

```
In [ ]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import math

np.random.seed(10)

data = pd.read_csv('Hws/HW5/Files/homework-5/data/Pokemon.csv')
data.columns = [d.strip().lower().replace(' ', '_').replace('.', '') for d in data.columns]
```

Exercise 1

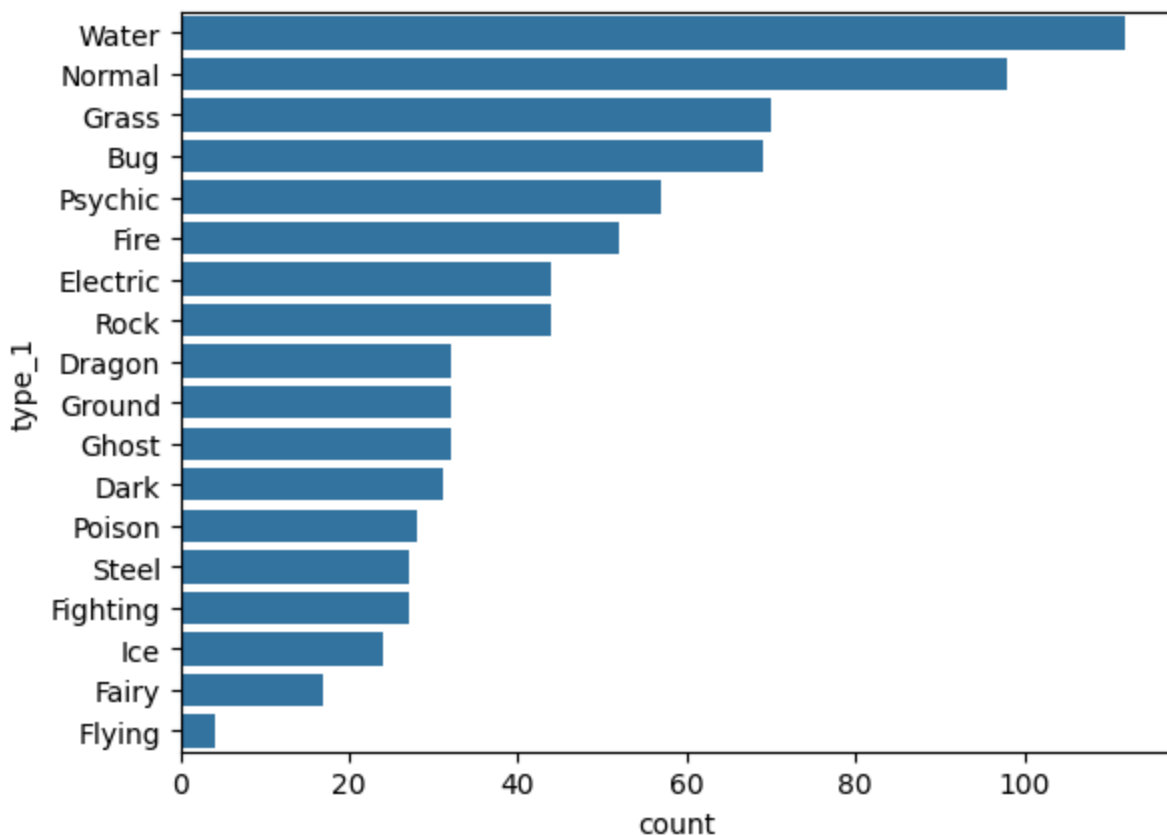
The column names were changed: spaces were replaced with underscores, first letters were converted to lower case, and other small things to make the columns match with the general naming conventions.

Exercise 2

```
In [ ]: data.type_1.unique()

Out[ ]: array(['Grass', 'Fire', 'Water', 'Bug', 'Normal', 'Poison', 'Electric',
        'Ground', 'Fairy', 'Fighting', 'Psychic', 'Rock', 'Ghost', 'Ice',
        'Dragon', 'Dark', 'Steel', 'Flying'], dtype=object)

In [ ]: sns.barplot(data.type_1.value_counts(), errorbar=None, orient='h')
plt.show()
```



I count 18 types of pokemon. There are definitely some with very few values, with the 12 lowest all below about 40.

```
In [ ]: value_counts = data.type_1.value_counts()
least_common = value_counts.nsmallest(12).index
data['type_1'] = data['type_1'].replace(least_common, 'Other')
data.type_1.value_counts()
```

```
Out[ ]: type_1
Other      342
Water      112
Normal      98
Grass       70
Bug         69
Psychic     57
Fire        52
Name: count, dtype: int64
```

```
In [ ]: from sklearn.preprocessing import LabelEncoder

le_t1 = LabelEncoder()
le_t1 = le_t1.fit(data['type_1'])
le_t1_transform = le_t1.transform(data['type_1'])
data['type_1'] = le_t1_transform

le_leg = LabelEncoder()
le_leg = le_leg.fit(data['legendary'])
le_leg_transform = le_leg.transform(data['legendary'])
data['legendary'] = le_leg_transform
```

Exercise 3

```
In [ ]: from sklearn.model_selection import train_test_split

X = data.drop('type_1', axis=1)
Y = data.type_1

x_train, x_test, y_train, y_test = train_test_split(X,Y, test_size=.3, stratify=Y)

x_train.reset_index(drop=True, inplace=True)
y_train.reset_index(drop=True, inplace=True)

train_len_check = (len(x_train) == len(y_train)) & (len(x_train) == len(data) * .7)
test_len_check = (len(x_test) == len(y_test)) & (len(x_test) == len(data) * .3)

print(f'Training Dataset Length Check: {train_len_check}')
print(f'Testing Dataset Length Check: {test_len_check}')
```

Training Dataset Length Check: True
Testing Dataset Length Check: True

```
In [ ]: from sklearn.model_selection import StratifiedKFold

# Perform 5-fold CV
skf = StratifiedKFold(n_splits=5, shuffle=True)

indicies = []
for _, (train_index, test_index) in enumerate(skf.split(x_train,y_train)):
    indicies.append(
        (train_index, test_index)
    )
```

Stratified sampling for cross validation will be useful here since we have so many different levels for the outcome level (7). Without this step, we would likely see class imbalances between the different folds, affecting our results.

