

SUPPLEMENTARY MATERIAL

Hyperparameter search space for individual models

Linear:

- 'fit_intercept': [True, False]
- 'positive': [True, False]

ENet:

- 'alpha': [float(10**x) for x in range(-6,2)]
- 'l1_ratio': [0.1, 0.3, 0.5, 0.7, 0.9]
- 'max_iter': [1000, 10000]
- 'warm_start': [False, True]

SVM:

- 'kernel': ['linear', 'rbf']
- 'C': [float(10**x) for x in range(-3, 3)]
- 'gamma': [float(10**x) for x in range(-3, 4)]

RandomForest:

- 'n_estimators': [100,250,500]
- 'max_features': [1.0, 3, 9, 15]
- 'max_depth': [int(x) for x in np.linspace(10, 110, num = 11)]+[None]
- 'min_samples_split': [2, 5, 10]
- 'min_samples_leaf': [1, 2, 4]
- 'bootstrap': [True, False]

XGBoost:

- 'n_estimators': [10, 100, 300, 600]
- 'min_child_weight': [1, 5, 10]
- 'gamma': [0.5, 1, 1.5, 2, 5]
- 'subsample': [0.6, 0.8, 1.0]
- 'colsample_bytree': [0.6, 0.8, 1.0]
- 'max_depth': [3,5,10,15,30,50]
- 'learning_rate': [1.0, 0.5, 0.3, 0.1, 0.05, 0.01]