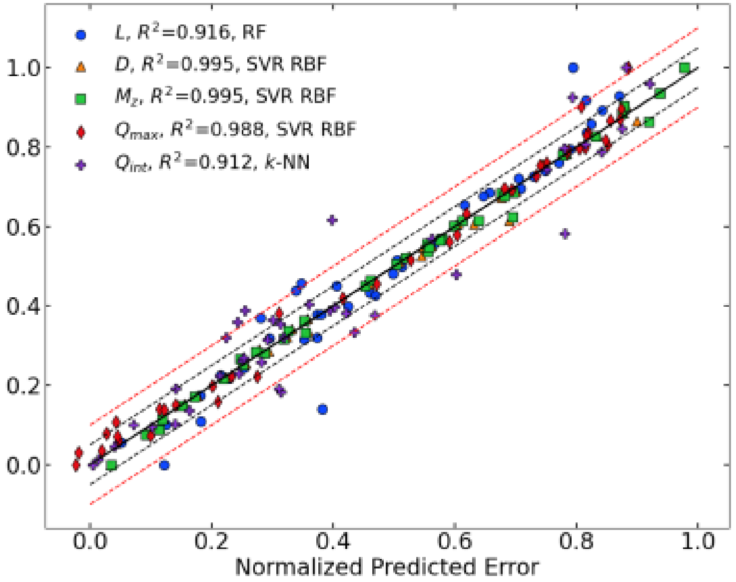


Distinct Training Set Normalized Error

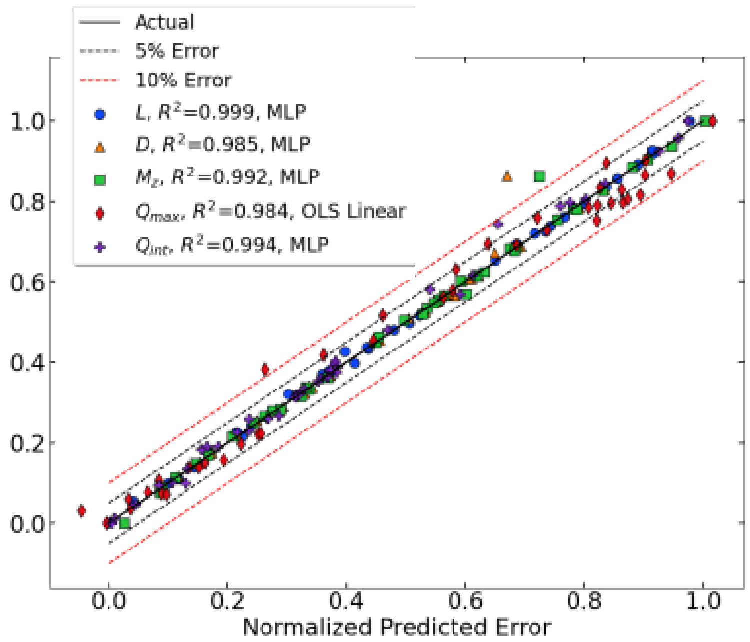
- D-Optimal and LHS sampling types produced best results
    - D-Optimal little bit better than LHS ($\bar{R}_D^2 = 0.991 > \bar{R}_{LHS}^2 = 0.990$)



LHS



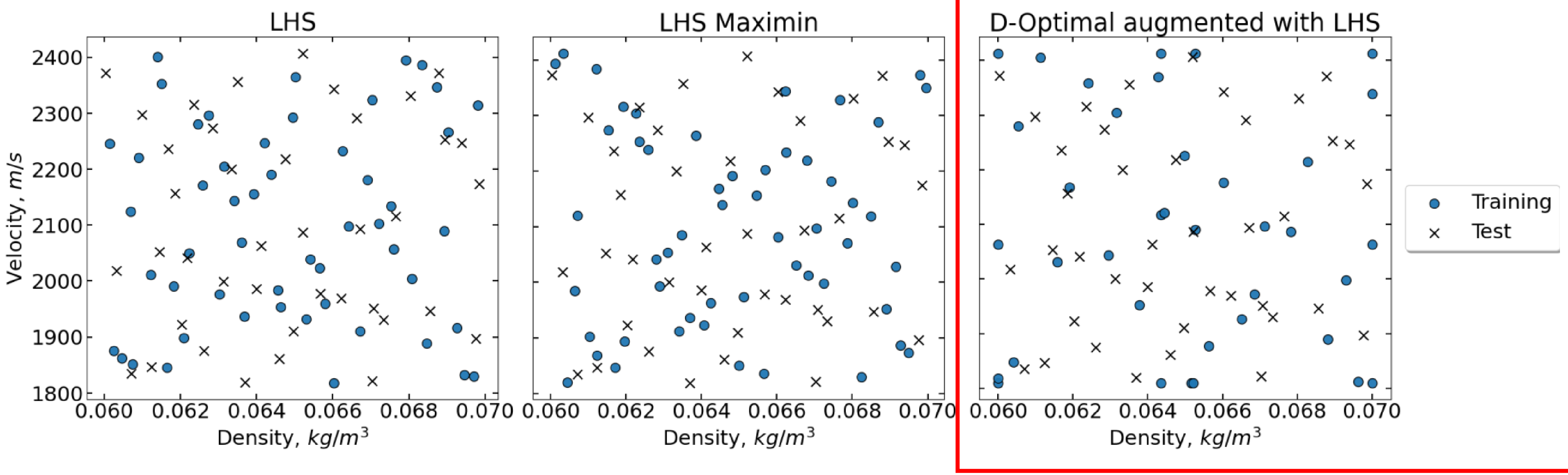
LHS Maximin



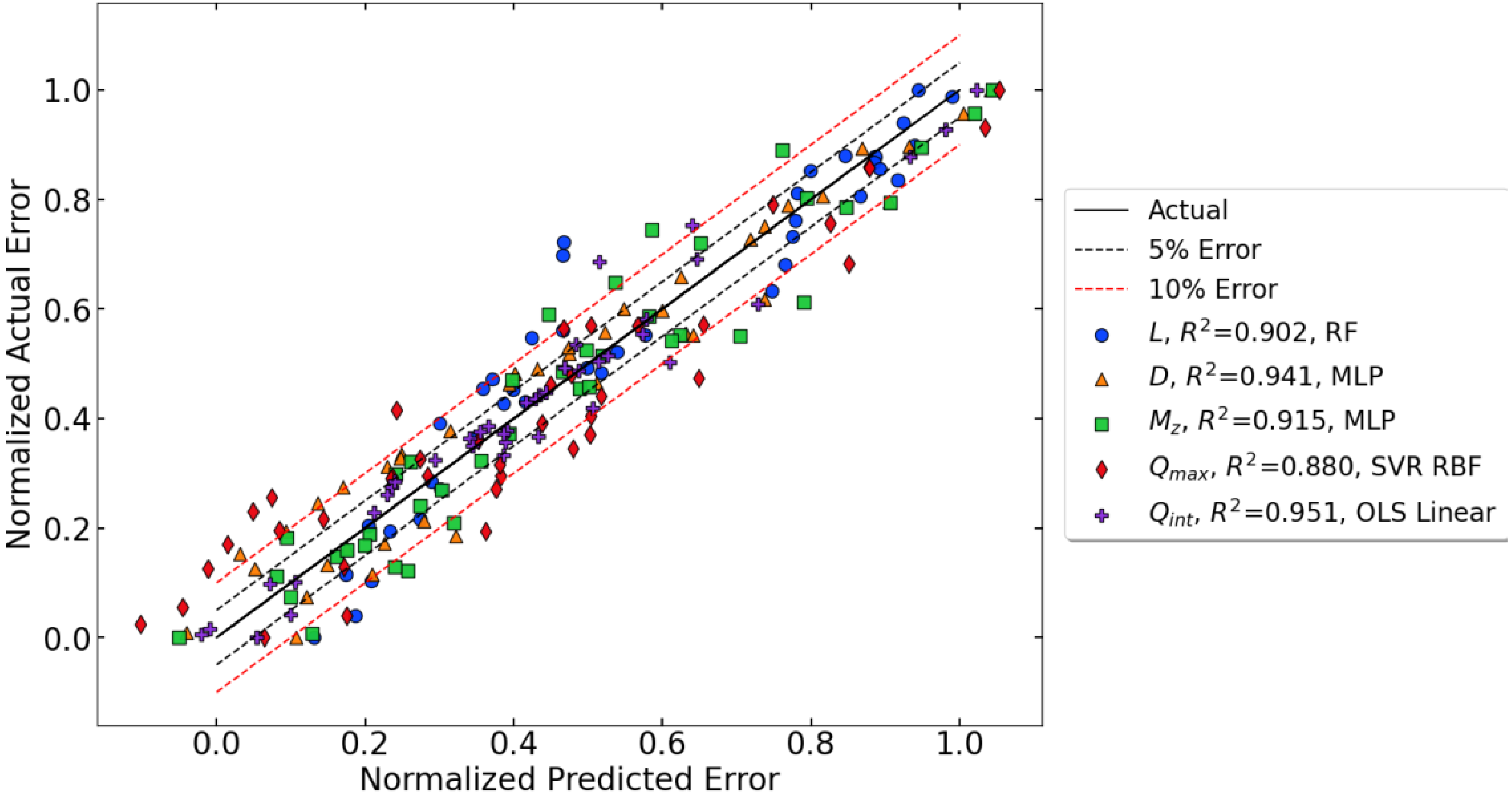
D-Optimal

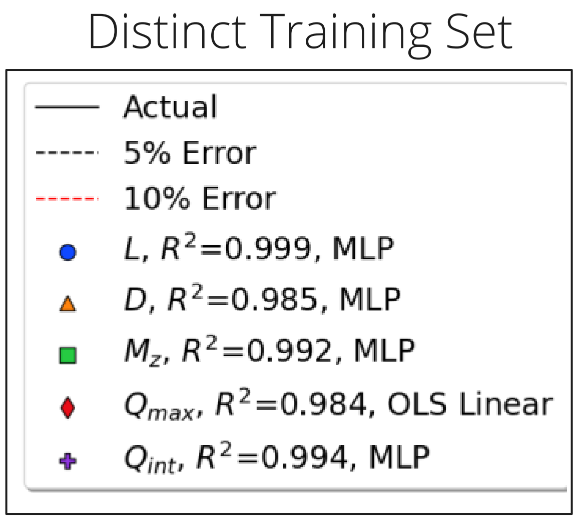
Single Training Set

- Leave-one-out cross validation (LOOCV)
  - Same training set for reduced-order model and error model



Single Training Set Normalized Error

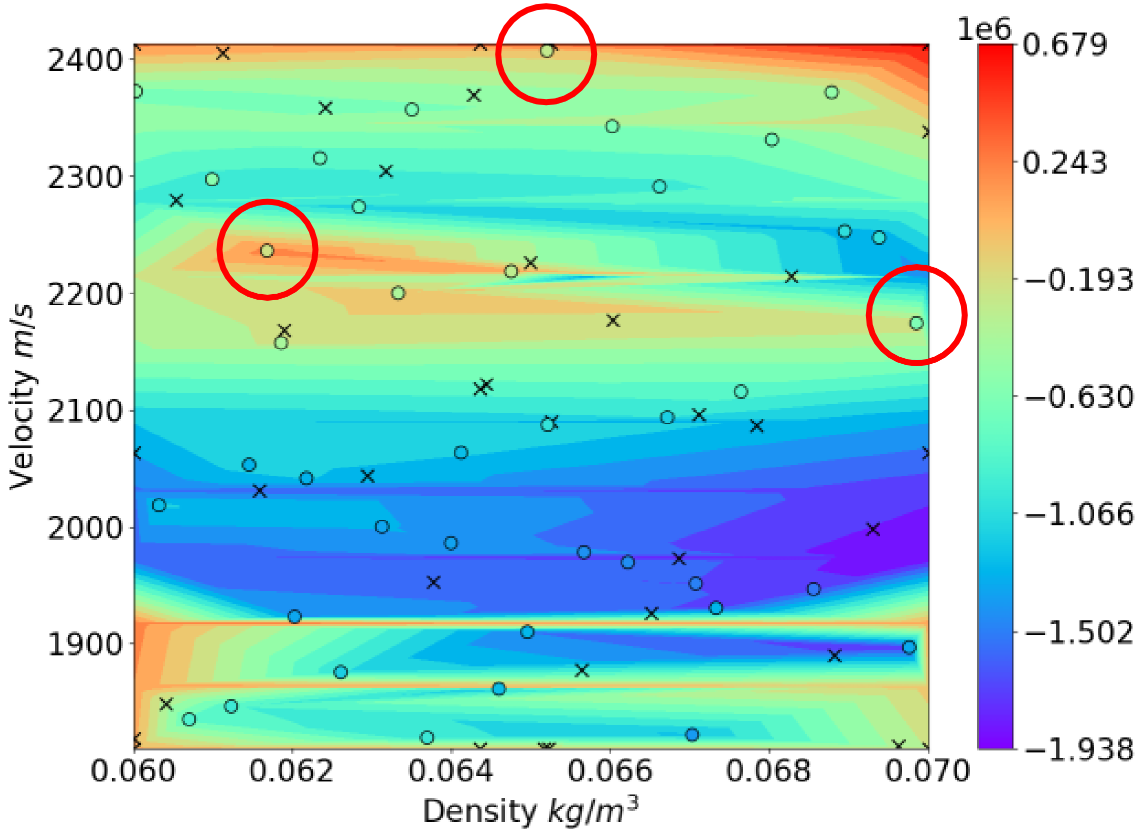




Single Training Set Error Contours

- Highly nonlinear error surface
- Large errors occur where
  - Few training points placed
  - Highly nonlinear areas
- Improve error model by improving spread of training points
  - D-Optimal design augmented with LHS
  - No distance constraint on augmented LHS points

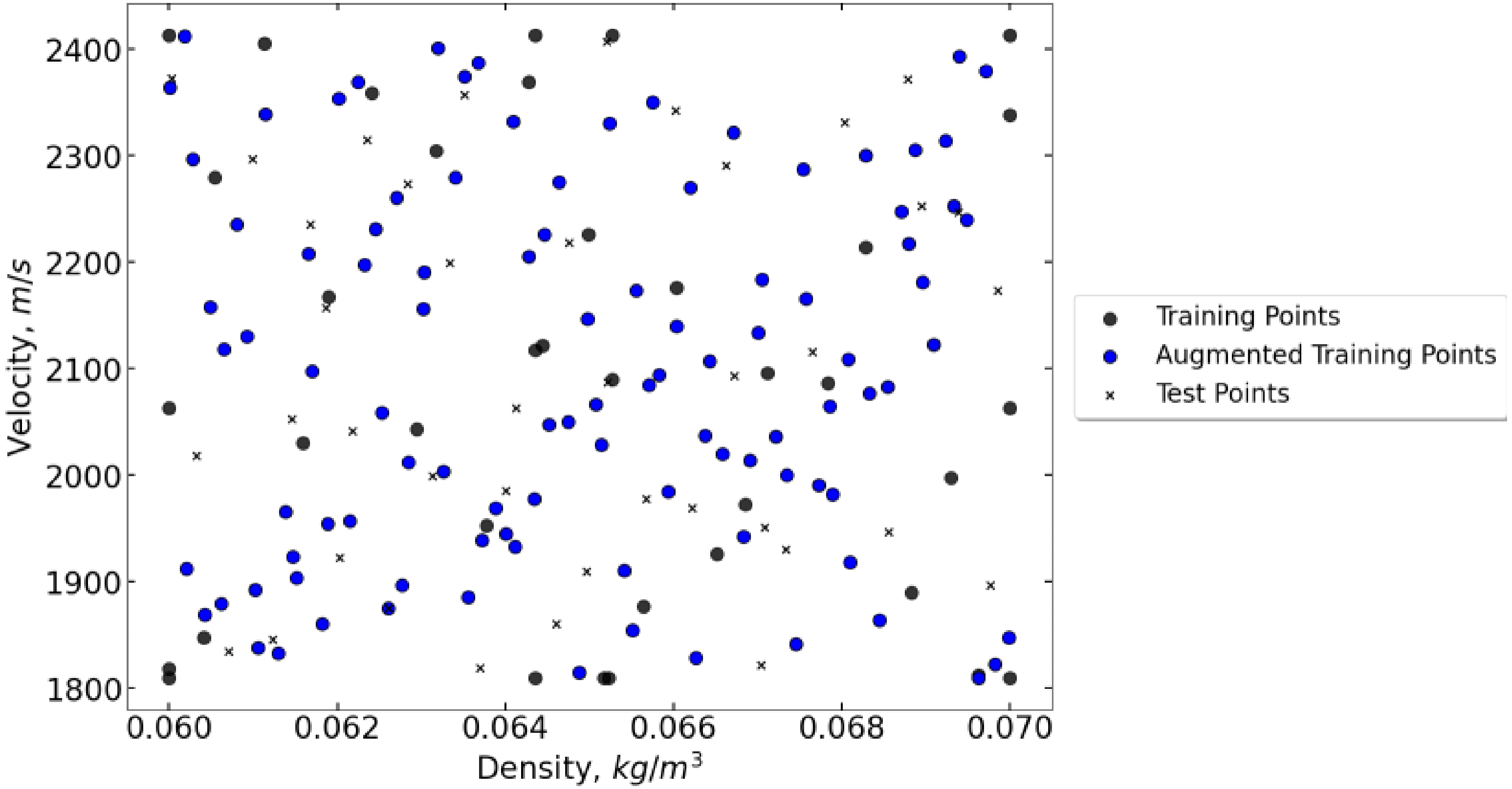
max , R 2 = 0.880



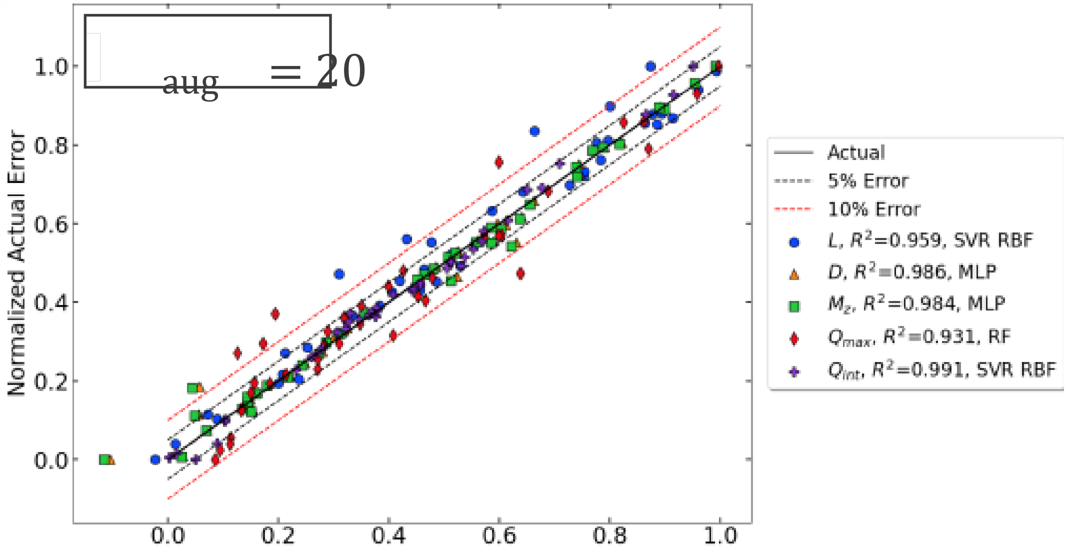
Augmented Training Set

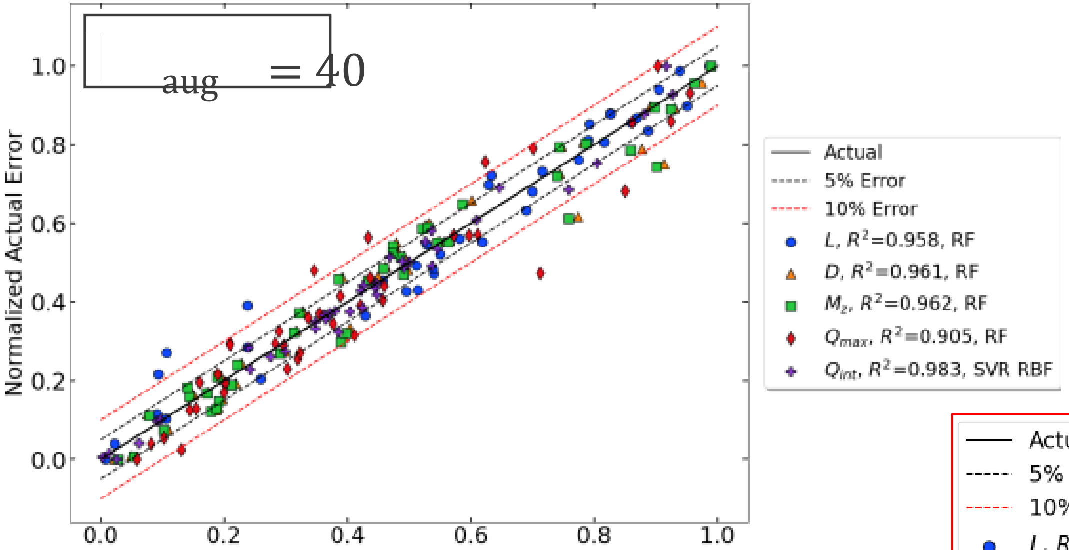
- Improve error model by augmenting with additional points

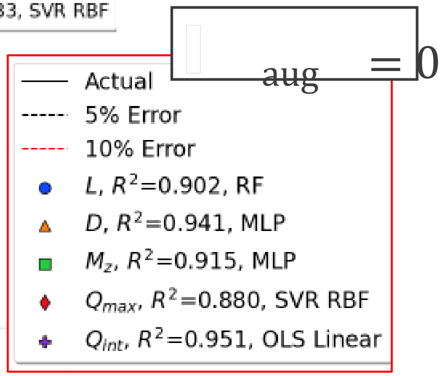
100 Augment Points

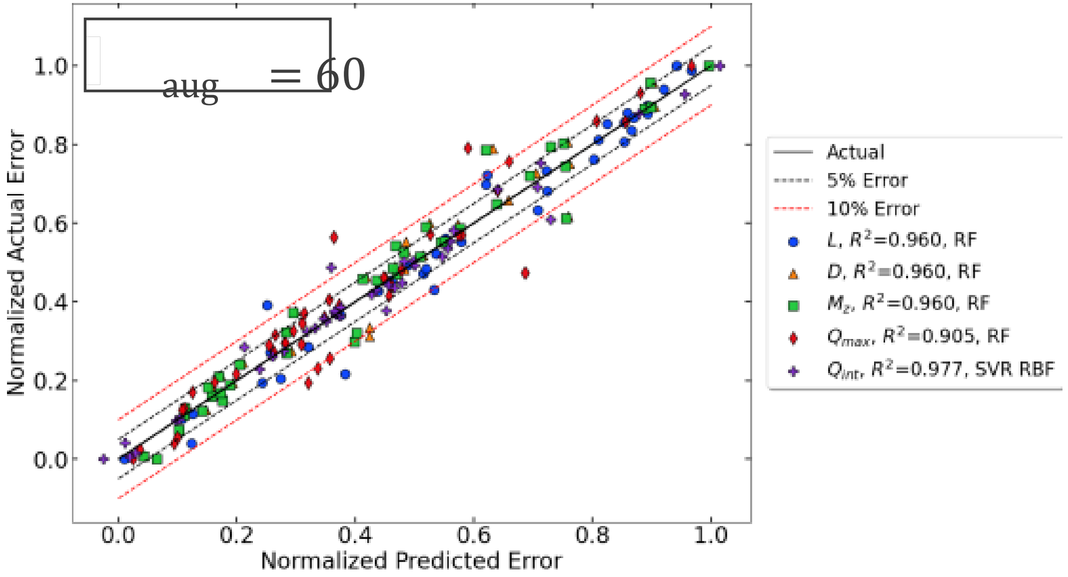


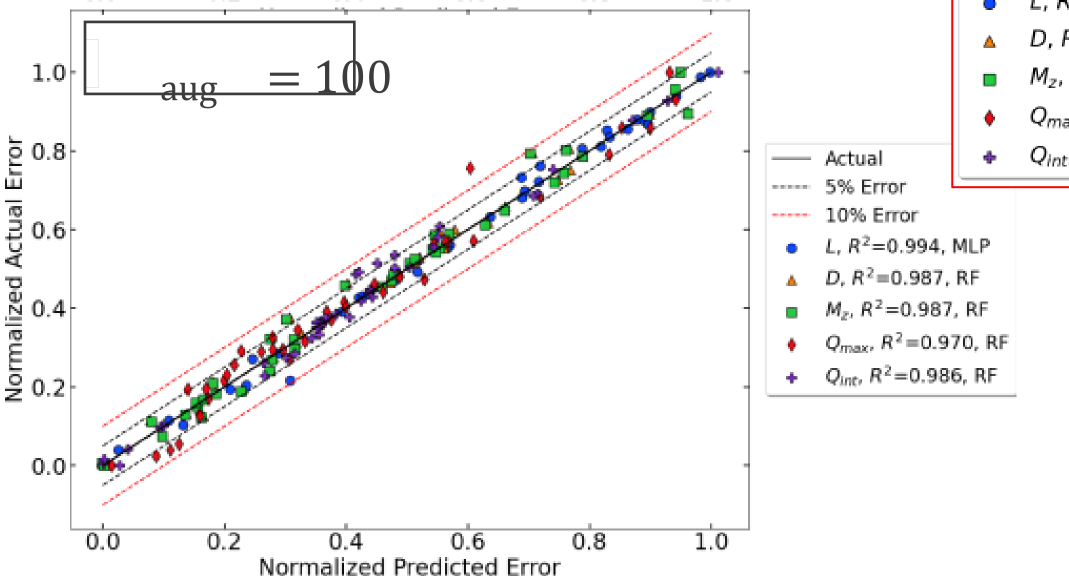
Augmented Training Set Normalized Error











Computational Runtime

- D-Optimal with LOOCV cuts computational expense by 64% compared to Distinct LHS
  - Design with 20 augmented points cuts computational expense by 44%

Category	Sampling Type	N_{train}	Total Time [s] $\times 10^6$	Relative Time to Distinct LHS	$\bar{R}^2$
Distinct	LHS	102	1.43	1.00	0.990
	LHS Maximin	103	1.44	1.01	0.961
	D-Optimal	87	1.22	0.85	0.991
Single Training Set	D-Optimal	37	0.52	0.36	0.918
Augmented Training Set	D-Optimal	57	0.80	0.56	0.970
		77	1.08	0.75	0.954
		97	1.36	0.95	0.952
		117	1.64	1.15	0.962
		137	1.91	1.34	0.985

Conclusions

- D-Optimal design reduces development cost of error model by 15%
  - Reduced total number of training points from 102 to 87
- LOOCV with D-Optimal design reduces development cost of error model by 64%
  - Adding 20 augment points improves accuracy from $\bar{R}^2 = 0.92$ to 0.97
  - Using 20 augment points reduces development cost by 44%
- May improve overall cost reduction by improving POD updates
  - Recalculating POD takes up 30% of overall cost with LOOCV
  - Possibility to use rank-1 updates to POD basis [1]

[2] Brand, M., "Fast low-rank modifications of the thin singular value decomposition," *Linear Algebra and its Applications*, Vol. 415, No. 1, 2006, pp. 20–30. https://doi.org/https://doi.org/10.1016/j.laa.2005.07.021, special Issue on Large Scale Linear and Nonlinear Eigenvalue Problems.

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Questions?