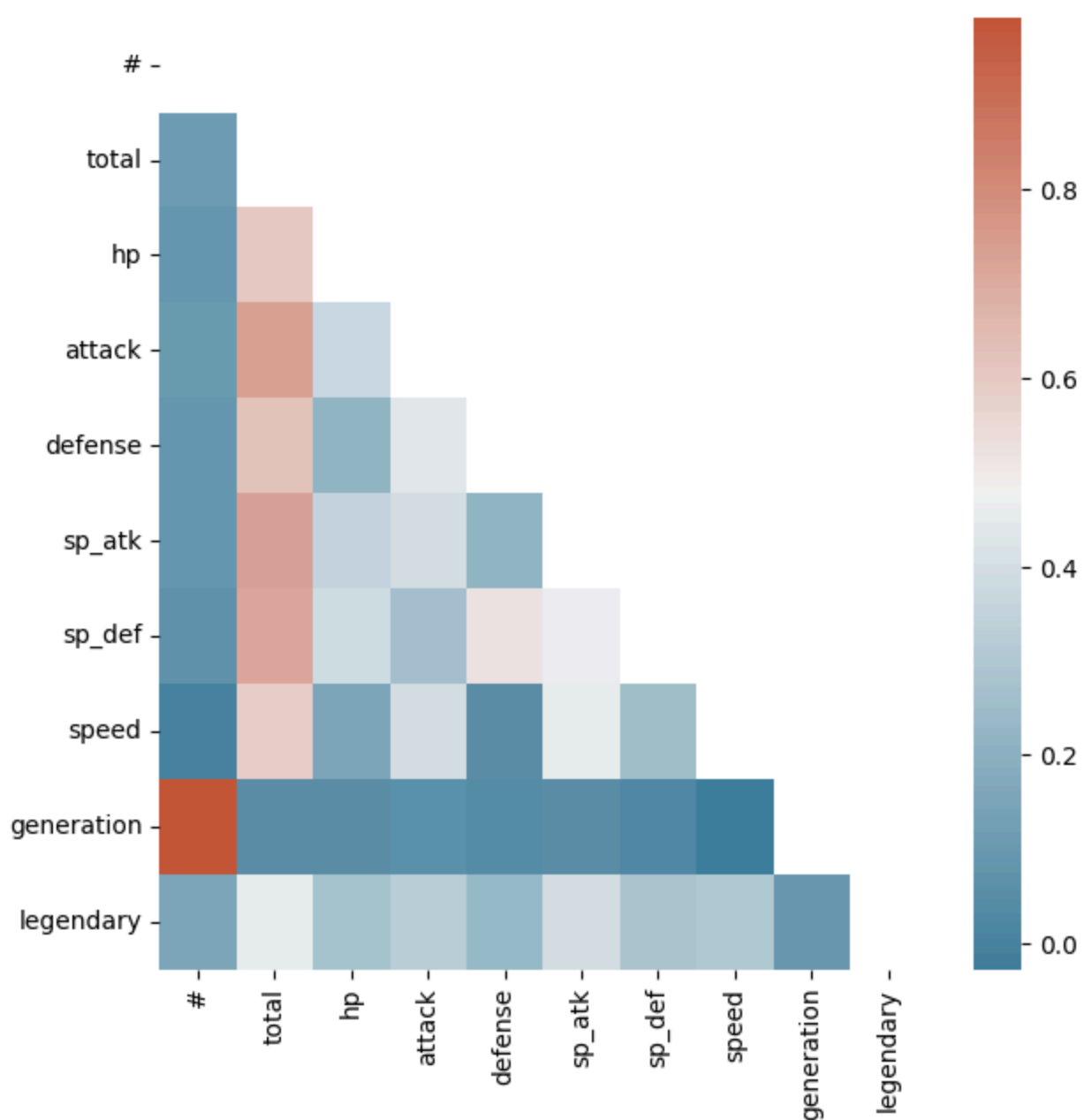
Exercise 4

I choose not to include the target variable here since the factor levels do not represent an ordering, and thus correlation of features with the numeric output are not important.

```
In [ ]: corr_df = x_train.select_dtypes(np.number).corr()
cmap = sns.diverging_palette(230, 20, as_cmap=True)
mask = np.triu(np.ones_like(corr_df, dtype=bool))

plt.figure(figsize=(7,7))

sns.heatmap(corr_df,
            mask=mask,
            cmap=cmap
            )
plt.show()
```



We can see that total has moderate/high correlation with many of the stats, which makes sense, since total represents the sum of all relevant stats. Also, the perfect correlation # and generation can likely be explained by the fact that smaller numbers were an earlier generation and larger numbers are more recent.

Outside of these obvious ones, we see that defense and sp_def are correlated, as is attack and some of the other attack stats.

Exercise 5

```
In [ ]: # Choose features

features = ['legendary', 'generation', 'sp_atk', 'attack',
            'speed', 'defense', 'hp', 'sp_def']

x_train, x_test = (x_train[features], x_test[features])

# Dummy encode two features
```

```
x_train = pd.get_dummies(x_train, columns=['legendary', 'generation'], dtype=int)
x_test = pd.get_dummies(x_test, columns=['legendary', 'generation'], dtype=int)
```

```
In [ ]: from sklearn.preprocessing import StandardScaler

# Center and scale all predictors
ss = StandardScaler()
x_train = pd.DataFrame(ss.fit_transform(x_train), columns=x_train.columns)
x_test = pd.DataFrame(ss.fit_transform(x_test), columns=x_test.columns)
```

Exercise 6

Setup Elastic Net Cross-Validation Grid

```
In [ ]: from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression

params_en = {'C': np.arange(.01,3.02,1/3),
              'l1_ratio': np.arange(0,1.01,1/9)}

en = LogisticRegression(penalty='elasticnet', solver='saga', max_iter=5000,tol=1e-3)
en_grid = GridSearchCV(
    estimator=en,
    param_grid=params_en,
    scoring='roc_auc_ovr',
    cv=indicies,
    verbose=1).fit(x_train,y_train)
```

Fitting 5 folds for each of 100 candidates, totalling 500 fits

```
In [ ]: en_grid.best_params_
```

```
Out[ ]: {'C': 0.6766666666666666, 'l1_ratio': 0.7777777777777777}
```

Exercise 7

Setup RF Cross-Validation Grid

```
In [ ]: from sklearn.ensemble import RandomForestClassifier

params_rf = {'n_estimators': np.arange(10,116,15),
              'min_samples_split': np.arange(2,18,2),
              'max_features': [1,2,3,4,6,8,11,14]}

rf = RandomForestClassifier()
rf_grid = GridSearchCV(
    estimator=rf,
    param_grid=params_rf,
    cv=indicies,
    scoring='roc_auc_ovr',
    verbose=1,
    n_jobs=-1).fit(x_train,y_train)
```

Fitting 5 folds for each of 512 candidates, totalling 2560 fits

```
In [ ]: rf_grid.best_params_
```

```
Out [ ]: {'max_features': 8, 'min_samples_split': 8, 'n_estimators': 85}
```

n_estimators: This represents how many trees are in the forest. Each tree is grown by taking a random sample of features and a random sample of the data to fit a decision tree on. In the end, the majority vote from all trees is taken as the output. More trees can result in better performance, but eventually diminishing returns are achieved.

min_samples_split: This represents how many samples are required for an internal node to be further split. Larger values can prevent overfitting by not letting the tree find patterns that apply to a small subset of the data.

max_features: This represents how many features each tree has access to while training. A smaller value allows trees to grow independently and mostly uncorrelated from each other since the trees have access to different features.

max_features (or mtry in R) cannot be less than one since then the trees would have no features to train on, or greater than 14 since that is how many features we have in total.

Exercise 8

Evaluate Cross-Validation Results; Interpret Parameters

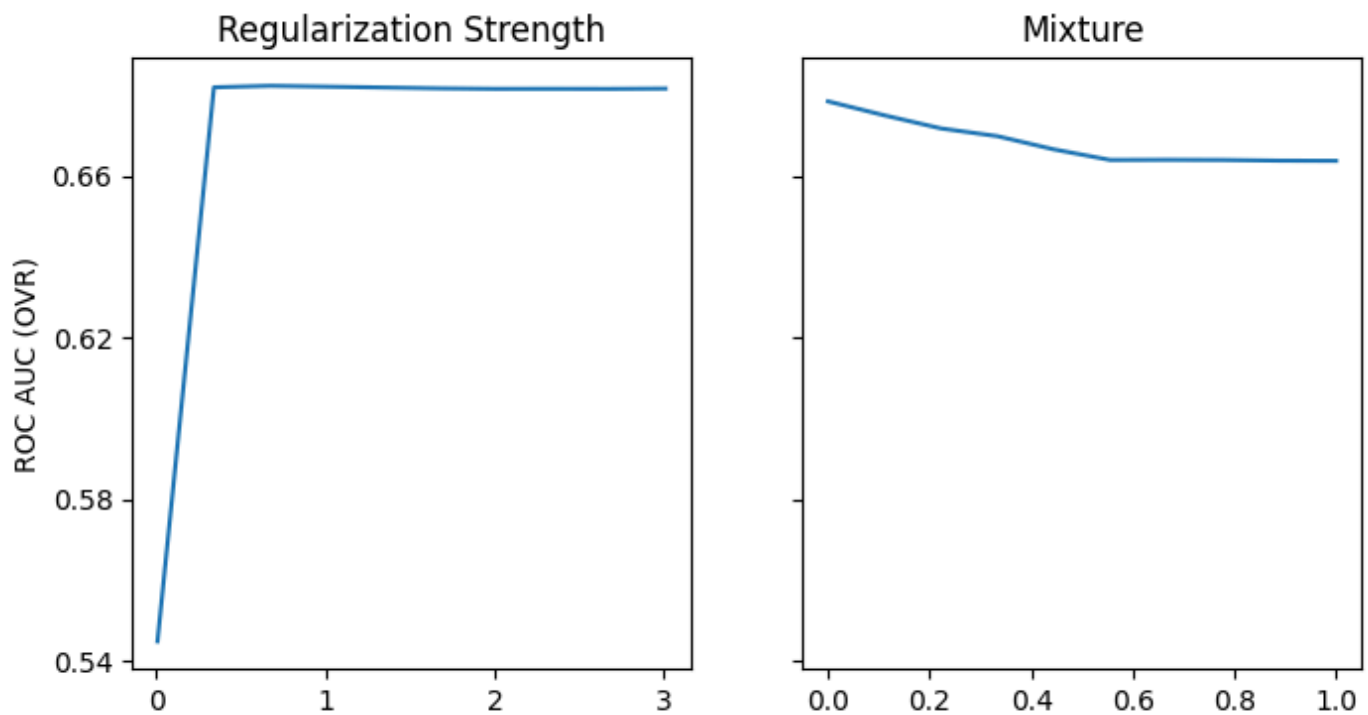
```
In [ ]: en_results_df = pd.DataFrame(en_grid.cv_results_)

en_results_c, en_results_l1 = ([], [])

for c in params_en['C']:
    en_results_c.append(
        en_results_df[en_results_df['param_C'] == c]['mean_test_score'].mean()
    )
for l in params_en['l1_ratio']:
    en_results_l1.append(
        en_results_df[en_results_df['param_l1_ratio'] == l]['mean_test_score'].mean()
    )

fig, ax = plt.subplots(1, 2, sharey=True, figsize=(8, 4))
ax[0].plot(params_en['C'], en_results_c)
ax[0].set_title('Regularization Strength')
ax[0].set_ylabel('ROC AUC (OVR)')
ax[0].set_yticks(np.arange(.54, .69, .04))

ax[1].plot(params_en['l1_ratio'], en_results_l1)
ax[1].set_title('Mixture', fontsize=12)
plt.show()
```



