CSU44061 Machine Learning - Week 3
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Dataset # id:16-16-16

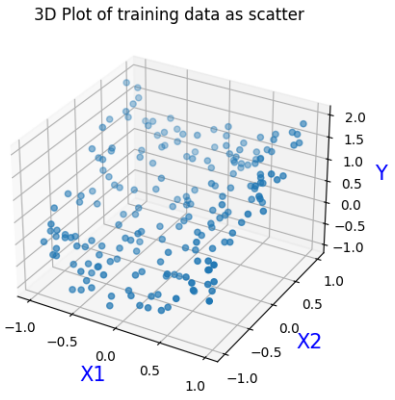
Question i

Code for all questions provided in the appendix.

Part a

Using code provided in the assignment, adding labels and titles, I obtain the following graph, displaying the training data and their associated output.

It seems that the data lies in a plane as it is quite flat.



Part b

As suggested, I used the PolynomialFeatures to create new features going up to the power of 5 for both our available features X_1 and X_2. Not that this method will generate all combinations of the 2 provided features up to the provided power (here 5). Thus we obtain a total of 21 features (ignoring the first factor that is always 0).

```
poly = PolynomialFeatures(5)
X_poly = poly.fit_transform(X)
```

Using these new features, we can train models. In this case, a Lasso model with C values of 1, 200 and 5000. I chose these as they seemed to give me a range interesting coefficients.

```
# Note that alpha = 1 / C
model = linear_model.Lasso(alpha=(1/C))
```

```
model.fit(X_poly, y)
ypred = model.predict(Xtest_poly)
```

Here are the parameters obtained from training a model with these 3 values for C:

C = 1
Intercept: 0.3866779957293107
Coefficients:

$$[0, 0, 0, 0, -0, -0, 0, 0, 0, 0, 0, -0, 0, -0, -0, 0, 0, 0, 0, 0, 0]$$

C = 200
Intercept: 0.051955900546351685
Coefficients:

$$[0, -0.00314985, 0.96742042, 0.87629499, -0.00654177, 0.00630364,$$
$$-0, 0, -0, 0, 0.06296949, -0, 0, -0, 0, -0, 0, -0, 0, -0, -0]$$

C = 5000
Intercept: −0.00883716709265242
Coefficients:

$$[0, 0, 1.00631362, 0.88266399, -0.07027632, 0.23958815,$$
$$0.30758898, 0, -0.44969477, -0.0277997, 0.14749331, -0.00335293,$$
$$-0.10920998, 0.05252247, -0.15571219, -0.36071504, 0.19936564,$$
$$0.22193872, -0.22696517, 0.32680584, -0.]$$

We notice that as C gets bigger, more and more coefficients come into play. For instance, using $C = 1$ resulted in all coefficients being 0. A greater value for C, such as $C = 200$ results in a model where some coefficients are non-zero. In our case that is 6 coefficients. Finally, a very big value for C such as $C = 5000$ makes most of our models parameters non-zero.

We can thus observe that a low value of C tends to set as many parameters as possible to 0.

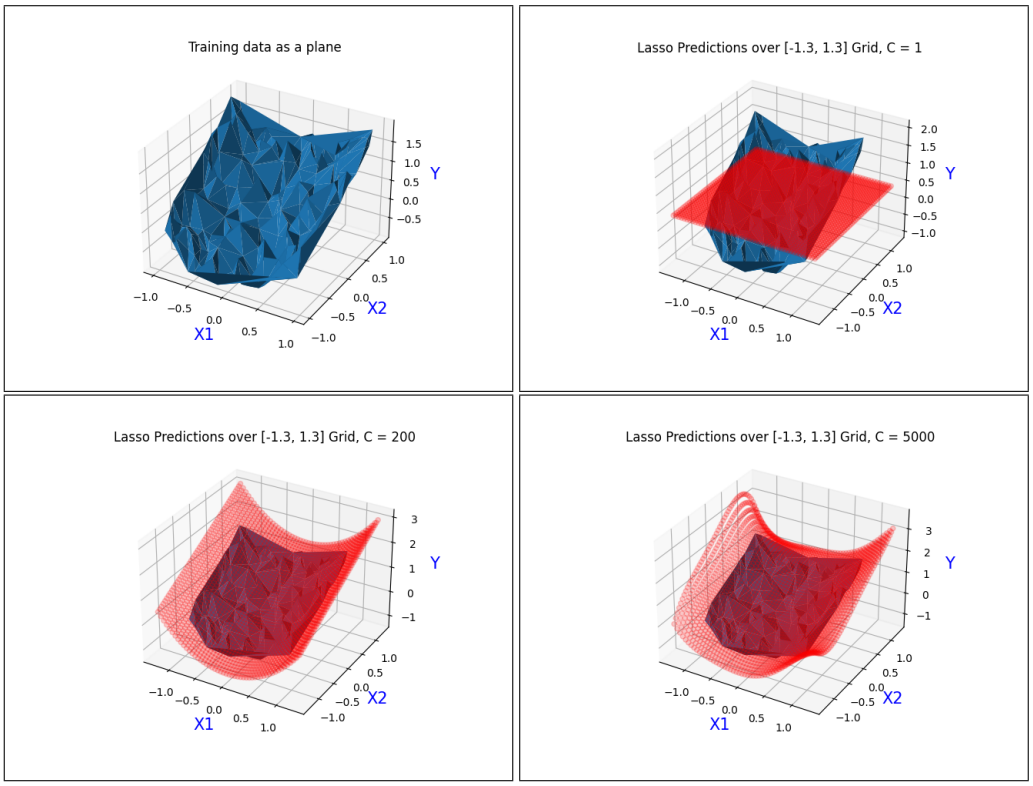
I picked these C values so that I found resulting model parameters organised as such, where we can clearly see the amount of non-zero parameters for each model.

Part c

For this section, I reduced the grid range to [-1.3, 1.3] since a bigger range made the predictions range too large for the y values, thus making it impossible to see the training data plane. I used the plot_trisurf command for plotting the training data as a surface. This yeilds the first plot (training data alone). Then, predictions use a simple scatter with a lower opacity such as not to hide the surface behind it. Adding the predictions to the plot we obtain the next 3 plots.

The code which implements the above explanation is the following:

```
ax = fig.add_subplot(111, projection='3d')
ax.scatter(Xtest[:, 0], Xtest[:, 1], ypred,
                                color="red", alpha=0.2)
ax.plot_trisurf(X[:, 0], X[:, 1], y)
```



We notice that a value of $C = 1$ yeilds a flat plane, this is expected as all of the models parameters are 0. Then, as we increase C and as more parameters come into play, the predictions become more and more complex. We can also notice that the more coefficents come into play, the more noise is taken into account by the model predictions.

Part d

Under-fitting is making a model so simple that it does not capture the true complexity of a training data. For example trying to predict a quadratic line using a linear model would be under-fitting as the predictions will be quite poor.

Over-fitting is the opposite. That is using too many features such that the model matches training data too closely and thus matches more noise that we likely do not want.

Taking this knowledge and comparing it to our models and plots above, we notice the following:

- The model with C = 1 is an example of underfitting. All of our coefficients are 0 thus none of the feature values are used to make predictions, our plot is a simple plane and we notice that it does not match accurately our training data.

- The model with C = 5000 is an example of over-fitting, we notice that all or almost all coefficients are used by the model thus making using of many features which may or may not be useful for predictions. Looking at the plot we notice how it is much more complex and fits noise from our training data with the many ups and downs that are noticeable on the predictions.

Part e

Similarly, I used the PolynomialFeatures to create the same features as with the previous questions up to a power of 5.

For the Ridge Regression model, I decided to use the following C values: 0.00001, 1, 200. I picked these C values so that we could observe the impact of a very small vs large C value. It allows to obtain a better idea of the impact of C on this sort of regression.

Training a Ridge regression model uses code very similar to the previous model:

```
# Note that alpha = 1 / 2C for Ridge regression
model = Ridge(alpha=(1/(2 * C)))
model.fit(X_poly, y)
ypred = model.predict(Xtest_poly)
```

We obtain the following coefficients:

C = 0.00001

Intercept: 0.38649423514736153

Coefficients:

$$[0.00000000e+00, 1.51458548e-04, 1.47029680e-03, 3.40428762e-04$$

$$-4.46143189e-05, -9.72722585e-06, 6.50007693e-05, 5.18327561e-04$$

$$1.43993794e-04, 9.12639486e-04, 3.19489175e-04, -2.50299601e-05$$

$$9.40108739e-05, -2.14996644e-05, -1.26054105e-05, 3.83327579e-05$$

$$3.23922402e-04, 6.38460692e-05, 3.09930239e-04, 1.35033294e-04$$
$$6.60283127e-04]$$

C = 1
Intercept: 0.02671319631416863
Coefficients:

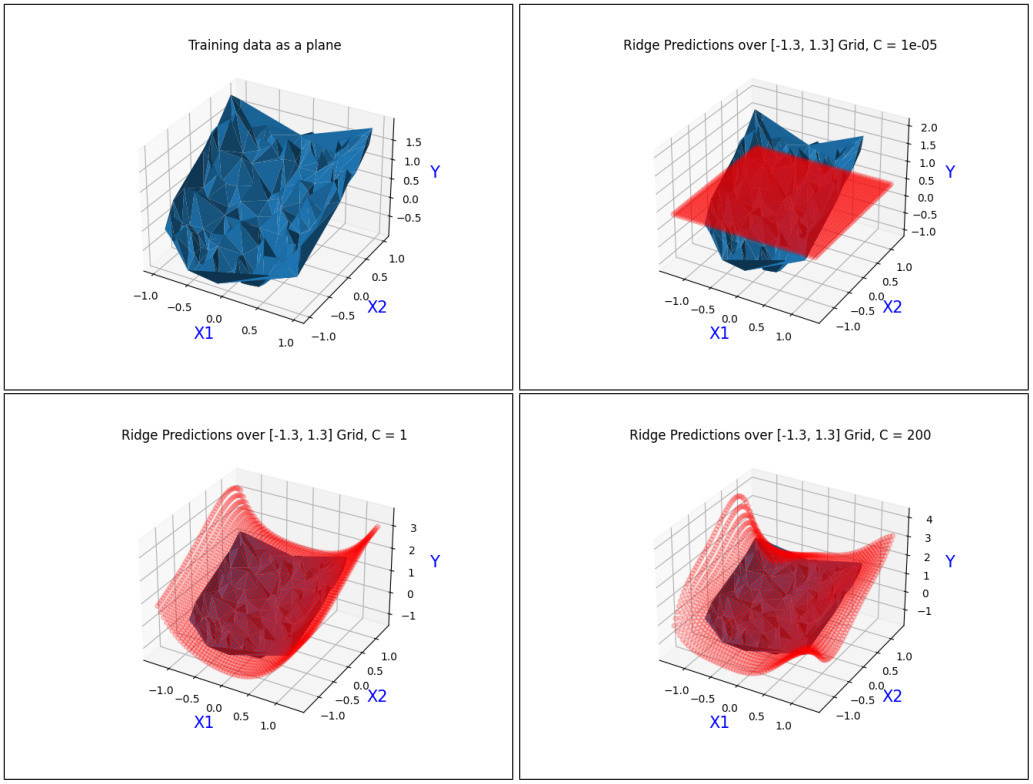
$$[0, 0.00897235, 0.93984335, 0.70409046, -0.05097339, 0.16709087$$
$$0.1100758, 0.09688451, -0.19635685, 0.07396169, 0.30812562, -0.04912464$$
$$-0.02268318, 0.05130517, -0.108326, -0.14242707, 0.06966072, 0.12227828$$
$$-0.16703029, 0.08436703, -0.04872375]$$

C = 200
Intercept: −0.02759728211480622
Coefficients:

$$[0, -0.00662543, 0.99248296, 0.89984203, -0.14267824, 0.3603547$$
$$0.57425937, 0.07124828, -0.79767503, 0.00522424, 0.1531058, 0.01859584$$
$$-0.20079551, 0.17207762, -0.2688553, -0.65605953, 0.27619337, 0.37207688$$
$$-0.45549789, 0.64632594, -0.00373098]$$

For this regression model, we notice that all coefficients are used for all values of C. However we also notice that when C tends to 0 so do the coefficients, on the opposite, the higher value for C the less impact the ridge term will have on its coefficients and thus that is why we only notice minor differences between C = 1 and C = 200.

For this section, I used the same grid range as in the previous question ([-1.3, 1.3]) such that it is easily visible and y values don't go into a range to large. since a bigger range made the predictions range too large for the y values, thus making it impossible to see the training data plane. I used the same plotting method as explained in the previous question. We obtain the following graphs:



We notice that a value of $C = 0.00001$ yeilds a flat plane, this is expected given all of the models parameters tend towards 0 as previously explained, this models is an example of underfitting. Then, as we increase C, the model takes the ridge term less and less into account, the more our model fits our data and goes into overfitting.

Comparing the variation in C values for both Lasso and Ridge regression, we notice that both yeild similar results in terms of predictions. Looking at our coefficients though, the Lasso regression uses less terms as it keeps the less important features coefficients to 0, while the Ridge regression uses most coefficients and plays on changing its impact to be more or less important. We can determine that Lasso regression is more useful for feature selection when we have a large amount of features (21 in this example) such as to avoid overfitting (by choosing an appropriate value for C).

Question ii

Part a

Using the provided fold values, we train a Lasso model for each of the folds, for each model we compute the mean square error (using sklearn's "mean_squared_error"

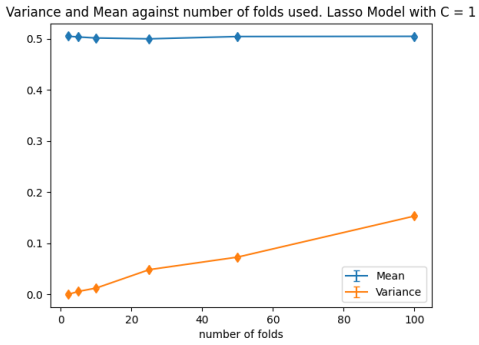
method). Then, for each fold we compute the variance and mean of the mean squarred error.

```
# For each fold, keep track of means, variances and folds
means = []
variances = []
C = 1
all_folds = [2, 5, 10, 25, 50, 100]
for f in all_folds:
    # Split the dataset into folds
    kf = KFold(n_splits=f)
    mse = []
    # Train a model using each fold
    for train, test in kf.split(X_poly):
        model = Lasso(alpha=(1/C))
        model.fit(X_poly[train], y[train])
        ypred = model.predict(X_poly[test])
        # Keep the MSE for each model
        mse.append(mean_squared_error(y[test], ypred))
    # Store the mean, variance for each model
    means.append(statistics.mean(mse))
    variances.append(statistics.variance(mse))
```

Executing this for all of the folds we then obtain a variance and mean for each computed fold. Creating the plot is quite simple, it uses the errorbar function with parameters uplims and lolims set such as to mark where a data point exists within the line.

```
fig = plt.figure()
ax = fig.add_subplot(111)
ax.errorbar(all_folds, means, label='Mean',
            yerr=all_folds, uplims=True, lolims=True)
ax.errorbar(all_folds, variances, label='Variance',
            yerr=all_folds, uplims=True, lolims=True)
```

We can obtain the following plot:



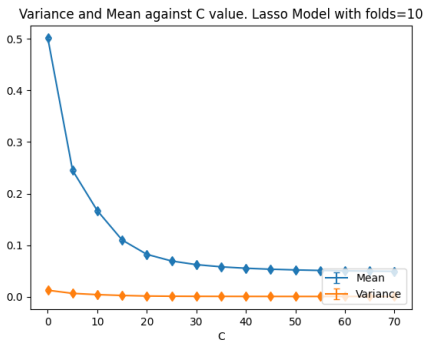
First of all, we notice that the mean is quite flat. That is to be expected, remember from the previous question, a lasso model with C = 1 yeilds a flat plane (ie all of its parameters are 0). Let's look at the variance, we notice that as the number of folds increases, so does the variance. That is to be expected given that our model is a baseline (constant model). Given that our dataset is quite small (200 entries or so), picking a k too large (such as 100) will make for a very low number of testing values for each fold thus making the variance bigger.

In this case, given the size of our dataset and taking into account that we do not want too big of a variance, picking k = 5 or k = 10 seem to be appropriate choices.

Part b

I decided to pick k = 10. We execute the same steps as with the previous question, only this time changing the value of C and keeping a constant number of folds. I decided to use a range of values for C going between 0.01 to 75 with a step size of 5. This is because these values seemed to give the section of variation we are interested in, making C go over 75 would give mostly the same values and similarly for going below 0.001.

