Gradient Descent, Regularization and Grid Search

Agenda

- Gradient Descent
  - Batch Gradient Descent
  - Stochastic Gradient Descent
  - Mini Batch Gradient Descent
- Overfitting
- Regularization
  - Ridge Regression
  - Lasso Regression
  - Elastic-Net Regression
- Grid Search

Supervised Linear Regression

In this session we shall cover:

- Gradient descent: obtain the model parameters
- Regularization: fine tune the model
- Grid Search: fine tune the hyperparameters

Gradient Descent

$$\underbrace{\text{Gradient}}_{\text{Slope}}\ \underbrace{\text{Descent}}_{\text{Moving Downwards}}$$

What is a cost function?

- A cost function tells how good the model performs at making predictions for a given set of parameters

- Cost function = Loss function = Error function

- For linear regression, the cost function is given by the sum of squares of residuals, i.e.

$$Error = \sum_{i=1}^{n} \left(y_{act} - y_{pred}\right)^2$$

where y_{act} is the actual value and y_{pred} is the predicted value

The gradient descent

- The gradient descent is an optimization technique which finds the parameters such that the error term is minimum

- It is an iterative method which converges to the optimum solution

- It takes large steps when it is away from the solution and takes smaller steps closer to the optimal solution

- The estimates of the parameter are updated at every iteration

Let us consider an example

- We consider the same example that we had for simple linear regression

- However, we shall consider only three observations

- In context with our example,

$$\text{Premium} = \beta_0 + \beta_1 \text{ Mileage} + \varepsilon$$

Mileage	Premium (in dollars)
10	120
13	115
14	135

Let us consider an example

- We shall first estimate for the intercept β_0 and assume a value for β_1

- Let $\beta_1 = 2.5$. This value will be constant in all the iterations

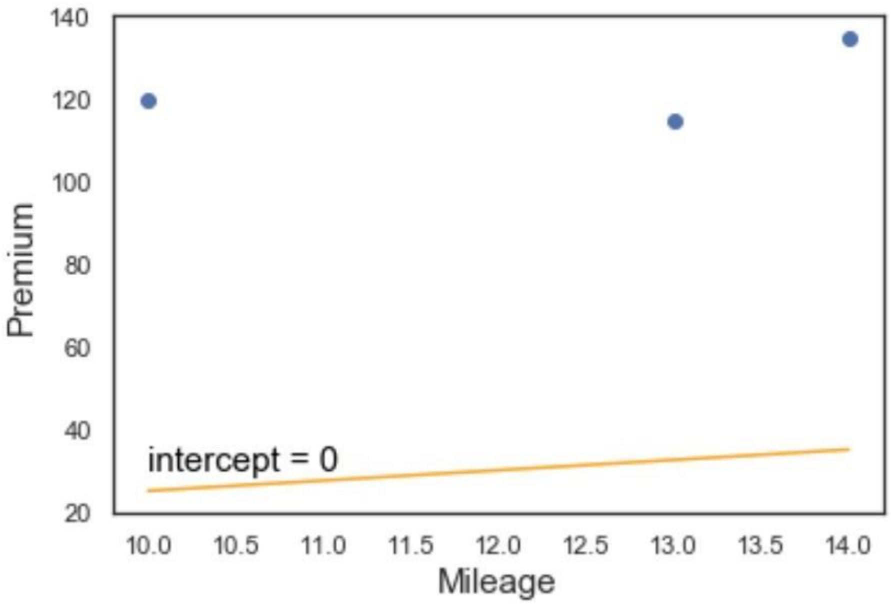
- In context with our example,

$$\text{Premium} = \beta_0 + 2.5 \text{ Mileage} + \varepsilon$$

Mileage	Premium (in dollars)
10	120
13	115
14	135

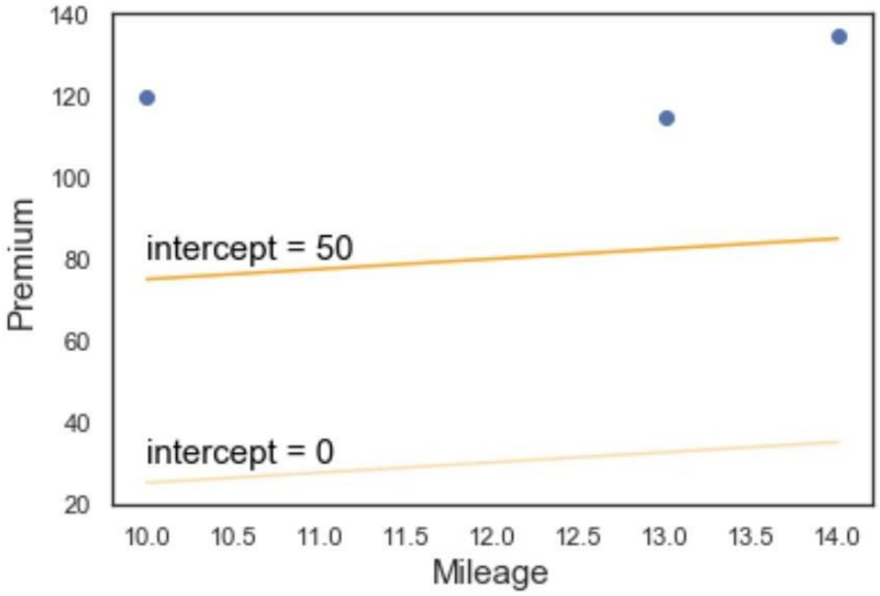
Example: gradient descent

- To estimate β_0, start with some initial value. Let $\beta_0 = 0$
- The line with intercept = 0 is obtained as shown
- We see it is far away from the data points, naturally the cost function value will be high
- The value cost function is 25831.25



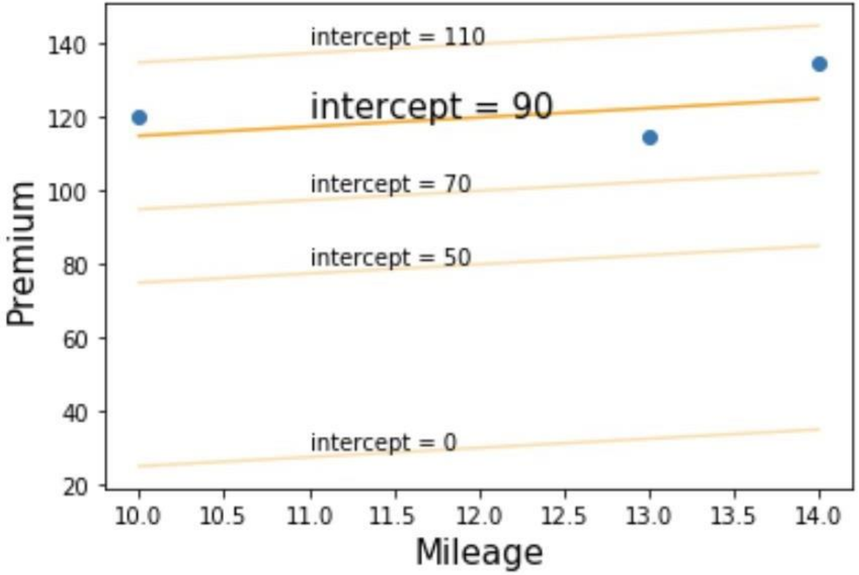
Example: gradient descent

- Now we increase the value of β_0 to 50
- The line with intercept = 50 obtained as shown
- The line has moved towards the data points as a result will have a lower cost function value
- The value cost function drops to 5581.25



Example: gradient descent

- We continue to increase until we obtain the lowest cost function
- The line with intercepts as 0, 50, 70, 90, 110 and 150 are shown
- Note the line with intercept 90 is the closest to points
- For intercept = 90, the value cost function to 181.25



The optimal solution

β_0 value	Cost function
0	25831.25
15	18181.25
30	11881.25
45	6931.25
60	3331.25
75	1081.25
90	181.25
105	631.25
120	1156.25
135	2131.25
150	10081.25

Is β_0= 90 the optimal solution?

The optimal solution

β_0 value	Cost function
0	25831.25
15	18181.25
30	11881.25
45	6931.25
60	3331.25
75	1081.25
90	181.25
105	631.25
120	1156.25
135	2131.25
150	10081.25

Is β_0= 90 the optimal solution?

Answer: Perhaps.

The optimal solution

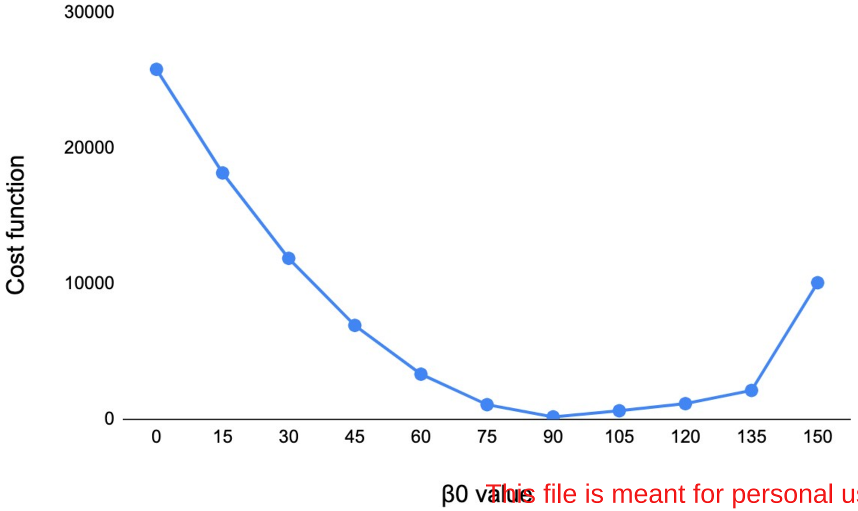
β_0 value	Cost function
88	223.25
88.5	210.5
90	181.25
90.5	174.5
91	169.25
91.5	165.5
92	163.25
92.5	162.5
93	163.25
93.5	165.5
94	164.25
94.5	174.5
95	181.25

- We now take small steps, around 90 to look for values which have minimum cost
- We see for β_0 = 92.5, the cost function is minimum
- In context with our example,

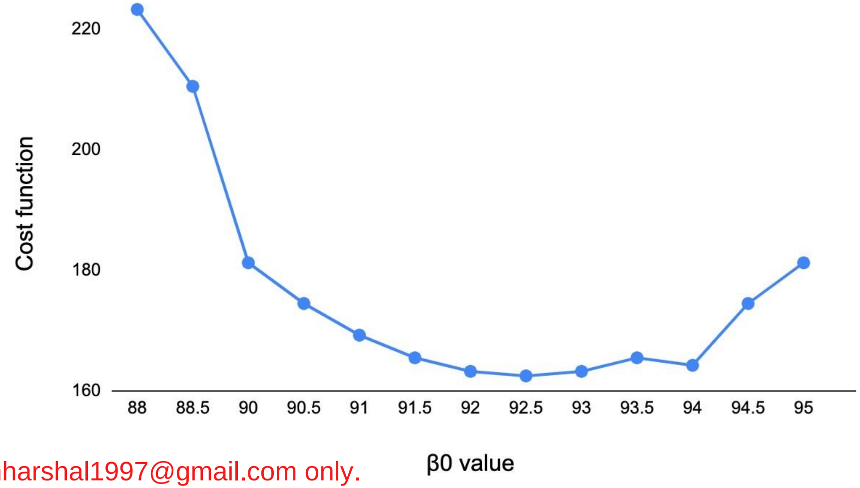
Premium = 92.5 + 2.5 Mileage

The step size

Large steps



Small steps



Gradient descent

Now we have the following questions:

- What should be the step size?
- How did we know the value of the intercept is to be increased?

Gradient descent

Now we have the following questions:

- What should be the step size?

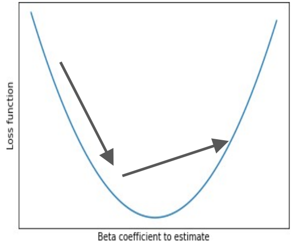
  The step size is the learning rate.

- How did we know the value of the intercept is to be increased?

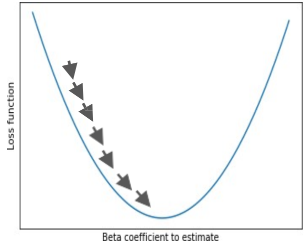
What is a learning rate?

- The gradient descent technique has a hyperparameter called learning rate, α
- It specifies the jumps the algorithm takes to move towards the optimal solution
- For very large α, the algorithm may skip the optimal solution and converges to suboptimal solution
- For very small α, the algorithm is more precise, however computationally expensive
- Thus, it is important to choose an appropriate learning rate

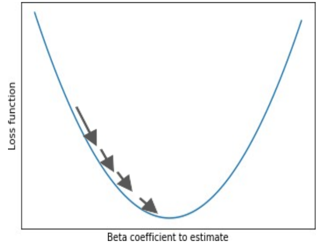
High learning rate



Low learning rate



Adequate learning rate



Gradient descent

Now we have the following questions:

- What should be the step size?

  The step size is the learning rate.

- How did we know the value of the intercept was to be increased?

  It is determined by the derivative of the cost function

Increase/decrease in the parameters

- The parameters are updated as

New parameter = old parameters - (learning rate x derivative)

$$\theta_{new} = \theta_{old} - (\alpha . \delta)$$

- The learning rate is always a positive number

- The gradient descent computes the derivative of the cost function at each iteration. This derivative value determines the increase/decrease in the parameter

Gradient descent procedure

- Start with some initial set of parameters
- Compute the cost function
- The derivative of the cost function (delta: δ) is calculated
- Update the parameters based on learning rate α and derivative δ
- Repeat the procedure until the derivative of cost function is zero

Why gradient descent?

The number of updates required for the algorithm to converge will increase with the increase in the training data.

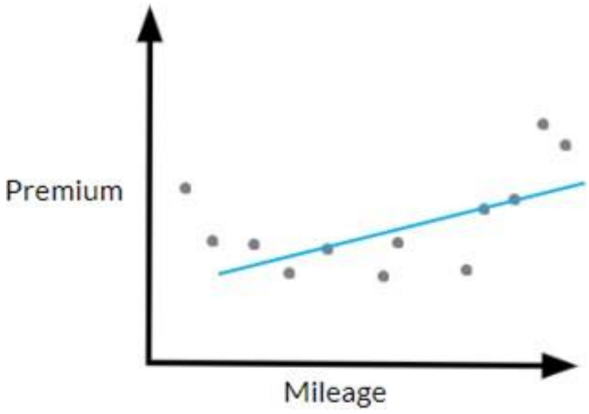
However, as the training data gets larger and larger, it is quite possible for the algorithm to converge much before every instance in the training data is learnt.

In other words, the increase in the training data size need not increase the training time needed to train the best possible model where the test error is at its least.

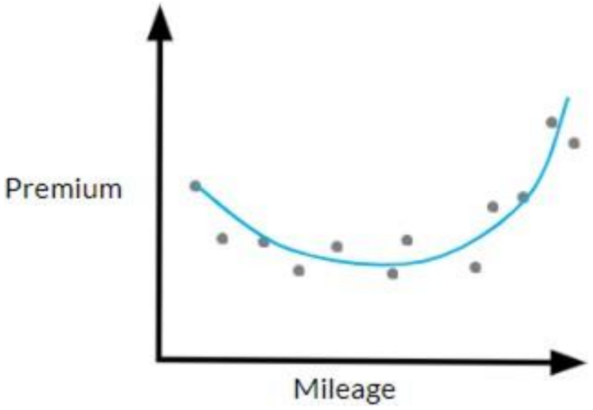
Revisiting Underfitting and Overfitting

Underfitting and overfitting

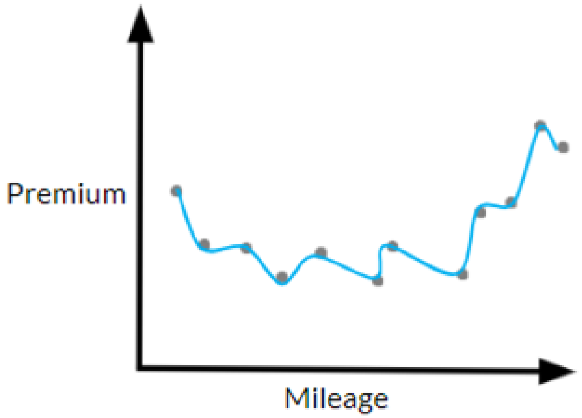
The plot that represents relationship between Premium and Mileage



Underfitted



Good fit/Robust



Overfitted

Overfitting

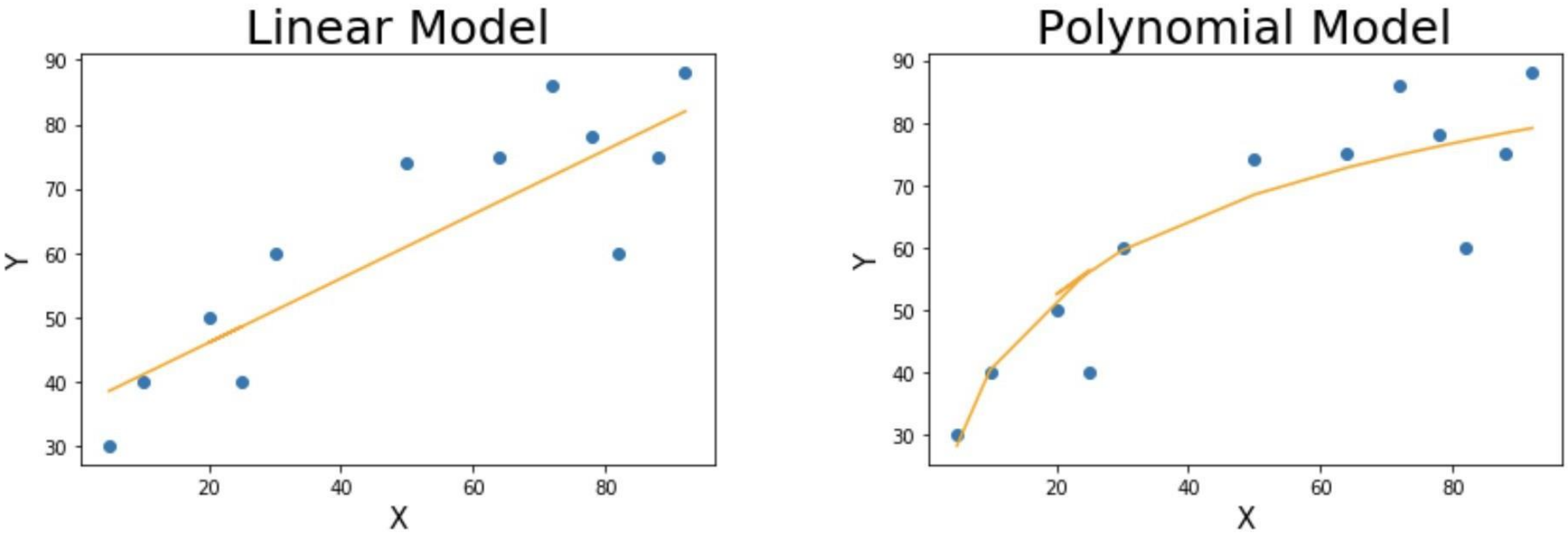
Generalization Error & Overfitting

- If a model performs very well on the training data but does not perform well on the testing data, it is said to have high generalization error

- High generalization error implies overfitting

- Generalization error can be reduced by avoiding overfitting in the model

Polynomial Model



Prevention of overfitting for Linear regression

To make our model more robust and fix the problem of overfitting, we need to:

- Shrink the coefficients or weights of features in model
- Eliminate high degree polynomial feature from a polynomial model

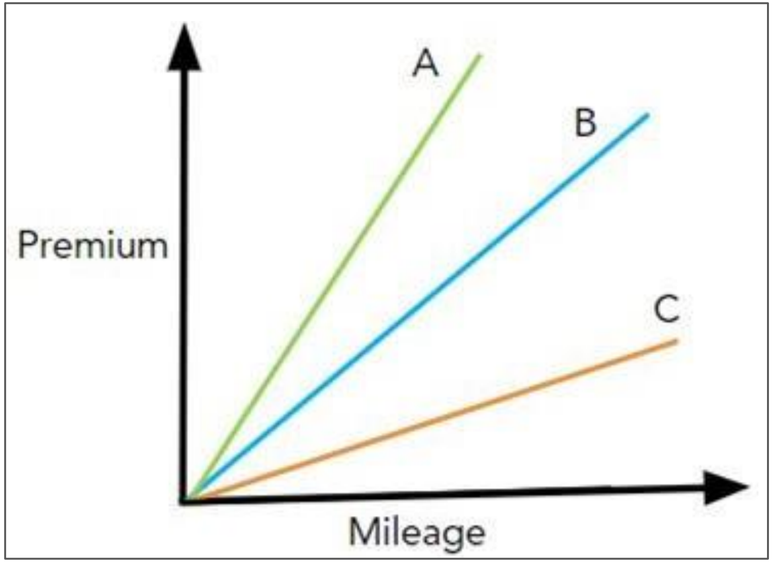
This can be achieved by using regularization.

Prevention of overfitting for Linear regression

To make our model more robust and fix the problem of overfitting, we need to shrink the coefficients or weights of features in model.

This can be achieved by using regularization.

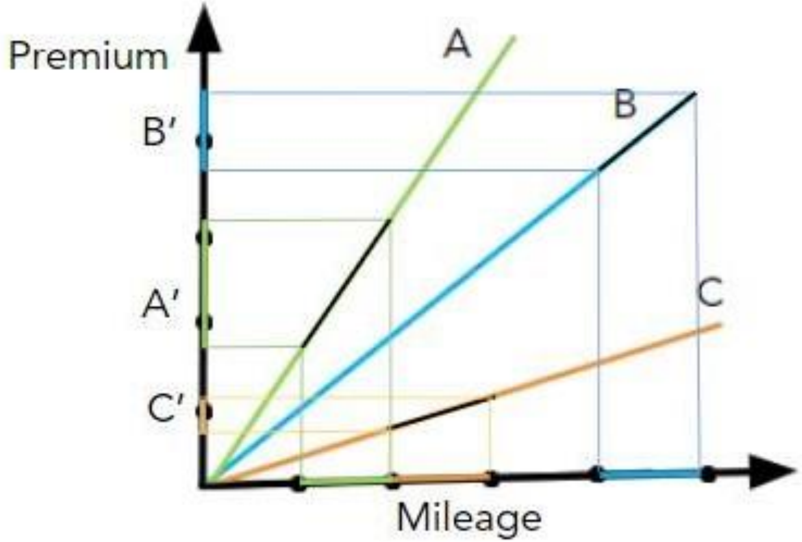
Example: Shrinking the β coefficients



Line A, B and C represent the relationships between Mileage and Premium for different cars.

We use them to study the influence of the regression coefficient on the target variable.

Example: Shrinking the β coefficients



A’ > B’ > C’

- A’, B’ and C’ represent the change in Premium per unit change in Mileage for the three different lines A, B and C respectively
- As we can see that as the slope decreases, the Premium become less sensitive to change in Mileage
- Thus, by reducing the sensitivity of the target variable with respect to the predictor variables, the bias increases

Why do we shrink the β coefficients?

- As we have seen from the Premium and Mileage example with decrease in slope, the dependent variable becomes less sensitive to change in independent variable
- Shrinking the slope introduces bias to the regression model
- With increase in bias, the variance decreases and the problem of overfitting can be fixed

Regularization

What is regularization?

- Regularization refers to the modifications we make to a learning algorithm, that help in reducing its generalization error but not its training error

- Regularization adds a penalty term to the cost function such that the model with higher variance receives a larger penalty

- It chooses a model with smaller parameter values (i.e. shrunk coefficients) that has less error

Regularization for linear regression

- On regularization, for linear regression there are two terms in the loss function
  - The OLS loss function
  - The penalty term

$$\text{Loss function}_{\text{regularization}} = \text{Loss function}_{\text{ols}} + \text{Penalty term}$$

- Regularization tries to balance the error from the loss function of OLS and the penalty term

Regularization for linear regression

- Regularization converges the beta coefficients of the linear regression model towards zero. This is known as shrinkage

- For linear regression the goal is to minimize,

$$\sum_{i=1}^{n} \left(y_{act} - y_{pred}\right)^2 + \text{penalty}$$

penalty = λ * w

λ = Regularization parameter

w = weight associated with the variables; generally considered to be the L-p norms

Regularization parameter

- Regularization parameter (λ) controls the strength of the penalty term

- If λ = 0, then there is no difference between a model with regularization and without regularization

- λ can take any values from 0 to infinity

- The best value for λ is determined by trying different values; the value that leads to least cross validation error is chosen

Types of regularization

- Ridge regression: Here, the w is the L2 norm

- Lasso regression: Here, the w is the L1 norm

- Elastic net regression: It is a combination of ridge and lasso regression

Ridge Regression

Ridge regression

- Ridge regression uses squared L-2 norm regularization i.e it adds a squared L-2 penalty
- Also known as L-2 regularization
- Squared L-2 penalty is equal to squares of magnitudes of β coefficients
- It diminishes the insignificant predictors but does not completely eliminate them

$$\text{cost function} = \underbrace{\sum_{i=1}^{n}\left(\mathrm{y}_{act} - \mathrm{y}_{pred}\right)^2}_{\text{least squares regression error}} + \underbrace{\lambda \cdot ||w||_2^2}_{\text{ridge regression penalty}}$$

Let us consider an example

- We consider the same example as earlier

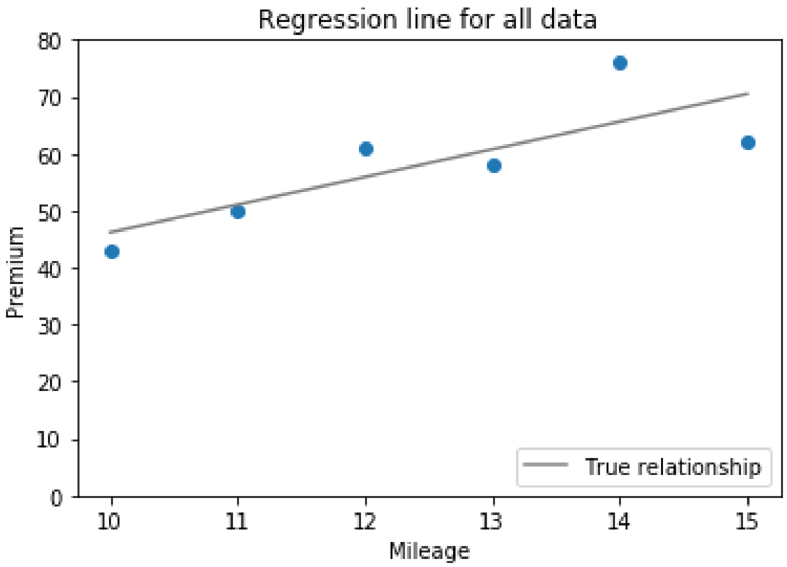
- However, we shall consider the six given observations

- In context with our example,

$$\text{Premium} = \beta_0 + \beta_1 \text{ Mileage} + \varepsilon$$

Mileage	Premium (in dollars)
11	50
14	76
10	43
15	62
13	58
12	61

Simple linear regression - OLS

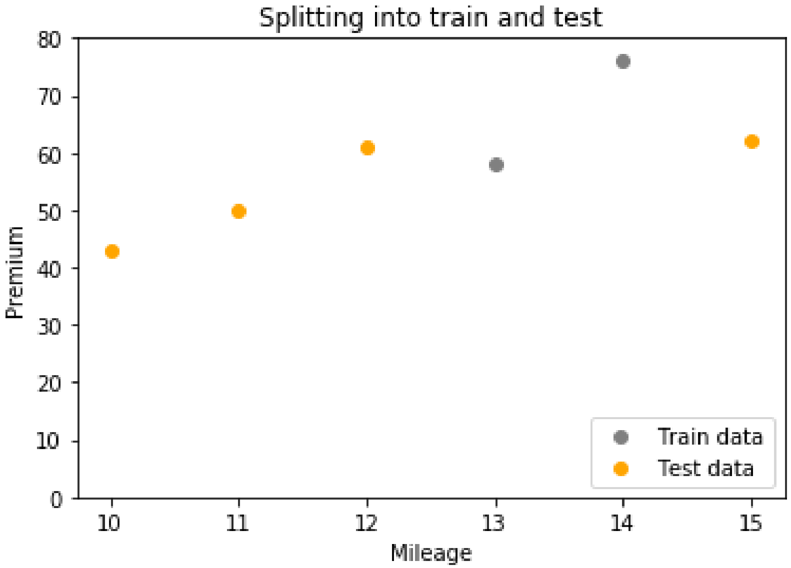


- We plot the graph of Premium against Mileage and estimate a regression line using all the data points, this captures the true relationship

- The equation is given by:

  Premium = -2.3809 + 4.8571 Mileage

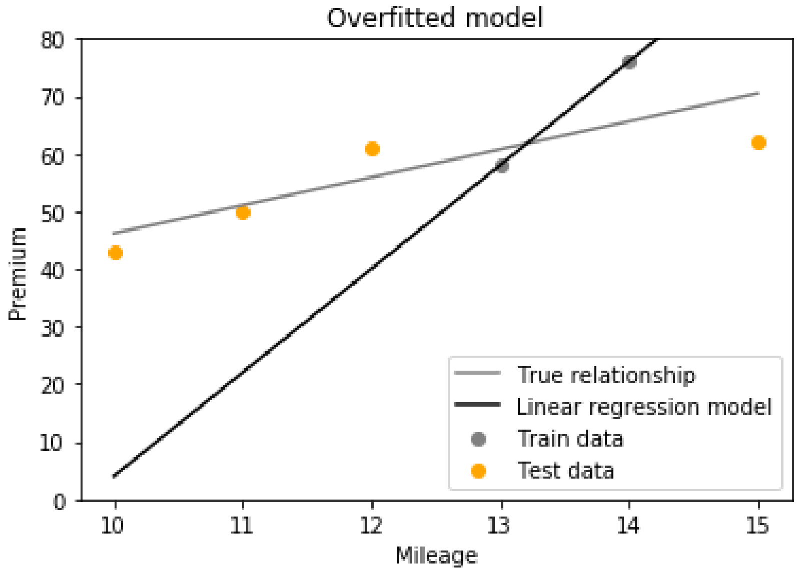
The train-test split



The entire data is split into:

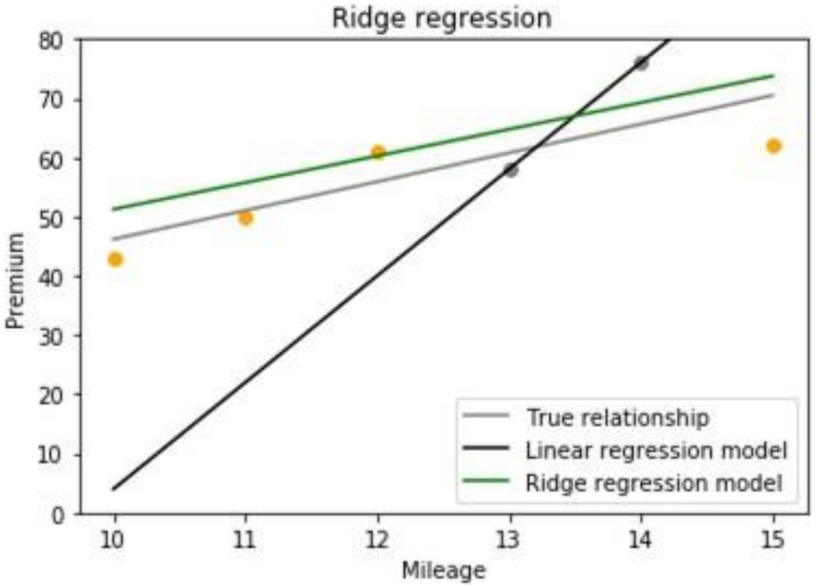
- Train data
- Test data

Overfitted model



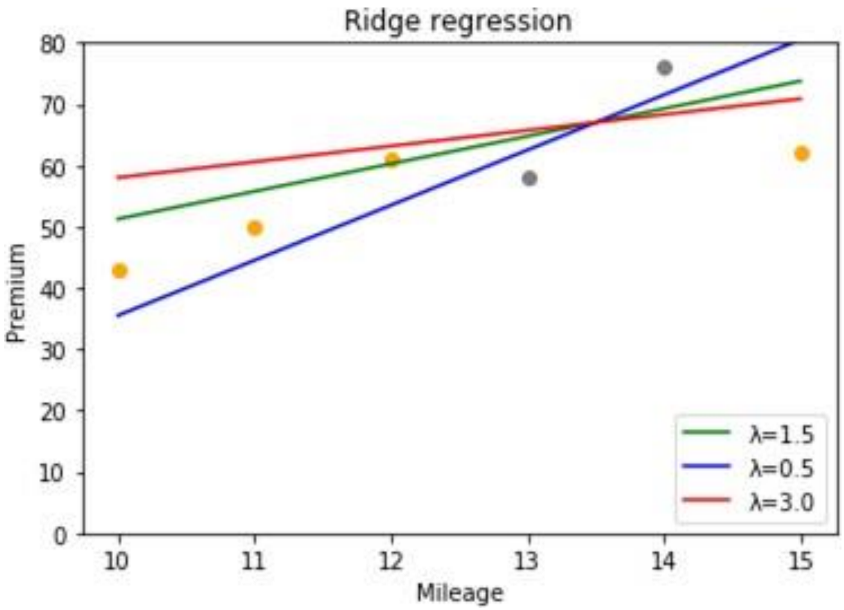
- Compared to the true relationship the black line performs very poorly on test data
- But it fits perfectly for train data, hence it is an overfitted model
- The black line has very high variance

Ridge regression



- Using ridge regression we get green line
- Compared to the black line, the green line is much closer to the line that captures the true relationship
- Hence, the green line performs much better on the test data than the black line

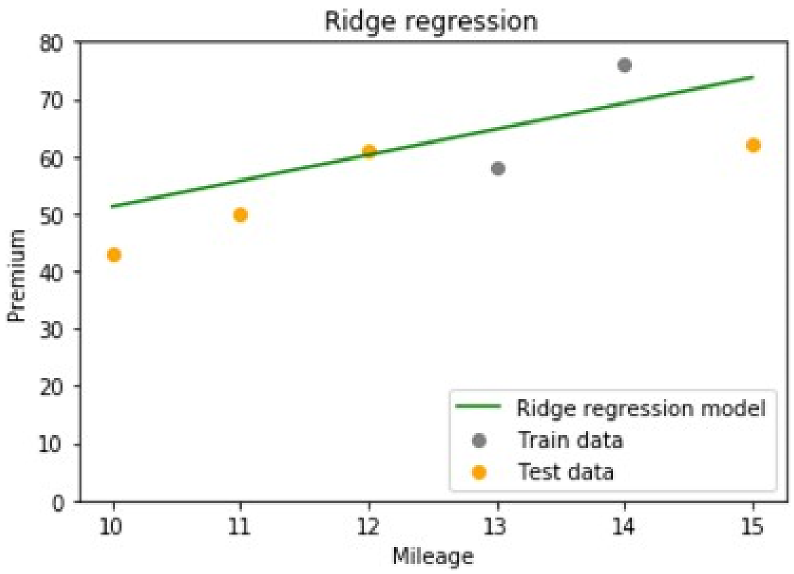
Regularization parameter



λ for model	1.5	0.5	3.0
RMSE	7.7419	11.0114	10.2444

When λ = 1.5, the RMSE value is least for test data, we choose this value

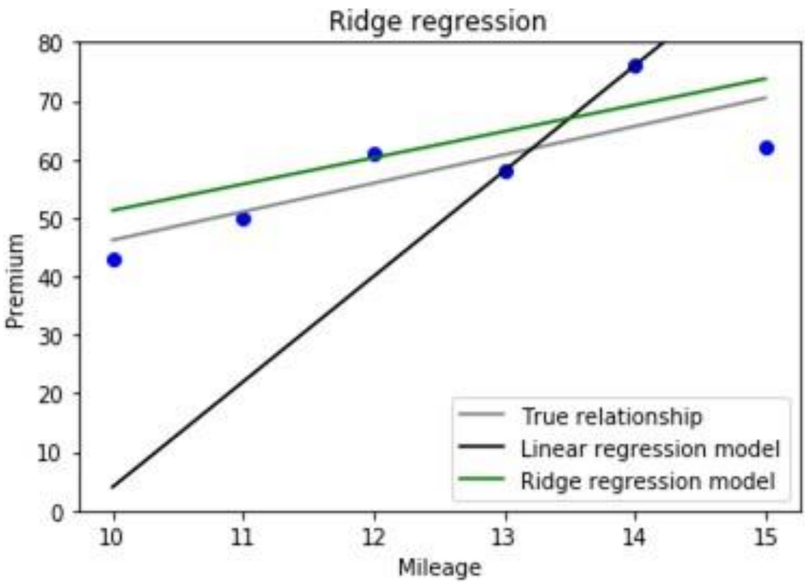
Ridge regression model



- This line introduces some bias to the model but decreases the variance
- The ridge regression line shrinks the β coefficients
- Equation of the green line is given by:

Premium = 6.25 + 4.6 Mileage

Ridge regression penalty

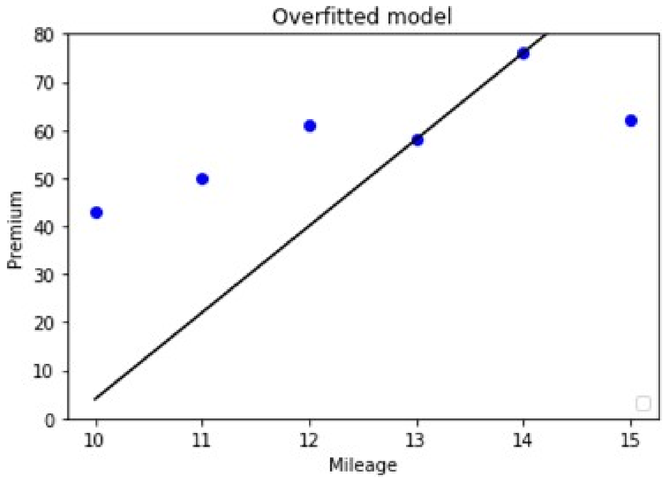


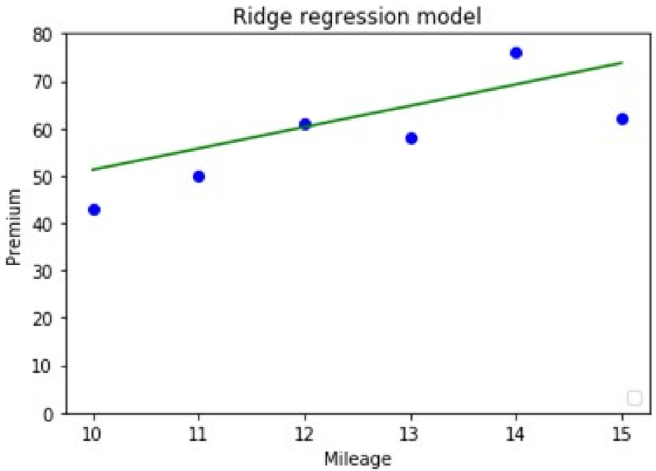
Ridge regression assigns a higher penalty to the model with higher variance

λ * $(\text{slope})^2$	**λ * $(\text{slope})^2$**
486	31.74

Here, λ = 1.5

Comparison of models





	β_0	$\beta_{mileage}$
β Coefficients	-176	18
Cost function	$\sum(\text{Actual Premium} - \text{Predicted Premium})^2$	

	β_0	$\beta_{mileage}$
β Coefficients	6.25	4.6
Cost function	$\sum(\text{Actual Premium} - \text{Predicted Premium})^2 + \lambda^* (\beta_{mileage})^2$	

Lasso Regression

Lasso regression

- Lasso regression uses L-1 norm regularization i.e it adds a L-1 penalty
- Also known as L-1 regularization
- L-1 penalty is equal to absolute value of β coefficients
- It extinguishes the insignificant predictors

$$\text{cost function} = \underbrace{\sum_{i=1}^{n} \left(y_{act} - y_{pred}\right)^2}_{\text{least squares regression error}} + \underbrace{\lambda \cdot ||w||_1}_{\text{lasso regression penalty}}$$

Data

Let us consider the following data.

Mileage	Engine_Capacity	Age	Premium (In dollars)
12.3	1.2	7.9	150
13.1	1.4	1.1	171
12.3	1.2	1.3	123
14.4	1.4	1.4	214
10.6	1.4	10.4	150
8.6	1.6	8.6	286
19.3	1.4	2.1	221
9.4	1.4	1.4	194
7.3	1.2	2.6	127
7.6	1.2	7	157
17.8	1.8	5	170
11.2	1.2	6.1	187
8.9	1.4	6.3	154
7.4	1.4	4	134
13	1.6	3	123
8	1.8	6	245

The train-test split

We divide the data into :

- **Train data**
- **Test data**

Mileage	Engine_Capacity	Age	Premium (In dollars)
12.3	1.2	7.9	150
13.1	1.4	1.1	171
12.3	1.2	1.3	123
14.4	1.4	1.4	214
10.6	1.4	10.4	150
8.6	1.6	8.6	286
19.3	1.4	2.1	221
9.4	1.4	1.4	194
7.3	1.2	2.6	127
7.6	1.2	7	157
17.8	1.8	5	170
11.2	1.2	6.1	187
8.9	1.4	6.3	154
7.4	1.4	4	134
13	1.6	3	123
8	1.8	6	245

PLEASE!! NOTE

Feature scaling before regularization

The regularization parameter (λ) imposes a higher penalty on the variable with higher magnitude values

To avoid this, we scale all the variables within same range of values

For the considered example, since all the variables in the data do not follow a gaussian distribution we have used min-max normalization

Regression line - OLS method

- We consider the training data and construct a linear regression model to see how the features influence the Premium value

- The equation of estimated line is given by :

$$Premium = 0.2211 - 0.1177\ Mileage + 0.5694\ Engine\_Capacity - 0.0187\ Age$$

Comparison of RMSE values

- We check the train accuracy and test accuracy on train and test data respectively

	Train data	Test data
RMSE	0.2315	0.3139

- A good model that generalizes well needs to have very similar errors on train and test sets

- Here, the difference between errors for train and test sets is significant, hence we can conclude that the model is overfitting the train data

Lasso regression

- We construct a lasso regression model on train data

- The equation of estimated line is given by :

  Premium = 0.3368 - 0 Mileage + 0.0112 Engine_Capacity + 0 Age

- The lasso regression shrinks the β coefficients of variables Mileage and Age to 0, thus eliminating them from the final model

- This is an instance of how lasso regression performs feature selection

Comparison of RMSE values

- We check the train accuracy and test accuracy on train and test data respectively

	Train data	Test data
RMSE	0.2776	0.2754

- The difference between errors for train and test sets is very insignificant
- We can conclude that the lasso regression model performs better at generalization compared to least squares model

Lasso regression penalty

- Lasso regression assigns a higher penalty to the model with higher variance

Penalty	Least squares regression model	Lasso regression model
$\lambda^*(\lvert\beta_0\rvert+\lvert\beta_{Mileage}\rvert+\lvert\beta_{Engine\_Capacity}\rvert+\lvert\beta_{Age}\rvert)$	0.0417	0.0157

- Here $\lambda = 0.045$, is calculated by trying different values

Comparison of models

Regression Model	β coefficients				Cost Function	RMSE	
	β_0	$\beta_{Mileage}$	$\beta_{Engine\_Capacity}$	β_{Age}		Train	Test
Least squares	0.2211	-0.1177	0.5694	-0.0187	$\Sigma(y_{act} - y_{pred})_2$	0.2315	0.3139
Lasso	0.3368	0	0.0112	0	$\Sigma(y_{act} - y_{pred})_2 + \lambda^*\Sigma\|\beta\|$	0.2776	0.2754

Elastic-net Regression

Elastic-net regression

- Elastic-net regression uses both L-1 and L-2 norm regularization

- Elastic-net regression is the combination of lasso and ridge regression

$$\text{cost function} = \underbrace{\sum_{i-1}^{n}\left(\mathrm{y}_{act} - \mathrm{y}_{pred}\right)^2}_{\text{least square regression error}} + \underbrace{\lambda_{\text{ridge}} \cdot ||w||_2^2}_{\text{ridge penalty}} + \underbrace{\lambda_{\text{lasso}} \cdot ||w||_1}_{\text{lasso penalty}}$$

PLEASE!! NOTE

L1 ratio

While implementing elastic net regression the regularization parameters are expressed in terms of λ and L1 ratio

$$\lambda = \lambda_{ridge} + \lambda_{lasso}$$

$$L1\_ratio = \frac{\lambda_{lasso}}{\lambda_{lasso} + \lambda_{ridge}}$$

	Penalty
L1_ratio = 0	L-2
L1_ratio = 1	L-1
0< L1_ratio <1	Combination of L-1 and L-2

Estimation of least squares regression

- We consider the same example considered for ridge regression

- Constructing a linear regression model on training data we get the following equation :

  Premium = 0.2211 - 0.1177 Mileage + 0.5694 Engine_Capacity - 0.0187 Age

Comparison of RMSE values

- We check the train accuracy and test accuracy on train and test data respectively

	Train data	Test data
RMSE	0.2315	0.3139

- A good model that generalizes well needs to have very similar errors on train and test sets
- Here, the difference between errors for train and test sets is significant, hence we can conclude that the model is overfitting the train data

Elastic-net regression

- We construct a elastic-net regression model on train data
- The equation of estimated line is given by :

  Premium = 0.3370 - 0 Mileage + 0.0106 Engine_Capacity + 0 Age

- The elastic-net regression shrinks the β coefficients of variables Mileage and Age to 0, thus eliminating them from the final model

Comparison of RMSE values

- We check performance of the elastic-net regression model trained on training data, on the entire data, (train and test)

	Train data	Test data
RMSE	0.2776	0.2754

- The difference between errors for train and test sets is very insignificant
- We can conclude that the elastic-net regression model performs better at generalization compared to least squares model

Elastic-net regression penalty

- Elastic-net regression assigns a higher penalty to the model with higher variance

Penalty	Least squares regression model	Elastic-net regression model
$\lambda_{lasso}*(\lvert\beta_0\rvert+\lvert\beta_{Mileage}\rvert+\lvert\beta_{Engine\_Capacity}\rvert+\lvert\beta_{Age}\rvert)$ $+$ $\lambda_{ridge}*((\beta_0)_2+(\beta_{Mileage})_2+(\beta_{Engine\_Capacity})_2+(\beta_{Age})_2)$	0.4190	0.0162

- $\lambda_{lasso} = 0.045$ and $\lambda_{ridge} = 0.05$, are calculated by trying different values

Comparison of models

Regression Model	β coefficients				Cost Function	RMSE	
	β_0	$\beta_{Mileage}$	$\beta_{Engine\_Capacity}$	β_{Age}		Train	Test
Least squares	0.2211	-0.1177	0.5694	-0.0187	$\Sigma(y_{act}-y_{pred})_2$	0.2315	0.3139
Elastic-net	0.3368	0	0.0112	0	$\Sigma(y_{act}-y_{pred})_2$ $+\lambda_{lasso}*\Sigma\lvert\beta\rvert$ $+\lambda_{ridge}*\Sigma(\beta)^2$	0.2776	0.2754

The two stage elastic net regularization

$$\Sigma(y_{act}-y_{pred})^2 + \lambda_{ridge} {}^{*}\Sigma(\beta) + \lambda_{lasso} {}^{*}\Sigma|\beta|$$

- First Stage: Ridge regression
- Second Stage: LASSO regression
- Note a double amount of shrinkage resulting in increased bias.
- In turn makes poor predictions. To improve the prediction performance, rescale the coefficients of elastic net by multiplying the estimated coefficients by $(1+\lambda_{ridge})$

When to use which regularization?

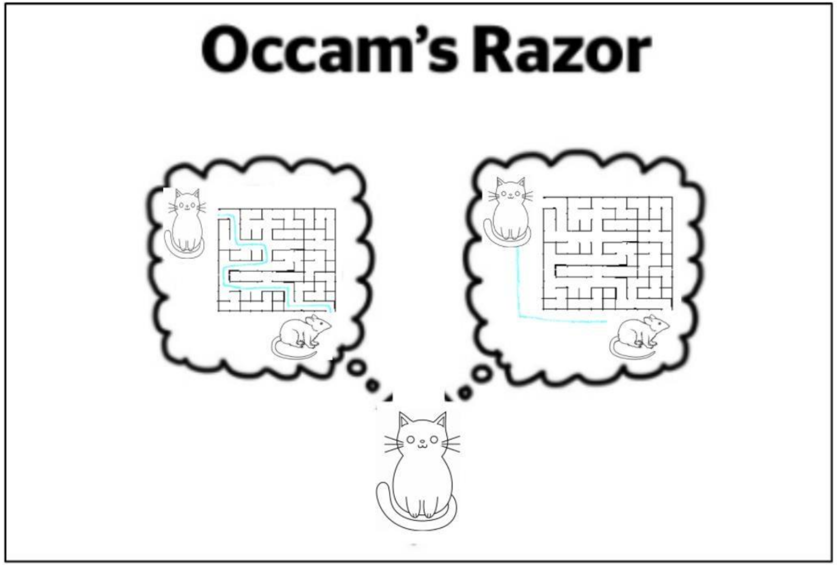
- If there are many interactions present or it is important to consider all the predictors in the model, ridge regression is used

- If the dataset contains some least significant independent variables that can be eliminated from the model, lasso regression is used

- If the dataset contains too many variables where it is practically impossible to determine whether to use ridge or lasso regression, elastic-net regression is used did you know?

Occam’s razor

Regularization is an application of occam’s razor, since it helps in choosing a simple model rather than an overly complex one



“When faced with two equally good hypotheses, always choose the simpler”

Grid Search

Hyperparameter

- The estimates of parameters are usually estimated from the data

- However, some parameters do not learn from the model; they are preset by the user. Such parameters are called hyperparameters

- As seen in the gradient descent, the learning rate (α) is a hyperparameter. Also the parameter lambda (λ) in regularization is a hyperparameter

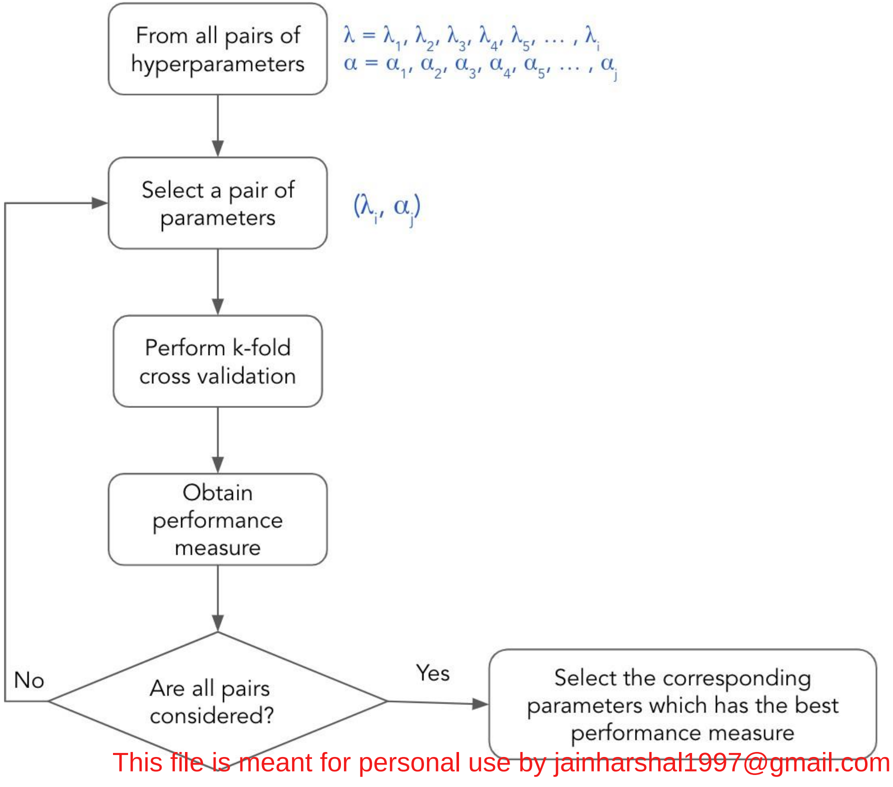
GridSearchCV

- The grid search is the process of tuning the hyperparameters to obtain the optimum values of the hyperparameters

- We use the the ‘GridSearchCV’ method to tune the hyperparameters

- Procedure:
  - Just as the name suggests, a grid of performance measure is obtained
  - Wherein each measure corresponds to a given hyperparameter values
  - Obtain the corresponding hyperparameters whose performance measure is highest

GridSearchCV



Hyperparameter λ

Hyperparameter α

	λ_1	λ_2	λ_3	λ_4	λ_5
α_1	.76	.35	.67	.76	.66
α_1	.76	.87	.82	.64	.71
α_1	.45	.56	.85	.72	.79
α_1	.78	.67	.34	.83	.91
α_1	.56	.44	.35	.65	.87

The RMSE values

Appendix

Types of gradient descent

- Batch gradient descent
- Stochastic gradient descent
- Mini batch gradient descent

Batch Gradient Descent

Batch Gradient Descent

$$\underbrace{\text{Batch}}_{\text{Complete Set}}\ \underbrace{\text{Gradient}}_{\text{Slope}}\ \underbrace{\text{Descent}}_{\text{Moving Downwards}}$$

Batch gradient descent

- The batch gradient descent computes the cost function with respect to the parameter for the entire data

- Also known as vanilla gradient descent

- In spite of being computationally expensive, it is efficient and gradually converges to the optimal solution

- In the premium example (slides 8-15), we used the batch gradient descent

Stochastic Gradient Descent

Stochastic Gradient Descent

Random Slope

Moving Downwards

Stochastic gradient descent (SGD)

- For data with many samples and many features, the batch gradient descent is slow
- The SGD works efficiently for large data as it works with only a single observation at each iteration, i.e. this one sample is used to calculate the derivative
- Advantage of SGD is that we can add more data to the train set. The estimated new parameters are based on the recent estimates and previous
- Specially useful in presence of clustered data

Mini Batch Gradient Descent

Mini Batch Gradient Descent

Small Set Slope

Moving Downwards

Mini batch gradient descent

- It is a combination of both Batch gradient descent and SGD
- Like in SGD where one sample is considered, mini batch uses a group of samples and in batch GD, all the sample are considered to obtain the cost function
- Hence it works faster than batch gradient descent and SGD
- Also known as vanilla mini batch gradient descent

To sum up...

	Batch GD	Mini Batch GD	Stochastic GD
Accuracy	High	Moderate	Low
Time required	High	Moderate	Low

Thank You