Exploring the Effectiveness of Machine Learning for Option Pricing

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DSO 530

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Executive Summary

Overview

The financial derivatives market has been in the spotlight for massive losses incurred by traders, leading to the bankruptcy of reputable institutions. Thest stories created a negative perception of derivatives, despite their importance in proper risk management when used correctly. So a good evaluation model is required. However, traditional parametric models, like Black-Scholes formula, for evaluating derivatives have limitations in terms of computational power and assumptions, which call for a data-driven approach based on non-parametric models. This study focuses on applying machine learning models to examine the option values of European call options for the S&P 500, as a means of improving the accuracy of risk assessment and management.

Problem Summary

The objective of this project is to build regression and classification models using training data that contains information on 1,680 options, with the aim of predicting the current option value (C) and whether the predicted value using Black-Scholes formula overestimates or underestimates the option value (BS). The goal is to select the most accurate approach for making predictions on the test dataset.

Methodology

We began our data analysis by performing data cleaning to ensure the quality of the dataset. We analyzed the distribution of variables and removed outliers. We also dropped records with missing values and ensured the completeness of the dataset. We then performed feature engineering, creating 10 new variables from the original four predictors to capture non-linear relationships and interactions to potentially improve model accuracy and generalization capabilities. Finally, we explored several regression and classification models for predicting the option value and determining the BS value. We trained the models with the original four variables and added new variables using feature selection to improve performance. Model performance was evaluated using cross-validation and train-test splitting, and the best-performing model was selected based on the results.

Result and Conclusion

In general, additive boosting algorithms have had the best performance on both regression and classification predictions. The XGBoost and CatBoost models were chosen as the most accurate and appropriate for predicting C (current option value) and BS (Black-Scholes label) respectively, based on their out-of-sample R squared scores and accuracy scores. Furthermore, to enhance the accuracy and reliability of predictions, we recommend incorporating all four predictor variables in the prediction. These models allow us to have reliable predictions for option price and BS label on testing data.

While machine learning models may outperform the Black-Scholes model in predicting option values due to their ability to capture complex and nonlinear patterns in market variables and their adaptability to changing market conditions, it's important to note that machine learning models are not a panacea and may also suffer from overfitting, data biases, and other modeling challenge. For example, the use of these models to predict the option values of highly volatile stocks like Tesla may not always be reliable, and further improvements in data collection and model training are needed to address this challenge.

Introduction and Description of the Variables

In this project, our aim is to build statistical and machine learning models to predict the values of European call options on the S&P 500. We will be using a training dataset that contains information on 1,680 options, including the current option value (C), current asset value (S), strike price (K), annual interest rate (r), time to maturity (tau), and BS, a categorical variable that indicates whether the predicted option value overestimates (1) or underestimates (0) the actual option value. A detailed explanation of these variables can be found at appendix 0-1.

The predictors used in our models will include S, K, r, and tau, while the numerical and categorical variables we aim to predict are C and BS, respectively. The test dataset is similar to the training dataset, except it lacks the value and BS variables. Our objective is to build regression models to predict the current option value (C) and classification models to predict whether the predicted value overestimates or underestimates current option value (BS). We will explore various regression and classification methods covered in the course and select the most accurate approach for making predictions on the test dataset.

Data Cleaning

The first step of our project is to ensure the quality of the data by cleaning it. We started this process by analyzing the distribution of the variables using a log scale. From this analysis, we identified two outliers in the current asset value variable: one over 40,000 and one at 0 (Appendix 1-2: Distribution of Current Asset Value). We determined that these outliers could potentially mislead the model, so we removed them from the dataset. Additionally, we removed two data points in the time to maturity variable with unrealistic values of 146 and 250 years (Appendix 1-7: Distribution of Time to Maturity). Finally, we dropped the data records that had missing values to ensure the completeness of the dataset.

Feature Engineering

We performed feature engineering on the data after cleaning, resulting in the creation of 10 new variables from the four original predictors. These new variables can improve the accuracy and generalization capability of the model and thus enhance its performance.

	New Variables	**Explanation**
1	S/K	Current asset value / Strike price of option, Relative asset value
2	log(S/K)	Logarithm of Relative asset value
3	(S/K)^2	Squared Relative asset value
4	r*tau	Annual interest rate * Time to maturity
5	(1+r)*tau	(1+Annual interest rate) * Time to maturity
6	(tau)^1/2	Square root of Time to maturity
7	S-K	Current asset value - Strike price of option
8	(S-K)*(r*tau)	Future interest value of (S - K)
	1+r*tau	Discount rate: 1 + Annual interest rate * Time to maturity
9	K*discount rate	Strike price of option * Discount rate
10	(S-K)*discount rate	(Current asset value - Strike price of option) * Discount rate

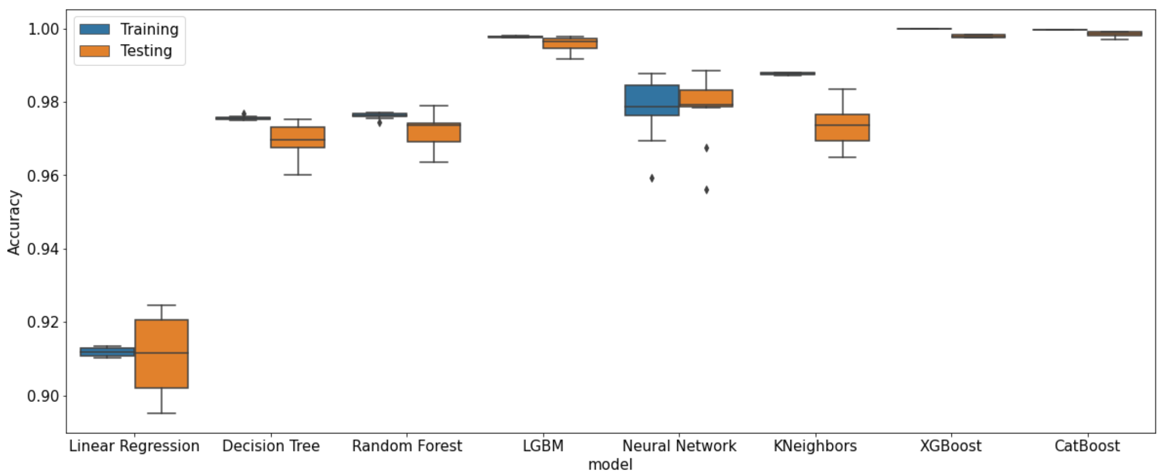
* Please refer to appendix 0-2 for a detailed explanation of these new variables.

Model Algorithms and Selection

1. **Predicting Current Option Value(C)**

The problem of predicting the current option value based on known variables is a case of supervised regression. Therefore, we explore several widely-used regression algorithms with diverse complexities. We use the following eight models for model exploration: Linear Regression, Decision Tree, Random Forest, LightGBM (LGBM), Neural Network, KNeighbors, XGBoost, and CatBoost.

First we use the original four variables(S, K, r, tau) to build and train the models, and the model performance is evaluated by the model's out-of-sample R square score respectively. 10-fold cross validation is applied to obtain relatively unbiased scores, ten results on the validation set are averaged to give the final validation score. The R square for all models are shown in Appendix 2-3. For each model, tuned hyperparameters are reported in the appendix.



From the results reported from cross-validation, we find that more complex non-linear models, especially boosting, perform better than simple ones, like linear regression. The XGBoost and CatBoost algorithm outperform others only marginally, in terms of both training and testing scores; but XGBoost also has least small standard deviation in test scores among all models, which means that XGBoost are more stable and robust.

To potentially improve the performance of the models; we then add the additional 10 featured variables to build the models. However, because of the high dimensionality, we perform feature selection before training the models. We first use best subset selection for linear model and forward selection for other models to filter the best model of each layer and then utilize cross-validation to select the optimal model.

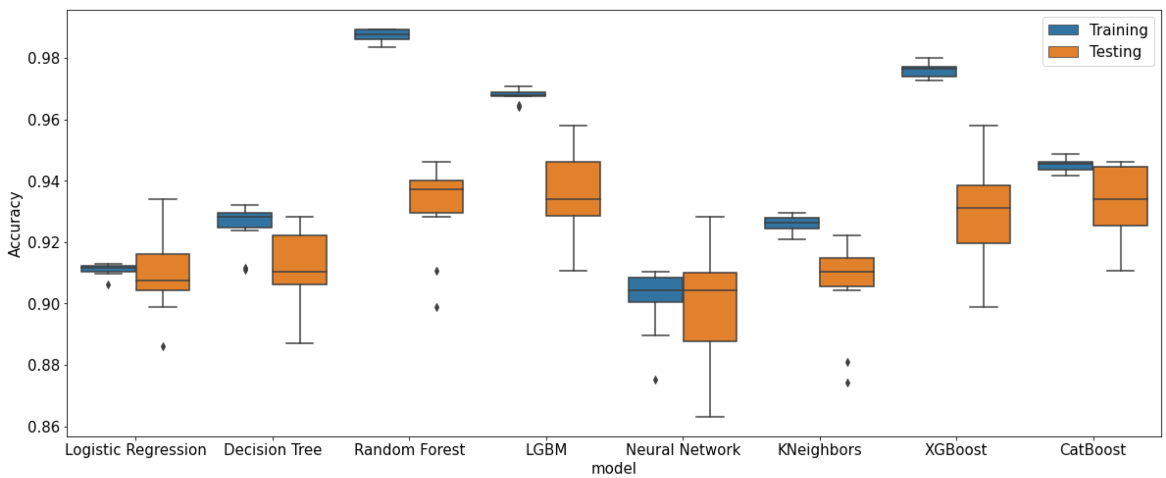
We then train additional eight models based on featured variables by repeating the steps we did for four variables above. The R square for all models are shown in Appendix 4-10.

While we see a significant performance improvement for Linear Regression, which increased the out-of-sample R square from 91.2% to 99.5%, improvements for other algorithms are minor or unnoticeable. Thus, it is preferable to choose models with fewer variables that can produce similar results. As a result, we choose XGBoost with the original four variables as our best model for prediction.

2. Predicting whether the Black-Scholes formula has underestimated or overestimated current option value (BS)

For the binary classification problem of using the BS label to classify option values as either overestimated or underestimated, we explored the below eight models: Logistic Regression, Decision Tree, Random Forest, LightGBM (LGBM), Neural Network, KNeighbors, XGBoost, and CatBoost.

Initially, we constructed models using the given four variables: S, K, r, and tau; and we evaluated the model performance using two techniques: cross-validation and training-testing splitting. For the cross-validation, we utilized stratified 10-fold to distribute the four variables evenly among folds, computed classification scores for both training and testing data, and obtained average classification scores for each fold. Then, we utilized the train-test splitting approach to fit various classification models and computed the accuracy scores for both the training and testing data. All model accuracy scores are exhibited in Appendix 3-3 , and the tuned hyperparameters for each model can be found in the appendix.



Based on the cross-validation results, we concluded that Catboost exhibited the best performance, as it showed neither overfitting nor underfitting patterns, had higher accuracy scores in both training and testing compared to other models, and displayed smaller variances in both testing and training scores. Although Random Forest yielded the highest training scores, it performed less well on testing data, which indicated an overfitting. Therefore, we selected Catboost as our best model, with accuracy scores of 0.9432 and 0.9343 for the training and testing data, respectively.
Similar to predicting the current option value, we attempted to improve our model performance by adding 10 new variables. However, we found that the original 4 variables resulted in better performance when we compared the accuracy scores between the models using the additional variables and the original 4 variables. As a result, we decided to choose CatBoost with only the original 4 variables to predict the BS label.

Business Insights

During our project, we used two models to predict option prices and BS labels for the testing data. Along the way, we gained valuable insights that can enhance the accuracy and reliability of such models. Achieving a balance between prediction accuracy and interpretation is crucial, but the relative importance of each depends on the specific goal of the predictions. For instance, if the aim is to make short-term trading decisions, prediction accuracy may take precedence over interpretation. In contrast, if the goal is to understand the factors that influence changes in stock prices over time, interpretation may be more important. In our case, we prioritize prediction accuracy over interpretation, given the limited information available.

Machine learning models may outperform the Black-Scholes model in predicting option values because they can capture more complex and nonlinear patterns in market variables, such as stock prices and volatility, and incorporate a wider range of input variables beyond the restrictive parametric assumptions of the Black-Scholes model. Additionally, machine learning models can adapt to changing market conditions and respond to structural changes in the data, which classical parametric models like Black-Scholes cannot. This makes machine learning models more robust and flexible for valuing a wide variety of derivatives even beyond options.

From a business perspective, including all four predictor variables in the prediction of option values could be beneficial for enhancing accuracy and adaptability. Each predictor provides distinct information and has a unique impact on the option's value and likelihood of exercise. Moreover, models including all four predictors can be more flexible and adaptable to highly volatile stock markets. By including all four relevant predictors, the models can better capture the dynamic relationships between the predictors and option values, resulting in more accurate and reliable predictions.

Moving on to the practical application of these insights, using our trained model to predict Tesla's stock option value can be risky and unreliable because of the high volatility of Tesla's stocks. It exhibits significant fluctuations over short periods in response to stock market changes. This can cause noise in the data, making the model less effective on new, unseen data. Additionally, the limited range of Tesla's option strike price and current stock price in the training data (between \$115-\$220 and around \$163, respectively) may not be representative of future values, leading to potential inaccuracies in the model's predictions. Using a larger and more diverse dataset could improve the model's accuracy and reliability.

Conclusion

In summary, the purpose of our project is to develop models using statistical and machine learning techniques to make predictions. The project began with data cleaning to ensure the quality of the dataset. Outliers and unrealistic values were removed, and missing data were dropped. Feature engineering was then performed, resulting in the creation of 10 new variables to capture non-linear relationships and interactions between the existing variables.

The project explored regression algorithms with various complexities and selected XGBoost with the original four variables as the best model with R-squared of 0.99 for both training and testing data. Binary classification methods were used to classify option values with the Catboost model selected as the best with accuracy scores of 0.94 and 0.93 for training and testing data respectively. Using these two models, we made predictions for option prices and BS labels for the test dataset. Overall, the project demonstrated the importance of data cleaning, feature engineering, and algorithm selection for accurate predictions in financial modeling.

Appendix

Appendix 0-1: Original Variables

Value (C):	Current option value, which refers to the estimated value of an option derived from its current trading price.
S:	Current asset value, which is the current trading price of a specific S&P 500 futures contract.
K:	Strike price of the option, which is the price at which an option holder can buy the underlying asset. It determines if an option is in-the-money, at-the-money, or out-of-the-money. A call option is in-the-money if the strike price is lower than the current market price of the underlying asset.
r:	Annual interest rate, which is the current risk free rate in the market, usually the treasury security yield with the matching tenor of the time to maturity with the specific option.
tau:	Time to maturity, which is the time between now and the maturity (expiration) date of the option.
BS:	The Black-Scholes formula was applied to this data to get C_pred. If C_pred – C > 0, i.e., the prediction overestimated the option value, we associate that option with (Over); otherwise, we associate that option with (Under).

Appendix 0-2: Explanation of New Variables

The first six new variables were designed to capture non-linear relationships and interactions between the existing variables. The first three of these involved the relative asset value and were calculated as the ratio of the current asset value to the strike price of the option, the logarithm of this ratio, and the square of this ratio. The fourth variable represented the cost of holding the option over the life of the contract. The fifth variable represents the discount factor applied to the future value of option price, commonly used to account for the time value of money. The sixth variable was intended to capture the effect of time decay on the option price.

The remaining four variables were created based on the concept of future value. The seventh variable was designed to measure the potential gain of the option, while the eighth variable represented the future interest value of the potential gain from the option. The ninth variable calculated the potential interest gain from holding the option until maturity. The last variable gave us the future value of gain from the option.

