# Regression Models with **Regularization**

#### **OVERVIEW**

- Norm of a vector
- Linear Regression Loss function
- Ridge and LASSO regression
- Example: Regression with regularization
- Logistic Regression Loss function
- Example: Logistic regression with regularization

#### **INTRODUCTION**

# Regression models with regularization

- Ridge regression (L2 regularization)
- LASSO regression (L1 regularization)
- Elastic net regression

# Norm of a Vector

Norm of a vector → a measure of the length of a vector

Vector 
$$\underline{b}' = [b_1, ..., b_m]$$

$$\ell_2$$
 norm

$$\ell_1$$
 norm

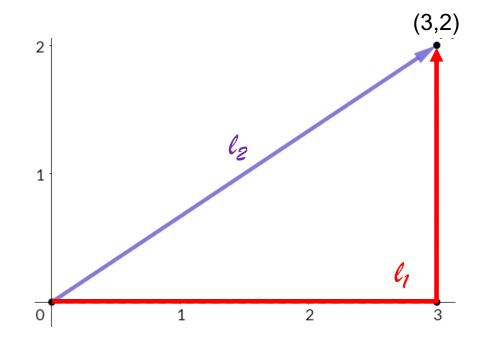
$$||b||_2 = \sqrt{b_1^2 + \dots + b_m^2}$$

$$||b||_1 = |b_1| + \cdots + |b_m|$$

# Norm of a vector a measure of the length of a vector

$$\|b\|_2 = \sqrt{3^2 + 2^2}$$

$$||b||_1 = |3| + |2|$$





# Ridge and LASSO Regression Models

#### **LOSS FUNCTION = COST FUNCTION**

# Linear Regression loss function (sum of squared errors)

$$\min_{b_0, \dots, b_p} SSE = \sum_{i=1}^n (y_i - \hat{y_i})^2$$

Find  $b_0, ..., b_p$ that minimize SSE

#### **LOSS FUNCTIONS**

# **Linear Regression** loss function

$$\min_{b_0,...,b_p} SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Find  $b_0, ..., b_p$ that minimize SSE

# Ridge Regression loss function

$$\underset{b_0, \dots, b_p}{\text{Min}} \quad SSE = \sum_{i=1}^{n} (y_i - \hat{y_i})^2 + \alpha \sum_{i=1}^{p} b_i^2$$

This term prevents large  $b_1, ..., b_p$ 

penalty

#### **RIDGE REGRESSION**

## Ridge Regression loss function

$$\min_{b_0, \dots, b_p} SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \alpha \sum_{i=1}^p b_i^2$$

- $\alpha$  is the *regularization* parameter
- If  $\alpha = 0$  (no regularization)

#### **RIDGE REGRESSION**

# Ridge Regression model

loss function

$$\min_{b_0,...,b_p} SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \alpha \sum_{i=1}^{p} b_i^2$$

with solution

$$\underline{b} = [X'X + \alpha I]^{-1} X'Y$$

#### **LASSO REGRESSION**

# **LASSO** Regression model

loss function

$$\min_{b_0, \dots, b_p} SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \alpha \sum_{i=1}^p |b_i|$$

- This loss function prevents large regression coefficients
- If  $\alpha$  is large, some regression coefficients are equal to zero resulting in a model with less predictors

#### **RIDGE AND LASSO LOSS FUNCTIONS**

.

$$\underset{b_0,...,b_p}{\text{Min}} \quad SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \alpha ||b||_2^2$$

$$\min_{b_0,...,b_p} SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \alpha ||b||_1$$



# Example Baseball Players

- The Hitters.csv file includes data about baseball players, such as their salary and 19 player's performance measures
- To predict the player's salary we will fit regression models with regularization
- We start by removing all rows with missing values in column Salary

- Fit 100 ridge regression models with  $10^{-2} < \alpha < 10^{10}$
- Show how the coefficients  $b_1, b_2, \dots, b_{19}$  shrink when  $\alpha$  increases
- Find the best value for  $\alpha$  using
  - holdout cross validation
  - 5-fold cross validation
- Use the best  $\alpha$  value to fit a ridge regression model
- Compute the test MSE
- Repeat with LASSO regression

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
# for holdout cv
from sklearn.model selection import train test split
# for K-fold cv
from sklearn.model_selection import GridSearchCV
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import MinMaxScaler
from sklearn.metrics import mean_squared_error
from sklearn.linear_model import Ridge, Lasso
```

```
df = pd.read_csv('Hitters.csv')
df.shape

(322, 20)

first 16 columns
```

df[:5]

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	CWalks	League	Division	PutOuts
0	293	66	1	30	29	14	1	293	66	1	30	29	14	Α	E	446
1	315	81	7	24	38	39	14	3449	835	69	321	414	375	N	W	632
2	479	130	18	66	72	76	3	1624	457	63	224	266	263	Α	W	880
3	496	141	20	65	78	37	11	5628	1575	225	828	838	354	N	Е	200
4	321	87	10	39	42	30	2	396	101	12	48	46	33	N	Е	805

```
df = pd.read_csv('Hitters.csv')
df.shape

(322, 20)

last 15 columns
```

df.iloc[:5,-15:]



	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	CWalks	League	Division	PutOuts	Assists	Errors	Salary	NewLeague
0	14	1	293	66	1	30	29	14	Α	Е	446	33	20	NaN	А
1	39	14	3449	835	69	321	414	375	N	W	632	43	10	475.0	N
2	76	3	1624	457	63	224	266	263	Α	W	880	82	14	480.0	А
3	37	11	5628	1575	225	828	838	354	N	Е	200	11	3	500.0	N
4	30	2	396	101	12	48	46	33	N	Е	805	40	4	91.5	N

```
# drop NAs
```

```
d0 = df.dropna()
d0.shape

(263, 20)
```

```
df = pd.read_csv('Hitters.csv')
df.shape

(322, 20)

df.iloc[:5,-15:]
```

	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	CWalks	League	Division	PutOuts	Assists	Errors	Salary	NewLeague
0	14	1	293	66	1	30	29	14	А	Е	446	33	20	NaN	А
1	39	14	3449	835	69	321	414	375	N	W	632	43	10	475.0	N
2	76	3	1624	457	63	224	266	263	Α	W	880	82	14	480.0	А
3	37	11	5628	1575	225	828	838	354	N	Е	200	11	3	500.0	N
4	30	2	396	101	12	48	46	33	N	Е	805	40	4	91.5	N

```
# drop NAs
```

```
d0 = df.dropna()
d0.shape
(263, 20)
```

```
y = d0.Salary
x0 = d0.drop(['Salary'],axis=1)
```

x0.dtypes	
AtBat	int64
Hits	int64
HmRun	int64
Runs	int64
RBI	int64
Walks	int64
Years	int64
CAtBat	int64
CHits	int64
CHmRun	int64
CRuns	int64
CRBI	int64
CWalks	int64
League	object
Division	object
PutOuts	int64
Assists	int64
Errors	int64
NewLeague	object

y = d0.Salary

x0 = d0.drop(['Salary'],axis=1)

#### Ridge Regression - One-hot Encoding with pd.get\_dummies()

Assists	Errors	League_N	Division_W	NewLeague_N
43	10	1	1	1
82	14	0	1	0
11	3	1	0	1
40	4	1	0	1

```
X = x.astype('float64')
```

x.dtypes	
AtBat	int64
Hits	int64
HmRun	int64
Runs	int64
RBI	int64
Walks	int64
Years	int64
CAtBat	int64
CHits	int64
CHmRun	int64
CRuns	int64
CRBI	int64
CWalks	int64
PutOuts	int64
Assists	int64
Errors	int64
League_N	uint8
Division_W	uint8
NewLeague N	uint8

#### **Ridge Regression** – Find 100 values in the interval $0.01 < \alpha < 10^{10}$

```
# Create a 1D array of 100 alpha values
# ranging from very small to very large
alphas = 10**np.linspace(10,-2,100)
                           split interval (10,-2) into
                           100 subintervals
alphas.shape
(100,)
# 10^{(-2)}
alphas.min()
0.01
# 10^10
alphas.max()
10000000000.0
```

```
# fit 100 Ridge regression models,
# one for each alpha (scaling all cols)

scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)

model = Ridge()

coefs = []
for a in alphas:
    model.set_params(alpha = a)
    model.fit(X_scaled, y)
    coefs.append(model.coef_)

coefs is a list of 1D arrays (vectors)
The arrays have the regression coefficients
```

#### **Ridge Regression** – Find 100 values in the interval $0.01 < \alpha < 10^{10}$

```
# Create a 1D array of 100 alpha values
# ranging from very small to very large
alphas = 10**np.linspace(10,-2,100)
                           split interval (10,-2) into
                           100 subintervals
alphas.shape
(100,)
# 10^{(-2)}
alphas.min()
0.01
# 10^10
alphas.max()
100000000000.0
```

```
# fit 100 Ridge regression models,
# one for each alpha (scaling all cols)
scaler = StandardScaler()
scaler.fit(X)
X scaled = scaler.transform(X)
model = Ridge()
coefs = []
for a in alphas:
    model.set params(alpha = a)
    model.fit(X scaled, y)
    coefs.append(model.coef )
# Store regression coeffs
df = pd.DataFrame(coefs)
df.columns = x.columns
df.index = alphas
df.index.name = 'alpha'
```

prodictors

 DataFrame with ridge regression coefficients

	predictors									
	PutOuts	Assists	Errors	League_N	Division_W	NewLeague_N				
alpha										
1.000000e+10	0.000	0.000	-0.000	-0.000	-0.000	-0.000				
7.564633e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000				
5.722368e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000				
4.328761e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000				
3.274549e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000				
3.053856e-02	78.762	53.500	-22.255	31.264	-58.504	-12.455				
2.310130e-02	78.762	53.557	-22.233	31.261	-58.482	-12.430				
1.747528e-02	78.762	53.600	-22.216	31.258	-58.466	-12.411				
1.321941e-02	78.762	53.632	-22.203	31.256	-58.453	-12.396				
1.000000e-02	78.761	53.657	-22.193	31.255	-58.444	-12.385				

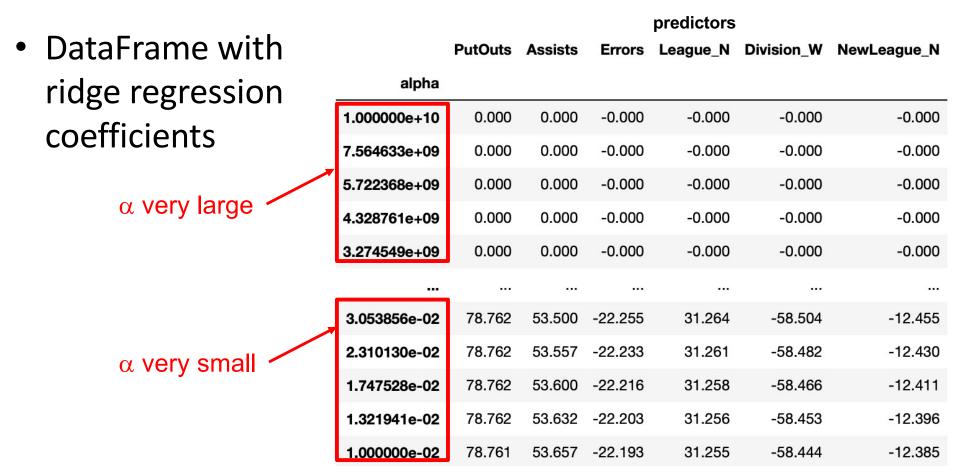
predictors

 DataFrame with ridge regression coefficients

model 1

model 100

	predictors								
	PutOuts	Assists	Errors	League_N	Division_W	NewLeague_N			
alpha									
1.000000e+10	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
7.564633e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
5.722368e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
4.328761e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
3.274549e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
•••									
3.053856e-02	78.762	53.500	-22.255	31.264	-58.504	-12.455			
2.310130e-02	78.762	53.557	-22.233	31.261	-58.482	-12.430			
1.747528e-02	78.762	53.600	-22.216	31.258	-58.466	-12.411			
1.321941e-02	78.762	53.632	-22.203	31.256	-58.453	-12.396			
1.000000e-02	78.761	53.657	-22.193	31.255	-58.444	-12.385			



 DataFrame with ridge regression coefficients

 $\alpha$  very large

		predictors									
	PutOuts	Assists	Errors	League_N	Division_W	NewLeague_N					
alpha											
1.000000e+10	0.000	0.000	-0.000	-0.000	-0.000	-0.000					
7.564633e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000					
5.722368e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000					
4.328761e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000					
3.274549e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000					
3.053856e-02	78.762	53.500	-22.255	31.264	-58.504	-12.455					
2.310130e-02	78.762	53.557	-22.233	31.261	-58.482	-12.430					
1.747528e-02	78.762	53.600	-22.216	31.258	-58.466	-12.411					
1.321941e-02	78.762	53.632	-22.203	31.256	-58.453	-12.396					
1.000000e-02	78.761	53.657	-22.193	31.255	-58.444	-12.385					
3.274549e+09  3.053856e-02 2.310130e-02 1.747528e-02 1.321941e-02	78.762 78.762 78.762 78.762 78.762	0.000  53.500 53.557 53.600 53.632	-0.000  -22.255 -22.233 -22.216 -22.203	-0.000  31.264 31.261 31.258 31.256	-0.000  -58.504 -58.482 -58.466 -58.453	-0.00 -12.45 -12.45 -12.35					

19 predictors

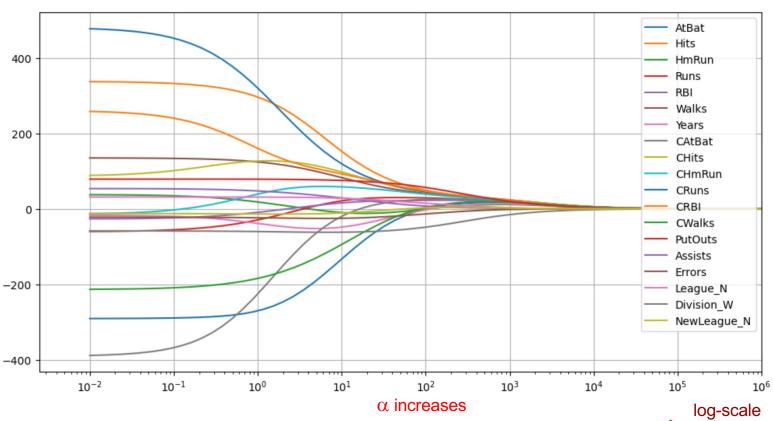
- DataFrame with ridge regression coefficients
- How does each ridge regression coefficient changes with alpha?

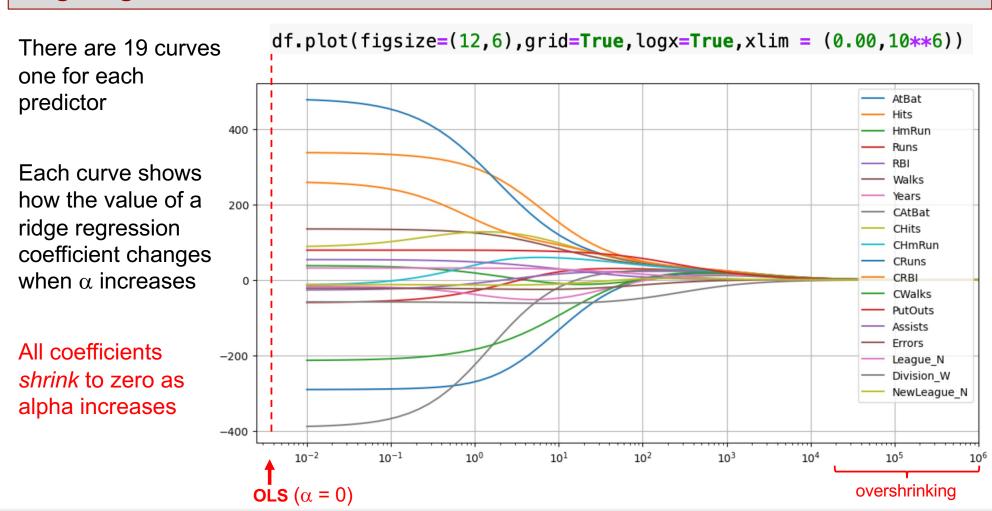
	predictors								
	PutOuts	Assists	Errors	League_N	Division_W	NewLeague_N			
alpha									
1.000000e+10	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
7.564633e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
5.722368e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
4.328761e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
3.274549e+09	0.000	0.000	-0.000	-0.000	-0.000	-0.000			
•••									
3.053856e-02	78.762	53.500	-22.255	31.264	-58.504	-12.455			
2.310130e-02	78.762	53.557	-22.233	31.261	-58.482	-12.430			
1.747528e-02	78.762	53.600	-22.216	31.258	-58.466	-12.411			
1.321941e-02	78.762	53.632	-22.203	31.256	-58.453	-12.396			
1.000000e-02	78.761	53.657	-22.193	31.255	-58.444	-12.385			

There are 19 curves one for each predictor

Each curve shows how the value of a ridge regression coefficient changes when α increases

df.plot(figsize=(12,6),grid=True,logx=True,xlim = (0.00,10\*\*6))







# **Holdout Cross Validation**

#### Ridge Regression - Holdout Cross Validation with fixed alpha

#### fit model with alpha = 4

```
ridge2 = Ridge(alpha=4)
ridge2.fit(X_train_scaled, y_train)
pred2 = ridge2.predict(X_test_scaled)
mspe = mean_squared_error(y_test, pred2)
mspe
```

102144.52395076505

#### fit model with huge alpha = 10<sup>9</sup>

```
ridge3 = Ridge(alpha=10**9)
ridge3.fit(X_train_scaled, y_train)
pred3 = ridge3.predict(X_test_scaled)
mspe = mean_squared_error(y_test, pred3)
mspe
```

172862.0826375247

Huge alpha makes coefficients very close to zero which increases MSPE

#### Ridge Regression - Holdout Cross Validation - Comparing test MSE

#### fit model with alpha = 4

```
ridge2 = Ridge(alpha=4)
ridge2.fit(X_train_scaled, y_train)
pred2 = ridge2.predict(X_test_scaled)
mspe = mean_squared_error(y_test, pred2)
mspe
```

102144.52395076505

#### **Linear Regression (alpha = 0)**

```
ols_model = Ridge(alpha=0)
ols_model.fit(X_train_scaled, y_train)
pred = ols_model.predict(X_test_scaled)
ols_mse = mean_squared_error(y_test, pred)
ols_mse
```

116690.468566612

#### fit model with huge alpha = 10<sup>9</sup>

```
ridge3 = Ridge(alpha=10**9)
ridge3.fit(X_train_scaled, y_train)
pred3 = ridge3.predict(X_test_scaled)
mspe = mean_squared_error(y_test, pred3)
mspe
```

172862.0826375247

Huge alpha makes coefficients very close to zero which increases MSPE

#### Ridge Regression - Holdout Cross Validation searching for alpha

#### Ridge Regression - Holdout Cross Validation searching for alpha

```
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_validation_scaled = scaler.transform(X_validation)

ridge_model = Ridge()

validation_mspes = []

for a in alphas:
    ridge_model.set_params(alpha = a)
    ridge_model.fit(X_train_scaled, y_train)
    yhat = ridge_model.predict(X_validation_scaled)
    mspe = mean_squared_error(y_validation,yhat)
    validation_mspes.append(mspe)
```

#### Valid MSE

```
alpha
1.000000e+10 161825.790184
7.564633e+09 161825.786925
5.722368e+09 161825.782617
4.328761e+09 161825.776922
3.274549e+09 161825.769393
```

**0.000000** 116690.468566 OLS

#### Ridge Regression - Holdout Cross Validation searching for alpha

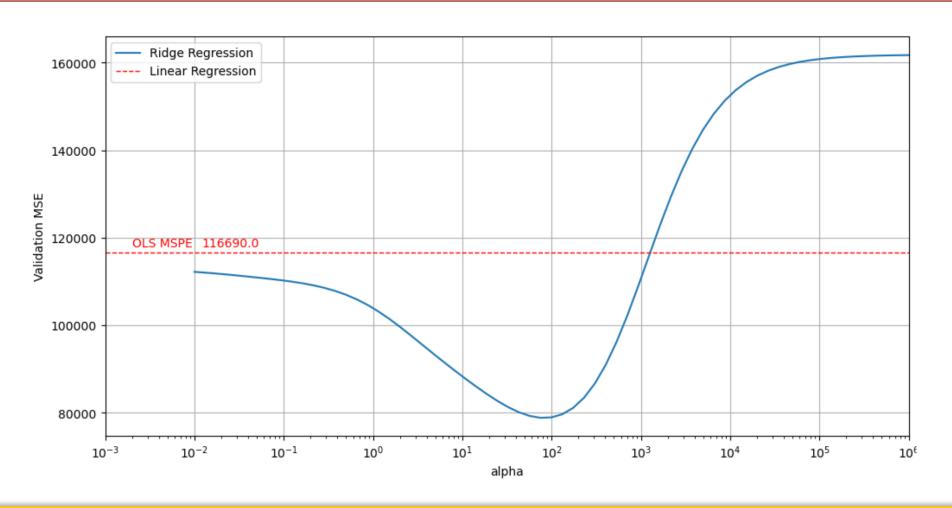
2.310130e-02 111577.207548

1.747528e-02 111800.332935

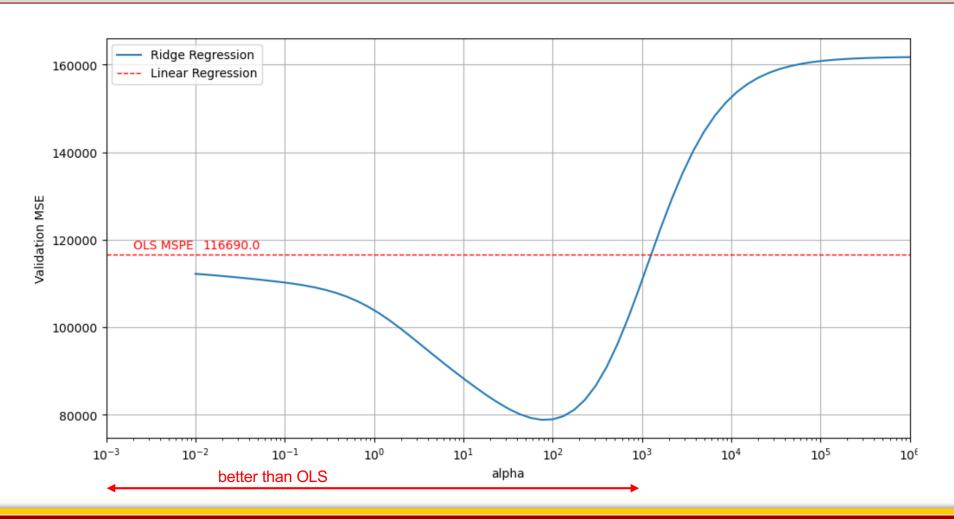
**1.321941e-02** 112003.332742

**1.000000e-02** 112182.439807

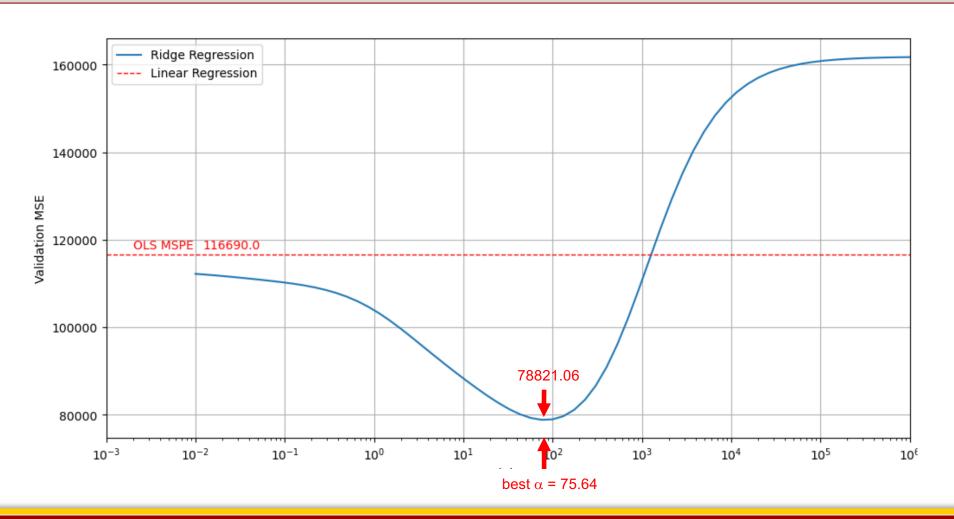
## **Ridge Regression – Validation Approach**



## **Ridge Regression Models better than OLS**



## **Ridge Regression best Model**



#### Ridge Regression – Test MSE from Holdout CV

```
min1 = df.Valid_MSE.min()
min1
                               ← Validation MSE
78821.05978981467
df[df.Valid_MSE == min1]
           Valid MSE
    alpha
 75.646333 78821.05979
# best alpha giving min Validation MSE
best alpha = df.Valid MSE.idxmin()
best alpha
75.64633275546291
```

```
scaler = StandardScaler()
scaler.fit(X_nontest)
X_nontest_scaled = scaler.transform(X_nontest)
X_test_scaled = scaler.transform(X_test)

ridge2 = Ridge(alpha = best_alpha)
ridge2.fit(X_nontest_scaled, y_nontest)
pred2 = ridge2.predict(X_test_scaled)
mspe = mean_squared_error(y_test, pred2)
mspe

99508.83201629658 ← Test MSE
```



# 5-fold Cross Validation

#### Ridge Regression 5-fold cross validation to find best alpha

#### Ridge Regression 5-fold cross validation to find best alpha

```
# best alpha (minimizing validation MSE)
X_train,X_test,\
                                                            ridgecv.best_params_
y_train,y_test = train_test_split(X,y,test_size=0.5,
                                 random state=1)
                                                            {'ridge alpha': 100.0}
scaler = StandardScaler()
                                                            alpha1 = ridgecv.best params ['ridge alpha']
scaler.fit(X_train)
                                                            alpha1
X_train_scaled = scaler.transform(X_train)
X test scaled = scaler.transform(X test)
                                                            100.0
scaler = StandardScaler()
                                                            # test MSE with best alpha
model = Ridge()
pipe1 = Pipeline([('scaler', scaler),('ridge', model)])
                                                            # fit RR model with best alpha
                                                            ridge1 = Ridge(alpha=alpha1)
param grid = {'ridge alpha': alphas}
                                                            ridge1.fit(X train scaled,y train);
ridgecv = GridSearchCV(pipe1,param grid,cv = 5,
                                                            yhat = ridge1.predict(X test scaled)
                       scoring = 'neg mean squared error')
                                                            best mspe = mean squared error(y test, yhat)
ridgecv.fit(X_train, y_train);
                                                            best_mspe
                                                                                    ← Test MSF
                                                            99586.56834382795
```

#### **PREDICTION**

	ridge_coeff		
AtBat	3.911359	CHmRun	41.512925
Hits	36.096360	CRuns	33.271936
HmRun	1.736680	CRBI	41.571334
Runs	19.611659	CWalks	25.535833
RBI	32.219132	PutOuts	75.761366
Walks	43.972410	Assists	-2.475953
Years	8.496447	Errors	-0.792667
CAtBat	17.992839	League_N	8.214298
CHits	32.545056	Division_W	-41.608368
CHmRun	41.512925	NewLeague_N	5.211955

#### **PREDICTION**

#### predict salary of first player in test set

```
X_test[:1]
    AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI CWalks
126 282.0 78.0
                 13.0
                      37.0 51.0
                                29.0
                                      5.0 1649.0 453.0
                                                         73.0
                                                               211.0 280.0
                                                                           138.0
newval = X_test_scaled[:1]
newval
array([[-0.75403349, -0.59086622, 0.20177987, -0.63314908, -0.00973381,
        -0.45405721, -0.50193827, -0.42197414, -0.40314783, 0.01162816,
        -0.43551916, -0.17330772, -0.4452582, 1.27997267, -0.33878194,
        -0.44171974, -1.03892496, 0.99239533, -1.00766295]])
ridge1.predict(newval)
array([461.60866494])
y_test[:1]
126
       500.0
Name: Salary, dtype: float64
```

Predicted Salary →

Actual Salary →