Cross Validation

- Is there a way we can achieve the following:
    - Train on **ALL** the data
    - Evaluate on **ALL** the data?

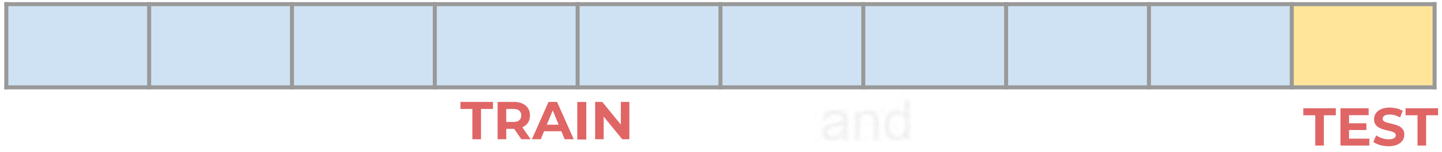
Consider this dataset:

	X		**y**
Area m^2	**Bedrooms**	**Bathrooms**	**Price**
200	3	2	$500,000
190	2	1	$450,000
230	3	3	$650,000
180	1	1	$400,000
210	2	2	$550,000

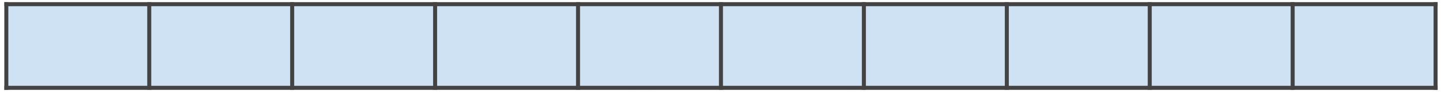
Consider training vs testing:

	X			**y**
	$\mathbf{x_1}$	$\mathbf{x_2}$	$\mathbf{x_3}$	$\mathbf{y}$
TRAIN	x^1_1	x^1_1	x^1_1	y_1
	x^2_1	x^2_1	x^2_1	y_2
	x^3_1	x^3_1	x^3_1	y_3
TEST	x^4_1	x^4_1	x^4_1	y_4
	x^5_1	x^5_1	x^5_1	y_5

Now we can represent full data and splits:

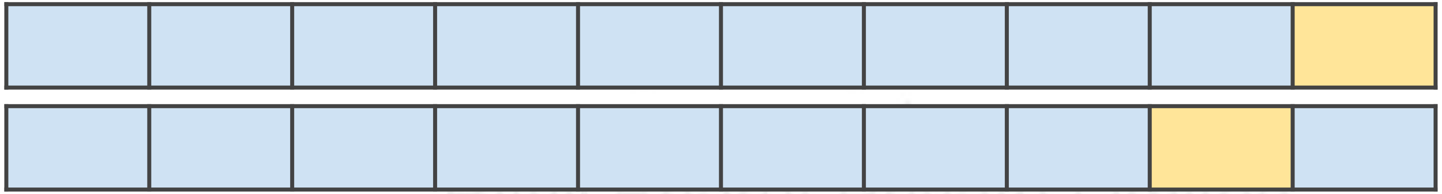


Split data into K equal parts:

