# A comprehensive guide to Feature Selection using Wrapper methods in Python

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## Introduction

In today's era of Big data and IoT, we are easily loaded with rich datasets having extremely *high dimensions*. In order to perform any machine learning task or to get insights from such *high dimensional* data, **feature selection** becomes very important. Since some features may be irrelevant or less significant to the dependent variable so their unnecessary inclusion to the model leads to

- Increase in **complexity** of a model and makes it **harder** to **interpret**.
- Increase in **time complexity** for a model to get trained.
- Result in a **dumb model** with inaccurate or less reliable predictions.

Hence, it gives an indispensable need to perform *feature selection*. **Feature selection** is very crucial and must component in machine learning and data science workflows especially while dealing with *high-dimensional* datasets.

## What is Feature selection?

As the name suggests, it is a process of selecting the most *significant* and *relevant* features from a vast set of features in the given dataset.

For a dataset with ***d*** input features, the ***feature selection*** process results in ***k*** features such that ***k* < *d***, where k is the smallest set of *significant* and *relevant* features.

So ***feature selection*** helps in finding the smallest set of features which results in

- **Training** a machine learning algorithm **faster**.
- Reducing the **complexity** of a model and making it easier to **interpret**.
- Building a **sensible model** with **better prediction power**.
- **Reducing over-fitting** by selecting the right set of features.

## Feature selection methods

For a dataset with **d features**, if we apply the hit and trial method with all possible combinations of features then total (**2^d – 1**) models need to be evaluated for a *significant* set of features. It is a time-consuming approach, therefore, we use *feature selection* techniques to find out the smallest set of features more efficiently.

There are three types of *feature selection* techniques :

1. Filter methods
2. Wrapper methods
3. Embedded methods

### Difference between Filter, Wrapper, and Embedded Methods for Feature Selection

| Filter methods | Wrapper methods | Embedded methods |
|---|---|---|
| Generic set of methods which do not incorporate a **specific machine learning algorithm.** | Evaluates on a **specific machine learning algorithm** to find optimal features. | Embeds (fix) features during **model building process.** Feature selection is done by observing each iteration of model training phase. |
| Much **faster** compared to Wrapper methods in terms of time complexity | **High computation time** for a dataset with many features | Sits **between Filter methods and Wrapper methods** in terms of time complexity |
| Less prone to **over-fitting** | High chances of **over-fitting** because it involves training of machine learning models with different combination of features | Generally used to reduce **over-fitting** by **penalizing** the coefficients of a model being too large. |
| Examples – **Correlation, Chi-Square test, ANOVA, Information gain** etc. | Examples - **Forward Selection, Backward elimination, Stepwise selection** etc. | Examples - **LASSO, Elastic Net, Ridge Regression** etc. |

Filter vs. Wrapper vs. Embedded methods

In this post, we will only discuss *feature selection* using ***Wrapper methods*** in Python.

## Wrapper methods

In *wrapper methods,* the *feature selection* process is based on a specific machine learning algorithm that we are trying to fit on a given dataset.

It follows a *greedy search approach* by evaluating all the possible combinations of features against the *evaluation criterion*. The *evaluation criterion* is simply the performance measure which depends on the type of problem, for e.g. For *regression* evaluation criterion can be p-values, R-squared, Adjusted R-squared, similarly for *classification* the evaluation criterion can be accuracy, precision, recall, f1-score, etc. Finally, it selects the combination of features that gives the optimal results for the specified machine learning algorithm.


Flow Chart – Wrapper methods

Most commonly used techniques under *wrapper methods* are:

1. Forward selection
2. Backward elimination
3. Bi-directional elimination(Stepwise Selection)

Too much theory so far. Now let us discuss *wrapper methods* with an example of ***the Boston house prices dataset*** available in sklearn. The dataset contains 506 observations of 14 different features. The dataset can be imported using the load_boston()function available in the sklearn.datasets module.

```
from sklearn.datasets import load_boston
boston = load_boston()
print(boston.data.shape)          # for dataset dimension
print(boston.feature_names)       # for feature names
print(boston.target)              # for target variable
print(boston.DESCR)               # for data description
```

Let's convert this raw data into a *data frame* including target variable and actual data along with feature names.

```
import pandas as pd
bos = pd.DataFrame(boston.data, columns = boston.feature_names)
bos['Price'] = boston.target
X = bos.drop("Price", 1)        # feature matrix
y = bos['Price']                # target feature
bos.head()
```

| | CRIM | ZN | INDUS | CHAS | NOX | RM | AGE | DIS | RAD | TAX | PTRATIO | B | LSTAT | Price |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.00632 | 18.0 | 2.31 | 0.0 | 0.538 | 6.575 | 65.2 | 4.0900 | 1.0 | 296.0 | 15.3 | 396.90 | 4.98 | 24.0 |
| 1 | 0.02731 | 0.0 | 7.07 | 0.0 | 0.469 | 6.421 | 78.9 | 4.9671 | 2.0 | 242.0 | 17.8 | 396.90 | 9.14 | 21.6 |
| 2 | 0.02729 | 0.0 | 7.07 | 0.0 | 0.469 | 7.185 | 61.1 | 4.9671 | 2.0 | 242.0 | 17.8 | 392.83 | 4.03 | 34.7 |
| 3 | 0.03237 | 0.0 | 2.18 | 0.0 | 0.458 | 6.998 | 45.8 | 6.0622 | 3.0 | 222.0 | 18.7 | 394.63 | 2.94 | 33.4 |
| 4 | 0.06905 | 0.0 | 2.18 | 0.0 | 0.458 | 7.147 | 54.2 | 6.0622 | 3.0 | 222.0 | 18.7 | 396.90 | 5.33 | 36.2 |

Here, the target variable is Price. We will be fitting a *regression model* to predict Price by selecting optimal features through *wrapper methods*.

### 1. Forward selection

In *forward selection*, we start with a null model and then start fitting the model with each individual feature one at a time and select the feature with the minimum *p-value*. Now fit a model with two features by trying combinations of the earlier selected feature with all other remaining features. Again select the feature with the minimum *p-value*. Now fit a model with three features by trying combinations of two previously selected features with other remaining features. Repeat this process until we have a set of selected features with a *p-value* of individual features less than the *significance level*.

In short, the steps for ***the forward selection*** technique are as follows :

1. Choose a *significance level* (e.g. SL = 0.05 with a 95% confidence).
2. Fit all possible *simple regression models* by considering one feature at a time. Total **'n'** models are possible. Select the feature with the lowest *p-value*.
3. Fit all possible models with one extra feature added to the previously selected feature(s).
4. Again, select the feature with a minimum *p-value*. if *p_value < significance level* then go to Step 3, otherwise terminate the process.

Now let us perform the same on Boston house price data.

```
def forward_selection(data, target, significance_level=0.05):
    initial_features = data.columns.tolist()
    best_features = []
    while (len(initial_features)>0):
        remaining_features = list(set(initial_features)-set(best_features))
        new_pval = pd.Series(index=remaining_features)
        for new_column in remaining_features:
            model = sm.OLS(target, sm.add_constant(data[best_features+
[new_column]])).fit()
            new_pval[new_column] = model.pvalues[new_column]
        min_p_value = new_pval.min()
        if(min_p_value<significance_level):
            best_features.append(new_pval.idxmin())
        else:
            break
    return best_features
```

This above function accepts data, target variable, and significance level as arguments and returns the final list of *significant features* based on *p-values* through ***forward selection***.

```
forward_selection(X,y)
```

```
#OUTPUT
['LSTAT',
'RM',
'PTRATIO',
'DIS',
'NOX',
'CHAS',
'B',
'ZN',
'CRIM',
'RAD',
'TAX']
```

### Implementing Forward selection using built-in functions in Python:

mlxtend library contains built-in implementation for most of the *wrapper methods* based feature selection techniques. SequentialFeatureSelector() function comes with various combinations of *feature selection* techniques.

```
#importing the necessary libraries
from mlxtend.feature_selection import SequentialFeatureSelector as SFS
from sklearn.linear_model import LinearRegression
# Sequential Forward Selection(sfs)
sfs = SFS(LinearRegression(),
          k_features=11,
          forward=True,
          floating=False,
          scoring = 'r2',
          cv = 0)
```

SequentialFeatureSelector() function accepts the following major arguments :

- LinearRegression() is an estimator for the entire process. Similarly, it can be any *classification* based algorithm.
- k_features indicates the number of features to be selected. It can be any random value, but the optimal value can be found by analyzing and visualizing the *scores* for different numbers of features.
- forward and floating arguments for different flavors of *wrapper methods*, here, forward = True and floating = False are for *forward selection* technique.
- The scoring argument specifies the *evaluation criterion* to be used. For *regression* problems, there is only r2 *score* in default implementation. Similarly for *classification*, it can be accuracy, precision, recall, f1-score, etc.
- cv argument is for *k-fold cross-validation*.

Now let's fit the above-defined *feature selector* on the Boston house price dataset.

```
sfs.fit(X, y)
sfs.k_feature_names_     # to get the final set of features
#OUTPUT
('CRIM',
'ZN',
'CHAS',
'NOX',
'RM',
'DIS',
'RAD',
'TAX',
'PTRATIO',
'B',
'LSTAT')
```

### 2. Backward elimination

In *backward elimination*, we start with the full model (including all the independent variables) and then remove the insignificant feature with the highest *p-value*(> *significance level*). This process repeats again and again until we have the final set of *significant* features.

In short, the steps involved in *backward elimination* are as follows:

1. Choose a *significance level* (e.g. SL = 0.05 with a 95% confidence).
2. Fit a full model including all the features.
3. Consider the feature with the highest *p-value*. If the *p-value* > *significance level* then go to Step 4, otherwise terminate the process.
4. Remove the feature which is under consideration.
5. Fit a model without this *feature*. Repeat the entire process from Step 3.

Now let us perform the same on Boston house price data.

```
def backward_elimination(data, target,significance_level = 0.05):
    features = data.columns.tolist()
    while(len(features)>0):
        features_with_constant = sm.add_constant(data[features])
        p_values = sm.OLS(target, features_with_constant).fit().pvalues[1:]
        max_p_value = p_values.max()
        if(max_p_value >= significance_level):
            excluded_feature = p_values.idxmax()
            features.remove(excluded_feature)
        else:
            break
    return features
```

This above function returns the final list of *significant features* based on *p-values* through ***backward elimination***.

```
# OUTPUT
['CRIM',
'ZN',
'CHAS',
'NOX',
'RM',
'DIS',
'RAD',
'TAX',
'PTRATIO',
'B',
'LSTAT']
```

### Implementing Backward elimination using built-in functions in Python:

The same SequentialFeatureSelector()function can be used to perform *backward elimination* by disabling the forward argument.

```
#Sequential backward selection(sbs)
sbs = SFS(LinearRegression(),
         k_features=11,
         forward=False,
         floating=False,
         cv=0)
sbs.fit(X, y)
sbs.k_feature_names_
# OUTPUT
('CRIM',
'ZN',
'CHAS',
'NOX',
'RM',
'DIS',
'RAD',
'TAX',
'PTRATIO',
'B',
'LSTAT')
```

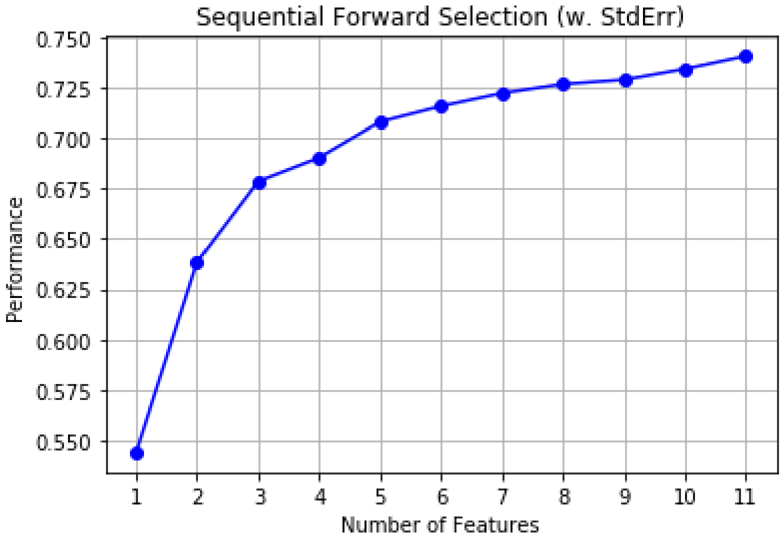
### Additional Note

Here we are directly using the optimal value of k_features argument in both *forward selection* and *backward elimination*. In order to find out the optimal number of *significant* features, we can use *the hit and trial* method for different values of k_features and make the final decision by plotting it against the model performance.

```
sfs1 = SFS(LinearRegression(),
         k_features=(3,11),
         forward=True,
         floating=False,
         cv=0)
sfs1.fit(X, y)
```

The same visualization can be achieved through plot_sequential_feature_selection()function available in mlxtend.plotting module.

```
from mlxtend.plotting import plot_sequential_feature_selection as plot_sfs
import matplotlib.pyplot as plt
fig1 = plot_sfs(sfs1.get_metric_dict(), kind='std_dev')
plt.title('Sequential Forward Selection (w. StdErr)')
plt.grid()
plt.show()
```




Here, on the y-axis, the performance label indicates the *R-squared* values for the different numbers of features.

### 3. Bi-directional elimination(Step-wise Selection)

It is similar to *forward selection* but the difference is while adding a new feature it also checks the *significance* of already added features and if it finds any of the already selected features insignificant then it simply removes that particular feature through *backward elimination*.

Hence, It is a combination of *forward selection* and *backward elimination*.

In short, the steps involved in *bi-directional elimination* are as follows:

1. Choose a *significance level* to enter and exit the model (e.g. SL_in = 0.05 and SL_out = 0.05 with 95% confidence).
2. Perform the next step of *forward selection* (newly added feature must have *p-value* < SL_in to enter).
3. Perform all steps of *backward elimination* (any previously added feature with *p-value*>SL_out is ready to exit the model).
4. Repeat steps 2 and 3 until we get a final *optimal* set of features.

Let us perform the same on Boston house price data.

```
def stepwise_selection(data, target,SL_in=0.05,SL_out = 0.05):
    initial_features = data.columns.tolist()
    best_features = []
    while (len(initial_features)>0):
        remaining_features = list(set(initial_features)-set(best_features))
        new_pval = pd.Series(index=remaining_features)
        for new_column in remaining_features:
            model = sm.OLS(target, sm.add_constant(data[best_features+
[new_column]])).fit()
            new_pval[new_column] = model.pvalues[new_column]
        min_p_value = new_pval.min()
        if(min_p_value<SL_in):
            best_features.append(new_pval.idxmin())
            while(len(best_features)>0):
                best_features_with_constant = sm.add_constant(data[best_features])
                p_values = sm.OLS(target,
best_features_with_constant).fit().pvalues[1:]
                max_p_value = p_values.max()
                if(max_p_value >= SL_out):
                    excluded_feature = p_values.idxmax()
                    best_features.remove(excluded_feature)
                else:
                    break
        else:
            break
    return best_features
```

This above function returns the final list of *significant* features based on *p-values* through *bi-directional elimination*.

```
stepwise_selection(X,y)

# OUTPUT
['LSTAT',
'RM',
'PTRATIO',
'DIS',
'NOX',
'CHAS',
'B',
'ZN',
'CRIM',
'RAD',
'TAX']
```

## Implementing bi-directional elimination using built-in functions in Python:

The same SequentialFeatureSelector()function can be used to perform *backward elimination* by enabling forward and floating arguments.

```
# Sequential Forward Floating Selection(sffs)
sffs = SFS(LinearRegression(),
         k_features=(3,11),
         forward=True,
         floating=True,
         cv=0)
sffs.fit(X, y)
sffs.k_feature_names_
# OUTPUT
('CRIM',
'ZN',
'CHAS',
'NOX',
'RM',
'DIS',
'RAD',
'TAX',
'PTRATIO',
'B',
'LSTAT')
```

## End Notes

In this article, we saw different kinds of Wrapper methods for feature selection with implementation using mlxtend library in Python.