1. Python Packages

In [1]:
```
!pip install xgboost
```

```
Defaulting to user installation because normal site-packages is not writeable
Requirement already satisfied: xgboost in c:\users\patron\appdata\roaming\python\pyt
hon39\site-packages (1.7.6)
Requirement already satisfied: numpy in c:\program files\anaconda\lib\site-packages
(from xgboost) (1.21.5)
Requirement already satisfied: scipy in c:\program files\anaconda\lib\site-packages
(from xgboost) (1.9.1)
```

In [2]:
```
import numpy as np
# Numpy stands for Numerical Python is a package for scientific computing
import pandas as pd
# Pandas stands for Panel Datas is a Python Data Analysis Library
import matplotlib.pyplot as plt
# Matplotlib is the plotting package that we'll use
import sklearn
# Scikit-Learn is a machine learning package, providing the backbone for our work
from sklearn import tree
from sklearn import metrics
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import KFold,RepeatedKFold
from sklearn.model_selection import cross_validate,GridSearchCV,ParameterGrid
from math import sqrt
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import PolynomialFeatures
from sklearn.neighbors import KNeighborsRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.svm import SVR
from sklearn.neural_network import MLPRegressor
from xgboost import XGBRegressor
from sklearn.tree import export_graphviz
```

2. Importing the DataFrame

In [3]:
```
df = pd.read_csv("compiled-set-1.csv")
df.head()
```

Out[3]:

	conc	micros	adc1
0	0	216	1.163245
1	0	1322716	1.163245
2	0	1346724	1.163245
3	0	1370732	1.163245
4	0	1394904	1.163245

3. Splitting Targets and Features

3.1. Export Features

In [4]:
```
x = df[['conc','micros']]
```

3.2. Read Features

In [5]:
```
x.head()
# First 5 sets are shown
```

Out[5]:

	conc	micros
0	0	216
1	0	1322716
2	0	1346724
3	0	1370732
4	0	1394904

3.3. Export Targets

In [6]:
```
y = df['adc1']
```

3.4. Read Targets

In [7]:
```
y.head()
# Outputs correspond to First 5 Feature sets are shown
```

Out[7]:
```
0    1.163245
1    1.163245
2    1.163245
3    1.163245
4    1.163245
Name: adc1, dtype: float64
```

4. Setting Up Model Evaluation

In [8]:
```
# Generate train/test split by reserving 20% of data as test set
x_train,x_test,y_train,y_test=train_test_split(x,y,test_size=0.2,random_state=1)
```

4.1. Fitting A Linear Regression Model

In [9]:
```
# Creating object for Linear Regression
LR = LinearRegression()
```

In [10]:
```
# fit/train the Linear regression model
LR.fit(x_train,y_train)
```

Out[10]:
```
LinearRegression()
```

In [11]:
```
# Make predictions on test data
LR_pred = LR.predict(x_test)
```

4.2. Multivariable Polynomial Regression

In [12]:
```
# Transforming Features into Polynomial Features
PF = PolynomialFeatures(degree=5)
```

In [13]:
```
x_train_poly = PF.fit_transform(x_train)
x_test_poly = PF.fit_transform(x_test)
```

In [14]:
```
# Fit the Linear Regression Model
LR.fit(x_train_poly,y_train)

# Make predictions on test and train data
x_test_predp = LR.predict(x_test_poly)
x_train_predp = LR.predict(x_train_poly)
```

In [15]:
```
# Accuracy of prediction for test data using LinearRegression model
LR.score(x_test_poly,y_test)
```

Out[15]:
```
0.3581898919450647
```

In [16]:
```
# Accuracy of prediction for train data using LinearRegression model
LR.score(x_train_poly,y_train)
```

