```
Simple Regression Dataset - Linear Regression vs XGBoost
Model is trained with XGBoost installed in notebook instance

In the later examples, we will train using SageMaker's XGBoost algorithm.

Training on SageMaker takes several minutes (even for simple dataset).

If algorithm is supported on Python, we will try them locally on notebook
instance

This allows us to quickly learn an algorithm, understand tuning options and
then finally train on SageMaker Cloud

In this exercise, let's compare XGBoost and Linear Regression for simple
regression dataset
```

In [2]:

```
import sys
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error, mean_absolute_error


# XGBoost
import xgboost as xgb
# Linear Regression
from sklearn.linear_model import LinearRegression
```

In [3]:

```
# All data
df = pd.read_csv(r'C:\Users\309962\Desktop\linear_all.csv')
```

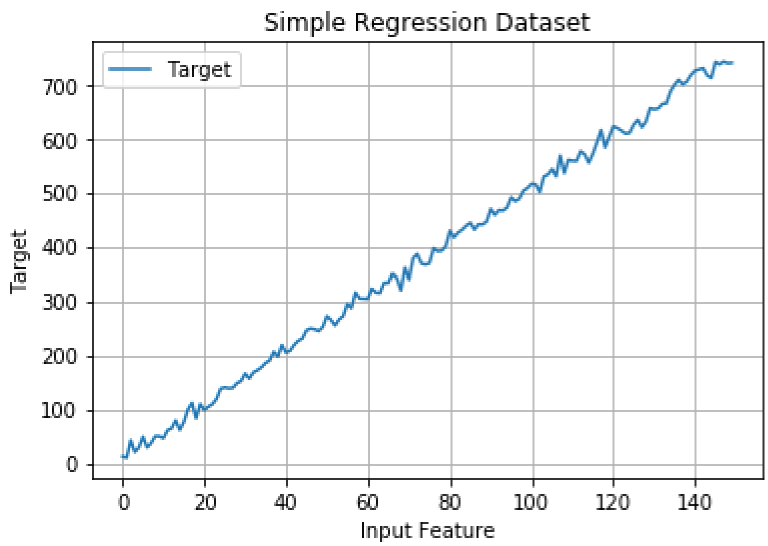
In [4]:

```
df.head()
```

Out[4]:

	x	y
0	0	12.412275
1	1	9.691298
2	2	42.307712
3	3	20.479079
4	4	29.096098

In [5]:
```
plt.plot(df.x,df.y,label='Target')
plt.grid(True)
plt.xlabel('Input Feature')
plt.ylabel('Target')
plt.legend()
plt.title('Simple Regression Dataset')
plt.show()
```



In [8]:
```
# Let's load Training and Validation Datasets
train_file = r'C:\Users\309962\Desktop\linear_train.csv'
validation_file = r'C:\Users\309962\Desktop\linear_validation.csv'

# Specify the column names as the file does not have column header
df_train = pd.read_csv(train_file,names=['y','x'])
df_validation = pd.read_csv(validation_file,names=['y','x'])
```

In [10]:
```
df_train.head()
```

Out[10]:

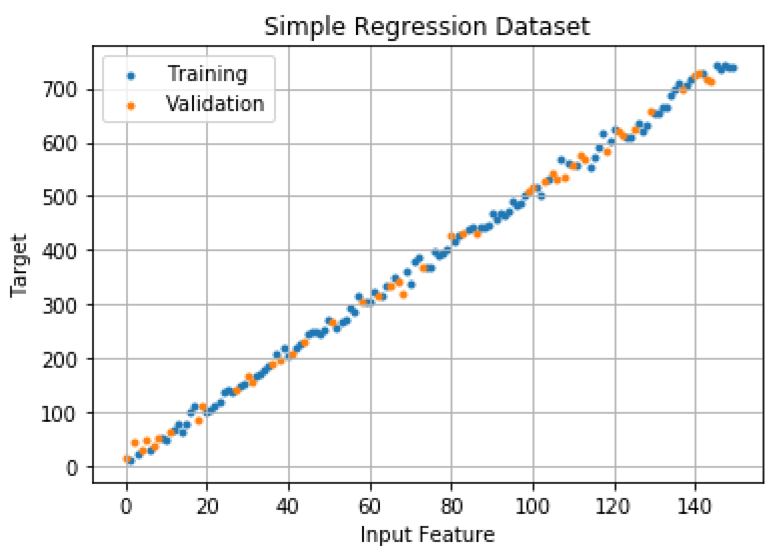
	y	x
0	425.457270	82
1	687.275162	134
2	554.643782	114
3	219.007382	42
4	560.269533	109

In [11]:
```
df_validation.head()
```

Out[11]:

	y	x
0	342.264067	67
1	60.951235	11
2	315.592889	62
3	700.097979	137
4	535.676139	108

In [12]:
```
plt.scatter(df_train.x,df_train.y,label='Training',marker='.')
plt.scatter(df_validation.x,df_validation.y,label='Validation',marker='.')
plt.grid(True)
plt.xlabel('Input Feature')
plt.ylabel('Target')
plt.title('Simple Regression Dataset')
plt.legend()
plt.show()
```



In [13]:
```

X_train = df_train.iloc[:,1:] # Features: 1st column onwards
y_train = df_train.iloc[:,0].ravel() # Target: 0th column

X_validation = df_validation.iloc[:,1:]
y_validation = df_validation.iloc[:,0].ravel()
```

In [14]:
```
# Create an instance of XGBoost Regressor
# XGBoost Training Parameter Reference:
#   https://github.com/dmlc/xgboost/blob/master/doc/parameter.md
regressor = xgb.XGBRegressor()
```

In [15]:

```
# Default Options
regressor
```

Out[15]:

```
XGBRegressor(base_score=None, booster=None, colsample_bylevel=None,
             colsample_bynode=None, colsample_bytree=None, gamma=None,
             gpu_id=None, importance_type='gain', interaction_constraints=None,
             learning_rate=None, max_delta_step=None, max_depth=None,
             min_child_weight=None, missing=nan, monotone_constraints=None,
             n_estimators=100, n_jobs=None, num_parallel_tree=None,
             objective='reg:squarederror', random_state=None, reg_alpha=None,
             reg_lambda=None, scale_pos_weight=None, subsample=None,
             tree_method=None, validate_parameters=False, verbosity=None)
```

In [16]:

```
# Train the model
# Provide Training Dataset and Validation Dataset
# XGBoost reports training and validation error
regressor.fit(X_train,y_train, eval_set = [(X_train, y_train), (X_validation, y_v
```

```
[90]    validation_0-rmse:0.48054       validation_1-rmse:15.02951
[91]    validation_0-rmse:0.46820       validation_1-rmse:15.02980
[92]    validation_0-rmse:0.46465       validation_1-rmse:15.03104

[93]    validation_0-rmse:0.46061       validation_1-rmse:15.03510
[94]    validation_0-rmse:0.44996       validation_1-rmse:15.04098
[95]    validation_0-rmse:0.43824       validation_1-rmse:15.05033
[96]    validation_0-rmse:0.43266       validation_1-rmse:15.05148
[97]    validation_0-rmse:0.41700       validation_1-rmse:15.05335
[98]    validation_0-rmse:0.40495       validation_1-rmse:15.05614
[99]    validation_0-rmse:0.39714       validation_1-rmse:15.06363
```

Out[16]:

```
XGBRegressor(base_score=0.5, booster=None, colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints=None,
             learning_rate=0.300000012, max_delta_step=0, max_depth=6,
             min_child_weight=1, missing=nan, monotone_constraints=None,
             n_estimators=100, n_jobs=0, num_parallel_tree=1,
             objective='reg:squarederror', random_state=0, reg_alpha=0,
             reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method=None,
```

In [17]:

```
# Get the Training RMSE and Evaluation RMSE
eval_result = regressor.evals_result()
```

In [18]:
```
eval_result
```

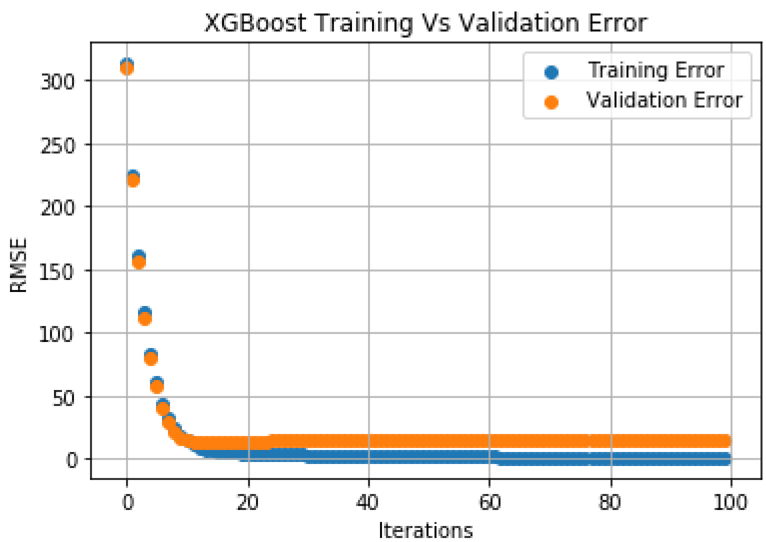
Out[18]:
```
{'validation_0': {'rmse': [312.592255,
   223.906281,
   160.909714,
   115.677025,
   83.50769,
   60.283211,
   43.793957,
   32.113873,
   23.797516,
   17.939562,
   13.833571,
   10.892591,
   8.737917,
   7.324715,
   6.226498,
   5.588068,
   5.027469,
   4.582295,
   4.258395,
```

In [19]:
```
training_rounds = range(len(eval_result['validation_0']['rmse']))
```

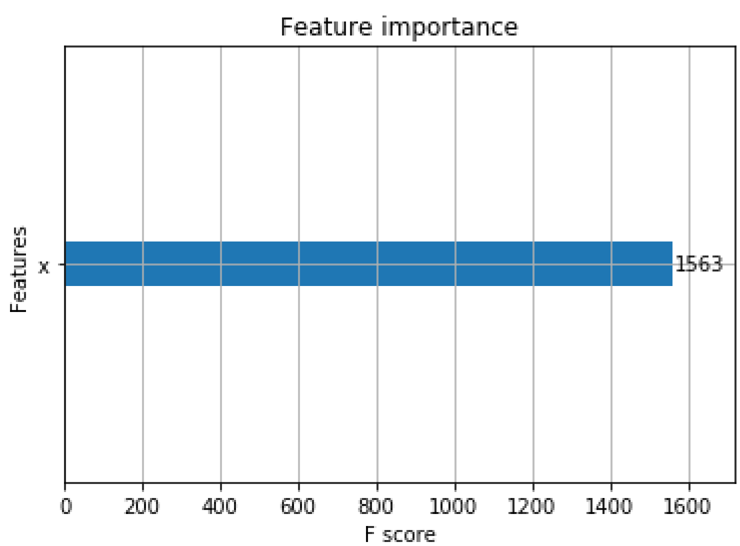
In [20]:
```
print(training_rounds)
```

```
range(0, 100)
```

In [21]:
```
plt.scatter(x=training_rounds,y=eval_result['validation_0']['rmse'],label='Traini
plt.scatter(x=training_rounds,y=eval_result['validation_1']['rmse'],label='Valida
plt.grid(True)
plt.xlabel('Iterations')
plt.ylabel('RMSE')
plt.title('XGBoost Training Vs Validation Error')
plt.legend()
plt.show()
```



