Introduction to Machine Learning: Supervised Learning Final Project

Ocean Acidification Prediction Using Machine Learning Algorithms

A growing concern in climate change and environmental science is Ocean Acidification. The ocean absorbs around 30 percent of the world's carbon dioxide emissions. Carbon dioxide in the air is dissolved into ocean water where it is broken into hydrogen ions and bicarbonate. This reaction in turn decreases the pH of the ocean making it more acidic. An increase in acidity posses a threat to marine life and biological processes. Over the last couple of decades, the National Ocean and Atmospheric Administration has set up carbon dioxide and pH monitoring systems on research cruise ships and water buoy observation stations along coastlines to gain a greater understanding of this issue.

Being able to predict and forecast ocean acidity trends could have a useful impact on policy and research. In my project I will compare the performance of three different machine learning regression algorithms in using ocean chemistry data to predict pH levels. I will look at Linear Regression, Gradient Boosting Regression and Decision Tree Regression.

Import Libraries

The following libraries will be used in my project.

In [285…

```
###############
# Importing Libraries used for the project
###############

%matplotlib inline
import numpy as np
import scipy as sp
import scipy.stats as stats
import pandas as pd
import glob
import os
import matplotlib.pyplot as plt
import seaborn as sns
sns.set()
import statsmodels.formula.api as smf
import statsmodels.api as sm
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
```

```python
from sklearn.datasets import make_regression
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.inspection import permutation_importance
```

Load Data

There are many ocean water quality sensors worldwide and many provide data freely accessible on the National Oceanic and Atmospheric Administration's website. In order to have more consistency in data and a manageable yet meaningful size, I chose one station, near La Parguera, Puerto Rico.

I pulled my data files from the NOAA's website under the National Centers for Environmental Information section. These files contained chemical, meteorological, physical and time sensor data from the La Parguera mooring located at 67W 18N in the Caribbean Sea near La Parguera, Puerto Rico.

The data I retrieved was in the form of csv files that were broken into approximately 12 month spans with several sensor readings per day. I choose to look at files starting from Dec 2012 (when the pH sensor was installed) until the most current, Oct 2021. The data totaled 5.2 MB in size. I stored the files in one folder and merged them into a single data frame. This dataframe had 29 columns and 22535 rows. The code below shows a summary of the column names and data types for the intial dataset.

The features I will be most interested in this analysis are:

Temperature- due to its ability to impact gas (such as CO_2) concentrations in water. Salinity- the salt concentration can affect the alkalinity (basic-ness) of the water. Dissolved Oxygen- impacts the chemical process. PH- measures the level of acidity, ranges from 0-14 and lower numbers are more acidic. Partial pressure of CO_2- relates to the concentration of CO_2 in water or air. Chlorophyll- also has the ability to absorb carbon dioxide.

Data Source Citation:

```
    Sutton, Adrienne J.; Sabine, Christopher L.; Morell,
Julio M.; Musielewicz, Sylvia; Maenner Jones, Stacy;
Dietrich, Colin; Bott, Randy; Osborne, John (2014). High-
resolution ocean and atmosphere pCO2 time-series measurements
from mooring La_Parguera_67W_18N in the Caribbean Sea (NCEI
Accession 0117354). NOAA National Centers for Environmental
Information. Dataset.
https://doi.org/10.3334/cdiac/otg.tsm_la_parguera_67w_18n.
Accessed Aug 3, 2024.
```

In [317…

```python
###############################################
# Load CSV files and merge into one data frame
###############################################
```

```
df = pd.concat(map(pd.read_csv, glob.glob(os.path.join('', "ocean data/La_Pa
df.head()

print("Original Data Frame Length:", len(df))
print(df.dtypes)
```

```
Original Data Frame Length: 22525
Mooring Name                   object
Latitude                      float64
Longitude                     float64
Date                           object
Time                           object
xCO2 SW (wet) (umol/mol)      float64
CO2 SW QF                       int64
H2O SW (mmol/mol)             float64
xCO2 Air (wet) (umol/mol)     float64
CO2 Air QF                      int64
H2O Air (mmol/mol)            float64
Licor Atm Pressure (hPa)      float64
Licor Temp (C)                float64
MAPCO2 %O2                    float64
SST (C)                       float64
Salinity                      float64
xCO2 SW (dry) (umol/mol)      float64
xCO2 Air (dry) (umol/mol)     float64
fCO2 SW (sat) (uatm)          float64
fCO2 Air (sat) (uatm)         float64
dfCO2                         float64
pCO2 SW (sat) (uatm)          float64
pCO2 Air (sat) (uatm)         float64
dpCO2                         float64
pH (total scale)              float64
pH QF                           int64
CHL (ug/l)                    float64
CHL QF                          int64
NTU (NTU)                     float64
NTU QF                          int64
DOXY (umol/kg)                float64
DOXY QF                         int64
dtype: object
```

Clean Data

I removed several columns such as location, date/time, mooring name, and other features that seemed redundant or unnecessary for modeling pH. Missing values were encoded as -999. I convert these to na's and then dropped any rows that contained na's. This had a drastic impact on the number of rows which brought it down to 2197. However, this is still large enough for modeling purposes. I also cleaned up column names in order to make it easier to work with. I viewed the statistical description of the data and created boxplot to verify significant outliers didn't exist. The final data frame contained 2197 rows with the following columns:

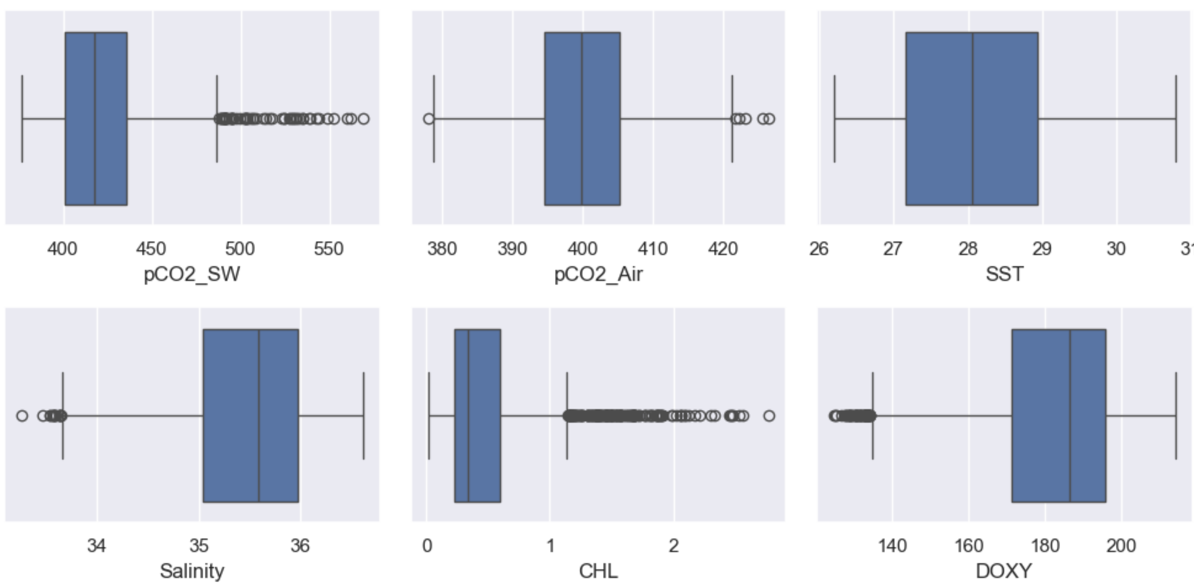
Variable	Description

Variable	Description
pCO2_SW	Partial Pressure of CO2 in sea water
pCO2_Air	CO2 of air four feet above sea level
SST	Sea Surface Temperature
Salinity	Portion of salt in water
CHL	Total Chlorophyll
DOXY	Dissolved Oxygen
pH	pH measurement of ocean water

In [287…

```
###################
# Cleaning the data
###################

# replace bad value with na
df = df.replace(to_replace = -999,value = np.nan)

# removed date, location, mooring, etc
# selecting only features needed for project
# and renaming columns

df_new = df[['pCO2 SW (sat) (uatm)','pCO2 Air (sat) (uatm)','SST (C)', 'Sali
df_new.rename(columns={'pCO2 SW (sat) (uatm)': 'pCO2_SW','pCO2 Air (sat) (ua

#drop any na's
df_new = df_new.dropna()
print("cleaned length", len(df_new))

#print stats summary to catch any usual data points
print(df_new.describe())

# look for outliers with boxplot
fig, axes = plt.subplots(2, 3, figsize=(10, 5))

# Plot on the first subplot
sns.boxplot(data=df_new, x="pCO2_SW", ax=axes[0,0])
sns.boxplot(data=df_new, x="pCO2_Air", ax=axes[0,1])
sns.boxplot(data=df_new, x="SST", ax=axes[0,2])
sns.boxplot(data=df_new, x="Salinity", ax=axes[1,0])
sns.boxplot(data=df_new, x="CHL", ax=axes[1,1])
sns.boxplot(data=df_new, x="DOXY", ax=axes[1,2])

plt.tight_layout()

# show the plot
plt.show()
```

```
cleaned length 1569
          pCO2_SW     pCO2_Air          SST     Salinity           pH  \
count  1569.000000  1569.000000  1569.000000  1569.000000  1569.000000   
mean    423.026769   399.988082    28.071955    35.464212     8.024362   
std      29.737656     7.702659     1.056878     0.690416     0.029680   
min     376.500000   377.900000    26.196000    33.261000     7.889000   
25%     401.000000   394.500000    27.159000    35.044000     8.005000   
50%     417.800000   399.800000    28.056000    35.589000     8.030000   
75%     435.600000   405.200000    28.944000    35.971000     8.048000   
max     569.000000   426.600000    30.803000    36.613000     8.092000   

               CHL         DOXY  
count  1569.000000  1569.000000  
mean      0.501581   180.855131  
std       0.442574    19.956333  
min       0.012000   125.000000  
25%       0.225000   171.400000  
50%       0.332000   186.400000  
75%       0.594000   195.800000  
max       2.778000   214.300000  
```



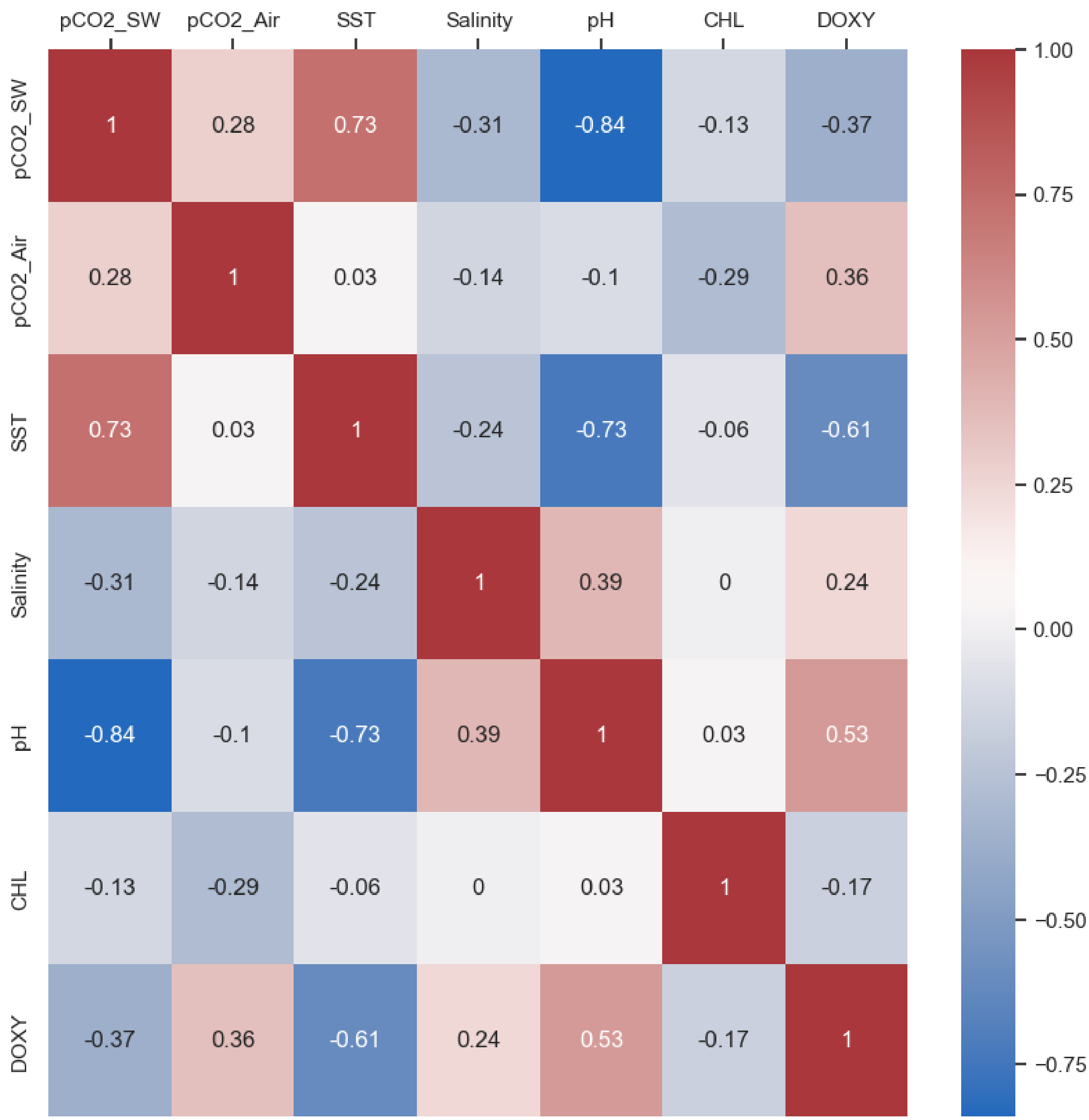
Exploratory Data Analysis

In my exploratory data analysis, I created correlation graphs and pairwise bivariate plots. The correlation graph shows the strongest correlation being between the pCO2_SW and pH (-0.84). Another strong correlation is pCO2_SW and SST (0.73) so this will be taken into consideration in the model. DOXY also shows some correlation with pH (0.53). The pairwise plot also shows a strong negative relationship between the partial pressure of the sea water (pCO2_SW) and the pH. As seawater CO2 increases, pH (acidity) decreases. A similar trend is seen with surface temperature (SST). The dissolved oxygen has a positive relationship. As dissolved O2 increased, pH increases. It's a little hard to see significant relationships between other features.

