MLPy Workshop 5

Student 1, Student 2

February 14, 2025

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.

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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).

[4]:
```
# Data libraries
import pandas as pd
```

```
import numpy as np
import matplotlib.pyplot as plt

# Plotting libraries
import matplotlib.pyplot as pltj
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.

[5]:
```
def get_coefs(m):
    """Returns the model coefficients from a Scikit-learn model object as an␣
 ↪array,
    includes the intercept if available.
    """

    # If pipeline, use the last step as the model
    if (isinstance(m, sklearn.pipeline.Pipeline)):
        m = m.steps[-1][1]


    if m.intercept_ is None:
        return m.coef_

    return np.concatenate([[m.intercept_], m.coef_])
```

[6]:
```
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.
↪DataFrame(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␣
↪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
- `lbph` - 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.

[7]:
```
prostate = pd.read_csv('prostate.csv')
prostate.head()
```

[7]:

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

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?

[8]:
```
# Part a
prostate.info()
prostate.describe()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 97 entries, 0 to 96
Data columns (total 10 columns):
 #   Column   Non-Null Count  Dtype
---  ------   --------------  -----
 0   lcavol   97 non-null     float64
```

```
 1   lweight  97 non-null     float64
 2   age      97 non-null     int64
 3   lbph     97 non-null     float64
 4   svi      97 non-null     int64
 5   lcp      97 non-null     float64
 6   gleason  97 non-null     int64
 7   pgg45    97 non-null     int64
 8   lpsa     97 non-null     float64
 9   train    97 non-null     object
dtypes: float64(5), int64(4), object(1)
memory usage: 7.7+ KB
```

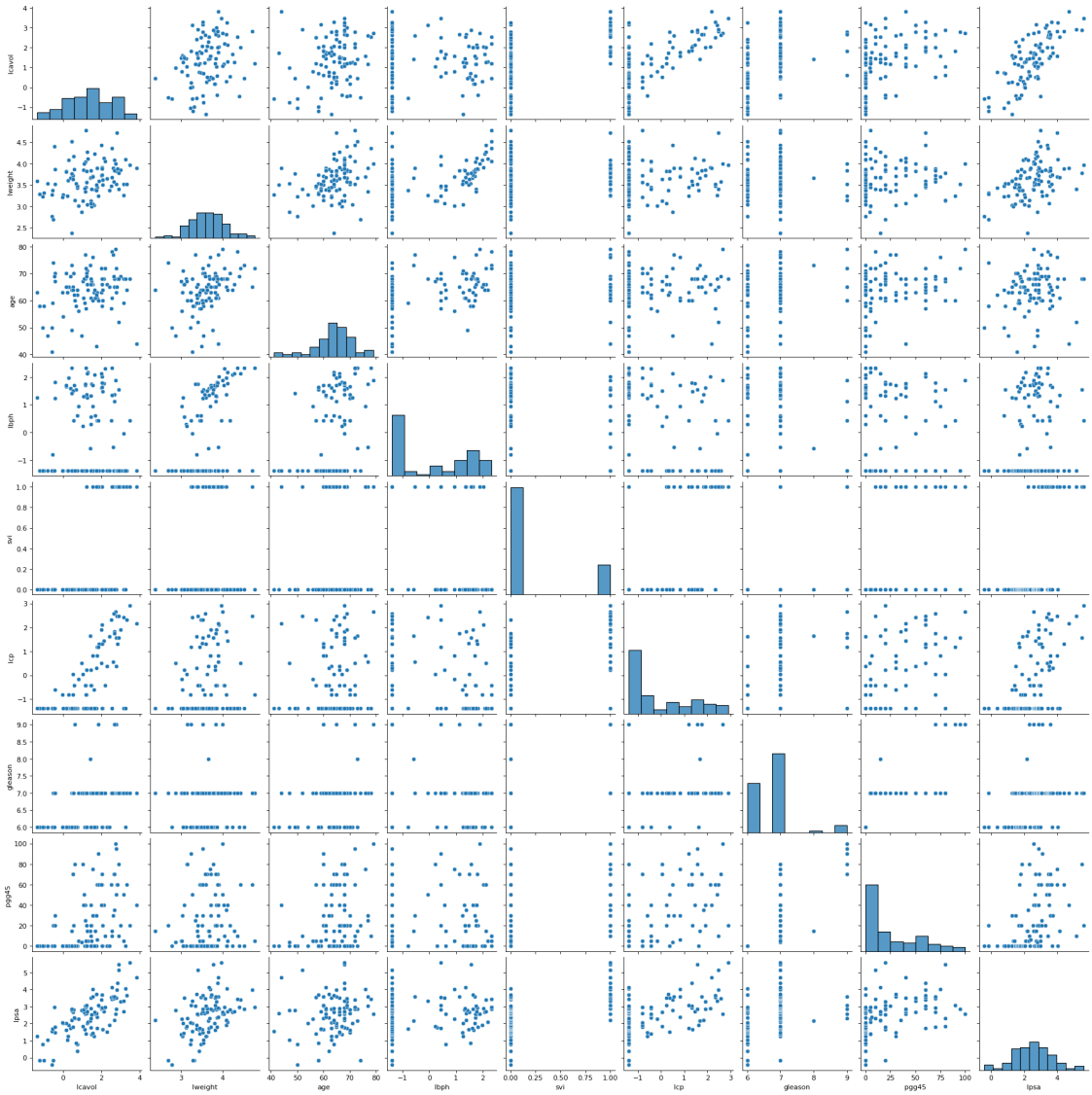
[8]:

	lcavol	lweight	age	lbph	svi	lcp
count	97.000000	97.000000	97.000000	97.000000	97.000000	97.000000
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
min	-1.347074	2.374906	41.000000	-1.386294	0.000000	-1.386294
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%	2.127041	3.876396	68.000000	1.558145	0.000000	1.178655
max	3.821004	4.780383	79.000000	2.326302	1.000000	2.904165

	gleason	pgg45	lpsa
count	97.000000	97.000000	97.000000
mean	6.752577	24.381443	2.478387
std	0.722134	28.204035	1.154329
min	6.000000	0.000000	-0.430783
25%	6.000000	0.000000	1.731656
50%	7.000000	15.000000	2.591516
75%	7.000000	40.000000	3.056357
max	9.000000	100.000000	5.582932

[9]:
```
# Part b
# pair plot prostate
sns.pairplot(prostate)
```

[9]:
```
<seaborn.axisgrid.PairGrid at 0x14455e750>
```



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`.

[10]:
```
# Create train and test data frames
train = prostate.query("train == 'T'").drop('train', axis=1)
test = prostate.query("train == 'F'").drop('train', axis=1)
```

[11]:
```
# 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,)
```

[12]:
```
# 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

[13]:
```
# 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.

[14]:
```
# 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.

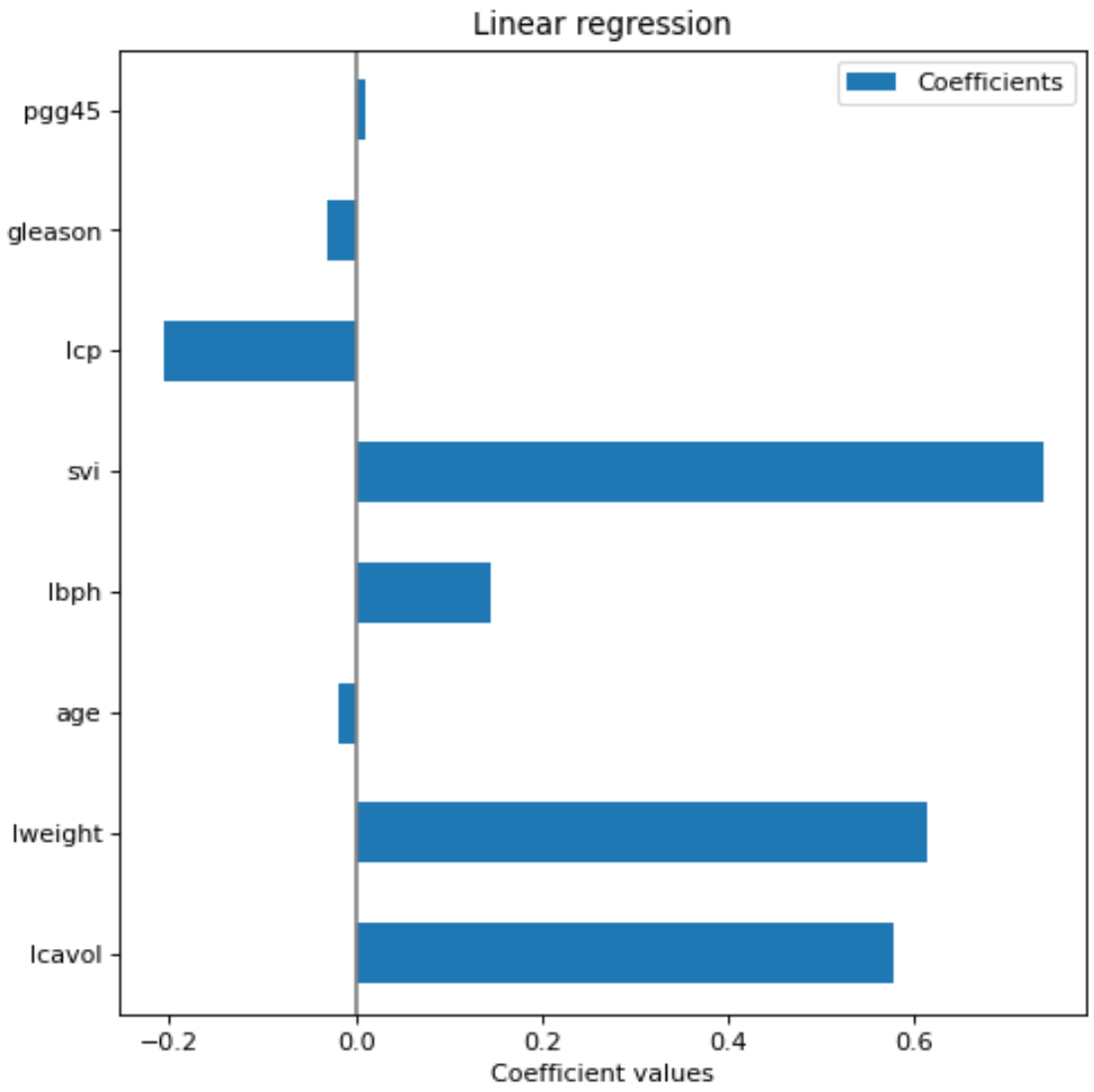
[15]:
```
# Create a data frame of the coeffcients
fe_names = lm.feature_names_in_

coefs = pd.DataFrame(
    np.copy(lm.coef_),
    columns=["Coefficients"],
    index=fe_names,
)

coefs

# To add intercept
# fe_names = np.append(['intercept'],lm.feature_names_in_)
```

```
# coefs = pd.DataFrame(
#     get_coefs(lm),
#     columns=["Coefficients"],
#     index=fe_names,
# )
```

[15]:

	Coefficients
lcavol	0.576543
lweight	0.614020
age	-0.019001
lbph	0.144848
svi	0.737209
lcp	-0.206324
gleason	-0.029503
pgg45	0.009465

[16]:
```
# 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)
```



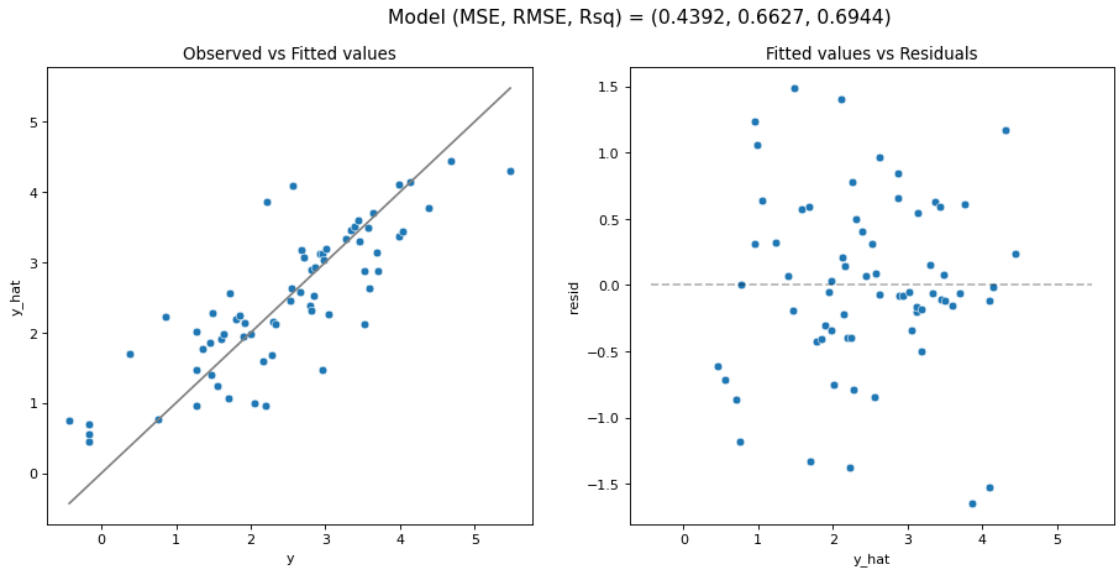
These coefficients have the typical regression interpretation, e.g. for each unit increase in `lcavol` we expect `lpsa` to increase by 0.5765 on average. To evaluate the predictive properities of our model, we will use the `model_fit` helper function.

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?

[17]:
```
model_fit(lm, X_train, y_train, plot=True)
```



[17]:
```
(0.4391997680583344, 0.6627214860394481, 0.6943711796768237)
```

The observed vs. fitted values showcase a good correlation. Additionally, their residuals are well spaced following the principal of homoscadasticity.

We would expect the test dataset to have a similar fit and correlation to the train dataset.

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 standaridize 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.

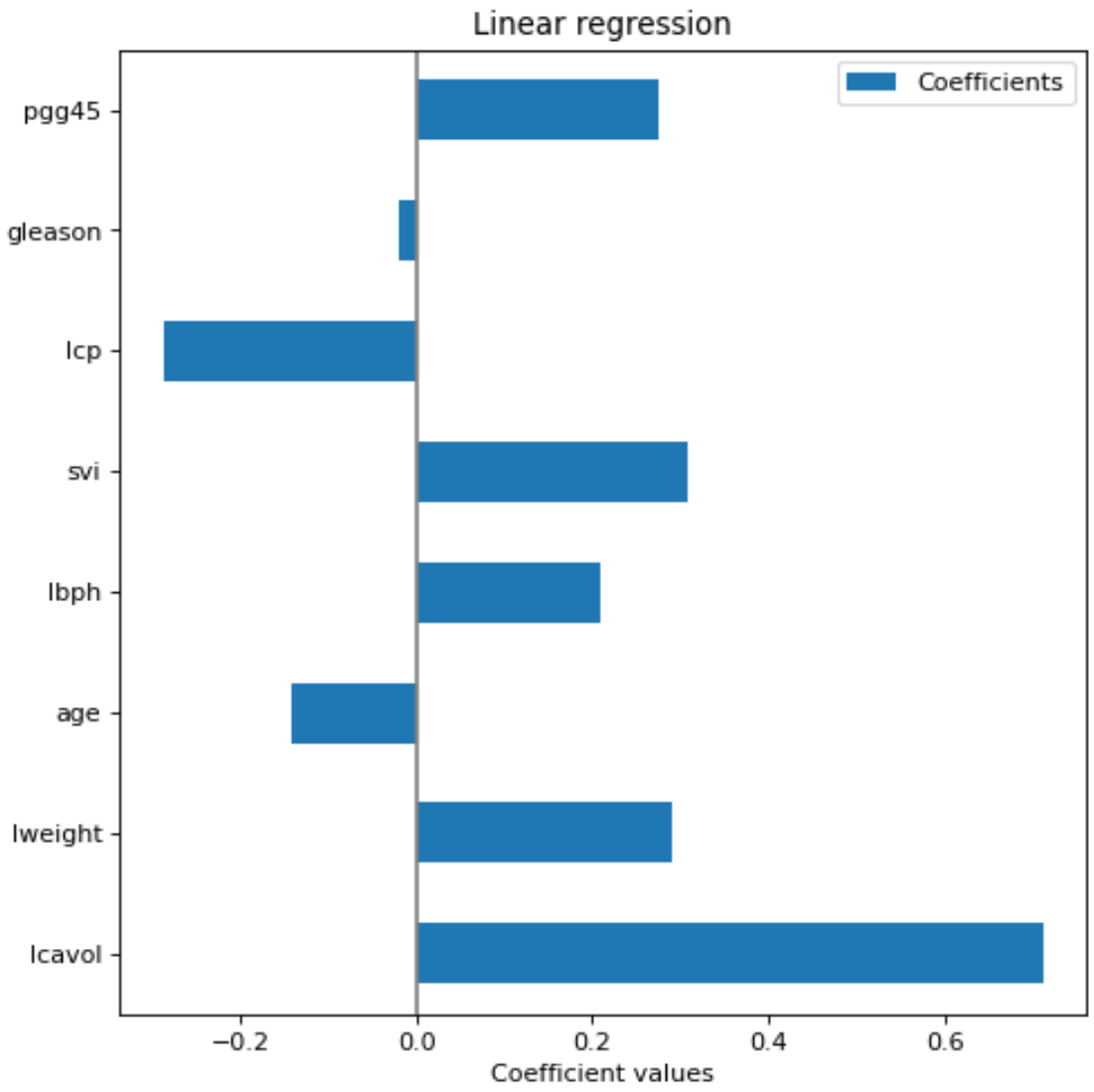
Keep in mind, that in order to get a realistic idea of the performance of model on the test data, **the mean and standard deviation used to standardize both the training and test sets should be computed from the training data only**. The best way to accomplish this is to include the StandardScaler in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

[18]:
```
# Linear regression pipeline, including standardization
from sklearn.preprocessing import StandardScaler

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

lm_s.fit(X_train, y_train)
fe_names = lm_s.feature_names_in_

coefs = pd.DataFrame(
    np.copy(lm_s.named_steps['linearregression'].coef_),
    columns=["Coefficients"],
    index=fe_names,
)

print(coefs)
# 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)
```

```
         Coefficients
lcavol       0.711041
lweight      0.290450
age         -0.141482
lbph         0.210420
svi          0.307300
lcp         -0.286841
gleason     -0.020757
pgg45        0.275268
```



After standardisation, we observe that `lcavol` has a greater correlation compared to other parameters.

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]:
```
# Extract and print the mean and std used in StandardScaler
ss = StandardScaler().fit(X_train)

ss_p = pd.DataFrame(
    np.c_[np.round(ss.mean_,4), np.round(ss.scale_,4)],
    columns=["Mean", "SD"],
    index=fe_names,
)
ss_p
```

[19]:

	Mean	SD
lcavol	1.3135	1.2333
lweight	3.6261	0.4730
age	64.7463	7.4460
lbph	0.0714	1.4527
svi	0.2239	0.4168
lcp	-0.2142	1.3902
gleason	6.7313	0.7036
pgg45	26.2687	29.0823

[20]:
```
print('After standardizing, the orginal value of 0 for svi is replaced with',np.
  ↪round(-ss.mean_[4]/ss.scale_[4],4) )
print('After standardizing, the orginal value of 1 for svi is replaced with',np.
  ↪round((1-ss.mean_[4])/ss.scale_[4],4) )
```

```
After standardizing, the orginal value of 0 for svi is replaced with -0.5371
After standardizing, the orginal 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 coeffcients when training with standardized features, we have that:

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

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:

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

Thus,

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

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]:
```
# unstandardized coeffs are obtained by dividing the estimated coeffs by the␣
 ↪standard deviations
# now we unstandardize the coefficients

coefs_unstd = pd.DataFrame(
    np.copy(lm_s.named_steps['linearregression'].coef_ / ss_p['SD']),
    columns=["Coefficients"],
    index=fe_names,
)

# create df of mean and SD of unstandardized coefs


print(coefs_unstd)
```

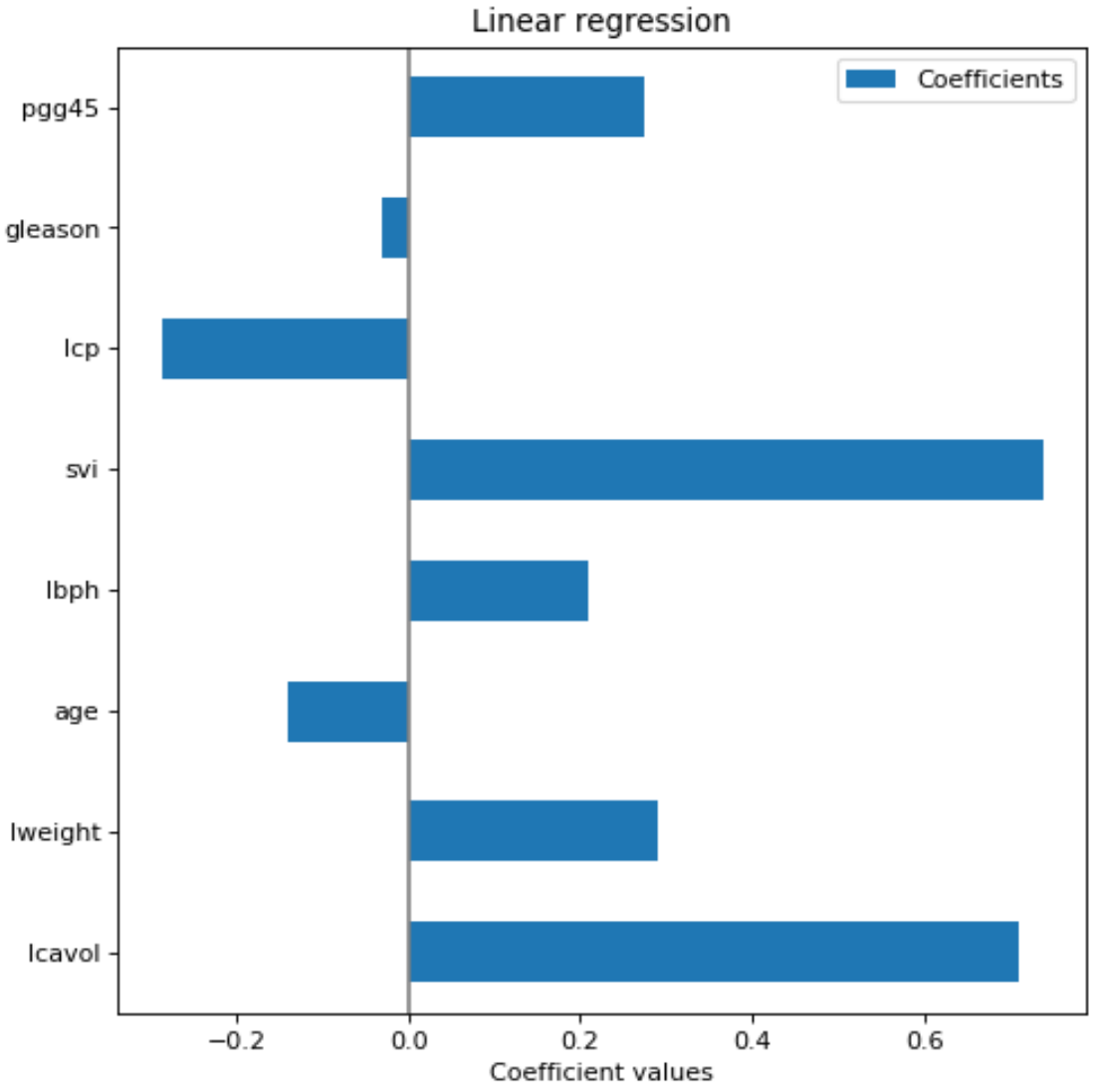
```
         Coefficients
lcavol       0.576535
lweight      0.614060
age         -0.019001
lbph         0.144847
svi          0.737285
lcp         -0.206331
gleason     -0.029501
pgg45        0.009465
```

The coefficients

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.

[22]:
```
# In our plot, we want to show the coefficients of the categorical features on␣
 ↪the original scale for improved interpretation
coefs = np.copy(lm_s[1].coef_)
coefs[[4,6]] = coefs[[4,6]]/lm_s['standardscaler'].scale_[[4,6]]

coefs = pd.DataFrame(
    coefs,
    columns=["Coefficients"],
    index=lm_s.feature_names_in_,
)
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)
plt.show()
```



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

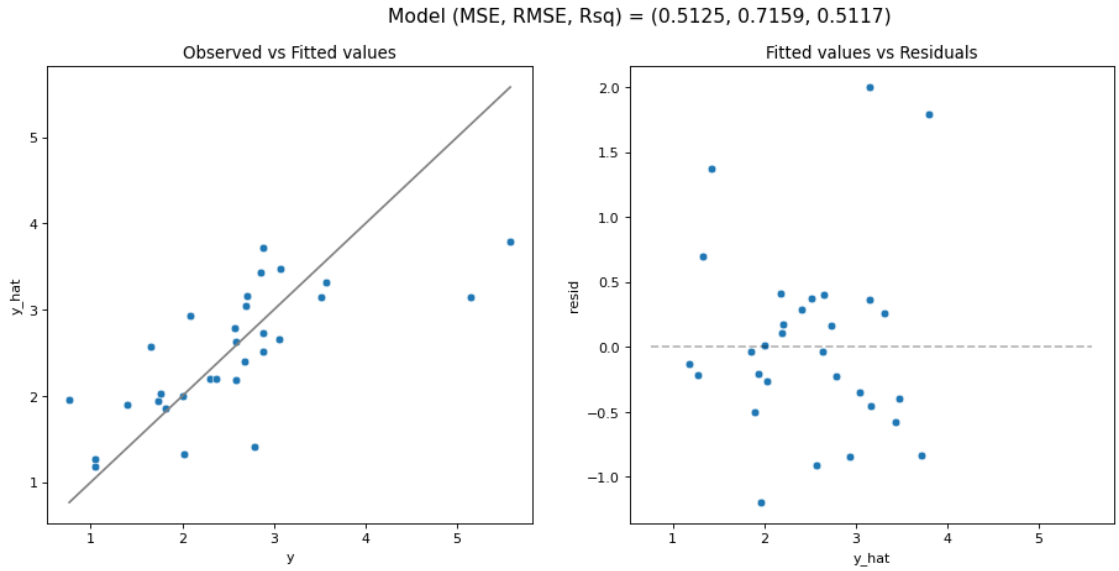
called, such as `.fit()` to fit the model and `.predict()` to make predictions.

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 = 1

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

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



[24]:
```
(0.5125174233583766, 0.715903222061737, 0.5117222864471656)
```

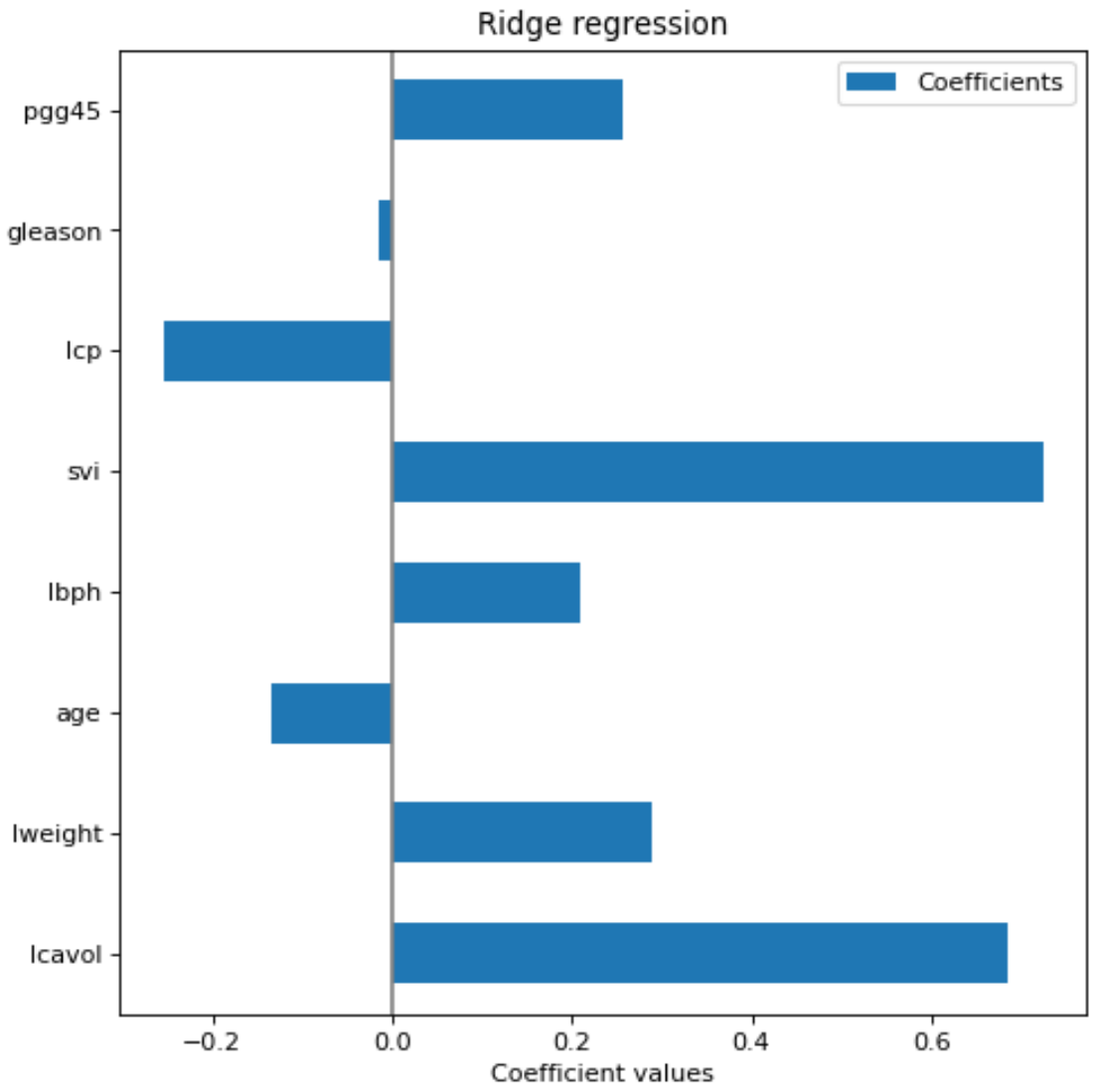
[25]:
```
# Create dataframe with coefficents, and unstandardize the binary coeffcients
rcoefs = np.copy(r[-1].coef_)
rcoefs[[4,6]] = rcoefs[[4,6]]/r[0].scale_[[4,6]]

rcoefs_ = pd.DataFrame(
    rcoefs,
```

```
    columns=["Coefficients"],
    index=r.feature_names_in_,
)

rcoefs_
```

[25]:

	Coefficients
lcavol	0.685410
lweight	0.289595
age	-0.134306
lbph	0.208411
svi	0.723594
lcp	-0.254532
gleason	-0.015993
pgg45	0.255985

[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()
```

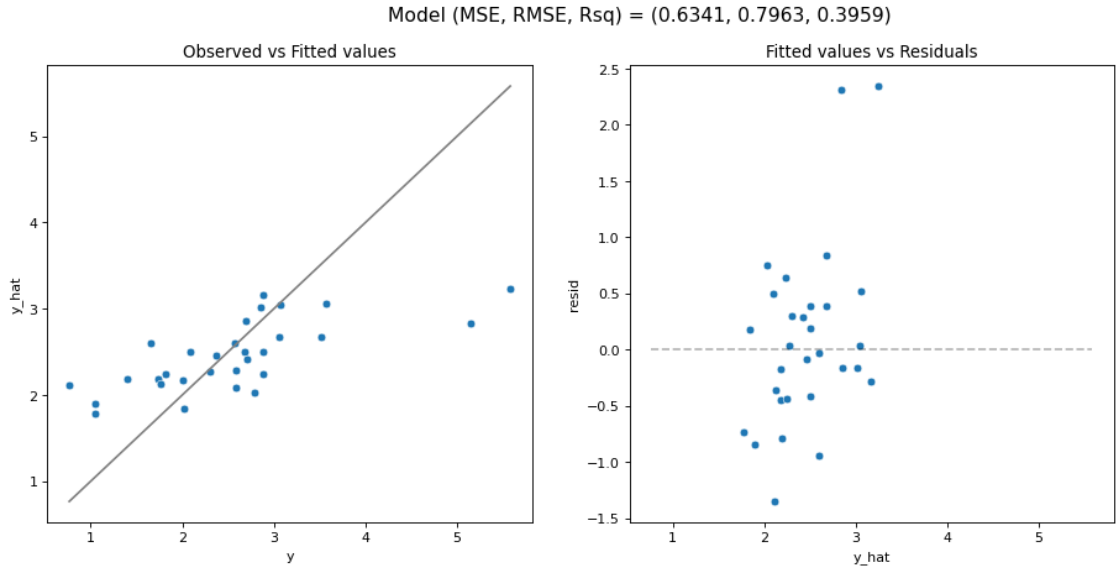


5.0.1 Exercise 5 (CORE)

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?

[32]:
```
# Selected alpha value
alpha_val = 200

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

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



[32]: (0.6341298259955314, 0.7963226896149145, 0.39586158943859795)

increasing `alpha` increases MSE

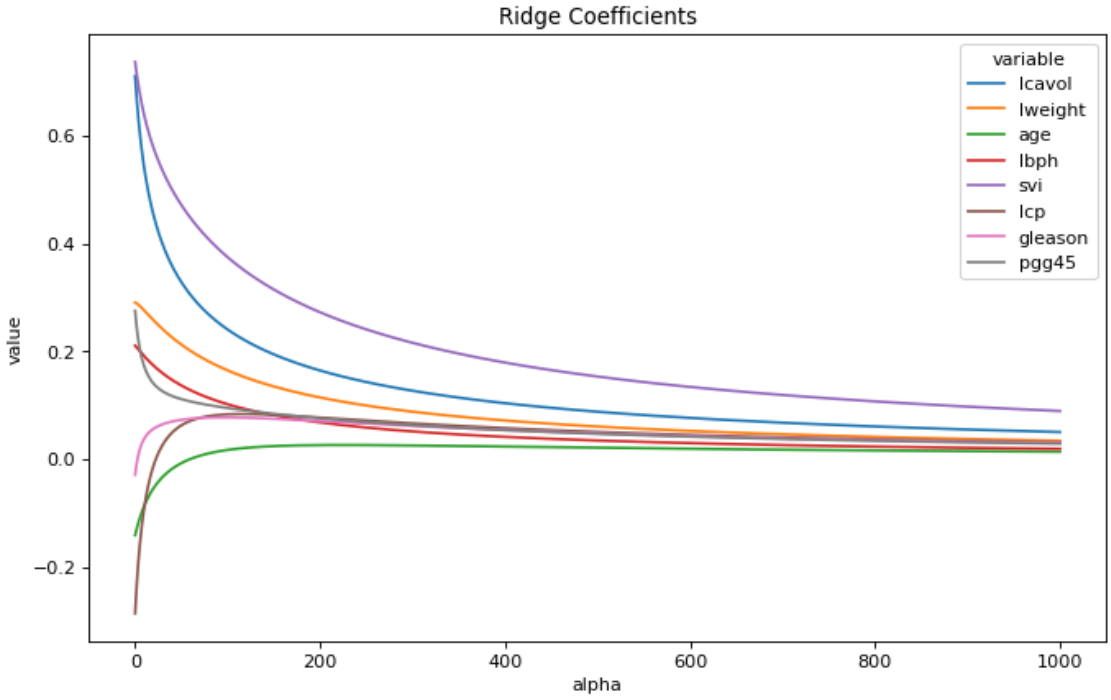
5.1 Solution path: Ridge coeffcients as a function of α

A useful way of examining the behavior of Ridge regression models is to plot the **solution path** of the coefficents $\mathbf{w}$ 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.

[33]:
```
# 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)))
```

[34]:
```
# 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)

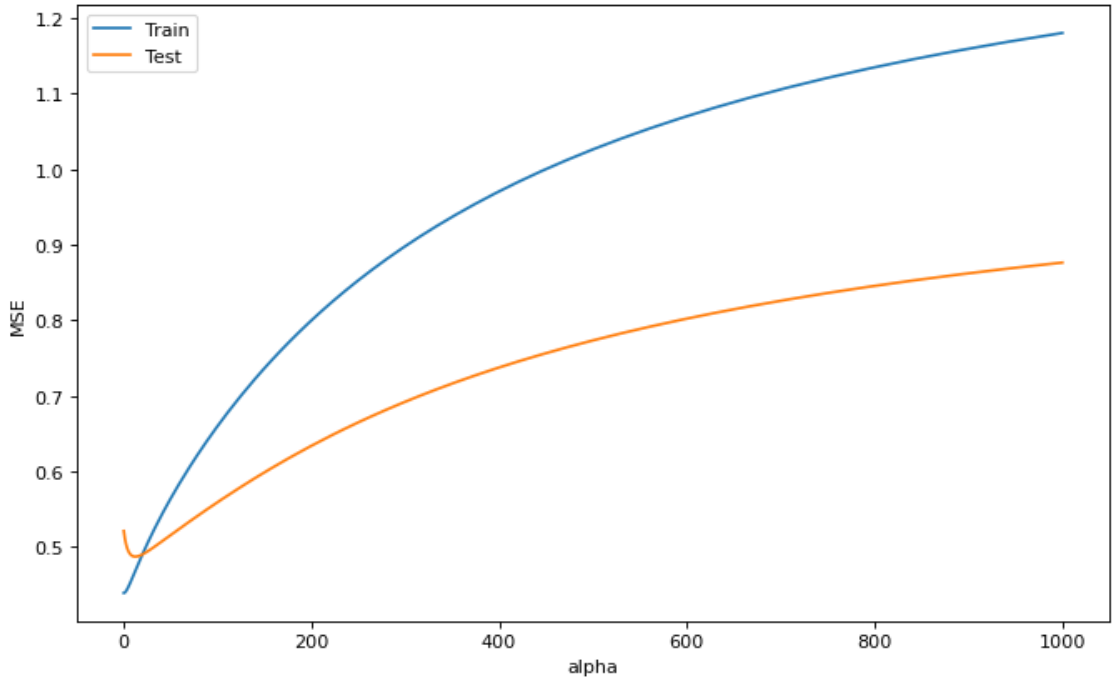
Based on this plot, which variable(s) seem to be the most important for predicting `lpsa`?

LCP and PGG45 have the sharpest drop as `alpha` increases suggesting they are importnat.

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?

[35]:
```
# Path of MSE as function of alpha
mses_path = pd.DataFrame(
    {'alpha': alphas, 'Train': np.asarray(mses_train), 'Test': np.
 ↪asarray(mses_test)}).melt(
    id_vars = ('alpha')
)

# Plot MSE path
plt.figure(figsize=(10,6))
ax = sns.lineplot(x='alpha', y='value', hue='variable', data=mses_path)
ax.set_ylabel("MSE")
# To remove legend title
handles, labels = ax.get_legend_handles_labels()
ax.legend(handles=handles[0:], labels=labels[0:])
plt.show()
```



There is an 'ideal' alpha value that minimises MSE for the test dataset.

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`.

[36]:
```
# Grid of tuning parameters
alphas = np.linspace(0, 15, num=151)

#Pipeline
m = make_pipeline(
        StandardScaler(),
        Ridge())
# 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={'ridge__alpha': alphas},
    cv=cv,
    scoring="neg_mean_squared_error")
gs.fit(X_train, y_train)
```

[36]:
```
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. ,  2.1,
        2.2,  2.3,  2.4,  2.5,  2.6,  2.7,  2.8,  2.9,  3. ,  3.1,  3.2,
        3.3,  3.4,  3.5,  3.6,  3.7,  3.8,  3.9,  4. ,  4.1,  4.2,  4…
        7.7,  7.8,  7.9,  8. ,  8.1,  8.2,  8.3,  8.4,  8.5,  8.6,  8.7,
        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 be-

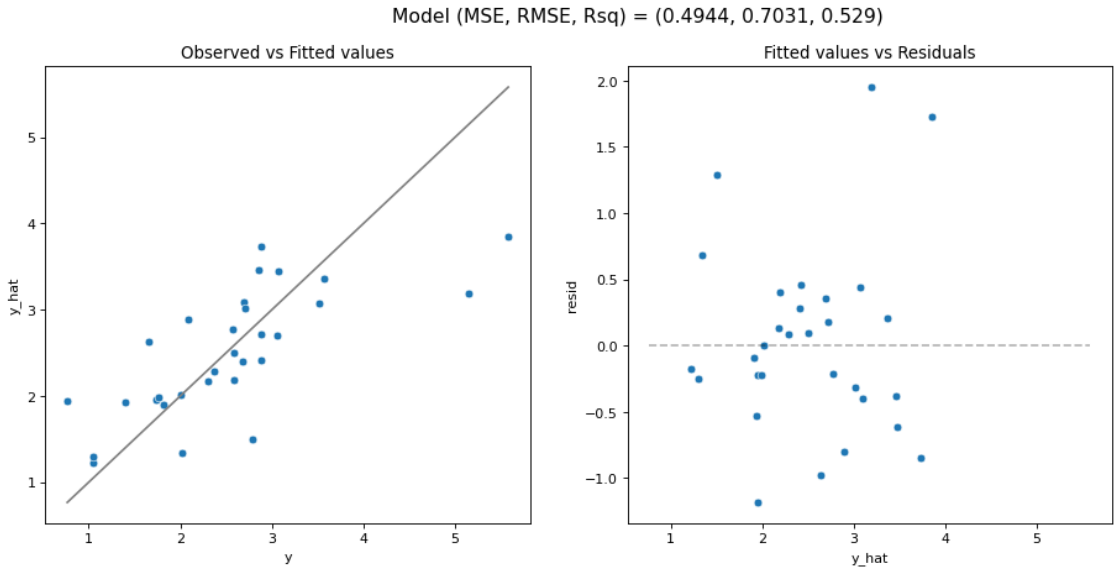
cause, while not obvious, the prostate data is structured (sorted by `lpsa` value) and this way we are able to ensure that the folds are properly shuffled. Failing to do this causes *very* unreliable results from the cross validation process.

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

[37]:
```
print(gs.best_params_)
print(-gs.best_score_)
```

```
{'ridge__alpha': 4.9}
0.7066011634399014
```

[38]:
```
model_fit(gs.best_estimator_, X_test, y_test, plot=True)
```



[38]:
```
(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 coeffcients for both models and comment on the results.

The plot above has a lower MSE compared to our previous models. suggesting that this is a better model.

[ ]:
```
# plot coeffs for the baseline model against coeffs for the ridge model.

# Baseline model
```

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_`.

[ ]:
```
cv_results = pd.DataFrame(gs.cv_results_)
cv_results.head()
```

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).

[39]:
```
# Extract only mean and split scores
cv_mse = pd.DataFrame(
    data = gs.cv_results_
).filter(
    # Extract the split#_test_score and mean_test_score columns
    regex = '(split[0-9]+|mean)_test_score'
).assign(
    # Add the alphas as a column
    alpha = alphas
)

cv_mse.update(
    # Convert negative mses to positive
    -1 * cv_mse.filter(regex = '_test_score')
)
```

[ ]:
```
# 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?

[ ]:
```
# Reshape the data frame for plotting
d = cv_mse.melt(
    id_vars=('alpha','mean_test_score'),
    var_name='fold',
    value_name='MSE'
)

# Plot the validation scores across folds
plt.figure(figsize=(10,7))
sns.lineplot(x='alpha', y='MSE', color='black', errorbar=None, data = d)  #␣
 ↪Plot the mean MSE in black.
sns.lineplot(x='alpha', y='MSE', hue='fold', data = d) # Plot the curves for␣
 ↪each fold in different colors
plt.show()
```

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.

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

# Selected alpha value
alpha_val = 0.15

# Lasso pipeline
```

```
l = make_pipeline(
    StandardScaler(),
    Lasso(alpha = alpha_val)
).fit(X_train, y_train)

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

[ ]:
```
# Create dataframe with coefficents, 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.

[44]:
```
# Part a: Compute and plot the solution path
alphas = np.linspace(0.01, 1, num=100) #We need smaller values of alpha in the␣
 ↪grid
```

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?

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

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

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

[ ]:
```
# Part c: extract the coefficients
```

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.

[49]:
```
# Lasso doesn't allow for alpha=0, so compute CV MSE for linear regression␣
 ↪model to compare with Lasso
gs_l = GridSearchCV(
    make_pipeline(
        StandardScaler(),
        LinearRegression()
    ),
    param_grid = {},
    cv=KFold(5, shuffle=True, random_state=1234),
    scoring="neg_mean_squared_error"
).fit(X_train, y_train)
```

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

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?

[51]:
```
from sklearn.compose import ColumnTransformer
alphas = np.linspace(0.01, 1, num=100)

ws = [] # Store coefficients
mses_train = [] # Store training mses
mses_test = [] # Store test mses

for a in alphas:
    m = make_pipeline(
        ColumnTransformer([
```

```
            ('num',StandardScaler(),[0,1,2,3,5,6,7]), # all variables except svi
            ('binary','passthrough',[4])]), # binary variable
        Lasso(alpha=a)
    ).fit(X_train, y_train)

    ws.append(m[1].coef_)
    mses_train.append(mean_squared_error(y_train, m.predict(X_train)))
    mses_test.append(mean_squared_error(y_test, m.predict(X_test)))
```

[ ]:
```
sol_path = pd.DataFrame(
    data = ws,
    columns = X_train.columns[np.array([0,1,2,3,5,6,7,4])] # Label columns w/␣
 ↪feature names
).assign(
    alpha = alphas,
).melt(
    id_vars = ('alpha')
)

# Plot the 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()
```

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 `l1_ratio`.

The following code plots the solution path for different choices of `l1_ratio` using the `.path()` method of `ElasticNet`. Notice how the solution paths resemble ridge and lasso for small and large values of `l1_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)`.

[ ]:
```
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 `l1_ratio`.

[ ]:
```
from sklearn.linear_model import ElasticNetCV

# Grid of tuning parameters
alphas = np.linspace(0.01, 10, num=50)
l1r = [0.01, .1, .5, .7, .9, .95, 1]

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

# Pipeline
m = make_pipeline(
        StandardScaler(),
        ElasticNet())

# Grid search
gs_enet = GridSearchCV(m,
                       param_grid={'elasticnet__alpha': alphas,␣
 ↪'elasticnet__l1_ratio': l1r},
                       cv = cv,
                       scoring="neg_mean_squared_error")
gs_enet.fit(X_train, y_train)

gs_enet.best_params_
```

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

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
```

```
[NbConvertApp] Converting notebook mlp_week05.ipynb to pdf
```

[ ]: