MLPy Workshop 5

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1 Week 5 - Regularization

1.1 Aims

By the end of this notebook you will be able to

- perform regulized regression in sklearn
- understand the role of tuning parameter(s)
- use cross-validation for model tuning and comparison.
- 1. Problem Definition and Setup
- 2. Exploratory Data Analysis
- 3. Baseline Model
- 4. Ridge Regression
- 5. Lasso Regression
- 6. ElasticNet Regression

During workshops, you will complete the worksheets together in teams of 2-3, using **pair programming**. You should aim to switch roles between driver and navigator approximately every 15 minutes. When completing worksheets:

- You will have tasks tagged by (CORE) and (EXTRA).
- Your primary aim is to complete the (CORE) components during the WS session, afterwards you can try to complete the (EXTRA) tasks for your self-learning process.

Instructions for submitting your workshops can be found at the end of worksheet. As a reminder, you must submit a pdf of your notebook on Learn by 16:00 PM on the Friday of the week the workshop was given.

2 Problem Definition and Setup

2.1 Packages

First, let's load some of the packages you wil need for this workshop (we will load others as we progress).

[1]: # Data libraries import pandas as pd

```
import numpy as np

# Plotting libraries
import matplotlib.pyplot as plt
import seaborn as sns

# Plotting defaults
plt.rcParams['figure.figsize'] = (10,6)
plt.rcParams['figure.dpi'] = 80

# sklearn modules
import sklearn
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV, KFold
```

2.2 User Defined Helper Functions

We will make use of the two helper functions that we used last week.

```
[3]: def model_fit(m, X, y, plot = False):

"""Returns the mean squared error, root mean squared error and R 2 value of

a fitted model based

on provided X and y values.

Args:

m: sklearn model object

X: model matrix to use for prediction

y: outcome vector to use to calculating rmse and residuals

plot: boolean value, should fit plots be shown

"""
```

```
y_hat = m.predict(X)
  MSE = mean_squared_error(y, y_hat)
  RMSE = np.sqrt(mean_squared_error(y, y_hat))
  Rsqr = r2_score(y, y_hat)
  Metrics = (round(MSE, 4), round(RMSE, 4), round(Rsqr, 4))
  res = pd.DataFrame(
      data = {'y': y, 'y_hat': y_hat, 'resid': y - y_hat}
  )
  if plot:
      plt.figure(figsize=(12, 6))
      plt.subplot(121)
      sns.lineplot(x='y', y='y_hat', color="grey", data = pd.
\rightarrowDataFrame(data={'y': [min(y),max(y)], 'y_hat': [min(y),max(y)]}))
      sns.scatterplot(x='y', y='y_hat', data=res).set_title("Observed vs_u
⇔Fitted values")
      plt.subplot(122)
      sns.scatterplot(x='y_hat', y='resid', data=res).set_title("Fitted_")
⇔values vs Residuals")
      plt.hlines(y=0, xmin=np.min(y), xmax=np.max(y), linestyles='dashed',__
⇔alpha=0.3, colors="black")
      plt.subplots_adjust(left=0.0)
      plt.suptitle("Model (MSE, RMSE, Rsq) = " + str(Metrics), fontsize=14)
      plt.show()
  return MSE, RMSE, Rsqr
```

2.3 Data

The data for this week's workshop comes from the Elements of Statistical Learning textbook. The data originally come from a study by Stamey et al. (1989) in which they examined the relationship between the level of prostate-specific antigen (psa) and a number of clinical measures in men who were about to receive a prostatectomy. The variables are as follows,

- lpsa log of the level of prostate-specific antigen
- lcavol log cancer volume
- lweight log prostate weight
- age patient age
- 1bph log of the amount of benign prostatic hyperplasia
- svi seminal vesicle invasion

- lcp log of capsular penetration
- gleason Gleason score
- pgg45 percent of Gleason scores 4 or 5
- train test / train split used in ESL

These data are available in prostate.csv, which is included in the workshop materials.

Let's start by reading in the data.

```
[4]: prostate = pd.read_csv('prostate.csv')
prostate.head()
```

```
[4]:
          lcavol
                    lweight
                                        lbph
                                                              gleason
                                                                                    lpsa
                              age
                                              svi
                                                         lcp
                                                                        pgg45
     0 -0.579818
                   2.769459
                               50 -1.386294
                                                0 -1.386294
                                                                     6
                                                                            0 - 0.430783
                                                0 -1.386294
     1 - 0.994252
                   3.319626
                               58 -1.386294
                                                                     6
                                                                            0 -0.162519
                                                                     7
     2 -0.510826
                               74 -1.386294
                                                0 -1.386294
                                                                           20 -0.162519
                   2.691243
     3 - 1.203973
                   3.282789
                               58 -1.386294
                                                0 - 1.386294
                                                                     6
                                                                            0 -0.162519
     4 0.751416
                   3.432373
                               62 -1.386294
                                                0 -1.386294
                                                                            0 0.371564
```

3 Exploratory Data Analysis

Before modelling, we will start with EDA to gain an understanding of the data, through descriptive statistics and visualizations.

3.0.1 Exercise 1 (CORE)

- a) Examine the data structure, look at the descriptive statistics, and create a pairs plot. Do any of our variables appear to be categorical / ordinal rather than numeric?
- b) Are there any interesting patterns in these data? Which variable appears likely to have the strongest relationship with lpsa? Why do you think we are exploring the relationship between these variables and lpsa (log of psa) rather than just psa?

```
[5]: # Part a
prostate.info()
prostate.describe()
```

```
1
          lweight
                   97 non-null
                                     float64
     2
                   97 non-null
                                     int64
          age
     3
          1bph
                   97 non-null
                                     float64
                   97 non-null
     4
          svi
                                     int64
     5
                   97 non-null
                                     float64
          lcp
     6
          gleason
                   97 non-null
                                     int64
     7
          pgg45
                   97 non-null
                                     int64
     8
                   97 non-null
                                     float64
          lpsa
     9
          train
                   97 non-null
                                     object
    dtypes: float64(5), int64(4),
                                    object(1)
    memory usage: 7.7+ KB
[5]:
                lcavol
                           lweight
                                                     1bph
                                                                   svi
                                                                              1cp
                                           age
                        97.000000
            97.000000
                                    97.000000
                                                97.000000
                                                            97.000000
                                                                        97.000000
     count
     mean
              1.350010
                         3.628943
                                    63.865979
                                                 0.100356
                                                             0.216495
                                                                        -0.179366
     std
              1.178625
                         0.428411
                                     7.445117
                                                 1.450807
                                                             0.413995
                                                                         1.398250
             -1.347074
                         2.374906
                                    41.000000
                                                -1.386294
                                                             0.000000
                                                                        -1.386294
     min
     25%
             0.512824
                         3.375880
                                    60.000000
                                                -1.386294
                                                             0.000000
                                                                        -1.386294
     50%
              1.446919
                         3.623007
                                    65.000000
                                                 0.300105
                                                             0.000000
                                                                        -0.798508
     75%
                                    68.000000
              2.127041
                         3.876396
                                                 1.558145
                                                             0.000000
                                                                         1.178655
             3.821004
                         4.780383
                                    79.000000
                                                 2.326302
                                                             1.000000
                                                                         2.904165
     max
               gleason
                              pgg45
                                           lpsa
            97.000000
     count
                         97.000000
                                     97.000000
     mean
             6.752577
                         24.381443
                                      2.478387
     std
             0.722134
                         28.204035
                                      1.154329
                                     -0.430783
     min
             6.000000
                           0.000000
     25%
             6.000000
                           0.000000
                                      1.731656
     50%
             7.000000
                         15.000000
                                      2.591516
     75%
             7.000000
                         40.000000
                                      3.056357
             9.000000
                        100.000000
     max
                                      5.582932
```