We notice that moderate regularization strength improves performance, and a higher `l1_ratio` (closer to lasso) perform better, **ALL ELSE CONSTANT**.

```
In [ ]: rf_results_df = pd.DataFrame(rf_grid.cv_results_)

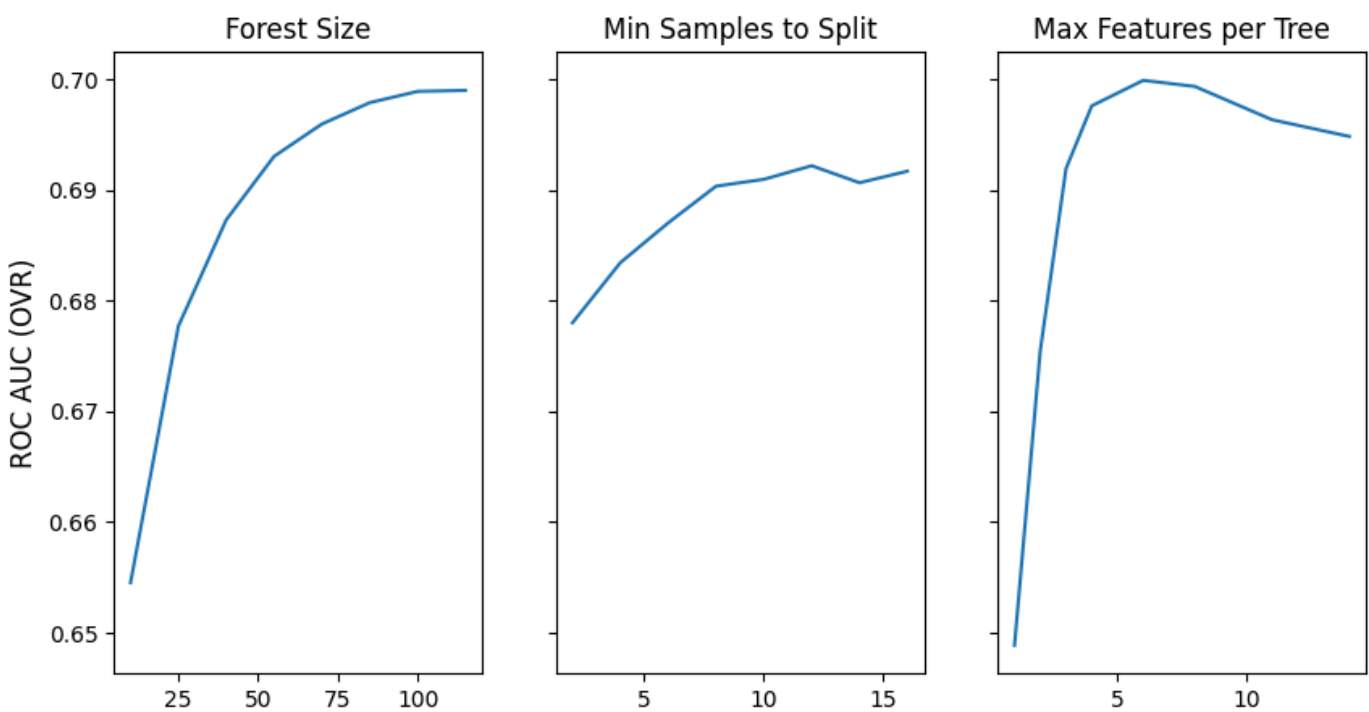
rf_results_trees, rf_results_mss, rf_results_max_feat = ([], [], [])

for n in params_rf['n_estimators']:
    rf_results_trees.append(
        rf_results_df[rf_results_df['param_n_estimators'] == n]['mean_test_score'].mean(
        )
    )
for m in params_rf['min_samples_split']:
    rf_results_mss.append(
        rf_results_df[rf_results_df['param_min_samples_split'] == m]['mean_test_score'].
    )
for f in params_rf['max_features']:
    rf_results_max_feat.append(
        rf_results_df[rf_results_df['param_max_features'] == f]['mean_test_score'].mean(
        )
    )

fig, ax = plt.subplots(1,3, sharey=True, figsize=(10,5))
ax[0].plot(params_rf['n_estimators'], rf_results_trees)
ax[0].set_title('Forest Size')
ax[0].set_ylabel('ROC AUC (OVR)', fontsize=12)

ax[1].plot(params_rf['min_samples_split'], rf_results_mss)
ax[1].set_title('Min Samples to Split')

ax[2].plot(params_rf['max_features'], rf_results_max_feat)
ax[2].set_title('Max Features per Tree')
plt.show()
```



We notice that more trees, more samples required to split an internal node, and more features available to each tree performed best, **ALL ELSE CONSTANT**.

```
In [ ]: print(f"The best model for Elastic Net: {en_grid.best_params}")
        print(f"The best model for Random Forests: {rf_grid.best_params}")
```

The best model for Elastic Net: {'C': 0.6766666666666666, 'l1_ratio': 0.7777777777777777}
The best model for Random Forests: {'max_features': 8, 'min_samples_split': 8, 'n_estimators': 85}

Exercise 9

Evaluation of RF Model on Test Set

```
In [ ]: from sklearn.metrics import roc_auc_score

rf_best = RandomForestClassifier(n_estimators=85, min_samples_split=12,
                               max_features=4).fit(x_train,y_train)

rf_pred = rf_best.predict_proba(x_test)
test_performance_rf = roc_auc_score(y_test.tolist(),rf_pred, multi_class='ovr')
print(f'RF Model Test ROC AUC: {round(test_performance_rf,3)}')
```