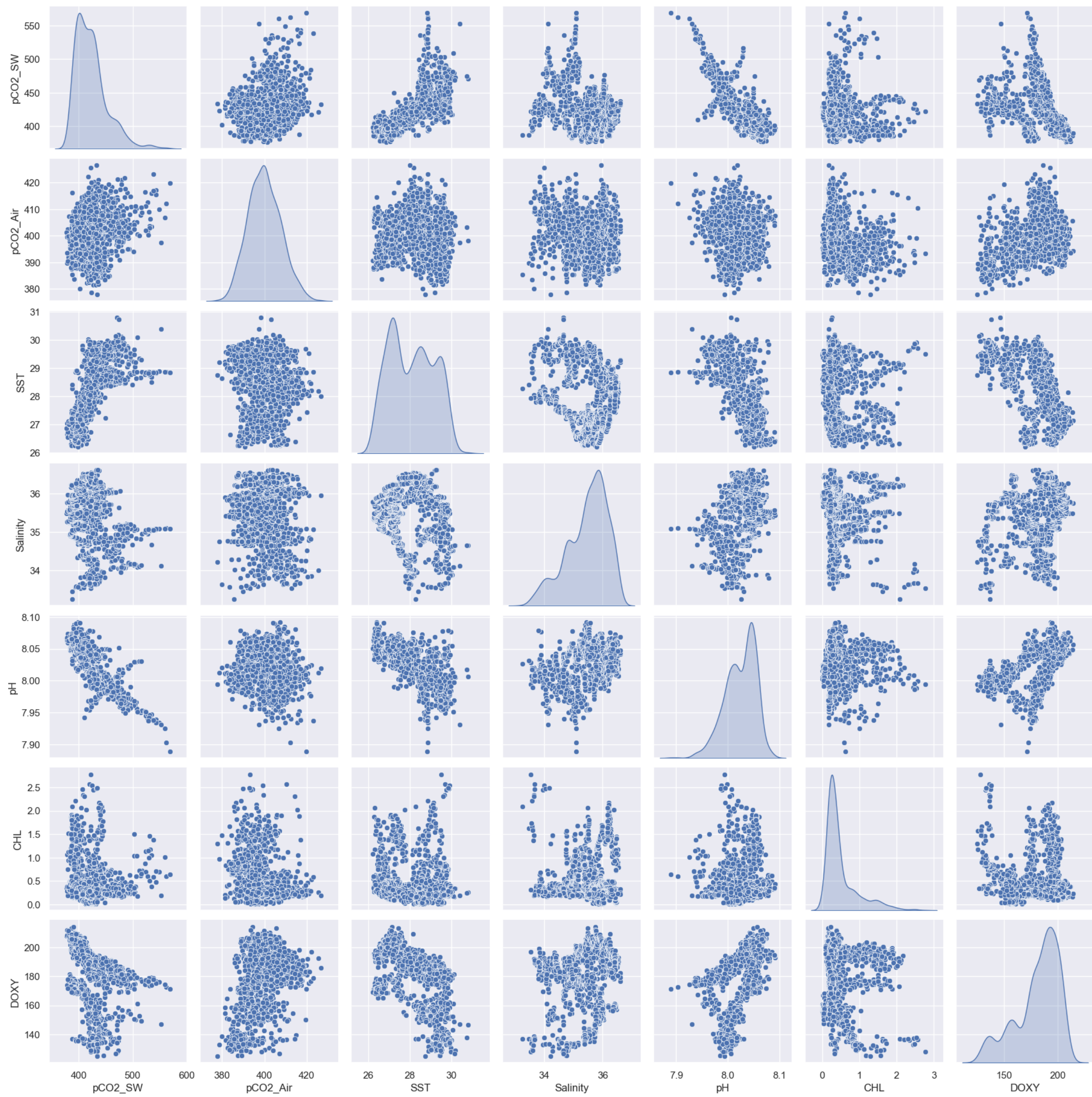
In [189…

```
##############
# EDA
```

```python
#############

# Correlation Matrix
matrix = df_new.corr().round(2)
plt.figure(figsize = (10,10))
heatmap = sns.heatmap(matrix, annot=True, cmap = 'vlag')
heatmap.xaxis.tick_top()

# Pairwise plot
plt.figure(figsize = (20,25))
pairplot = sns.pairplot(df_new, diag_kind = 'kde')
```




```
&lt;Figure size 2000x2500 with 0 Axes&gt;
```



Models

In this project I will compare three different types of regression models to make predictions. Before running the models I did an 80/20 split of the data into train and test datasets. Below I create regression models using statsmodels and sklearn. I use Linear, Decision Tree and Gradient Boost Regression algorithms.

Linear Regression

I initially ran a linear regression model for all features. In the full model, the CHL feature had a p-value > 0.05 and can be considered insignificant. I removed CHL and also the SST feature due the the collinearity seen in the EDA above. These were removed from the test and training sets and were not used for the proceeding algorithms as well (done in next block of code). I looked at several model options with the remaining features and compared the adjusted R squared values. The model with the best adjusted R squared was one that included the features: pCO2_SW, pCO2_Air, Salinity and DOXY. I then plotted partial regression plots that model relationships between pH and a single parameter while keeping the parameters constant.

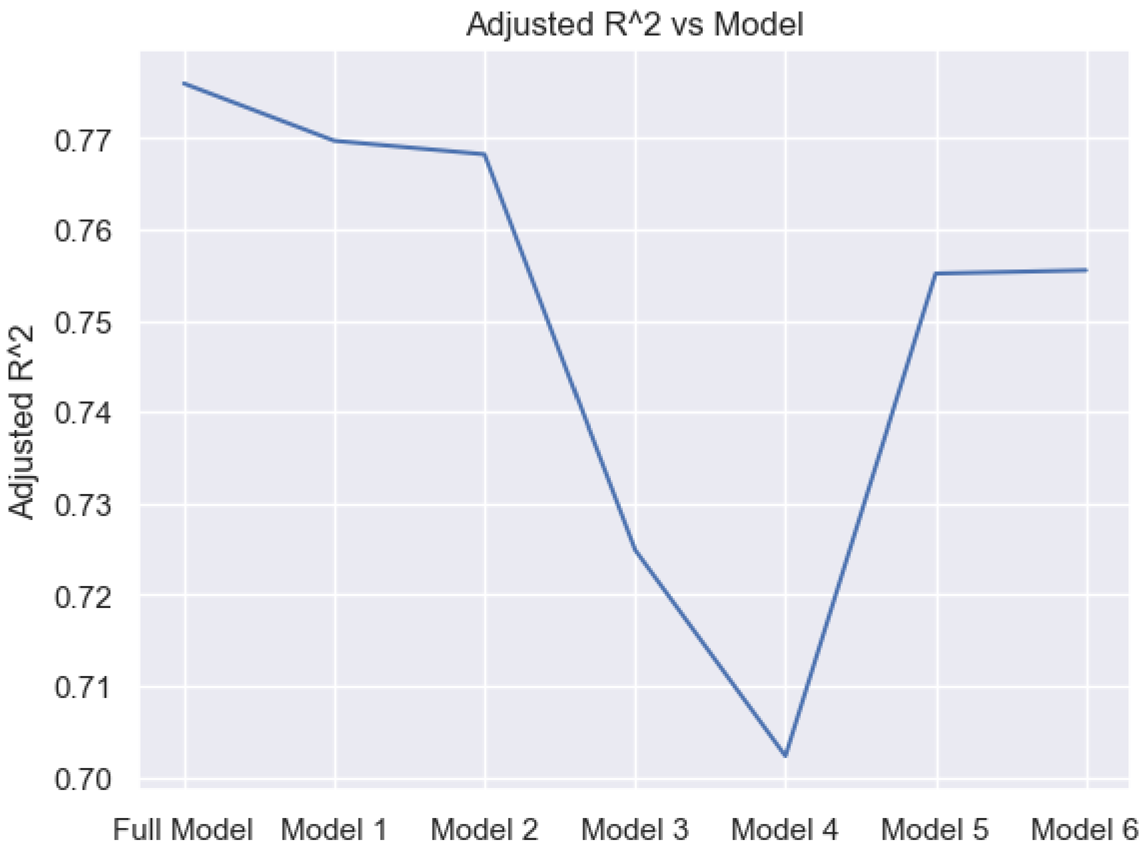
In [340…

```
#############
# Modeling
#############

#create test and training data
train_ocean, test_ocean = train_test_split(df_new, train_size = 0.8, random_

#slpit y (pH) data apart
train_ocean_y = train_ocean["pH"]
train_ocean_x = train_ocean.drop("pH", axis=1)

test_ocean_y = test_ocean["pH"]
test_ocean_x = test_ocean.drop("pH", axis=1)

##########################
# Linear Regression
##########################

model_full = smf.ols(formula = 'pH ~ pCO2_SW+pCO2_Air+SST+Salinity+CHL+DOXY'
print(model_full.summary())
print()


# Calculate Adjusted R-squared for different model options
print("Full Model R2:" ,model_full.rsquared_adj)

model_1 = smf.ols(formula = 'pH ~ pCO2_SW+pCO2_Air+Salinity+DOXY', data=trai
print("Model 1 Adj R2: ", model_1.rsquared_adj)
model_2 = smf.ols(formula = 'pH ~ pCO2_SW+Salinity+DOXY', data=train_ocean).
print("Model 2 Adj R2: ", model_2.rsquared_adj)
model_3 = smf.ols(formula = 'pH ~ pCO2_SW+Salinity', data=train_ocean).fit()
print("Model 3 Adj R2: ", model_3.rsquared_adj)
model_4 = smf.ols(formula = 'pH ~ pCO2_SW', data=train_ocean).fit()
print("Model 4 Adj R2: ", model_4.rsquared_adj)
model_5 = smf.ols(formula = 'pH ~ pCO2_SW+DOXY', data=train_ocean).fit()
print("Model 5 Adj R2: ", model_5.rsquared_adj)
model_6 = smf.ols(formula = 'pH ~ pCO2_SW+pCO2_Air+DOXY', data=train_ocean).
print("Model 6 Adj R2: ", model_6.rsquared_adj)


x = ["Full Model", "Model 1", "Model 2", "Model 3", "Model 4", "Model 5", "M
adjr2_train = [model_full.rsquared_adj, model_1.rsquared_adj, model_2.rsquar


# Plotting Different Model Adj R squared
plt.plot(x, adjr2_train)
plt.ylabel("Adjusted R^2")
plt.title("Adjusted R^2 vs Model")
plt.show()
```

```python
# Using Best Model to Predict and Evaluate Test Data
y_lm_pred_train = model_1.predict(train_ocean_x)
y_lm_pred_test = model_1.predict(test_ocean_x)

# Calculate R-squared
r2_lm_train = r2_score(train_ocean_y , y_lm_pred_train)
r2_lm_test = r2_score(test_ocean_y , y_lm_pred_test)

# Calculate Mean Squared Error
mse_lm_train = mean_squared_error(train_ocean_y, y_lm_pred_train)
mse_lm_test = mean_squared_error(test_ocean_y, y_lm_pred_test)

#Print Chosen model summary
print(model_1.summary())

#Plotting Partial Regression Plots
fig = sm.graphics.plot_partregress_grid(model_1)
fig.tight_layout(pad=1.0)


print()
print()
print("Linear Regression:")
print('Train Mean Squared Error:', mse_lm_train)
print('Train R-squared:', r2_lm_train)
print('Test Mean Squared Error:', mse_lm_test)
print('Test R-squared:', r2_lm_test)
```

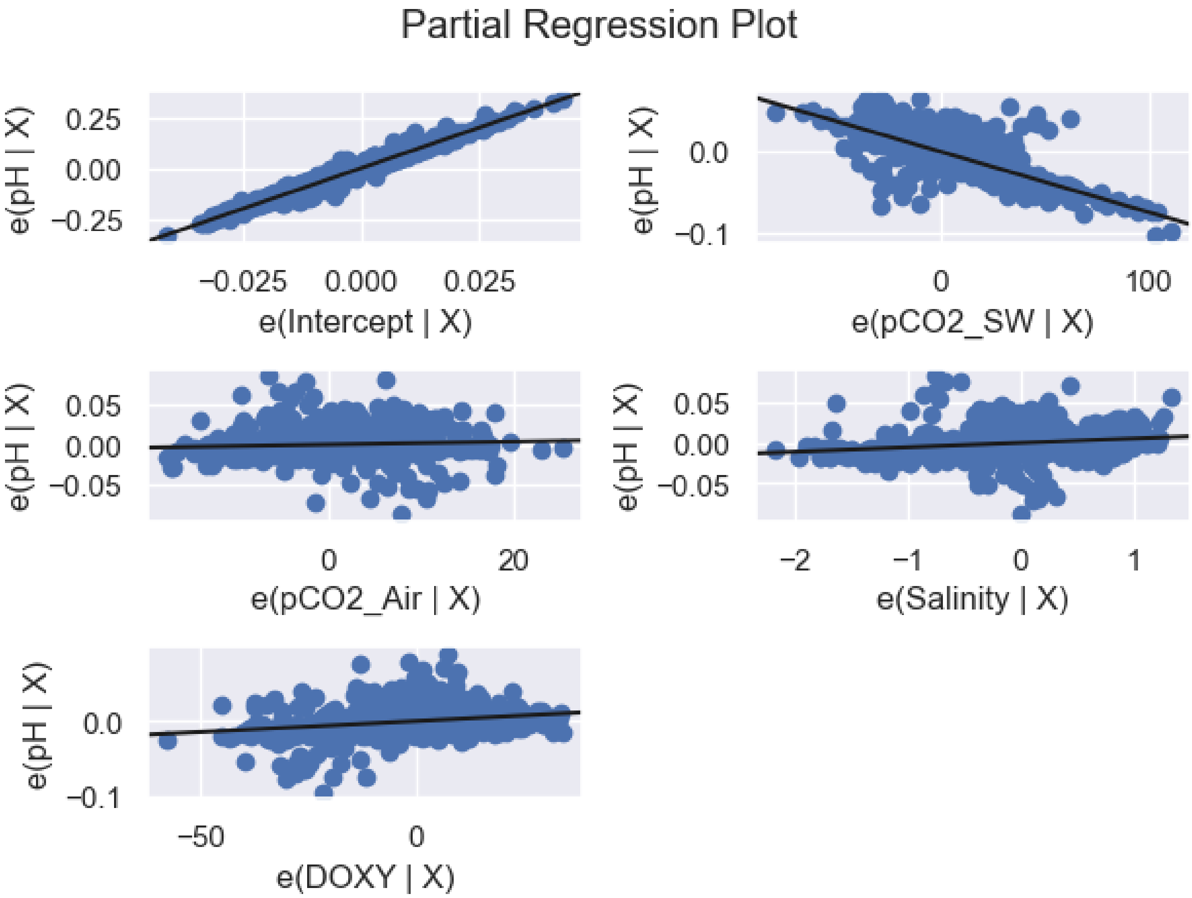
```
                            OLS Regression Results
==============================================================================
=
Dep. Variable:                     pH   R-squared:                       0.77
7
Model:                            OLS   Adj. R-squared:                  0.77
6
Method:                 Least Squares   F-statistic:                     725.
1
Date:                Thu, 15 Aug 2024   Prob (F-statistic):               0.0
0
Time:                        08:50:24   Log-Likelihood:                 3584.
0
No. Observations:                1255   AIC:                            -715
4.
Df Residuals:                    1248   BIC:                            -711
8.
Df Model:                           6

Covariance Type:            nonrobust

==============================================================================
=
                 coef    std err          t      P>|t|      [0.025      0.97
5]
------------------------------------------------------------------------------
-
Intercept      8.0991      0.036    223.136      0.000       8.028       8.17
0
pCO2_SW       -0.0007   2.19e-05    -30.048      0.000      -0.001      -0.00
1
pCO2_Air       0.0002    6.4e-05      2.858      0.004    5.73e-05       0.00
0
SST           -0.0039      0.001     -5.973      0.000      -0.005      -0.00
3
Salinity       0.0058      0.001      9.320      0.000       0.005       0.00
7
CHL           -0.0016      0.001     -1.701      0.089      -0.003       0.00
0
DOXY           0.0002   2.94e-05      6.917      0.000       0.000       0.00
0
==============================================================================
=
Omnibus:                      295.455   Durbin-Watson:                   2.02
2
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             2825.88
5
Skew:                           0.804   Prob(JB):                         0.0
0
Kurtosis:                      10.173   Cond. No.                     5.63e+0
4
==============================================================================
=

Notes:
```

```
[1] Standard Errors assume that the covariance matrix of the errors is correc
tly specified.
[2] The condition number is large, 5.63e+04. This might indicate that there a
re
strong multicollinearity or other numerical problems.

Full Model R2: 0.7760052190380093
Model 1 Adj R2:  0.76972923556961
Model 2 Adj R2:  0.7682432708818645
Model 3 Adj R2:  0.7249098774922522
Model 4 Adj R2:  0.7023277392157959
Model 5 Adj R2:  0.7551708150835477
Model 6 Adj R2:  0.7555312941959244
```



```
                            OLS Regression Results

==============================================================================
=
Dep. Variable:                     pH   R-squared:                       0.77
0
Model:                            OLS   Adj. R-squared:                  0.77
0
Method:                 Least Squares   F-statistic:                     104
9.
Date:                Thu, 15 Aug 2024   Prob (F-statistic):               0.0
0
Time:                        08:50:24   Log-Likelihood:                3565.
6
No. Observations:                1255   AIC:                            -712
1.
Df Residuals:                    1250   BIC:                            -709
6.
Df Model:                           4

Covariance Type:            nonrobust

==============================================================================
=
                 coef    std err          t      P>|t|      [0.025      0.97
5]
------------------------------------------------------------------------------
-
Intercept      8.0114      0.033    239.581      0.000       7.946       8.07
7
pCO2_SW       -0.0007   1.69e-05    -43.665      0.000      -0.001      -0.00
1
pCO2_Air       0.0002   6.39e-05      3.012      0.003    6.71e-05       0.00
0
Salinity       0.0055      0.001      8.839      0.000       0.004       0.00
7
DOXY           0.0003   2.59e-05     11.329      0.000       0.000       0.00
0
==============================================================================
=
Omnibus:                      263.804   Durbin-Watson:                   2.03
0
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             3210.64
0
Skew:                           0.603   Prob(JB):                         0.0
0
Kurtosis:                      10.742   Cond. No.                     5.11e+0
4
==============================================================================
=

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correc
tly specified.
[2] The condition number is large, 5.11e+04. This might indicate that there a
re
```

```
strong multicollinearity or other numerical problems.


Linear Regression:
Train Mean Squared Error: 0.00019940616413150898
Train R-squared: 0.7704637515646034
Test Mean Squared Error: 0.00020546814728600324
Test R-squared: 0.7766998490460703
```

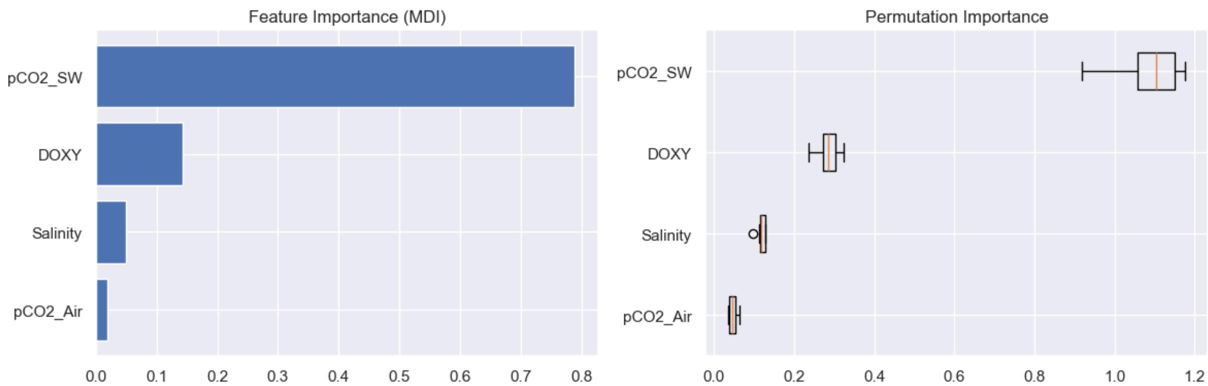


Decision Tree Regression

Next I created a Decision Tree Regression model. I set a max depth of 5 and used the default criterion of squared error. I calculated the mean squared error for the training and testing datasets. I also created Feature and Permutation Importance charts.

In [314…
```
##########################
# Decision Tree Regression
##########################

## drop SST and CHL due to colinearity and low significance
##
train_ocean_x = train_ocean_x.drop(['SST', 'CHL'], axis=1)
test_ocean_x = test_ocean_x.drop(['SST', 'CHL'], axis=1)


dtr = tree.DecisionTreeRegressor(max_depth=5)
dtr = dtr.fit(train_ocean_x, train_ocean_y)
```

```
# Predict using train/test data
y_dtr_pred_train = dtr.predict(train_ocean_x)
y_dtr_pred_test = dtr.predict(test_ocean_x)


# Calculate Mean Squared Error
mse_dtr_train = mean_squared_error(train_ocean_y , y_dtr_pred_train)
mse_dtr_test = mean_squared_error(test_ocean_y, y_dtr_pred_test)

# Calculate R-squared
r2_dtr_train = r2_score(train_ocean_y , y_dtr_pred_train)
r2_dtr_test = r2_score(test_ocean_y , y_dtr_pred_test)


# Graph Feature and Permutation Importance
feature_importance_dtr = dtr.feature_importances_
sorted_idx_dtr = np.argsort(feature_importance_dtr)
pos_dtr = np.arange(sorted_idx_dtr.shape[0]) + 0.5
fig = plt.figure(figsize=(12, 4))
plt.subplot(1, 2, 1)

plt.barh(pos_dtr, feature_importance_dtr[sorted_idx_dtr], align="center")
plt.yticks(pos_dtr, np.array(train_ocean_x.columns)[sorted_idx_dtr])
plt.title("Feature Importance (MDI)")

result_dtr = permutation_importance(
    dtr, test_ocean_x, test_ocean_y, n_repeats=10, random_state=42, n_jobs=2
)
sorted_idx_dtr = result_dtr.importances_mean.argsort()
plt.subplot(1, 2, 2)
plt.boxplot(
    result.importances[sorted_idx_dtr].T,
    vert=False,
    tick_labels=np.array(train_ocean_x.columns)[sorted_idx_dtr],
)
plt.title("Permutation Importance")
fig.tight_layout()
plt.show()


print("Decision Tree Regression:")
print('Train Mean Squared Error:', mse_dtr_train)
print('Train R-squared:', r2_dtr_train)
print('Test Mean Squared Error:', mse_dtr_test)
print('Test R-squared:', r2_dtr_test)
```




```
Decision Tree Regression:
Train Mean Squared Error: 9.398634562506831e-05
Train R-squared: 0.8918124057353458
Test Mean Squared Error: 0.00023353813142905152
Test R-squared: 0.7461937497834324
```

