Introduction:

For this exercise I experimented with different preprocessing methods and their effect on various ML models as well as with and without hyperparameter optimization. I went with numerical preprocessors because every categorical preprocessor I tried had extremely long runtimes that I would just cancel after 15+ minutes of running.

Dataset Description:

I used the wine quality dataset[1] for this and picked the white wine dataset because it has more entries than the red dataset. This data includes 11 features and a target value called "quality" that is between 0 and 10.

[1]: https://archive-beta.ics.uci.edu/dataset/186/wine+quality

Experimental Setup:

For these experiments I picked a few models to test on, Random Forest because it has been the most accurate in every test on the wine dataset, K Nearest Neighbors because I wanted to how much preprocessing would improve it, and Support Vector Machine because I wanted a third model, and it was used in all the examples on scikit-learn's documentation.

Then I picked a couple preprocessing methods, I decided to use two different scaler methods because I thought those would have the most impact and I used the basic scaler and a minmax scaler.

Then I ran some tests on all the models with default parameters and optimized parameters with and without preprocessing and compared the results.

Parameters of the preprocessing methods are all default.

The hyperparameter optimizations will both use cross validation with 5 folds and have n_iter set to 15 which is the number of hyperparameter settings sampled.

The hyperparameters optimized are:

Random Forest:

bootstrap:

The default value for this is true, and I also tested false, this parameter either uses bootstrap samples for true or uses the whole dataset for each tree for false.

max_depth:

The default value for this is None, and I tested this with values 25, 50 and None, this parameter sets the max depth of the tree.

n_estimators:

The default value for this is 100, and I tested this with values 25, 50, 75, 100, 125 and 150, this parameter sets how many random trees the algorithm will generate.

min_samples_split:

The default value for this is 2, and I tested this with values 2, 4, 6, 8, this parameter determines the minimum amount of samples before a node can split.

min_samples_leaf:

The default value for this is 1, and I tested this with 1, 3, 5, 7, this parameter determines the minimum number of samples in a leaf.

K-Nearest-Neighbors:

n_neighbors:

The default value for this is 5, and I tested this with values 3, 4, 5, 6, 10, this parameter sets the number of neighbors.

leaf_size:

The default value for this is 30, and I tested this with values 10, 30, 50, 100, 200, this parameter sets the leaf size passed into the balltree and kdtree algorithms.

algorithm:

The default value for this is ‘auto’ and I tested this with 'ball_tree', 'kd_tree', 'brute', 'auto', this parameter changes which algorithm is being used.

p:

The default value for this is 2, and I tested this with both 1 and 2, it changes which distance formula is used.

weights:

The default value for this is ‘uniform’ and I also tested ‘distance’, uniform weighs all points in each ‘neighborhood’ equally, whereas distance weights points by the inverse of their distance.

Support Vector Machine:

C:

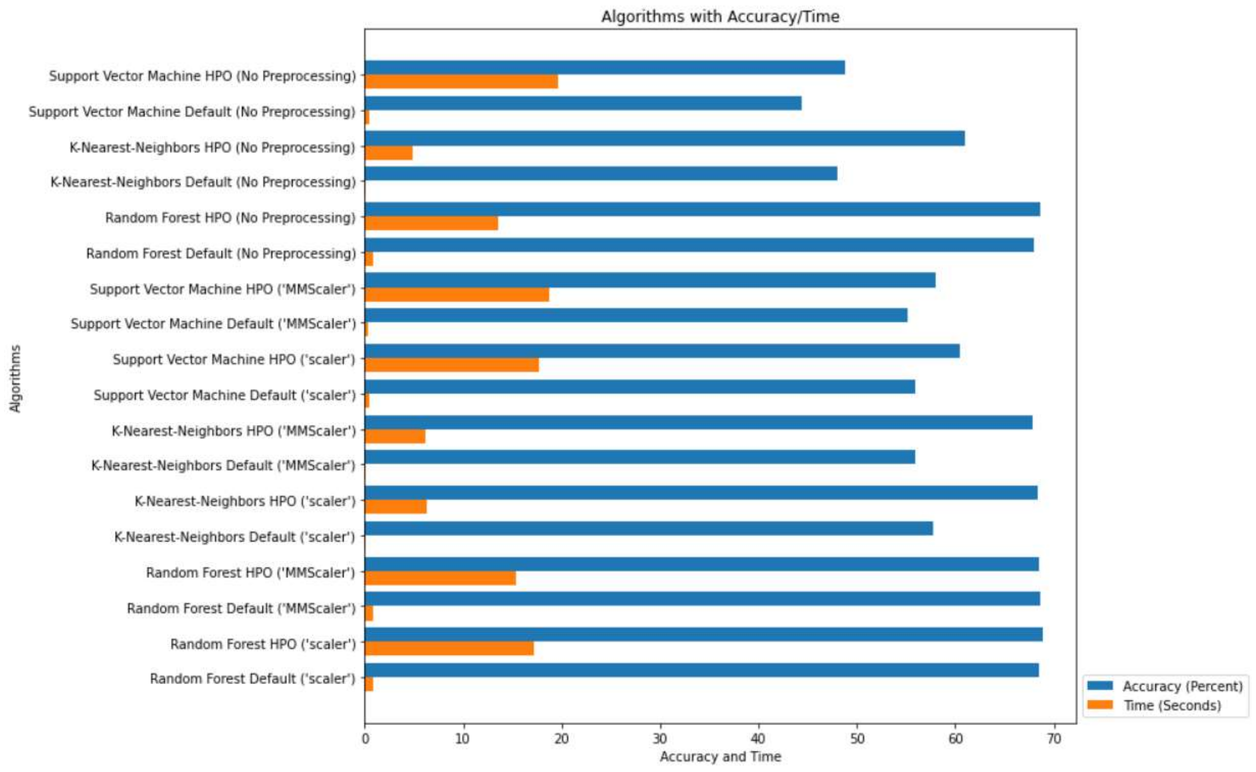
The default value for this is 1, I tested this with values 1, 10, 100, this parameter changes the regularization parameter.

kernel:

The default value for this is ‘rbf’ and I also tried ‘sigmoid’, I only went with these two because the other ones would never finish even when I left it running by itself for about 15 minutes, and they change how boundaries are calculated for classification.

I then output the results sorting by accuracy first and time second then labeling the best one.

Results:



Best Algorithm by accuracy and time is: Random Forest HPO ('scaler')

List of algorithms sorted best to worst:
Random Forest HPO ('scaler'): 68.87755% accuracy, 17.22775 seconds
Random Forest HPO (No Preprocessing): 68.67347% accuracy, 13.49371 seconds
Random Forest Default ('MMScaler'): 68.57143% accuracy, 0.86074 seconds
Random Forest Default ('scaler'): 68.46939% accuracy, 0.87675 seconds
Random Forest HPO ('MMScaler'): 68.46939% accuracy, 15.33215 seconds
K-Nearest-Neighbors HPO ('scaler'): 68.36735% accuracy, 6.33886 seconds
Random Forest Default (No Preprocessing): 67.95918% accuracy, 0.86174 seconds
K-Nearest-Neighbors HPO ('MMScaler'): 67.85714% accuracy, 6.19089 seconds
K-Nearest-Neighbors HPO (No Preprocessing): 61.02041% accuracy, 4.86061 seconds
Support Vector Machine HPO ('scaler'): 60.51020% accuracy, 17.67231 seconds
Support Vector Machine HPO ('MMScaler'): 58.06122% accuracy, 18.71609 seconds
K-Nearest-Neighbors Default ('scaler'): 57.75510% accuracy, 0.01001 seconds
K-Nearest-Neighbors Default ('MMScaler'): 55.91837% accuracy, 0.01001 seconds
Support Vector Machine Default ('scaler'): 55.91837% accuracy, 0.40435 seconds
Support Vector Machine Default ('MMScaler'): 55.20408% accuracy, 0.38883 seconds
Support Vector Machine HPO (No Preprocessing): 48.77551% accuracy, 19.68513 seconds
K-Nearest-Neighbors Default (No Preprocessing): 48.06122% accuracy, 0.00851 seconds
Support Vector Machine Default (No Preprocessing): 44.38776% accuracy, 0.40885 seconds

List of best hyperparameters per algorithm:
Best Paremeters found for Random Forest ('scaler'): OrderedDict([('classifier__bootstrap', False), ('classifier__max_depth', 25), ('classifier__min_samples_leaf', 3), ('classifier__min_samples_split', 4), ('classifier__n_estimators', 100)])

Best Paremeters found for Random Forest ('MMScaler'): OrderedDict([('classifier__bootstrap', False), ('classifier__max_depth', 25), ('classifier__min_samples_leaf', 3), ('classifier__min_samples_split', 6), ('classifier__n_estimators', 125)])

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Best Paremeters found for K-Nearest-Neighbors ('scaler'): OrderedDict([('classifier__algorithm', 'auto'), ('classifier__leaf_s
ize', 200), ('classifier__n_neighbors', 10), ('classifier__p', 1), ('classifier__weights', 'distance')])

Best Paremeters found for K-Nearest-Neighbors ('MMScaler'): OrderedDict([('classifier__algorithm', 'kd_tree'), ('classifier
__leaf_size', 200), ('classifier__n_neighbors', 10), ('classifier__p', 1), ('classifier__weights', 'distance')])

Best Paremeters found for Support Vector Machine ('scaler'): OrderedDict([('classifier__C', 100), ('classifier__kernel', 'rbf
')])

Best Paremeters found for Support Vector Machine ('MMScaler'): OrderedDict([('classifier__C', 100), ('classifier__kernel', '
rbf')])

Best Paremeters found for Random Forest (No Preprocessing): OrderedDict([('classifier__bootstrap', False), ('classifier__
max_depth', 50), ('classifier__min_samples_leaf', 1), ('classifier__min_samples_split', 8), ('classifier__n_estimators', 50)])

Best Paremeters found for K-Nearest-Neighbors (No Preprocessing): OrderedDict([('classifier__algorithm', 'kd_tree'), ('cla
ssifier__leaf_size', 200), ('classifier__n_neighbors', 10), ('classifier__p', 1), ('classifier__weights', 'distance')])

Best Paremeters found for Support Vector Machine (No Preprocessing): OrderedDict([('classifier__C', 100), ('classifier__k
ernel', 'rbf')])
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The results show some improvements for random forest with preprocessed data and huge improvements for the support vector and k nearest neighbors algorithms when the data is preprocessed. Also that performance is improved across the board when the data is preprocessed for this dataset.

Code:

Main.py