In [1]:
```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
import statsmodels.api as sm
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import KFold
import time
import itertools
from sklearn.tree import DecisionTreeRegressor
from sklearn import tree
import lightgbm as lgb
import xgboost as xgb
from sklearn.ensemble import RandomForestRegressor
from sklearn.neural_network import MLPRegressor
from sklearn.neighbors import KNeighborsRegressor
from catboost import CatBoostRegressor
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import StratifiedKFold
from sklearn.metrics import accuracy_score
from catboost import CatBoostClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.neural_network import MLPClassifier
from sklearn.neighbors import KNeighborsClassifier
```

1. Data Cleaning

1.1 Import the Data

In [2]:
```python
data = pd.read_csv("option_train.csv")
```

In [3]:
```python
data.head(5)
```

Out[3]:

	Value	S	K	tau	r	BS
0	21.670404	431.623898	420.0	0.341270	0.03013	Under
1	0.125000	427.015526	465.0	0.166667	0.03126	Over
2	20.691244	427.762336	415.0	0.265873	0.03116	Under
3	1.035002	451.711658	460.0	0.063492	0.02972	Over
4	39.553020	446.718974	410.0	0.166667	0.02962	Under

1.2 Data Exploring

In [4]:
```python
data.describe()
```

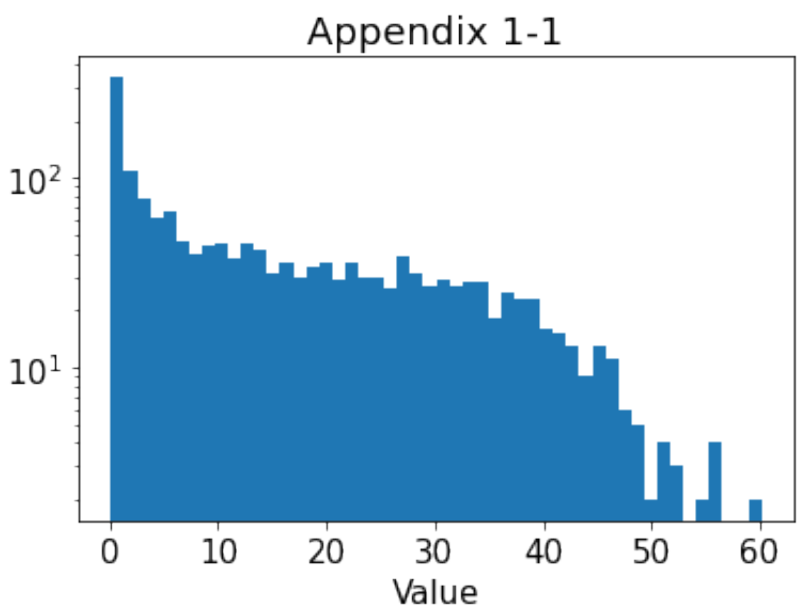
Out[4]:

	Value	S	K	tau	r
count	1678.000000	1679.000000	1678.000000	1679.000000	1680.000000
mean	15.068709	464.402535	438.241955	0.437519	0.030235
std	14.040023	973.652179	23.408989	7.057555	0.000557
min	0.125000	0.000000	375.000000	0.003968	0.029510
25%	2.255001	433.863864	420.000000	0.119048	0.029820
50%	11.190967	442.634081	440.000000	0.202381	0.030130
75%	25.747434	447.320414	455.000000	0.285714	0.030540
max	60.149367	40333.000000	500.000000	250.000000	0.031880

1.2.1 Explore Extreme Value

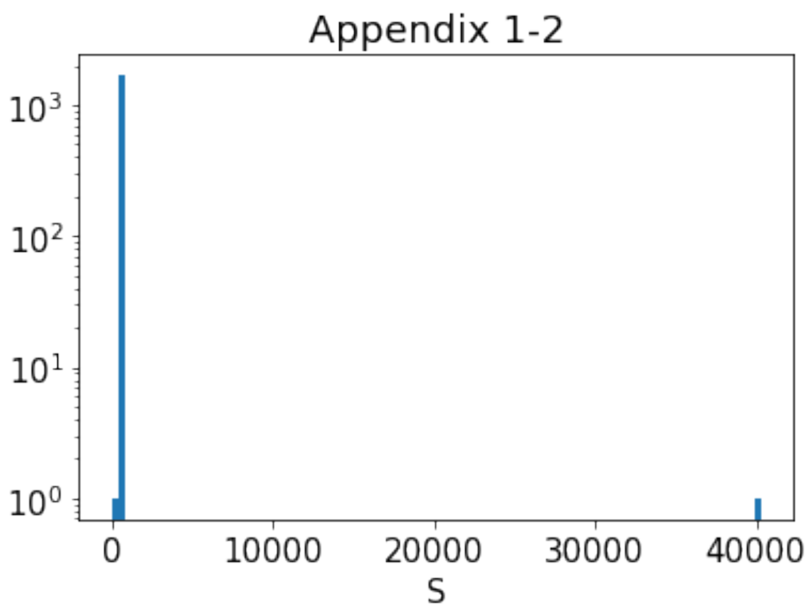
1.2.1.1 Value: current option value

In [5]:
```
plt.rcParams.update({'figure.figsize':(6,4)})
plt.rcParams.update({'font.size':15})
plt.hist(data['Value'], bins = 50)
plt.yscale('log')
plt.xlabel('Value')
plt.title ('Appendix 1-1')
plt.show()
```



1.2.1.2 S: current asset value

In [6]:
```
plt.hist(data['S'], bins = 100)
plt.yscale('log')
plt.xlabel('S')
plt.title ('Appendix 1-2')
plt.show()
```



In [7]:
```
data[data['S'] > 5000]
```

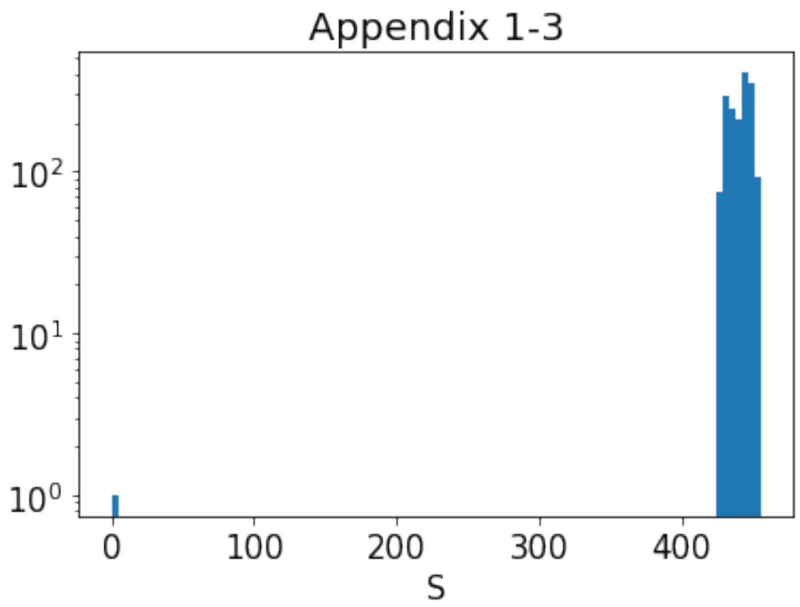
Out[7]:

	Value	S	K	tau	r	BS
47	11.451273	40333.0	425.0	0.043651	0.03147	Under

When the asset value is extremely high, we examine the observation carefully and think the difference between asset value and strike price is extremely high and the value of option doesn't match the difference. Therefore we treat the observation as an outlier.

In [8]:
```
data.drop(labels = data[data['S'] > 5000].index, axis = 0, inplace = True)
```

In [9]:
```
plt.hist(data['S'], bins = 100)
plt.yscale('log')
plt.xlabel('S')
plt.title ('Appendix 1-3')
plt.show()
```



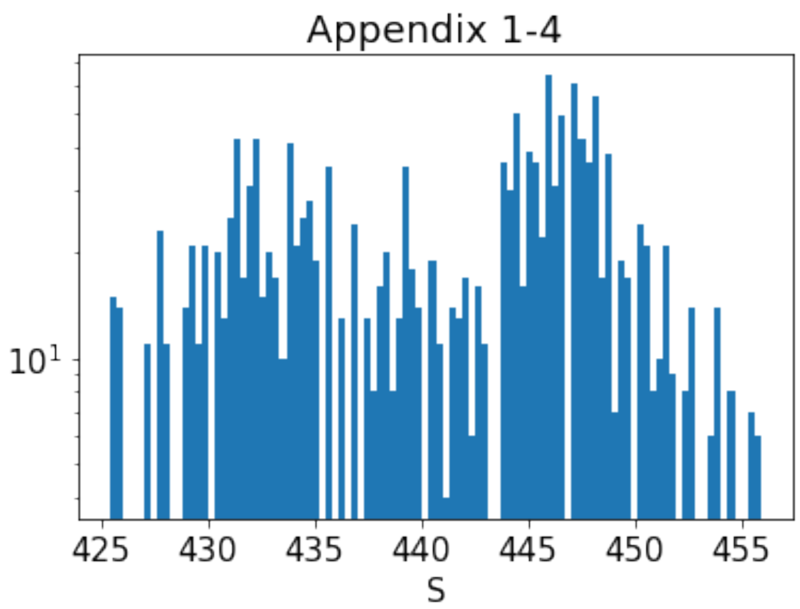

```
In [10]: data[data['S'] == 0]
```

Out[10]:

	Value	S	K	tau	r	BS
879	4.125	0.0	455.0	0.170635	0.03003	Over

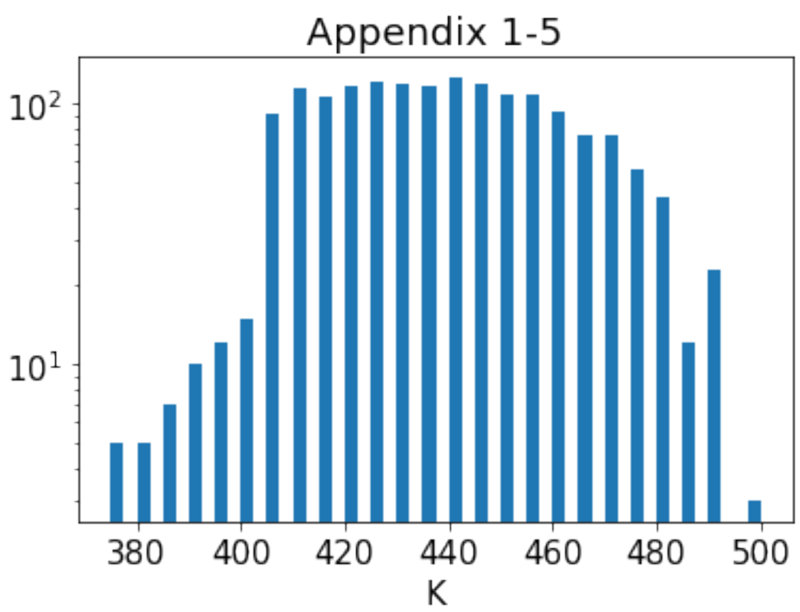
```
In [11]: data.drop(labels = data[data['S'] == 0].index, axis = 0, inplace = True)
```

```
In [12]: plt.hist(data['S'], bins = 100)
         plt.yscale('log')
         plt.xlabel('S')
         plt.title ('Appendix 1-4')
         plt.show()
```



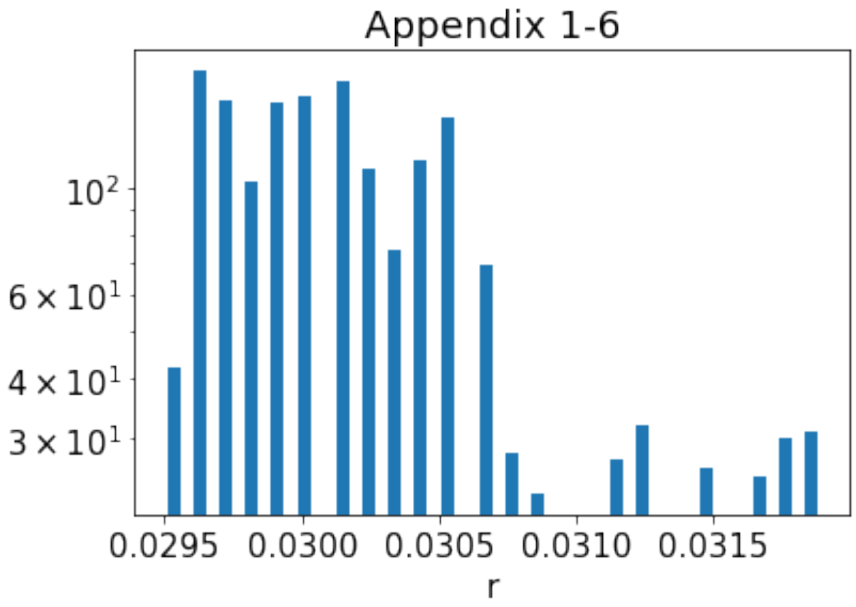
1.2.1.3 K: strike price of option

```
In [13]: plt.hist(data['K'], bins = 50)
         plt.yscale('log')
         plt.xlabel('K')
         plt.title ('Appendix 1-5')
         plt.show()
```



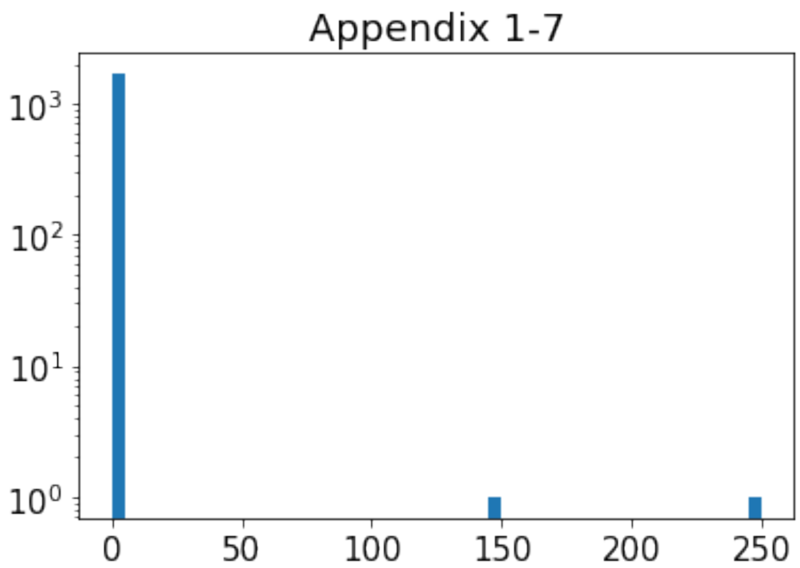
1.2.1.4 r: annual interest rate

In [14]:
```
plt.hist(data['r'], bins = 50)
plt.yscale('log')
plt.xlabel('r')
plt.title ('Appendix 1-6')
plt.show()
```



1.2.1.5 tau: time to maturity

In [15]:
```
plt.hist(data['tau'], bins = 50)
plt.yscale('log')
plt.title ('Appendix 1-7')
plt.show()
```



In [16]:
```
data[data['tau'] > 1]
```

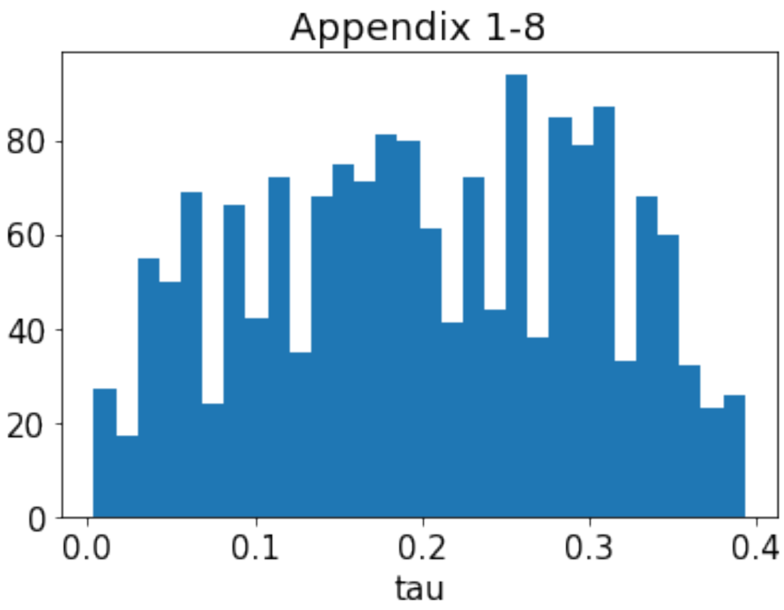
Out[16]:

	Value	S	K	tau	r	BS
12	2.315001	448.688109	470.0	250.0	0.03013	Over
33	2.565000	445.042240	455.0	146.0	0.03003	Over

We notcie that time to maturity of 2 observations extremely exceeds 1 year (250 years and 146 years respectively). In reality, time to maturity of options usually won't exceed 1 year. Therefore, we identify these two observations as outliers and remove them from the dataset.

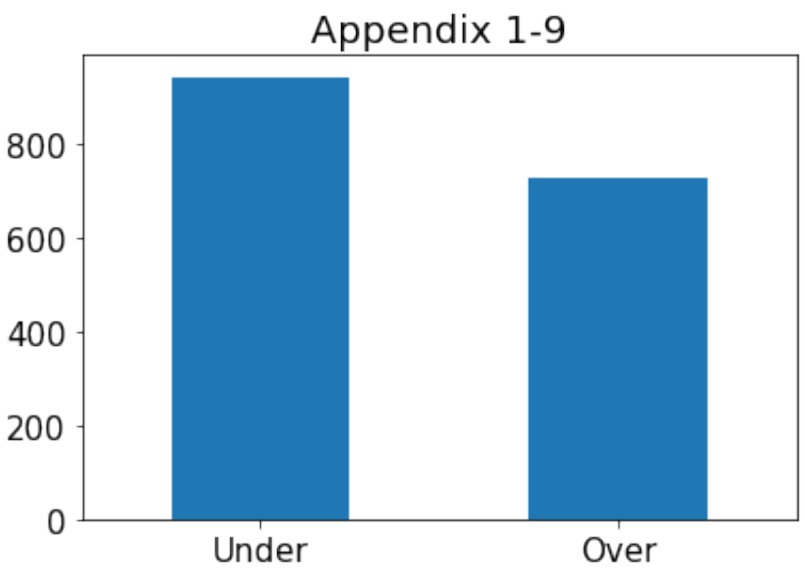
In [17]:
```
data.drop(labels = data[data['tau'] > 1].index, axis = 0, inplace = True)
```

In [18]:
```
plt.hist(data['tau'], bins =30)
plt.xlabel("tau")
plt.title ('Appendix 1-8')
plt.show()
```



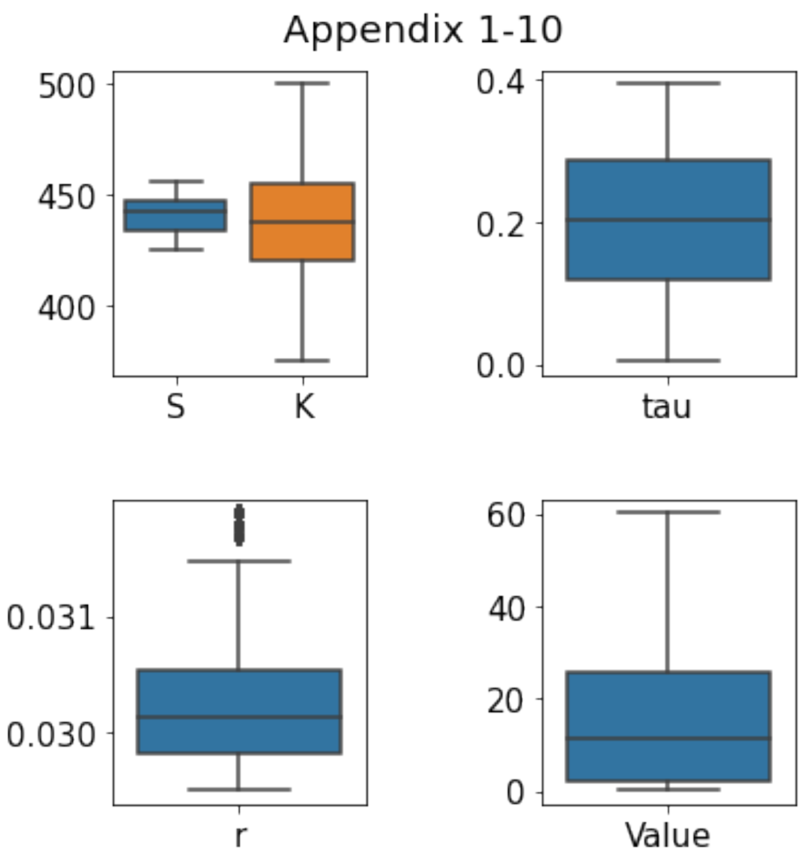
1.2.1.6 BS: Black-Scholes

In [19]:
```
data['BS'].value_counts().plot(kind = 'bar')
plt.xticks(rotation=0)
plt.title ('Appendix 1-9')
plt.show()
```



1.2.1.7 Boxplot of Each Variable

In [20]:
```
fig, axs = plt.subplots(2,2, figsize = (6,6))
fig.tight_layout(pad = 2)
sns.boxplot(ax = axs[0,0], data = data[['S', 'K']])
sns.boxplot(ax = axs[0,1], data = data[['tau']])
sns.boxplot(ax = axs[1,0], data = data[['r']])
sns.boxplot(ax = axs[1,1], data = data[['Value']])
fig.suptitle ('Appendix 1-10')
plt.show()
```



1.2.2 Remove Missing Value

In [21]:
```
np.sum(data.isnull())
```

Out[21]:
```
Value    2
S        1
K        2
tau      1
r        0
BS       0
dtype: int64
```

In [22]:
```
data.drop(labels = data[data['Value'].isnull()].index, axis = 0, inplace = True)
data.drop(labels = data[data['S'].isnull()].index, axis = 0, inplace = True)
data.drop(labels = data[data['K'].isnull()].index, axis = 0, inplace = True)
data.drop(labels = data[data['tau'].isnull()].index, axis = 0, inplace = True)
```

1.2.3 Encoding Categorical Variable

Encoding BS into categorical variable where 1 = Over, 0 = Under

In [23]:
```
mapping = {'Under': 0, 'Over': 1}
data['BS'] = data['BS'].map(mapping)
```

In [24]:
```
data.set_index(pd.Series([x for x in range(data.shape[0])]), inplace = True)
```

2. Feature Engineering

2.1 Non-Linear and Interaction Variables

$\frac{S}{K}$, $log(\frac{S}{K})$, $r*tau$, $(\frac{S}{K})^2$, $(1+r)*tau$, $\sqrt{tau}$

In [25]:
```
data['S/K'] = data['S']/data['K']
data['log(S/K)'] = np.log(data['S/K'])
data['(S/K)^2'] = data['S/K']**2
data['r*tau'] = data['r']*data['tau']
data['(1+r)*tau'] = data['tau'] + data['r*tau']
data['(tau)^1/2'] = data['tau']**2
```

2.2 Future Value

(S-K), (S-K)/(r*tau), (S-K)/tau, 1/(1 + r/tau), K/discount rate

In [26]:
```
data['(S-K)'] = data['S'] - data['K']
data['(S-K)*(r*tau)'] = data['(S-K)']*data['r*tau']
data['discount rate'] = 1 + data['r*tau']
data['K*discount rate'] = data['K']*data['discount rate']
data['(S-K)*discount rate'] = data['(S-K)']*data['discount rate']
```

3. Model Exploration - With Initial Variables

3.1 For Value (C)

3.1.1 Linear Regression

In [27]:
```
y = data[['Value', 'BS']]
y_value = data['Value']
y_BS = data['BS']
X = data.drop(['Value', 'BS','discount rate'], axis = 1)
kfolds = KFold(n_splits = 10, random_state = 1, shuffle = True)

value_score = pd.DataFrame(columns = ['Training CV', 'Testing CV',
                           'Training Validation Set Approach', 'Testing Validation Set Approach'])
value_compare = pd.DataFrame(columns = ['model','Training', 'Testing'])
```

In [28]:
```
# Use cross validation to get Mean out of sample R-squared
cv_score_train = []
cv_score_test = []
original_var = ['K', 'S', 'tau', 'r']
for train_index, test_index in kfolds.split(X, y_value):
    X1 = X.iloc[train_index][original_var]
    X1 = sm.add_constant(X1)
    y_train = y_value.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    X_test = sm.add_constant(X_test)
    y_test = y_value.iloc[test_index]

    # Train the model
    model = sm.OLS(y_train, X1)
    regression = model.fit()

    # Return the score
    r2_train = regression.rsquared
    TSS_test = ((y_test - y_test.mean())**2).sum()
    RSS_test = ((regression.predict(X_test) - y_test)**2).sum()
    r2_test = (TSS_test - RSS_test)/TSS_test

    cv_score_train.append(r2_train)
    cv_score_test.append(r2_test)
```

In [29]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X, y_value, test_size=0.2,random_state=5)

X1 = sm.add_constant(X_train[original_var])
X2 = sm.add_constant(X_test[original_var])

# Train the model
model = sm.OLS(y_train, X1)
regression = model.fit()

# Return the score
r2_train = regression.rsquared
TSS_test = ((y_test - y_test.mean())**2).sum()
RSS_test = ((regression.predict(X2) - y_test)**2).sum()
r2_test = (TSS_test - RSS_test)/TSS_test
```

In [30]:
```
# store score for each model
value_score.loc['Linear Regression'] = [np.mean(cv_score_train), np.mean(cv_score_test), r2_train, r2_test]
df = pd.DataFrame({'model': ['Linear Regression']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.2 Decision Tree Regression

In [31]:
```
def tree_cost_complexity_pruning(X, y_value):
    clf_tree = DecisionTreeRegressor(random_state=0)
    path = clf_tree.cost_complexity_pruning_path(X, y_value)
    ccp_alphas = path.ccp_alphas
    score = []
    ccp_alphas = ccp_alphas[ccp_alphas >=0]
    for ccp_alpha in ccp_alphas:
        score_for_alpha = []
        for train_index, test_index in kfolds.split(X, y_value):
            X_train = X.iloc[train_index][original_var]
            y_train = y_value.iloc[train_index]
            X_test = X.iloc[test_index][original_var]
            y_test = y_value.iloc[test_index]

            clf = DecisionTreeRegressor(random_state=0, ccp_alpha=ccp_alpha)
            clf.fit(X_train, y_train)

            TSS_test = ((y_test - y_test.mean())**2).sum()
            RSS_test = ((clf.predict(X_test) - y_test)**2).sum()
            r2_test = (TSS_test - RSS_test)/TSS_test
            score_for_alpha.append(r2_test)
        score.append(sum(score_for_alpha)/len(score_for_alpha))

    alpha_cv = ccp_alphas[np.argmax(score)]
    return alpha_cv
```

In [32]:
```
def cv(var,model):
    cv_score_train = []
    cv_score_test = []
    model_name = model
    if model == 'Random Forest':
        model = RandomForestRegressor(random_state=9, n_estimators =100, max_depth = 100, min_samples_split=10,
                                      min_samples_leaf=10)
    if model == 'Decision Tree':
        model = DecisionTreeRegressor(random_state=9, max_depth = 100, min_samples_split=30,min_samples_leaf=20,
                                      ccp_alpha = alpha_cv)
    elif model == 'Linear':
        model = LinearRegression()
    elif model == 'LGBM':
        model = lgb.LGBMRegressor(random_state = 5, num_leaves=20,n_estimators=100, max_depth = 50)
    elif model == 'NN':
        model = MLPRegressor(random_state = 5,hidden_layer_sizes=(18,18,18), activation = 'relu', solver = 'adam'
                             learning_rate= 'constant',
                          learning_rate_init = 0.01)
    elif model == 'KNeighbors':
        model = KNeighborsRegressor(n_neighbors=3)
    elif model == 'XGBoost':
        model = xgb.XGBRegressor(random_state = 5,max_depth=25, n_estimators=30)
    elif model == 'CatBoost':
        model = CatBoostRegressor(random_state = 5,verbose=0, max_depth=8, iterations=200, learning_rate = 0.1)
    for train_index, test_index in kfolds.split(X, y_value):
        X_train = X.iloc[train_index][list(var)]
        y_train = y_value.iloc[train_index]
        X_test = X.iloc[test_index][list(var)]
        y_test = y_value.iloc[test_index]
        # Train the model
        regression = model.fit(X_train, y_train)
        # Return the score
        # rsquared for train data
        TSS_train = ((y_train - y_train.mean())**2).sum()
        RSS_train = ((regression.predict(X_train) - y_train)**2).sum()
        r2_train = (TSS_train - RSS_train)/TSS_train
        # rsquared for test data
        TSS_test = ((y_test - y_test.mean())**2).sum()
        RSS_test = ((regression.predict(X_test) - y_test)**2).sum()
        r2_test = (TSS_test - RSS_test)/TSS_test

        cv_score_train.append(r2_train)
        cv_score_test.append(r2_test)

    value_score.loc[model_name,['Training CV', 'Testing CV']] = [np.mean(cv_score_train), np.mean(cv_score_test)]
    return {"model": model, "r2_train": cv_score_train, "r2_test": cv_score_test, "variable": var}
```

In [33]:
```
def validation_set_approach(var, model):
    # Use Train Test Split to test the model performance
    X_train, X_test, y_train, y_test = train_test_split(X[var], y_value, test_size=0.2,random_state=5)
    model_name = model
    if model == 'Random Forest':
        model = RandomForestRegressor(random_state=9, n_estimators =100, max_depth = 100, min_samples_split=10,
                                      min_samples_leaf=10)
    if model == 'Decision Tree':
        model = DecisionTreeRegressor(random_state=9, max_depth = 100, min_samples_split=30,min_samples_leaf=20,
                                      ccp_alpha = alpha_cv)
    elif model == 'Linear':
        model = LinearRegression()
    elif model == 'LGBM':
        model = lgb.LGBMRegressor(random_state = 5, num_leaves=20,n_estimators=100, max_depth = 50)
    elif model == 'NN':
        model = MLPRegressor(random_state = 5,hidden_layer_sizes=(18,18,18), activation = 'relu', solver = 'adam'
                             learning_rate= 'constant',
                          learning_rate_init = 0.01)
    elif model == 'KNeighbors':
        model = KNeighborsRegressor(n_neighbors=3)
    elif model == 'XGBoost':
        model = xgb.XGBRegressor(random_state = 5,max_depth=25, n_estimators=30)
    elif model == 'CatBoost':
        model = CatBoostRegressor(random_state = 5,verbose=0, max_depth=8, iterations=200, learning_rate = 0.1)
    # Train the model
    regression = model.fit(X_train, y_train)
    # Return the score
    # rsquared for train data
    TSS_train = ((y_train - y_train.mean())**2).sum()
    RSS_train = ((regression.predict(X_train) - y_train)**2).sum()
    r2_train = (TSS_train - RSS_train)/TSS_train
    # rsquared for test data
    TSS_test = ((y_test - y_test.mean())**2).sum()
    RSS_test = ((regression.predict(X_test) - y_test)**2).sum()
    r2_test = (TSS_test - RSS_test)/TSS_test
    value_score.loc[model_name,['Training Validation Set Approach', 'Testing Validation Set Approach']] /=
        [r2_train, r2_test]
```

In [34]:
```
original_var = ['K', 'S', 'tau', 'r']
alpha_cv = tree_cost_complexity_pruning(X[original_var],y_value)
result = cv(original_var, model = 'Decision Tree')
validation_set_approach(original_var, 'Decision Tree')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [35]:
```
# store score for each model
df = pd.DataFrame({'model': ['Decision Tree']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.3 Random Forest Regression

In [36]:
```
result = cv(original_var, model = 'Random Forest')
validation_set_approach(original_var, 'Random Forest')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [37]:
```
# store score for each model
df = pd.DataFrame({'model': ['Random Forest']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.4 LGBM Regression

In [38]:
```
result = cv(original_var, model = 'LGBM')
validation_set_approach(original_var, 'LGBM')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [39]:
```
# store score for each model
df = pd.DataFrame({'model': ['LGBM']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.5 Nerual Network Regression

In [40]:
```
result = cv(original_var, model = 'NN')
validation_set_approach(original_var, 'NN')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [41]:
```
# store score for each model
df = pd.DataFrame({'model': ['Neural Network']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.6 KNeighbors Regression

In [42]:
```
result = cv(original_var, model = 'KNeighbors')
validation_set_approach(original_var, 'KNeighbors')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [43]:
```
# store score for each model
df = pd.DataFrame({'model': ['KNeighbors']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.7 XGBoost Regression

In [44]:
```
result = cv(original_var, model = 'XGBoost')
validation_set_approach(original_var, 'XGBoost')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

In [45]:
```
# store score for each model
df = pd.DataFrame({'model': ['XGBoost']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

3.1.8 CatBoost Regression

In [46]:
```
result = cv(original_var, model = 'CatBoost')
validation_set_approach(original_var, 'CatBoost')
cv_score_train = result['r2_train']
cv_score_test = result['r2_test']
```

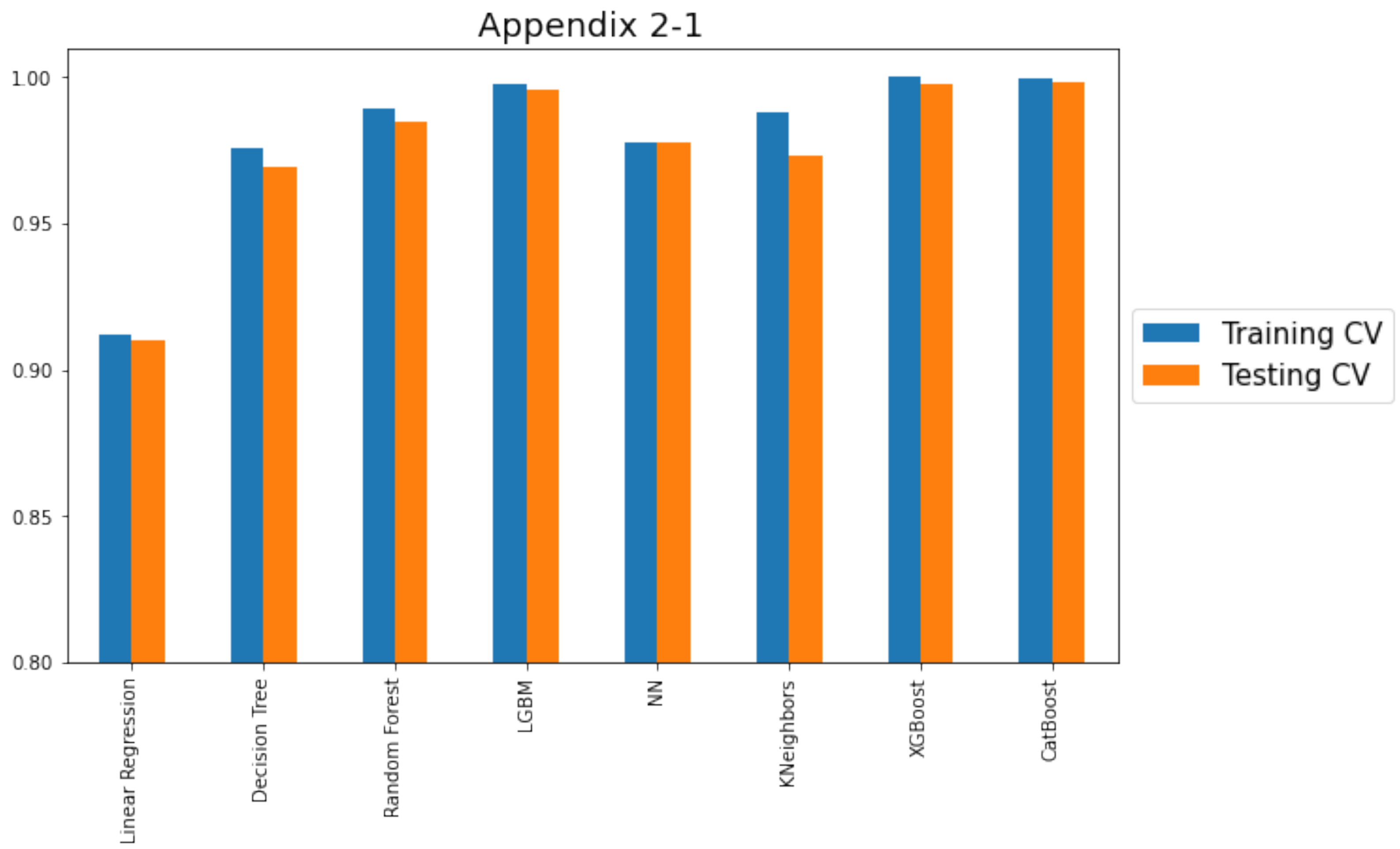
In [47]:
```
# store score for each model
df = pd.DataFrame({'model': ['CatBoost']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

In [48]:
```
value_score
```

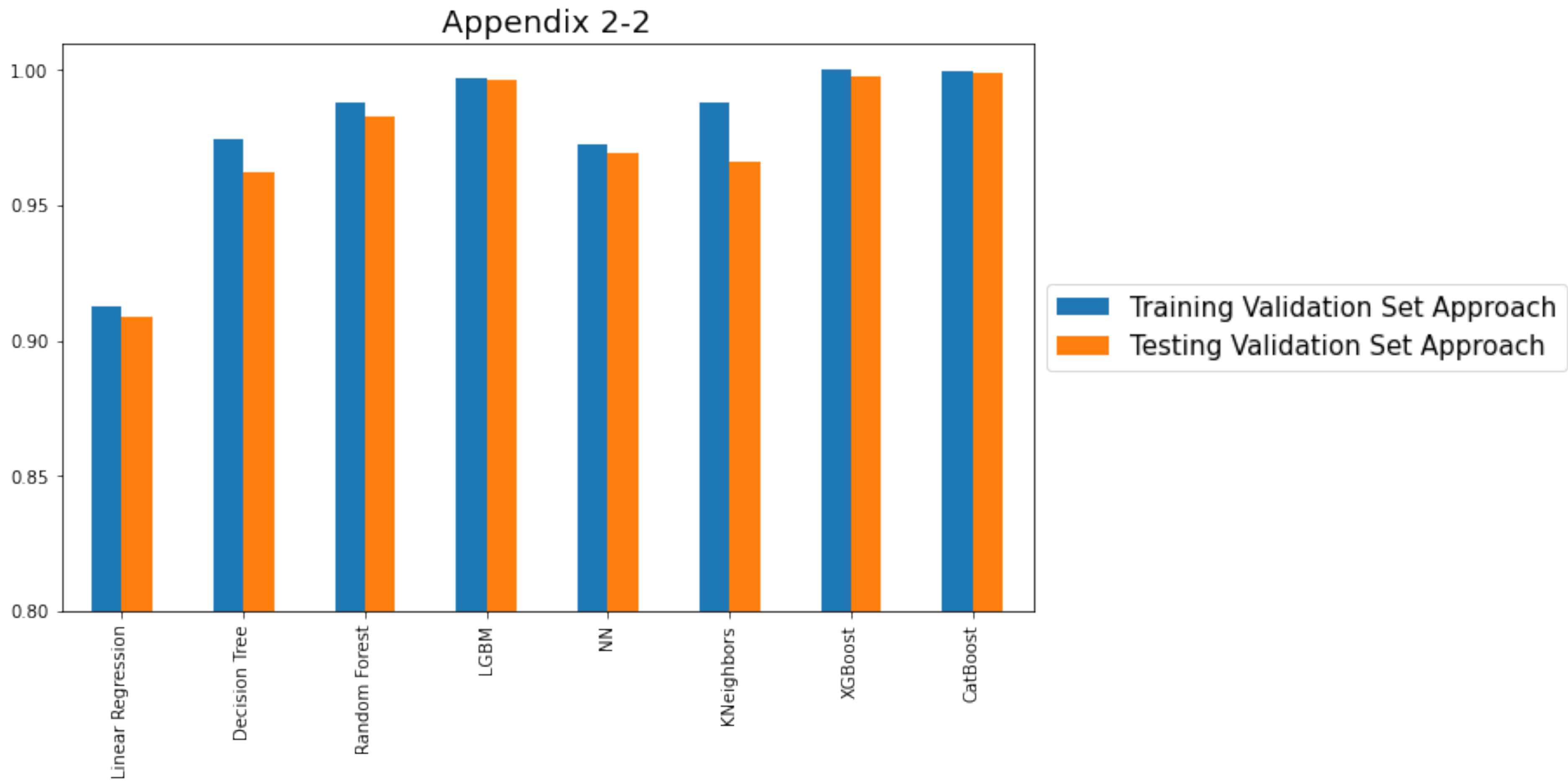
Out[48]:

	Training CV	Testing CV	Training Validation Set Approach	Testing Validation Set Approach
Linear Regression	0.911910	0.910002	0.912325	0.908975
Decision Tree	0.975635	0.969149	0.974508	0.962396
Random Forest	0.989055	0.984696	0.987830	0.982893
LGBM	0.997700	0.995823	0.997175	0.996120
NN	0.977895	0.977544	0.972457	0.969199
KNeighbors	0.987691	0.973050	0.987685	0.966178
XGBoost	0.999999	0.997885	0.999999	0.997799
CatBoost	0.999615	0.998490	0.999629	0.998905

In [49]:
```
value_score[['Training CV', 'Testing CV']].plot(kind = 'bar', figsize = (10,6), fontsize = 10)
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.8, 1.01)
plt.yticks([0.8, 0.85, 0.9, 0.95,1.0])
plt.title ('Appendix 2-1')
plt.show()
```

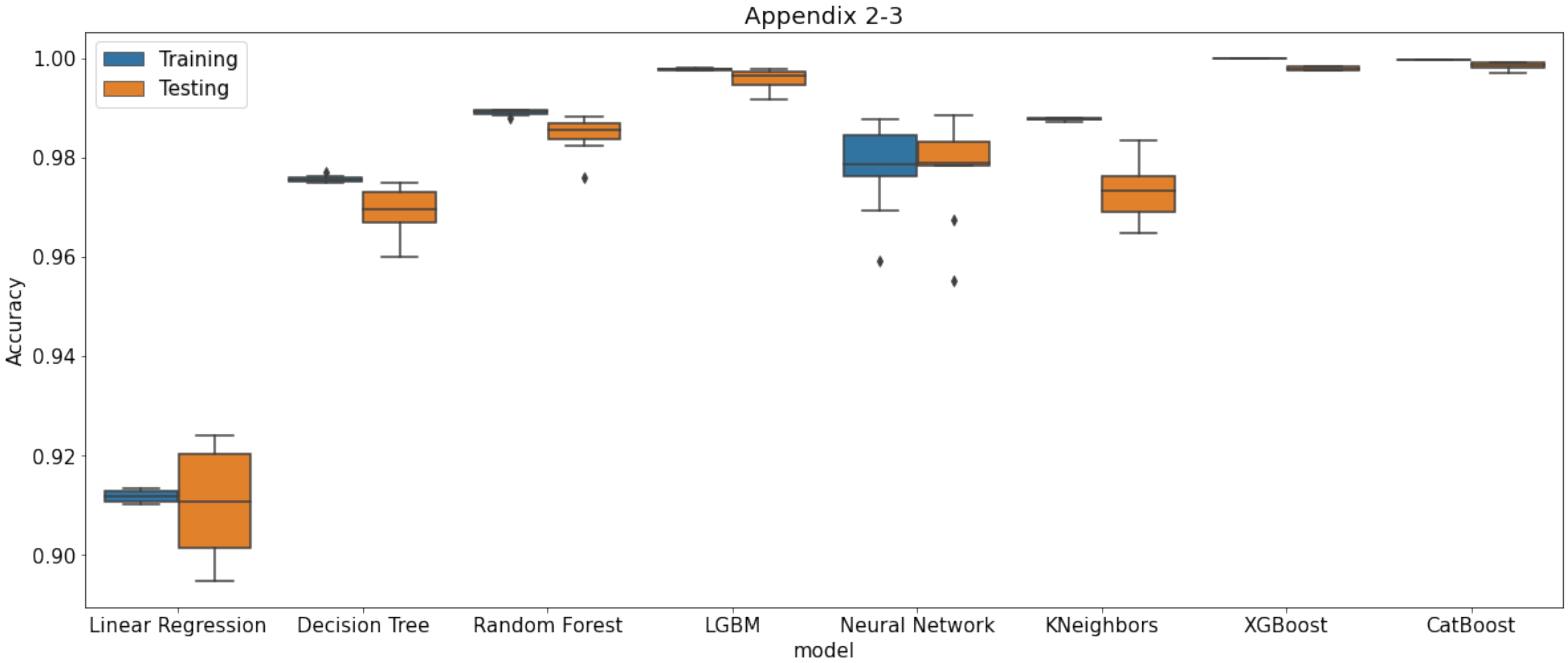


In [50]:
```
value_score[['Training Validation Set Approach', 'Testing Validation Set Approach']].plot(kind = 'bar',
                                                                        figsize = (10,6), fontsize = 10)
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.8, 1.01)
plt.yticks([0.8, 0.85, 0.9, 0.95,1.0])
plt.title ('Appendix 2-2')
plt.show()
```

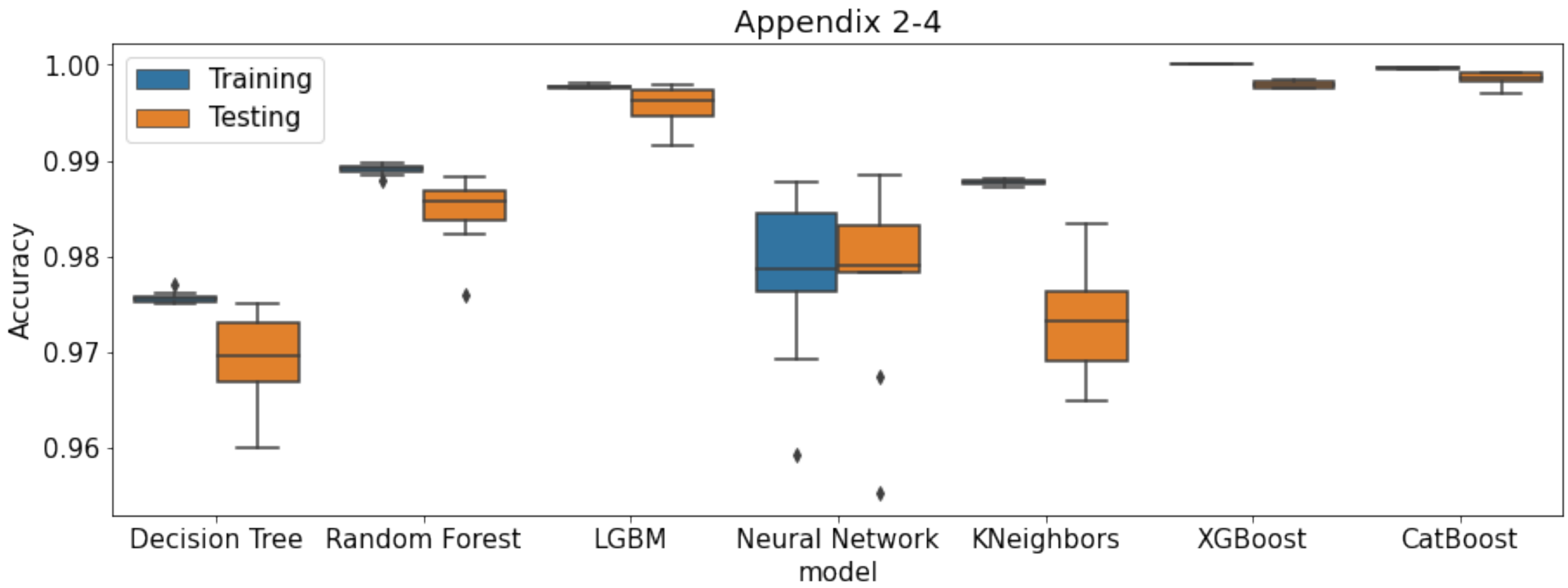


In [51]:
```
value_compare = value_compare.melt(id_vars = ['model'])
```

In [52]:
```
plt.figure(figsize = (20,8))
sns.boxplot(x='model',y='value',hue='variable', data=value_compare)
plt.ylabel('Accuracy')
plt.legend(title = '')
plt.title ('Appendix 2-3')
plt.show()
```



In [53]:
```
plt.figure(figsize = (15,5))
sns.boxplot(x='model',y='value',hue='variable', data = value_compare[value_compare['model'] != 'Linear Regression
plt.ylabel('Accuracy')
plt.legend(title = '')
plt.title ('Appendix 2-4')
plt.show()
```



3.2 For BS

3.2.1 Logistic Regression

In [54]:
```
kfolds = StratifiedKFold(n_splits = 10, random_state = 1, shuffle = True)
BS_score = pd.DataFrame(columns = ['Training CV', 'Testing CV',
                                   'Training Validation Set Approach', 'Testing Validation Set Approach'])
BS_compare = pd.DataFrame(columns = ['model','Training', 'Testing'])
```

In [55]:
```
cv_classification_score_train = []
cv_classification_score_test = []

for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]

    # Fit the model
    model = LogisticRegression(penalty='none', max_iter=10000).fit(X1,y_train)

    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [56]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=5)

# Train the model
model = LogisticRegression(penalty='none', max_iter=10000)
model = model.fit(X_train, y_train)

# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)

# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [57]:
```
# store accuracy score for each model
BS_score.loc['Logistic Regression'] = [np.mean(cv_classification_score_train),
                                       np.mean(cv_classification_score_test),score_train, score_test]
df = pd.DataFrame({'model': ['Logistic Regression']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.2 Decision Tree Classification

In [58]:
```
from sklearn.tree import DecisionTreeClassifier
```

In [59]:
```
def tree_cost_complexity_pruning(X, y_BS):
    clf_tree = DecisionTreeClassifier(random_state=0)
    path = clf_tree.cost_complexity_pruning_path(X, y_BS)
    ccp_alphas = path.ccp_alphas
    accuracies = []
    ccp_alphas = ccp_alphas[ccp_alphas >=0]
    for ccp_alpha in ccp_alphas:
        score_for_alpha = []
        for train_index, test_index in kfolds.split(X, y_BS):
            clf = DecisionTreeClassifier(random_state=0, ccp_alpha=ccp_alpha)
            clf.fit(X.iloc[train_index], y_BS.iloc[train_index])
            y_pred = clf.predict(X.iloc[test_index])
            score = accuracy_score(y_pred, y_BS.iloc[test_index])
            score_for_alpha.append(score)
        accuracies.append(sum(score_for_alpha)/len(score_for_alpha))
    alpha_cv = ccp_alphas[np.argmax(accuracies)]
    return alpha_cv
```

In [60]:
```
cv_classification_score_train = []
cv_classification_score_test = []
alpha_cv = tree_cost_complexity_pruning(X,y_BS)
for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]
    # Fit the model
    model = DecisionTreeClassifier(random_state=8, max_depth = 80, min_samples_split=10,min_samples_leaf=20,
                                   ccp_alpha = alpha_cv)
    model.fit(X1,y_train)
    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [61]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)
# Train the model
model = DecisionTreeClassifier(random_state=8, max_depth = 80, min_samples_split=10,min_samples_leaf=20,
                               ccp_alpha = alpha_cv)
model = model.fit(X_train, y_train)
# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)
# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [62]:
```
BS_score.loc['Decision Tree'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                 score_train, score_test]
df = pd.DataFrame({'model': ['Decision Tree']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.3 Random Forest Classification

In [63]:
```
cv_classification_score_train = []
cv_classification_score_test = []
for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]

    # Fit the model
    model = RandomForestClassifier(random_state=3, n_estimators =100, max_depth = 100, min_samples_split= 2,
                                   min_samples_leaf=2).fit(X1,y_train)

    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [64]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)
# Train the model
model = RandomForestClassifier(random_state=3, n_estimators =100, max_depth = 100, min_samples_split= 2,
                               min_samples_leaf=2)
model = model.fit(X_train, y_train)
# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)
# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [65]:
```
BS_score.loc['Random Forest'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                          score_train, score_test]
df = pd.DataFrame({'model': ['Random Forest']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.4 LGBM Classification

In [66]:
```
cv_classification_score_train = []
cv_classification_score_test = []

for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]

    # Fit the model
    model = lgb.LGBMClassifier(num_leaves=25,n_estimators=30, max_depth = 30).fit(X1,y_train)

    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [67]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)

# Train the model
model = lgb.LGBMClassifier(num_leaves=25,n_estimators=30, max_depth = 30)
model = model.fit(X_train, y_train)

# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)

# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [68]:
```
BS_score.loc['LGBM'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                          score_train, score_test]
df = pd.DataFrame({'model': ['LGBM']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.5 Neural Network Classification

In [69]:
```
cv_classification_score_train = []
cv_classification_score_test = []
for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]
    # Fit the model
    model = MLPClassifier(random_state = 5, hidden_layer_sizes=(15,15,15,15,15), activation = 'relu',
                          solver = 'adam', learning_rate= 'adaptive',
                          learning_rate_init = 0.01).fit(X1,y_train)
    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [70]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)
# Train the model
model = MLPClassifier(random_state = 5, hidden_layer_sizes=(15,15,15,15,15), activation = 'relu',
                      solver = 'adam', learning_rate= 'adaptive',
                          learning_rate_init = 0.01).fit(X_train, y_train)
# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)

# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [71]:
```
BS_score.loc['Neural Network'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                          score_train, score_test]
df = pd.DataFrame({'model': ['Neural Network']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.6 KNeighbors Classification

In [72]:
```
cv_classification_score_train = []
cv_classification_score_test = []

for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]

    # Fit the model
    model = KNeighborsClassifier(n_neighbors = 8).fit(X1,y_train)

    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [73]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)

# Train the model
model = KNeighborsClassifier(n_neighbors = 8).fit(X_train, y_train)

# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)

# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [74]:
```
BS_score.loc['KNeighbors'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                          score_train, score_test]
df = pd.DataFrame({'model': ['KNeighbors']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.7 XGBoost Classification

In [75]:
```
cv_classification_score_train = []
cv_classification_score_test = []

for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]
    # Fit the model
    model = xgb.XGBClassifier(random_state = 5, max_depth=10, n_estimators=5).fit(X1,y_train)
    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [76]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)
# Train the model
model = xgb.XGBClassifier(random_state = 4, max_depth=10, n_estimators=5).fit(X_train, y_train
# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)
# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [77]:
```
BS_score.loc['XGBoost'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                                          score_train, score_test]
df = pd.DataFrame({'model': ['XGBoost']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

3.2.8 Catboost Classification

In [78]:
```
cv_classification_score_train = []
cv_classification_score_test = []
for train_index, test_index in kfolds.split(X, y_BS):
    X1 = X.iloc[train_index][original_var]
    y_train = y_BS.iloc[train_index]
    X_test = X.iloc[test_index][original_var]
    y_test = y_BS.iloc[test_index]
    # Fit the model
    model = CatBoostClassifier(random_state = 5, verbose=0, max_depth=5, iterations=100,
                               learning_rate = 0.1).fit(X1,y_train)
    # Store the score
    cv_classification_score_train.append(model.score(X1, y_train))
    cv_classification_score_test.append(model.score(X_test[original_var], y_test))
```

In [79]:
```
# Use Train Test Split to test the model performance
X_train, X_test, y_train, y_test = train_test_split(X[original_var], y_BS, test_size=0.2,random_state=4)
# Train the model
model = CatBoostClassifier(random_state = 5, verbose=0, max_depth=5, iterations=100,
                           learning_rate = 0.1).fit(X_train, y_train)
# Return the score
# accuracy score for train data
score_train = accuracy_score(model.predict(X_train), y_train)
# accuracy score for test data
score_test = accuracy_score(model.predict(X_test), y_test)
```

In [80]:
```
BS_score.loc['CatBoost'] = [np.mean(cv_classification_score_train), np.mean(cv_classification_score_test),
                            score_train, score_test]
df = pd.DataFrame({'model': ['CatBoost']*10,
              'Training': cv_classification_score_train,
              'Testing': cv_classification_score_test})
BS_compare = pd.concat([BS_compare, df])
```

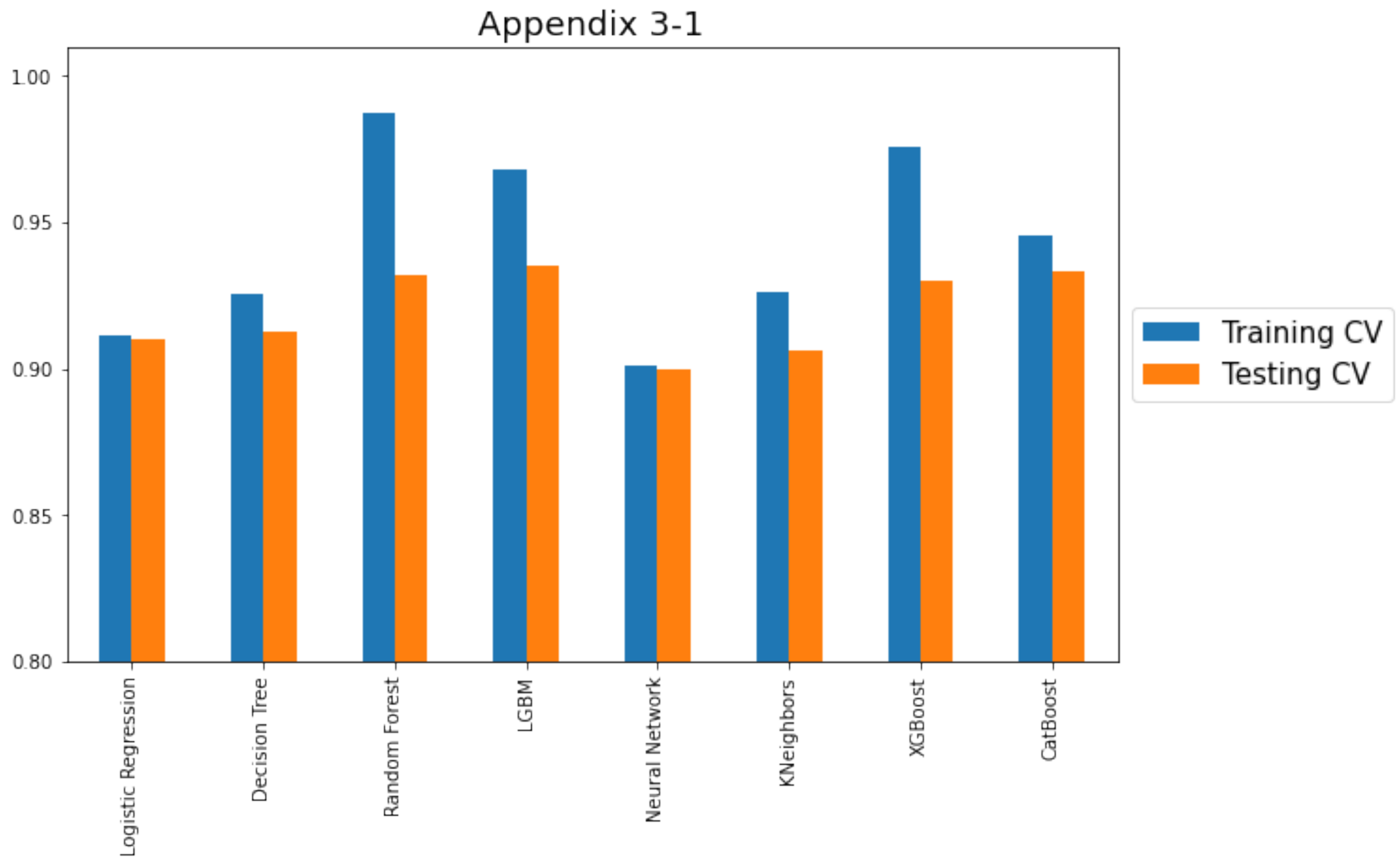
In [81]:
```
# store score for each model
value_score.loc['CatBoost'] = [np.mean(cv_score_train), np.mean(cv_score_test), r2_train, r2_test]
df = pd.DataFrame({'model': ['CatBoost']*10,
              'Training': cv_score_train,
              'Testing': cv_score_test})
value_compare = pd.concat([value_compare, df])
```

In [82]:
```
BS_score
```

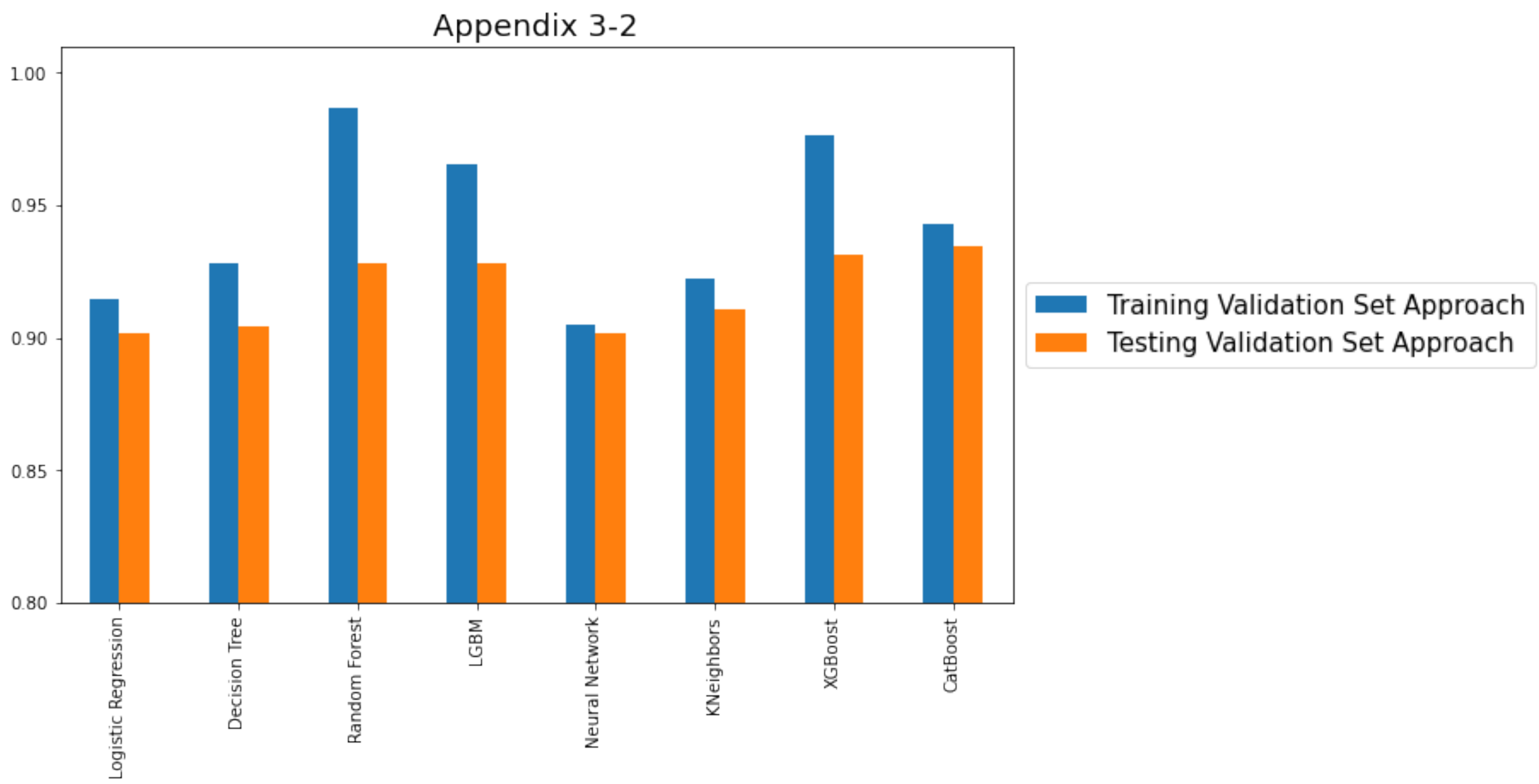
Out[82]:

	Training CV	Testing CV	Training Validation Set Approach	Testing Validation Set Approach
Logistic Regression	0.911071	0.910340	0.914798	0.901493
Decision Tree	0.925218	0.912753	0.928251	0.904478
Random Forest	0.987381	0.931890	0.986547	0.928358
LGBM	0.967723	0.934870	0.965620	0.928358
Neural Network	0.901109	0.899604	0.905082	0.901493
KNeighbors	0.925882	0.906166	0.922272	0.910448
XGBoost	0.975958	0.930101	0.976084	0.931343
CatBoost	0.945142	0.933084	0.943199	0.934328

In [83]:
```
BS_score[['Training CV', 'Testing CV']].plot(kind = 'bar', figsize = (10,6), fontsize = 10)
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.8, 1.01)
plt.yticks([0.8, 0.85, 0.9, 0.95,1.0])
plt.title ('Appendix 3-1')
plt.show()
```

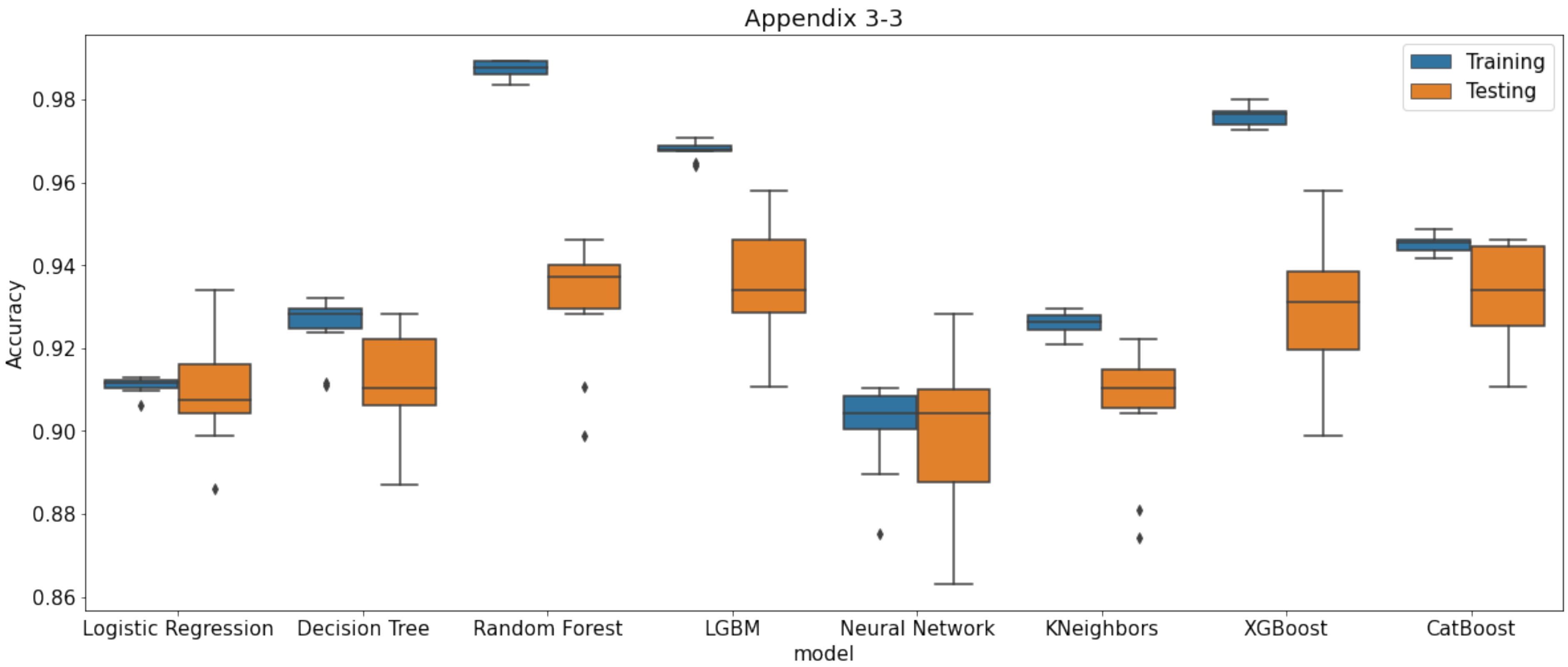


In [84]:
```python
BS_score[['Training Validation Set Approach', 'Testing Validation Set Approach']].plot(
    kind = 'bar', figsize = (10,6), fontsize = 10)
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.8, 1.01)
plt.yticks([0.8, 0.85, 0.9, 0.95,1.0])
plt.title ('Appendix 3-2')
plt.show()
```



In [85]:
```python
BS_compare = BS_compare.melt(id_vars = ['model'])
```

In [86]:
```python
plt.figure(figsize = (20,8))
sns.boxplot(x='model',y='value',hue='variable', data = BS_compare)
plt.ylabel('Accuracy')
plt.legend(title = '')
plt.title ('Appendix 3-3')
plt.show()
```



4.1 For Value (C) - With Created Variables

4.1.1 Linear Regression

In [87]:
```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
import statsmodels.api as sm
from sklearn.preprocessing import StandardScaler
import time
import itertools
```

In [88]:
```
value_score = pd.DataFrame(columns = ['r2_train', 'r2_test'])
kfolds = KFold(n_splits = 10, shuffle = True, random_state = 1)
```

In [89]:

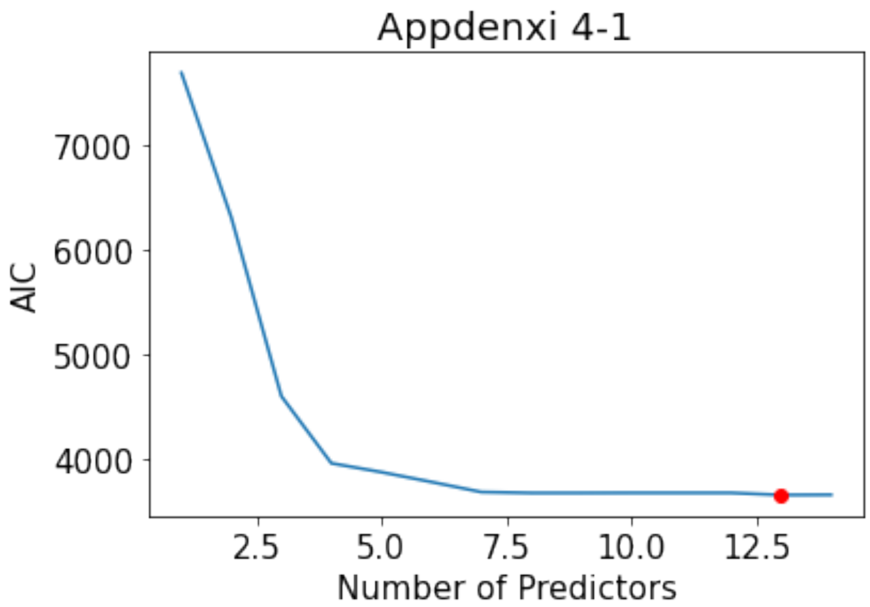
```python
def cv(var,model):
    cv_score_train = []
    cv_score_test = []
    if model == 'Random Forest':
        model = RandomForestRegressor(random_state=9, n_estimators =100, max_depth = 100,
                                      min_samples_split=10,min_samples_leaf=10)
    elif model == 'Linear':
        model = LinearRegression()
    elif model == 'LGBM':
        model = lgb.LGBMRegressor(random_state = 5, num_leaves=20,n_estimators=100, max_depth = 50)
    elif model == 'NN':
        model = MLPRegressor(random_state = 5,hidden_layer_sizes=(18,18,18), activation = 'relu',
                             solver = 'adam', learning_rate= 'constant',
                          learning_rate_init = 0.01)
    elif model == 'KNeighbors':
        model = KNeighborsRegressor(n_neighbors=3)
    elif model == 'XGBoost':
        model = xgb.XGBRegressor(random_state = 5,max_depth=25, n_estimators=30)
    elif model == 'CatBoost':
        model = CatBoostRegressor(random_state = 5,verbose=0, max_depth=8, iterations=200, learning_rate = 0.1)
    for train_index, test_index in kfolds.split(X, y_value):
        X_train = X.iloc[train_index][list(var)]
        y_train = y_value.iloc[train_index]
        X_test = X.iloc[test_index][list(var)]
        y_test = y_value.iloc[test_index]
        # Train the model
        regression = model.fit(X_train, y_train)
        # Return the score
        # rsquared for train data
        TSS_train = ((y_train - y_train.mean())**2).sum()
        RSS_train = ((regression.predict(X_train) - y_train)**2).sum()
        r2_train = (TSS_train - RSS_train)/TSS_train
        # rsquared for test data
        TSS_test = ((y_test - y_test.mean())**2).sum()
        RSS_test = ((regression.predict(X_test) - y_test)**2).sum()
        r2_test = (TSS_test - RSS_test)/TSS_test
        cv_score_train.append(r2_train)
        cv_score_test.append(r2_test)
    return {"model": model, "r2_train": np.mean(cv_score_train),
            "r2_test": np.mean(cv_score_test), "variable": var}

def subset(var):
    X_train, X_test, y_train, y_test = train_test_split(X, y_value, test_size=0.2,random_state=2)
    X1 = sm.add_constant(X_train[list(var)])
    model = sm.OLS(y_train, X1)
    regression = model.fit()

    #rsquared for train data
    r2_train = regression.rsquared

    # rsquared for test data
    X2_test = sm.add_constant(X_test[list(var)])
    TSS = ((y_test - y_test.mean())**2).sum()
    RSS_test = ((regression.predict(X2_test) - y_test)**2).sum()
    r2_test = (TSS - RSS_test)/TSS

    return {"model": regression, "r2_train": r2_train, "r2_test": r2_test,'variable': var}

def getBest(k):
    results = []

    for combo in itertools.combinations(X.columns, k):
        results.append(subset(combo))

    # Wrap everything in a dataframe
    models = pd.DataFrame(results)

    # Choose the model with the smallest RSS
    best_model = models.loc[models['r2_test'].idxmax()]

    return best_model
```

In [90]:

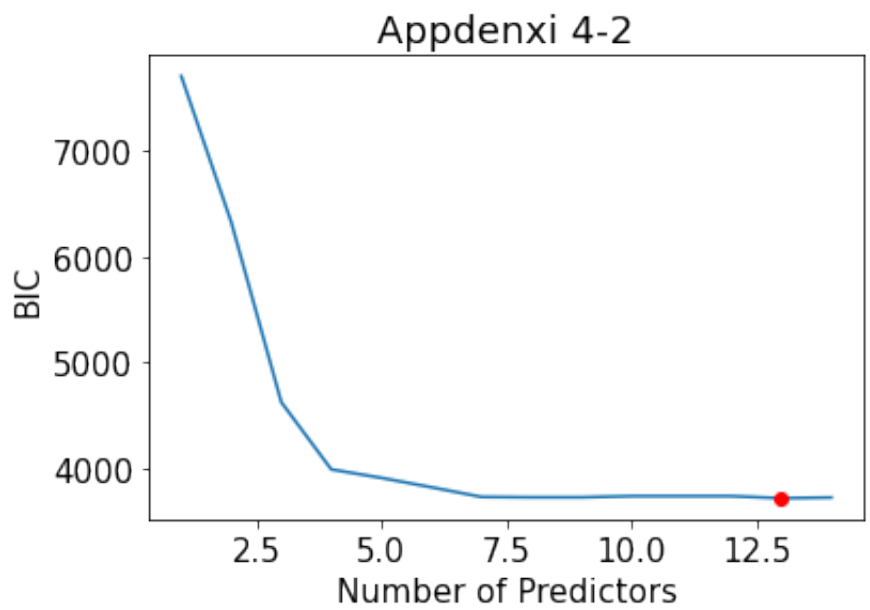
```python
models = pd.DataFrame(columns = ["model","r2_train", "r2_test",'variable'])
ct = time.time()
for i in range(1, X.shape[1]+1):
    models.loc[i] = getBest(i)
```

In [91]:

```python
aic = models.apply(lambda row: row['model'].aic, axis = 1)
plt.plot(aic)
plt.plot(aic.idxmin(), aic.min(), "or")
plt.ylabel('AIC')
plt.xlabel('Number of Predictors')
plt.title("Appdenxi 4-1")
plt.show()
```



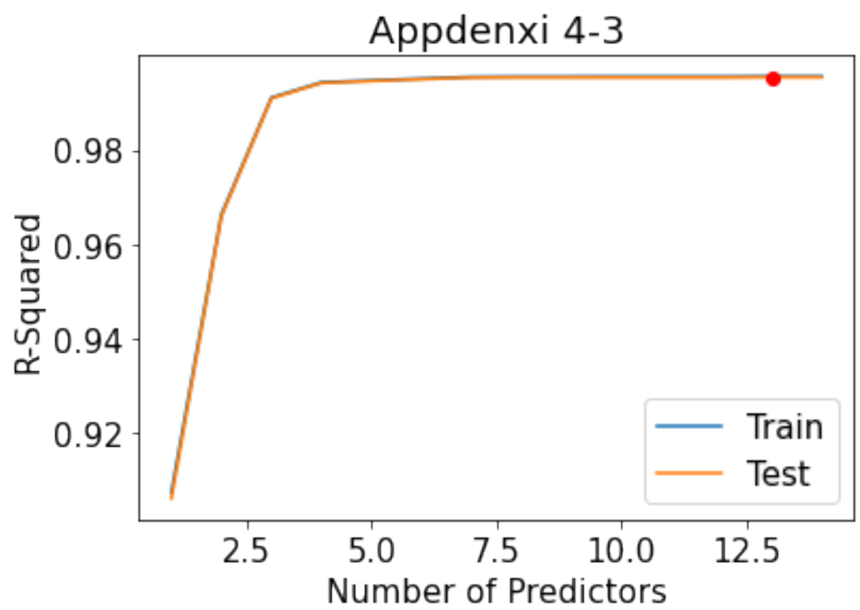

```
In [92]: bic = models.apply(lambda row: row[0].bic, axis = 1)
         plt.plot(bic)
         plt.plot(bic.idxmin(), bic.min(), "or")
         plt.ylabel('BIC')
         plt.xlabel('Number of Predictors')
         plt.title("Appdenxi 4-2")
         plt.show()
```




```
In [93]: for i in range(1, X.shape[1]+1):
             models.loc[i] = cv(models.loc[i, 'variable'], 'Linear')
         models['r2_test'] = models['r2_test'].astype("float")
         value_score.loc['Linear Regression'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```

```
In [94]: def plot_score(models,title):
             models['r2_test'] = models['r2_test'].astype("float")
             plt.plot(models['r2_train'])
             plt.plot(models['r2_test'])
             plt.plot(models['r2_test'].idxmax(), models['r2_test'].max(),"or")
             plt.ylabel('R-Squared')
             plt.xlabel('Number of Predictors')
             plt.title("R-Squared for Training/Testing Data")
             plt.legend(['Train', 'Test'])
             plt.title(title)
             plt.show()
```

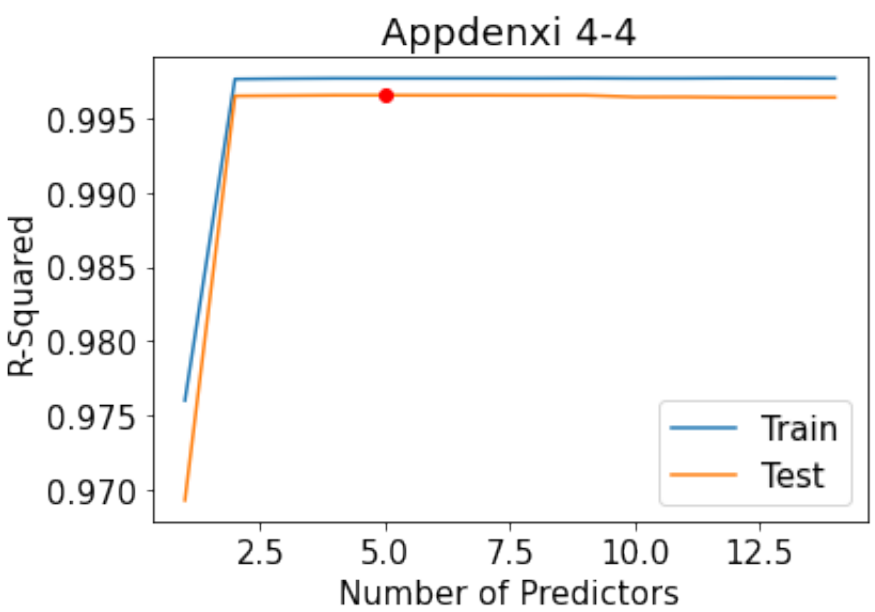
```
In [95]: plot_score(models, 'Appdenxi 4-3')
```



4.1.2 Random Forest Regression

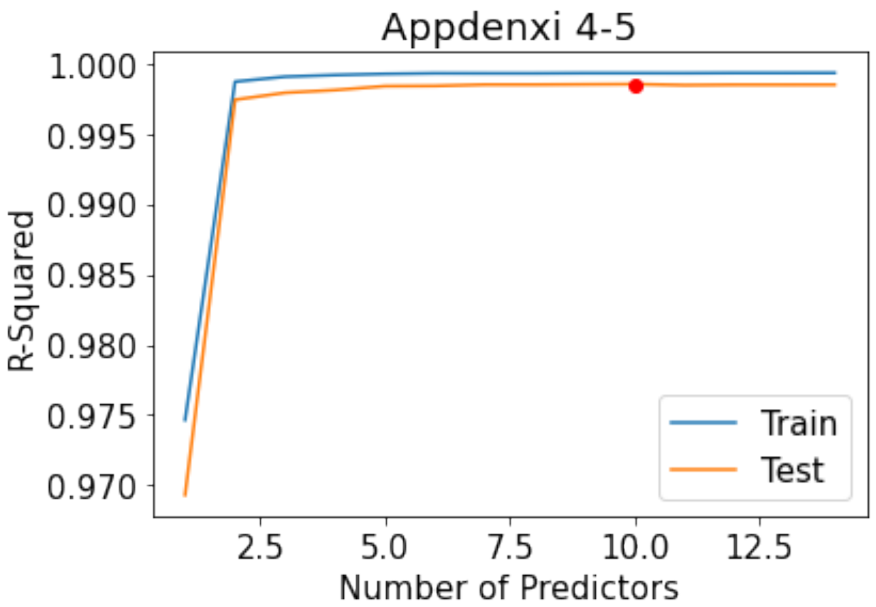
```
In [96]: def subset(var, model):
    X_train, X_test, y_train, y_test = train_test_split(X, y_value, test_size=0.2,random_state=2)
    X1 = X_train[list(var)]
    if model == 'Random Forest':
        model = RandomForestRegressor(random_state=9, n_estimators =100, max_depth = 100,
                                      min_samples_split=10,min_samples_leaf=10)
    elif model == 'LGBM':
        model = lgb.LGBMRegressor(random_state = 5, num_leaves=20,n_estimators=100, max_depth = 50)
    elif model == 'NN':
        model = MLPRegressor(random_state = 5,hidden_layer_sizes=(18,18,18), activation = 'relu',
                             solver = 'adam', learning_rate= 'constant',
                          learning_rate_init = 0.01, max_iter= 300)
    elif model == 'KNeighbors':
        model = KNeighborsRegressor(n_neighbors=3)
    elif model == 'XGBoost':
        model = xgb.XGBRegressor(random_state = 5,max_depth=25, n_estimators=30)
    elif model == 'CatBoost':
        model = CatBoostRegressor(random_state = 5,verbose=0, max_depth=8, iterations=200, learning_rate = 0.1)
    regression = model.fit(X1, y_train)
    X2_test = X_test[list(var)]
    # rsquared for train data
    TSS = ((y_train - y_train.mean())**2).sum()
    RSS_train = ((regression.predict(X1) - y_train)**2).sum()
    r2_train = (TSS - RSS_train)/TSS
    # rsquared adj for test data
    TSS = ((y_test - y_test.mean())**2).sum()
    RSS_test = ((regression.predict(X2_test) - y_test)**2).sum()
    r2_test = (TSS - RSS_test)/TSS
    return {"model": regression, "r2_train": r2_train, "r2_test": r2_test,"variable": var}

def forward(predictors,model):
    ct = time.time()
    results = []
    remaining = X.columns.drop(predictors)
    for pred in remaining:
        results.append(subset(predictors + [pred],model))
    # Wrap everything up in a dataframe
    models = pd.DataFrame(results)
    best_model = models.loc[models['r2_test'].idxmax()]
    return best_model
```

```
In [97]: forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'Random Forest')
    models.loc[i] = cv(models.loc[i, 'variable'], 'Random Forest')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-4')
value_score.loc['Random Forest'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```



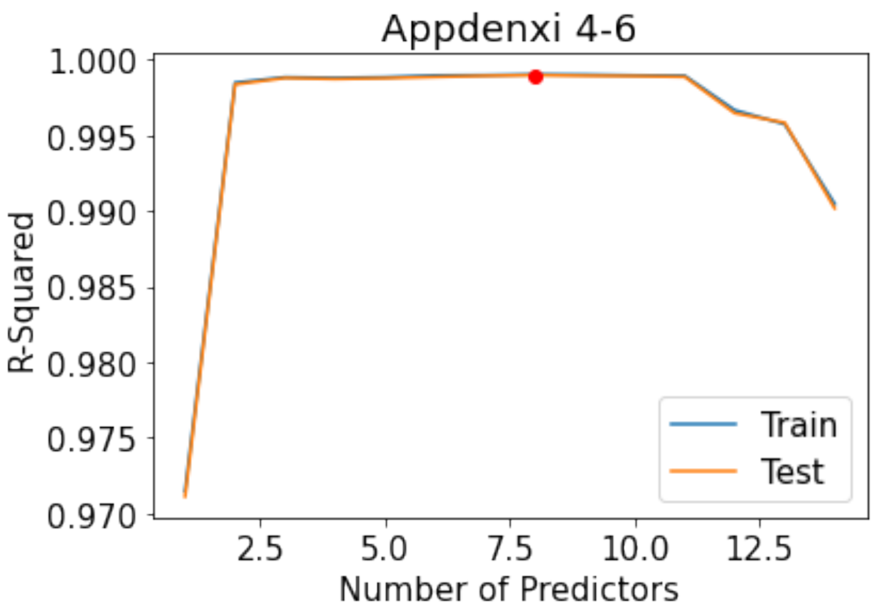
4.1.3 LGBM Regression

```
In [98]: forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'LGBM')
    models.loc[i] = cv(models.loc[i, 'variable'], 'LGBM')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-5')
value_score.loc['LGBM'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```



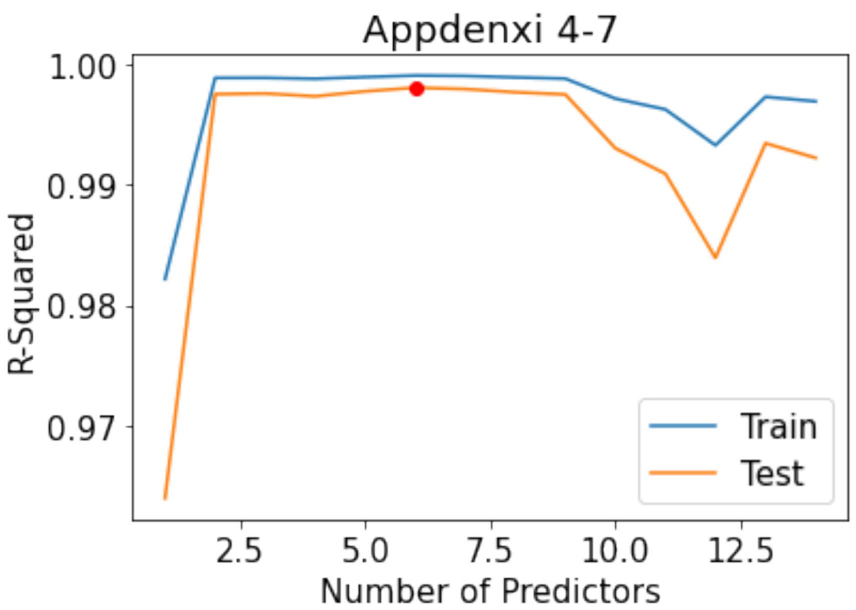
4.1.4 Neural Network Regression

In [99]:
```
forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'NN')
    models.loc[i] = cv(models.loc[i, 'variable'], 'NN')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-6')
value_score.loc['Neural Network'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```



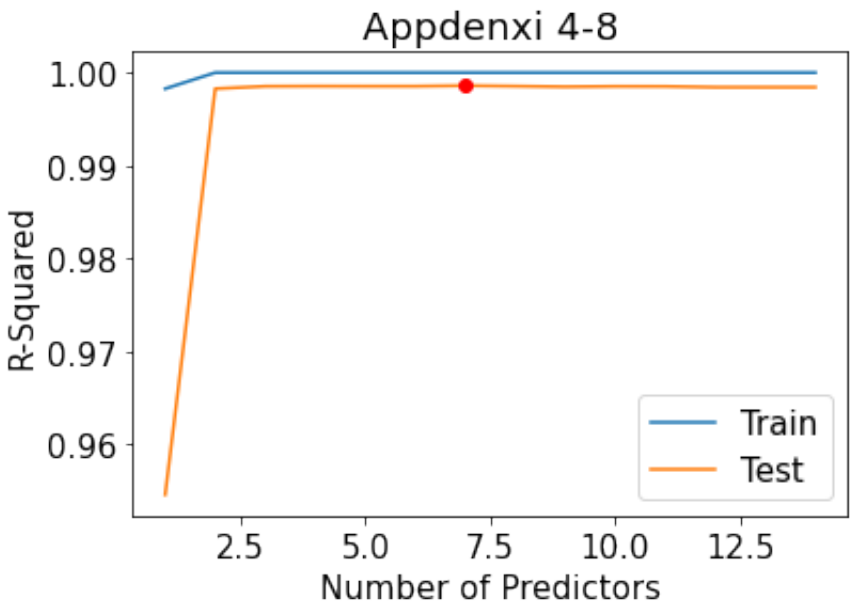
4.1.5 KNeighbors Regression

In [100…
```
forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'KNeighbors')
    models.loc[i] = cv(models.loc[i, 'variable'], 'KNeighbors')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-7')
value_score.loc['KNeighbors'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```



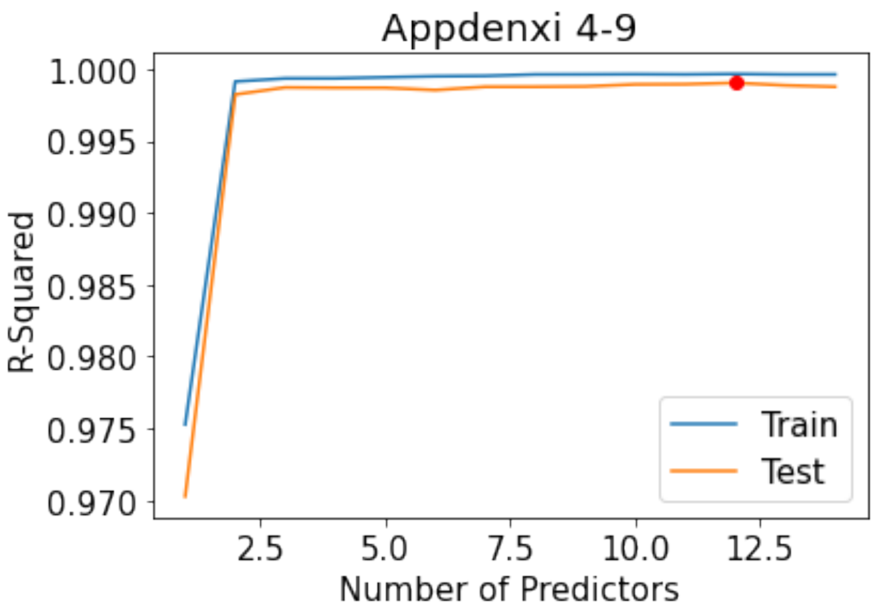
4.1.6 XGBoost Regression

In [101…
```
forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'XGBoost')
    models.loc[i] = cv(models.loc[i, 'variable'], 'XGBoost')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-8')
value_score.loc['XGBoost'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```



4.1.7 CatBoost Regression

In [102…
```
forward_num = X.shape[1]
models = pd.DataFrame(columns = ["model",'r2_train', "r2_test","variable"])
predictors = []
for i in range(1, forward_num + 1):
    models.loc[i] = forward(predictors, model = 'CatBoost')
    models.loc[i] = cv(models.loc[i, 'variable'], 'CatBoost')
    predictors = models.loc[i]['variable']
plot_score(models,'Appdenxi 4-9')
value_score.loc['CatBoost'] = models.loc[models['r2_test'].idxmax(),['r2_train', 'r2_test']]
```

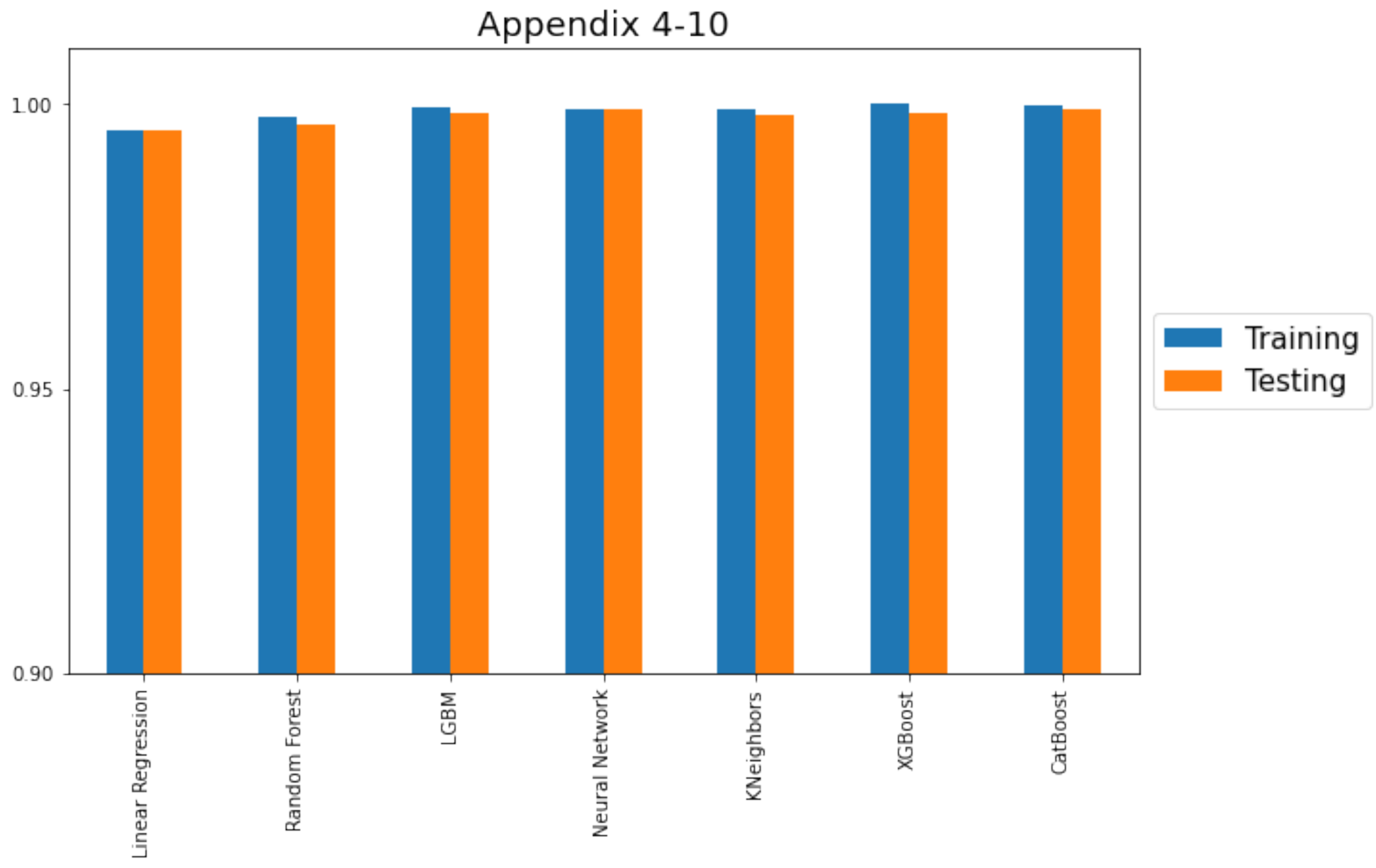


In [103…
```
value_score
```

Out[103]:

	r2_train	r2_test
Linear Regression	0.995506	0.995352
Random Forest	0.997706	0.996568
LGBM	0.999313	0.998528
Neural Network	0.999029	0.99898
KNeighbors	0.99906	0.998048
XGBoost	0.999999	0.998595
CatBoost	0.99967	0.99905

In [104…
```
value_score.plot(kind = 'bar', figsize = (10,6), fontsize = 10)
plt.legend(['Training', 'Testing'],loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.9, 1.01)
plt.yticks([0.9, 0.95,1.0])
plt.title ('Appendix 4-10')
plt.show()
```



4.2 For BS

4.2.1 Logistic Regression

In [105…

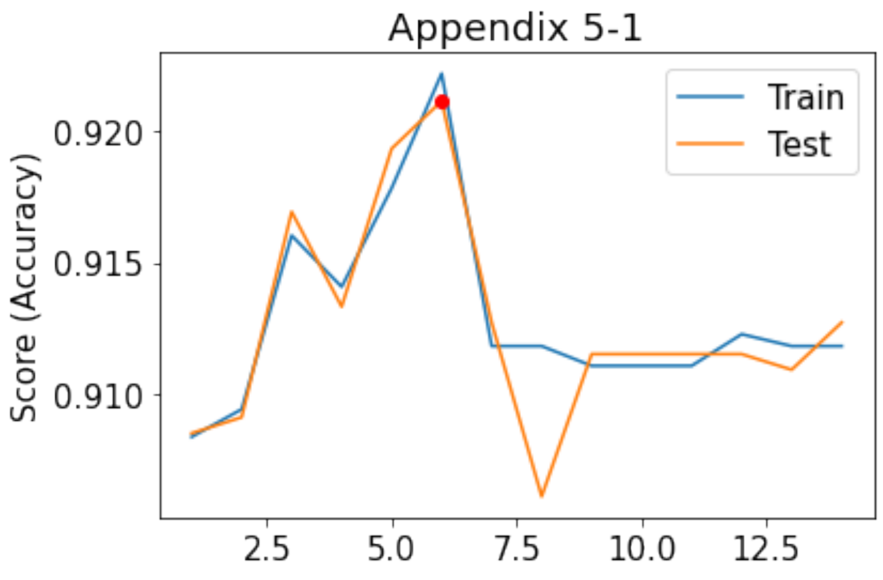
```
kfolds = StratifiedKFold(n_splits = 5, random_state = 1, shuffle = True)
BS_score = BS_score = pd.DataFrame(columns = ['score_train', 'score_test'])
```

In [106…

```
def cv(var,model_name):
    cv_classification_score_train = []
    cv_classification_score_test = []
    if model_name == 'Logistics':
        model = LogisticRegression(penalty='none', max_iter=10000)
    elif model_name == 'Random Forest':
        model = RandomForestClassifier(random_state=3, n_estimators =100, max_depth = 100,
                                       min_samples_split= 2, min_samples_leaf=2)
    elif model_name == 'LGBM':
        model = lgb.LGBMClassifier(num_leaves=25,n_estimators=30, max_depth = 30)
    elif model_name == 'NN':
        model = MLPClassifier(random_state = 5, hidden_layer_sizes=(15,15,15,15,15),
                              activation = 'relu', solver = 'adam', learning_rate= 'adaptive',
                          learning_rate_init = 0.01)
    elif model_name == 'KNeighbors':
        model = KNeighborsClassifier(n_neighbors = 8)
    elif model_name == 'XGBoost':
        model = xgb.XGBClassifier(random_state = 5, max_depth=10, n_estimators=5)
    elif model_name == 'CatBoost':
        model = CatBoostClassifier(random_state = 5, verbose=0, max_depth=5, iterations=100, learning_rate = 0.1)
    elif model_name == 'Decision Tree':
        model = DecisionTreeClassifier(random_state=3, max_depth=20,min_samples_split=20,min_samples_leaf=20)

    for train_index, test_index in kfolds.split(X, y_BS):
        X1 = X.iloc[train_index][var]
        y_train = y_BS.iloc[train_index]
        X_test = X.iloc[test_index][var]
        y_test = y_BS.iloc[test_index]
        model = model.fit(X1,y_train)
        cv_classification_score_train.append(model.score(X1, y_train))
        cv_classification_score_test.append(model.score(X_test[var], y_test))

    return {"model": model, "score_train": np.mean(cv_classification_score_train),
            "score_test": np.mean(cv_classification_score_test), "variable": var}

def subset(var, model_name):
    X_train, X_test, y_train, y_test = train_test_split(X[var], y_BS, test_size=0.2,random_state=4)
    if model_name == 'Logistics':
        model = LogisticRegression(penalty='none', max_iter=10000)
    elif model_name == 'Random Forest':
        model = RandomForestClassifier(random_state=3, n_estimators =100, max_depth = 100,
                                       min_samples_split= 2, min_samples_leaf=2)
    elif model_name == 'LGBM':
        model = lgb.LGBMClassifier(num_leaves=25,n_estimators=30, max_depth = 30)
    elif model_name == 'NN':
        model = MLPClassifier(random_state = 5, hidden_layer_sizes=(15,15,15,15,15),
                              activation = 'relu', solver = 'adam', learning_rate= 'adaptive',
                          learning_rate_init = 0.01)
    elif model_name == 'KNeighbors':
        model = KNeighborsClassifier(n_neighbors = 8)
    elif model_name == 'XGBoost':
        model = xgb.XGBClassifier(random_state = 5, max_depth=10, n_estimators=5)
    elif model_name == 'CatBoost':
        model = CatBoostClassifier(random_state = 5, verbose=0, max_depth=5, iterations=100, learning_rate = 0.1)
    elif model_name == 'Decision Tree':
        model = DecisionTreeClassifier(random_state=3, max_depth=20,min_samples_split=20,min_samples_leaf=20)

    model = model.fit(X_train, y_train)

    # Return the score
    # accuracy score for train data
    score_train = accuracy_score(model.predict(X_train), y_train)

    # accuracy score for test data
    score_test = accuracy_score(model.predict(X_test), y_test)

    return {"model": regression, "score_train": score_train, "score_test": score_test,'variable': var}

def forward(predictor, model_name):
    results = []
    remaining = X.columns.drop(predictors)
    for pred in remaining:
        results.append(subset(predictors + [pred], model_name))

    # Wrap everything up in a dataframe
    models = pd.DataFrame(results)

    best_model = models.loc[models['score_test'].idxmax()]

    return best_model
```

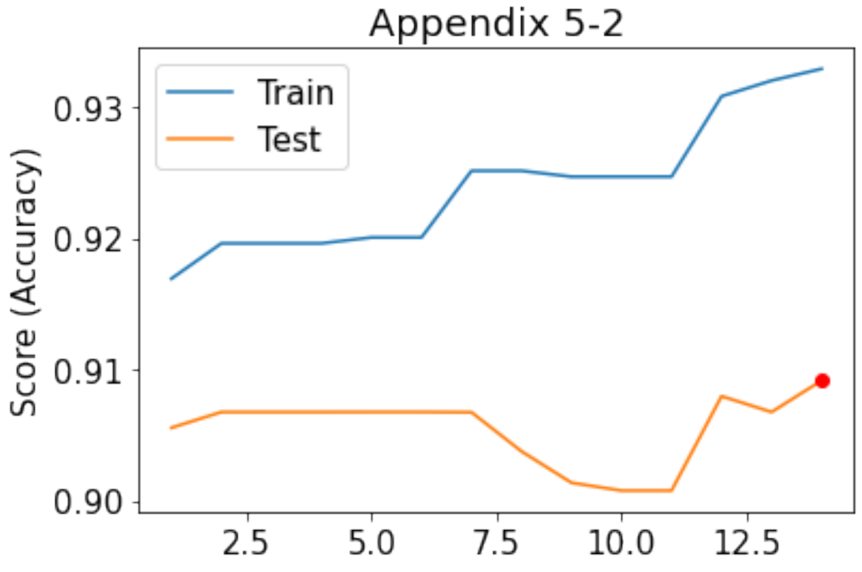
In [107…
```
forward_num = X.shape[1]
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors,'Logistics')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'Logistics')
```

In [108…
```
def plot_score(models2,title):
    models2['score_test'] = models2['score_test'].astype("float")
    plt.plot(models2['score_train'])
    plt.plot(models2['score_test'])
    plt.plot(models2['score_test'].idxmax(), models2['score_test'].max(),"or")
    plt.ylabel('Score (Accuracy)')
    plt.legend(['Train', 'Test'])
    plt.title(title)
    plt.show()
plot_score(models2, 'Appendix 5-1')
BS_score.loc['Logistic Regression'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



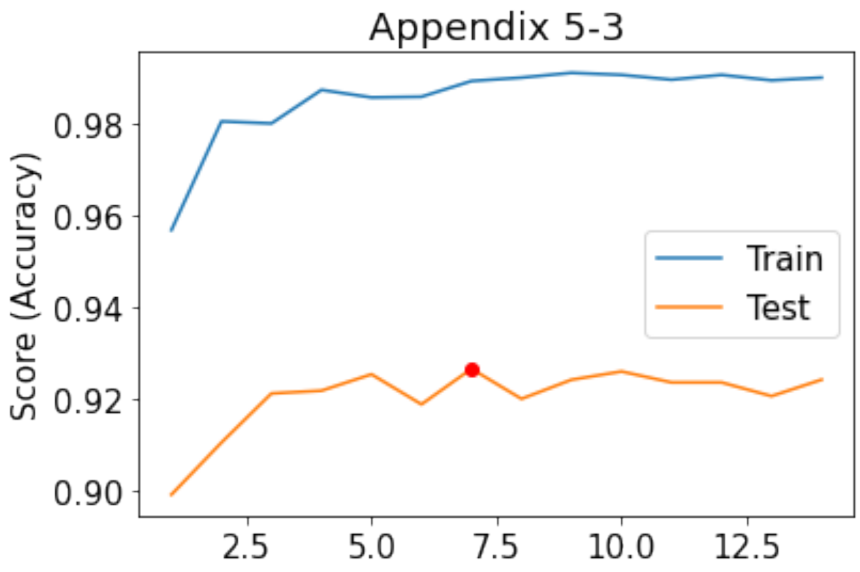
3.2.2 Decision Tree

In [109…
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'Decision Tree')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'Decision Tree')
plot_score(models2, 'Appendix 5-2')
BS_score.loc['Decision Tree'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



4.2.3 Random Forest

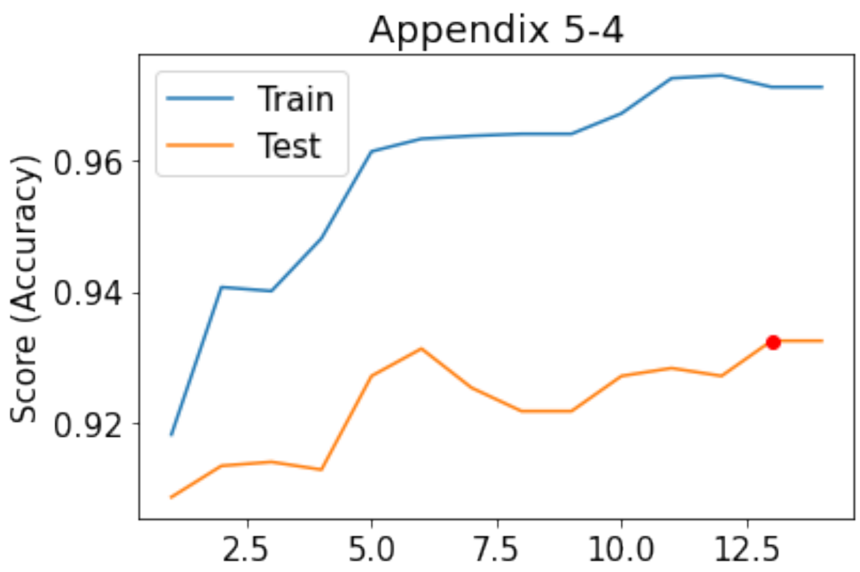
In [110…
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'Random Forest')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'Random Forest')
plot_score(models2,'Appendix 5-3')
BS_score.loc['Random Forest'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



4.2.4 LGBM Classification

In [111…

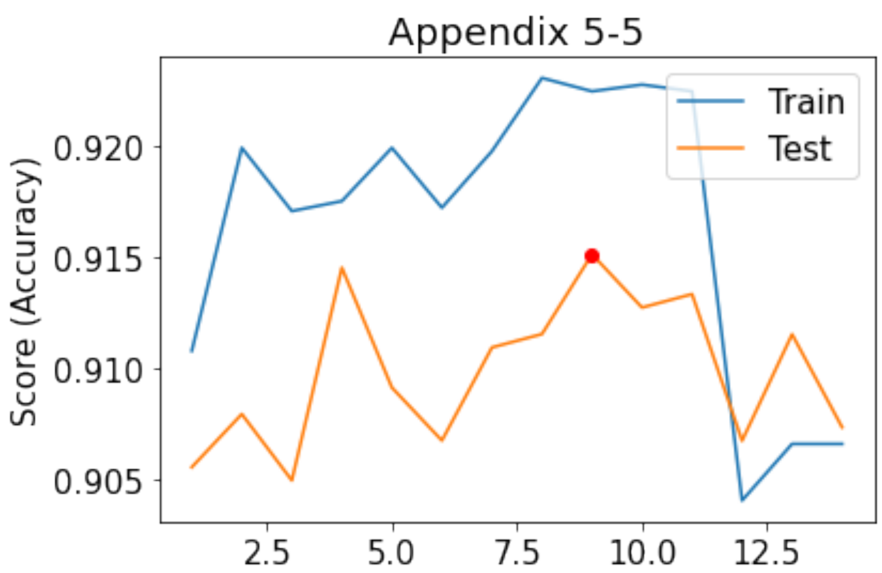
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'LGBM')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'LGBM')
plot_score(models2,'Appendix 5-4')
BS_score.loc['LGBM'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



4.2.5 Neural Network Classification

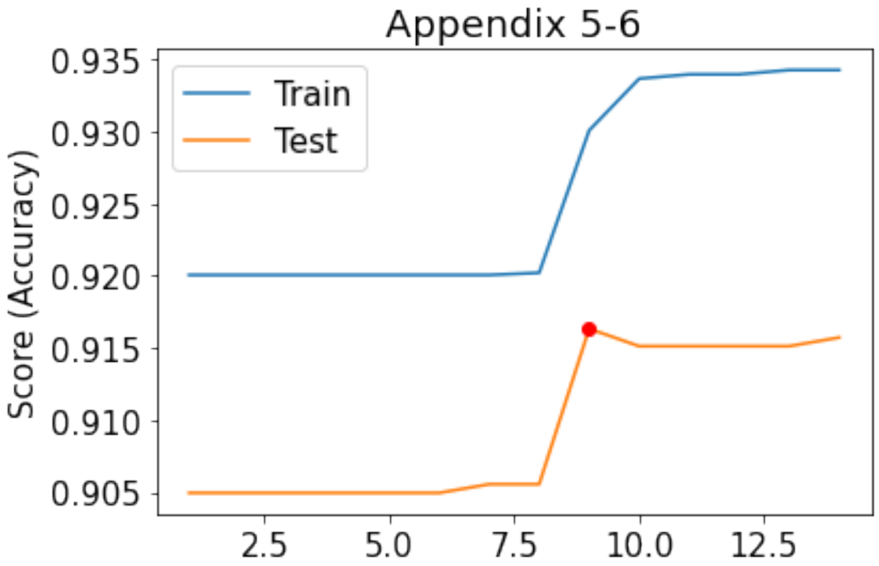
In [112…

```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'NN')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'NN')
plot_score(models2,'Appendix 5-5')
BS_score.loc['Neural Network'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



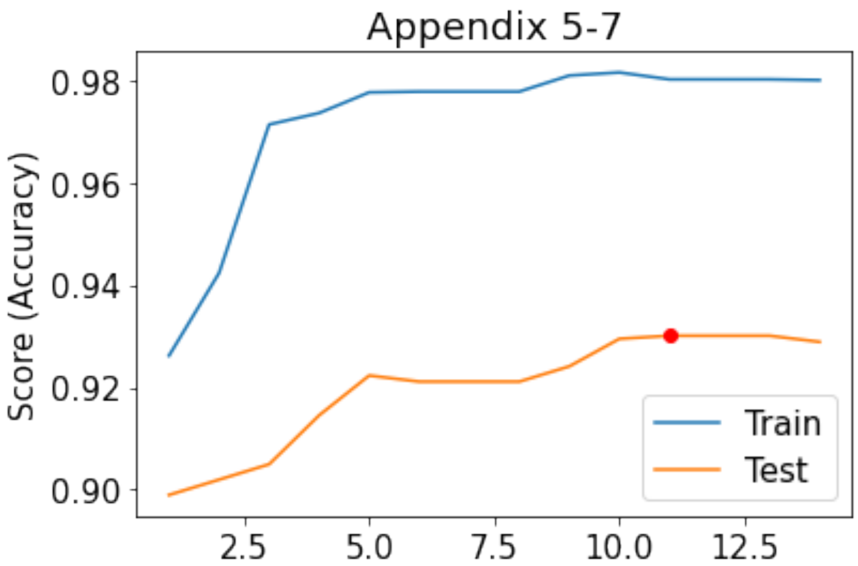
4.2.6 KNeighbors Classification

In [113…
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'KNeighbors')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'KNeighbors')
plot_score(models2,'Appendix 5-6')
BS_score.loc['KNeighbors'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



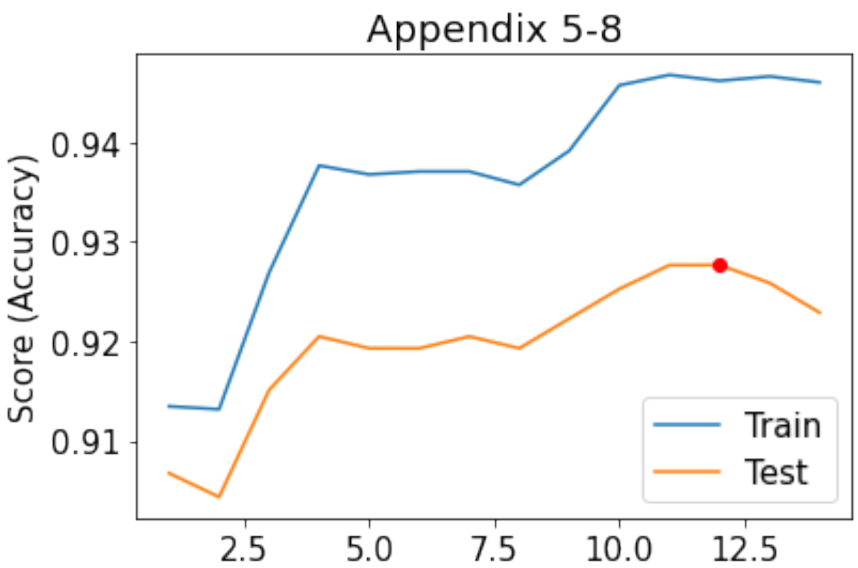
4.2.7 XGBoost Classification

In [114…
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'XGBoost')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'XGBoost')
plot_score(models2,'Appendix 5-7')
BS_score.loc['XGBoost'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



4.2.8 CatBoost Classification

In [115…
```
models2 = pd.DataFrame(columns = ['model', 'score_train', 'score_test', 'variable'])
predictors = []
for i in range(1, forward_num + 1):
    models2.loc[i] = forward(predictors, 'CatBoost')
    predictors = models2.loc[i]['variable']
    models2.loc[i] = cv(models2.loc[i, 'variable'], 'CatBoost')
plot_score(models2,'Appendix 5-8')
BS_score.loc['CatBoost'] = models2.loc[models2['score_test'].idxmax(),['score_train', 'score_test']]
```



In [116…

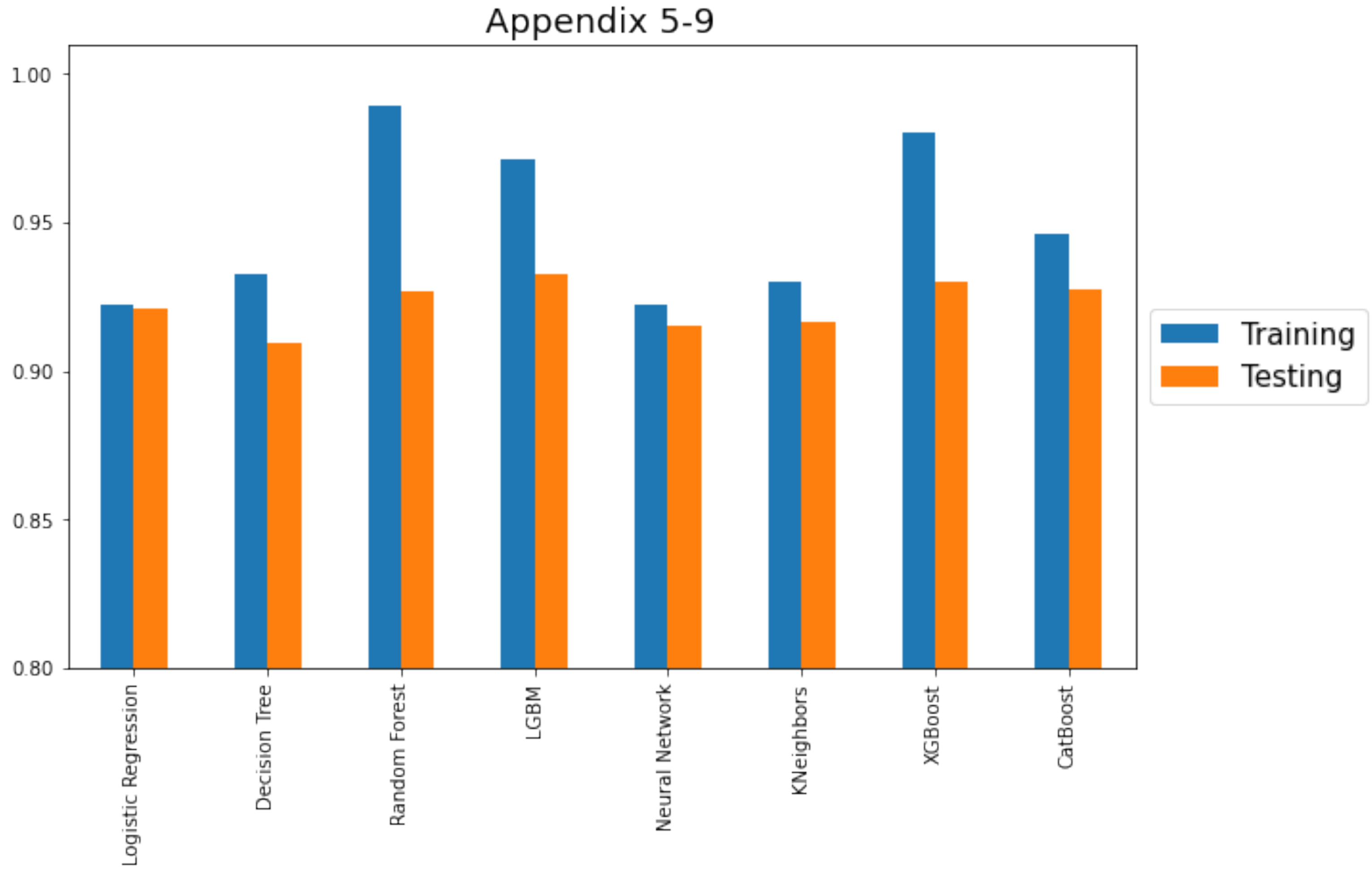
```
BS_score
```

Out[116]:

	score_train	score_test
Logistic Regression	0.922146	0.921108
Decision Tree	0.932905	0.909148
Random Forest	0.98939	0.926485
LGBM	0.971309	0.932462
Neural Network	0.922445	0.915124
KNeighbors	0.930067	0.916329
XGBoost	0.980124	0.930067
CatBoost	0.946204	0.927684

In [117…

```
BS_score.plot(kind = 'bar', figsize = (10,6), fontsize = 10)
plt.legend(['Training', 'Testing'],loc='center left', bbox_to_anchor=(1, 0.5))
plt.ylim(0.8, 1.01)
plt.yticks([0.8, 0.85, 0.9, 0.95,1.0])
plt.title ('Appendix 5-9')
plt.show()
```



5. Predict the Option Value and BS with Selected Models

In [118…

```
data_test = pd.read_csv('option_test_wolabel.csv')
```

In [119…

```
original_var = ['S', 'K', 'tau', 'r']
model = xgb.XGBRegressor(random_state = 5,max_depth=25, n_estimators=30)
model = model.fit(X[original_var], y_value)
test_value = model.predict(data_test)

model = CatBoostClassifier(random_state = 5, verbose=0, max_depth=5, iterations=100, learning_rate = 0.1)
model = model.fit(X[original_var], y_BS)
test_BS = model.predict(data_test)
pd.DataFrame({'Value': test_value,'BS':test_BS}).to_csv('group_11_prediction.csv')
```