In [22]:
```
xgb.plot_importance(regressor)
plt.show()
```



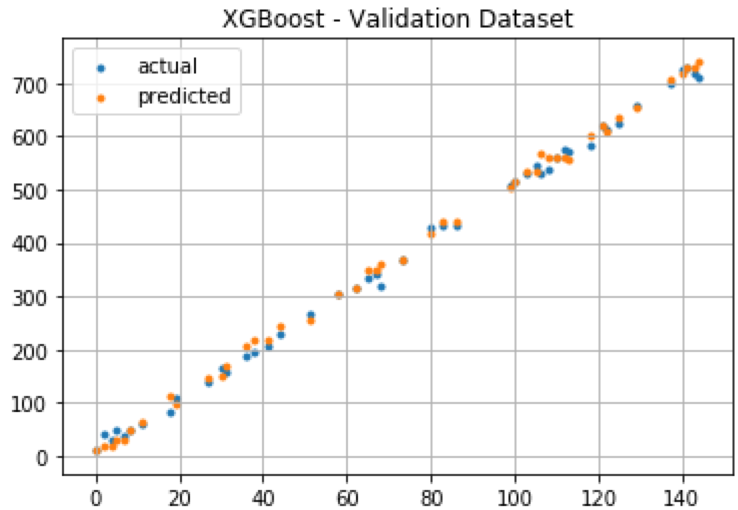
In [23]:
```
result = regressor.predict(X_validation)
```

In [24]:
```
result[:5]
```

Out[24]:
```
array([350.00354,  64.40639, 314.84644, 705.8229 , 560.227  ],
      dtype=float32)
```

In [25]:
```

plt.title('XGBoost - Validation Dataset')
plt.scatter(df_validation.x,df_validation.y,label='actual',marker='.')
plt.scatter(df_validation.x,result,label='predicted',marker='.')
plt.grid(True)
plt.legend()
plt.show()
```

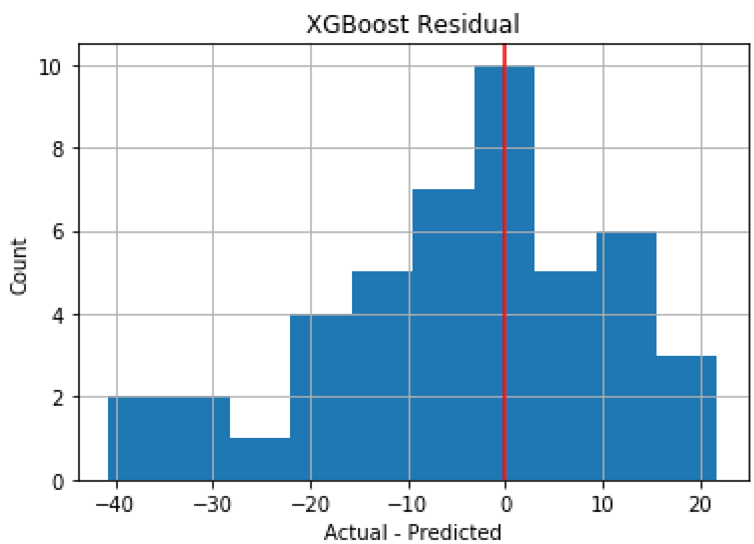


In [26]:
```
# RMSE Metrics
print('XGBoost Algorithm Metrics')
mse = mean_squared_error(df_validation.y,result)
print(" Mean Squared Error: {0:.2f}".format(mse))
print(" Root Mean Square Error: {0:.2f}".format(mse**.5))
```

```
XGBoost Algorithm Metrics
 Mean Squared Error: 226.91
 Root Mean Square Error: 15.06
```

In [27]:

```
# Residual
# Over prediction and Under Prediction needs to be balanced
# Training Data Residuals
residuals = df_validation.y - result
plt.hist(residuals)
plt.grid(True)
plt.xlabel('Actual - Predicted')
plt.ylabel('Count')
plt.title('XGBoost Residual')
plt.axvline(color='r')
plt.show()
```



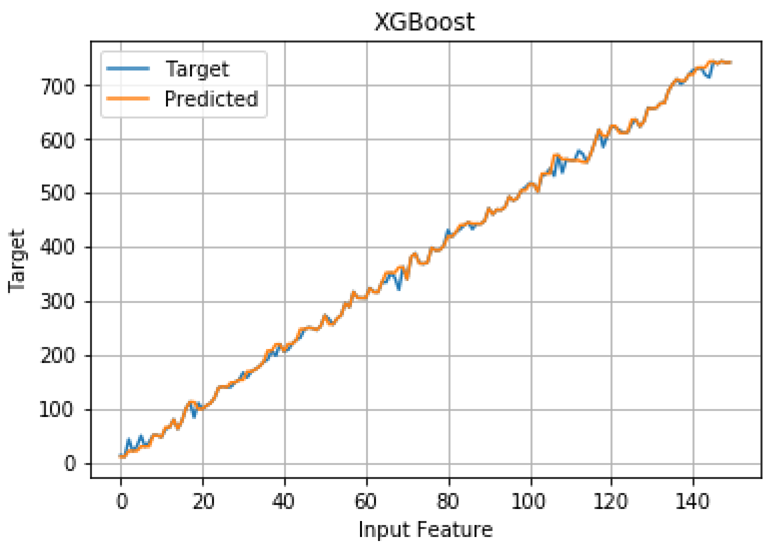
In [28]:

```
# Count number of values greater than zero and less than zero
value_counts = (residuals > 0).value_counts(sort=False)

print(' Under Estimation: {0}'.format(value_counts[True]))
print(' Over  Estimation: {0}'.format(value_counts[False]))
```

```
 Under Estimation: 22
 Over  Estimation: 23
```

In [29]:
```
# Plot for entire dataset
plt.plot(df.x,df.y,label='Target')
plt.plot(df.x,regressor.predict(df[['x']]) ,label='Predicted')
plt.grid(True)
plt.xlabel('Input Feature')
plt.ylabel('Target')
plt.legend()
plt.title('XGBoost')
plt.show()
```



Linear Regression Algorithm

In [30]:
```
lin_regressor = LinearRegression()
```

In [31]:
```
lin_regressor.fit(X_train,y_train)
```

Out[31]:
```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize=False)
```

In [32]:
```
lin_regressor.coef_
```

Out[32]:
```
array([4.99777227])
```

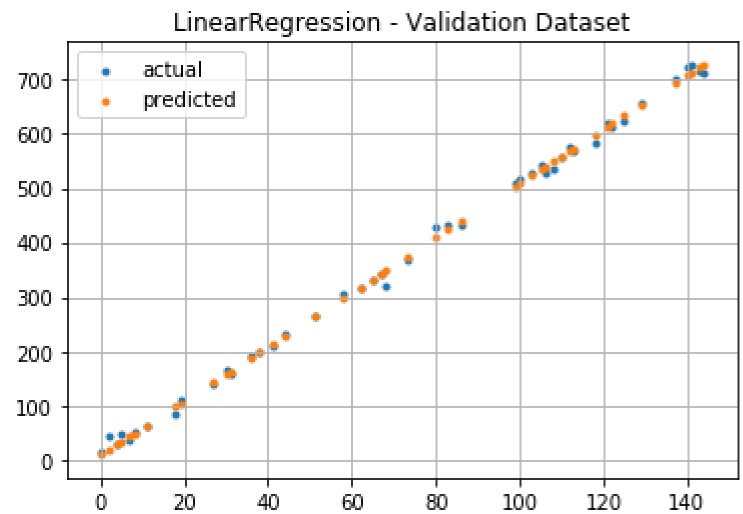
In [33]:
```
lin_regressor.intercept_
```

Out[33]:
```
8.683965388503339
```

In [34]:
```
result = lin_regressor.predict(df_validation[['x']])
```

In [35]:

```
plt.title('LinearRegression - Validation Dataset')
plt.scatter(df_validation.x,df_validation.y,label='actual',marker='.')
plt.scatter(df_validation.x,result,label='predicted',marker='.')
plt.grid(True)
plt.legend()
plt.show()
```

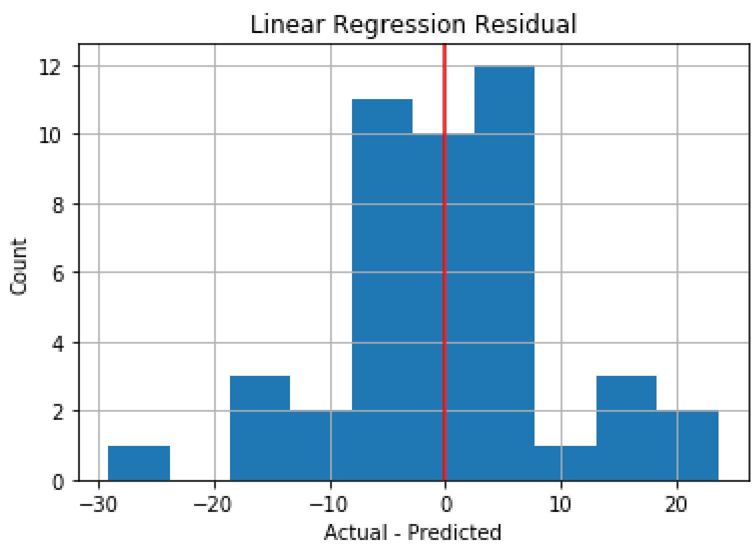


In [36]:

```
# RMSE Metrics
print('Linear Regression Metrics')
mse = mean_squared_error(df_validation.y,result)
print(" Mean Squared Error: {0:.2f}".format(mse))
print(" Root Mean Square Error: {0:.2f}".format(mse**.5))
```

```
Linear Regression Metrics
 Mean Squared Error: 99.10
 Root Mean Square Error: 9.95
```

In [37]:
```
# Residual
# Over prediction and Under Prediction needs to be balanced
# Training Data Residuals
residuals = df_validation.y - result
plt.hist(residuals)
plt.grid(True)
plt.xlabel('Actual - Predicted')
plt.ylabel('Count')
plt.title('Linear Regression Residual')
plt.axvline(color='r')
plt.show()
```



In [38]:
```
# Count number of values greater than zero and less than zero
value_counts = (residuals > 0).value_counts(sort=False)

print(' Under Estimation: {0}'.format(value_counts[True]))
print(' Over  Estimation: {0}'.format(value_counts[False]))
```

```
 Under Estimation: 24
 Over  Estimation: 21
```

In [39]:
```
# Plot for entire dataset
plt.plot(df.x,df.y,label='Target')
plt.plot(df.x,lin_regressor.predict(df[['x']]) ,label='Predicted')
plt.grid(True)
plt.xlabel('Input Feature')
plt.ylabel('Target')
plt.legend()
plt.title('LinearRegression')
plt.show()
```

Input Features - Outside range used for training

XGBoost Prediction has an upper and lower bound (applies to tree based algorithms)

Linear Regression extrapolates

In [40]:
```
# True Function
def straight_line(x):
    return 5*x + 8
```

In [41]:
```
# X is outside range of training samples
X = np.array([-100,-5,160,1000,5000])
y = straight_line(X)

df_tmp = pd.DataFrame({'x':X,'y':y})
df_tmp['xgboost']=regressor.predict(df_tmp[['x']])
df_tmp['linear']=lin_regressor.predict(df_tmp[['x']])
```

In [42]:

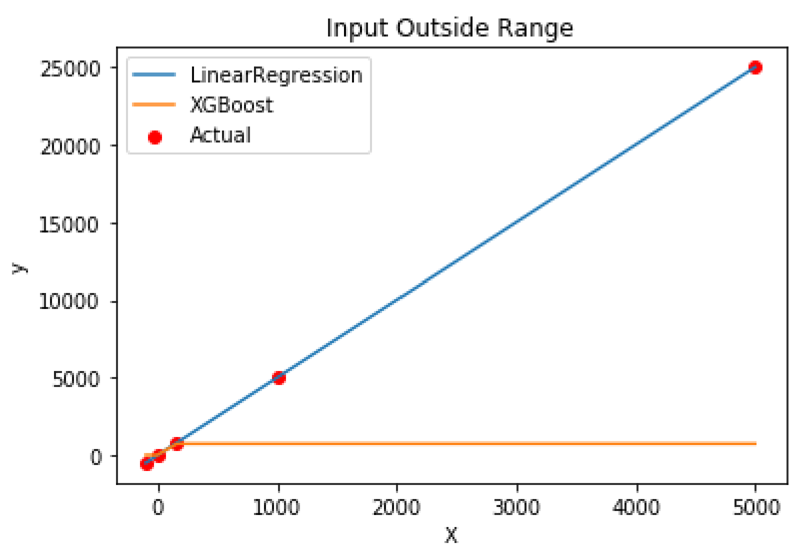
```
df_tmp
```

Out[42]:

	x	y	xgboost	linear
0	-100	-492	9.905086	-491.093262
1	-5	-17	9.905086	-16.304896
2	160	808	739.950562	808.327528
3	1000	5008	739.950562	5006.456235
4	5000	25008	739.950562	24997.545312

In [43]:

```
# XGBoost Predictions have an upper bound and lower bound
# Linear Regression Extrapolates
plt.scatter(df_tmp.x,df_tmp.y,label='Actual',color='r')
plt.plot(df_tmp.x,df_tmp.linear,label='LinearRegression')
plt.plot(df_tmp.x,df_tmp.xgboost,label='XGBoost')
plt.legend()
plt.xlabel('X')
plt.ylabel('y')
plt.title('Input Outside Range')
plt.show()
```



In [44]:

```
# X is inside range of training samples
X = np.array([0,1,3,5,7,9,11,15,18,125])
y = straight_line(X)

df_tmp = pd.DataFrame({'x':X,'y':y})
df_tmp['xgboost']=regressor.predict(df_tmp[['x']])
df_tmp['linear']=lin_regressor.predict(df_tmp[['x']])
```

In [45]:

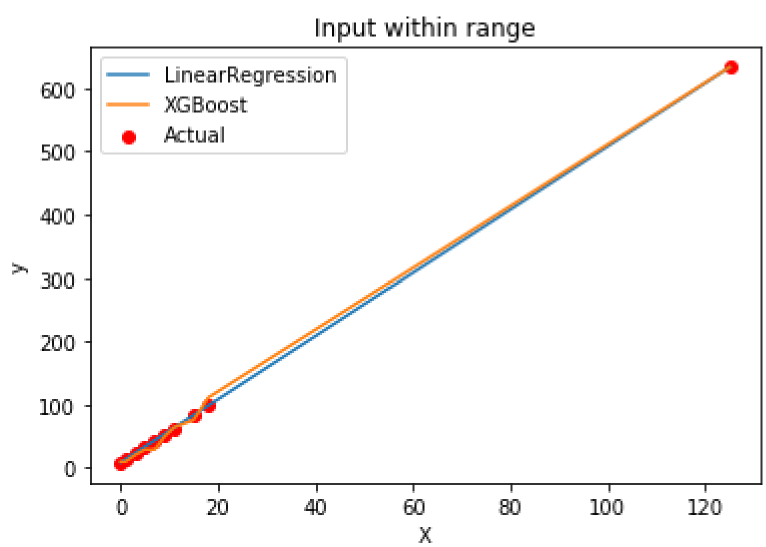
```
df_tmp
```

Out[45]:

	x	y	xgboost	linear
0	0	8	9.905086	8.683965
1	1	13	9.905086	13.681738
2	3	23	20.523394	23.677282
3	5	33	28.935297	33.672827
4	7	43	28.935297	43.668371
5	9	53	49.514168	53.663916
6	11	63	64.406387	63.659460
7	15	83	75.930733	83.650549
8	18	98	111.305298	98.643866
9	125	633	633.698364	633.405499

In [46]:

```
# XGBoost Predictions have an upper bound and lower bound
# Linear Regression Extrapolates
plt.scatter(df_tmp.x,df_tmp.y,label='Actual',color='r')
plt.plot(df_tmp.x,df_tmp.linear,label='LinearRegression')
plt.plot(df_tmp.x,df_tmp.xgboost,label='XGBoost')
plt.legend()
plt.xlabel('X')
plt.ylabel('y')
plt.title('Input within range')
plt.show()
```



Summary

1.Use sagemaker notebook as your own server on the cloud 2.Install python packages 3.Train directly on SageMaker Notebook (for small datasets, it takes few seconds). 4.Once happy with algorithm and performance, you can train on sagemaker cloud (takes several minutes even for small datasets) 5.Not all algorithms are available for installation (for example: AWS algorithms like DeepAR are available only in SageMaker) 6.In this exercise, we installed XGBoost and compared performance of XGBoost model and Linear Regression

In [ ]:

```

```