Feature Selection for Machine Learning

This section lists 4 feature selection recipes for machine learning in Python

This post contains recipes for feature selection methods.

Each recipe was designed to be complete and standalone so that you can copy-and-paste it directly into you project and use it immediately.

Recipes uses the Pima Indians onset of diabetes dataset to demonstrate the feature selection method . This is a binary classification problem where all of the attributes are numeric.

Dataset File. Dataset Details.

Univariate Selection

Statistical tests can be used to select those features that have the strongest relationship with the output variable.

The scikit-learn library provides the SelectKBest class that can be used with a suite of different statistical tests to select a specific number of features.

Many different statistical test scan be used with this selection method. For example the ANOVA F-value method is appropriate for numerical inputs and categorical data, as we see in the Pima dataset. This can be used via the f_classif() function. We will select the 4 best features using this method in the example below.

```
In [ ]: # Feature Selection with Univariate Statistical Tests
        from pandas import read csv
        from numpy import set printoptions
        from sklearn.feature selection import SelectKBest
        from sklearn.feature selection import f classif
        # load data
        filename = './pima-indians-diabetes.csv'
        names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'cla
        dataframe = read csv(filename, names=names)
        array = dataframe.values
        X = array[:,0:8]
        Y = array[:,8]
        # feature extraction
        test = SelectKBest(score func=f classif, k=4)
        fit = test.fit(X, Y)
        # summarize scores
        set printoptions(precision=3)
        print(fit.scores )
        features = fit.transform(X)
```

```
# summarize selected features
print(features[0:5,:])
[ 39.67 213.162
                 3.257
                        4.304 13.281 71.772 23.871 46.1411
[[ 6. 148.
            33.6 50. ]
  1.
       85.
             26.6 31. ]
 [ 8. 183. 23.3 32.]
   1.
       89.
             28.1 21. ]
   0. 137.
             43.1 33.]]
 Γ
```

For help on which statistical measure to use for your data, see the tutorial:

How to Choose a Feature Selection Method For Machine Learning Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

You can see the scores for each attribute and the 4 attributes chosen (those with the highest scores). Specifically features with indexes 0 (preq), 1 (plas), 5 (mass), and 7 (age).

Recursive Feature Elimination

The Recursive Feature Elimination (or RFE) works by recursively removing attributes and building a model on those attributes that remain.

It uses the model accuracy to identify which attributes (and combination of attributes) contribute the most to predicting the target attribute.

You can learn more about the RFE class in the scikit-learn documentation.

The example below uses RFE with the logistic regression algorithm to select the top 3 features. The choice of algorithm does not matter too much as long as it is skillful and consistent.

```
In [ ]: from pandas import read csv
        from sklearn.feature selection import RFE
        from sklearn.linear model import LogisticRegression
        # load data
        url = "./pima-indians-diabetes.csv"
        names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'cla
        dataframe = read csv(url, names=names)
        array = dataframe.values
        X = array[:,0:8]
        Y = array[:,8]
        # feature extraction
        model = LogisticRegression(solver='lbfgs', max iter=1000)
        rfe = RFE(model, n features to select=3)
        fit = rfe.fit(X, Y)
        print("Num Features: %d" % fit.n features )
        print("Selected Features: %s" % fit.support )
        print("Feature Ranking: %s" % fit.ranking )
```

```
Num Features: 3
Selected Features: [ True False False False False True True False]
Feature Ranking: [1 2 4 6 5 1 1 3]
```

You can see that RFE chose the top 3 features as preg, mass and pedi.

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

These are marked True in the support_ array and marked with a choice "1" in the ranking_ array.

Principal Component Analysis

Principal Component Analysis (or PCA) uses linear algebra to transform the dataset into a compressed form.

Generally this is called a data reduction technique. A property of PCA is that you can choose the number of dimensions or principal component in the transformed result.

In the example below, we use PCA and select 3 principal components.

Learn more about the PCA class in scikit-learn by reviewing the PCA API. Dive deeper into the math behind PCA on the Principal Component Analysis Wikipedia article.

```
In [ ]: # Feature Extraction with PCA
        import numpy
        from pandas import read csv
        from sklearn.decomposition import PCA
        # load data
        url = "./pima-indians-diabetes.csv"
        names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'cla
        dataframe = read csv(url, names=names)
        array = dataframe.values
        X = array[:,0:8]
        Y = array[:,8]
        # feature extraction
        pca = PCA(n components=3)
        fit = pca.fit(X)
        # summarize components
        print("Explained Variance: %s" % fit.explained variance ratio )
        print(fit.components )
        Explained Variance: [0.889 0.062 0.026]
        [[-2.022e-03 9.781e-02 1.609e-02 6.076e-02 9.931e-01 1.401e-02
           5.372e-04 -3.565e-03]
         [-2.265e-02 -9.722e-01 -1.419e-01 5.786e-02 9.463e-02 -4.697e-02
          -8.168e-04 -1.402e-01]
         [-2.246e-02 1.434e-01 -9.225e-01 -3.070e-01 2.098e-02 -1.324e-01
          -6.400e-04 -1.255e-01]]
```

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

You can see that the transformed dataset (3 principal components) bare little resemblance to the source data.

Feature Importance

Bagged decision trees like Random Forest and Extra Trees can be used to estimate the importance of features.

In the example below we construct a ExtraTreesClassifier classifier for the Pima Indians onset of diabetes dataset. You can learn more about the ExtraTreesClassifier class in the scikit-learn API.

```
In []: from pandas import read_csv
    from sklearn.ensemble import ExtraTreesClassifier
    # load data
    url = "./pima-indians-diabetes.csv"
    names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'cladataframe = read_csv(url, names=names)
    array = dataframe.values
    X = array[:,0:8]
    Y = array[:,8]
    # feature extraction
    model = ExtraTreesClassifier(n_estimators=10)
    model.fit(X, Y)
    print(model.feature_importances_)
```

[0.106 0.244 0.105 0.085 0.08 0.141 0.109 0.129]

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

You can see that we are given an importance score for each attribute where the larger score the more important the attribute. The scores suggest at the importance of plas, age and mass.

Summary

In this post you discovered feature selection for preparing machine learning data in Python with scikit-learn.

You learned about 4 different automatic feature selection techniques:

Univariate Selection. Recursive Feature Elimination. Principle Component Analysis. Feature Importance. If you are looking for more information on feature selection, see these related posts:

Feature Selection with the Caret R Package Feature Selection to Improve Accuracy and Decrease Training Time An Introduction to Feature Selection Feature Selection in Python with Scikit-Learn Do you have any questions about feature selection or this post? Ask your questions in the comment and I will do my best to answer them.