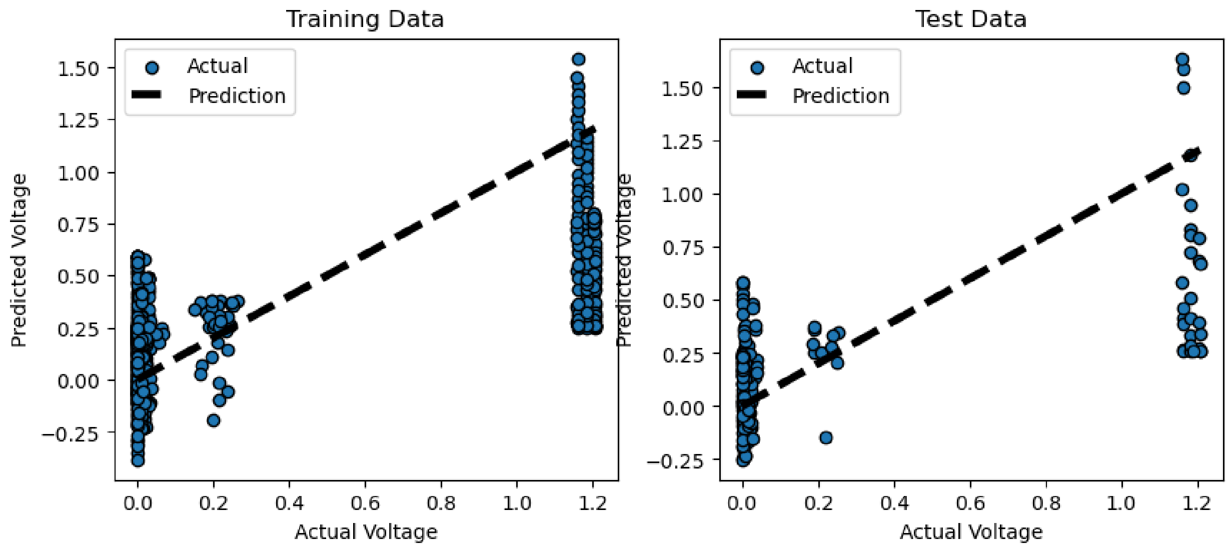
Out[16]:
```
0.42573947918886523
```

In [17]:
```
def rmse(y_true, Y_predictions): return round(np.sqrt(metrics.mean_squared_error(y_tr
def rmse_std(y_true, Y_predictions): return round(rmse(y_true, Y_predictions)/np.std(
def mae(y_true, Y_predictions): return round(metrics.mean_absolute_error(y_true, Y_pr
def r2(y_true, Y_predictions): return round(metrics.r2_score(y_true, Y_predictions),4
```

In [18]:
```
def parity_stats(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    rmse_left = rmse(y_left_true,Y_left_predictions)
    rmse_std_left = rmse_std(y_left_true,Y_left_predictions)
    mae_left = mae(y_left_true,Y_left_predictions)
    r2_left = r2(y_left_true,Y_left_predictions)
    rmse_right = rmse(y_right_true,Y_right_predictions)
    rmse_std_right = rmse_std(y_right_true,Y_right_predictions)
    mae_right = mae(y_right_true,Y_right_predictions)
    r2_right = r2(y_right_true,Y_right_predictions)
    stats_df = pd.DataFrame({'Error Metric' : ['RMSE', 'RMSE/std', 'MAE', 'R2'],
    title_left : [str(rmse_left), rmse_std_left, str(mae_left), r2_left], title_right
    return stats_df
```

In [19]:
```
def parity_plots(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    fig1, (ax1,ax2) = plt.subplots(1,2,figsize=(10,4))
    ax1.scatter(y_left_true, Y_left_predictions, edgecolors=(0, 0, 0))
    ax1.plot([y_left_true.min(), y_left_true.max()], [y_left_true.min(),y_left_true.ma
    ax1.legend(["Actual", "Prediction"])
    ax1.set_xlabel('Actual Voltage')
    ax1.set_ylabel('Predicted Voltage')
    ax1.set_title(title_left)
    ax2.scatter(y_right_true, Y_right_predictions, edgecolors=(0, 0, 0))
    ax2.plot([y_right_true.min(), y_right_true.max()], [y_right_true.min(), y_right_tr
    ax2.legend(["Actual", "Prediction"])
    ax2.set_xlabel('Actual Voltage')
    ax2.set_ylabel('Predicted Voltage')
    ax2.set_title(title_right)
    plt.savefig("parity_rf.jpg",dpi=300)
    plt.show()
```

In [20]:
```
parity_plots(y_train,x_train_predp,y_test,x_test_predp,title_left="Training Data",tit
parity_stats(y_train,x_train_predp,y_test,x_test_predp,"Training Data","Test Data")
# print error metrics for training data
```