RF Model Test ROC AUC: 0.729

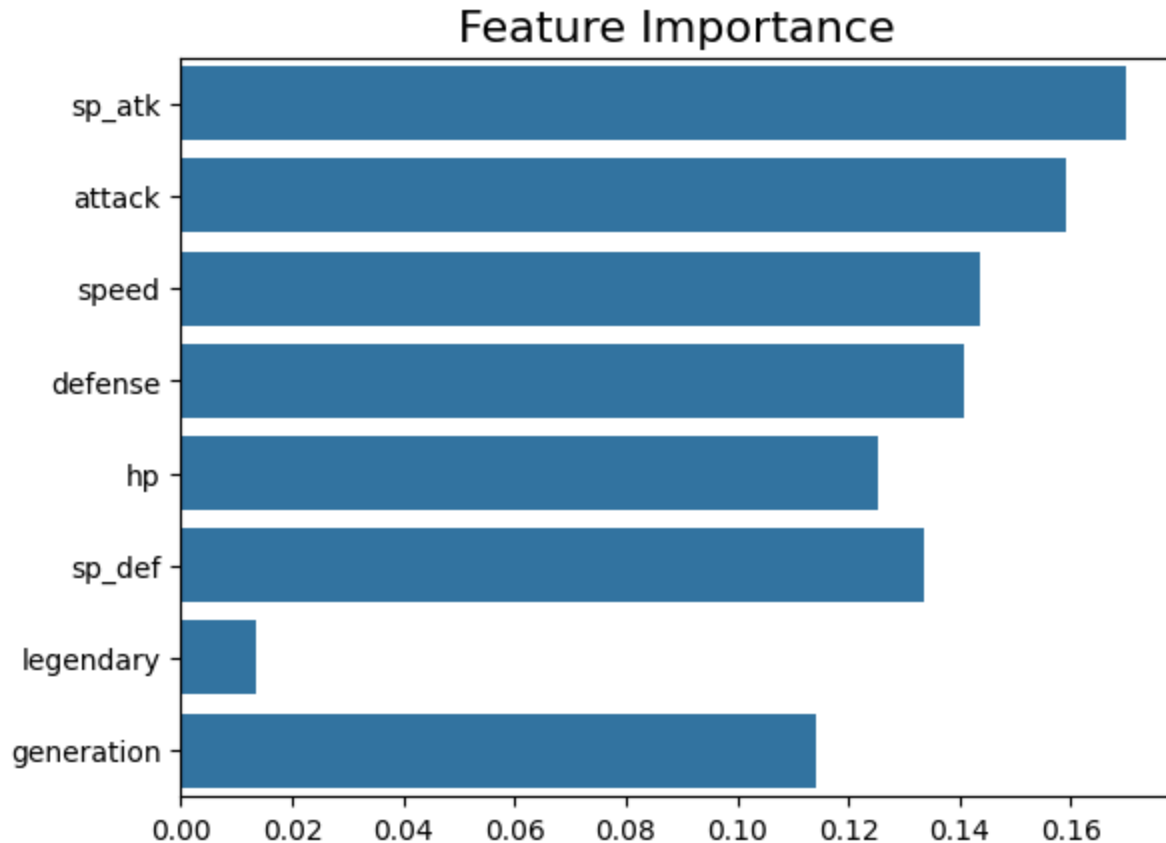
```
In [ ]: feat_imp = pd.DataFrame(rf_best.feature_importances_, index=x_train.columns.values)
        feat_imp.loc['legendary'] = feat_imp.loc['legendary_0'] + feat_imp.loc['legendary_1']

        gen_sum = 0
        for j in range(1,7):
            gen_sum += feat_imp.loc[f'generation_{j}']
        feat_imp.loc['generation'] = gen_sum

        feat_imp.drop(['legendary_0', 'legendary_1', 'generation_1', 'generation_2',
                       'generation_3', 'generation_4', 'generation_5',
                       'generation_6'], axis=0, inplace=True)
```



```
sns.barplot(feats_imp[0], orient='h')
plt.xlabel('')
plt.title('Feature Importance', fontsize=16)
plt.show()
```



We notice that the features were all equally importance except for legendary. This could happen because there are an equal number of legendaries for each type, making it a not useful predictor of pokemon type.

```
In [ ]: from sklearn.metrics import roc_curve, auc, confusion_matrix, ConfusionMatrixDisplay
ivt = le_t1.inverse_transform([0,1,2,3,4,5,6])
n_classes = rf_pred.shape[1]
fpr = dict()
tpr = dict()
roc_auc = dict()

for i in range(n_classes):
    fpr[i], tpr[i], _ = roc_curve(y_test == i, rf_pred[:, i])
    roc_auc[i] = auc(fpr[i], tpr[i])

# Plot all ROC curves
fig, axes = plt.subplots(3, 3, figsize=(15, 15))
ax = axes.ravel() # Flatten the 3x3 matrix into an array for easy indexing

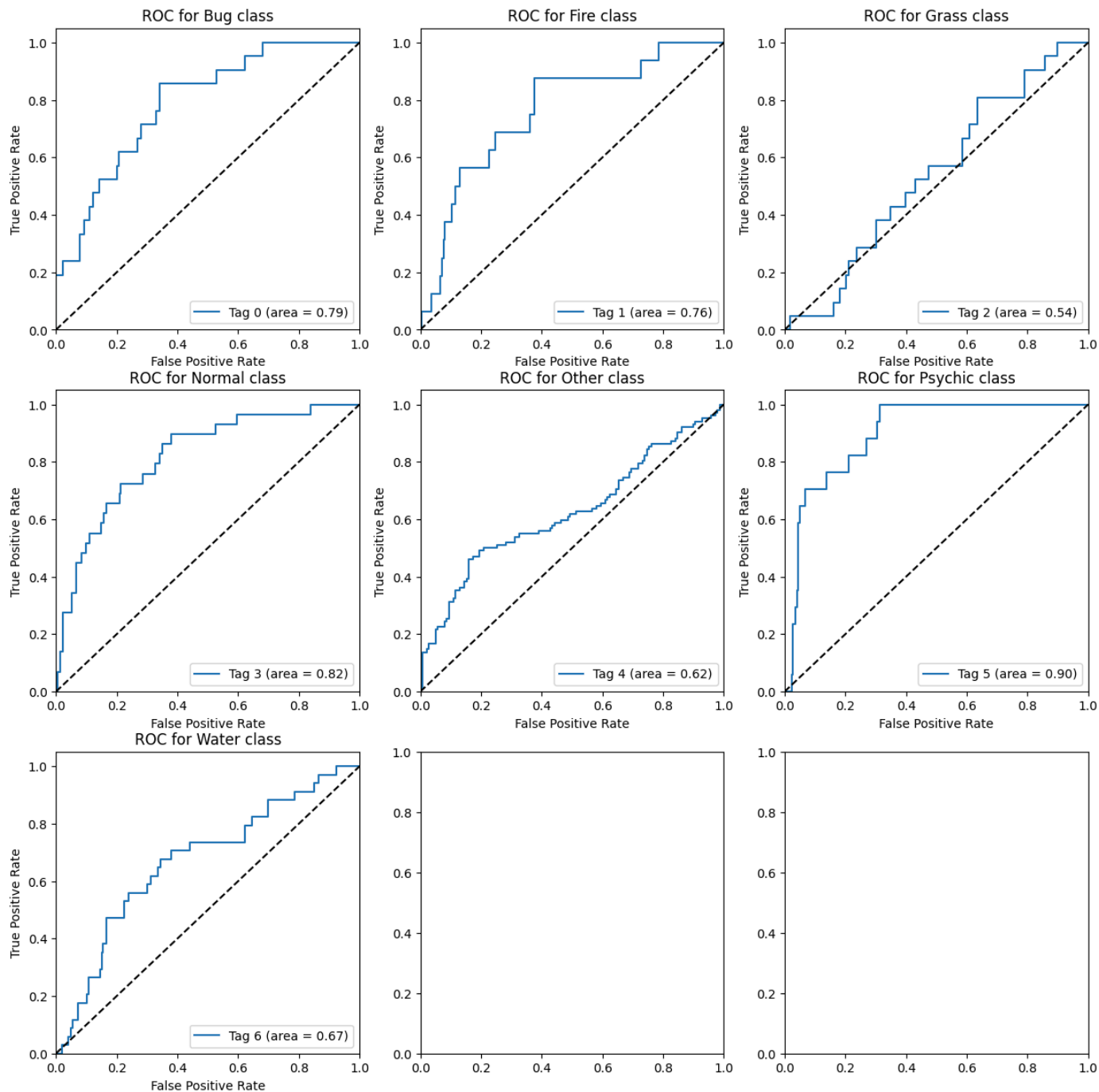
for i in range(n_classes):
    ax[i].plot(fpr[i], tpr[i], label=f'Tag {i} (area = {roc_auc[i]:.2f})')
    ax[i].plot([0, 1], [0, 1], 'k--')
    ax[i].set_xlim([0.0, 1.0])
    ax[i].set_ylim([0.0, 1.05])
    ax[i].set_xlabel('False Positive Rate')
    ax[i].set_ylabel('True Positive Rate')
    ax[i].set_title(f'ROC for {ivt[i]} class')
    ax[i].legend(loc="lower right")
```

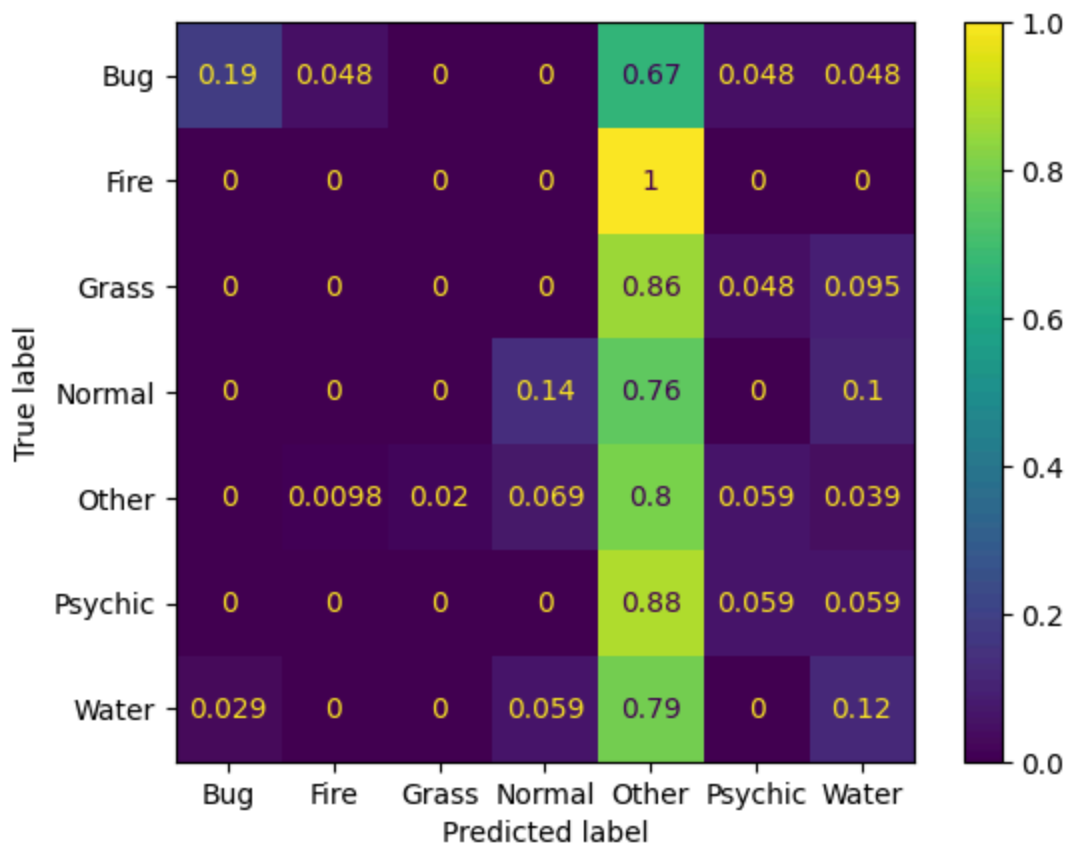
```
plt.show()
```

```
fig.tight_layout()
```

```
# Confusion matrix
```

```
inverse_transform = {i: val for i, val in enumerate(le_t1.inverse_transform(range(7)))}  
y_test_transform = [inverse_transform[num] for num in y_test]  
y_pred_transform = [inverse_transform[num] for num in rf_best.predict(x_test)]  
cm = confusion_matrix(y_test_transform, y_pred_transform, normalize='true')  
cm_display = ConfusionMatrixDisplay(cm, display_labels=[j for j in inverse_transform.values()])  
plt.show()
```





The model did well for predicting "Other", with an 86% success rate. We can see that the model did poorly for predicting classes besides "Other"; in fact, it predicted "Other" for almost every test point. This could be for a few reasons. First, there is a significant class imbalance in the data. As shown below, there are far more in the "Other" category than the rest. Even though we stratified for the train/test split and for the CV Splitting, the model is mostly seeing "Other" as the correct outcome. Hence, it makes sense that with seven possible outcomes, the outcome with the highest predicted probability is the one with the most data points.

The least accurate was for the "Grass" class, which we can see by looking at the ROC AUC curves. At certain thresholds, the model actually did worse than chance at predicting these outcomes.

```
In [ ]: data['type_1'].value_counts()
```

```
Out[ ]: type_1
4      342
6      112
3       98
2       70
0       69
5       57
1       52
Name: count, dtype: int64
```

Exercise 11

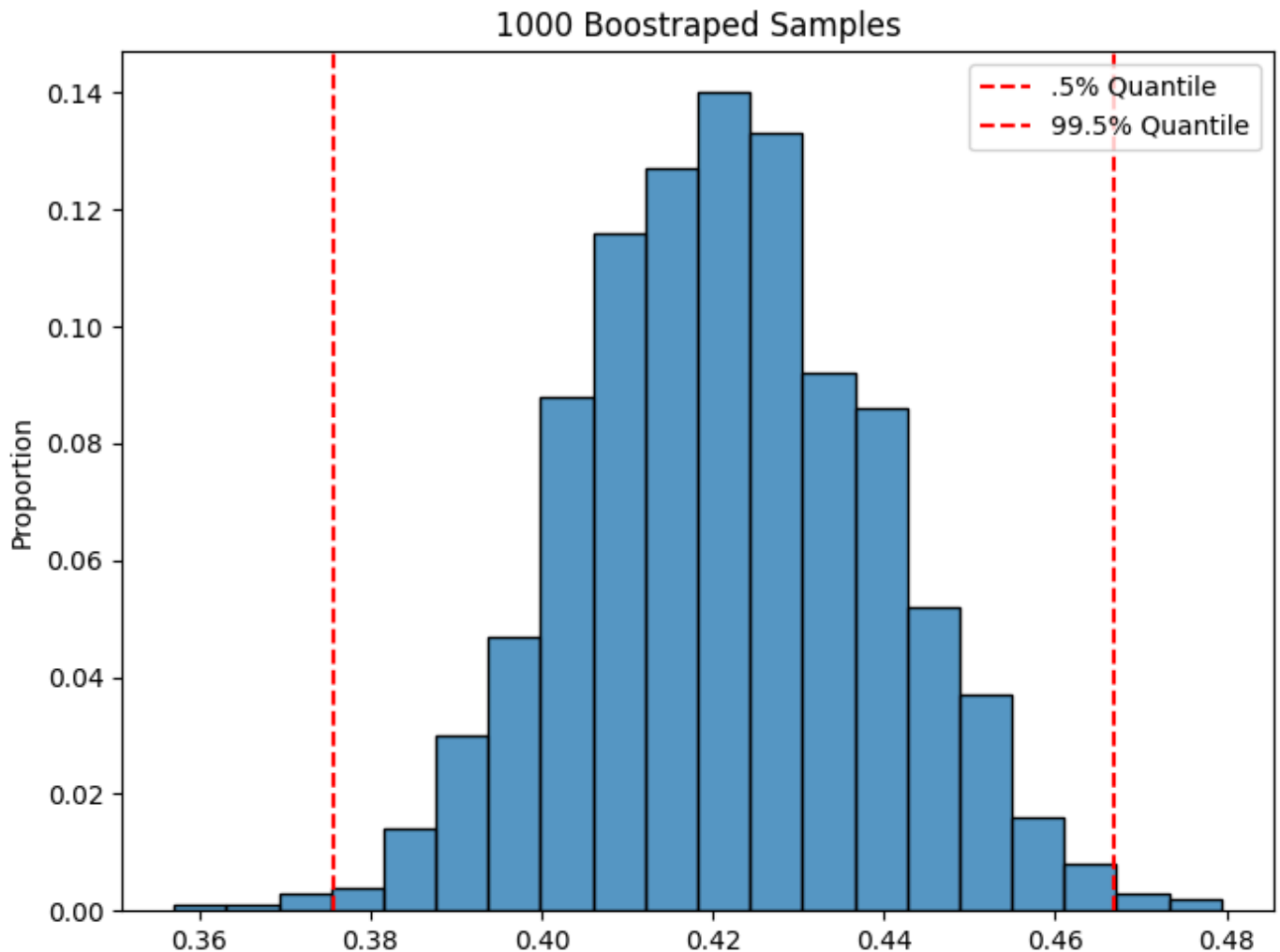
Bootstrap resampling of Steph Curry's 2020-2021 3 point attempts

```
In [ ]: data2 = np.concatenate((np.ones(337), np.zeros(464)))
```

```
In [ ]: from sklearn.utils import resample
```

```
emperical_means = []  
for _ in range(1000):  
    emperical_means.append(  
        np.mean(resample(data2))  
    )
```

```
In [ ]: plt.figure(figsize=(8,6))  
sns.histplot(emperical_means, bins=20, stat='proportion')  
plt.title('1000 Boostaped Samples')  
plt.axvline(np.quantile(emperical_means,.005), ls='--', c='r', label='.5% Quantile')  
plt.axvline(np.quantile(emperical_means,.995), ls='--', c='r', label='99.5% Quantile')  
plt.legend()  
plt.show()
```



```
In [ ]: print(f"99% Confidence Interval (Quantiles): {round(np.quantile(emperical_means,.005),3)}  
99% Confidence Interval (Quantiles): 0.376 - 0.467
```

Exercise 12

Random Forest for Abalone Data

```
In [ ]: data = pd.read_csv('HWs/HW5/Files/homework-5/data/abalone.csv')  
data['age'] = data['rings'] + 1.5
```

```

data = pd.get_dummies(data, columns=['type'],dtype=int, drop_first=True)
# Create interaction terms
data['shucked_weight*longest_shell'] = data['shucked_weight'] * data['longest_shell']
data['longest_shell*diameter'] = data['longest_shell'] * data['diameter']
data['shucked_weight*shell_weight'] = data['shucked_weight'] * data['shell_weight']

# Center and Scale Data
ss = StandardScaler()
pd.DataFrame(ss.fit_transform(data), columns=data.columns)

X = data.drop(['age', 'rings'], axis=1)
Y = data['age']

# Create train / test split
x_train, x_test, y_train, y_test = train_test_split(X,Y, test_size=.3, random_state=10)

x_train.reset_index(drop=True,inplace=True)
y_train.reset_index(drop=True, inplace=True)

print(f"Train data length check: {(len(x_train) == len(y_train)) and (len(x_train) == ma
print(f"Test data length check: {(len(x_test) == len(y_test)) and (len(x_test) == math.c

from sklearn.model_selection import KFold
kf = KFold(n_splits=5, shuffle=True,random_state=10)
indicies = []
for i, (train_index, test_index) in enumerate(kf.split(x_train)):
    indicies.append(
        (train_index,test_index)
    )

```

Train data length check: True

Test data length check: True

```

In [ ]: from sklearn.ensemble import RandomForestRegressor

params_rf = {'n_estimators': np.arange(10,116,15),
             'min_samples_split': np.arange(2,18,2),
             'max_features': [1,2,3,4,6,8,10,12]}

rf = RandomForestRegressor(n_jobs=-1,random_state=10)
rf_grid = GridSearchCV(
    estimator=rf,
    cv=indicies,
    param_grid=params_rf,
    scoring='neg_mean_squared_error',
    verbose=1).fit(x_train,y_train)

```

Fitting 5 folds for each of 512 candidates, totalling 2560 fits

```

In [ ]: rf_results_df = pd.DataFrame(rf_grid.cv_results_)

rf_results_trees, rf_results_mss, rf_results_max_feat = ([],[],[])

for trees in params_rf['n_estimators']:
    rf_results_trees.append(
        rf_results_df[rf_results_df['param_n_estimators'] == trees]['mean_test_score'].m
    )

for m in params_rf['min_samples_split']:
    rf_results_mss.append(
        rf_results_df[rf_results_df['param_min_samples_split'] == m]['mean_test_score'].
    )

for mf in params_rf['max_features']:

```

```

rf_results_max_feat.append(
    rf_results_df[rf_results_df['param_max_features'] == mf]['mean_test_score'].mean
)

```

```

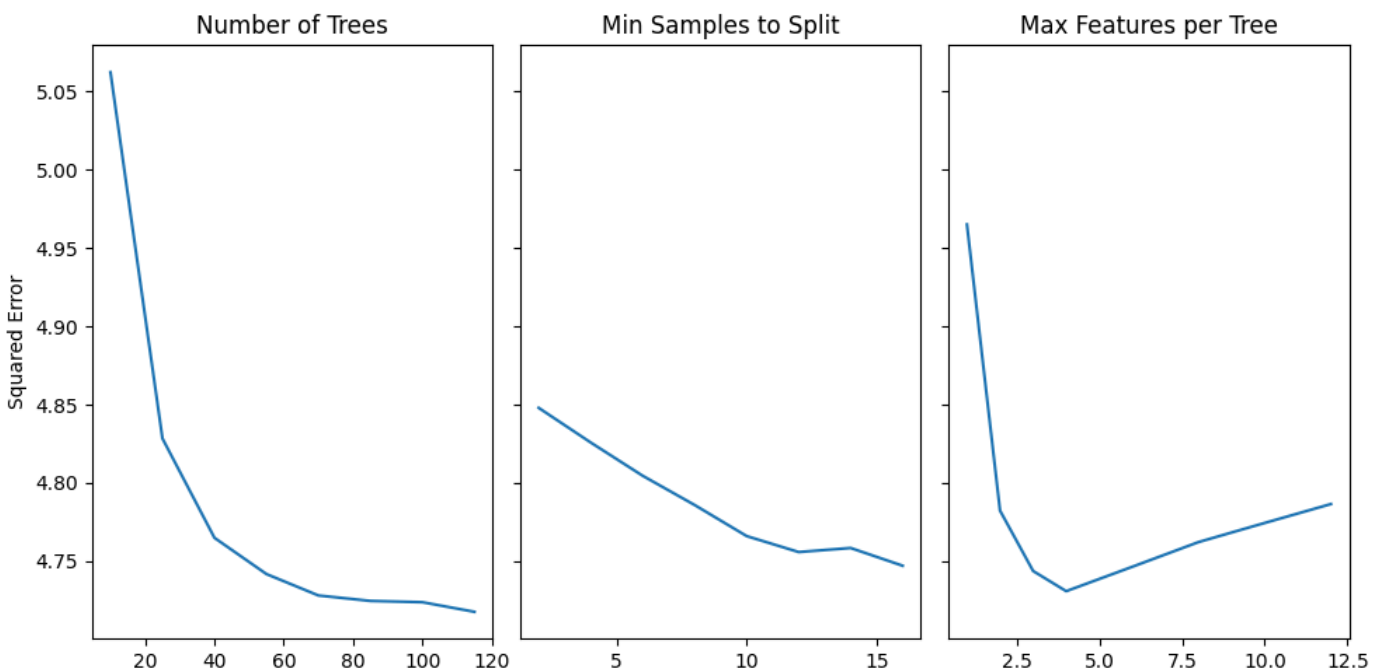
In [ ]: fig, ax = plt.subplots(1,3, sharey=True, figsize=(10,5))

plots = [rf_results_trees, rf_results_mss, rf_results_max_feat]
x_vals = [params_rf['n_estimators'], params_rf['min_samples_split'], params_rf['max_features']]
titles = ['Number of Trees', 'Min Samples to Split', 'Max Features per Tree']

for i in range(3):
    if i == 0: ax[i].set_ylabel('Squared Error')
    ax[i].plot(x_vals[i], plots[i])
    ax[i].set_title(titles[i])

fig.tight_layout()
plt.show()

```



Here we can see that for the training-set cross-validation results, more trees, more samples required to split an internal node, and a moderate amount of max features allowed per tree gave the best results.

```

In [ ]: print(f'The best parameter combination was" {rf_grid.best_params_}')

The best parameter combination was" {'max_features': 4, 'min_samples_split': 16, 'n_estimators': 70}

```

Now we will fit to the entire training set with these parameters and evaluate on the testing set.

```

In [ ]: from sklearn.metrics import mean_squared_error

rf = RandomForestRegressor(n_estimators=70, min_samples_split=16, max_features=4, n_jobs=-1)
rf_pred = rf.predict(x_test)

print(f"The final models RMSE on the test set was: {round(mean_squared_error(y_test, rf_pred), 3)}")

The final models RMSE on the test set was: 2.095

```