Feature importance

This notebook is part of the following blogpost: https://medium.com/bigdatarepublic/feature-importance-whats-in-a-name-79532e59eea3

#Install non-standard packages (assuming jupyter notebook)

Install dependencies

!pip install shap

```
!pip install lime
!pip install eli5
    Looking in indexes: <a href="https://pypi.org/simple">https://us-python.pkg.dev/colab-w</a>
    Collecting lime
      Downloading lime-0.2.0.1.tar.gz (275 kB)
                                                - 275.7/275.7 KB 4.4 MB/s eta 0:00:
      Preparing metadata (setup.py) ... done
    Requirement already satisfied: matplotlib in /usr/local/lib/python3.9/dist-pac
    Requirement already satisfied: numpy in /usr/local/lib/python3.9/dist-packages
    Requirement already satisfied: scipy in /usr/local/lib/python3.9/dist-packages
    Requirement already satisfied: tqdm in /usr/local/lib/python3.9/dist-packages
    Requirement already satisfied: scikit-learn>=0.18 in /usr/local/lib/python3.9/
    Requirement already satisfied: scikit-image>=0.12 in /usr/local/lib/python3.9/
    Requirement already satisfied: networkx>=2.2 in /usr/local/lib/python3.9/dist-
    Requirement already satisfied: pillow!=7.1.0,!=7.1.1,!=8.3.0,>=6.1.0 in /usr/l
    Requirement already satisfied: imageio>=2.4.1 in /usr/local/lib/python3.9/dist
    Requirement already satisfied: packaging>=20.0 in /usr/local/lib/python3.9/dis
    Requirement already satisfied: tifffile>=2019.7.26 in /usr/local/lib/python3.9
    Requirement already satisfied: PyWavelets>=1.1.1 in /usr/local/lib/python3.9/d
    Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.
    Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.9/dist-
    Requirement already satisfied: cycler>=0.10 in /usr/local/lib/python3.9/dist-p
    Requirement already satisfied: contourpy>=1.0.1 in /usr/local/lib/python3.9/di
    Requirement already satisfied: importlib-resources>=3.2.0 in /usr/local/lib/py
    Requirement already satisfied: kiwisolver>=1.0.1 in /usr/local/lib/python3.9/d
    Requirement already satisfied: pyparsing>=2.3.1 in /usr/local/lib/python3.9/di
    Requirement already satisfied: python-dateutil>=2.7 in /usr/local/lib/python3.
    Requirement already satisfied: fonttools>=4.22.0 in /usr/local/lib/python3.9/d
    Requirement already satisfied: zipp>=3.1.0 in /usr/local/lib/python3.9/dist-pa
    Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.9/dist-packa
    Building wheels for collected packages: lime
      Building wheel for lime (setup.py) ... done
      Created wheel for lime: filename=lime-0.2.0.1-py3-none-any.whl size=283859 s
```

Successfully built lime

Stored in directory: /root/.cache/pip/wheels/ed/d7/c9/5a0130d06d6310bc6cbe55

```
Successibly putil time
Installing collected packages: lime
Successfully installed lime-0.2.0.1
Looking in indexes: <a href="https://pypi.org/simple">https://us-python.pkg.dev/colab-w</a>
Collecting eli5
  Downloading eli5-0.13.0.tar.gz (216 kB)
                                           - 216.2/216.2 KB 4.6 MB/s eta 0:00:
  Preparing metadata (setup.py) ... done
Requirement already satisfied: attrs>17.1.0 in /usr/local/lib/python3.9/dist-p
Requirement already satisfied: jinja2>=3.0.0 in /usr/local/lib/python3.9/dist-
Requirement already satisfied: numpy>=1.9.0 in /usr/local/lib/python3.9/dist-p
Requirement already satisfied: scipy in /usr/local/lib/python3.9/dist-packages
Requirement already satisfied: six in /usr/local/lib/python3.9/dist-packages (
Requirement already satisfied: scikit-learn>=0.20 in /usr/local/lib/python3.9/
Requirement already satisfied: graphviz in /usr/local/lib/python3.9/dist-packa
Requirement already satisfied: tabulate>=0.7.7 in /usr/local/lib/python3.9/dis
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.9/dis
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.
Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.9/dist-
Building wheels for collected packages: eli5
  Building wheel for eli5 (setup.py) ... done
  Created wheel for eli5: filename=eli5-0.13.0-py2.py3-none-any.whl size=10774
  Stored in directory: /root/.cache/pip/wheels/7b/26/a5/8460416695a992a2966b41
Successfully built eli5
Installing collected packages: eli5
```

Import packages

```
#Imports
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import itertools
#scikit-learn package (https://pypi.org/project/scikit-learn)
from sklearn.model selection import train test split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, confusion_matrix, roc_curve, auc, roc_auc
from sklearn.metrics import make scorer
#eli5 package (https://eli5.readthedocs.io/en/latest)
import eli5
from eli5.sklearn import PermutationImportance
#lime package (https://github.com/marcotcr/lime)
import lime
import lime.lime tabular
#shap package (https://github.com/slundberg/shap)
import shap
```

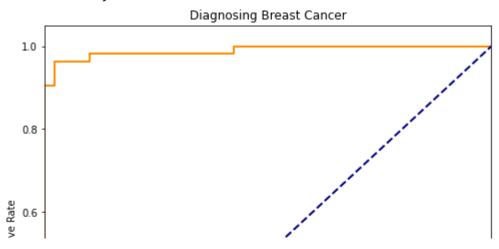
Load data and train model

```
#Load Wisconsin diagnostic breast cancer data from UCI #
url prefix = "https://archive.ics.uci.edu/ml/machine-learning-databases/"
#if url url does not work you can use this mirror instead:
#url_prefix = "http://mlr.cs.umass.edu/ml/machine-learning-databases/"
data url = url prefix + "breast-cancer-wisconsin/wdbc.data"
#Define column labels
id status = ["ID", "diagnosis"]
#Mean, standard error and maximum ('worst') values are available for features
#computed on a collection of cells in a tissue
column labels = itertools.product(["radius", "texture", "perimeter", "area",
                                  "smoothness", "compactness", "concavity",
                                  "concave_points", "symmetry", "fractal_dim"],
                                 ["mean", "std", "max"])
column_labels = id_status + [f"{t}_{f}" for f, t in column_labels]
#Read into pandas DataFrame
df = pd.read csv(data url, header=None, names = column labels)
#Define feature set
X = df.drop('ID', axis=1).drop('diagnosis', axis=1)
#Define diagnosis as integer: malignant (1) or benign (0)
y = (df['diagnosis'] == "M")*1
#Split train and test set.
RANDOM STATE = 123
X train, X test, y train, y test = train test split(X, y, test size=0.25,
                                                     stratify=y,
                                                     random state=RANDOM STATE)
#Train random forest classification model
model = RandomForestClassifier(max depth=4, random state=RANDOM STATE)
model.fit(X_train, y_train)
# Diagnosis prediction
y predict = model.predict(X test)
# Probability of malignant tissue produced by the model
y prob = [probs[1] for probs in model.predict proba(X test)]
```

Evaluate model

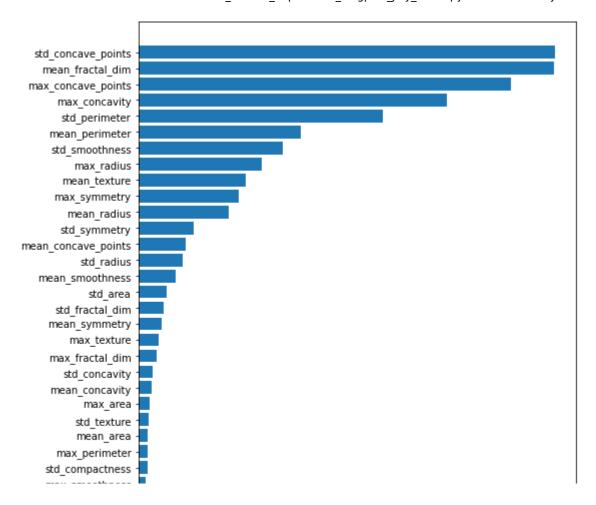
```
#Accuracy on test set
print(f"Test accuracy: {accuracy_score(y_test, y_predict).round(2)}")
# Confusion matrix test set
pd.DataFrame(
    confusion_matrix(y_test, y_predict),
    columns=['Predicted Benign', 'Predicted Malignant'],
    index=['Benign', 'Malignant']
)
# Compute area under the curve
fpr, tpr, _ = roc_curve(y_test, y_prob)
roc_auc = auc(fpr, tpr)
#Set default figure size
plt.rcParams['figure.figsize'] = (8,8)
# Plot ROC curve
plt.figure()
lw = 2
plt.plot(fpr, tpr, color='darkorange',
         lw=lw, label='ROC curve (area = %0.2f)' % roc_auc)
plt.plot([0, 1], [0, 1], color='navy', lw=lw, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title("Diagnosing Breast Cancer")
plt.legend(loc="lower right")
plt.show()
```

Test accuracy: 0.97



Model-specific feature importance

```
# Feature importance dataframe
imp_df = pd.DataFrame({'feature': X_train.columns.values,
                        'importance': model.feature_importances_})
# Reorder by importance
ordered_df = imp_df.sort_values(by='importance')
imp_range=range(1,len(imp_df.index)+1)
## Barplot with confidence intervals
height = ordered_df['importance']
bars = ordered_df['feature']
y_pos = np.arange(len(bars))
# Create horizontal bars
plt.barh(y_pos, height)
# Create names on the y-axis
plt.yticks(y_pos, bars)
plt.xlabel("Mean reduction in tree impurity in random forest")
plt.tight layout()
# Show graphic
plt.show()
```

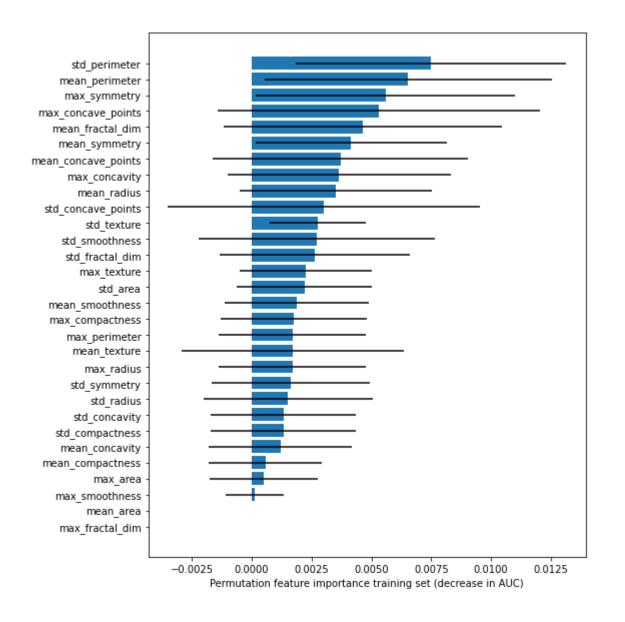


Permutation feature importance

ci = 1.96 * ordered df['std']

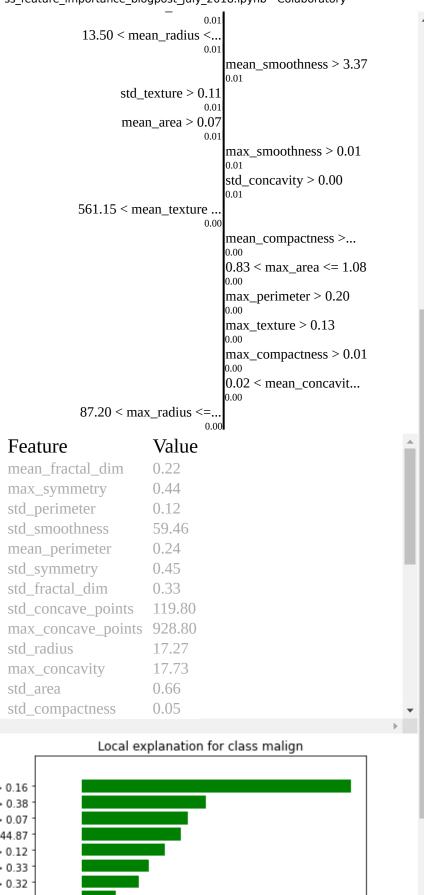
```
0.08
                                                     0.10
                                                             0.12
                                                                    0.14
# Feature importance based on TRAINING set
perm test = PermutationImportance(model, scoring=make scorer(roc auc score),
                                    n_iter=50, random_state=RANDOM_STATE, cv="prefit")
# fit and see the permuation importances
perm_test.fit(X_train, y_train)
imp_df = eli5.explain_weights_df(perm_test)
label_df = pd.DataFrame({'feature': [ "x" + str(i) for i in range(len(X_test.columns)
imp_df = pd.merge(label_df, imp_df, on='feature', how='inner', validate="one_to_one")
# Reorder by importance
ordered_df = imp_df.sort_values(by='weight')
imp_range=range(1,len(imp_df.index)+1)
## Barplot with confidence intervals
height = ordered_df['weight']
bars = ordered_df['feature_name']
```

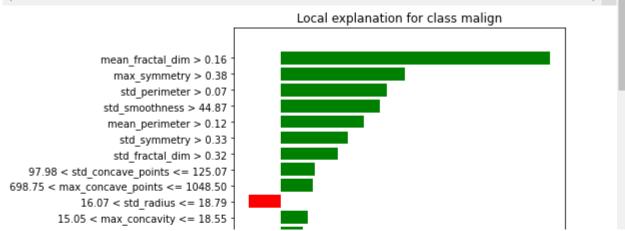
```
y_pos = np.arange(len(bars))
# Create horizontal bars
plt.barh(y_pos, height, xerr=ci)
# Create names on the y-axis
plt.yticks(y_pos, bars)
plt.xlabel("Permutation feature importance training set (decrease in AUC)")
plt.tight_layout()
# Show graphic
plt.show()
```



- LIME

```
#Explain samples in test set
X_{explain} = X_{test}
explainer = lime.lime tabular.LimeTabularExplainer(training data=X train.values,
                                                    feature_names=X_train.columns.valu
                                                    discretize continuous=True,
                                                    class_names=["benign", "malign"],
                                                    mode="classification",
                                                    verbose=True,
                                                    random_state=RANDOM_STATE)
#Explaining first subject in test set using all 30 features
exp = explainer.explain_instance(X_explain.values[0,:],model.predict_proba,
                                 num_features=30)
#Plot local explanation
plt = exp.as_pyplot_figure()
plt.tight_layout()
exp.show_in_notebook(show_table=True)
```





explain the model's predictions on test set using SHAP values

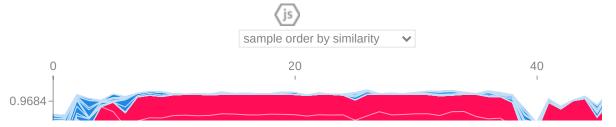
same syntax works for xgboost, LightGBM, CatBoost, and some scikit-learn models
explainer = shap.TreeExplainer(model)

- # shap_values consists of a list of two matrices of dimension samplesize x #features
 # The first matrix uses average nr of benign samples as base value
- # The second matrix which is used below uses average nr of malignant samples as base shap_values = explainer.shap_values(X_explain)
- # Interactive visualization of the explanation of the first subject
- # in the test set (X_explain).
- # It shows the relative contribution of features to get from the base value of malign
- # samples(average value)
- # to the output value (1 in case of malignant sample)
- # the numbers at the bottom show the actual values for this sample.
- shap.initjs() #initialize javascript in cell
- shap.force_plot(explainer.expected_value[1], shap_values[1][0,:], X_explain.iloc[0,:]

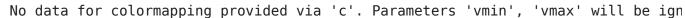


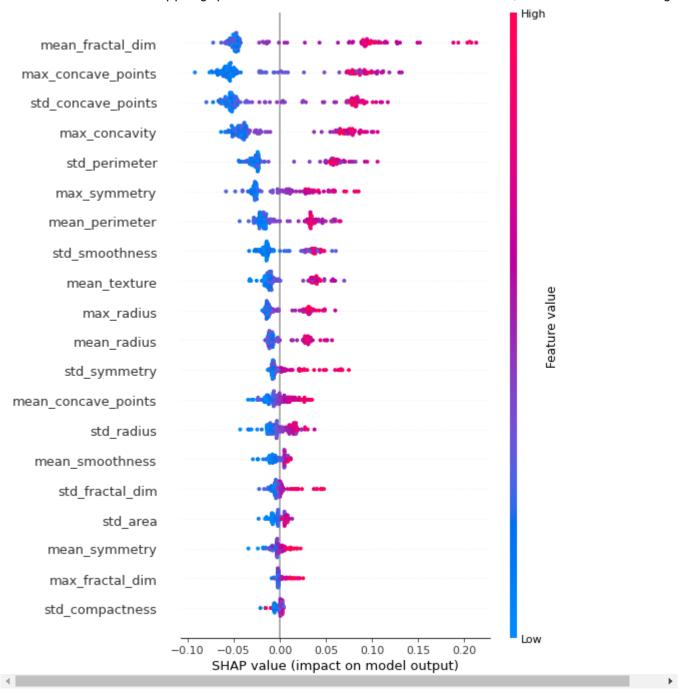
#Interactive visualization of all sample/feature Shapley values
#It is possible to show the relative contribution of individual features for all
samples on the y-axis as well.
shap.initjs()

shap.force plot(explainer.expected value[1], shap values[1], X explain)



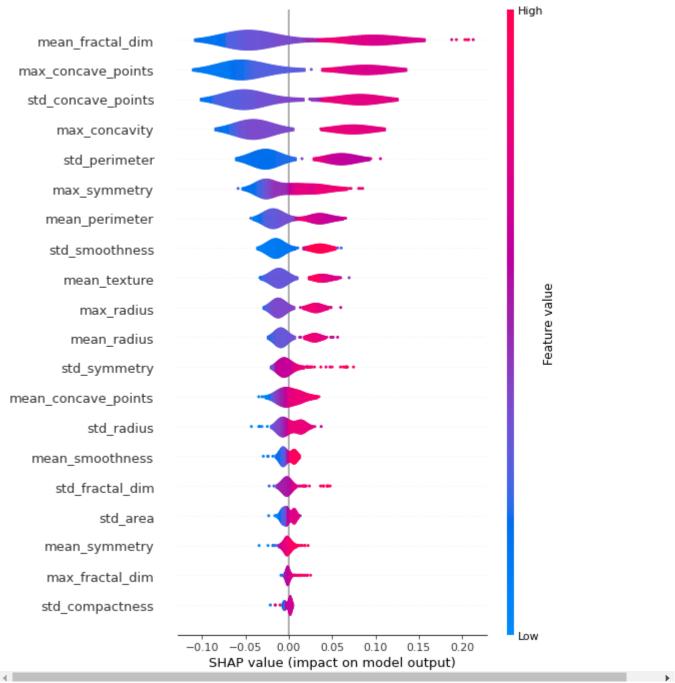
#A summary plot with the shapley value (feature importance)
shap.summary_plot(shap_values[1], X_explain)





#Same as above, but with violin plots to better see the distribution of shapley value shap.summary_plot(shap_values[1], X_explain, plot_type="violin")

