Elastic Net (degree=1)

Data processing
Degree 1 polynomial: X (133, 297)
Split Train | Test = 70% | 30%
5-fold, n_repeats=2

GridSearch

- SelectKBest:
  - k=all
- ElasticNet:
  - alpha=0.1
  - l1_ratio = 0.0001

Results
Best_score_MAE: 2.674
Train_MAE: 0.186
Test_MAE: 2.935

Elastic Net (degree=2)

Data processing
Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 2

GridSearch

- SelectKBest:
  - k=all
- ElasticNet:
  - alpha=0.001
  - l1_ratio = 0.1584

Results
Best_score_MAE: 2.635
Train_MAE: 0.00044
Test_MAE: 2.473

Random Forest (degree=1)

Data processing
Degree 1 polynomial: X (133, 297)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = 100
- RandomForest:
  - max_depth = 15

Results
Best_score_MAE: 2.708
Train_MAE: 0.998
Test_MAE: 2.453

Random Forest (degree=2)

Data processing
Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch
- SelectKBest:
  - k = all
- RandomForest:
  - max_depth = 5

Results
Best_score_MAE: 2.747
Train_MAE: 1.018
Test_MAE: 2.862

KRR RBF (degree=1)

Data processing
Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch
- SelectKBest:
  - k = 5
- KernelRidge:
  - alpha = 0.01
  - gamma = 0.01

Results
Best_score_MAE: 3.11
Train_MAE: 2.322
Test_MAE: 3.412

KRR RBF (degree=2)

Data processing
Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = 5
- KernelRidge:
  - alpha = 0.001
  - gamma = 0.01

Results
Best_score_MAE: 3.863
Train_MAE: 1.945
Test_MAE: 2.686

KRR Polynomial (degree=1)

Data processing
Degree 1 polynomial: X (133, 297)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = all
- KernelRidge:
  - alpha = 0.001
  - degree = 2

Results
Best_score_MAE: 2.866
Train_MAE: 0.0015
Test_MAE: 2.779

KRR Polynomial (degree=2)

Data processing
Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = 1000
- KernelRidge:
  - alpha = 0.001
  - degree = 2

Results

Best_score_MAE: 2.871
Train_MAE: 0.0016
Test_MAE: 3.372

KRR Sigmoid (degree=1)

Data processing

Degree 1 polynomial: X (133, 297)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = all
- KernelRidge:
  - alpha = 0.1
  - gamma = 0.001

Results

Best_score_MAE: 2.482
Train_MAE: 1.66
Test_MAE: 2.639

KRR Sigmoid (degree=2)

Data processing

Degree 2 polynomial: X (133, 44253)
Split Train | Test = 70% | 30%
5-fold, n_repeats = 3

GridSearch

- SelectKBest:
  - k = all
- KernelRidge:
  - alpha = 1
  - gamma = 0.01

Results

Best_score_MAE: 2.761

Train_MAE: 2.769
Test_MAE: 2.690

Comparing KRR Sigmoid with Elastic Net

Both with degree 1 polynomial features: X(133, 297)

- KernelRidge:
  - kernel: sigmoid
  - alpha: 0.1
  - gamma: 0.001
- ElasticNet:
  - alpha: 0.1
  - l1_ratio: 0.0001

RepeatedKFold(n_splits=5, n_repeats=3, random_state=42)

	KernelRidge	ElasticNet
Average train_score	**1.86**	**0.24**
Best	*1.62*	*0.18*
Worst	*2.12*	*0.27*
Average test_score	**2.67**	**2.73**
Best	*1.8*	*1.99*
Worse	*3.36*	*3.5*
Global score	**2.17**	**0.35**