Regression (Continued) III

Today's Outline

- Cross-Validation
- Bootstrapping
- Transformations
- Boruta and Mallow's CP

K-Fold Cross Validation

- K-fold cross validation splits our data up into k subsets
- Train our model on k-1 subsets and predict on the one that's left out
- Repeat over all combinations of subsets
- Helpful to measure overfitting and optimizing model parameters
- On the right I show the first step of 5-fold cross validation where the first 20 observations are used to train and the last 5 are used to test

 Train

 (step 1)

1095 20 27595.000000 6.998509 1122 578 6.359574 1368 0 7.221105 1145 1078 6.997596 1237 567 933 11 6.838405 12 1339 0 7.199678 10.597809 937 2513 800049 22 299999 2011 0 7.606388 1585 0 7.368340 1058 922 759 6.632002 1414 7.254178 23 1041

1 ceo[:25]

Test (Step 1)

K-Fold Cross Validation (sklearn)



- Sklearn is the premiers ML library for most models
- Includes tools for testing, tuning, and cross validation
- The kfold submodule will automatically split your data into k subsets
- This is a generator function that we can iterate through in a loop
- Can be combined with other compatible functions
- We can also set shuffle = True if we suspect our data isn't arranged randomly

```
1 from sklearn, model selection import KFold # import KFold
  for train index, test_index in kf.split(ceo):
       print("TRAIN:", train index, "TEST:", test index)
158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175
176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193
194 195 196 197 198 199 200 201 202 203 204 205 206 207 208
```

Manual Cross Validation

- Cross validation can be implemented manually in the following steps:
 - Train model over training indices
 - Make predictions over the test indices
 - Calculate a test metric (MSE, MAPE, RMSE, etc) to evaluate the model's performance against the observed testing values
 - Store the performance for each fold

```
# split the data into 5 subsets
kf = KFold(n_splits = 5)

mse = []
for train_index, test_index in kf.split(ceo):
    # train data over training set
    results = smf.ols('np.log(salary) ~ np.log(sales)', ceo.iloc[train_index]).fit()

# test over last split
s = ((np.log(ceo.iloc[test_index]["salary"]) - results.predict(ceo.iloc[test_index]))**2).mean()

# append test metric
mse.append(s)
```

```
1 mse

[0.12340491612500952,

0.13110902468036287,

0.2573800924128631,

0.34446212923335046,

0.4873535250351009]
```

Sklearn Cross Validation

- Cross validation is straightforward in sklearn
- Requires us to use the sklearn regression functions for compatibility
- Cross_val_score has us specify:
 - The model
 - Dependent/independent variables
 - The scoring method
 - Number of folds
- Sklearn seeks to maximize each metric, so this is why the negative is taken of some metrics (like MSE and RMSE)
- Why do we square? Why prefer MSE over RMSE?

```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score

x = np.log(ceo[['sales']])
y = np.log(ceo[['salary']])

regr = LinearRegression()
scores = cross_val_score(regr, x, y, cv=5, scoring='neg_mean_squared_error')
print('5-Fold CV MSE Scores:', scores)

5-Fold CV MSE Scores: [-0.12340492 -0.13110902 -0.25738009 -0.34446213 -0.48735353]
```

```
Regression
                                      metrics.explained variance score
'explained_variance'
'max error'
                                     metrics.max error
'neg_mean_absolute_error'
                                     metrics.mean absolute error
'neg_mean_squared_error'
                                     metrics.mean squared error
'neg_root_mean_squared_error'
                                     metrics.mean_squared_error
'neg_mean_squared_log_error'
                                     metrics.mean_squared_log_error
'neg_median_absolute_error'
                                     metrics.median_absolute error
                                     metrics.r2 score
'neg_mean_poisson_deviance'
                                      metrics.mean poisson deviance
'neg_mean_gamma_deviance'
                                     metrics.mean gamma deviance
'neg_mean_absolute_percentage_error
                                     metrics.mean absolute percentage error
'd2_absolute_error_score'
                                     metrics.d2 absolute error score
'd2_pinball_score'
                                     metrics.d2 pinball score
'd2_tweedie_score'
                                     metrics.d2 tweedie score
```

Bootstrapping

- The standard errors, intervals, and other properties of some estimators make be difficult or impossible to calculate (for example the CI on a lowess smoother)
- Bootstrapping gives us a very powerful way to use resampling to estimate these properties
- The algorithm is straightforward:
 - Get a representative sample from your population of size N
 - Generate B bootstrap samples of size N with replacement from your original sample
 - Calculate your desired statistic over each bootstrap sample
 - Use the distribution of your bootstrap sample statistics to find the moments, confidence intervals, etc. of the original sample statistic
- Also can be used in machine learning to create ensemble models

Manual Bootstrapping

- On the right I show the algorithm for bootstrapping regression coefficients
- This framework can be applied for other statistics and ML models as well
- Here we calculate the percentile confidence interval
 - Note that the percentile method tends to be more vulnerable to bias and skew (not a first choice)

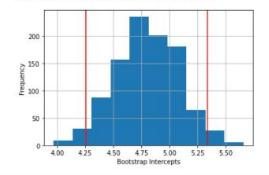
```
# build dataframe to store sample statistics
   coefs = pd.DataFrame(columns = ["B0","B1"])
   # we will generate 1000 bootstrap samples
   for i in range(1000):
       # sample from the data with replacement N times
       sample = ceo.sample(ceo.shape[0] ,replace = True)
       # fit model on bootstrap sample
       results = smf.ols('np.log(salary) ~ np.log(sales)', sample).fit()
11
12
13
       # pull out the bootstrap sample statistics
       b0,b1 = results.params
15
16
       # store the bootstrap sample statistics for later use
17
       coefs = coefs.append({"B0":b0, "B1":b1}, ignore index = True)
18
   # below I calculate the percentile bootstraps for a 95% confidence interval
20
   # the 97.5 percentile of thebootstrap sample statistics
   b0 u, b1 u = coefs.quantile(.975)
23
  # the 2.5 percentile of the bootstrap sample statistics
   b0 1, b1 1 = coefs.quantile(.025)
```

Plotting Bootstraps

- On the right we plot the bootstrap sample statistics for the slope and intercepts of the regression
- We also include the 95% percentile confidence interval for each statistic

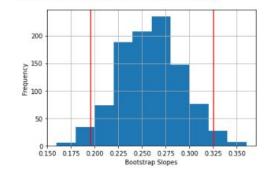
```
1 coefs.B0.hist()
2
3 plt.xlabel("Bootstrap Intercepts")
4 plt.ylabel("Frequency")
5 plt.axvline(b0_u, color = "red")
6 plt.axvline(b0_1, color = "red")
```

: <matplotlib.lines.Line2D at 0x1dbfe7b9be0>



```
1 coefs.B1.hist()
2 plt.xlabel("Bootstrap Slopes")
3 plt.ylabel("Frequency")
4 plt.axvline(b1_u, color = "red")
5 plt.axvline(b1_l, color = "red")
```

: <matplotlib.lines.Line2D at 0x1dbfe977400>



Basic Bootstrap Confidence Interval

 Bootstrap standard errors can also be computed using the following basic estimator:

$$SE_{bt}\Big(\hat{ heta}\Big) = \sqrt{\left(B-1
ight)^{-1}\sum_{b=1}^{B}\left(\hat{ heta}^{*,b}-ar{\hat{ heta}^{*}}
ight)^{2}}$$

$$\left[\hat{ heta}-SE_{bt}\Big(\hat{ heta}\Big)z_{1-lpha/2},\hat{ heta}+SE_{bt}\Big(\hat{ heta}\Big)z_{1-lpha/2}
ight]$$

```
# calculate the bootstrap standard error over the bootstrap statistics for betal
se_bt = coefs.B1.std(ddof = 1)

# calculate the basic CI
[b1-1.96*se_bt, b1+1.96*se_bt]
```

[0.19157312824957456, 0.3217702550787261]

Scipy Stats Bootstrap

- No convenient function similar to R for bootstrap regression
- However, we can write our own function for the "statistic" argument and use the scipy.stats.bootstrap() function to get similar results
- BCa (bias-corrected CI) is the preferred method for calculating bootstrap confidence intervals and si complicated to implement manually
- BCa can be used with this method

```
statistic : callable
```

Statistic for which the confidence interval is to be calculated. *statistic* must be a callable that accepts len(data) samples as separate arguments and returns the resulting statistic. If *vectorized* is set True, *statistic* must also accept a keyword argument *axis* and be vectorized to compute the statistic along the provided *axis*.

```
scipy.stats.bootstrap(data, statistic, *, n_resamples=9999, batch=None,
vectorized=True, paired=False, axis=0, confidence_level=0.95, method='BCa',
random_state=None) # [source]
```

```
1 from scipy.stats import bootstrap
   # Note that you have to write your own functions that will work with
 2 # scipv.stats bootstrap
   # The first one takes in x and y, returns beta1
   def reg boot b1(x,v):
       # bootstrap function gives us a 1d array, need 2d
       x = x.reshape((len(x),1))
9
       y = y.reshape((len(y),1))
       reg = LinearRegression().fit(x,y)
10
11
12
       # Pul.L out heta1
13
       return reg.coef [0][0]
14
   # The first one takes in x and y, returns beta0
   def reg_boot_intercept(x,y):
17
       # bootstrap function gives us a 1d array, need 2d
18
19
       x = x.reshape((len(x),1))
20
       y = y.reshape((len(y),1))
       reg = LinearRegression().fit(x,y)
21
22
23
        # Pull out beta0
24
       return reg.intercept [0]
```

Scipy Stats Bootstrap (Continued)

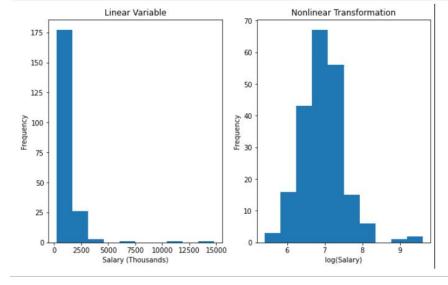
- Function is specified as follows:
 - X, y are taken as arguments
 - We feed in the statistic and confidence intervals we want to calculate
 - Vectorized = False says the axis doesn't matter (for example mean can be calculated over rows or columns)
 - Method can be percentile, basic, or BCa
 - Paired says we need to line up the x and y observations

ConfidenceInterval(low=0.192185058916601, high=0.3190080132891142)

Log-Linear Models

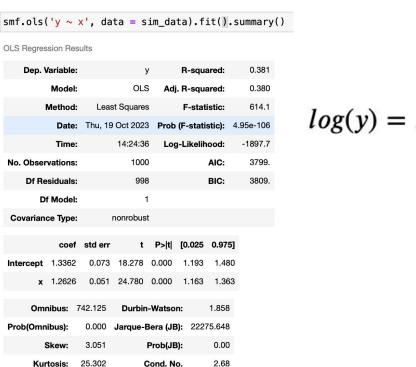
- Log-linear models regress the logarithm of the dependent variable on a linear expression of the dependent variable
- Log stands for the natural logarithm which is calculated by default in np.log()
- Log transformation tends to make skewed distributions more 'normal'
- This transformation might help us meet conditions such as
 - Error normality for hypothesis testing
 - Constant variance
- These models are also convenient to interpret

```
fig, ax = plt.subplots(1, 2, figsize = (10, 6))
ax[0].hist(ceo.salary)
ax[0].set_title("Linear Variable")
ax[0].set_xlabel("Salary (Thousands)")
ax[0].set_ylabel("Frequency")
ax[1].hist(np.log(ceo.salary))
ax[1].set_title("Nonlinear Transformation")
ax[1].set_xlabel("log(Salary)")
ax[1].set_ylabel("Frequency")
plt.show()
```

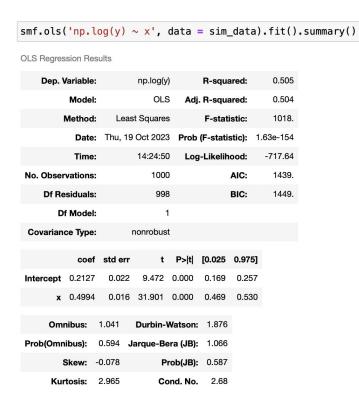


Log-Linear Model Example

Transformations can also linearize a relationship between two variables

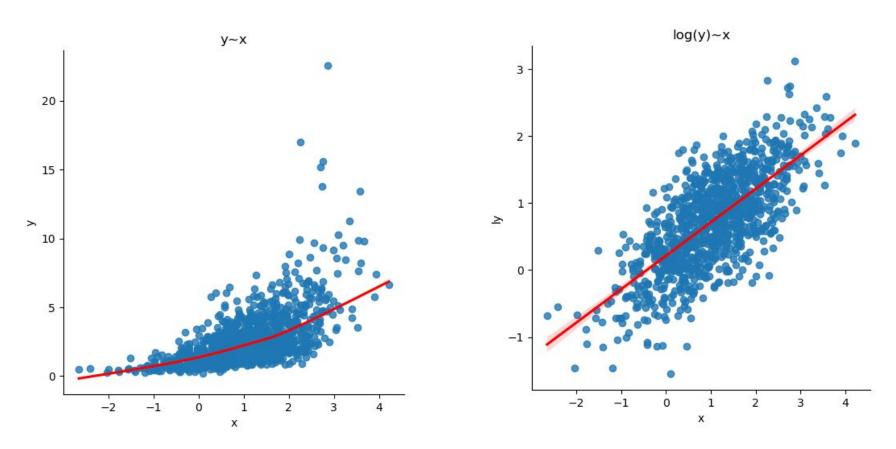


$$log(y) = .2 + .5x + e$$



Log-Linear Model Example (Plotted)

• Transformations can also linearize a relationship between two variables



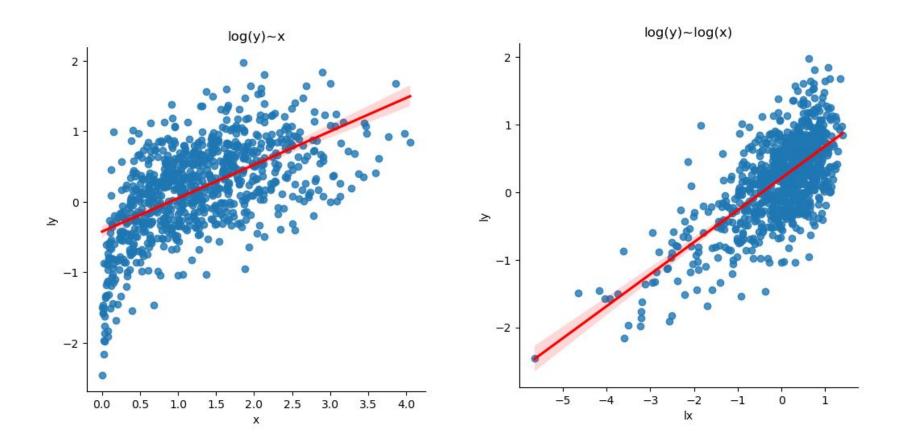
Log-Log Model Example

$$log(y) = .2 + .5 * log(x) + e$$

```
smf.ols('np.log(y) ~ x', data = sim_data).fit().summary()
OLS Regression Results
    Dep. Variable:
                           np.log(y)
                                         R-squared:
                                                        0.333
                                     Adj. R-squared:
           Model:
                              OLS
                                                        0.332
                     Least Squares
                                                        417.3
         Method:
                                          F-statistic:
            Date: Thu, 19 Oct 2023 Prob (F-statistic):
                                                     1.54e-75
            Time:
                          15:09:56
                                     Log-Likelihood:
                                                       -663.46
 No. Observations:
                               837
                                                AIC:
                                                        1331.
                               835
                                                        1340.
     Df Residuals:
                                                BIC:
        Df Model:
                                 1
 Covariance Type:
                         nonrobust
             coef std err
                                 t P>|t|
                                          [0.025 0.975]
                     0.035
                           -12.117 0.000
 Intercept -0.4239
                                           -0.493
                                                 -0.355
        x 0.4749
                     0.023
                            20.428 0.000
                                           0.429
                                                  0.521
      Omnibus:
                 9.767
                          Durbin-Watson:
                                            2.026
                 0.008
                        Jarque-Bera (JB):
                                            9.773
 Prob(Omnibus):
         Skew:
                 -0.246
                                Prob(JB):
                                          0.00755
      Kurtosis:
                 3.197
                               Cond. No.
                                             3.84
```

```
smf.ols('np.log(y) \sim np.log(x)', data = sim_data).fit().summary()
OLS Regression Results
                                                         0.465
    Dep. Variable:
                          np.log(y)
                                         R-squared:
           Model:
                              OLS
                                     Adj. R-squared:
                                                         0.465
                     Least Squares
         Method:
                                         F-statistic:
                                                         726.9
            Date: Thu, 19 Oct 2023 Prob (F-statistic):
                                                     1.15e-115
                          15:09:57
                                     Log-Likelihood:
                                                       -571.01
            Time:
 No. Observations:
                              837
                                               AIC:
                                                         1146.
     Df Residuals:
                              835
                                               BIC:
                                                         1155.
        Df Model:
 Covariance Type:
                         nonrobust
            coef std err
                               t P>|t| [0.025 0.975]
 Intercept 0.2068
                    0.017 12.468
                                  0.000
                                                0.239
 np.log(x) 0.4738
                    0.018 26.961 0.000 0.439
                         Durbin-Watson: 2.092
      Omnibus: 0.288
 Prob(Omnibus): 0.866
                       Jarque-Bera (JB): 0.192
         Skew: 0.024
                               Prob(JB): 0.908
                              Cond. No.
       Kurtosis:
                3.057
                                         1.08
```

Log-Log Model Example (Plotted)



Log-Linear Statsmodels

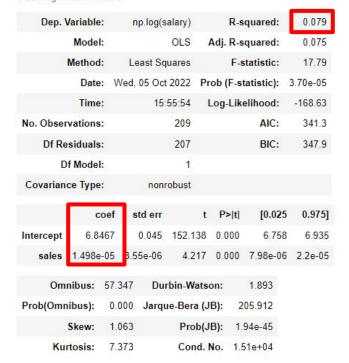
- Non-linear regressions can be fit using statsmodels
- Add np.log(variable) for each variable you want to take the log of in the model
- Here log(salary) is the dependent variable
- I can then print out a summary of the regression results using the result.summary() method

$$\ln(salary) = \beta_0 + \beta_1 sales + u$$

```
# log-linear model
reg1 = smf.ols('np.log(salary) ~ sales', data = ceo)
results1 = reg1.fit()

# look at parameters
results1.summary()
```

OLS Regression Results



Log-Log Statsmodels

- Add np.log(variable) for each variable you want to take the log of in the model
- Here log(salary) is the dependent variable
- log (sales) is the predictor
- I can then print out a summary of the regression results using the result.summary() method

$$\ln(salary) = \beta_0 + \beta_1 \ln(sales) + u$$

```
# Log-Log model | reg2 = smf.ols('np.log(salary) ~ np.log(sales)', data = ceo) results2 = reg2.fit() | results2.summary() |

OLS Regression Results | Dep. Variable: np.log(salary) | R-squared: 0.211 |

Model: OLS Adi. R-squared: 0.207
```

Dep. Variable:			np.log(salary)			R-squared:			
Model:			OLS			Adj. R-squared:		.207	
Method:			Least Squares			F-statistic:		55.30	
Date:		Wed, 05 Oct 2022			Prob (F-statistic):): 2.70	2.70e-12	
T	15:56:28			Log-Likelihood:		d: -15	-152.50		
No. Observations:			209		AIC:		309.0		
Df Residuals:			207			BIC	C: 3	15.7	
Df Mo	del:			1					
Covariance T	ype:		nor	robust					
	С	oef :	std err	t	P> t	[0.025	0.975]		
Intercept	4.82	220	0.288	16.723	0.000	4.254	5.390		
np.log(sales)	0.25	67	0.035	7.436	0.000	0.189	0.325		
Omnibu	ıs:	34.15	D.	ırbin-Wa	tson:	1.860			
Prob(Omnibu	s):	0.000	Jarq	ue-Bera	(JB):	403.831			
Skew:		1.507		Prob(JB):		2.04e-88			
Kurtosis:		9.106		Cond. No.		70.0			

Interpreting log-linear and log-log coefficients

- The slope associated with a given independent variable log linear model is interpreted as a semi-elasticity
- The slope associated with a given independent variable log-log model is the elasticity

We interpret this model using semi-elasticity, such that a 1 unit move in x is associated with a $(100 * \beta_1)\%$ rise in y (approximately).

```
# Log-linear models
r1_b1 = results1.params[1]
print("A one unit increase in sales is associated with a", str(r1_b1*100)+"%", "increase in ceo salary.")

A one unit increase in sales is associated with a 0.0014982498318048918% increase in ceo salary.
```

We interpret this model using elasticity, such that a 1% unit move in x is associated with a β_1 % rise in y.

```
# log-log models
r2_b1 = results2.params[1]

Print("A one percent increase in sales is associated with a", str(r2_b1)+"%", "increase in ceo salary.")

A one percent increase in sales is associated with a 0.2566716916641503% increase in ceo salary.
```

Exercises Bootstrap and Cross-Validation

- Fit the following two regressions
 - log(wage) ~educ
 - log(wage) ~exper
- Use 5-fold cross validation to determine which model produces the best out of sample predictions using "neg_mean_squared_error"
- Create a bootstrap confidence interval for the slope parameter (b1) in the log(wage) ~ educ regression

Box-Cox Power Transform

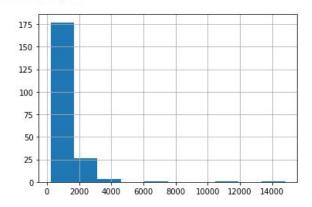
- Like a log transformation, the box-cox transformation can help us meet normality assumptions
- Simple to implement manually
- Manual implementation does not find the best lambda

$$T_{BC}(x,\lambda) = x^{(\lambda)} = \begin{cases} \frac{x^{\lambda} - 1}{\lambda} & \text{when } \lambda \neq 0; \\ log_e x & \text{when } \lambda = 0. \end{cases}$$

```
def box_cox(x, 1 = 0):
    if 1 == 0:
        bc = np.log(x)
    else:
        bc = (x**l-1)/l
    return bc
8
```

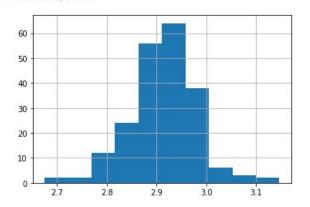
```
M 1 ceo.salary.hist()
```

(0]: <AxesSubplot:>



```
■ 1 box_cox(ceo.salary, -.3).hist()
```

2]: <AxesSubplot:>

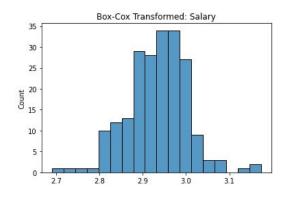


Scipy Box-Cox

- The scipy.stats.boxcox() function finds the value of lambda that maximizes the log-likelihood function
- Returns the desired lambda and the transformed data

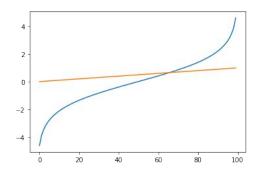
```
b  bc_salary, lambda_salary = stats.boxcox(ceo["salary"])
  print(lambda_salary)
  sns.histplot(bc_salary)
  plt.title("Box-Cox Transformed: Salary")
  plt.show()
```

-0.2970139553908451



Restricted Range Transformation: Logit

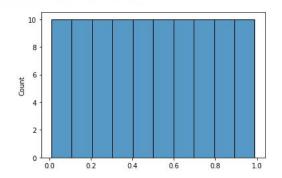
- The arcsin square root transformation (shown in 430 notes) and logit transformation are used on variables with ranges restricted between 0 and 1
- These variables often have values that cluster at 0 and
- Transformation stretches out these values towards the ends and makes relationships easier to understand
- Also stabilizes the variance and tends to make the data more normal



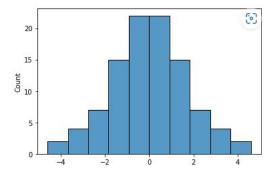
$$T_{logit} = logit(x) = ln\left(\frac{x}{1-x}\right)$$

```
M 1 original = np.linspace(0.01, .99, 100)
2 sns.histplot(original, bins = 10)
```

: <AxesSubplot:ylabel='Count'>



- transformed = np.log(original/(1-original))
 sns.histplot(transformed, bins = 10)
- : <AxesSubplot:ylabel='Count'>



Boruta

- BorutaShap <u>uses random forest to measure variable importance</u>
- The runtime of Borutashap scales linearly with the number of observations, and thus can take a very long time to run with large datasets

```
# susbet non-redundant predictors (dont keep salary or varaibales and their log versions)

| boruta_data = ceo[["salary", "roe", "ros", "indus", "finance",
| "consprod", "utility", "lsales"]].copy()

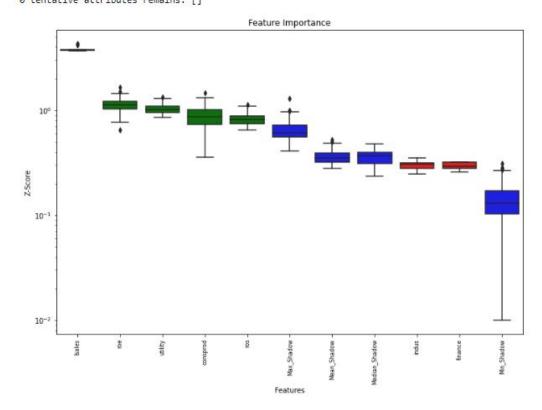
| from BorutaShap import BorutaShap
| x = boruta_data.iloc[:, 1:]
| y = np.log(boruta_data['salary'])

| # if model is not specified in BroutaShap(): default = random forest (just like R and BorutaPy)
| Feature_Selector = BorutaShap(importance_measure='shap', classification=False)
| Feature_Selector.fit(X=x, y=y, n_trials=50, random_state=0)
| Feature_Selector.plot(which_features='all')

| 100% | 50/50 [00:24<00:00, 2.06it/s]
```

Boruta

```
5 attributes confirmed important: ['consprod', 'utility', 'lsales', 'ros', 'roe']
2 attributes confirmed unimportant: ['finance', 'indus']
0 tentative attributes remains: []
```



N 1 # Returns a subset of the original data with the selected features 2 Feature_Selector.Subset()

1:						
		utility	roe	consprod	Isales	ros
1	0	0	14.1	0	10.225389	191
	1	0	10.9	0	9.206132	13
	2	0	23.5	0	8.720281	14
	3	0	5.9	0	9.695602	-21
	4	0	13.8	0	9.988894	56

Mallows CP

- Mallows CP is another metric that we can use to tell us the best subset of features to include in our model
- The mallow() function from RegscorePy allows us to make this calculation by plugging in:
 - The observed values (y)
 - The fitted values from the full regression (y_pred)
 - The fitted values from a regression on a feature subset (y_sub)
 - The number of parameters in the full regression (k)
 - The number of parameters in the subset regression (p)

```
from RegscorePy import mallow

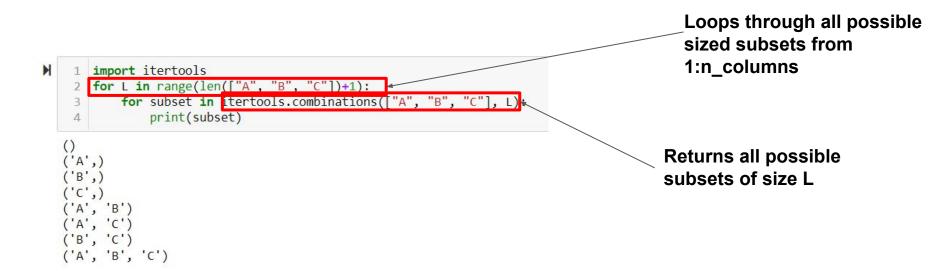
model = smf.ols(formula='np.log(salary) ~ roe + np.log(sales) + consprod +ros + utility + finance + utility', data=ceo)
results = model.fit()
y = np.log(ceo['salary'])
y_pred=results.fittedvalues

# You need to run each sub regression individually, and get the score for each subset
# Using subset size =1
mr_sub = smf.ols(formula='np.log(salary) ~ lsales +consprod', data=ceo)
mr_sub_fit = mr_sub.fit()
y_sub=mr_sub_fit.fittedvalues

k = 8 # number of parameters in orginal model (includes y-intercept)
p = 3 # number of parameters in the subset model (includes y-intercept)
mallow.mallow(y, y_pred,y_sub, k, p)
```

Subsets Loop

- Every subset of features needs to be run individually
- This can be done in a for loop
- The itertools.combinations() function will generate all possible subsets of an iterable object (like a list)
- Then we can combine this with the code in the previous slide to calculate Mallow's CP on all subsets
- Note that we have to cut out the empty set in the full code



Mallows CP Loop

```
subdat = ceo[['salary', 'roe', 'ros', 'indus', 'finance', 'consprod', 'utility', 'lsales']].copy()
```

```
1 import itertools
 3 # get the base model, y and its fitted values
 4 model = smf.ols(formula='np.log(salary) ~ roe + lsales + consprod +ros + utility + finance + utility', data=ceo)
 5 results = model.fit()
 6 y = np.log(ceo['salary'])
 7 y pred=results.fittedvalues
10 storage cp = pd.DataFrame(columns = ["Variables", "CP"])
11 k = 8 # number of parameters in orginal model (includes y-intercept)
12
for L in range(1, len(subdat.columns[1:]) + 1):
       for subset in itertools.combinations(subdat.columns[1:], L):
14
15
16
           # join the strings in the data together
17
           formula1 = 'np.log(salary)~'+'+'.join(subset)
18
           # get the cp
19
           results = smf.ols(formula=formula1, data = ceo).fit()
20
21
           y sub = results.fittedvalues
           p = len(subset)+1 # number of parameters in the subset model (includes y-intercept)
22
23
           cp = mallow.mallow(y, y pred,y sub, k, p)
24
26
           # add to the dataframe
27
           storage cp = storage cp.append({'Variables': subset, 'CP': cp}, ignore index = True)
```

Exercises Boruta and Mallow's CP

- Use the boruta algorithm to select the optimal subset of variables
- Use the following to get started:

```
boruta_data = data[["wage", "exper", "tenure", "female", "nonwhite"]].copy()

from BorutaShap import BorutaShap
    x = boruta_data.iloc[:, 1:]
    y = np.log(boruta_data['wage'])
```

 Calculate Mallow's CP for a regression using the full model above and a sub-regression containing only education as a regressor