□ No data for colormapping provided via 'c'. Parameters 'vmin', 'vmax' will be ign



```
!pip install numpy
!pip install pandas
!pip install sklearn
!pip install seaborn
!pip install rfpimp
!pip install eli5
!pip install xgboost
!pip install matplotlib
```

```
Defaulting to user installation because normal site-packages is not writeab
Requirement already satisfied: numpy in /home/deepcode/.local/lib/python3.
9/site-packages (1.24.2)
Defaulting to user installation because normal site-packages is not writeab
Requirement already satisfied: pandas in /home/deepcode/.local/lib/python3.
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Requirement already satisfied: python-dateutil>=2.8.1 in /home/deepcode/.lo
cal/lib/python3.9/site-packages (from pandas) (2.8.2)
Requirement already satisfied: pytz>=2020.1 in /home/deepcode/.local/lib/py
thon3.9/site-packages (from pandas) (2022.7.1)
Requirement already satisfied: six>=1.5 in /usr/lib/python3/dist-packages
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Defaulting to user installation because normal site-packages is not writeab
le
Collecting sklearn
 Using cached sklearn-0.0.post1.tar.gz (3.6 kB)
 Preparing metadata (setup.py) ... done
Building wheels for collected packages: sklearn
 Building wheel for sklearn (setup.py) ... done
 Created wheel for sklearn: filename=sklearn-0.0.post1-py3-none-any.whl si
ze=2342 sha256=c32631bb64cc7e59f09b292901f6c16e70cbdd4f2b6c9030d874059649a0
9f22
  Stored in directory: /home/deepcode/.cache/pip/wheels/f8/e0/3d/9d0c2020c4
4a519b9f02ab4fa6d2a4a996c98d79ab2f569fa1
Successfully built sklearn
Installing collected packages: sklearn
Successfully installed sklearn-0.0.post1
Defaulting to user installation because normal site-packages is not writeab
le
Requirement already satisfied: seaborn in /home/deepcode/.local/lib/python
3.9/site-packages (0.12.2)
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Requirement already satisfied: matplotlib!=3.6.1,>=3.1 in /usr/lib/python3/
dist-packages (from seaborn) (3.3.4)
Requirement already satisfied: numpy!=1.24.0,>=1.17 in /home/deepcode/.loca
l/lib/python3.9/site-packages (from seaborn) (1.24.2)
Requirement already satisfied: pytz>=2020.1 in /home/deepcode/.local/lib/py
thon3.9/site-packages (from pandas>=0.25->seaborn) (2022.7.1)
Requirement already satisfied: python-dateutil>=2.8.1 in /home/deepcode/.lo
cal/lib/python3.9/site-packages (from pandas>=0.25->seaborn) (2.8.2)
Requirement already satisfied: six>=1.5 in /usr/lib/python3/dist-packages
(from python-dateutil>=2.8.1->pandas>=0.25->seaborn) (1.16.0)
Defaulting to user installation because normal site-packages is not writeab
le
Collecting rfpimp
 Downloading rfpimp-1.3.7.tar.gz (10 kB)
 Preparing metadata (setup.py) ... done
Requirement already satisfied: matplotlib in /usr/lib/python3/dist-packages
(from rfpimp) (3.3.4)
Requirement already satisfied: numpy in /home/deepcode/.local/lib/python3.
9/site-packages (from rfpimp) (1.24.2)
```

```
Requirement already satisfied: pandas in /home/deepcode/.local/lib/python3.
9/site-packages (from rfpimp) (1.5.3)
Requirement already satisfied: scikit-learn in /home/deepcode/.local/lib/py
thon3.9/site-packages (from rfpimp) (1.2.2)
Requirement already satisfied: pytz>=2020.1 in /home/deepcode/.local/lib/py
thon3.9/site-packages (from pandas->rfpimp) (2022.7.1)
Requirement already satisfied: python-dateutil>=2.8.1 in /home/deepcode/.lo
cal/lib/python3.9/site-packages (from pandas->rfpimp) (2.8.2)
Requirement already satisfied: threadpoolctl>=2.0.0 in /home/deepcode/.loca
l/lib/python3.9/site-packages (from scikit-learn->rfpimp) (3.1.0)
Requirement already satisfied: joblib>=1.1.1 in /home/deepcode/.local/lib/p
ython3.9/site-packages (from scikit-learn->rfpimp) (1.2.0)
Requirement already satisfied: scipy>=1.3.2 in /usr/lib/python3/dist-packag
es (from scikit-learn->rfpimp) (1.6.0)
Requirement already satisfied: six>=1.5 in /usr/lib/python3/dist-packages
(from python-dateutil>=2.8.1->pandas->rfpimp) (1.16.0)
Building wheels for collected packages: rfpimp
 Building wheel for rfpimp (setup.py) ... done
 Created wheel for rfpimp: filename=rfpimp-1.3.7-py3-none-any.whl size=106
66 sha256=263e4b317e46897c05ee0a7bb89677d4bd6a89ce0b8f6421f38e359b0c63e72c
 Stored in directory: /home/deepcode/.cache/pip/wheels/d9/f2/53/6d8c73011f
73fc347598d683ff8b2343605ad43474ae083816
Successfully built rfpimp
Installing collected packages: rfpimp
Successfully installed rfpimp-1.3.7
Defaulting to user installation because normal site-packages is not writeab
le
Collecting eli5
 Downloading eli5-0.13.0.tar.gz (216 kB)
                                           - 216.2/216.2 kB 2.1 MB/s eta 0:
00:00a 0:00:01
 Preparing metadata (setup.py) ... done
Requirement already satisfied: attrs>17.1.0 in /usr/lib/python3/dist-packag
es (from eli5) (20.3.0)
Collecting graphviz
 Downloading graphviz-0.20.1-py3-none-any.whl (47 kB)
                                         ---- 47.0/47.0 kB 4.6 MB/s eta 0:0
0:00
Requirement already satisfied: jinja2>=3.0.0 in /home/deepcode/.local/lib/p
ython3.9/site-packages (from eli5) (3.1.2)
Requirement already satisfied: numpy>=1.9.0 in /home/deepcode/.local/lib/py
thon3.9/site-packages (from eli5) (1.24.2)
Requirement already satisfied: scikit-learn>=0.20 in /home/deepcode/.local/
lib/python3.9/site-packages (from eli5) (1.2.2)
Requirement already satisfied: scipy in /usr/lib/python3/dist-packages (fro
m eli5) (1.6.0)
Requirement already satisfied: six in /usr/lib/python3/dist-packages (from
eli5) (1.16.0)
Requirement already satisfied: tabulate>=0.7.7 in /usr/lib/python3/dist-pac
kages (from eli5) (0.8.7)
Requirement already satisfied: MarkupSafe>=2.0 in /home/deepcode/.local/li
b/python3.9/site-packages (from jinja2>=3.0.0->eli5) (2.1.2)
Requirement already satisfied: joblib>=1.1.1 in /home/deepcode/.local/lib/p
ython3.9/site-packages (from scikit-learn>=0.20->eli5) (1.2.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in /home/deepcode/.loca
l/lib/python3.9/site-packages (from scikit-learn>=0.20->eli5) (3.1.0)
```

```
Building wheels for collected packages: eli5
          Building wheel for eli5 (setup.py) ... done
          Created wheel for eli5: filename=eli5-0.13.0-py2.py3-none-any.whl size=10
        7727 sha256=2697ee93142ad720efb5c93c959d69388971a2760199906adab4da583c92048
          Stored in directory: /home/deepcode/.cache/pip/wheels/7b/26/a5/8460416695
        a992a2966b41caa5338e5e7fcea98c9d032d055c
        Successfully built eli5
        Installing collected packages: graphviz, eli5
        Successfully installed eli5-0.13.0 graphviz-0.20.1
        Defaulting to user installation because normal site-packages is not writeab
        Collecting xgboost
          Downloading xgboost-1.7.4-py3-none-manylinux2014 x86 64.whl (193.6 MB)
                                                   - 193.6/193.6 MB 2.3 MB/s eta 0:
        00:0000:0100:02
        Requirement already satisfied: scipy in /usr/lib/python3/dist-packages (fro
        m xgboost) (1.6.0)
        Requirement already satisfied: numpy in /home/deepcode/.local/lib/python3.
        9/site-packages (from xgboost) (1.24.2)
        Installing collected packages: xgboost
        Successfully installed xgboost-1.7.4
        Defaulting to user installation because normal site-packages is not writeab
        Requirement already satisfied: matplotlib in /usr/lib/python3/dist-packages
        (3.3.4)
In [ ]: import numpy as np
        import pandas as pd
        import seaborn as sns
        from sklearn.model selection import train test split
        from sklearn.ensemble import RandomForestRegressor
        from xqboost import XGBClassifier
        from xgboost import plot importance
        from matplotlib import pyplot as plt
        np.random.seed(seed = 42)
In [ ]: # Read CSV
        task file = 'task data.csv'
        with open(task file, mode = 'rb') as f:
            data = pd.read csv(f)
        # Extract names of each column (using pandas)
        headers = np.array(list(data.columns.values))
        names = headers[2:]
        y = data.class label
        X = pd.DataFrame(data,columns=names)
In [ ]: print(headers)
        ['sample index' 'class_label' 'sensor0' 'sensor1' 'sensor2' 'sensor3'
         'sensor4' 'sensor5' 'sensor6' 'sensor7' 'sensor8' 'sensor9']
        print(names)
In [ ]:
```

```
['sensor0' 'sensor1' 'sensor2' 'sensor3' 'sensor4' 'sensor5' 'sensor6'
'sensor7' 'sensor8' 'sensor9']
```