Gradient Boost Regression

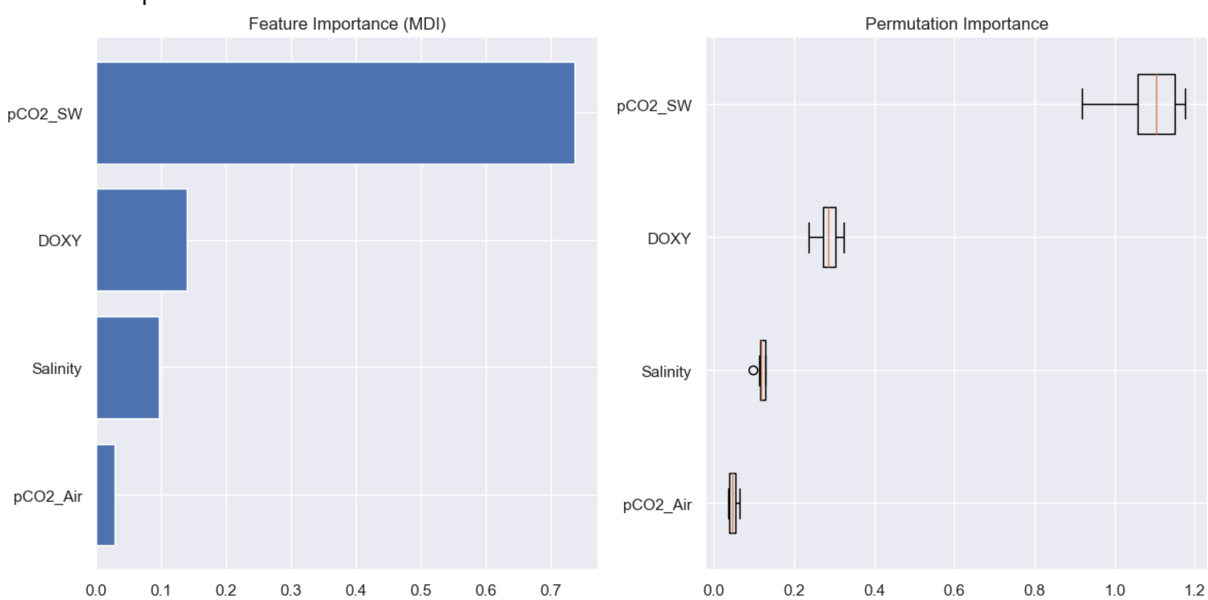
Finally, I used a similar approach with a Gradient Boost Regression model. I computed mean squared error and r squared values for the model and created Feature and Permutation Importance charts.

In [315…

```
##########################
# Gradient Boost Regressor
##########################

reg = GradientBoostingRegressor(random_state=0)
reg = reg.fit(train_ocean_x, train_ocean_y)

y_gbr_pred_test = reg.predict(test_ocean_x)
y_gbr_pred_train = reg.predict(train_ocean_x)


#Calculate Mean Squared Error
mse_gbr_train = mean_squared_error(train_ocean_y, y_gbr_pred_train)
mse_gbr_test = mean_squared_error(test_ocean_y, y_gbr_pred_test)

# Calculate R-squared
r2_gbr_train = r2_score(train_ocean_y, y_gbr_pred_train)
r2_gbr_test = r2_score(test_ocean_y, y_gbr_pred_test)

print("Gradient Boost Regressor: ")
print('Train Mean Squared Error:', mse_gbr_train)
print('Train R-squared:', r2_gbr_train)
print('Test Mean Squared Error:', mse_gbr_test)
print('Test R-squared:', r2_gbr_test)

feature_importance = reg.feature_importances_

sorted_idx = np.argsort(feature_importance)
pos = np.arange(sorted_idx.shape[0]) + 0.5
fig = plt.figure(figsize=(12, 6))
plt.subplot(1, 2, 1)
```

```
plt.barh(pos, feature_importance[sorted_idx], align="center")
plt.yticks(pos, np.array(train_ocean_x.columns)[sorted_idx])
plt.title("Feature Importance (MDI)")

result = permutation_importance(
    reg, test_ocean_x, test_ocean_y, n_repeats=10, random_state=42, n_jobs=2
)
sorted_idx = result.importances_mean.argsort()
plt.subplot(1, 2, 2)
plt.boxplot(
    result.importances[sorted_idx].T,
    vert=False,
    tick_labels=np.array(train_ocean_x.columns)[sorted_idx],
)
plt.title("Permutation Importance")
fig.tight_layout()
plt.show()
```

```
Gradient Boost Regressor:
Train Mean Squared Error: 5.7963666148998377e-05
Train R-squared: 0.9332780782813297
Test Mean Squared Error: 0.00012132408609850814
Test R-squared: 0.8681465370764554
```



Results and Analysis

Looking at the Partial Regression plots from the linear model, it is clear that the feature that has the greatest impact on pH in the model is the sea water partial pressure (pCO2_SW). There is a greater slope in the regression line as CO2_SW increases. The Decision Tree and Gradient Boost Regression plots for feature and permuation importance also both indicate the stregth of the relationship in the model. Both show dissolved oxygen (DOXY) to be the next greatest feature of importance.

The metrics used in comparing the three alogrithms were mean squared error and R squared score. These are good metrics to use when evaluating regression model performance. Mean squared values were computed for test an train sets for each algorithm. All algorithms performed decently well, however, the Gradient Boost Regression algorithm did the best, it had the lowest mean squared error and highest R squared values. The code below graphs this information.

Mean Squared Error

	Train	Test
Linear Regression	0.00019	0.00021
Decision Tree Regression	0.00009	0.00023
Gradient Boost Regression	0.00006	0.00012

R-Squared

	Train	Test
Linear Regression	0.7704	0.7767
Decision Tree Regression	0.8918	0.7462
Gradient Boost Regression	0.9333	0.8681

Due to the observation that the sea water CO2 partial pressure showed such importance in the models, I went back and created a single parameter model using the three algorithms. Below are the performance metrics:

Mean Squared Error

	Train	Test
Linear Regression	0.00026	0.00026
Decision Tree Regression	0.00021	0.00031
Gradient Boost Regression	0.00019	0.00030

R-Squared

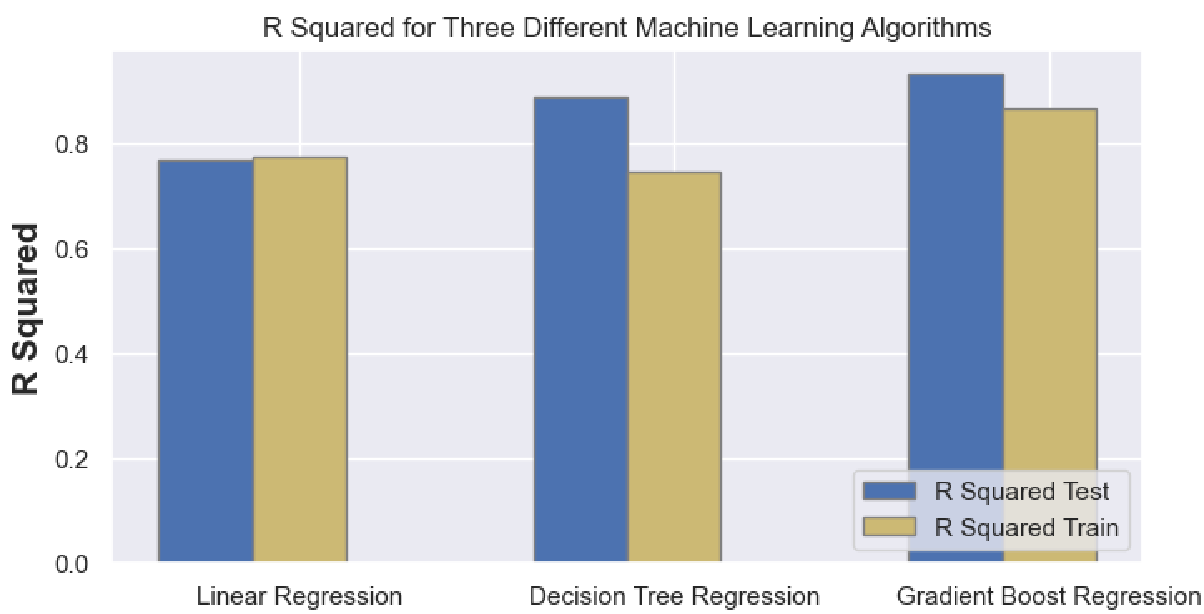
	Train	Test
Linear Regression	0.7026	0.7179
Decision Tree Regression	0.7551	0.6634
Gradient Boost Regression	0.7767	0.6762

The performance was not as good with the single parameter model, and it is a little less obvious which algorithm had the optimum performance. Looking at the test data, the Linear Regression algorithm gave the lowest MSE and the highest R-squared value. The code and a comparison chart for this analysis are below.

In [334…

```
##############################
# Create Bar Chart for MSE and R squared Comparison
##############################
```

```
# Store Metrics from 3 models for test and train
algo = ["Linear Regression","Decision Tree Regression","Gradient Boost Regre
mse_test = [mse_lm_test, mse_dtr_test, mse_gbr_test]
mse_train = [mse_lm_train, mse_dtr_train, mse_gbr_train]
r2_test = [r2_lm_test, r2_dtr_test, r2_gbr_test]
r2_train = [r2_lm_train, r2_dtr_train, r2_gbr_train]

# Create Bar Chart for MSE
# set width of bar
barWidth = 0.25
fig = plt.subplots(figsize =(8, 4))

# Set position of bar on X axis
br1 = np.arange(len(mse_test))
br2 = [x + barWidth for x in br1]

# Make the plot
plt.bar(br1, mse_train, color ='r', width = barWidth,
        edgecolor ='grey', label ='MSE Train')
plt.bar(br2, mse_test, color ='g', width = barWidth,
        edgecolor ='grey', label ='MSE Test')

# Adding Labels
plt.ylabel('Mean Squared Error', fontweight ='bold', fontsize = 15)
plt.xticks([r + barWidth for r in range(len(mse_test))],algo)
plt.title("Mean Square Error for Three Different Machine Learning Algorithms

plt.legend()
plt.show()


# Create Bar Chart for R squared

# set width of bar
barWidth = 0.25
fig = plt.subplots(figsize =(8, 4))

# Set position of bar on X axis
br1 = np.arange(len(r2_test))
br2 = [x + barWidth for x in br1]

# Make the plot
plt.bar(br1, r2_train, color ='b', width = barWidth,
        edgecolor ='grey', label ='R Squared Train')
plt.bar(br2, r2_test, color ='y', width = barWidth,
        edgecolor ='grey', label ='R Squared Test')

# Adding Labels
plt.ylabel('R Squared', fontweight ='bold', fontsize = 15)
plt.xticks([r + barWidth for r in range(len(r2_test))],algo)
plt.title("R Squared for Three Different Machine Learning Algorithms")
plt.legend(loc='lower right')
plt.show()
```



In [349…

```
######################
# Running models with only pCO_SW parameter
######################

train_ocean_x_pCO2SW = train_ocean_x['pCO2_SW']
test_ocean_x_pCO2SW = test_ocean_x['pCO2_SW']


#plt.scatter(train_ocean_x_pCO2SW, train_ocean_y)
# Linear Reg
lm_pCO2SW = smf.ols(formula = 'pH ~ pCO2_SW', data=train_ocean).fit()
print(lm_pCO2SW.summary())

# LM Predict
y_lm_pred_train_pCO2SW = lm_pCO2SW.predict(train_ocean_x_pCO2SW)
y_lm_pred_test_pCO2SW = lm_pCO2SW.predict(test_ocean_x_pCO2SW)

train_ocean_x_pCO2SW = train_ocean_x_pCO2SW.to_numpy()
test_ocean_x_pCO2SW = test_ocean_x_pCO2SW.to_numpy()
```

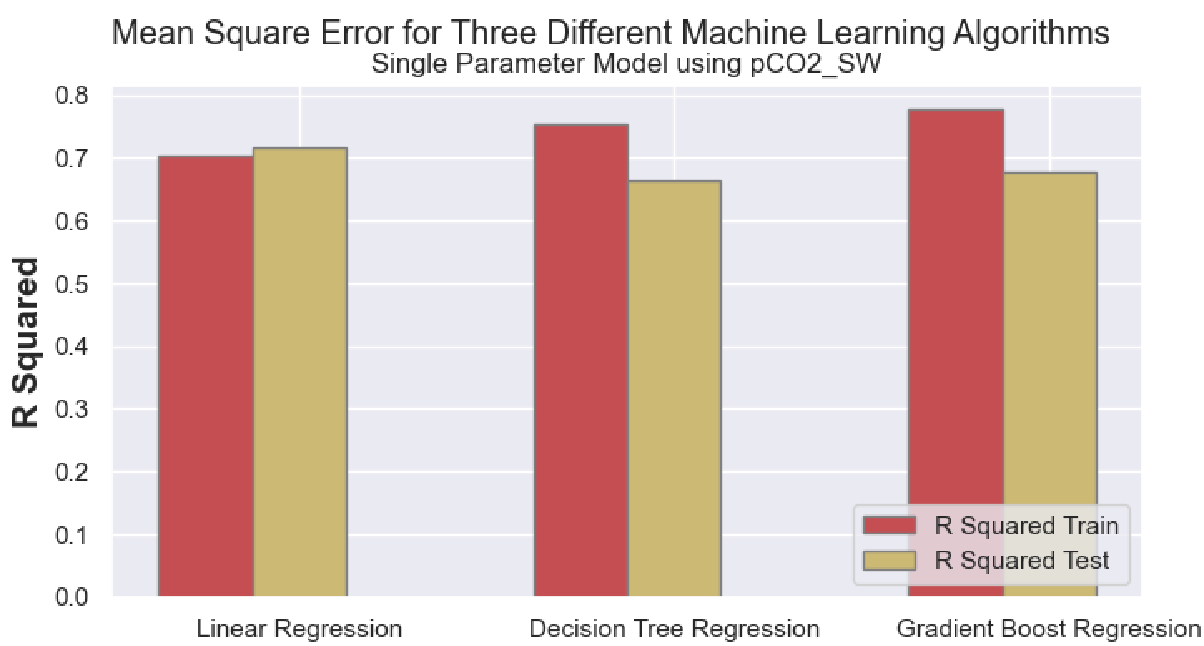
```
# LM R-squared / Mean Squared Error
r2_lm_train_pCO2SW = r2_score(train_ocean_y , y_lm_pred_train_pCO2SW)
r2_lm_test_pCO2SW = r2_score(test_ocean_y , y_lm_pred_test_pCO2SW)
mse_lm_train_pCO2SW = mean_squared_error(train_ocean_y, y_lm_pred_train_pCO2
mse_lm_test_pCO2SW = mean_squared_error(test_ocean_y, y_lm_pred_test_pCO2SW)


#Decision Tree Reg
dtr_pCO2SW = tree.DecisionTreeRegressor()
dtr_pCO2SW = dtr.fit(train_ocean_x_pCO2SW.reshape(-1, 1), train_ocean_y)

# DTR Predict
y_dtr_pred_train_pCO2SW = dtr_pCO2SW.predict(train_ocean_x_pCO2SW.reshape(-1
y_dtr_pred_test_pCO2SW = dtr_pCO2SW.predict(test_ocean_x_pCO2SW.reshape(-1,


# DTR R-squared / Mean Squared Error
mse_dtr_train_pCO2SW = mean_squared_error(train_ocean_y , y_dtr_pred_train_p
mse_dtr_test_pCO2SW = mean_squared_error(test_ocean_y, y_dtr_pred_test_pCO2S
r2_dtr_train_pCO2SW = r2_score(train_ocean_y , y_dtr_pred_train_pCO2SW)
r2_dtr_test_pCO2SW = r2_score(test_ocean_y , y_dtr_pred_test_pCO2SW)

# Gradient Boost Reg
reg_pCO2SW = GradientBoostingRegressor(random_state=0)
reg_pCO2SW = reg_pCO2SW.fit(train_ocean_x_pCO2SW.reshape(-1, 1), train_ocean

# GBR Predict
y_gbr_pred_train_pCO2SW = reg_pCO2SW.predict(train_ocean_x_pCO2SW.reshape(-1
y_gbr_pred_test_pCO2SW = reg_pCO2SW.predict(test_ocean_x_pCO2SW.reshape(-1,


# GBE R-squared / Mean Squared Error
mse_gbr_train_pCO2SW = mean_squared_error(train_ocean_y , y_gbr_pred_train_p
mse_gbr_test_pCO2SW = mean_squared_error(test_ocean_y, y_gbr_pred_test_pCO2S
r2_gbr_train_pCO2SW = r2_score(train_ocean_y , y_gbr_pred_train_pCO2SW)
r2_gbr_test_pCO2SW = r2_score(test_ocean_y , y_gbr_pred_test_pCO2SW)

print()
print()
print("Single Parameter Performance- pCO2_SW")
print("Linear Regression")
print("MSE train/test: ", mse_lm_train_pCO2SW, mse_lm_test_pCO2SW)
print("R squared train/test: " ,r2_lm_train_pCO2SW, r2_lm_test_pCO2SW)
print("Decision Tree Regression")
print("MSE train/test: ", mse_dtr_train_pCO2SW, mse_dtr_test_pCO2SW)
print("R squared train/test: " ,r2_dtr_train_pCO2SW, r2_dtr_test_pCO2SW)
print("Gradient Boost Regression")
print("MSE train/test: ", mse_gbr_train_pCO2SW, mse_gbr_test_pCO2SW)
print("R squared train/test: " ,r2_gbr_train_pCO2SW, r2_gbr_test_pCO2SW)


#####
# Plotting Results for single parameter model
#####
```

```
############################
# Create Bar Chart for MSE and R squared Comparison
############################

# Store Metrics from 3 models for test and train
mse_test_pCO2SW = [mse_lm_test_pCO2SW, mse_dtr_test_pCO2SW, mse_gbr_test_pCO
mse_train_pCO2SW = [mse_lm_train_pCO2SW, mse_dtr_train_pCO2SW, mse_gbr_train
r2_test_pCO2SW = [r2_lm_test_pCO2SW, r2_dtr_test_pCO2SW, r2_gbr_test_pCO2SW]
r2_train_pCO2SW = [r2_lm_train_pCO2SW, r2_dtr_train_pCO2SW, r2_gbr_train_pCO

# Create Bar Chart for MSE
# set width of bar
barWidth = 0.25
fig = plt.subplots(figsize =(8, 4))

# Set position of bar on X axis
br1 = np.arange(len(mse_test_pCO2SW))
br2 = [x + barWidth for x in br1]

# Make the plot
print()
print()
plt.bar(br1, mse_train_pCO2SW, color ='b', width = barWidth,
        edgecolor ='grey', label ='MSE Train')
plt.bar(br2, mse_test_pCO2SW, color ='g', width = barWidth,
        edgecolor ='grey', label ='MSE Test')

# Adding Labels
plt.ylabel('Mean Squared Error', fontweight ='bold', fontsize = 15)
plt.xticks([r + barWidth for r in range(len(mse_test))],algo)
plt.suptitle("Mean Square Error for Three Different Machine Learning Algorit
plt.title("Single Parameter Model using pCO2_SW")
plt.legend()
plt.show()


# Create Bar Chart for R squared

# set width of bar
barWidth = 0.25
fig = plt.subplots(figsize =(8, 4))

# Set position of bar on X axis
br1 = np.arange(len(r2_test_pCO2SW))
br2 = [x + barWidth for x in br1]

# Make the plot
plt.bar(br1, r2_train_pCO2SW, color ='r', width = barWidth,
        edgecolor ='grey', label ='R Squared Train')
plt.bar(br2, r2_test_pCO2SW, color ='y', width = barWidth,
        edgecolor ='grey', label ='R Squared Test')

# Adding Labels
plt.ylabel('R Squared', fontweight ='bold', fontsize = 15)
```

```
plt.xticks([r + barWidth for r in range(len(r2_test_pCO2SW))],algo)
plt.suptitle("Mean Square Error for Three Different Machine Learning Algorit
plt.title("Single Parameter Model using pCO2_SW")
plt.legend(loc='lower right')
plt.show()
```

```
                            OLS Regression Results
==============================================================================
=
Dep. Variable:                     pH   R-squared:                       0.70
3
Model:                            OLS   Adj. R-squared:                  0.70
2
Method:                 Least Squares   F-statistic:                     296
0.
Date:                Thu, 15 Aug 2024   Prob (F-statistic):               0.0
0
Time:                        09:33:03   Log-Likelihood:                 3403.
0
No. Observations:                1255   AIC:                            -680
2.
Df Residuals:                    1253   BIC:                            -679
2.
Df Model:                           1

Covariance Type:            nonrobust

==============================================================================
=
                 coef    std err          t      P>|t|      [0.025      0.97
5]
------------------------------------------------------------------------------
-
Intercept      8.3791      0.007   1284.148      0.000       8.366       8.39
2
pCO2_SW       -0.0008   1.54e-05    -54.403      0.000      -0.001      -0.00
1
==============================================================================
=
Omnibus:                      128.117   Durbin-Watson:                   2.03
1
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              945.16
3
Skew:                           0.048   Prob(JB):                    5.76e-20
6
Kurtosis:                       7.250   Cond. No.                    6.08e+0
3
==============================================================================
=

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correc
tly specified.
[2] The condition number is large, 6.08e+03. This might indicate that there a
re
strong multicollinearity or other numerical problems.


Single Parameter Performance- pCO2_SW
Linear Regression
MSE train/test:  0.00025839208151053967 0.00025953543761073555
```

```
R squared train/test:  0.7025651174141884 0.7179402103835517
Decision Tree Regression
MSE train/test:  0.00021272393124125016 0.0003097232527305104
R squared train/test:  0.7551336823402125 0.6633967356877196
Gradient Boost Regression
MSE train/test:  0.0001940240926737965 0.00029793308304906416
R squared train/test:  0.7766590489697519 0.6762101410958811
```



Conclusion

In this project I used three different machine learning algorithms to model the affect of different variables on ocean water pH. I used Linear Regression, Decision Tree Regression and Gradient Boost Regression and computed mean squared error and R squared scores as a means for evaluation. All models performed well, but the Gradient

Boost Regression algorithm showed to be very good a predicting pH levels with a multi-parametric model. The Linear Regression algorithm did well with one parameter. These algorithms could be effective tools in forecasting trends and help researchers and policy makers gain understanding in ocean acidification. In my analysis, the partial pressure of CO2 in the sea water was shown to be the most crucial parameter for the models. For future improvements, a more scientific knowledge set of additional parameters and interaction to investigate may be needed. Another future improvement could be to fund projection data for ocean water pCO2 levels and use the models to predict changes in ocean water pH levels.

This project shows the potential and relatively easiness of these algorithms to be useful tools for forecasting, whether for environmental causes or other regression prediction applications.