M6-HW2

October 16, 2023

1 Problem 7 (30 Points)

Data-driven field prediction models can be used as a substitute for performing expensive calculations/simulations in design loops. For example, after being trained on finite element solutions for many parts, they can be used to predict nodal von Mises stress for a new part by taking in a mesh representation of the part geometry.

Consider the plane-strain compression problem shown in "data/plane-strain.png".

In this problem you are given node features for 100 parts. These node features have been extracted by processing each part shape using a neural network. You will perform feature selection to determine which of these features are most relevant using feature selection tools in sklearn.

You are welcome to use any of the code provided in the lecture activities.

Summary of deliverables: SciKit-Learn Models: Print Train and Test MSE - `LinearRegression()` with all features - `DecisionTreeRegressor()` with all features - `LinearRegression()` with features selected by `RFE()` - `DecisionTreeRegressor()` with features selected by `RFE()`

Feature Importance/Coefficient Visualizations - Feature importance plot for Decision Tree using all features - Feature coefficient plot for Linear Regression using all features - Feature importance plot for DT showing which features RFE selected - Feature coefficient plot for LR showing which features RFE selected

Stress Field Visualizations: Ground Truth vs. Prediction - Test dataset shape index 8 for decision tree and linear regression with all features - Test dataset shape index 16 for decision tree and linear regression with RFE features

Questions - Respond to the 5 prompts at the end

Imports and Utility Functions:

```
[ ]: import numpy as np
     import matplotlib.pyplot as plt
     from sklearn.tree import DecisionTreeRegressor
     from sklearn.linear_model import LinearRegression
     from sklearn.metrics import mean_squared_error
     from sklearn.feature_selection import RFE

     def plot_shape(dataset, index, model=None, lims=None):
```

```
    x = dataset["coordinates"][index][:,0]
    y = dataset["coordinates"][index][:,1]

    if model is None:
        c = dataset["stress"][index]
    else:
        c = model.predict(dataset["features"][index])

    if lims is None:
        lims = [min(c),max(c)]

    plt.scatter(x,y,s=5,c=c,cmap="jet",vmin=lims[0],vmax=lims[1])
    plt.colorbar(orientation="horizontal", shrink=.75, pad=0,ticks=lims)
    plt.axis("off")
    plt.axis("equal")

def plot_shape_comparison(dataset, index, model, title=""):
    plt.figure(figsize=[6,3.2], dpi=120)
    plt.subplot(1,2,1)
    plot_shape(dataset,index)
    plt.title("Ground Truth",fontsize=9,y=.96)
    plt.subplot(1,2,2)
    c = dataset["stress"][index]
    plot_shape(dataset, index, model, lims = [min(c), max(c)])
    plt.title("Prediction",fontsize=9,y=.96)
    plt.suptitle(title)
    plt.show()

def load_dataset(path):
    dataset = np.load(path)
    coordinates = []
    features = []
    stress = []
    N = np.max(dataset[:,0].astype(int)) + 1
    split = int(N*.8)
    for i in range(N):
        idx = dataset[:,0].astype(int) == i
        data = dataset[idx,:]
        coordinates.append(data[:,1:3])
        features.append(data[:,3:-1])
        stress.append(data[:,-1])
    dataset_train = dict(coordinates=coordinates[:split], features=features[:
 ↪split], stress=stress[:split])
    dataset_test = dict(coordinates=coordinates[split:],␣
 ↪features=features[split:], stress=stress[split:])
    X_train, X_test = np.concatenate(features[:split], axis=0), np.
 ↪concatenate(features[split:], axis=0)
```

```
    y_train, y_test = np.concatenate(stress[:split], axis=0), np.
  ↪concatenate(stress[split:], axis=0)
    return dataset_train, dataset_test, X_train, X_test, y_train, y_test

def get_shape(dataset,index):
    X = dataset["features"][index]
    y = dataset["stress"][index]
    return X, y

def plot_importances(model, selected = None, coef=False, title=""):
    plt.figure(figsize=(6,2),dpi=150)
    y = model.coef_ if coef else model.feature_importances_
    N = 1+len(y)
    x = np.arange(1,N)

    plt.bar(x,y)

    if selected is not None:
        plt.bar(x[selected],y[selected],color="red",label="Selected Features")
        plt.legend()

    plt.xlabel("Feature")

    plt.ylabel("Coefficient" if coef else "Importance")
    plt.xlim(0,N)
    plt.title(title)
    plt.show()
```

1.1 Loading the data

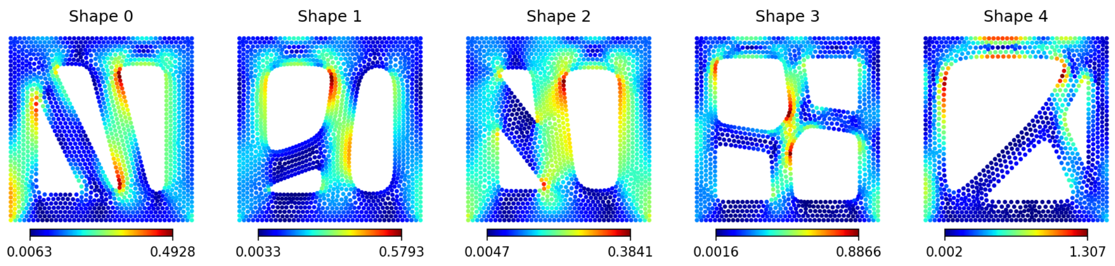
First, complete the code below to load the data and plot the von Mises stress fields for a few shapes. You'll need to input the path of the data file, the rest is done for you.

All training node features and outputs are in `X_train` and `y_train`, respectively. Testing nodes are in `X_test`, `y_test`.

`dataset_train` and `dataset_test` contain more detailed information such as node coordinates, and they are separated by shape.
Get features and outputs for a shape by calling `get_shape(dataset,index)`. `N_train` and `N_test` are the number of training and testing shapes in each of these datasets.

[ ]:
```
dataset_train, dataset_test, X_train, X_test, y_train, y_test =␣
  ↪load_dataset("data/stress_nodal_features.npy")
N_train = len(dataset_train["stress"])
N_test = len(dataset_test["stress"])

plt.figure(figsize=[15,3.2], dpi=150)
for i in range(5):
    plt.subplot(1,5,i+1)
    plot_shape(dataset_train,i)
    plt.title(f"Shape {i}")
plt.show()
```



1.2 Fitting models with all features

Create two models to fit the training data `X_train`, `y_train`: 1. A `LinearRegression()` model 2. A `DecisionTreeRegressor()` model with a `max_depth` of 20

Print the training and testing MSE for each.

[ ]:
```
linear_regression_model = LinearRegression()
linear_regression_model.fit(X_train, y_train)

decision_tree_regressor_model = DecisionTreeRegressor(max_depth=20)
decision_tree_regressor_model.fit(X_train, y_train)

print("Linear Regression Model")
print(f"\tTrain MSE: {mean_squared_error(y_train, linear_regression_model.
 ↪predict(X_train))}")
print(f"\tTest MSE: {mean_squared_error(y_test, linear_regression_model.
 ↪predict(X_test))}")
print()

print("Decision Tree Regressor Model")
print(f"\tTrain MSE: {mean_squared_error(y_train, decision_tree_regressor_model.
 ↪predict(X_train))}")
print(f"\tTest MSE: {mean_squared_error(y_test, decision_tree_regressor_model.
 ↪predict(X_test))}")
print()
```

```
Linear Regression Model
        Train MSE: 0.00811060145497322
        Test MSE: 0.009779482148587704

Decision Tree Regressor Model
        Train MSE: 0.0004944875978805109
```

```
Test MSE: 0.008197317473637781
```

1.3 Visualization

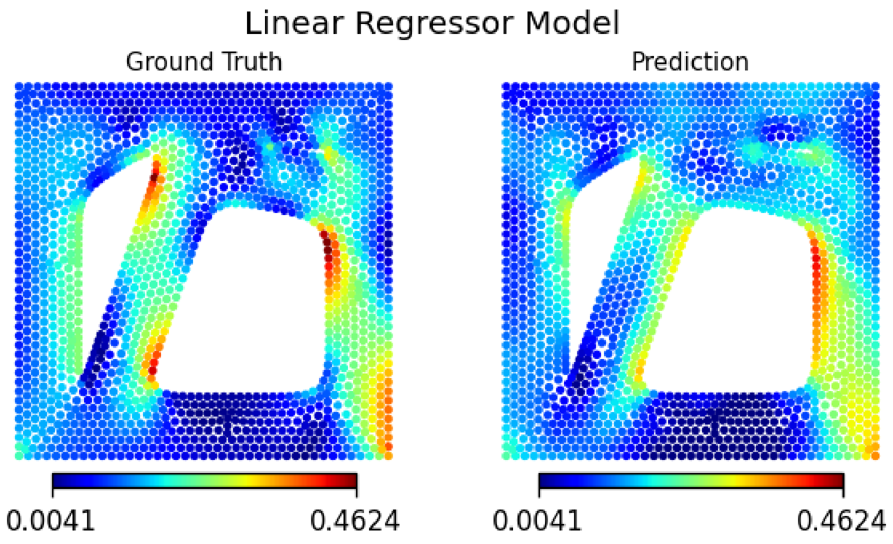
Use the `plot_shape_comparison()` function to plot the index 8 shape results in `dataset_test` for each model.

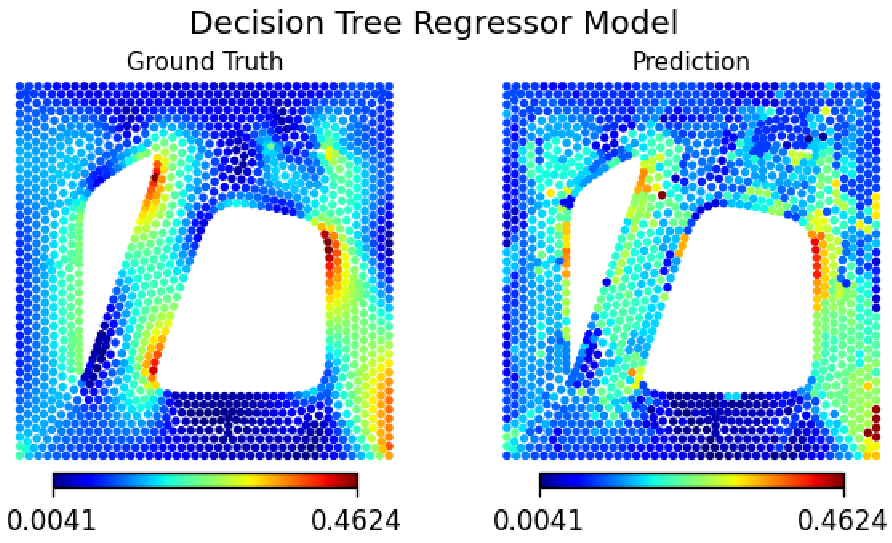
Include titles to indicate which plot is which, using the `title` argument.

```
[ ]: test_idx = 8

     plot_shape_comparison(dataset_test, test_idx, linear_regression_model, "Linear␣
      ↪Regressor Model")

     plot_shape_comparison(dataset_test, test_idx, decision_tree_regressor_model,␣
      ↪"Decision Tree Regressor Model")
```



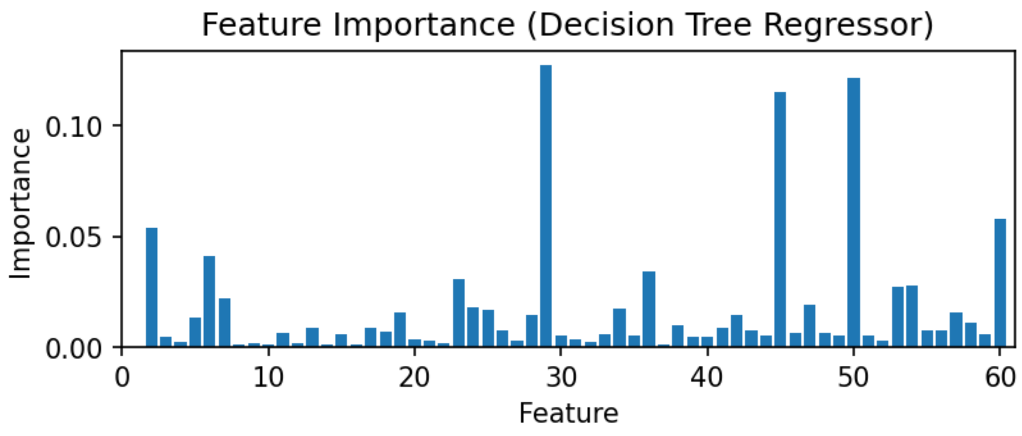


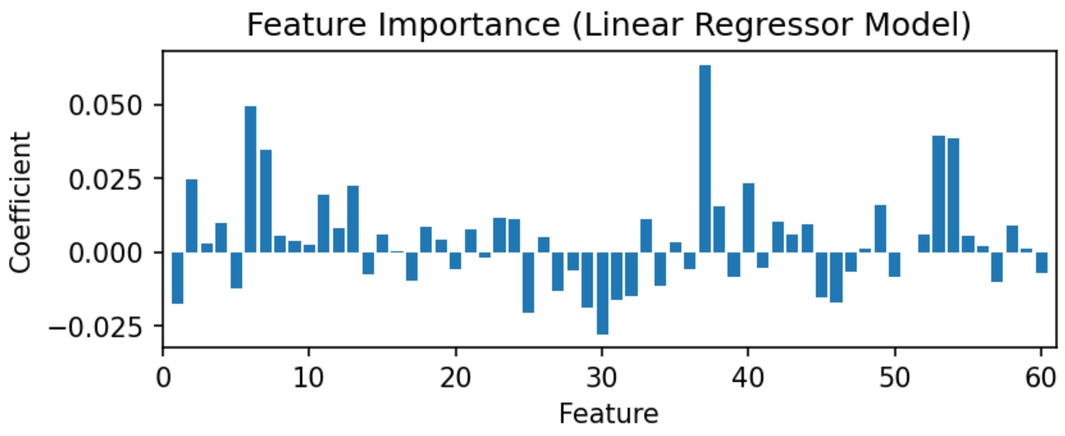
1.4 Feature importance

For a tree methods, "feature importance" can be computed, which can be done for an sklearn model using `.feature_importances_`.

Use the provided function `plot_importances()` to visualize which features are most important to the final decision tree prediction.
Then create another plot using the same function to visualize the linear regression coefficients by setting the "coef" argument to `True`.

```
[ ]: plot_importances(decision_tree_regressor_model, title="Feature Importance␣
       ↪(Decision Tree Regressor)")
     plot_importances(linear_regression_model, coef=True, title="Feature Importance␣
       ↪(Linear Regressor Model)")
```





1.5 Feature Selection by Recursive Feature Elimination

Using `RFE()` in sklearn, you can iteratively select a subset of only the most important features.

For both linear regression and decision tree (depth 20) models: 1. Create a new model. 2. Create an instance of `RFE()` with `n_features_to_select` set to 30. 3. Fit the RFE model as you would a normal sklearn model. 4. Report the train and test MSE.

Note that the decision tree RFE model may take a few minutes to train.
Visit https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.RFE.html for more information.

```
[ ]: linear_regression_RFE = RFE(LinearRegression(), n_features_to_select=30)
     decision_tree_RFE = RFE(DecisionTreeRegressor(max_depth=20),␣
      ↪n_features_to_select=30)

     linear_regression_RFE.fit(X_train, y_train)
     decision_tree_RFE.fit(X_train, y_train)

     print("Linear Regression RFE")
     print(f"\tTrain MSE: {mean_squared_error(y_train, linear_regression_RFE.
      ↪predict(X_train))}")
     print(f"\tTest MSE: {mean_squared_error(y_test, linear_regression_RFE.
      ↪predict(X_test))}")
     print()

     print("Decision Tree RFE")
     print(f"\tTrain MSE: {mean_squared_error(y_train, decision_tree_RFE.
      ↪predict(X_train))}")
     print(f"\tTest MSE: {mean_squared_error(y_test, decision_tree_RFE.
      ↪predict(X_test))}")
```

```
print()
```

```
Linear Regression RFE
        Train MSE: 0.008508717641234398
        Test MSE: 0.01015037577599287

Decision Tree RFE
        Train MSE: 0.0005351821126843501
        Test MSE: 0.009160064414859462
```

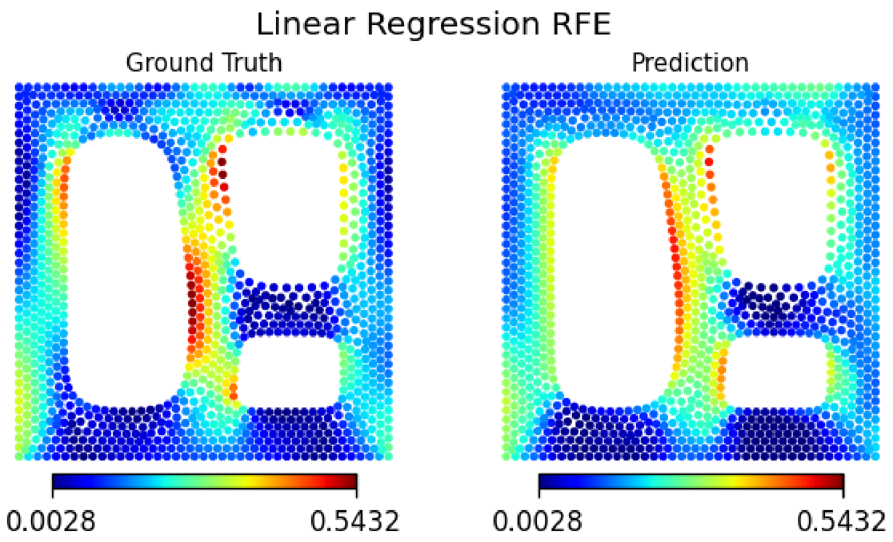
1.6 Visualization

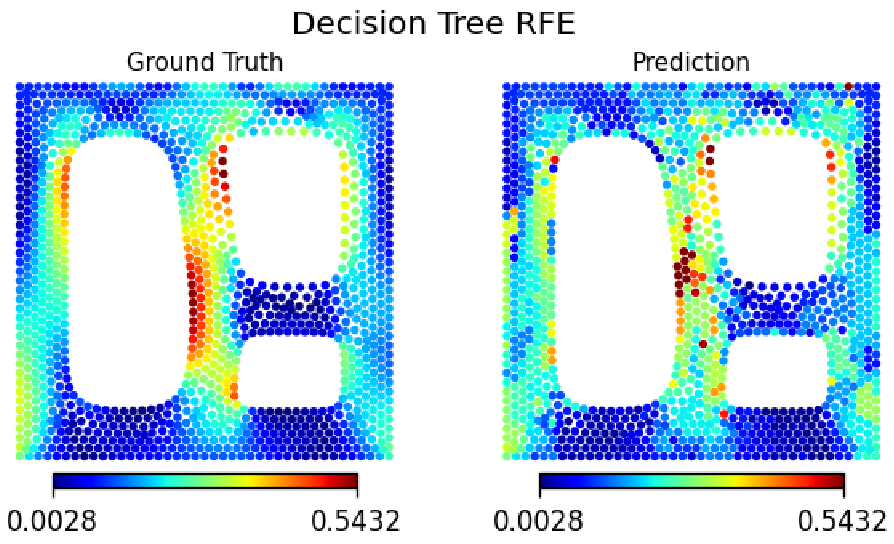
Use the `plot_shape_comparison()` function to plot the index 16 shape results in `dataset_test` for each model.

As before, include titles to indicate which plot is which, using the `title` argument.

```
[ ]: test_idx = 16

plot_shape_comparison(dataset_test, test_idx, linear_regression_RFE, "Linear␣
↪Regression RFE")
plot_shape_comparison(dataset_test, test_idx, decision_tree_RFE, "Decision Tree␣
↪RFE")
```





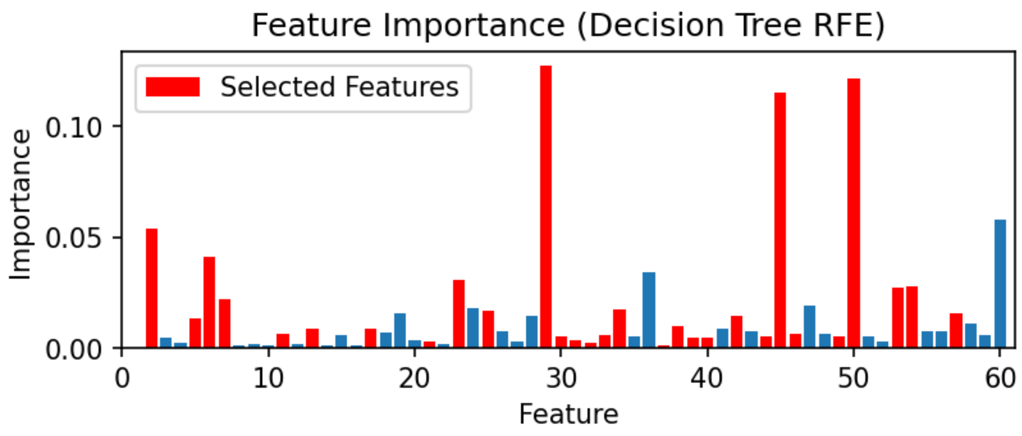
1.7 Feature importance with RFE

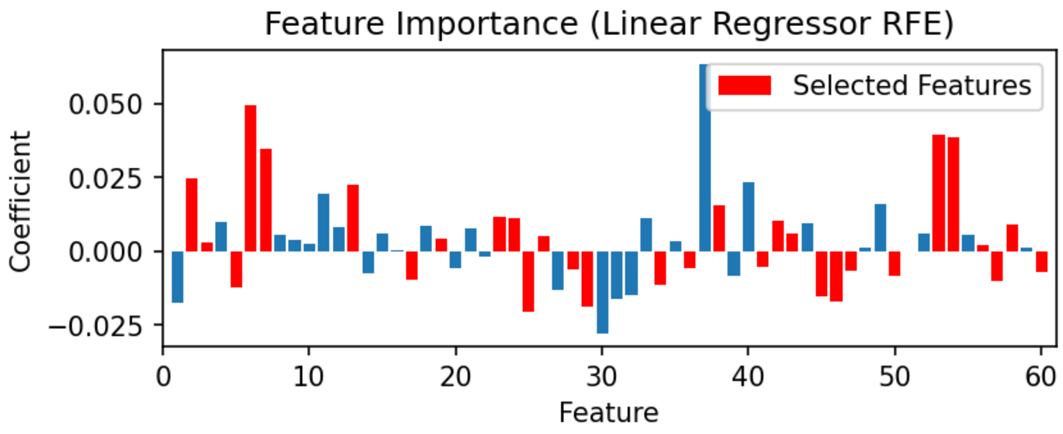
Recreate the 2 feature importance/coefficent plots from earlier, but this time highlight which features were ultimately selected after performing RFE by coloring those features red. You can do this by setting the `selected` argument equal to an array of selected indices.

For an RFE model `rfe`, the selected feature indices can be obtained via `rfe.get_support(indices=True)`.

[ ]:
```
linear_regression_indices = linear_regression_RFE.get_support(indices=True)
decision_tree_indices = decision_tree_RFE.get_support(indices=True)

plot_importances(decision_tree_regressor_model,␣
 ↪selected=linear_regression_indices, coef=False, title="Feature Importance␣
 ↪(Decision Tree RFE)")
plot_importances(linear_regression_model, selected=decision_tree_indices,␣
 ↪coef=True, title="Feature Importance (Linear Regressor RFE)")
```





1.8 Questions

1. Did the MSE increase or decrease on test data for the Linear Regression model after performing RFE?

   The MSE decreased after performing RFE but only by a marginal amount.

2. Did the MSE increase or decrease on test data for the Decision Tree model after performing RFE?

   The MSE decreased after performing RFE but only by a marginal amount.

3. Describe the qualitative differences between the Linear Regression and the Decision Tree predictions.

   The linear regression model has a much more smooth profile of stress concentration change across the surface whereas the decision tree model has very sharp changes in the stress concentration predictions. In addition, the decision tree model is able to predict higher stress concentrations than the linear regressor model is able to do.

4. Describe how the importance of features that were selected by RFE compare to that of features that were eliminated (for the decision tree).

   In general it seems that the higher importance features had larger coefficients for the decision tree model. While this isn't a perfect match to the data, in general the model chose features with high coefficients as more important.

5. Describe how the coefficients that were selected by RFE compare to that of features that were eliminated (for linear regression).

   This model seemed to choose a variety of features with a range of coefficients seemingly around the average of the whole of the coefficients. This is much different to the decision tree feature importance because it doesn't seem to care too much about how large a feature's coefficient is in determining importance.