In []:

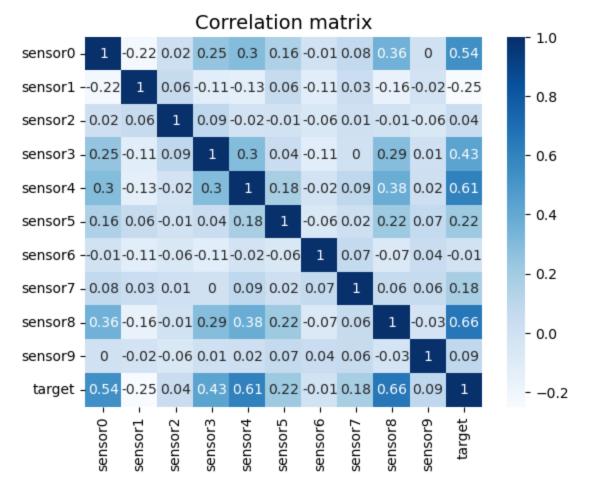
As per problem statement, the emphasis is on identifying the importance of a particular feature in the machine learning model. This is a classification problem wherein we need to identify the important feature and we need to justify the reasons by showing why we have chosen a specific feature and how it turns out to be important feature. Identifying the important features is very important due to the following reasons: 1. It will help us improve the model's by concentrating on important features (variables) 2. It will help us get rid of features that are not relevant or which don not contribute the model's performance.

Feature importance can be implemented using various model's the popular among them being Random forest, XGBoost, Linear Regression. My idea here is that the better the model is, the more we can rely on the feature importance and how to interepret the problem. I will explain the reason for chosing the model as we proceed.

Exploratory data analysis

]:	print(data.describe	2())				
		class_label	sensor0	sensor1	sensor2	sensor3	\
	count	400.000000	400.000000	400.000000	400.000000	400.000000	
	mean	0.000000	0.523661	0.509223	0.481238	0.509752	
	std	1.001252	0.268194	0.276878	0.287584	0.297712	
	min	-1.000000	0.007775	0.003865	0.004473	0.001466	
	25%	-1.000000	0.299792	0.283004	0.235544	0.262697	
	50%	0.000000	0.534906	0.507583	0.460241	0.510066	
	75%	1.000000	0.751887	0.727843	0.734937	0.768975	
	max	1.000000	0.999476	0.998680	0.992963	0.995119	
		sensor4	sensor5	sensor6	sensor7	sensor8	senso
	r9						
	count 00	400.000000	400.000000	400.000000	400.000000	400.000000	400.0000
	mean 33	0.497875	0.501065	0.490480	0.482372	0.482822	0.5419
	std	0.288208	0.287634	0.289954	0.282714	0.296180	0.2724
	90						
	min	0.000250	0.000425	0.000173	0.003322	0.003165	0.0004
	52						
	25%	0.249369	0.269430	0.226687	0.242848	0.213626	0.3212
	64						
	50%	0.497842	0.497108	0.477341	0.463438	0.462251	0.5783
	89						
	75%	0.743401	0.738854	0.735304	0.732483	0.740542	0.7689
	90						
	max 65	0.999412	0.997367	0.997141	0.998230	0.996098	0.9994





From the correlation matrix we can note that there is no correlation between the features.

Models:

a) Random Forest

Since Decision trees can be used for better interpretability of the model, the downside is that it works well if the depth is very small. Since the current dataset has only 400 data points, it might be easy to interpret the model using Decision tree, but if the aspect of scalebility is considered it might not be a best approach and this is where Random Forest comes into picture. In Random forest the subset of data is chosen which is also called as bootstrap. These bootstrap are fed to decision trees with large depths randomly. The final result is obtained by counting the majority of the vote from all the decision trees. This technique is called as boot strapping or bagging. This also helps in overcoming bais.

In order to validate the Random forest model, I have used oob_score . Out of bag score(oob_score) is used when the dataset is smaller in size. Since validation score requires

us to keep apart certain part of da ta, it is good to use oob_score since it works only on subset of decision trees and while the validation score is calculated on all the decision trees.

Out[]:

RandomForestClassifier

RandomForestClassifier(n_jobs=-1, oob_score=True, random_state=42)

```
In [ ]: #print('Score :', rf.score(X_test,y_test))
print('Out of bag error:', rf.oob_score_)
```

Out of bag error: 0.985

As we can obersve that the model performed well on the training set. The oob_score obtained is also good. I will now check which feature is more important and try to visulaize it. This will help us understand which feature has to be given more importance.

In Scikit learn, we can use the feature importance by just using the decision tree which can help us in give some prior intution of th features. Decision Tree is one of the machine learning algorithms that is used for a range of classification and regression problems and more specifically in the decision analysis problems. Decision tree provides a tree-like structure which comprises od decisions that can be made based on a hypothesis. A decision tree is represented in an upside-down where each node represents a feature also called attribute and each brach also called link to the nodes is represents a decision or condition for selecting the specific node. The top node of the tree is called the root node and the bottom-most nodes are called the leaf nodes. The main idea behind using a decision tree is to represent the whole data in the form of a tree.

It has some advantages such as it is faster and it is easier to implement. The downside is it suffers from bias problem due to high cardinality and inflate the importance of continous featues.

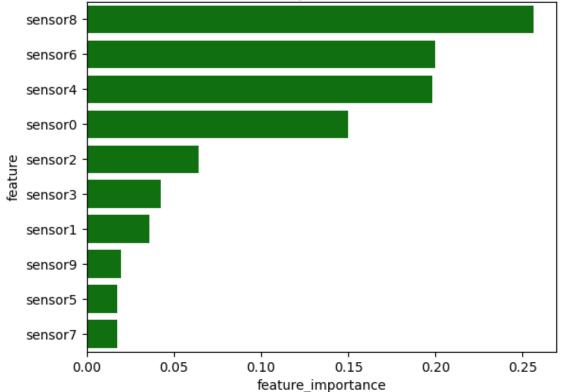
```
# plotting a feature importance dataframe (horizontal barchart)
def var_imp_plot(imp_df, title):
   imp_df.columns = ['feature', 'feature_importance']
   sns.barplot(x = 'feature_importance', y = 'feature', data = imp_df, orie
   .set_title(title, fontsize = 20)
```

In []:	<pre>base_imp = imp_df(X.columns, rf.feature_importances_)</pre>
	base_imp

Out[]:		feature	feature_importance
	0	sensor8	0.256427
	1	sensor6	0.199622
	2	sensor4	0.198249
	3	sensor0	0.149611
	4	sensor2	0.063839
	5	sensor3	0.042247
	6	sensor1	0.036030
	7	sensor9	0.019462
	8	sensor5	0.017295
	9	sensor7	0.017217

```
In [ ]: var_imp_plot(base_imp, 'Default feature importance (scikit-learn)')
```

Default feature importance (scikit-learn)



Using the default feature importance of Scikit-learn we can get the below mentioned graph. As we can notice that the top features are from Sensor8, Sensor4 and Sensor6.

[Reference : https://scikit-learn.org/stable/modules/feature selection.html]

This default feature importance doesn't gives a proper picture of feature importance. This is because the there is bias involved in this method .[Reference https://www.stat.berkeley.edu/~breiman/RandomForests/cc_home.htm#varimp]. Another issue is the collinearity and the inflation towards the continous values.

Hence we need to find a better method.

Other method to check the feature importance.

There are other ways to check the feature importance and I have chosen the following:

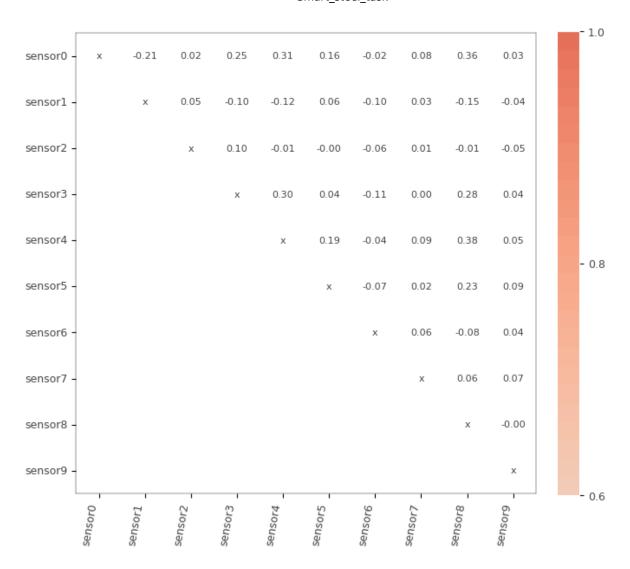
1. Permutation feature importance :

In this method we first train the model and calculate the score by passing validation set (or 00B set in case of Random Forest). We call this score as benchmark result. We then re shuffle the values from one feature in the dataset and then pass it to the model to calcualte the score again. We then calculate the feature importance score which the the difference between the score obtained after shuffling the data and benchmark result. We repeat this process for all the features.

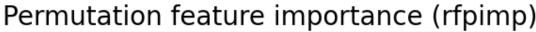
This method has advantages like it is applicable to any model, reasonably efficient, reliable technique and no need to retrain the model at each modification of the dataset. The downside is it is more computationally expensive than default feature_importances permutation importance overestimates the importance of correlated predictors - Strobl et al (2008)

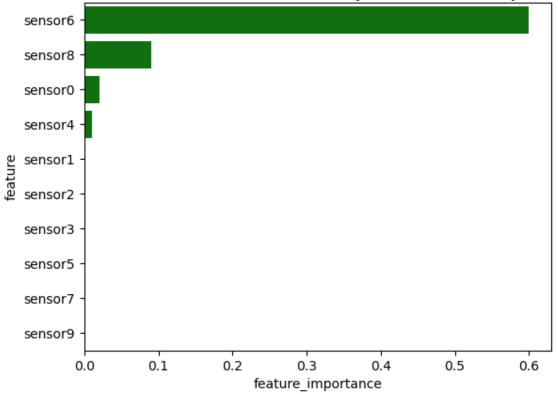
```
[ Reference :https://explained.ai/rf-
importance/index.html#5 ]
```

```
In [ ]: from rfpimp import plot_corr_heatmap
   viz = plot_corr_heatmap(X, figsize=(7,7))
   viz.view()
```



```
In [ ]: #Referring the code from https://explained.ai/rf-importance/index.html#5
        from sklearn.metrics import r2 score
        from rfpimp import permutation importances
        def r2(rf, X, y):
            return r2 score(y, rf.predict(X))
        perm imp rfpimp = permutation importances(rf, X, y, r2)
        perm imp rfpimp.reset index(drop = False, inplace = True)
In [ ]: #Referring the code from https://explained.ai/rf-importance/index.html#5
        from rfpimp import *
        rf pimp = RandomForestClassifier(n estimators=100, n jobs=-1)
        %time I = oob_importances(rf_pimp, X, y)
        CPU times: user 504 ms, sys: 28.2 ms, total: 532 ms
        Wall time: 482 ms
In [ ]: %time I = cv importances(rf pimp, X, y, k=5)
        CPU times: user 4.42 s, sys: 414 ms, total: 4.83 s
        Wall time: 6.28 s
```





As we can notice that the permutation method gives a different result when compared to the Scikit learn's default feature importance. In this result the sensor 6 turned out to be more important. Even though sensor 8 is still an important feature and is among the top 4 values, this helped us to overcome the issue of collinearity which the default feature importance method suffer's with

As we can notice that the time take to get the feature importance using permutation method is much less. This will be beneficial when the dataset is very small as in this case. However this method will suffer badly when compared to default feature importance method when the size of the data increases. Hence its not scalable.

Another feature importance method is using eli5 which is another option present in scikit learn. [Reference:

http://eli5.readthedocs.io/en/latest/blackbox/permutation_importance.html]

This method shows us a way where in we can check how the score will reduce if a particular feature is not present. Since the number of features present is not more for this problem, this

3/19/23, 3:29 PM Smart steel task

method is not power intensive(resource consumption), otherwise it might suffer if the number of features increase.

```
In []: import eli5
    from eli5.sklearn import PermutationImportance

    perm = PermutationImportance(rf, cv = None, refit = False, n_iter = 50).fit(
        perm_imp_eli5 = imp_df(X.columns, perm.feature_importances_)
        var_imp_plot(perm_imp_eli5, 'Permutation feature importance (eli5)')
```

2023-03-19 15:25:08.935289: I tensorflow/core/platform/cpu_feature_guard.c c:193] This TensorFlow binary is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the following CPU instructions in performance-critical operations: AVX2 FMA

To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.

2023-03-19 15:25:09.088763: W tensorflow/compiler/xla/stream_executor/platf orm/default/dso_loader.cc:64] Could not load dynamic library 'libcudart.so. 11.0'; dlerror: libcudart.so.11.0: cannot open shared object file: No such file or directory

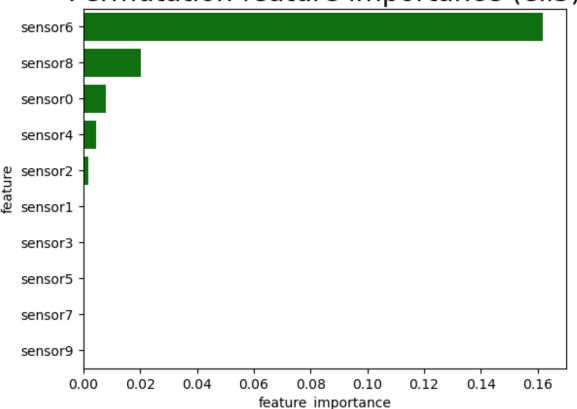
2023-03-19 15:25:09.088784: I tensorflow/compiler/xla/stream_executor/cuda/cudart_stub.cc:29] Ignore above cudart dlerror if you do not have a GPU set up on your machine.