Code to plot these values is the exact same as for the previous question, with the difference that the C value is plotted on the X axis instead of the number of folds. We then obtain the following plot:



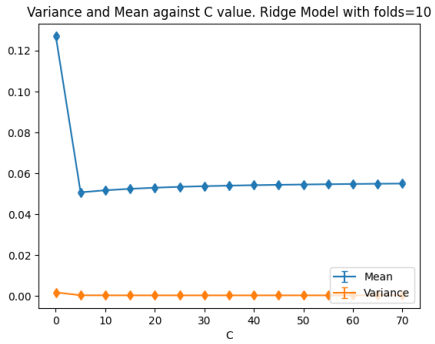
Part c

Using the plot we obtain in part b, we notice that a low value for C (such as C = 1) yeilds a mean of 0.5 which is very high, for such scenarios when C is very low, we have all coefficients set to 0 which explains we obtain such a high mean value. On the opposite when C is too high, we essentially have a linear regression.

In this case it seems like the sweet spot is at C = 45 as it seems the be where the mean squared error is stabilising.

Part d

Using the same values and justification as with part b of this question, we obtain the following plot:



We notice that a low value for C (such as C = 1) yeilds a mean of 0.12 which is the highest on this plot, for such scenarios when C is very low, we have all coefficients close to 0 which explains we obtain such a high mean value. On the opposite when C is too high, the ridge term is essentially not taken into account.

In this case it seems like the sweet spot is at C = 5 as it seems the be where the mean squared error is stabilising (and the lowest)

Appendix

Question 1

```
from sklearn.linear_model import Ridge
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.preprocessing import PolynomialFeatures
from sklearn import linear_model

# Read in data
df = pd.read_csv("week3.csv", comment='#')
X1 = df.iloc[:, 0]
X2 = df.iloc[:, 1]
X = np.column_stack((X1, X2))
y = np.array(df.iloc[:, 2])

# Plot Q1 a - 3D figure.
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.scatter(X[:, 0], X[:, 1], y)
```

```
ax.set_xlabel('X1', color='blue', size=15)
ax.set_ylabel('X2', color='blue', size=15)
ax.set_zlabel('Y', color='blue', size=15)
ax.set_title("3D Plot of training data as scatter")

# Q1 b training lasso models
# Grab the powers up to 5.
poly = PolynomialFeatures(5)
X_poly = poly.fit_transform(X)
# Generate the [-5,5] grid for predictions.
Xtest = []
grid = np.linspace(-1.3, 1.3)
for i in grid:
    for j in grid:
        Xtest.append([i, j])
# Grab the powers up to 5 for the grid data.
Xtest = np.array(Xtest)
Xtest_poly = poly.fit_transform(Xtest)

# Plot the plan with training data alone
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.plot_trisurf(X[:, 0], X[:, 1], y)
ax.set_xlabel('X1', color='blue', size=15)
ax.set_ylabel('X2', color='blue', size=15)
ax.set_zlabel('Y', color='blue', size=15)
ax.set_title("Training data as a plane")

# Question 1 b and c - using C = 1 200 and 500
for C in [1, 200, 5000]:
    # Note that alpha = 1 / C
    model = linear_model.Lasso(alpha=(1/C))
    model.fit(X_poly, y)
    ypred = model.predict(Xtest_poly)
    # Print model parameters
    print("c = ", C)
    print(model.intercept_)
    print(model.coef_)
    # Plot model predictions.
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(Xtest[:, 0], Xtest[:, 1], ypred,
                        color="red", alpha=0.2)
    ax.plot_trisurf(X[:, 0], X[:, 1], y)
    ax.set_xlabel('X1', color='blue', size=15)
    ax.set_ylabel('X2', color='blue', size=15)
```

```
    ax.set_zlabel('Y', color='blue', size=15)
    ax.set_title("Lasso Predictions over " +
                 "[-1.3, 1.3] Grid, C = " + str(C))

# Question e - Ridge Model
for C in [0.00001, 1, 200]:
    # Note that alpha = 1 / 2C for Ridge regression
    model = Ridge(alpha=(1/(2 * C)))
    model.fit(X_poly, y)
    ypred = model.predict(Xtest_poly)
    # Print model parameters.
    print("c = ", C)
    print(model.intercept_)
    print(model.coef_)
    # Plot model predictions.
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(Xtest[:, 0], Xtest[:, 1],
            ypred, color="red", alpha=0.2)
    ax.plot_trisurf(X[:, 0], X[:, 1], y)
    ax.set_xlabel('X1', color='blue', size=15)
    ax.set_ylabel('X2', color='blue', size=15)
    ax.set_zlabel('Y', color='blue', size=15)
    ax.set_title("Ridge Predictions over " +
            "[-1.3, 1.3] Grid, C = " + str(C))
plt.show()
```

Question 2

```
from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import PolynomialFeatures
from sklearn.model_selection import KFold
from sklearn.linear_model import Ridge, Lasso
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import statistics

# Read in data
df = pd.read_csv("week3.csv", comment='#')
X1 = df.iloc[:, 0]
X2 = df.iloc[:, 1]
X = np.column_stack((X1, X2))
y = np.array(df.iloc[:, 2])

# Get polynomials for features
poly = PolynomialFeatures(5)
```

```
X_poly = poly.fit_transform(X)

# Question a
# For each fold, keep track of means, variances and folds
means = []
variances = []
C = 1
all_folds = [2, 5, 10, 25, 50, 100]
for f in all_folds:
    # Split the dataset into folds
    kf = KFold(n_splits=f)
    mse = []
    # Train a model using each fold
    for train, test in kf.split(X_poly):
        model = Lasso(alpha=(1/C))
        model.fit(X_poly[train], y[train])
        ypred = model.predict(X_poly[test])
        # Keep the MSE for each model
        mse.append(mean_squared_error(y[test], ypred))
    # Store the mean, variance for each model
    means.append(statistics.mean(mse))
    variances.append(statistics.variance(mse))

# Plot the means and variances
fig = plt.figure()
ax = fig.add_subplot(111)
ax.errorbar(all_folds, means, label='Mean',
            yerr=all_folds, uplims=True, lolims=True)
ax.errorbar(all_folds, variances, label='Variance',
            yerr=all_folds, uplims=True, lolims=True)
ax.set_xlabel("number of folds")
ax.set_title(
    "Variance and Mean against number of folds used." +
    "Lasso Model with C = 1")
ax.legend(loc='lower right')

# Question b - Lasso model using 10-fold
means = []
variances = []
num_folds = 10
# Using a range of Cs between 1 and 75
# with a 5 increment per step.
C_range = np.arange(0.01, 75, 5)
for C in C_range:
    # Split the dataset in 10 folds
    kf = KFold(n_splits=num_folds)
```

```
    mse = []
    # Train a model for each fold
    for train, test in kf.split(X_poly):
        model = Lasso(alpha=(1/C))
        model.fit(X_poly[train], y[train])
        ypred = model.predict(X_poly[test])
        # Keep the MSE for each model
        mse.append(mean_squared_error(y[test], ypred))
    # Store all models folds variances and means.
    means.append(statistics.mean(mse))
    variances.append(statistics.variance(mse))

# Plot the means and variances
fig = plt.figure()
ax = fig.add_subplot(111)
ax.errorbar(C_range, means, label='Mean',
            yerr=C_range, uplims=True, lolims=True)
ax.errorbar(C_range, variances, label='Variance',
            yerr=C_range, uplims=True, lolims=True)
ax.set_xlabel("mean/variance")
ax.set_xlabel("C")
ax.set_title(
    "Variance and Mean against C value." +
    "Lasso Model with folds=10")
ax.legend(loc='lower right')

# Question d - Ridge model using 10 folds.
means = []
variances = []
num_folds = 10
for C in C_range:
    # Split the dataset in 10 folds
    kf = KFold(n_splits=num_folds)
    mse = []
    # Train a model for each fold
    for train, test in kf.split(X_poly):
        model = Ridge(alpha=(1/(2 * C)))
        model.fit(X_poly[train], y[train])
        ypred = model.predict(X_poly[test])
        # Keep the MSE for each model
        mse.append(mean_squared_error(y[test], ypred))
    # Store all models folds variances and means.
    means.append(statistics.mean(mse))
    variances.append(statistics.variance(mse))

# Plot the means and variances
```

```
fig = plt.figure()
ax = fig.add_subplot(111)
ax.errorbar(C_range, means, label='Mean',
            yerr=C_range, uplims=True, lolims=True)
ax.errorbar(C_range, variances, label='Variance',
            yerr=C_range, uplims=True, lolims=True)
ax.set_xlabel("mean/variance")
ax.set_xlabel("C")
ax.set_title(
    "Variance and Mean against C value." +
    "Ridge Model with folds=10")
ax.legend(loc='lower right')
plt.show()
```