

1

Dataset
(one output variable)

FEM dataset

Inputs: window thicknesses
Output: target variable y

$t_{w,1}$	$t_{w,2}$	...	t_{w,N_w}	y
...	...	...	...	...
...	...	...	...	...
...	...	...	...	...
...	...	...	...	...
...	...	...	...	...
...	...	...	...	...

2

Cross-validation
(adapted to dataset size)

CV strategy

Select number of folds K
based on dataset size N

If $N \leq 20$

Leave-One-Out ($K = N$)

(*) Reduced search space for
tree-based models to mitigate
overfitting

If $21 \leq N \leq 80$

Repeated K-Fold CV
($K = 4, 5$ times)

If $N > 80$

K-Fold CV ($K = 5$)

Example: 5-fold CV

Fold 1 2 3 4 5

Split 1

Split 2

...

...

Split 5

Training data

Validation data

3

Model training and performance
evaluation

For each
candidate model

Random Forest
(RF)

Gradient Boosting
(GBR)

XGBoost

Support Vector
Regression (SVR)

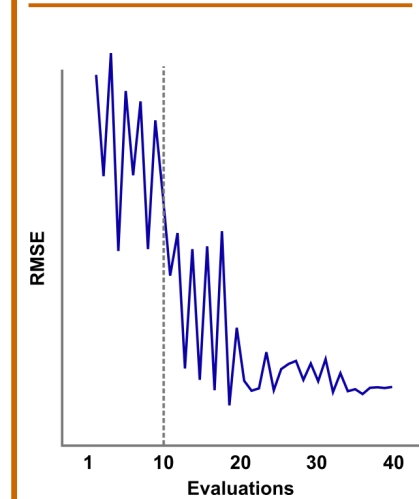
Gaussian Process
Regression (GPR)

Multi-Layer
Perceptron (MLP)

Bayesian
optimization

(40 evaluations)

Cross-validated RMSE
for each configuration



Best configuration:
min. mean RMSE

4

Model selection

Model ranking

Model	Mean RMSE
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Model A	0.100
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Model B	0.103
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Model C	0.106
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Model D	0.120
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...

...

1 Competitive threshold:
 $\leq 5\%$ above best RMSE
($0.100 \times 1.05 = 0.105$)

2 Among competitive models,
select by lowest relative
RMSE dispersion

3 Tie breaker:
lower mean RMSE

Selected best model