2023-03-19 15:25:09.721479: W tensorflow/compiler/xla/stream_executor/platf orm/default/dso_loader.cc:64] Could not load dynamic library 'libnvinfer.s o.7'; dlerror: libnvinfer.so.7: cannot open shared object file: No such file or directory

2023-03-19 15:25:09.721543: W tensorflow/compiler/xla/stream_executor/platf orm/default/dso_loader.cc:64] Could not load dynamic library 'libnvinfer_pl ugin.so.7'; dlerror: libnvinfer_plugin.so.7: cannot open shared object fil e: No such file or directory

2023-03-19 15:25:09.721550: W tensorflow/compiler/tf2tensorrt/utils/py_util s.cc:38] TF-TRT Warning: Cannot dlopen some TensorRT libraries. If you would like to use Nvidia GPU with TensorRT, please make sure the missing libraries mentioned above are installed properly.





In []:	eli5.show_weights(pe		
Out[]:	Weight	Feature	
out[].	0.1619 ± 0.0242	x6	
	0.0203 ± 0.0100	x8	
	0.0078 ± 0.0054	x0	
	0.0046 ± 0.0047	x4	
	0.0016 ± 0.0034	x2	
	0 ± 0.0000	x9	
	0 ± 0.0000	x7	
	0 ± 0.0000	x5	
	0 ± 0.0000	x3	
	0 ± 0.0000	x1	

As we can notice that by using this method we got the similar result as we obtained via rfpimp. This gives us a better undertanding that the sensor 6 is an important feature. It has more weightage.

There are other feature selection methods mentioned in Scikit learn such as lasso but I haven't used them.

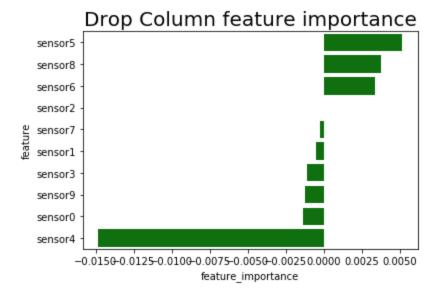
[Reference: https://scikit-

 $learn.org/stable/auto_examples/feature_selection/plot_select_from_model_boston.html\#sphx-glr-auto-examples-feature-selection-plot-select-from-model-boston-py\]$

2. Check the feature importance by dropping a column

I will now check how the model behaves if we drop certain coloumn features for training. This helps us justify our previous benchamarks and results that we have obtained. We will check if the sensor6 feature turns out to be the important one which we have see above.

```
In [ ]: from sklearn.base import clone
        def drop col feat imp(model, X train, y train, random state = 42):
            # clone the model to have the exact same specification as the one initial
            model clone = clone(model)
            # set random state for comparability
            model clone.random state = random state
            # training and scoring the benchmark model
            model clone.fit(X train, y train)
            benchmark score = model clone.score(X train, y train)
            # list for storing feature importances
            importances = []
            # iterating over all columns and storing feature importance (difference
            for col in X train.columns:
                model clone = clone(model)
                model clone.random_state = random_state
                model clone.fit(X train.drop(col, axis = 1), y train)
                drop col score = model clone.score(X train.drop(col, axis = 1), y tr
                importances.append(benchmark score - drop col score)
            importances df = imp df(X train.columns, importances)
            return importances df
In [ ]: from sklearn.ensemble import RandomForestRegressor
        X train, X test, y train, y test = train test split(X, y, test size = 0.8, r
        rf 1 = RandomForestRegressor(n estimators = 100,
                                   n jobs = -1,
                                   oob score = True,
                                   bootstrap = True, random state=42)
        rf 1.fit(X train, y train)
        %time drop imp = drop col feat imp(rf 1, X train, y train)
        print(drop imp)
        var imp plot(drop imp, 'Drop Column feature importance')
        Wall time: 2.69 s
           feature feature importance
        0 sensor5
                              0.005149
        1 sensor8
                            0.003756
        2 sensor6
                             0.003359
        3 sensor2
                            -0.000010
        4 sensor7
                            -0.000256
        5 sensor1
                           -0.000508
        6 sensor3
                            -0.001101
        7 sensor9
                            -0.001242
        8 sensor0
                            -0.001343
        9 sensor4
                            -0.014849
```



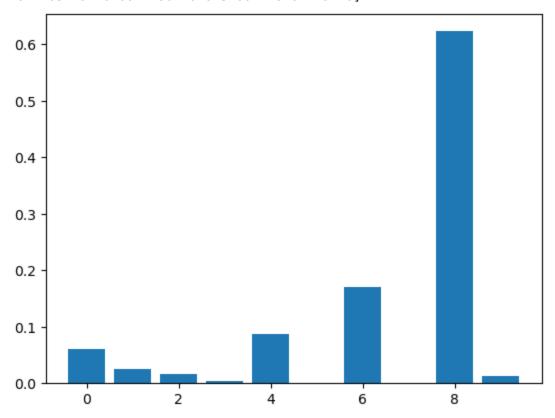
Now as we can see that certain features if dropped causes high impact both positively and negatively. As we can see sensors 8,5,6 and sensors 4,0,9 causes high impact on the overall model performance. This is one of the most important and accuracte feature selection method. The negative importance in this case means the model performance will improve if we remove these features. Another surprising thing to note is that sensor 4 which was one of the important features in observed previously, turns out to be a negative impacting feature.

This method has one downfall which is comptutation cost. The reason for chosing random forest regressor in this method was that I wanted to see how dropping each feature causes the impact on the model. If we use the random forest classification, it will simply classify either 1 or -1 and we cannot derive any meaning out of it.

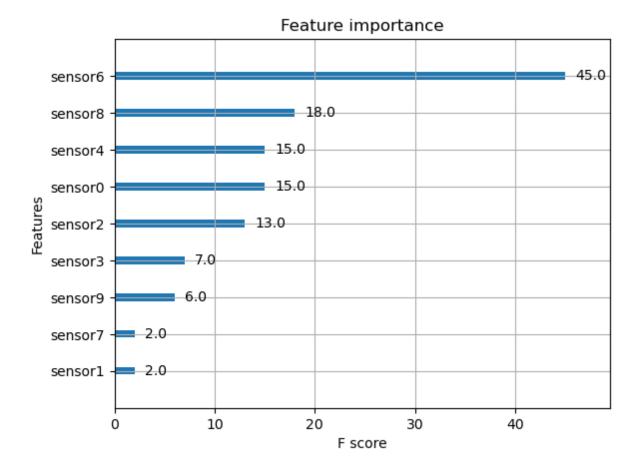
b) XGBoost classifier

[15:28:50] WARNING: ../src/learner.cc:767:
Parameters: { "bootstrap", "oob_score" } are not used.

[0.06006592 0.02580716 0.01665014 0.00399834 0.08641388 0. 0.17037797 0.00122901 0.6231604 0.01229716]



In []: # plot feature importance using XGBOOST
 plot_importance(xgb)
 plt.show()



Conclusion:

From the above I can conclude that sensor 6 turns out to be an important feature. I have also explained the reasons for chosing the models and methods. The permutation method helps us to identify the feature importance by eliminating bias, on the other hand I explained the downside of it as well.

BAlternatively, I have used XGBoost feature importance and it turned out that the scikit learn default feature_importance gives the same result as previous ones but surprisingly, XGBOOST feature importance gives similar results as seen in the permuatation method because in boosting as we saw there is not much correlation between the features , boosting will use the feature that is not correlated since correlated feature will not be used in the splitting process.

In []: