In [ ]:

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Laboratory 28: Assessing Fitness; Prediction Intervals

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ENGR 1330 Laboratory 28 - In Lab

Background

In Lab 26 we examined regression, both using primative python and packages. In this lab we will put these ideas into practice, and look at measures of fitness and uncertainty.

Lets start with an example.

A polymeric material contains a solvent that dissolves as a function of time. The concentration of the solvent, expressed as a percentage of the total weight of the polymer, is shown in the table below.

Solvent Concentration (w%)	Time(sec)
55.5	0
44.7	2
38.0	4
34.7	6
30.6	8
27.2	10
22.0	12
15.9	14
8.1	16
2.9	18
1.5	20

Fit a linear data model to the data, plot the data and model. Determine the equation of the data model and the corresponding RMSE and R^2 value.

In [1]:
```
# Load the necessary packages
import numpy as np
```

```
import pandas as pd
import statistics
import math
from matplotlib import pyplot as plt
import statsmodels.formula.api as smf
```

In [2]:

```
# make a dataframe
concentration = [55.5,44.7,38.0,34.7,30.6,27.2,22.0,15.9,8.1,2.9,1.5]
time = [0,2,4,6,8,10,12,14,16,18,20]
polymer = pd.DataFrame({'Time':time, 'Conc':concentration})
polymer.head() # check if dataframe is as anticipated
```

Out[2]:

	Time	Conc
0	0	55.5
1	2	44.7
2	4	38.0
3	6	34.7
4	8	30.6

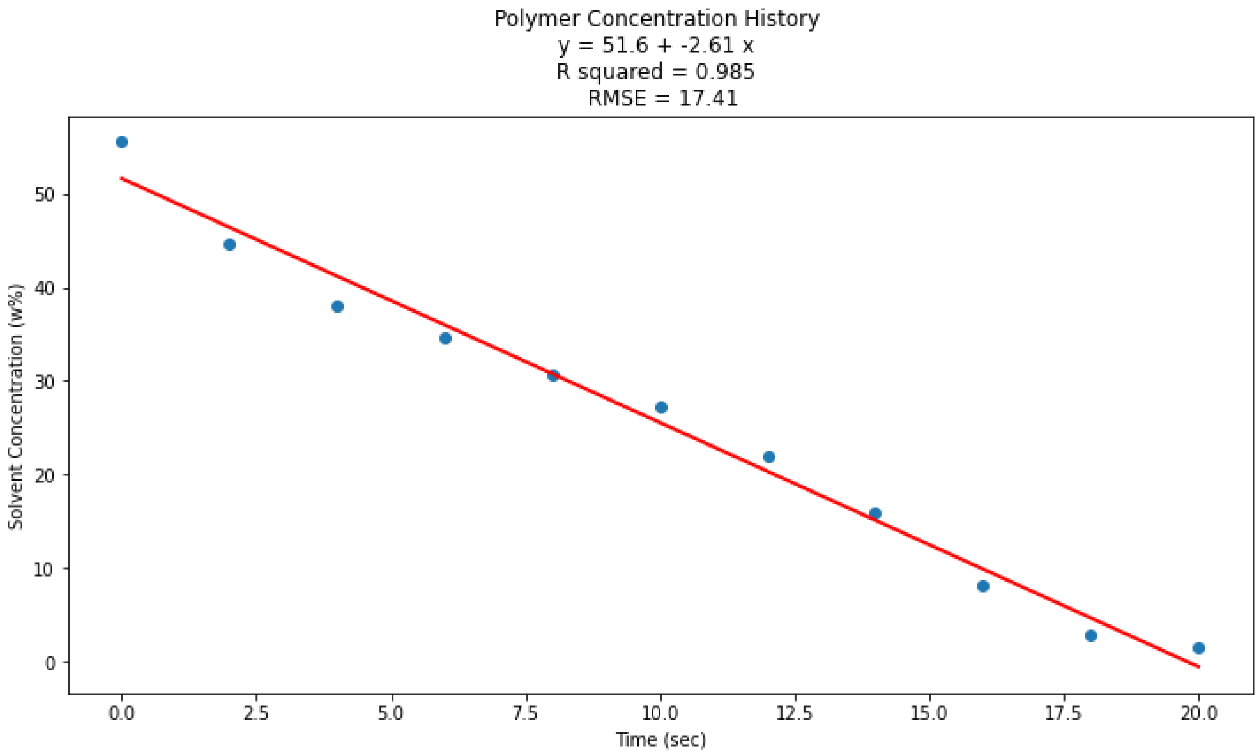
In [3]:

```
# Initialise and fit linear regression model using `statsmodels`
model = smf.ols('Conc ~ Time', data=polymer)
model = model.fit()
#print(model.summary())
# dir(model) # activate to find attributes
intercept = model.params[0]
slope = model.params[1]
Rsquare = model.rsquared
RMSE = math.sqrt(model.mse_total)
```

To find the various values a visit to Here is useful! Below we will construct a title line that contains the equation, RMSE, and R-square using type casting and concatenation, then pass it to the plot.

In [4]:

```
# Predict values
NP_pred = model.predict()

titleline = 'Polymer Concentration History \n' + 'y = ' + str(round(intercept,2)) + ' +
# Plot regression against actual data - What do we see?
plt.figure(figsize=(12, 6))
plt.plot(polymer['Time'], polymer['Conc'], 'o')          # scatter plot showing actual
plt.plot(polymer['Time'], NP_pred, 'r', linewidth=2)   # regression line
plt.xlabel('Time (sec)')
plt.ylabel('Solvent Concentration (w%)')
plt.title(titleline)

plt.show()
```

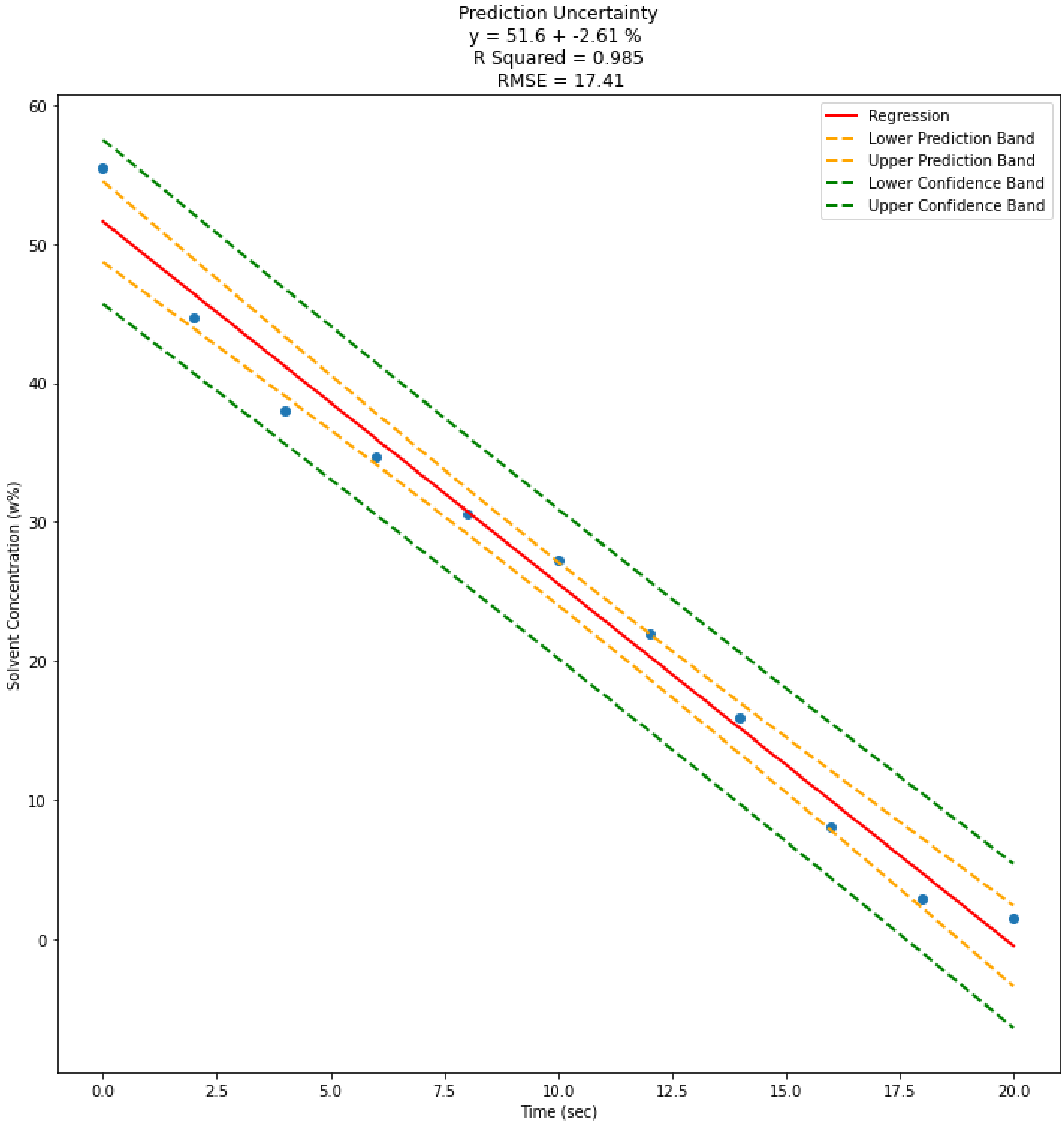


Now suppose we want to get an idea of prediction uncertainty, we can use ideas from the lesson;

The API calls are explained Here

In [8]:
```
from statsmodels.sandbox.regression.predstd import wls_prediction_std   #needed to get
prstd, iv_l, iv_u = wls_prediction_std(model) #iv_l and iv_u give you the limits of the
#print(iv_l)
#print(iv_u)
from statsmodels.stats.outliers_influence import summary_table

st, data, ss2 = summary_table(model, alpha=0.05)

fittedvalues = data[:, 2]
predict_mean_se  = data[:, 3]
predict_mean_ci_low, predict_mean_ci_upp = data[:, 4:6].T
predict_ci_low, predict_ci_upp = data[:, 6:8].T

polymer['FittedConc']=fittedvalues
polymer['PD-Low']=predict_ci_low
polymer['PD-Upp']=predict_ci_upp
polymer['CI-Low']=predict_mean_ci_low
polymer['CI-Upp']=predict_mean_ci_upp
ddf = polymer.sort_values('Time')

newtitleline= 'Prediction Uncertainty\n'+'y = '+str(round(intercept,2))+ ' + '+str(roun
plt.figure(figsize=(12, 12))
plt.plot(ddf['Time'], ddf['Conc'], 'o') # observation scatterplot
plt.plot(ddf['Time'], ddf['FittedConc'], 'r', linewidth=2, label = 'Regression')   # re
plt.plot(ddf['Time'], ddf['CI-Low'],'--', color='orange',lw=2 , label ='Lower Predictio
plt.plot(ddf['Time'], ddf['CI-Upp'],'--',  color='orange',lw=2 , label = 'Upper Predict
plt.plot(ddf['Time'], ddf['PD-Low'],'--', color='green',  lw=2, label = 'Lower Confiden
plt.plot(ddf['Time'], ddf['PD-Upp'], '--',color='green', lw=2, label = 'Upper Confidenc

#MY CODE
plt.xlabel('Time (sec)')
```

```
plt.ylabel('Solvent Concentration (w%)')
plt.legend(loc='upper right')
plt.title(newtitleline)

plt.show()
```



Exercise 1:

Fix the plot above to include a title, x and y axis labels and a legend.

Exercise 2:

A polymeric material contains a solvent that dissolves as a function of time. The concentration of the solvent, expressed as a percentage of the total weight of the polymer, is shown in the table below.

Solvent Concentration (w%)	Time(sec)
30.2	0
44.7	2
22.5	4
41.3	6
28.8	8
14.0	10
26.2	12
11.0	14
23.4	16
14.5	18
4.2	20

Fit a linear data model to the data, plot the data and model. Determine the equation of the data model and the corresponding RMSE and R^2 value. Compare the results for this data with the example, which data set produces a better fit? Why?

In [9]:

```
concentration2 = [30.2, 44.7, 22.5, 41.3, 28.8, 14.0, 26.2, 11.0, 23.4,14.5,4.2]
time2 = [0,2,4,6,8,10,12,14,16,18,20]

polymer2 = pd.DataFrame({'Time':time2, 'Conc':concentration2})
polymer2.head()
```

Out[9]:

