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Ch6 hw 1, 8, 9 (no f), 11

```
In [ ]: import numpy as np
import pandas as pd
from matplotlib.pyplot import subplots
from statsmodels.api import OLS
import sklearn.model_selection as skm
import sklearn.linear_model as skl
from sklearn.preprocessing import StandardScaler
from ISLP import load_data
from ISLP.models import ModelSpec as MS
from functools import partial

from sklearn.pipeline import Pipeline
from sklearn.decomposition import PCA
from sklearn.cross_decomposition import PLSRegression
from ISLP.models import \
     (Stepwise,
      sklearn_selected,
      sklearn_selection_path)
# !pip install l0bnb
from l0bnb import fit_path # fit_path is a function that fits the l0bnb mode

from sklearn.feature_selection import SequentialFeatureSelector as SFS
```

1

We perform best subset, forward stepwise, and backward stepwise selection on a single data set. For each approach, we obtain p + 1 models, containing 0, 1, 2, . . . , p predictors. Explain your answers:

- a) Which of the three models with k predictors has the smallest training RSS?

The model with k predictors that has the smallest training RSS will be the one that used best subset selection. This is because best subset selection considers all possible models with k predictors and selects the best one. Forward and backward stepwise selection do not consider all possible models with k predictors, so they may miss the best model.

- b) Which of the three models with k predictors has the smallest test RSS?

Best subset selection would most likely have the smallest test RSS. This is because best subset selection considers all possible models with k predictors and selects the best one. Forward and backward stepwise selection do not consider all possible models, however they may still find the best model by chance.

- c) True or False:

- - i. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the (k +1)-variable model identified by forward stepwise selection.

True. The model with k+1 is an augmented version of the model with k predictors.

- - ii. The predictors in the k-variable model identified by back- ward stepwise are a subset of the predictors in the (k + 1)- variable model identified by backward stepwise selection.

True. The model with k is created by removing a predictor from the model with k+1 predictors.

- - iii. The predictors in the k-variable model identified by back- ward stepwise are a subset of the predictors in the (k + 1)- variable model identified by forward stepwise selection.

False. There is no connection here.

- - iv. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the (k +1)-variable model identified by backward stepwise selection.

False. No connection.

- - v. The predictors in the k-variable model identified by best subset are a subset of the predictors in the (k + 1)-variable model identified by best subset selection.

False. The model with k+1 selects from all possible models with k+1 predictors, so it may not be a subset of the model with k predictors (predictors may be added or removed).

8

In this exercise, we will generate simulated data, and will then use this data to perform forward and backward stepwise selection.

- a) Create a random number generator and use its normal() method to generate a predictor X of length n = 100, as well as a noise vector " of length n = 100.

In [ ]:
```
def numGen(n):
    np.random.seed(42)
    return np.random.normal(size=n)

n = 100
X = numGen(n)
noise = numGen(n)
```

- b) Generate a response vector Y of length n = 100 according to the model

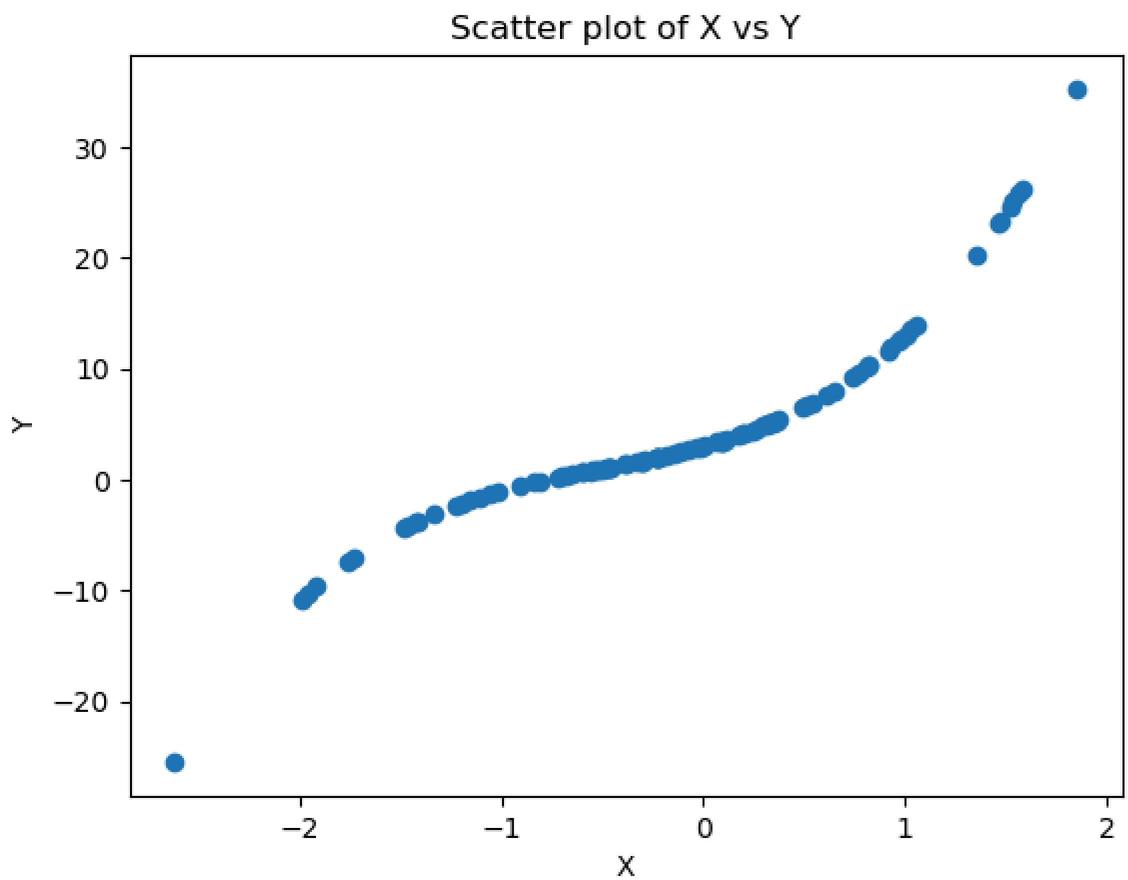
$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$$

, where β_0, β_1, β_2, and β_3 are constants of your choice.

In [ ]:
```
beta = np.array([3, 4, 3, 2])
Y = beta[0] + beta[1]*X + beta[2]*X**2 + beta[3]*X**3 + noise
```

In [ ]:
```
# plot the data
fig, ax = subplots()
ax.scatter(X, Y)
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_title('Scatter plot of X vs Y')
fig.show()
```

```
/tmp/ipykernel_22045/1526155891.py:7: UserWarning: FigureCanvasAgg is non-in
teractive, and thus cannot be shown
  fig.show()
```



- c) Use forward stepwise selection to select a model containing the predictors $X, X^2, \ldots, X^{10}$. What is the model obtained according to C_p? Report the coeffecients of the model obtained.

In [ ]:
```
def nCp(sigma2, estimator, X, Y): # negative Cp statistic
    "Negative Cp statistic"
    n, p = X.shape
    Yhat = estimator.predict(X)
    RSS = np.sum((Y - Yhat)**2)
    return -(RSS + 2 * p * sigma2) / n
```

In [ ]:
```
# create a dataframe with the predictors and the response
df = pd.DataFrame({'Y': Y})
for i in range(1, 11):
    df[f'X^{i}'] = X**i
# move the response to the last column
df = df[['X^1', 'X^2', 'X^3', 'X^4', 'X^5', 'X^6', 'X^7', 'X^8', 'X^9', 'X^1

design = MS(df.columns.drop('Y')).fit(df) # fit a model spec to the data (MS
Yc = np.array(df['Y']) # the response variable
Xc = design.transform(df) # the design matrix with predictors
sigma2 = OLS(Yc,Xc).fit().scale # the residual variance of the OLS model, .s

neg_Cp = partial(nCp, sigma2)

strategy = Stepwise.first_peak(design,
```

```python
                                direction='forward',
                                max_terms=len(design.terms))

df_Cp = sklearn_selected(OLS,
                                strategy,
                                scoring=neg_Cp)
df_Cp.fit(df, Yc)
df_Cp.selected_state_
```

Out[ ]:

```
('X^1', 'X^2', 'X^3')
```

The coefs from forward selection are the ones that were used to generate the data. The added predictors are not significant, so they are not included in the model.

- d) Repeat (c), using backwards stepwise selection. How does your answer compare to the results in (c)?

In [ ]:

```python
# use SFS for backward selection
# will need linear regression as the estimator

from sklearn.linear_model import LinearRegression

sfs = SFS(LinearRegression(),
            n_features_to_select=3,
            direction='backward',
            scoring=neg_Cp,
            cv=5)

sfs.fit(Xc, Yc)
# get the selected features
# use the boolean array sfs.get_support() to get the selected features from
selected_features = Xc.columns[sfs.get_support()]
selected_features
```

Out[ ]:

```
Index(['X^1', 'X^2', 'X^3'], dtype='object')
```

The coefs from backward selection are the same as the coefs from forward selection.

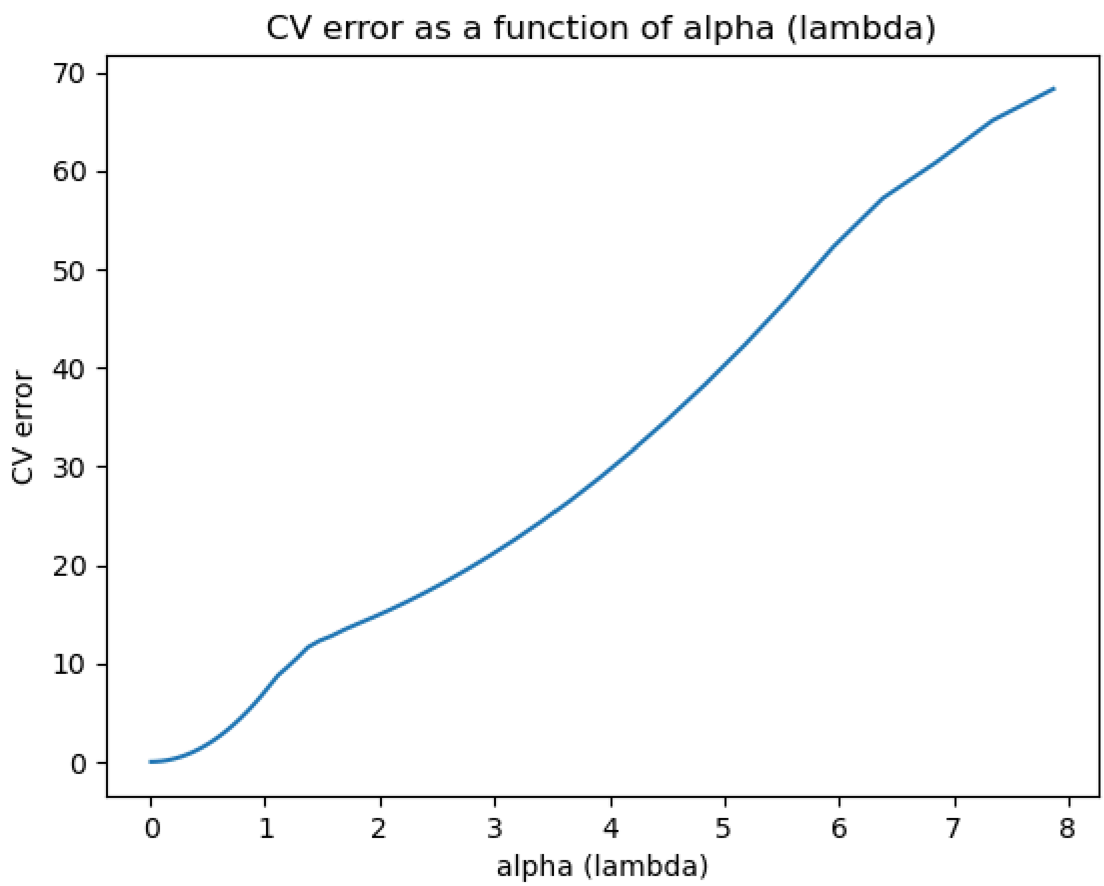
- e) Now fit a lasso model to the simulated data, again using $X, X^2, \ldots, X^{10}$ as predictors. Use cross-validation to select the optimal value of λ. Create plots of the cross-validation error as a function of λ. Report the resulting coefficient estimates, and discuss the results obtained.

In [ ]:

```python
kfold = skm.KFold(n_splits=5, shuffle=True, random_state=42)
scaler = StandardScaler()

lassoCV = skl.ElasticNetCV(n_alphas=100,
                           l1_ratio=1,
                           cv=kfold)
pipeCV = Pipeline(steps=[('scaler', scaler),
                         ('lasso', lassoCV)])
```

```python
# create a dataframe with the predictors and the response
df = pd.DataFrame({'Y': Y})
for i in range(1, 11):
    df[f'X^{i}'] = X**i
# move the response to the last column
df = df[['X^1', 'X^2', 'X^3', 'X^4', 'X^5', 'X^6', 'X^7', 'X^8', 'X^9', 'X^1

pipeCV.fit(df.drop(columns=['Y']), df.Y)
tuned_lasso = pipeCV.named_steps['lasso']
print("optimal lambda (alpha): {}".format(tuned_lasso.alpha_))
# get coef names from df using tuned_lasso.coef_
coef_names = df.drop(columns=['Y']).columns
# get the non-zero coefficients
non_zero_coef = coef_names[tuned_lasso.coef_ != 0]
print("non-zero coefficients and their values: \n{}".format(pd.Series(tuned_
# intercept
print("intercept: {}".format(tuned_lasso.intercept_))

# create plot of the CV error as a function of alpha
fig, ax = subplots()
ax.plot(tuned_lasso.alphas_, tuned_lasso.mse_path_.mean(axis=1))
# ax.set_xscale('log')
ax.set_xlabel('alpha (lambda)')
ax.set_ylabel('CV error')
ax.set_title('CV error as a function of alpha (lambda)');
```

```
optimal lambda (alpha): 0.007870977285052191
non-zero coefficients and their values:
X^1    4.522824
X^2    3.426460
X^3    5.344180
dtype: float64
intercept: 4.19305560215925
```



- f) Now generate a response vector Y according to the model

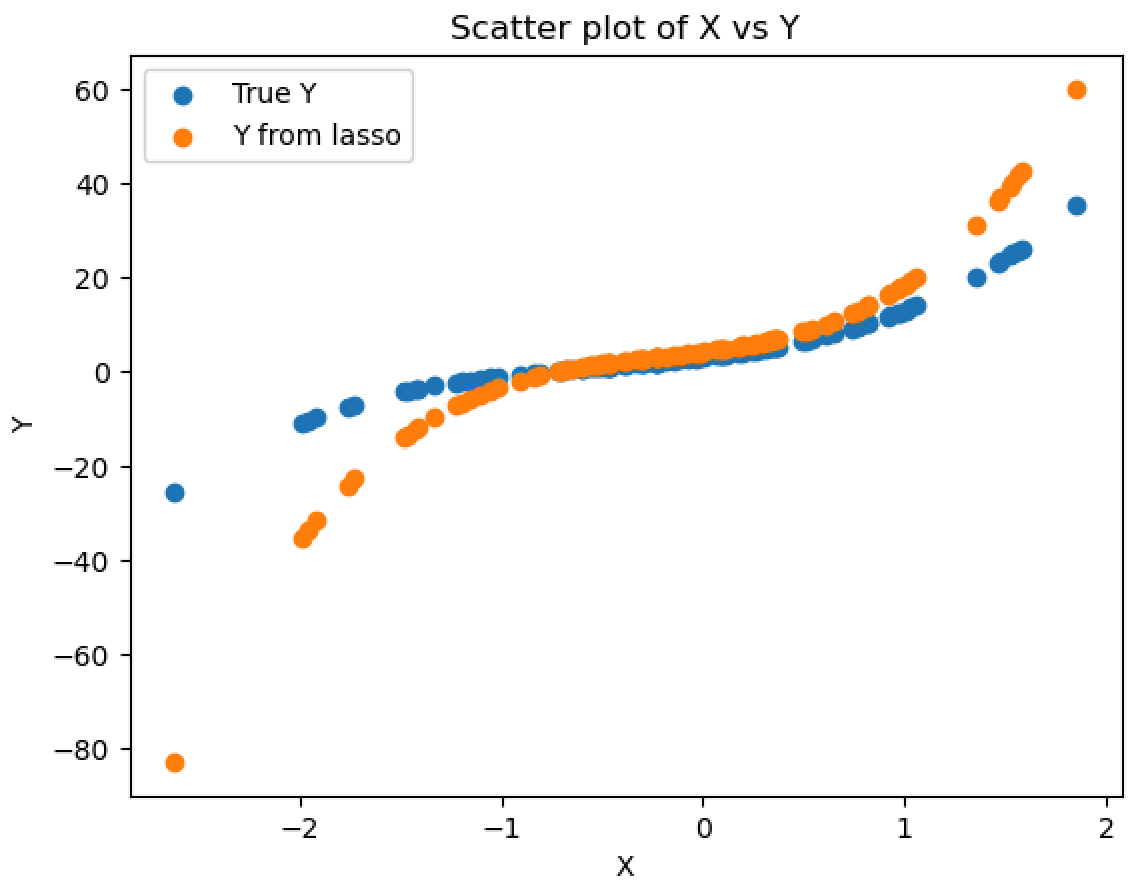
$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$$

and perform stepwise selection and the lasso. Discuss the results obtained.

In [ ]:
```
# create new reponse vector using results from lasso
b0 = tuned_lasso.intercept_
b1 = tuned_lasso.coef_[0]
b2 = tuned_lasso.coef_[1]
b3 = tuned_lasso.coef_[2]

Y_lasso = b0 + b1*X + b2*X**2 + b3*X**3 + noise
```

In [ ]:
```
# plot the data
fig, ax = subplots()
ax.scatter(X, Y, label='True Y')
ax.scatter(X, Y_lasso, label='Y from lasso')
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_title('Scatter plot of X vs Y')
ax.legend()
```

Out[ ]: `<matplotlib.legend.Legend at 0x7b964c515e10>`



In [ ]:
```
# perform stepwise selection and lasso
# create a dataframe with the predictors and the response
df = pd.DataFrame({'Y': Y_lasso})
for i in range(1, 4):
    df[f'X^{i}'] = X**i
# move the response to the last column
df = df[['X^1', 'X^2', 'X^3', 'Y']]
design = MS(df.columns.drop('Y')).fit(df) # fit a model spec to the data (MS
Y = np.array(df['Y']) # the response variable
X = design.transform(df) # the design matrix with predictors
sigma2 = OLS(Y,X).fit().scale # the residual variance of the OLS model, .sca

neg_Cp = partial(nCp, sigma2)

strategy = Stepwise.first_peak(design,
                               direction='forward',
                               max_terms=len(design.terms))

df_Cp = sklearn_selected(OLS,
                         strategy,
                         scoring=neg_Cp)
df_Cp.fit(df, Y)
df_Cp.selected_state_
```

Out[ ]: ('X^1', 'X^2', 'X^3')

9

In this exercise, we will predict the number of applications received using the other variables in the College data set.

In [ ]:
```
# load college data
college = load_data('College')
college
```

Out[ ]:

	Private	Apps	Accept	Enroll	Top10perc	Top25perc	F.Undergrad	P.Undergrad	O
0	Yes	1660	1232	721	23	52	2885	537	
1	Yes	2186	1924	512	16	29	2683	1227	
2	Yes	1428	1097	336	22	50	1036	99	
3	Yes	417	349	137	60	89	510	63	
4	Yes	193	146	55	16	44	249	869	
...	...	...	...	...	...	...	...	...	
772	No	2197	1515	543	4	26	3089	2029	
773	Yes	1959	1805	695	24	47	2849	1107	
774	Yes	2097	1915	695	34	61	2793	166	
775	Yes	10705	2453	1317	95	99	5217	83	
776	Yes	2989	1855	691	28	63	2988	1726	

777 rows × 18 columns

(a) Split the data set into a training set and a test set.

In [ ]:
```
# train test split
X = college.drop(columns=['Apps'])
Y = college['Apps']
# cast Private to 0 and 1
X['Private'] = X['Private'].map({'Yes': 1, 'No': 0})
X_train, X_test, Y_train, Y_test = skm.train_test_split(X, Y, test_size=0.2,
```

(b) Fit a linear model using least squares on the training set, and report the test error obtained.

In [ ]:
```
lm = OLS(Y_train.to_numpy(), X_train.to_numpy()).fit()
Yhat = lm.predict(X_test)
test_error = np.mean((Y_test - Yhat)**2)
print("Test error OLS: {}".format(test_error))
# R^2
R2 = lm.rsquared
print("R^2: {}".format(R2))
```

```
Test error OLS: 1494664.5933117634
R^2: 0.9586161124350168
```

(c) Fit a ridge regression model on the training set, with λ chosen by cross-validation. Report the test error obtained.

In [ ]:
```
alphas = np.logspace(-3, 3, 100)
ridgeCV = skl.RidgeCV(alphas=alphas, cv=5)
ridgeCV.fit(X_train, Y_train)
Yhat = ridgeCV.predict(X_test)
test_error = np.mean((Y_test - Yhat)**2)
print("Test error Ridge: {}".format(test_error))
# R^2
R2 = ridgeCV.score(X_test, Y_test)
print("R^2: {}".format(R2))
```

```
Test error Ridge: 1475450.1731708471
R^2: 0.8890363191118873
```

(d) Fit a lasso model on the training set, with λ chosen by cross-validation. Report the test error obtained, along with the number of non-zero coefficient estimates.

In [ ]:
```
lassoCV = skl.LassoCV(n_alphas=100, cv=5)
lassoCV.fit(X_train, Y_train)
Yhat = lassoCV.predict(X_test)
test_error = np.mean((Y_test - Yhat)**2)
print("Test error Lasso: {}".format(test_error))
print("Number of non-zero coefficients: {}".format(np.sum(lassoCV.coef_ != 0
# R^2
R2 = lassoCV.score(X_test, Y_test)
print("R^2: {}".format(R2))
```

```
Test error Lasso: 1587020.0176529174
Number of non-zero coefficients: 7
R^2: 0.8806455236482635
```

(e) Fit a PCR model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.

In [ ]:
```
pca = PCA()
X_train_pca = pca.fit_transform(X_train)
X_test_pca = pca.transform(X_test)
# fit a linear regression model on the transformed data
lm = OLS(Y_train, X_train_pca).fit()
Yhat = lm.predict(X_test_pca)
test_error = np.mean((Y_test - Yhat)**2)
print("Test error PCR: {}".format(test_error))
# R^2
R2 = lm.rsquared
print("R^2: {}".format(R2))
```

```
Test error PCR: 9977075.391008932
R^2: 0.6001928194338894
```

(g) Comment on the results obtained. How accurately can we predict the number of college applications received? Is there much difference among the test errors resulting from these five approaches?

The best approach based on error appears to be the ridge regression model. Based on R^2, the best approach is standard linear regression. We cannot very accurtaely predict the number of college applications received. The test errors are all very similar, with the exception of PCR being much higher.

11

We will now try to predict per capita crime rate in the Boston dataset.

In [ ]:
```
# import Boston data
boston = load_data('Boston')
boston
```

Out[ ]:

	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	lstat	mec
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296	15.3	4.98	24
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	9.14	21
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242	17.8	4.03	34
3	0.03237	0.0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	2.94	33
4	0.06905	0.0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	5.33	36
...	...	...	...	...	...	...	...	...	...	...	...	...	
501	0.06263	0.0	11.93	0	0.573	6.593	69.1	2.4786	1	273	21.0	9.67	22
502	0.04527	0.0	11.93	0	0.573	6.120	76.7	2.2875	1	273	21.0	9.08	20
503	0.06076	0.0	11.93	0	0.573	6.976	91.0	2.1675	1	273	21.0	5.64	23
504	0.10959	0.0	11.93	0	0.573	6.794	89.3	2.3889	1	273	21.0	6.48	22
505	0.04741	0.0	11.93	0	0.573	6.030	80.8	2.5050	1	273	21.0	7.88	11

506 rows × 13 columns

(a) Try out some of the regression methods explored in this chapter, such as best subset selection, the lasso, ridge regression, and PCR. Present and discuss results for the approaches that you consider.

In [ ]:
```
# Try out some of the regression methods explored in this chapter, such as b
X = boston.drop(columns=['crim'])
Y = boston['crim']
X_train, X_test, Y_train, Y_test = skm.train_test_split(X, Y, test_size=0.2,

# best subset selection
```

```python
design = MS(X.columns).fit(X)
Y = Y_train.to_numpy()
X = design.transform(X_train)
sigma2 = OLS(Y,X).fit().scale
neg_Cp = partial(nCp, sigma2)
strategy = Stepwise.first_peak(design,
                                 direction='forward',
                                 max_terms=len(design.terms))
df_Cp = sklearn_selected(OLS,
                             strategy,
                             scoring=neg_Cp)
df_Cp.fit(X_train, Y_train)
print("Selected features best subset selection: {}".format(df_Cp.selected_st
# test error
Y = Y_test.to_numpy()
X = design.transform(X_test)
Yhat = df_Cp.predict(X_test)
test_error = np.mean((Y - Yhat)**2)
print("Test error best subset selection: {}".format(test_error))
# selected features

# lasso
alphas = np.logspace(-3, 3, 100)
lassoCV = skl.LassoCV(n_alphas=100, cv=5)
lassoCV.fit(X_train, Y_train)
Yhat = lassoCV.predict(X_test)
test_error = np.mean((Y_test - Yhat)**2)
# select non-zero coefficients
non_zero_coef = X_train.columns[lassoCV.coef_ != 0]
print("Selected features Lasso: {}".format(non_zero_coef))
print("Test error Lasso: {}".format(test_error))

# ridge
alphas = np.logspace(-3, 3, 100)
ridgeCV = skl.RidgeCV(alphas=alphas, cv=5)
ridgeCV.fit(X_train, Y_train)
Yhat = ridgeCV.predict(X_test)
test_error = np.mean((Y_test - Yhat)**2)
# selected features
print("Selected features Ridge: {}".format(X_train.columns[abs(ridgeCV.coef_
print("Test error Ridge: {}".format(test_error))

# PCR
pca = PCA()
X_train_pca = pca.fit_transform(X_train)
X_test_pca = pca.transform(X_test)
# fit a linear regression model on the transformed data
lm = OLS(Y_train, X_train_pca).fit()
Yhat = lm.predict(X_test_pca)
test_error = np.mean((Y_test - Yhat)**2)
print("Test error PCR: {}".format(test_error))
# selected features
print("Selected features PCR: {}".format(X_train.columns[abs(pca.components_
```

```
Selected features best subset selection: ('dis', 'medv', 'nox', 'ptratio',
'rad', 'zn')
Test error best subset selection: 25.916708095673883
Selected features Lasso: Index(['zn', 'age', 'dis', 'rad', 'tax', 'lstat',
'medv'], dtype='object')
Test error Lasso: 26.763407229661542
Selected features Ridge: Index(['indus', 'rm', 'dis', 'rad', 'ptratio', 'lst
at', 'medv'], dtype='object')
Test error Ridge: 25.676539805879067
Test error PCR: 33.65738415899526
Selected features PCR: Index(['zn', 'indus', 'age', 'rad', 'tax', 'lstat',
'medv'], dtype='object')
```

(b) Propose a model (or set of models) that seem to perform well on this data set, and justify your answer. Make sure that you are evaluating model performance using validation set error, cross-validation, or some other reasonable alternative, as opposed to using training error.

In [ ]:
```
# it appears the ridge regression was the best from above
# Propose a model (or set of models) that seem to perform well on this data
# import Boston data
boston = load_data('Boston')
# Try out some of the regression methods explored in this chapter, such as b
X = boston.drop(columns=['crim'])
Y = boston['crim']
X_train, X_test, Y_train, Y_test = skm.train_test_split(X, Y, test_size=0.2,

# define model
alphas = np.logspace(-3, 3, 100)
model = skl.RidgeCV(alphas=alphas, cv=5)
# fit model
model.fit(X_train, Y_train)
# predict
Yhat = model.predict(X_test)
# test error
test_error = np.mean((Y_test - Yhat)**2)
print("Test error Ridge: {}".format(test_error))
print("Selected features Ridge: {}".format(X_train.columns[abs(model.coef_)
```

```
Test error Ridge: 25.676539805879067
Selected features Ridge: Index(['indus', 'rm', 'dis', 'rad', 'ptratio', 'lst
at', 'medv'], dtype='object')
```

(c) Does your chosen model involve all of the features in the dataset? Why or why not?

The ridge model did not involve all features. Technically it did, but their coefficients were shrunk to near zero. The reason for this is that the model is trying to avoid overfitting by reducing the number of predictors.