Out[20]:

	Error Metric	Training Data	Test Data	Note
0	RMSE	0.3451	0.3654	(0.0 for perfect prediction)
1	RMSE/std	0.7578	0.801	(0.0 for perfect prediction)
2	MAE	0.2597	0.2668	(0.0 for perfect prediction)
3	R2	0.4257	0.3582	(1.0 for perfect prediction)

4.3. Support Vector Regression

In [21]:
```
# Creating object for Support Vector Regression
SV = SVR()
```

In [22]:
```
# fit/train the Support Vector Regression model
SV.fit(x_train,y_train)
```

Out[22]: SVR()

In [23]:
```
# Make predictions on test and train data
SV_test_pred = SV.predict(x_test)
SV_train_pred = SV.predict(x_train)
```

In [24]:
```
# Accuracy of prediction for test data using current model
SV.score(x_test,y_test)
```

Out[24]: -0.09822820105166397

In [25]:
```
def rmse(y_true, Y_predictions): return round(np.sqrt(metrics.mean_squared_error(y_tr
def rmse_std(y_true, Y_predictions): return round(rmse(y_true, Y_predictions)/np.std(
def mae(y_true, Y_predictions): return round(metrics.mean_absolute_error(y_true, Y_pr
def r2(y_true, Y_predictions): return round(metrics.r2_score(y_true, Y_predictions),4
```

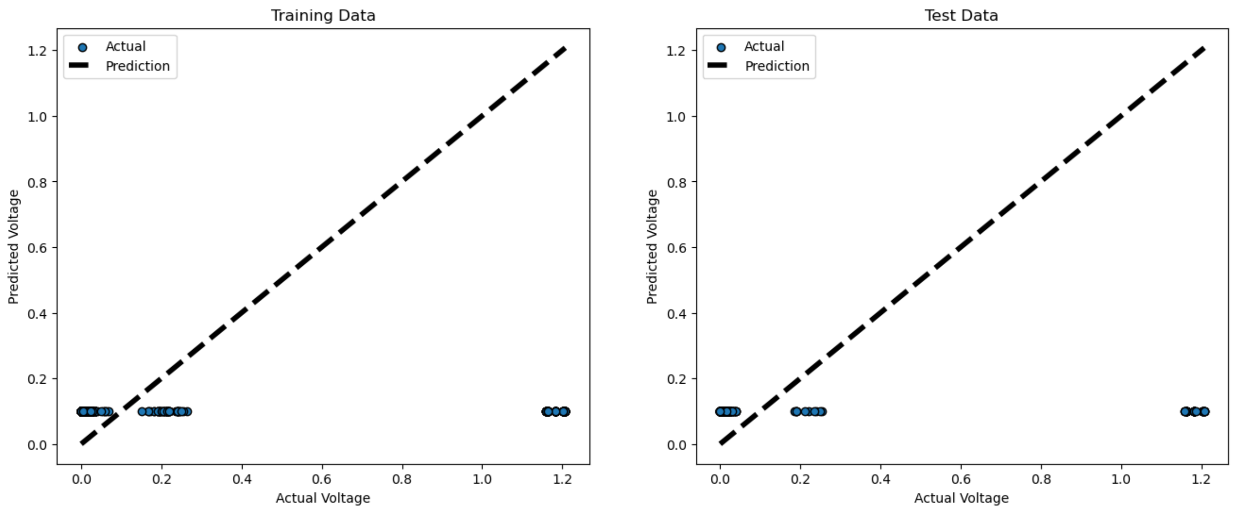
In [26]:
```
def parity_stats(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    rmse_left = rmse(y_left_true,Y_left_predictions)
    rmse_std_left = rmse_std(y_left_true,Y_left_predictions)
    mae_left = mae(y_left_true,Y_left_predictions)
    r2_left = r2(y_left_true,Y_left_predictions)

    rmse_right = rmse(y_right_true,Y_right_predictions)
    rmse_std_right = rmse_std(y_right_true,Y_right_predictions)
    mae_right = mae(y_right_true,Y_right_predictions)
    r2_right = r2(y_right_true,Y_right_predictions)

    stats_df = pd.DataFrame({'Error Metric' : ['RMSE','RMSE/std','MAE','R2'], title_l
    return stats_df
```

In [27]:
```
def parity_plots(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    fig1, (ax1,ax2) = plt.subplots(1,2,figsize=(16,6))
    ax1.scatter(y_left_true, Y_left_predictions, edgecolors=(0, 0, 0))
    ax1.plot([y_left_true.min(), y_left_true.max()], [y_left_true.min(),y_left_true.m
    ax1.legend(["Actual", "Prediction"])
    ax1.set_xlabel('Actual Voltage')
    ax1.set_ylabel('Predicted Voltage')
    ax1.set_title(title_left)
    ax2.scatter(y_right_true, Y_right_predictions, edgecolors=(0, 0, 0))
    ax2.plot([y_right_true.min(), y_right_true.max()], [y_right_true.min(),y_right_tr
    ax2.legend(["Actual", "Prediction"])
    ax2.set_xlabel('Actual Voltage')
    ax2.set_ylabel('Predicted Voltage')
    ax2.set_title(title_right)
    plt.savefig("parity.jpg",dpi=300)
    plt.show()
```

In [28]:
```
parity_plots(y_train, SV_train_pred, y_test, SV_test_pred, title_left="Training Data"
parity_stats(y_train, SV_train_pred, y_test, SV_test_pred, "Training Data", "Test Dat
```



Out[28]:

	Error Metric	Training Data	Test Data	Note
0	RMSE	0.4765	0.478	(0.0 for prefect prediction)
1	RMSE/std	1.0463	1.0479	(0.0 for prefect prediction)
2	MAE	0.2788	0.2802	(0.0 for perfect prediction)
3	R2	-0.095	-0.0982	(1.0 for perfect prediction)

4.4. K-Nearest Neighbors Regression

In [29]:
```
# Creating object for KNN Regression
knn = KNeighborsRegressor(n_neighbors=4)
```

In [30]:
```
# fit/train the KNN Regression model
knn.fit(x_train,y_train)
```

Out[30]: `KNeighborsRegressor(n_neighbors=4)`

In [31]:
```
# Accuracy of prediction for test data using KNN Regression model
knn.score(x_test,y_test)
```

Out[31]: `0.33429697766021704`

In [32]:
```
# Accuracy of prediction for train data using KNN Regression model
knn.score(x_train,y_train)
```

Out[32]: `0.6560104549430679`

In [33]:
```
# Make predictions on test and train data
knn_test_pred = knn.predict(x_test)
knn_train_pred = knn.predict(x_train)
```

In [34]:
```python
def rmse(y_true, Y_predictions): return round(np.sqrt(metrics.mean_squared_error(y_tr
def rmse_std(y_true, Y_predictions): return round(rmse(y_true, Y_predictions)/np.std(
def mae(y_true, Y_predictions): return round(metrics.mean_absolute_error(y_true, Y_pr
def r2(y_true, Y_predictions): return round(metrics.r2_score(y_true, Y_predictions),4
```

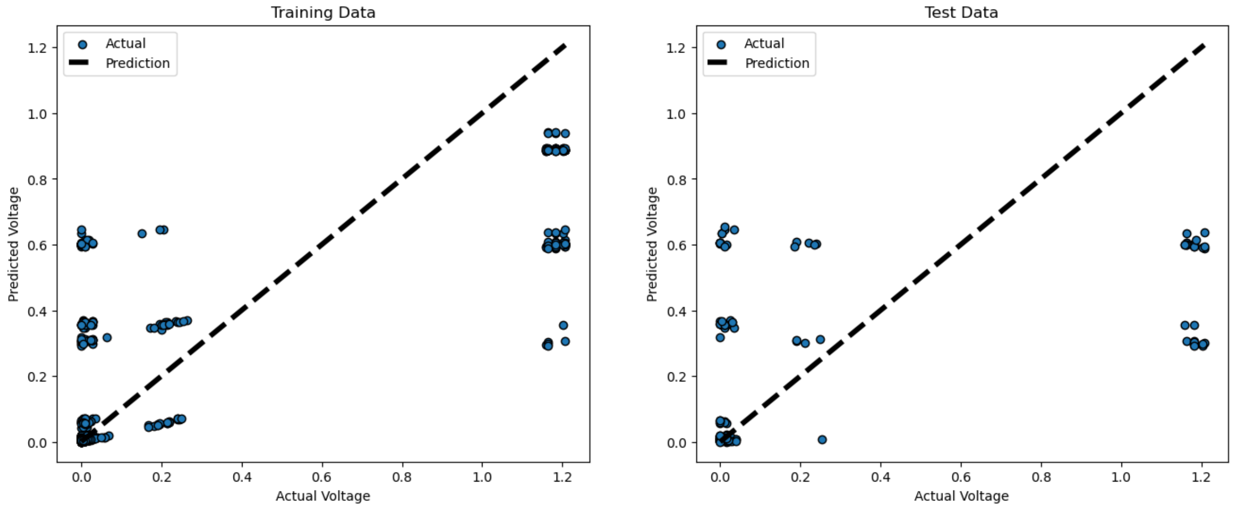
In [35]:
```python
def parity_stats(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    rmse_left = rmse(y_left_true,Y_left_predictions)
    rmse_std_left = rmse_std(y_left_true,Y_left_predictions)
    mae_left = mae(y_left_true,Y_left_predictions)
    r2_left = r2(y_left_true,Y_left_predictions)

    rmse_right = rmse(y_right_true,Y_right_predictions)
    rmse_std_right = rmse_std(y_right_true,Y_right_predictions)
    mae_right = mae(y_right_true,Y_right_predictions)
    r2_right = r2(y_right_true,Y_right_predictions)

    stats_df = pd.DataFrame({'Error Metric' : ['RMSE','RMSE/std','MAE','R2'], title_l
    return stats_df
```

In [36]:
```python
def parity_plots(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    fig1, (ax1,ax2) = plt.subplots(1,2,figsize=(16,6))
    ax1.scatter(y_left_true, Y_left_predictions, edgecolors=(0, 0, 0))
    ax1.plot([y_left_true.min(), y_left_true.max()], [y_left_true.min(),y_left_true.m
    ax1.legend(["Actual", "Prediction"])
    ax1.set_xlabel('Actual Voltage')
    ax1.set_ylabel('Predicted Voltage')
    ax1.set_title(title_left)
    ax2.scatter(y_right_true, Y_right_predictions, edgecolors=(0, 0, 0))
    ax2.plot([y_right_true.min(), y_right_true.max()], [y_right_true.min(),y_right_tr
    ax2.legend(["Actual", "Prediction"])
    ax2.set_xlabel('Actual Voltage')
    ax2.set_ylabel('Predicted Voltage')
    ax2.set_title(title_right)
    plt.savefig("parity.jpg",dpi=300)
    plt.show()
```

In [37]:
```
parity_plots(y_train, knn_train_pred, y_test, knn_test_pred, title_left="Training Dat
parity_stats(y_train, knn_train_pred, y_test, knn_test_pred, "Training Data", "Test D
```



Out[37]:

	Error Metric	Training Data	Test Data	Note
0	RMSE	0.2671	0.3722	(0.0 for prefect prediction)
1	RMSE/std	0.5865	0.8159	(0.0 for prefect prediction)
2	MAE	0.1569	0.2302	(0.0 for perfect prediction)
3	R2	0.656	0.3343	(1.0 for perfect prediction)

4.5. Fitting A Decision Tree Model

4.5.1. Using Extreme Gradient Boosting Algorithm

In [38]:
```
# Creating object for Extreme Gradient Boosting Regression
XGB = XGBRegressor(base_score=0.5, booster='gbtree', callbacks=None,
             colsample_bylevel=1, colsample_bynode=1,
             colsample_bytree=1, early_stopping_rounds=None,
             enable_categorical=False, eval_metric=None, gamma=0, gpu_id=1, grow_poli
             interaction_constraints='', learning_rate=0.300000012, max_bin=256,
             max_cat_to_onehot=4,
             max_delta_step=0, max_depth=6, max_leaves=0,
             min_child_weight=1, monotone_constraints='()',
             n_estimators=100, n_jobs=0, num_parallel_tree=1,
             predictor='auto', random_state=0, reg_alpha=0, reg_lambda=1)
```

In [39]:
```
# fit/train the Decision Tree model
XGB.fit(x_train,y_train)
```

```
[21:55:54] WARNING: C:\buildkite-agent\builds\buildkite-windows-cpu-autoscaling-grou
p-i-0fdc6d574b9c0d168-1\xgboost\xgboost-ci-windows\src\learner.cc:347: Only 1 GPUs a
re visible, setting `gpu_id` to 0
```

Out[39]:
```
XGBRegressor(base_score=0.5, booster='gbtree', callbacks=None,
             colsample_bylevel=1, colsample_bynode=1, colsample_bytree=1,
             early_stopping_rounds=None, enable_categorical=False,
             eval_metric=None, feature_types=None, gamma=0, gpu_id=1,
             grow_policy='depthwise', importance_type=None,
             interaction_constraints='', learning_rate=0.300000012, max_bin=256,
             max_cat_threshold=None, max_cat_to_onehot=4, max_delta_step=0,
             max_depth=6, max_leaves=0, min_child_weight=1, missing=nan,
             monotone_constraints='()', n_estimators=100, n_jobs=0,
             num_parallel_tree=1, predictor='auto', random_state=0, ...)
```

In [40]:
```
Train_predictions = XGB.predict(x_train)
# Make predictions on training data
Test_predictions = XGB.predict(x_test)
# Make predictions on testing data
```

In [41]:
```
def rmse(y_true, Y_predictions): return round(np.sqrt(metrics.mean_squared_error(y_tr
def rmse_std(y_true, Y_predictions): return round(rmse(y_true, Y_predictions)/np.std(
def mae(y_true, Y_predictions): return round(metrics.mean_absolute_error(y_true, Y_pr
def r2(y_true, Y_predictions): return round(metrics.r2_score(y_true, Y_predictions),4
```

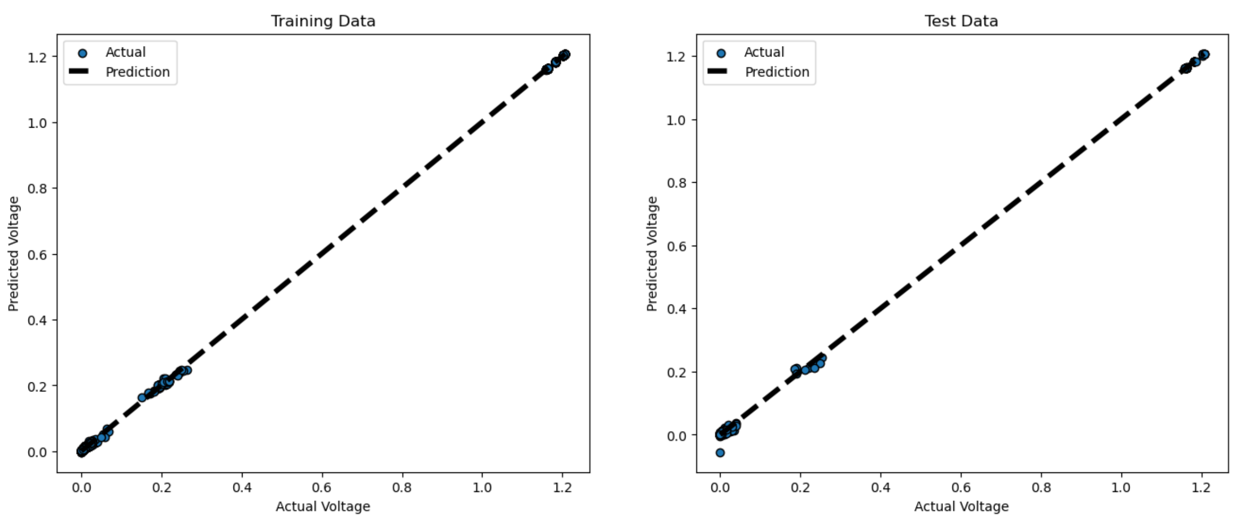
In [42]:
```
def parity_stats(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    rmse_left = rmse(y_left_true,Y_left_predictions)
    rmse_std_left = rmse_std(y_left_true,Y_left_predictions)
    mae_left = mae(y_left_true,Y_left_predictions)
    r2_left = r2(y_left_true,Y_left_predictions)

    rmse_right = rmse(y_right_true,Y_right_predictions)
    rmse_std_right = rmse_std(y_right_true,Y_right_predictions)
    mae_right = mae(y_right_true,Y_right_predictions)
    r2_right = r2(y_right_true,Y_right_predictions)

    stats_df = pd.DataFrame({'Error Metric' : ['RMSE','RMSE/std','MAE','R2'], title_l
    return stats_df
```

In [43]:
```
def parity_plots(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    fig1, (ax1,ax2) = plt.subplots(1,2,figsize=(16,6))
    ax1.scatter(y_left_true, Y_left_predictions, edgecolors=(0, 0, 0))
    ax1.plot([y_left_true.min(), y_left_true.max()], [y_left_true.min(),y_left_true.m
    ax1.legend(["Actual", "Prediction"])
    ax1.set_xlabel('Actual Voltage')
    ax1.set_ylabel('Predicted Voltage')
    ax1.set_title(title_left)
    ax2.scatter(y_right_true, Y_right_predictions, edgecolors=(0, 0, 0))
    ax2.plot([y_right_true.min(), y_right_true.max()], [y_right_true.min(),y_right_tr
    ax2.legend(["Actual", "Prediction"])
    ax2.set_xlabel('Actual Voltage')
    ax2.set_ylabel('Predicted Voltage')
    ax2.set_title(title_right)
    plt.savefig("parity.jpg",dpi=300)
    plt.show()
```

In [44]:
```
parity_plots(y_train, Train_predictions, y_test, Test_predictions, title_left="Traini
parity_stats(y_train, Train_predictions, y_test, Test_predictions, "Training Data", "
```



Out[44]:

	Error Metric	Training Data	Test Data	Note
0	RMSE	0.0028	0.0072	(0.0 for prefect prediction)
1	RMSE/std	0.0061	0.0158	(0.0 for prefect prediction)
2	MAE	0.0016	0.0039	(0.0 for perfect prediction)
3	R2	1.0	0.9997	(1.0 for perfect prediction)

4.5.2. Random Forest Regressor Class

In [45]:
```
# Creating object for Linear Regression
RF=RandomForestRegressor(random_state=1,n_estimators=1,bootstrap=False)
```

In [46]:
```
# fit/train the Decision Tree model
RF.fit(x_train,y_train)
```

Out[46]:
```
RandomForestRegressor(bootstrap=False, n_estimators=1, random_state=1)
```

In [47]:
```
# Make predictions on test data
RF_pred = RF.predict(x_test)
```

In [48]:
```
# Accuracy of prediction for test data using current model
RF.score(x_train,y_train)
```

Out[48]:
```
1.0
```

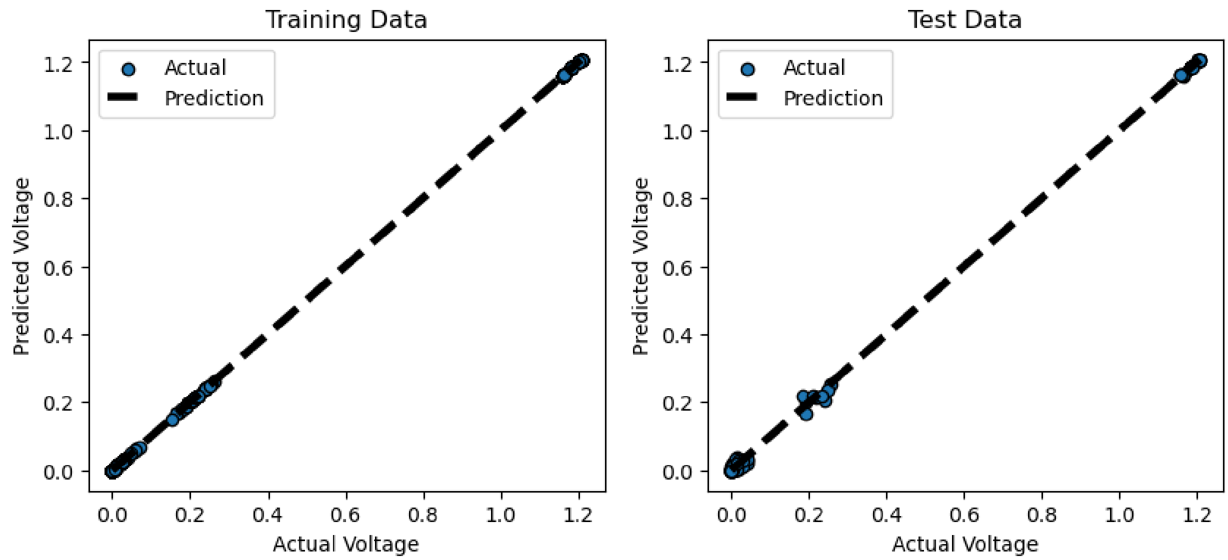
In [49]:
```
Train_predictions = RF.predict(x_train)
# Make predictions on training data
Test_predictions = RF.predict(x_test)
# Make predictions on testing data
```

In [50]:
```
def rmse(y_true, Y_predictions): return round(np.sqrt(metrics.mean_squared_error(y_tr
def rmse_std(y_true, Y_predictions): return round(rmse(y_true, Y_predictions)/np.std(
def mae(y_true, Y_predictions): return round(metrics.mean_absolute_error(y_true, Y_pr
def r2(y_true, Y_predictions): return round(metrics.r2_score(y_true, Y_predictions),4
```

In [51]:
```
def parity_stats(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    rmse_left = rmse(y_left_true,Y_left_predictions)
    rmse_std_left = rmse_std(y_left_true,Y_left_predictions)
    mae_left = mae(y_left_true,Y_left_predictions)
    r2_left = r2(y_left_true,Y_left_predictions)
    rmse_right = rmse(y_right_true,Y_right_predictions)
    rmse_std_right = rmse_std(y_right_true,Y_right_predictions)
    mae_right = mae(y_right_true,Y_right_predictions)
    r2_right = r2(y_right_true,Y_right_predictions)
    stats_df = pd.DataFrame({'Error Metric' : ['RMSE', 'RMSE/std', 'MAE', 'R2'],
    title_left : [str(rmse_left), rmse_std_left, str(mae_left), r2_left], title_right
    return stats_df
```

In [52]:
```
def parity_plots(y_left_true,Y_left_predictions,y_right_true,Y_right_predictions,titl
    fig1, (ax1,ax2) = plt.subplots(1,2,figsize=(10,4))
    ax1.scatter(y_left_true, Y_left_predictions, edgecolors=(0, 0, 0))
    ax1.plot([y_left_true.min(), y_left_true.max()], [y_left_true.min(),y_left_true.ma
    ax1.legend(["Actual", "Prediction"])
    ax1.set_xlabel('Actual Voltage')
    ax1.set_ylabel('Predicted Voltage')
    ax1.set_title(title_left)
    ax2.scatter(y_right_true, Y_right_predictions, edgecolors=(0, 0, 0))
    ax2.plot([y_right_true.min(), y_right_true.max()], [y_right_true.min(), y_right_t
    ax2.legend(["Actual", "Prediction"])
    ax2.set_xlabel('Actual Voltage')
    ax2.set_ylabel('Predicted Voltage')
    ax2.set_title(title_right)
    plt.savefig("parity_rf.jpg",dpi=300)
    plt.show()
```

In [53]:
```
parity_plots(y_train,Train_predictions,y_test,Test_predictions,title_left="Training Da
parity_stats(y_train,Train_predictions,y_test,Test_predictions,"Training Data","Test I
# print error metrics for training data
```



Out[53]:

	Error Metric	Training Data	Test Data	Note
0	RMSE	0.0	0.0074	(0.0 for perfect prediction)
1	RMSE/std	0.0	0.0162	(0.0 for perfect prediction)
2	MAE	0.0	0.0036	(0.0 for perfect prediction)
3	R2	1.0	0.9997	(1.0 for perfect prediction)

5. Making Prediction

In [54]:
```
 # Make predictions
RF.predict([[50,2000000]])
# Predict voltage generated at a concentration of 50 mg/dL and after 2 seconds|
```

```
C:\Program Files\Anaconda\lib\site-packages\sklearn\base.py:450: UserWarning: X does
not have valid feature names, but RandomForestRegressor was fitted with feature name
s
  warnings.warn(
```

Out[54]: array([1.207234])

5.1. Visualization of Decision Tree

In [*]:
```
plt.figure(figsize=(600,200))
tree.plot_tree(RF.estimators_[0], filled=True)
plt.savefig("tree.pdf",dpi=600)
```