	Time	Conc
0	0	30.2
1	2	44.7
2	4	22.5
3	6	41.3
4	8	28.8

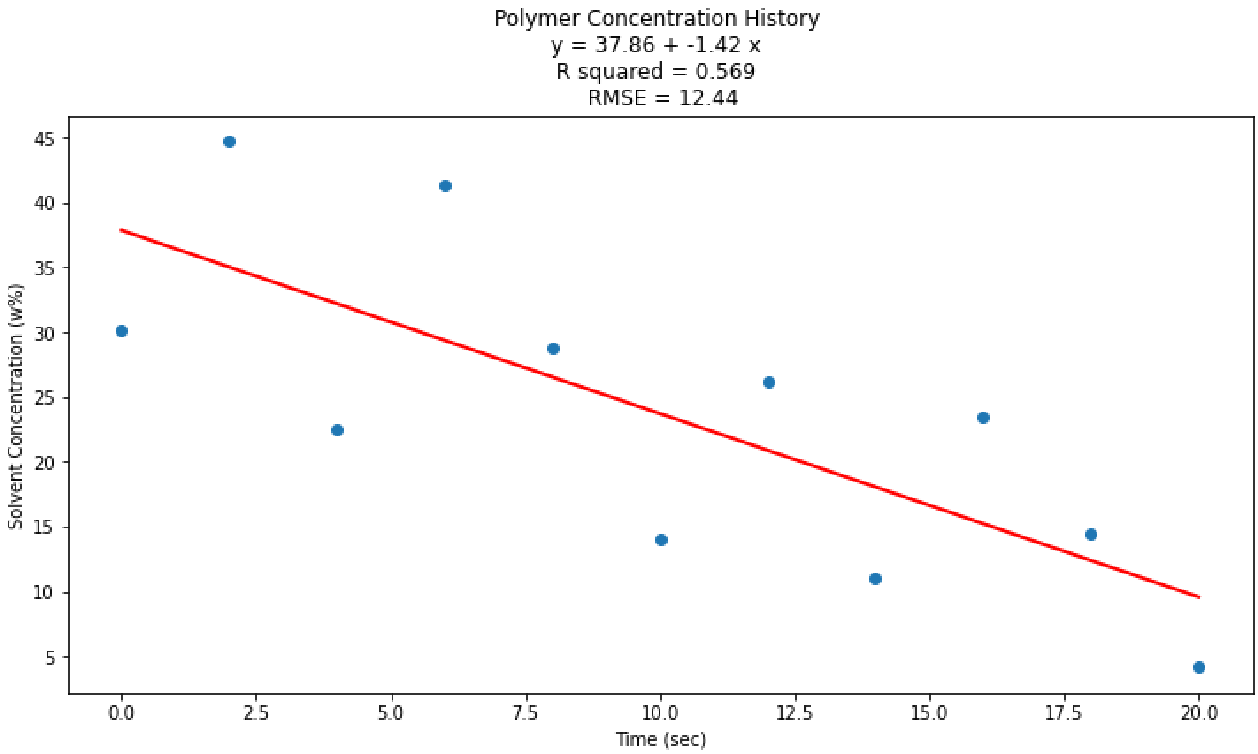
In [10]:

```
# Initialise and fit linear regression model using `statsmodels`
model2 = smf.ols('Conc ~ Time', data=polymer2)
model2 = model2.fit()
#print(model.summary())
# dir(model) # activate to find attributes
intercept2 = model2.params[0]
slope2 = model2.params[1]
Rsquare2 = model2.rsquared
RMSE2 = math.sqrt(model2.mse_total)
```

In [11]:

```
# Predict values
```

```
NP_pred2 = model2.predict()

titleline = 'Polymer Concentration History \n' + 'y = ' + str(round(intercept2,2)) + '
# Plot regression against actual data - What do we see?
plt.figure(figsize=(12, 6))
plt.plot(polymer2['Time'], polymer2['Conc'], 'o')          # scatter plot showing actu
plt.plot(polymer2['Time'], NP_pred2, 'r', linewidth=2)   # regression line
plt.xlabel('Time (sec)')
plt.ylabel('Solvent Concentration (w%)')
plt.title(titleline)

plt.show()
```



In [13]:

```
from statsmodels.sandbox.regression.predstd import wls_prediction_std   #needed to get 
prstd, iv_l, iv_u = wls_prediction_std(model2) #iv_l and iv_u give you the limits of th
#print(iv_l)
#print(iv_u)
from statsmodels.stats.outliers_influence import summary_table

st, data, ss2 = summary_table(model2, alpha=0.05)

fittedvalues = data[:, 2]
predict_mean_se  = data[:, 3]
predict_mean_ci_low, predict_mean_ci_upp = data[:, 4:6].T
predict_ci_low, predict_ci_upp = data[:, 6:8].T

polymer2['FittedConc']=fittedvalues
polymer2['PD-Low']=predict_ci_low
polymer2['PD-Upp']=predict_ci_upp
polymer2['CI-Low']=predict_mean_ci_low
polymer2['CI-Upp']=predict_mean_ci_upp
ddf = polymer2.sort_values('Time')

newtitleline= 'Prediction Uncertainty\n'+'y = '+str(round(intercept2,2))+ ' + '+str(rou
plt.figure(figsize=(12, 12))
```

```
plt.plot(ddf['Time'], ddf['Conc'], 'o') # observation scatterplot
plt.plot(ddf['Time'], ddf['FittedConc'], 'r', linewidth=2, label = 'Regression')   # re
plt.plot(ddf['Time'], ddf['CI-Low'],'--', color='orange',lw=2 , label ='Lower Predictio
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plt.plot(ddf['Time'], ddf['PD-Low'],'--', color='green',  lw=2, label = 'Lower Confiden
plt.plot(ddf['Time'], ddf['PD-Upp'], '--',color='green', lw=2, label = 'Upper Confidenc

#MY CODE
plt.xlabel('Time (sec)')
plt.ylabel('Solvent Concentration (w%)')
plt.legend(loc='upper right')
plt.title(newtitleline)

plt.show()
```

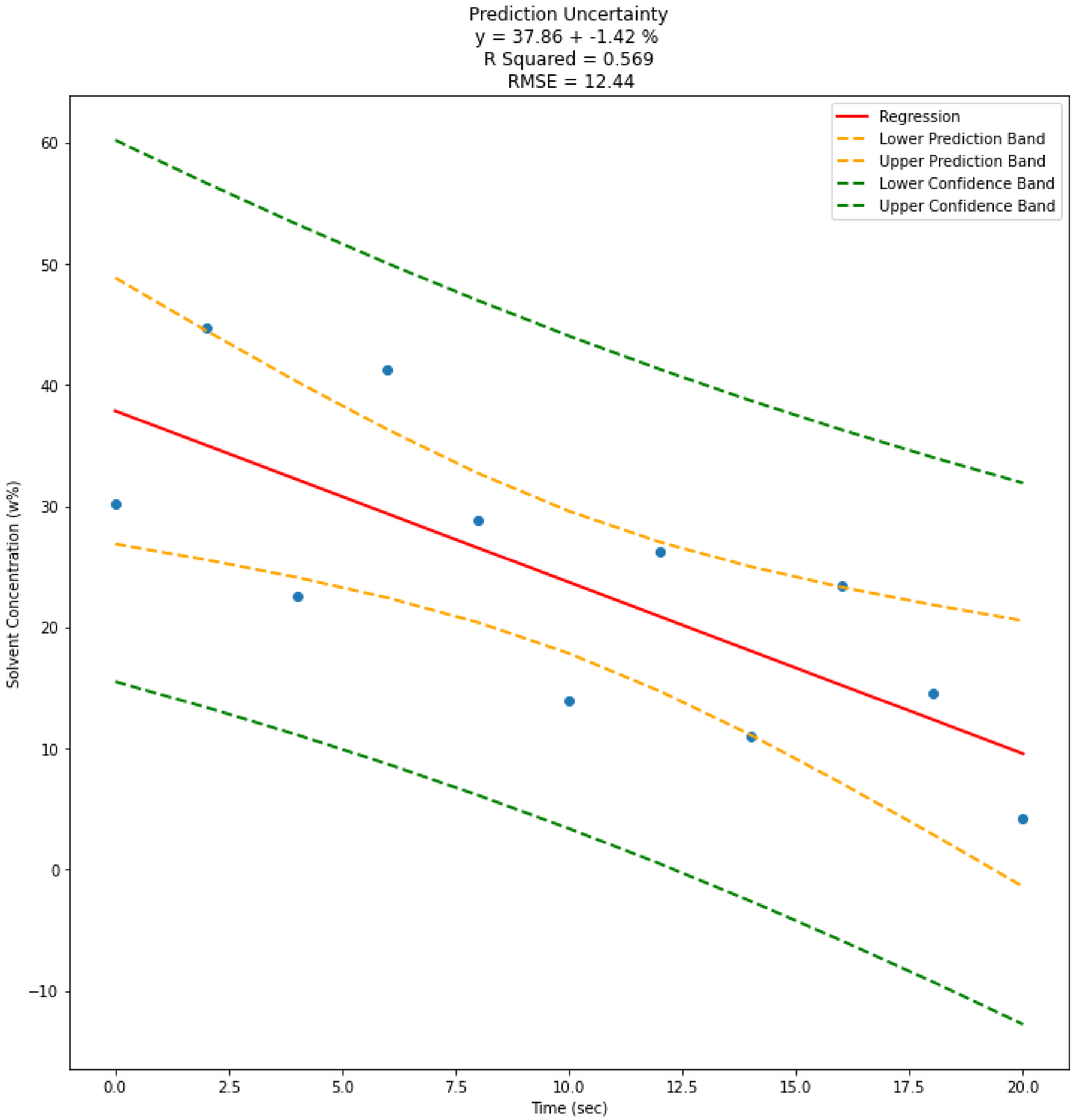

In [ ]: