Python Tutorial 9

March 27, 2022

This tutorial is for Dr. Xin Tong's DSO 530 class at the University of Southern California in Spring 2022. It aims to give you some supplementary code to implement Subset Selection in Python.

1 Linear Model Subset Selection

```
[1]: %matplotlib inline
import pandas as pd
import numpy as np
import itertools
import time
import statsmodels.api as sm
import matplotlib.pyplot as plt
```

1.1 Best Subset Selection

Here we apply the best subset selection approach to the Hitters data. We wish to predict a baseball player's Salary on the basis of various statistics associated with performance in the previous year. Let's take a quick look:

```
[2]: df = pd.read_csv('Hitters.csv')
df.head()
```

[2]:			Player	AtB	at 1	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	\
0	-An	.dy	Allanson	n 2	93	66	1	30	29	14	1	293	
1		-Al	an Ashby	₇ 3	15	81	7	24	38	39	14	3449	
2	_	Alv	in Davis	s 4	79	130	18	66	72	76	3	1624	
3	-A	ndr	e Dawson	n 4	96	141	20	65	78	37	11	5628	
4	-Andre	s G	alarraga	a 3	21	87	10	39	42	30	2	396	
	CHits		CRuns	CRBI	CWa.	lks	League	Divisi	on Pu	ıt0uts	Assists	Errors	\
0	66		30	29		14	A		E	446	33	20	
1	835		321	414	;	375	N		W	632	43	10	
2	457		224	266	:	263	A		W	880	82	14	
3	1575		828	838	;	354	N		E	200	11	3	
4	101	•••	48	46		33	N		Ε	805	40	4	

Salary NewLeague

```
0 NaN A
1 475.0 N
2 480.0 A
3 500.0 N
4 91.5 N
```

[5 rows x 21 columns]

First, we note that the Salary variable is missing for some of the players. The isnull() function can be used to identify the missing observations. It returns a vector of the same length as the input vector, with a TRUE value for any missing element, and a FALSE value for a non-missing element. The sum() function can then be used to count the missing elements:

```
[3]: print(df["Salary"].isnull().sum())
```

59

We see that Salary is missing for 59 players. The dropna() function removes all of the rows that have missing values in any variable:

```
before dropna(): (322, 20)
after dropna(): (263, 20)
check the number of missing salary after dropna(): 0
```

Here, we use pd.get_dummies function to transform the original categorical variable League, Division and NewLeague into the usable "1/0" format.

```
[5]: df[['League', 'Division', 'NewLeague']].head()
```

```
[5]: League Division NewLeague
1 N W N
```

```
2 A W A
3 N E N
4 N E N
5 A W A
```

```
[6]: dummies = pd.get_dummies(df[['League', 'Division', 'NewLeague']])
```

```
[7]: dummies.head()
```

```
League_A League_N Division_E Division_W NewLeague_A NewLeague_N
[7]:
     1
                0
                           1
                                                      1
     2
                1
                           0
                                        0
                                                      1
                                                                    1
                                                                                  0
     3
                0
                           1
                                        1
                                                      0
                                                                    0
                                                                                  1
     4
                0
                           1
                                        1
                                                      0
                                                                    0
                                                                                  1
     5
                1
                           0
                                         0
                                                      1
                                                                    1
                                                                                  0
```

Note that for every categorical variable with K categories, we only need K-1 dummies to represent it.

```
# Drop the column with the dependent variable (Salary), and columns for which → we created dummy variables

X_ = df.drop(['Salary', 'League', 'Division', 'NewLeague'], axis=1)

# Define the feature set X.

X = pd.concat([X_, dummies[['League_N', 'Division_W', 'NewLeague_N']]], axis=1)

## Note that alternatively, you can use drop_first=True in .get_dummies to → directly get K-1 dummies

## for a categorical variable with K categories.
```

We can perform best subset selection by identifying the best model that contains a given number of predictors, where **best** is quantified as having the smallest RSS. We'll define a helper function to output the best set of variables for each model size:

```
[9]: def processSubset(feature_set):
    # Fit model on feature_set and calculate RSS
    X1 = sm.add_constant(X[list(feature_set)])
    model = sm.OLS(y,X1)
    regr = model.fit()
    RSS = ((regr.predict(X1) - y) ** 2).sum()
    return {"model":regr, "RSS":RSS}
```

Here, we calculate the RSS along with the process of model building.

```
[10]: def getBest(k):
    tic = time.time()
```

Note that getting the smallest RSS is the same as getting the highest R^2 .

