

1

Dataset
(one output variable)

FEM dataset

Inputs: window thicknesses
Output: target variable y

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

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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

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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

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Model selection

Model ranking

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

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