float64

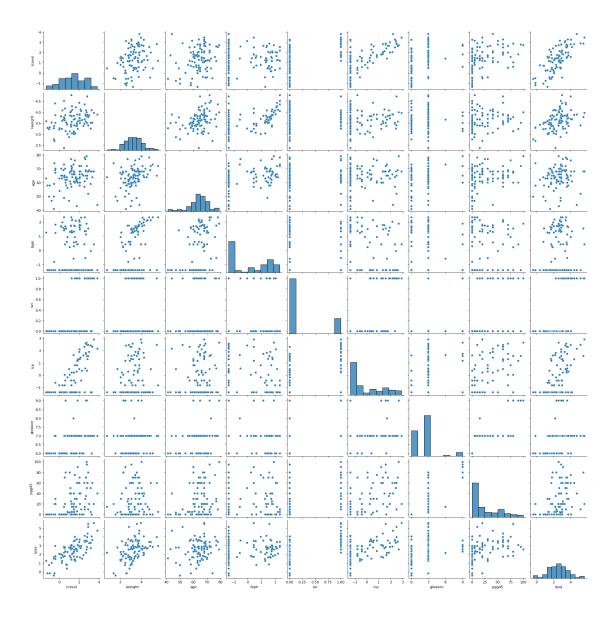
0

lcavol

97 non-null

All the columns contain numerical data, except for the train column which indicates if the datapoint is to be included in the training set or the test set. Of the numerical data, gleason and svi behave like ordinal/binary variables.

```
[6]: # Part b
sns.pairplot(data=prostate)
plt.show()
```



lpsa appears to have the strongest linear relation with lcavol, but also with lweight. We are using the logs because of the choice of the model/regression we might try to fit.

3.1 Train-Test Set

For these data we have already been provided a column to indicate which values should be used for the training set and which for the test set. This is encoded by the values in the train column - we can use these columns to separate our data and generate our training data: X_train and y_train as well as our test data X_test and y_test.

```
[6]: # Create train and test data frames
train = prostate.query("train == 'T'").drop('train', axis=1)
test = prostate.query("train == 'F'").drop('train', axis=1)
```

```
[7]: # Training data
X_train = train.drop(['lpsa'], axis=1)
y_train = train.lpsa

print('X_train:', X_train.shape)
print('y_train:', y_train.shape)

X_train: (67, 8)
y_train: (67,)

[8]: # Test data
X_test = test.drop('lpsa', axis=1)
y_test = test.lpsa

print("X_test:", X_test.shape)
print("y_test:", y_test.shape)

X_test: (30, 8)
y_test: (30,)
```

Let's also fix the random seed to make this notebook's output identical at every run

```
[9]: # Fix seed rng = np.random.seed(0)
```

4 Baseline model

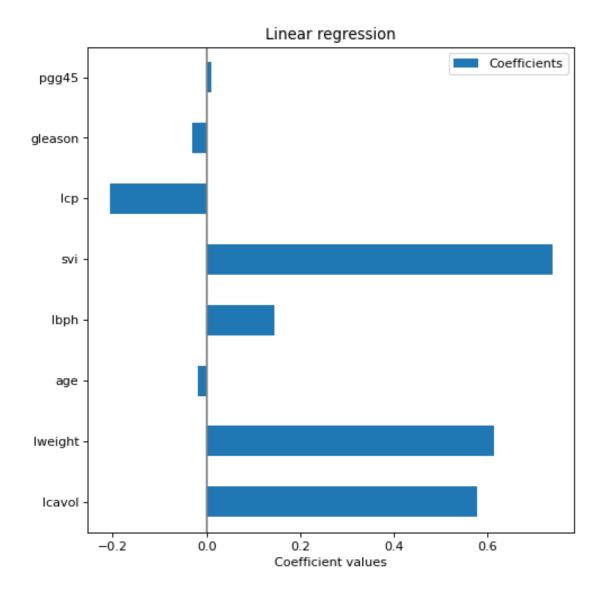
Our first task is to fit a baseline model which we will be able to use as a point of comparison for our subsequent models. A good candidate for this is a simple linear regression model that includes all of our features.

```
[10]: # Train a linear regression model
from sklearn.linear_model import LinearRegression
lm = LinearRegression().fit(X_train, y_train)
```

We can extract the coefficients for the model, which correspond to the variables: lcavol, lweight, age, lbph, svi, lcp, gleason, and pgg45 respectively.

```
# To add intercept
# fe_names = np.append(['intercept'],lm.feature_names_in_)
# coefs = pd.DataFrame(
# get_coefs(lm),
# columns=["Coefficients"],
# index=fe_names,
# )
```

```
[11]:
              Coefficients
     lcavol
                  0.576543
     lweight
                  0.614020
     age
                 -0.019001
     lbph
                  0.144848
     svi
                  0.737209
                -0.206324
     lcp
      gleason
                 -0.029503
                  0.009465
     pgg45
[12]: # Plot of the coefficients
      coefs.plot.barh(figsize=(9, 7))
      plt.title("Linear regression")
      plt.axvline(x=0, color=".5")
      plt.xlabel("Coefficient values")
      plt.subplots_adjust(left=0.3)
```



These coefficients have the typical regression interpretation, e.g. for each unit increase in lcavol we expect lpsa to increase by 0.5765 on average. To evaluate the predictive properities of our model, we will use the model_fit helper function.

4.0.1 Exercise 2 (CORE)

Use the model_fit function to evaluate both the model fit on the training data and the predictions on the test data.

- Based on these plots do you see anything in the fit or residual plot that is potentially concerning?
- Do you expect the MSE on test data to be better or worse than the MSE on the training data?

[14]: model_fit(lm, X_train, y_train, True)

Model (MSE, RMSE, Rsq) = (0.4392, 0.6627, 0.6944)

Observed vs Fitted values

1.5

1.0

0.5

2

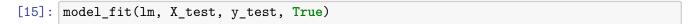
1.0

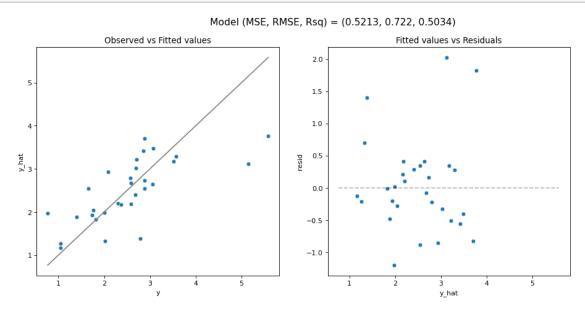
-0.5

-1.0

-1.5

[14]: (0.43919976805833433, 0.662721486039448, 0.6943711796768238)





[15]: (0.5212740055076021, 0.7219930785731966, 0.503379850238179)

Of concern in the plots above we observe of 2 high-leverage outliers in the test data, which may

affect the slope of the fit significantly. As expected, we obtain lower MSE and better R^2 on the TRAINING data versus the TEST data.

4.1 Standardization

In subsequent sections we will be exploring the use of the Ridge and Lasso regression models which both penalize larger values of \mathbf{w} . While not particularly bad, our baseline model had coefficients that ranged from the smallest at 0.0095 to the largest at 0.737 which is about a 78x difference in magnitude. This difference can be made even worse if we were to change the units of one of our features, e.g. changing a measurement in kg to grams would change that coefficient by 1000 which has no effect on the fit of our linear regression model (predictions and other coefficients would be unchanged) but would have a meaningful impact on the estimates given by a Ridge or Lasso regression model, since that coefficient would now dominate the penalty term.

To deal with this issue, the standard approach is to standardize all features. Additionally, the feature values can now be interpreted as the number of standard deviations each observation is away from that column's mean. Using sklearn we can perform this transformation using the StandardScaler transformer from the preprocessing submodule.

Keep in mind, that in order to get a realistic idea of the performance of model on the test data, the mean and standard deviation used to standardize both the training and test sets should be computed from the training data only. The best way to accomplish this is to include the StandardScaler in a modeling pipeline for your data

4.1.1 Exercise 3 (CORE)

Consider the following pipeline that first standardizes the features before linear regression. Fit the model to the training data. Using this new model what has changed about our model results? Comment on both the model's coefficients as well as its predictive performance. How has the interpretation of coefficients changed?

```
[16]: # Linear regression pipeline, including standardization
from sklearn.preprocessing import StandardScaler

lm_s = make_pipeline(
    StandardScaler(),
    LinearRegression()
)

lmst = lm_s.fit(X_train, y_train)

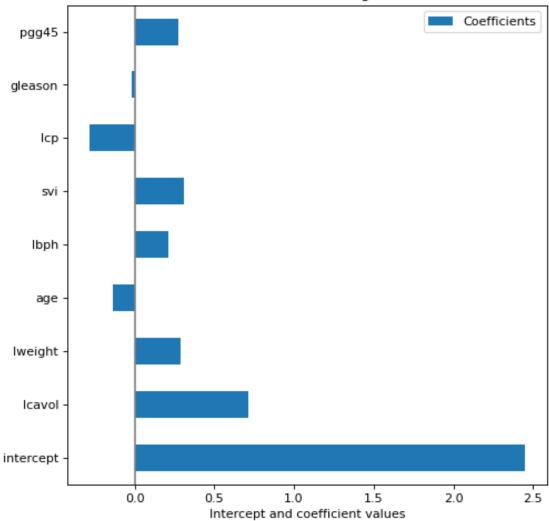
fe_names = np.concatenate([['intercept'], lmst.feature_names_in_])

coefs = pd.DataFrame(
    np.copy(get_coefs(lmst)),
    columns=["Coefficients"],
    index=fe_names,
)
```

coefs

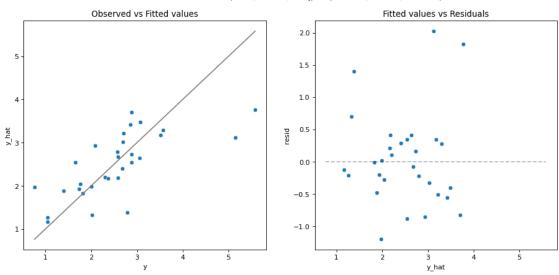
```
[16]:
                 Coefficients
      intercept
                     2.452345
      lcavol
                     0.711041
      lweight
                     0.290450
      age
                    -0.141482
      lbph
                     0.210420
      svi
                     0.307300
      lcp
                    -0.286841
      gleason
                    -0.020757
                     0.275268
     pgg45
[17]: coefs.plot.barh(figsize=(9, 7))
      plt.title("Standardized Linear regression")
      plt.axvline(x=0, color=".5")
      plt.xlabel("Intercept and coefficient values")
     plt.subplots_adjust(left=0.3)
```





[18]: model_fit(lmst, X_test, y_test, True)





[18]: (0.5212740055076005, 0.7219930785731955, 0.5033798502381805)

While the fit and quality of the model has not changed, the interpretation of the intercept and coefficient values has changed: higher values of the coefficient after using the StandardScaler() does indeed indicate a measure of the sensitivity of the predicted variable with respect to a given feature RELATIVE to the other features in the linear model we are fitting.

Note that by simply adding the StandardScaler() step in the pipeline, we have standardized all features, including the binary and ordinal features. This makes interpreting the coefficients of the binary and ordinal features more challenging. Because of this, typically it is preferred to only standardize the numerical variables; in that case, you can use ColumnTransformer() to apply standardization only to the numerical variables.

We can check the mean and standard deviation used to standardize the features by accessing the .mean_ and .scale_ attributes of the StandardScaler(). Notice the values used to transform the binary variable svi.

```
[19]:
                   Mean
                               SD
      lcavol
                 1.3135
                           1.2333
      lweight
                 3.6261
                           0.4730
                64.7463
                           7.4460
      age
      1bph
                 0.0714
                           1.4527
      svi
                 0.2239
                           0.4168
      lcp
                -0.2142
                           1.3902
      gleason
                 6.7313
                           0.7036
      pgg45
                26.2687
                          29.0823
```

After standardizing, the orignal value of 0 for svi is replaced with -0.5371 After standardizing, the orignal value of 1 for svi is replaced with 1.8619

When standardizing all features, if we are interested in interpreting the value of the coefficients of the categorical inputs, we should **unstandardize** the coefficients. Letting $\tilde{\mathbf{x}}$ denote the standardized features and $\hat{\mathbf{w}}$ denote the estimated coefficients when training with standardized features, we have that:

$$\mathbf{E}[y|\tilde{\mathbf{x}}] = \hat{w}_0 + \hat{w}_1 \tilde{x}_1 + \dots + \hat{w}_D \tilde{x}_D.$$

Noting that $\tilde{x}_d = (x_d - \bar{x}_d)/s_d$ (where \bar{x}_d and s_d represent the sample mean and standard deviation), we can transform back to the original space:

$$\mathbf{E}[y|\mathbf{x}] = \hat{w}_0 + \hat{w}_1(x_1 - \bar{x}_1)/s_1 + \ldots + \hat{w}_D(x_D - \bar{x}_D)/s_D.$$

Thus,

$$\mathbf{E}[y|\mathbf{x}] = \left(\hat{w}_0 - \sum_d \bar{x}_d/s_d\right) + \hat{w}_1/s_1x_1 + \ldots + \hat{w}_D/s_Dx_D.$$

And, the *unstandardized* coefficients are obtain by dividing $\hat{\mathbf{w}}$ by the standard deviations.

4.1.2 Exercise 4 (CORE)

Unstandardize the coefficients and interpret the effect of the binary variable svi.

```
[21]: # Unstandardize the coefficients
unst_coef = coefs[1:]['Coefficients'] / ss_p['SD']
unst_coef
```

```
[21]: lcavol 0.576535
lweight 0.614060
age -0.019001
```

```
lbph 0.144847

svi 0.737285

lcp -0.206331

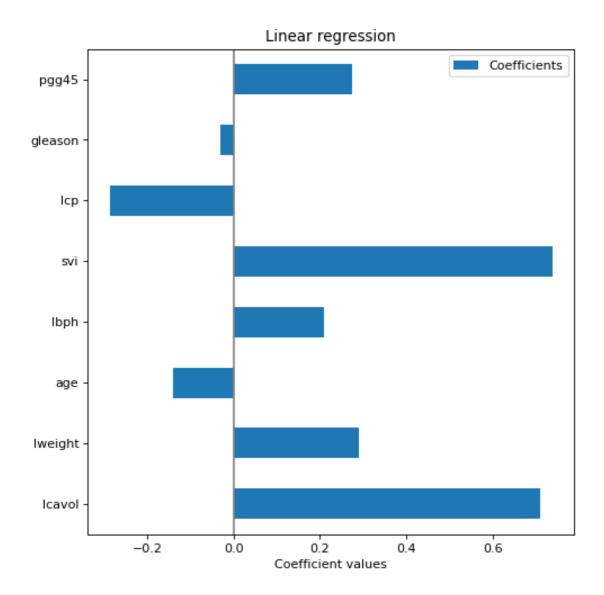
gleason -0.029501

pgg45 0.009465

dtype: float64
```

The unstandardized coefficient associated to svi is 0.737, which is the largest among all the unstandardized coefficients, followed by lcavol and lweight. This indicates the effect of binary variable svi is strongly positive when trying to predict lpsa, svi being TRUE significantly increasing the lpsa prediction in our model in addition to the positive effects of the numerical lcavol & lweight.

Note that in our plot of the coefficients, we want to show the coefficients of the categorical features on the original scale but the coefficients of the numerical features after standardization, for improved interpretation and comparison.



5 Ridge Regression

Ridge regression is a natural extension to linear regression which introduces an ℓ_2 penalty on the coefficients in a standard least squares problem.

The Ridge model is provided by the linear_model submodule. Note that the penalty parameter (referred to as λ in the lecture notes) is called alpha is sklearn, and, as discussed in lectures, this parameter crucially determines the amount of shrinkage towards zero and the weight of the ℓ_2 penalty.

After defining the ridge regression model via, e.g. Ridge(alpha = 1), the usual methods can be called, such as .fit() to fit the model and .predict() to make predictions.

As for the LinearRegression(), after fitting, the intercept and coefficients are stored separately in

the attributes .intercept_ and .coef_. In Ridge, this is helpful as it highlights how the penalty is only applied to the coefficient (i.e. we do not want to shrink the intercept).

Let's start by fitting a ridge regression model with $\alpha = 1$.

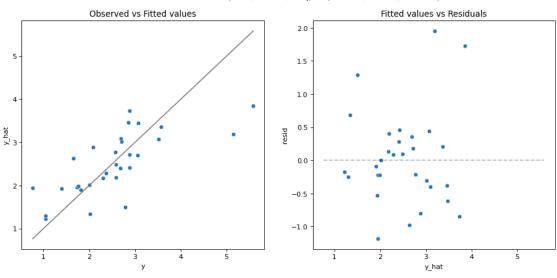
[23]: from sklearn.linear_model import Ridge

```
[24]: # Selected alpha value
alpha_val = 5

# Ridge pipeline
r = make_pipeline(
    StandardScaler(),
    Ridge(alpha = alpha_val)
).fit(X_train, y_train)

model_fit(r, X_test, y_test, plot = True)
```

Model (MSE, RMSE, Rsq) = (0.4942, 0.703, 0.5292)

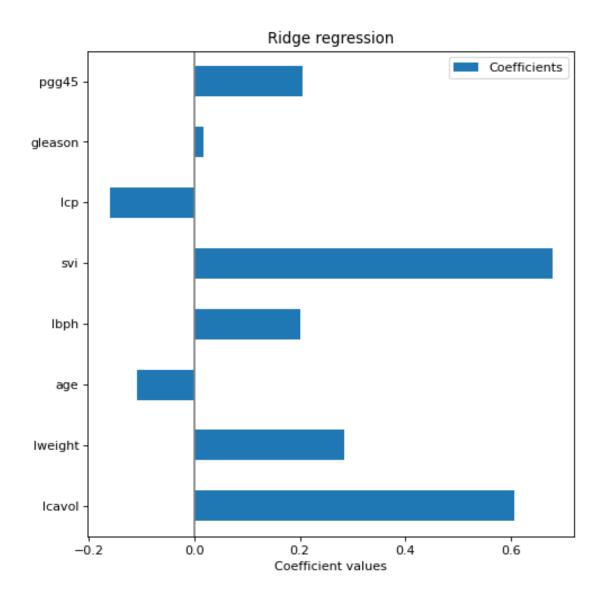


[24]: (0.4941537530376167, 0.7029607051874356, 0.5292174398761034)

```
[25]: # Create dataframe with coefficients, and unstandardize the binary coeffcients
    rcoefs = np.copy(r[-1].coef_)
    rcoefs[[4,6]] = rcoefs[[4,6]]/r[0].scale_[[4,6]]

rcoefs_ = pd.DataFrame(
    rcoefs,
    columns=["Coefficients"],
    index=r.feature_names_in_,
)
```

```
rcoefs
[25]:
               Coefficients
     lcavol
                   0.606103
      lweight
                   0.284181
      age
                  -0.109822
      lbph
                   0.200299
      svi
                   0.678658
      lcp
                  -0.160521
      gleason
                   0.017698
                   0.205013
     pgg45
[26]: # Plot of the coefficients
      rcoefs_.plot.barh(figsize=(9, 7))
      plt.title("Ridge regression")
      plt.axvline(x=0, color=".5")
      plt.xlabel("Coefficient values")
      plt.subplots_adjust(left=0.3)
      plt.show()
```



5.0.1 Exercise 5 (CORE)

Adjust the value of alpha in the cell above and rerun it. Qualitatively, how does the model fit change as alpha changes? How does the MSE change?

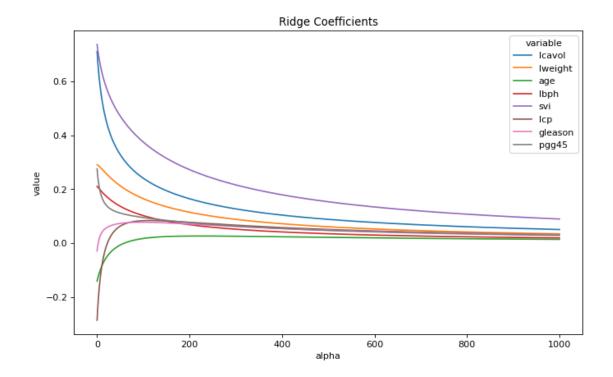
I have changed the value of alpha to alpha = 5. Qualitatively, the MSE has decreased if we perform this change compared to alpha = 1, and the fit has improved as we get a better R^2 value.

5.1 Solution path: Ridge coefficients as a function of α

A useful way of examining the behavior of Ridge regression models is to plot the **solution path** of the coefficients \mathbf{w} as a function of the penalty parameter α . Since Ridge regression is equivalent to linear regression when $\alpha = 0$, we can see that as we increase the value of α , we are shrinking all of the coefficients in \mathbf{w} towards zero asymptotically α approaches infinity.

```
[27]: # Grid of alpha values
      alphas = np.logspace(-2, 3, num=200) # from 10^-2 to 10^3
      ws = [] # Store coefficients
      mses_train = [] # Store training mses
      mses_test = [] # Store test mses
      for a in alphas:
          m = make_pipeline(
              StandardScaler(),
              Ridge(alpha=a)
          ).fit(X_train, y_train)
          w_temp = np.copy(m[1].coef_)
          w_{temp}[[4,6]] = w_{temp}[[4,6]]/m[0].scale_[[4,6]]
          ws.append(w_temp)
          mses_train.append(mean_squared_error(y_train, m.predict(X_train)))
          mses_test.append(mean_squared_error(y_test, m.predict(X_test)))
[28]: # Create a data frame for plotting
      sol_path = pd.DataFrame(
          data = ws,
          columns = X_train.columns # Label columns w/ feature names
      ).assign(
          alpha = alphas,
      ).melt(
          id_vars = ('alpha')
      )
      # Plot solution path of the weights
      plt.figure(figsize=(10,6))
      ax = sns.lineplot(x='alpha', y='value', hue='variable', data=sol_path)
      ax.set_title("Ridge Coefficients")
```

plt.show()



5.1.1 Exercise 6 (CORE)

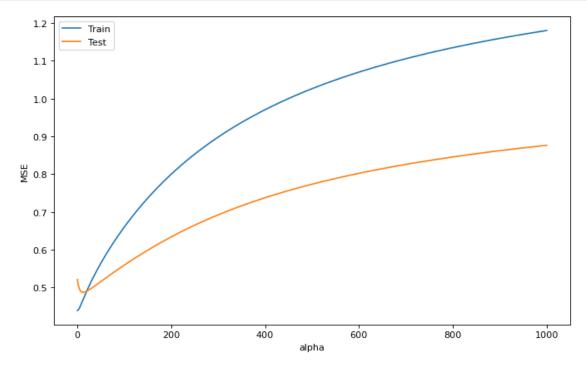
Based on this plot, which variable(s) seem to be the most important for predicting lpsa?

Based on the plot above, we note that the variables which seem most important in predicting are lpsa are: primarily, svi, and secondarily lcavol.

5.1.2 Exercise 7 (CORE)

Run the code below to also plot both the training and test MSE as a function of α . What do you notice about the MSE as we increase α ? Which value of α seems better regarding the changes on training and testing MSE values?

```
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles=handles[0:], labels=labels[0:])
plt.show()
```



For the training data, increasing the alpha always increases the MSE, however when we look at the test data, we see that the optimal/minimal MSE is obtained for a value of alpha around 5. Increasing alpha further results in overfitting.

5.2 Tuning the penalty parameter with cross-validation

We see that the value of α crucially determines the performance of the ridge regression model. While RidgeRegression() uses the default value of alpha=1, this should never be used in practice. Instead, this parameter can be tuned using cross-validation.

As with the polynomial models from last week, we can use GridSearchCV to employ k-fold cross validation to determine an optimal α . Remember, you can use the method $.get_params()$ on your pipeline to list the parameters names to specify in GridSearchCV.

```
# m.get_params()

# CV strategy
cv = KFold(5, shuffle=True, random_state=1234)

# Grid search
gs = GridSearchCV(m,
    param_grid={'ridge__alpha': alphas},
    cv=cv,
    scoring="neg_mean_squared_error")
gs.fit(X_train, y_train)
```

```
[30]: GridSearchCV(cv=KFold(n splits=5, random state=1234, shuffle=True),
                 estimator=Pipeline(steps=[('standardscaler', StandardScaler()),
                                          ('ridge', Ridge())]),
                 param_grid={'ridge__alpha': array([ 0. , 0.1, 0.2, 0.3, 0.4,
     0.5, 0.6, 0.7, 0.8, 0.9, 1.,
             1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.
             2.2, 2.3, 2.4, 2.5, 2.6,
                                         2.7, 2.8,
                                                    2.9, 3.,
                                                               3.1,
             3.3, 3.4, 3.5, 3.6,
                                   3.7,
                                         3.8, 3.9, 4.,
                                                          4.1,
                                                               4.2,
                                   8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.7,
             7.7, 7.8, 7.9, 8.,
             8.8, 8.9, 9., 9.1, 9.2, 9.3, 9.4, 9.5, 9.6, 9.7, 9.8,
             9.9, 10., 10.1, 10.2, 10.3, 10.4, 10.5, 10.6, 10.7, 10.8, 10.9,
            11. , 11.1, 11.2, 11.3, 11.4, 11.5, 11.6, 11.7, 11.8, 11.9, 12. ,
            12.1, 12.2, 12.3, 12.4, 12.5, 12.6, 12.7, 12.8, 12.9, 13. , 13.1,
            13.2, 13.3, 13.4, 13.5, 13.6, 13.7, 13.8, 13.9, 14., 14.1, 14.2,
            14.3, 14.4, 14.5, 14.6, 14.7, 14.8, 14.9, 15. ])},
                 scoring='neg mean squared error')
```

Note that we are passing sklearn.model_selection.KFold(5, shuffle=True, random_state=1234) to the cv argument rather than leaving it to its default. This is because, while not obvious, the prostate data is structured (sorted by lpsa value) and this way we are able to ensure that the folds are properly shuffled. Failing to do this causes *very* unreliable results from the cross validation process.

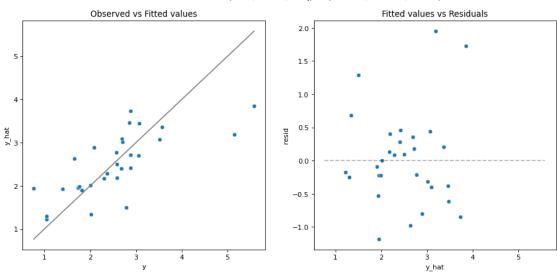
Once fit, we can examine the results to determine what value of α was chosen as well as examine the results of cross validation.

```
[31]: print(gs.best_params_)
    print(-gs.best_score_)

{'ridge__alpha': 4.9}
    0.7066011634399013

[32]: model_fit(gs.best_estimator_, X_test, y_test, plot=True)
```





[32]: (0.4944100876726734, 0.7031430065588887, 0.528973228686775)

5.2.1 Exercise 8 (CORE)

- How does this model compare to the performance of our baseline model? Is it better or worse?
- How do the model coefficients for this model compare to the baseline model? To answer this plot the coefficients for the baseline model against the coefficients for the ridge model. Are they always higher or lower? Now, use np.linalg.norm to compute the ℓ_2 norm of the coefficients for both models and comment on the results.

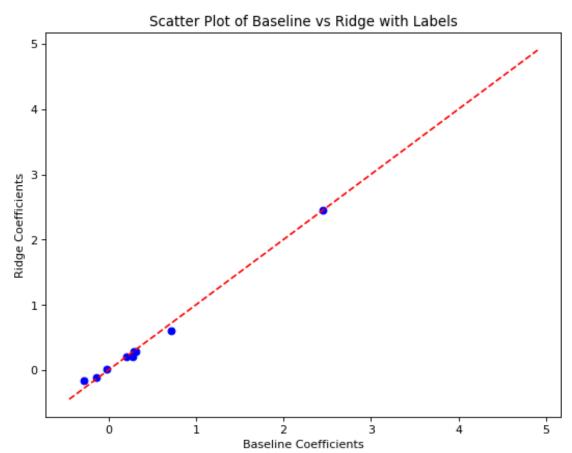
It is clear that the previously obtained model is BETTER than the baseline model we used originally, because its R^2 is better: 0.52 vs. 0.5.

```
[33]: fe_names = np.concatenate([['intercept'], lm.feature_names_in_])

baseline_coefs = pd.DataFrame(
    np.copy(get_coefs(lmst)),
    columns=["Coefficients"],
    index=fe_names,
)

ridge_coefs = pd.DataFrame(
    np.copy(get_coefs(gs.best_estimator_)),
    columns=["Coefficients"],
    index=fe_names,
)

coefs = pd.concat([baseline_coefs, ridge_coefs], axis=1)
```



```
[34]: print(np.linalg.norm(ridge_coefs['Coefficients'][1:]))
print(np.linalg.norm(baseline_coefs['Coefficients'][1:]))
```

- 0.807318313759715
- 0.9524432722339893

4

-0.778793

As we can see sometimes the Ridge coefficients are larger than the baseline ones and viceversa, however they are all relatively close to each other, lying close to x = y. Meanwhile, the l2 norm for the baseline model is 0.95, while for the Ridge model it is 0.80, indicating that the Ridge coefficients are closer among each other, as expected as that is the point behind the correction.

As we saw last week, it is also recommend to plot the CV scores. Although the grid search may report a best value for the parameter corresponding to the maximum CV score (e.g. min CV MSE), if the curve is relatively flat around the minimum, we may prefer the simpler model.

Recall from last week that we can access the cross-validated scores (along with other results for each split) in the attribute cv_results_.

```
[35]: cv_results = pd.DataFrame(gs.cv_results_)
      cv_results.head()
[35]:
         mean_fit_time
                         std_fit_time
                                        mean_score_time
                                                          std_score_time
      0
              0.003351
                             0.000333
                                                0.001473
                                                                0.000074
      1
              0.003003
                             0.000150
                                               0.001348
                                                                0.000024
      2
              0.002902
                             0.000046
                                               0.001338
                                                                0.000031
      3
              0.003818
                             0.001588
                                               0.001371
                                                                0.000065
      4
              0.002897
                             0.000019
                                                0.001309
                                                                0.000012
         param_ridge__alpha
                                                               params
      0
                         0.0
                                                {'ridge_alpha': 0.0}
      1
                         0.1
                                                {'ridge__alpha': 0.1}
      2
                         0.2
                                                {'ridge__alpha': 0.2}
                               {'ridge_alpha': 0.30000000000000004}
      3
                         0.3
      4
                         0.4
                                                {'ridge__alpha': 0.4}
         split0_test_score
                             split1_test_score
                                                  split2_test_score
                                                                      split3_test_score
      0
                  -0.933523
                                      -0.684212
                                                          -0.732690
                                                                               -0.424796
      1
                  -0.934023
                                      -0.685383
                                                          -0.733913
                                                                               -0.422857
      2
                  -0.934523
                                      -0.686515
                                                          -0.735152
                                                                               -0.420989
      3
                  -0.935022
                                      -0.687609
                                                          -0.736407
                                                                               -0.419188
      4
                  -0.935519
                                      -0.688668
                                                          -0.737675
                                                                               -0.417453
         split4_test_score
                             mean_test_score
                                               std_test_score
                                                                rank_test_score
      0
                  -0.789296
                                    -0.712903
                                                      0.166571
                                                                             134
      1
                  -0.786632
                                    -0.712561
                                                      0.167126
                                                                             130
      2
                  -0.783993
                                    -0.712234
                                                      0.167674
                                                                             126
      3
                  -0.781380
                                    -0.711921
                                                      0.168215
                                                                             123
```

0.168750

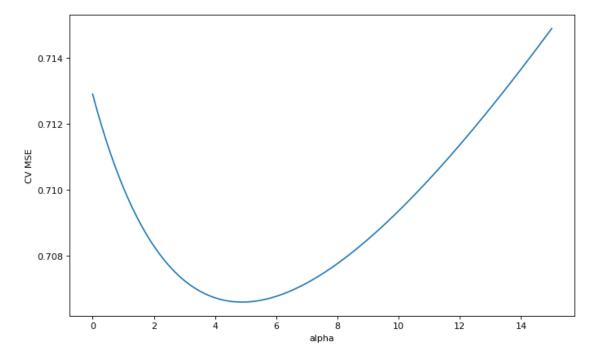
119

-0.711622

In particular, let's examining the mean_test_score and the split#_test_score keys since these are used to determine the optimal α .

In the code below we extract these data into a data frame by selecting our columns of interest along with the α values used (and transform negative MSE values into positive values).

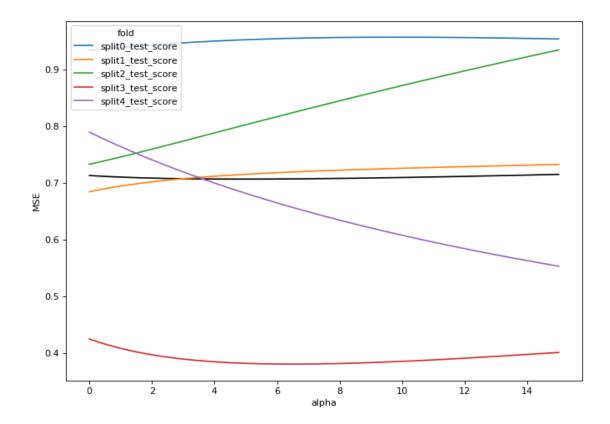
```
[37]: # Plot CV MSE
plt.figure(figsize=(10,6))
ax = sns.lineplot(x='alpha', y='mean_test_score', data=cv_mse)
ax.set_ylabel('CV MSE')
plt.show()
```



This plot shows that the value of $\alpha=4.9$ corresponds to the minimum of this curve. However, this plot gives us an overly confident view of this particular value of α . Specifically, if instead of just plotting the mean MSE across all of the validation sets, we also examine the MSE for each fold individually and the corresponding optimal value of α , we see that there is a lot of noise in the MSE and we should take the value $\alpha=4.9$ with a grain of salt.

5.2.2 Exercise 9 (CORE)

Run the code below to plot the MSE for each validation set in the 5-fold cross validation. Why do you think that our cross validation results are unstable?



Unstability occurs due to several factors, in particular the small dataset size and potential class imbalance.

Note: Due to the importance of tuning the value of α in ridge regression, sklearn provides a function called RidgeCV which combines Ridge with GridSearchCV. However, we will avoid using this function for two reasons:

- it does not allow us to account for additional steps in our pipeline such as standardization when carrying out cross validation, resulting in data leakage
- it only allows storing all results of the cross-validation in the attribute .cv_results_ in the case of the default leave-one-out cross validation, with option store_cv_results=True. So, if you want to access all results and use a cross-validation strategy other than leave-one-out, you will need to use GridSearchCV.

6 Lasso Regression

We saw that ridge regression with a wise choice of α can outperform our baseline linear regression. We can now investigate if lasso can yield a more accurate or interpretable solution. Recall that lasso uses an ℓ_1 penalty on the coefficients, as opposed to the ℓ_2 penalty of ridge.

The Lasso model is also provided by the linear_model submodule and similarly requires the choice of the tuning parameter alpha to determine the weight of the ℓ_1 penalty.

Try running the code below with different values of α to see how it effects sparsity in the coefficients

and model performance.

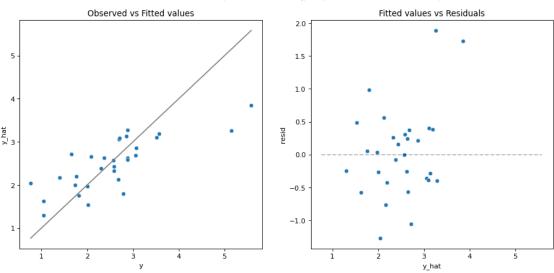
```
[39]: from sklearn.linear_model import Lasso

# Selected alpha value
alpha_val = 0.15

# Lasso pipeline
1 = make_pipeline(
    StandardScaler(),
    Lasso(alpha = alpha_val)
).fit(X_train, y_train)

model_fit(1, X_test, y_test, plot = True)
```





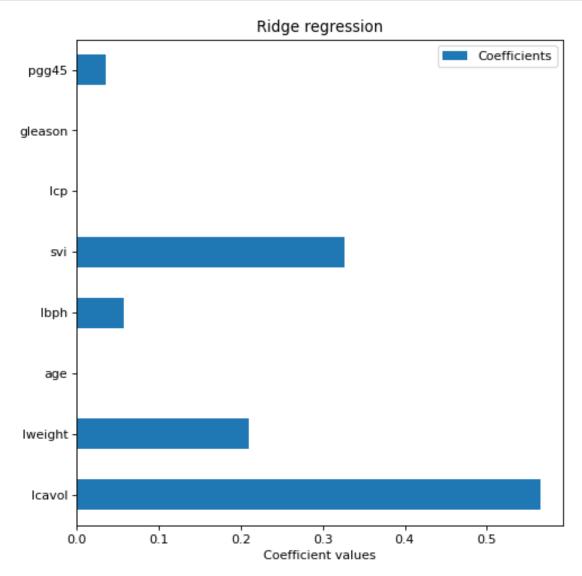
[39]: (0.4564332868640818, 0.6755984657058376, 0.565153902009766)

```
[40]: # Create dataframe with coefficients, and unstandardize the binary coeffcients
lcoefs = np.copy(l[-1].coef_)
lcoefs[[4,6]] = lcoefs[[4,6]]/l[0].scale_[[4,6]]

lcoefs_ = pd.DataFrame(
    lcoefs,
    columns=["Coefficients"],
    index=r.feature_names_in_,
)

# Plot of the coefficients
```

```
lcoefs_.plot.barh(figsize=(9, 7))
plt.title("Ridge regression")
plt.axvline(x=0, color=".5")
plt.xlabel("Coefficient values")
plt.subplots_adjust(left=0.3)
plt.show()
```

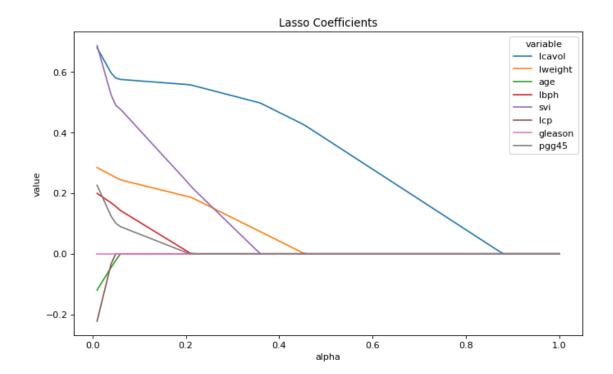


6.0.1 Exercise 10 (CORE)

- a) Plot the solution path of the coefficients as a function of α .
- b) How does this differ between the solution path for Ridge for large α ? for small α ?
- c) Which variable seems to be the most important for predicting lpsa?

Note that $\alpha=0$ causes a warning due to the fitting method (coordinate descent) not converging well without regularization (the ℓ_1 penalty here). So, the grid of α values needs to start at some small positive constant.

```
[43]: # Part a: Compute and plot the solution path
      alphas = np.linspace(0.01, 1, num=100) #We need smaller values of alpha in the
       \hookrightarrow qrid
      ws = [] # Store coefficients
      mses_train = [] # Store training mses
      mses_test = [] # Store test mses
      for a in alphas:
          m = make_pipeline(
              StandardScaler(),
              Lasso(alpha=a)
          ).fit(X_train, y_train)
          w_temp = np.copy(m[1].coef_)
          w_{temp}[[4,6]] = w_{temp}[[4,6]]/m[0].scale_[[4,6]]
          ws.append(w_temp)
          mses_train.append(mean_squared_error(y_train, m.predict(X_train)))
          mses_test.append(mean_squared_error(y_test, m.predict(X_test)))
      # Create a data frame for plotting
      sol_path = pd.DataFrame(
          data = ws,
          columns = X_train.columns # Label columns w/ feature names
      ).assign(
          alpha = alphas,
      ).melt(
          id_vars = ('alpha')
      )
      # Plot solution path of the weights
      plt.figure(figsize=(10,6))
      ax = sns.lineplot(x='alpha', y='value', hue='variable', data=sol_path)
      ax.set_title("Lasso Coefficients")
      plt.show()
```



This differs significantly from the solution path from Ridge as the coefficients converge to zero much faster than in the Ridge case. In fact all coefficients converge to zero before the value of alpha hits 1. We again note that the most significant predictors are leavel, svi and lweight, with leavel being the most significant in the Lasso case.

6.1 Tuning the Lasso penalty parameter

Again, we can use the GridSearchCV function to tune our Lasso model and optimize the α hyperparameter (or use LassoCV, which combines Lasso and GridSearchCV but we will focus on the former).

6.1.1 Exercise 11 (CORE)

- a) Use GridSearchCV to find the optimal value of α .
- b) Plot the CV MSE and MSE for each fold. Comment on the stability and uncertainty of α across the different folds.
- c) Which variables are included with this optimal value of α ?

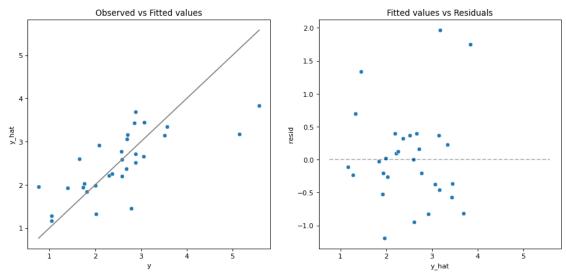
```
[45]: # Part a: optimal alpha

# Grid of tuning parameters
alphas = np.linspace(0.01, 1, num=100)

#Pipeline
```

```
m = make_pipeline(
              StandardScaler(),
              Lasso())
      # To get the parameter name for grid search
      # m.get_params()
      # CV strategy
      cv = KFold(5, shuffle=True, random_state=1234)
      # Grid search
      gs = GridSearchCV(m,
          param_grid={'lasso__alpha': alphas},
          cv=cv,
          scoring="neg_mean_squared_error")
      gs.fit(X_train, y_train)
[45]: GridSearchCV(cv=KFold(n_splits=5, random_state=1234, shuffle=True),
                   estimator=Pipeline(steps=[('standardscaler', StandardScaler()),
                                             ('lasso', Lasso())]),
                   param_grid={'lasso__alpha': array([0.01, 0.02, 0.03, 0.04, 0.05,
      0.06, 0.07, 0.08, 0.09, 0.1, 0.11,
             0.12, 0.13, 0.14, 0.15, 0.16, 0.17, 0.18, 0.19, 0.2, 0.21, 0.22,
             0.23, 0.24, 0.25, 0.26, 0.27, 0.28, 0.29, 0.3, 0.31, 0.32, 0.33,
             0.34, 0...6, 0.37, 0.38, 0.39, 0.4, 0.41, 0.42, 0.43, 0.44,
             0.45, 0.46, 0.47, 0.48, 0.49, 0.5, 0.51, 0.52, 0.53, 0.54, 0.55,
             0.56, 0.57, 0.58, 0.59, 0.6, 0.61, 0.62, 0.63, 0.64, 0.65, 0.66,
            0.67, 0.68, 0.69, 0.7, 0.71, 0.72, 0.73, 0.74, 0.75, 0.76, 0.77,
             0.78, 0.79, 0.8, 0.81, 0.82, 0.83, 0.84, 0.85, 0.86, 0.87, 0.88,
            0.89, 0.9, 0.91, 0.92, 0.93, 0.94, 0.95, 0.96, 0.97, 0.98, 0.99,
             1. ])},
                   scoring='neg_mean_squared_error')
[46]: print(gs.best params)
      print(-gs.best_score_)
     {'lasso__alpha': 0.01}
     0.7200836927253956
[47]: model_fit(gs.best_estimator_, X_test, y_test, plot=True)
```

Model (MSE, RMSE, Rsq) = (0.4987, 0.7062, 0.5249)



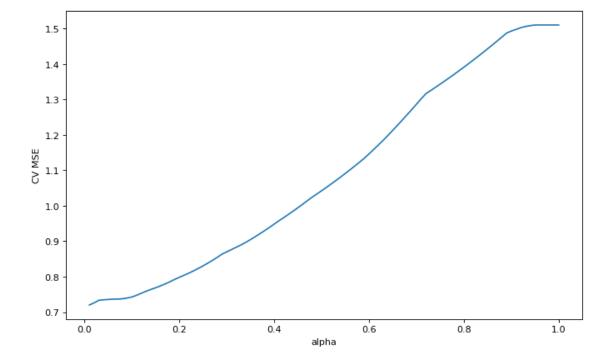
[47]: (0.49871501409473484, 0.7061975744044544, 0.5248719054252093)

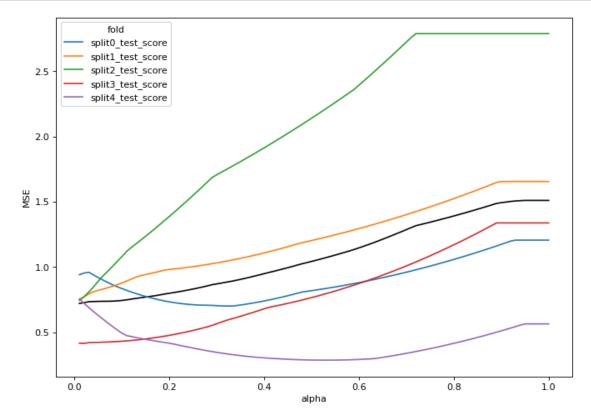
```
[48]: cv_results = pd.DataFrame(gs.cv_results_)
      cv_results.head()
[48]:
         mean_fit_time
                        std_fit_time
                                      mean_score_time
                                                        std_score_time
      0
              0.003688
                            0.000692
                                              0.001650
                                                               0.000227
                                              0.001371
      1
              0.003089
                            0.000174
                                                               0.000048
      2
                            0.000224
              0.003064
                                              0.001415
                                                               0.000026
      3
                            0.000119
              0.003031
                                              0.001381
                                                               0.000042
      4
              0.002938
                             0.000081
                                              0.001400
                                                               0.000069
         param_lasso__alpha
                                                      split0_test_score
                                              params
      0
                       0.01
                             {'lasso_alpha': 0.01}
                                                               -0.940161
      1
                       0.02 {'lasso_alpha': 0.02}
                                                               -0.953103
      2
                       0.03
                             {'lasso_alpha': 0.03}
                                                               -0.958974
      3
                       0.04 {'lasso_alpha': 0.04}
                                                               -0.937995
      4
                       0.05 {'lasso_alpha': 0.05}
                                                               -0.917877
         split1_test_score
                            split2_test_score
                                                split3_test_score
                                                                    split4_test_score
      0
                 -0.740926
                                     -0.749231
                                                         -0.415599
                                                                            -0.754501
                 -0.770968
                                     -0.772592
                                                        -0.413556
                                                                            -0.720210
      1
      2
                 -0.793434
                                     -0.808020
                                                        -0.419270
                                                                            -0.687614
      3
                 -0.810282
                                     -0.847646
                                                        -0.420746
                                                                            -0.656808
      4
                 -0.820705
                                     -0.891464
                                                        -0.420835
                                                                            -0.627757
         mean_test_score
                          std_test_score rank_test_score
      0
               -0.720084
                                 0.169478
```

```
2
1
         -0.726086
                           0.175171
2
         -0.733463
                           0.179349
                                                     3
3
                           0.181346
                                                     4
         -0.734695
                                                     5
4
         -0.735728
                           0.187333
```

```
[51]: # Part b: plot the CV MSE and MSE for each fold as a function of alpha
# Plot CV MSE

plt.figure(figsize=(10,6))
ax = sns.lineplot(x='alpha', y='mean_test_score', data=cv_mse)
ax.set_ylabel('CV MSE')
plt.show()
```





Note that CV MSE is increasing with alpha, while the MSEs for each fold are again unstable for the reasons previously mentioned. Additionally, MSE for each CV is in general increasing for increasing alpha.

```
[54]:
                  Coefficients
                      2.452345
      intercept
      lcavol
                      0.680148
      lweight
                      0.284639
      age
                     -0.120078
      1bph
                      0.199373
      svi
                      0.286585
                     -0.222663
      lcp
                     -0.00000
      gleason
                      0.226124
      pgg45
```

Included variables: lcavol, lweight, age, lbph, svi, lcp, pgg45

6.1.2 Exercise 12 (CORE)

Run the following code to compute the CV MSE for the linear model and compare with the CV MSE of the lasso model to suggest an optimal value of α .

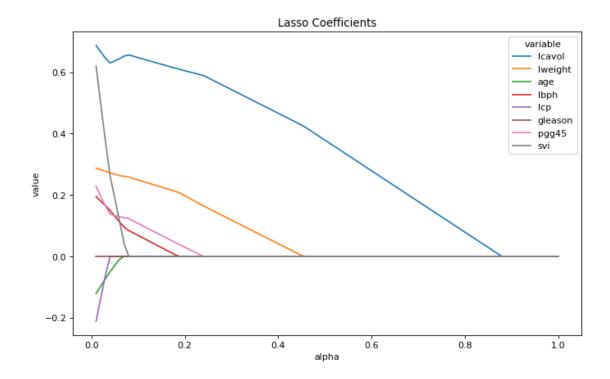
```
[56]: print('CV MSE for baseline linear model', round(gs_l.best_score_ * -1,4))
```

CV MSE for baseline linear model 0.7129

The CV MSE of the lasso model was 0.72 for a value of a lasso alpha = 0.01 (versus the CV MSE for the baseline linear model of 0.7129). This indicates that unlike Ridge regression, Lasso regression may be unable to provide us with a better model compared to the baseline.

6.1.3 Exercise 13 (EXTRA)

In the following code, use ColumnTransfomer to apply standarization to all variables except the binary variable svi. How does the affect the lasso solution path and the importance of svi relative to the other variables?



7 ElasticNet Regression

Lastly, we can use elastic net regression, which is hybrid between lasso and ridge, including both an ℓ_1 and ℓ_2 penalty. The ElasticNet model is again provided by the linear_model submodule and minimizes the objective:

$$\frac{1}{2N}||\mathbf{y}-\mathbf{X}\mathbf{w}||_2^2 + \alpha\rho||\mathbf{w}||_1 + 0.5\alpha(1-\rho)||\mathbf{w}||_2^2.$$

In this parameterization, ρ determines relative strength of the ℓ_1 penalty compared to the ℓ_2 and is referred to as l1_ratio in ElasticNet. Thus, we can also fit ridge and lasso regression models with ElasticNet through appropriate choice of l1_ratio: - ridge corresponds to l1_ratio=0 - lasso corresponds to l1_ratio=1

The parameter α is referred to as alpha in ElasticNet and controls the overall penalty relative the residual sum of squares.

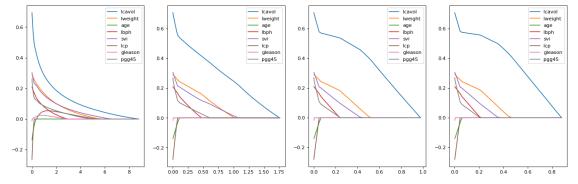
The general ElasticNet requires tuning of both alpha and 11_ratio.

The following code plots the solution path for different choices of 11_ratio using the .path() method of ElasticNet. Notice how the solution paths resemble ridge and lasso for small and large values of 11_ratio respectively.

In this case, .path() by default automatically selects a range of alpha values, except for the case when l1_ratio = 0, i.e. ridge regression. For ridge, you need to supply your own grid of alpha values through the option path(...,alphas=myalphas).

```
[59]: from sklearn.linear_model import ElasticNet

Xs = StandardScaler().fit_transform(X_train)
    l1r = [.1, .5, .9, 1]
    fig, ax = plt.subplots(1,4,figsize= (20,6))
    for i, l in enumerate(l1r):
        sol_path = ElasticNet.path(Xs, y_train, l1_ratio=l)
        d = pd.DataFrame( data = sol_path[1].T, columns = X_train.columns, index = sol_path[0])
        d.plot(ax=ax[i])
```



Again, we can use GridSearchCV (or ElasticNetCV) to tune the parameters. In the following code, we use GridSearchCV to tune both alpha and 11_ratio.

```
gs_enet.fit(X_train, y_train)
gs_enet.best_params_

[60]: {'elasticnet__alpha': 0.01, 'elasticnet__l1_ratio': 0.01}
```

```
[61]: print('CV MSE for elasticnet model', round(-gs_enet.best_score_,4))
print('CV MSE for ridge model',round(-gs.best_score_,4))
```

```
CV MSE for elasticnet model 0.7113
CV MSE for ridge model 0.7201
```

7.0.1 Exercise 15 (EXTRA)

Comment on the optimal values of ElasticNet compared with our basineline, ridge, and lasso models. How does the performance of the models compare on the test data?

[]:

8 Competing the Worksheet

At this point you have hopefully been able to complete all the CORE exercises and attempted the EXTRA ones. Now is a good time to check the reproducibility of this document by restarting the notebook's kernel and rerunning all cells in order.

Before generating the PDF, please go to Edit -> Edit Notebook Metadata and change 'Student 1' and 'Student 2' in the **name** attribute to include your name. If you are unable to edit the Notebook Metadata, please add a Markdown cell at the top of the notebook with your name(s).

Once that is done and you are happy with everything, you can then run the following cell to generate your PDF. Once generated, please submit this PDF on Learn page by 16:00 PM on the Friday of the week the workshop was given.

```
[]: !jupyter nbconvert --to pdf mlp_week05.ipynb
```