This returns a *DataFrame* containing the best model that we generated, along with the RSS.

What function itertools.combinations(iterable, r) does is to return r length subsequences of elements from the input iterable. For example:

```
[11]: print(list(itertools.combinations('12345',2)))
        [('1', '2'), ('1', '3'), ('1', '4'), ('1', '5'), ('2', '3'), ('2', '4'), ('2', '5'), ('3', '4'), ('3', '5'), ('4', '5')]

[12]: print(list(itertools.combinations('12345',3)))
        [('1', '2', '3'), ('1', '2', '4'), ('1', '2', '5'), ('1', '3', '4'), ('1', '3', '5'), ('1', '4', '5'), ('2', '3', '4'), ('2', '3', '5'), ('2', '4', '5'), ('3', '4', '5')]
        Now we want to call that function for each number of predictors k:
```

```
[13]: # Could take quite awhile to complete...

models = pd.DataFrame(columns=["RSS", "model"])

tic = time.time()
for i in range(0,8):
    models.loc[i] = getBest(i)
```

```
toc = time.time()
print("Total elapsed time:", (toc-tic), "seconds.")
```

Processed 1 models on 0 predictors in 0.02093195915222168 seconds.

Processed 19 models on 1 predictors in 0.05792999267578125 seconds.

Processed 171 models on 2 predictors in 0.37050867080688477 seconds.

Processed 969 models on 3 predictors in 2.239161729812622 seconds.

Processed 3876 models on 4 predictors in 10.45738697052002 seconds.

Processed 11628 models on 5 predictors in 29.638815879821777 seconds.

Processed 27132 models on 6 predictors in 80.33709907531738 seconds.

Processed 50388 models on 7 predictors in 158.28794288635254 seconds.

Total elapsed time: 282.6905539035797 seconds.

Now we have one big *DataFrame* that contains the best models of sizes 0 to 7. Note that to save computation time, we did not look at models of sizes 8 to 19.

[14]: models

const

```
[14]:
                    RSS
                                                                            model
          5.331911e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
          3.617968e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
          3.064656e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
      3 2.924930e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
      4 2.797085e+07
                          <statsmodels.regression.linear model.Regressio...</pre>
      5 2.714990e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
      6 2.619490e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
         2.590655e+07
                          <statsmodels.regression.linear_model.Regressio...</pre>
```

55.982

If we want to access the details of each model, we can get a full rundown of a single model using the summary() function:

[15]: print(models.loc[2, "model"].summary())

-47.9559

OLS Regression Results

=======================================	=======================================		
Dep. Variable:	Salary	R-squared:	0.425
Model:	OLS	Adj. R-squared:	0.421
Method:	Least Squares	F-statistic:	96.17
Date:	Sun, 27 Mar 2022	<pre>Prob (F-statistic):</pre>	5.43e-32
Time:	17:21:38	Log-Likelihood:	-1907.2
No. Observations:	263	AIC:	3820.
Df Residuals:	260	BIC:	3831.
Df Model:	2		
Covariance Type:	nonrobust		
=======================================	=======================================		=======================================
С	oef std err	t P> t	[0.025 0.975]

-0.857

0.392

-158.193

62.281

Hits	3.3008	0.482	6.851	0.000	2.352	4.250
CRBI	0.6899	0.067	10.262	0.000	0.558	0.822
Omnibus:		117.6	673 Durbi	n-Watson:		1.927
Prob(Omnibus):	0.0	000 Jarqu	e-Bera (JB):		700.819
Skew:		1.7	704 Prob(JB):		6.59e-153
Kurtosis:		10.2	235 Cond.	No.		1.24e+03
========	========	.=======				

Notes:

- [1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
- [2] The condition number is large, 1.24e+03. This might indicate that there are strong multicollinearity or other numerical problems.

This output indicates that the best two-variable model contains only Hits and CRBI.

Here, as a digression, we recall a key difference between df.loc() and df.iloc():

loc() gets rows (or columns) with particular labels from the index.

iloc() gets rows (or columns) at particular positions in the index (so it only takes integers).

For example:

```
[16]: data = pd.Series(np.arange(10), index=[20, 21, 22, 23, 24, 1, 2, 3, 4, 5]) data
```

[17]: data.loc[:3]

3

7

dtype: int64

[18]: data.iloc[:3]

[18]: 20 0 21 1 22 2

dtype: int64

You can use the functions we defined above to explore as many variables as are desired.

[19]: print(getBest(19)["model"].summary())

Processed 1 models on 19 predictors in 0.007917642593383789 seconds. $\hbox{OLS Regression Results}$

==========	===========		
Dep. Variable:	Salary	R-squared:	0.546
Model:	OLS	Adj. R-squared:	0.511
Method:	Least Squares	F-statistic:	15.39
Date:	Sun, 27 Mar 2022	Prob (F-statistic):	7.84e-32
Time:	17:21:38	Log-Likelihood:	-1876.2
No. Observations:	263	AIC:	3792.
Df Residuals:	243	BIC:	3864.

Df Model: 19 Covariance Type: nonrobust

========	coef	std err	 t	P> t	[0.025	0.975]
const	163.1036	90.779	1.797	0.074	-15.710	341.917
AtBat	-1.9799	0.634	-3.123	0.002	-3.229	-0.731
Hits	7.5008	2.378	3.155	0.002	2.818	12.184
HmRun	4.3309	6.201	0.698	0.486	-7.885	16.546
Runs	-2.3762	2.981	-0.797	0.426	-8.248	3.495
RBI	-1.0450	2.601	-0.402	0.688	-6.168	4.078
Walks	6.2313	1.829	3.408	0.001	2.630	9.833
Years	-3.4891	12.412	-0.281	0.779	-27.938	20.960
CAtBat	-0.1713	0.135	-1.267	0.206	-0.438	0.095
CHits	0.1340	0.675	0.199	0.843	-1.195	1.463
CHmRun	-0.1729	1.617	-0.107	0.915	-3.358	3.013
CRuns	1.4543	0.750	1.938	0.054	-0.024	2.933
CRBI	0.8077	0.693	1.166	0.245	-0.557	2.172
CWalks	-0.8116	0.328	-2.474	0.014	-1.458	-0.165
PutOuts	0.2819	0.077	3.640	0.000	0.129	0.434
Assists	0.3711	0.221	1.678	0.095	-0.065	0.807
Errors	-3.3608	4.392	-0.765	0.445	-12.011	5.290
League_N	62.5994	79.261	0.790	0.430	-93.528	218.727
Division_W	-116.8492	40.367	-2.895	0.004	-196.363	-37.335
NewLeague_N	-24.7623	79.003	-0.313	0.754	-180.380	130.855

87.414	Durbin-Watson:	2.018
0.000	Jarque-Bera (JB):	452.923
1.236	Prob(JB):	4.46e-99
8.934	Cond. No.	2.09e+04
	0.000 1.236	87.414 Durbin-Watson: 0.000 Jarque-Bera (JB): 1.236 Prob(JB): 8.934 Cond. No.

Notes:

- [1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
- [2] The condition number is large, 2.09e+04. This might indicate that there are strong multicollinearity or other numerical problems.

In addition to using the summary function to print to the screen, we can access just the parts we need using the model's attributes. For example, if we want the R^2 value:

```
[20]: models.loc[2, "model"].rsquared
```

[20]: 0.42522374646677885

In addition to the verbose output, we get when we print the summary to the screen, fitting the \mathtt{OLS} also produced many other useful statistics such as adjusted- R^2 , AIC, and BIC. We can examine these to try to select the best overall model across different model sizes. Let's start by looking at R^2 across all our models:

```
[21]: # Gets the second element from each row ('model') and pulls out its R rsquared

→ attribute

models.apply(lambda row: row[1].rsquared, axis=1)
```

- [21]: 0 0.000000
 - 1 0.321450
 - 2 0.425224
 - 3 0.451429
 - 4 0.475407
 - 5 0.490804
 - 6 0.508715
 - 7 0.514123

dtype: float64

As expected, the R^2 statistic increases monotonically as more variables are included.

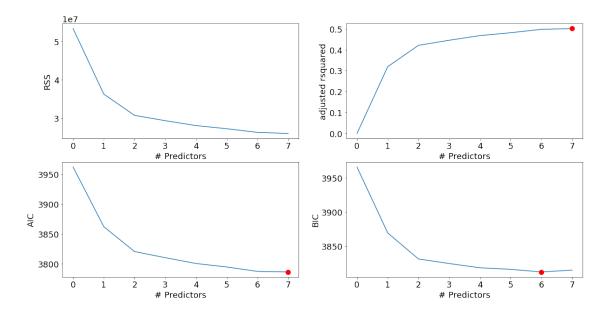
Plotting RSS, adjusted- R^2 , AIC, and BIC for all of the models at once will help us decide which model to select.:

```
[22]: plt.figure(figsize=(20,10))
plt.rcParams.update({'font.size': 18, 'lines.markersize': 10})

# Set up a 2x2 grid so we can look at 4 plots at once
plt.subplot(2, 2, 1)
```

```
# We will now plot a curve to show the relationship between the number of \Box
\rightarrowpredictors and the RSS
plt.plot(models["RSS"])
plt.xlabel('# Predictors')
plt.ylabel('RSS')
# We will now plot a red dot to indicate the model with the largest adjusted_{\sqcup}
\rightarrow R^2 statistic.
# The idxmax() function can be used to identify the location of the maximum
→point of a vector
rsquared_adj = models.apply(lambda row: row[1].rsquared_adj, axis=1)
plt.subplot(2, 2, 2)
plt.plot(rsquared_adj)
plt.plot(rsquared_adj.idxmax(), rsquared_adj.max(), "or")
plt.xlabel('# Predictors')
plt.ylabel('adjusted rsquared')
# We'll do the same for AIC and BIC, this time looking for the models with the
\hookrightarrowSMALLEST statistic
aic = models.apply(lambda row: row[1].aic, axis=1)
plt.subplot(2, 2, 3)
plt.plot(aic)
plt.plot(aic.idxmin(), aic.min(), "or")
plt.xlabel('# Predictors')
plt.ylabel('AIC')
bic = models.apply(lambda row: row[1].bic, axis=1)
plt.subplot(2, 2, 4)
plt.plot(bic)
plt.plot(bic.idxmin(), bic.min(), "or")
plt.xlabel('# Predictors')
plt.ylabel('BIC')
```

[22]: Text(0, 0.5, 'BIC')



Recall that in the second step of our selection process, we narrowed the field down to just one model of each size $k \leq p$. According to BIC, the best performer is the model with 6 variables. According to AIC and adjusted- R^2 something a bit more complex might be better.

1.2 Forward Stepwise Selection (optional)

We can also use a similar approach to perform forward stepwise or backward stepwise selection, using a slight modification of the functions we defined above:

```
[23]: def forward(predictors):
    # Pull out predictors we still need to process
    remaining_predictors = [p for p in X.columns if p not in predictors]

    tic = time.time()

    results = []

    for p in remaining_predictors:
        results.append(processSubset(predictors+[p]))

# Wrap everything up in a nice dataframe
models = pd.DataFrame(results)

# Choose the model with the highest RSS
best_model = models.loc[models['RSS'].idxmin]

toc = time.time()
```

```
print("Processed ", models.shape[0], "models on", len(predictors)+1,□
→"predictors in", (toc-tic), "seconds.")

# Return the best model, along with some other useful information about the□
→model
return best_model
```

Except for the null model, forward stepwise regression can be implemented as below.

```
[24]: models2 = pd.DataFrame(columns=["RSS", "model"])

tic = time.time()
predictors = []

for i in range(1,len(X.columns)+1):
    models2.loc[i] = forward(predictors)
    predictors = models2.loc[i]["model"].model.exog_names.copy()
    predictors.remove('const')

toc = time.time()
print("Total elapsed time:", (toc-tic), "seconds.")
```

```
Processed 19 models on 1 predictors in 0.04671430587768555 seconds.
Processed 18 models on 2 predictors in 0.039489030838012695 seconds.
Processed 17 models on 3 predictors in 0.03871488571166992 seconds.
Processed 16 models on 4 predictors in 0.03974795341491699 seconds.
Processed 15 models on 5 predictors in 0.04239082336425781 seconds.
Processed 14 models on 6 predictors in 0.04398989677429199 seconds.
Processed 13 models on 7 predictors in 0.041918039321899414 seconds.
Processed 12 models on 8 predictors in 0.0393519401550293 seconds.
Processed 11 models on 9 predictors in 0.03719592094421387 seconds.
Processed 10 models on 10 predictors in 0.03577899932861328 seconds.
Processed 9 models on 11 predictors in 0.033032894134521484 seconds.
Processed 8 models on 12 predictors in 0.03284788131713867 seconds.
Processed 7 models on 13 predictors in 0.029610157012939453 seconds.
Processed 6 models on 14 predictors in 0.02554774284362793 seconds.
Processed 5 models on 15 predictors in 0.02216792106628418 seconds.
Processed 4 models on 16 predictors in 0.018649816513061523 seconds.
Processed 3 models on 17 predictors in 0.015812158584594727 seconds.
Processed 2 models on 18 predictors in 0.01139521598815918 seconds.
Processed 1 models on 19 predictors in 0.006227970123291016 seconds.
Total elapsed time: 0.6431300640106201 seconds.
```

Clearly, forward stepwise selection runs faster than best subset selection.

Let's see how the forward stepwise selection models stack up against best subset selection for models with 7 predictors:

```
[25]: print("Best Subset Selection:\n", models.loc[7, "model"].summary())
print("\n\nForward Stepwise Selection:\n", models2.loc[7, "model"].summary())
```

Best Subset Selection:

OLS Regression Results

Dep. Variable:	Salary	R-squared:	0.514
Model:	OLS	Adj. R-squared:	0.501
Method:	Least Squares	F-statistic:	38.55
Date:	Sun, 27 Mar 2022	Prob (F-statistic):	1.19e-36
Time:	17:21:39	Log-Likelihood:	-1885.1
No. Observations:	263	AIC:	3786.
Df Residuals:	255	BIC:	3815.
Df Model:	7		
Covariance Type:	nonrobust		
			===========

	coef	std err	t	P> t	[0.025	0.975]
const Hits Walks CAtBat CHits CHmRun PutOuts	79.4509 1.2834 3.2274 -0.3752 1.4957 1.4421 0.2367	63.794 0.584 1.203 0.097 0.334 0.422 0.075	1.245 2.196 2.684 -3.866 4.480 3.420 3.161	0.214 0.029 0.008 0.000 0.000 0.001 0.002	-46.179 0.133 0.859 -0.566 0.838 0.612 0.089	205.081 2.434 5.596 -0.184 2.153 2.272 0.384
Division_W	-129.9866	39.499	-3.291	0.001	-207.773	-52.200
Omnibus: Prob(Omnibus): Skew: Kurtosis:		0	.000 Jarq .440 Prob	======== in-Watson: ue-Bera (JB) (JB): . No.):	2.022 681.266 1.16e-148 1.23e+04

Notes:

- [1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
- [2] The condition number is large, 1.23e+04. This might indicate that there are strong multicollinearity or other numerical problems.

Forward Stepwise Selection:

OLS Regression Results

Dep. Variable:	Salary	R-squared:	0.513			
Model:	OLS	Adj. R-squared:	0.500			
Method:	Least Squares	F-statistic:	38.41			
Date:	Sun, 27 Mar 2022	Prob (F-statistic):	1.50e-36			

Time: No. Observations: Df Residuals: Df Model: Covariance Type:			263 AIC: 255 BIC: 7	kelihood:		-1885.4 3787. 3815.
	coef	std err	t	P> t	[0.025	0.975]
PutOuts Division_W AtBat Walks	0.8538 7.4499 0.2533 -127.1224 -1.9589 4.9131	0.151 1.661 0.075 39.807 0.529 1.443	1.666 5.640 4.485 3.382 -3.193 -3.701 3.405 -1.538	0.000 0.000 0.001 0.002 0.000 0.001	0.556 4.179 0.106 -205.515 -3.001 2.072	1.152 10.721 0.401 -48.730
Omnibus: Prob(Omnibus) Skew: Kurtosis:	ıs):	1.			:	1.988 609.074 5.51e-133 2.58e+03

Notes:

- [1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
- [2] The condition number is large, 2.58e+03. This might indicate that there are strong multicollinearity or other numerical problems.

The results above indicate that the best seven-variable models are different between the best subset selection and forward stepwise selection.

1.3 Backward Stepwise Selection (optional)

We only need a minor change to implement backward stepwise selection: loop through the predictors in reverse.

```
[26]: def backward(predictors):
    tic = time.time()
    results = []
    for combo in itertools.combinations(predictors, len(predictors)-1):
        results.append(processSubset(combo))

# Wrap everything up in a nice dataframe
models = pd.DataFrame(results)
```

```
# Choose the model with the highest RSS
best_model = models.loc[models['RSS'].idxmin]

toc = time.time()
print("Processed ", models.shape[0], "models on", len(predictors)-1,__

"predictors in", (toc-tic), "seconds.")

# Return the best model, along with some other useful information about the__

model
return best_model
```

```
Processed 1 models on 19 predictors in 0.00609278678894043 seconds.
Processed 19 models on 18 predictors in 0.07275176048278809 seconds.
Processed 18 models on 17 predictors in 0.06374907493591309 seconds.
Processed 17 models on 16 predictors in 0.05979299545288086 seconds.
Processed 16 models on 15 predictors in 0.05682206153869629 seconds.
Processed 15 models on 14 predictors in 0.0506129264831543 seconds.
Processed 14 models on 13 predictors in 0.046527862548828125 seconds.
Processed 13 models on 12 predictors in 0.04227089881896973 seconds.
Processed 12 models on 11 predictors in 0.03786587715148926 seconds.
Processed 11 models on 10 predictors in 0.034002065658569336 seconds.
Processed 10 models on 9 predictors in 0.03050708770751953 seconds.
Processed 9 models on 8 predictors in 0.027508974075317383 seconds.
Processed 8 models on 7 predictors in 0.02334117889404297 seconds.
Processed 7 models on 6 predictors in 0.019824981689453125 seconds.
Processed 6 models on 5 predictors in 0.016820907592773438 seconds.
Processed 5 models on 4 predictors in 0.014647960662841797 seconds.
Processed 4 models on 3 predictors in 0.012042999267578125 seconds.
Processed 3 models on 2 predictors in 0.008568763732910156 seconds.
Processed 2 models on 1 predictors in 0.005591869354248047 seconds.
```

Total elapsed time: 0.649940013885498 seconds.

For this data, the best 7-variable models identified by forward stepwise selection, backward stepwise selection, and best subset selection are different.

```
[28]: print("Best Subset Selection:\n",models.loc[7, "model"].params)
print("\nForward Stepwise Selection:\n",models2.loc[7, "model"].params)
print("\nBackward Stepwise Selection:\n",models3.loc[7, "model"].params)
```

Best Subset Selection:

const 79.450947 Hits 1.283351 Walks 3.227426 CAtBat -0.375235 CHits 1.495707 CHmRun 1.442054 PutOuts 0.236681 Division_W -129.986643

dtype: float64

Forward Stepwise Selection:

const 109.787306 CRBI 0.853762 Hits 7.449877 PutOuts 0.253340 Division_W -127.122393 AtBat -1.958885 Walks 4.913140 CWalks -0.305307

dtype: float64

Backward Stepwise Selection:

const 105.648749 AtBat -1.976284Hits 6.757491 Walks 6.055869 CRuns 1.129309 CWalks -0.716335 PutOuts 0.302885 Division_W -116.169217

dtype: float64