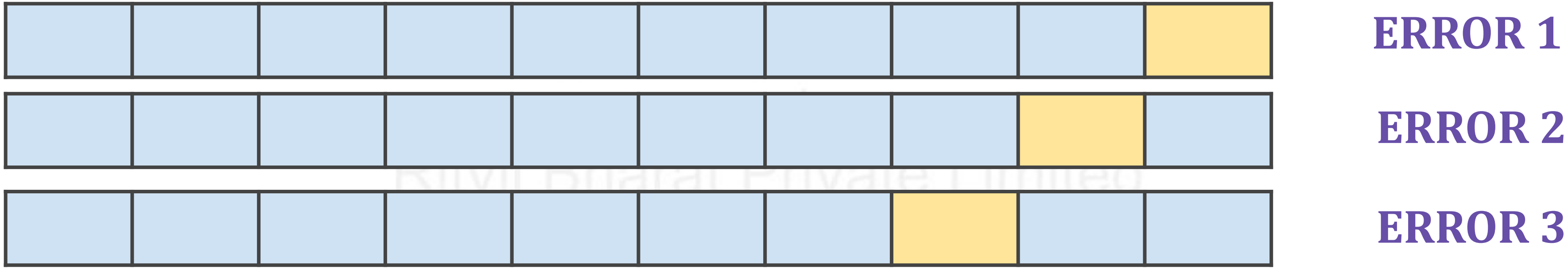


- 1/K left as test set
- Train model and get error metric for split:

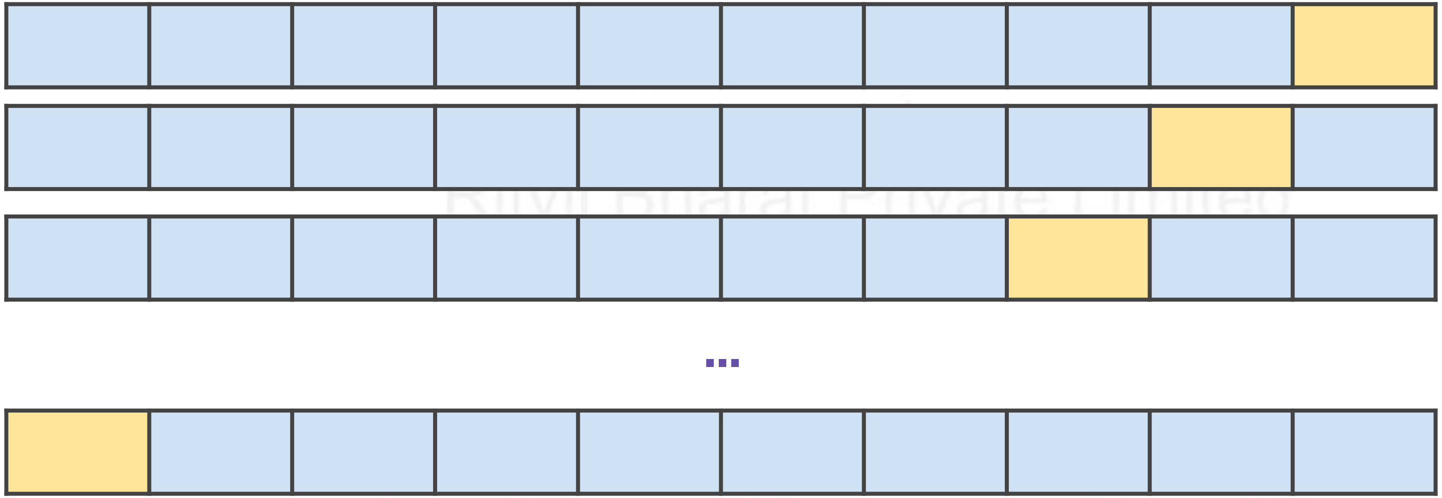
Repeat for another 1/K split



And again



Do it for all possible splits



ERROR 1

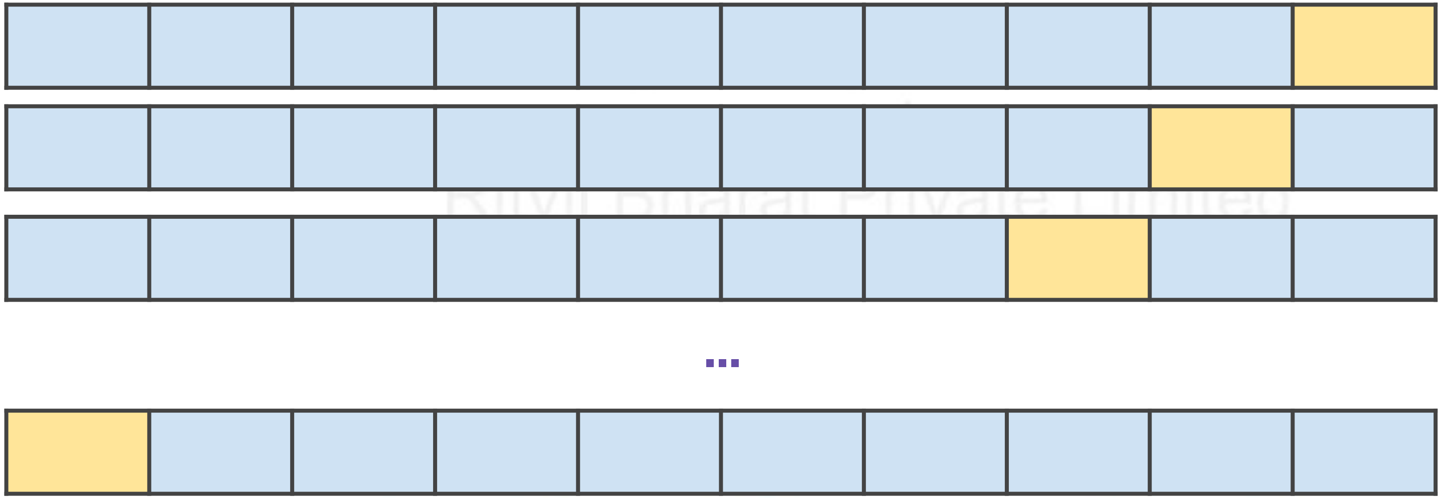
ERROR 2

ERROR 3

...

ERROR K

Get average error



ERROR 1

ERROR 2

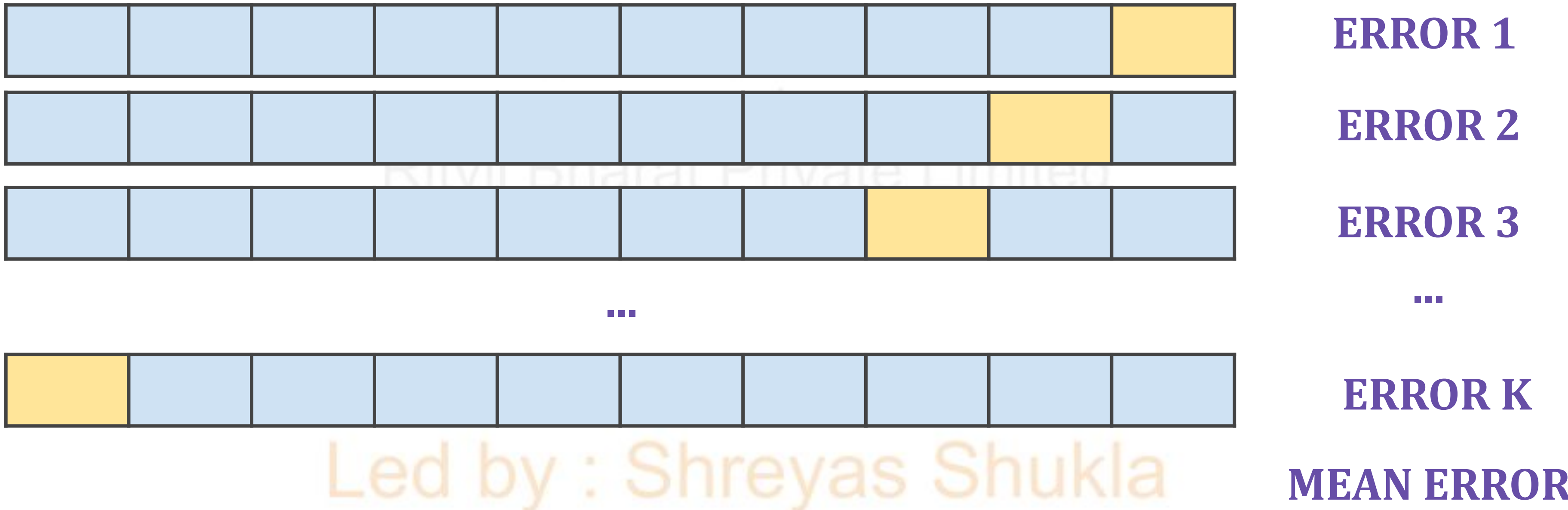
ERROR 3

...

ERROR K

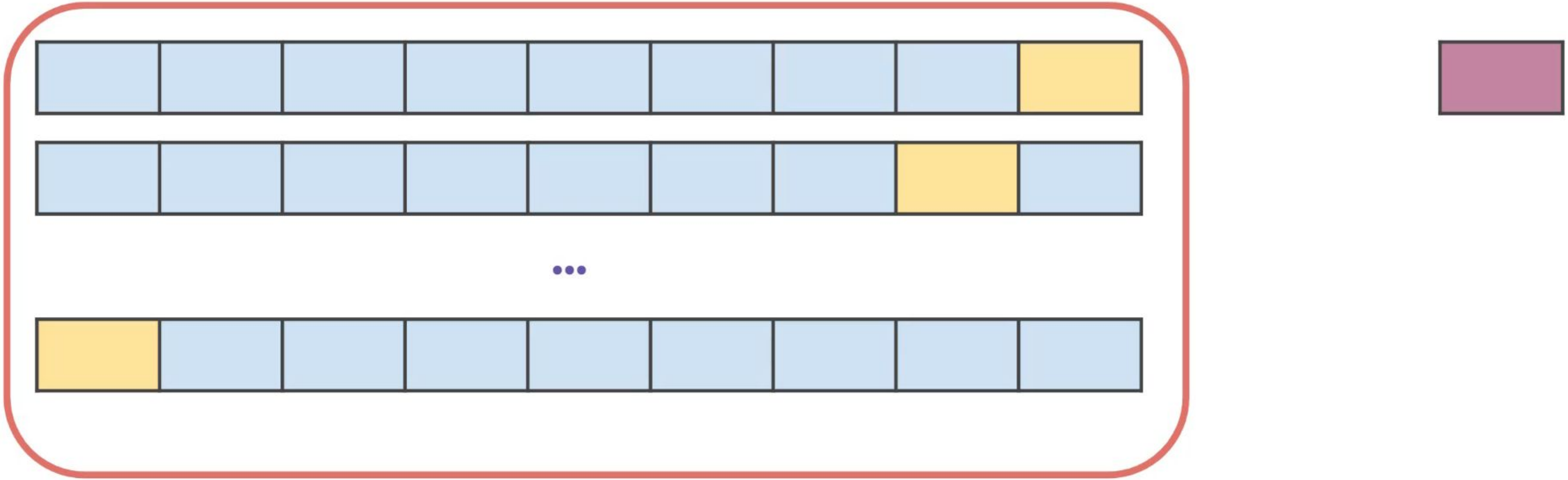
MEAN ERROR

Average error is the expected performance



- We were able to train on all data **and** evaluate on all data!
- Better sense of true performance across multiple potential splits.
- What is the cost of this?
  - We have to repeat computations K number of times!
- Common choice for K is 10 so each test set is 10% of your total data.
- Largest K possible would be K equal to the number of number of rows.
  - This is known as **leave one out** cross validation.

Hold-Out Test Set: Train | Validation Split | Test



Regularization for Linear Regression

Jupiter Exercise

Ridge Regression

- Help reduce the potential for overfitting to the training data.
- Adds a penalty term to the error based on the squared value of the coefficients.
- Ridge Regression is a regularization method for Linear Regression.

General formula for the regression line:

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p$$

These Beta coefficients were solved by minimizing the residual sum of squares (RSS).

$$\text{RSS} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

We could substitute our regression equation for **ŷ**:

$$
\begin{aligned}
\mathrm{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2
\end{aligned}
$$

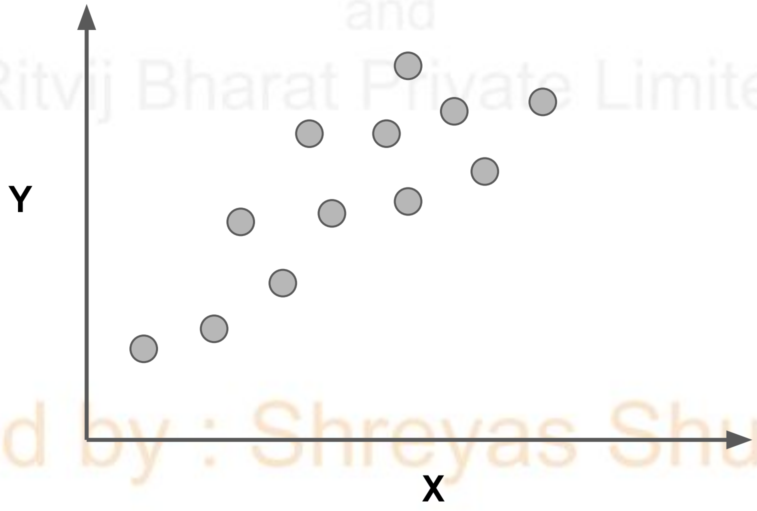
Summarize RSS:

$$\mathrm{RSS} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

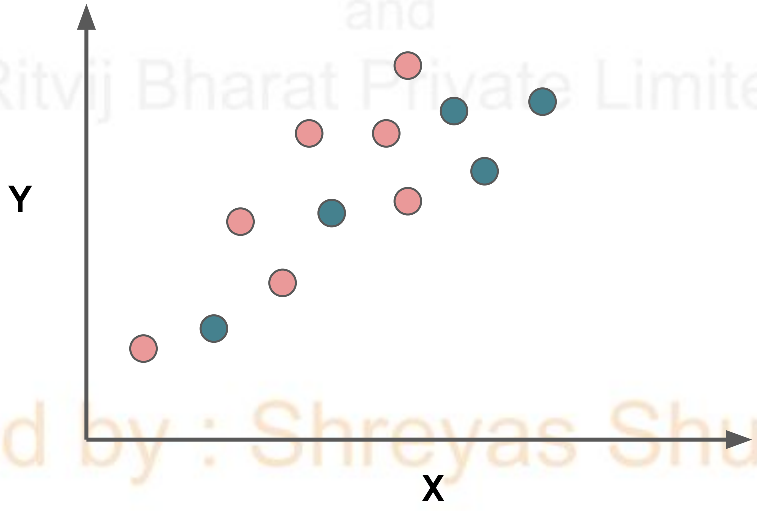
- Ridge Regression adds a **shrinkage penalty**
- Ridge Regression seeks to minimize this entire error term **RSS + Penalty**.
- **Shrinkage penalty** based off the squared coefficient:
- **Shrinkage penalty** has a **tunable lambda parameter which determines how severe the penalty is. Theoretically,** it can be any value from 0 to positive infinity.

$$\text{Error} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 \boxed{+ \lambda \sum_{j=1}^{p}\beta_j^2}$$

Thought experiment

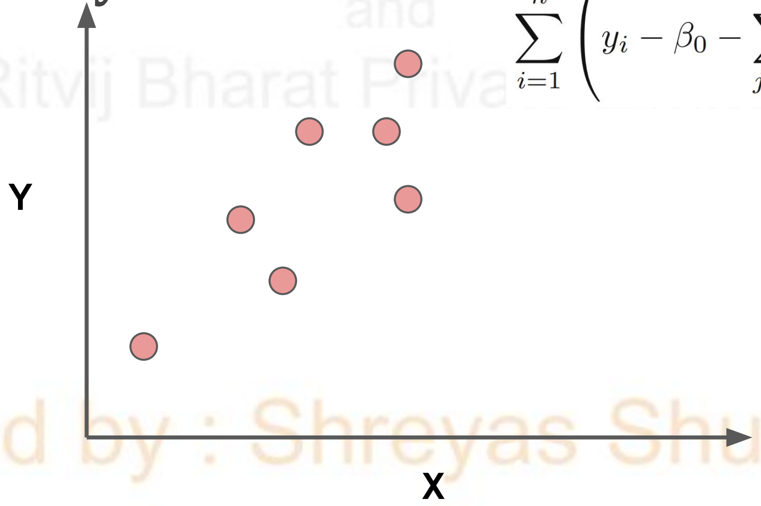


Split the dataset into a training set and test set:



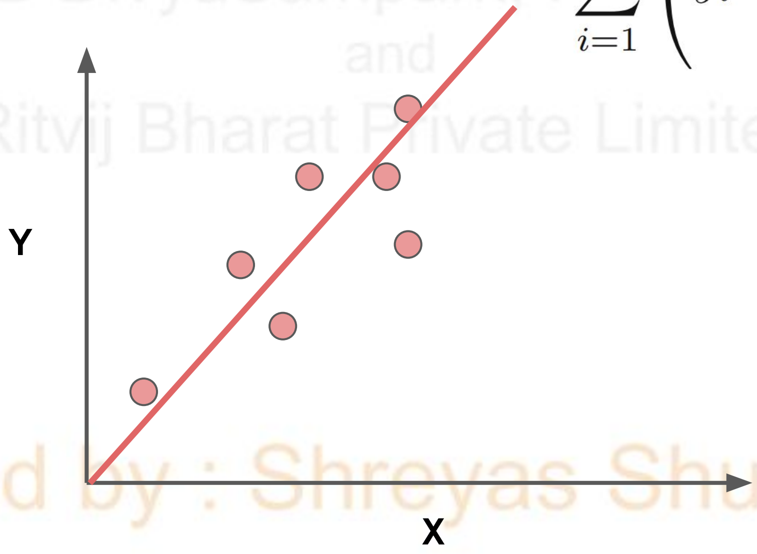
- Now we can fit on the training data to produce the line: $\hat{y} = \boldsymbol{\beta_1} \mathbf{x} + \boldsymbol{\beta_0}$
- Regardless of RSS or Ridge error, we're still trying to create a line: $\hat{y} = \boldsymbol{\beta_1} \mathbf{x} + \boldsymbol{\beta_0}$
- The only difference would be the coefficients found.
- **First let's fit using only RSS...**

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2$$



- Our fitted $\hat{y} = \beta_1 x + \beta_0$
- Appears to have over fit to training data.

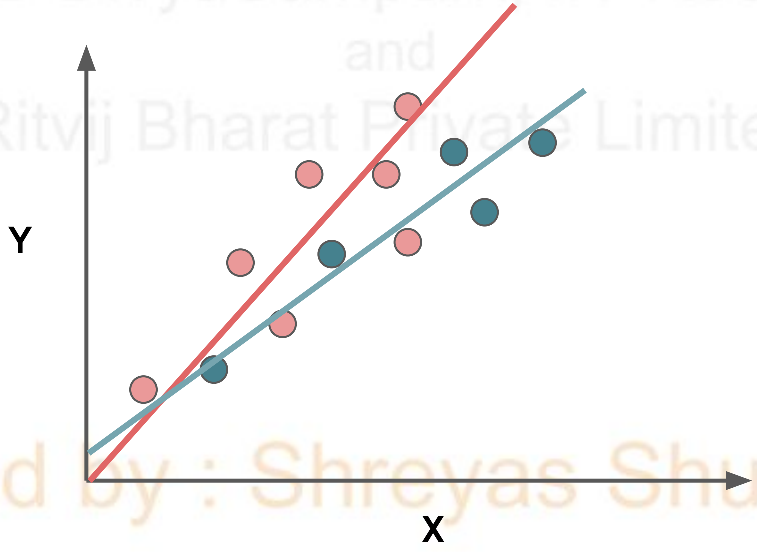
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2$$



This means we have high **variance.**

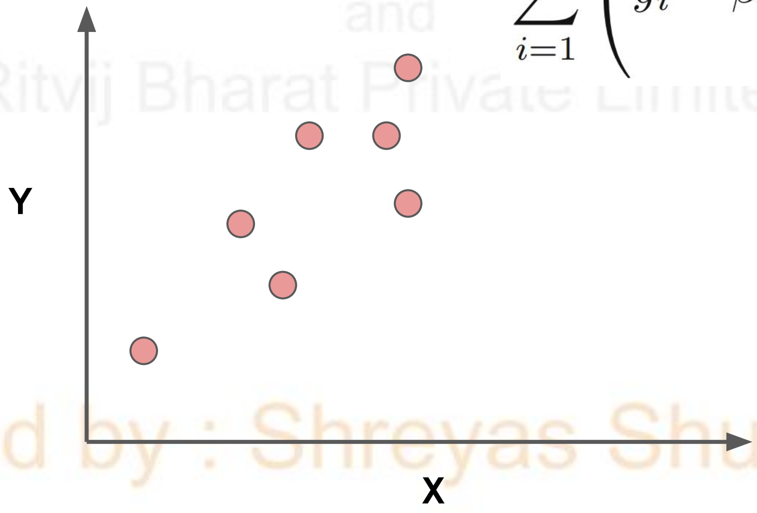
Could we introduce a little more **bias** to significantly **reduce** variance?

- Would adding the penalty term help generalize with more **bias**?
- Adding bias can help generalize $\hat{y} = \beta_1 x + \beta_0$



- Let's imagine trying to reduce the Ridge Regression error term:
- There is λ and the squared slope coefficient.

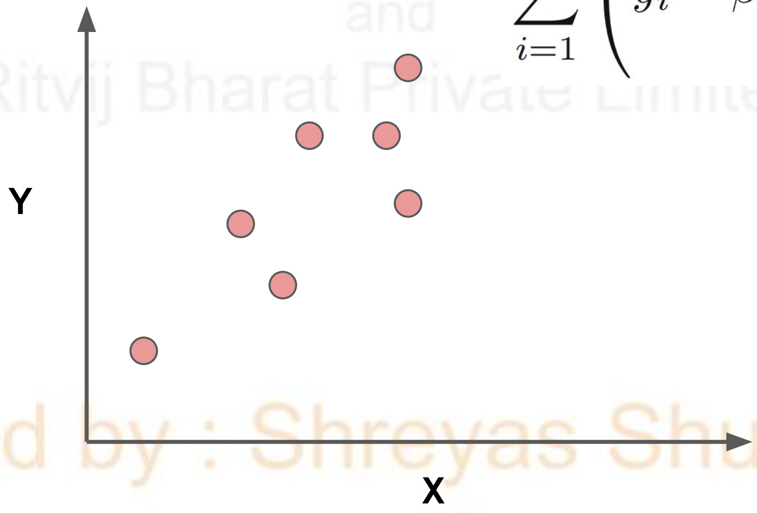
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \boxed{\lambda \sum_{j=1}^{p}\beta_j^2}$$



Assume **λ = 1**

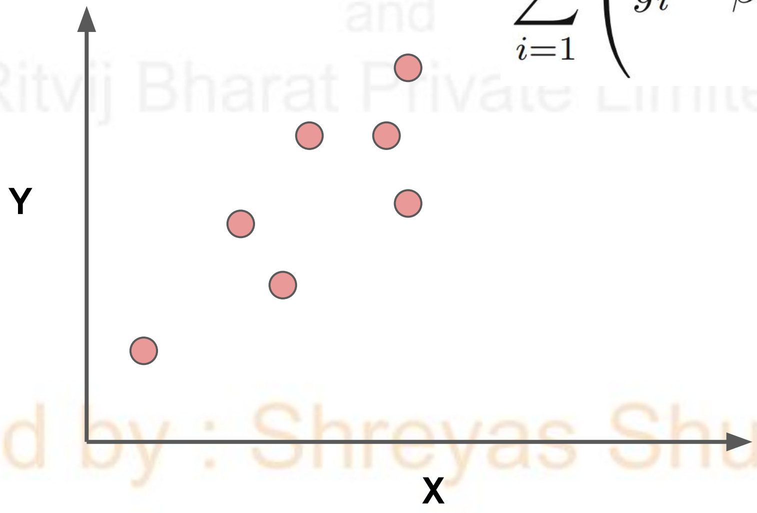
Then essentially, we're trying to minimize is the beta coefficient and the beta coefficient squared.

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$



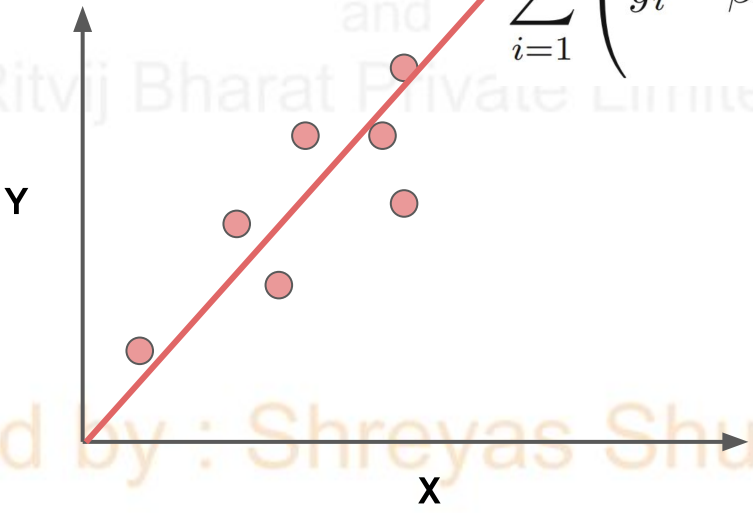
This punishes a large slope for $\hat{y} = \beta_1 x + \boxed{\beta_0}$

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \boxed{\lambda\sum_{j=1}^{p}\beta_j^2}$$



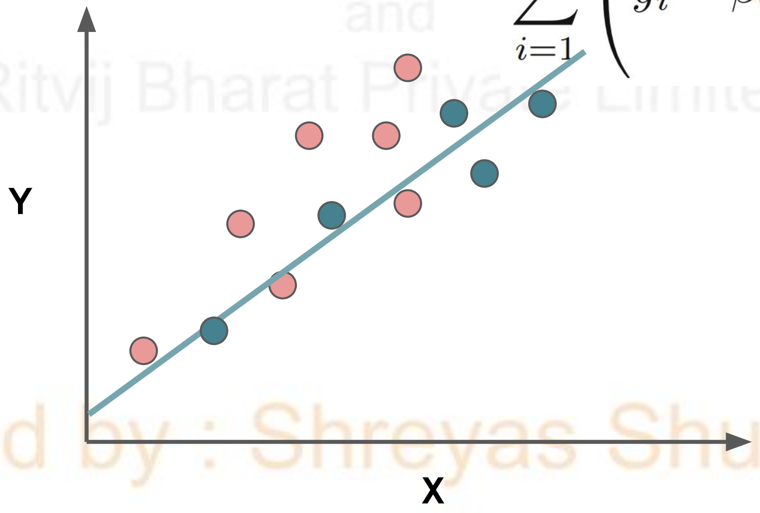
For single feature this lowers slope at the cost of some additional bias.

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \boxed{\lambda \sum_{j=1}^{p} \beta_j^2}$$



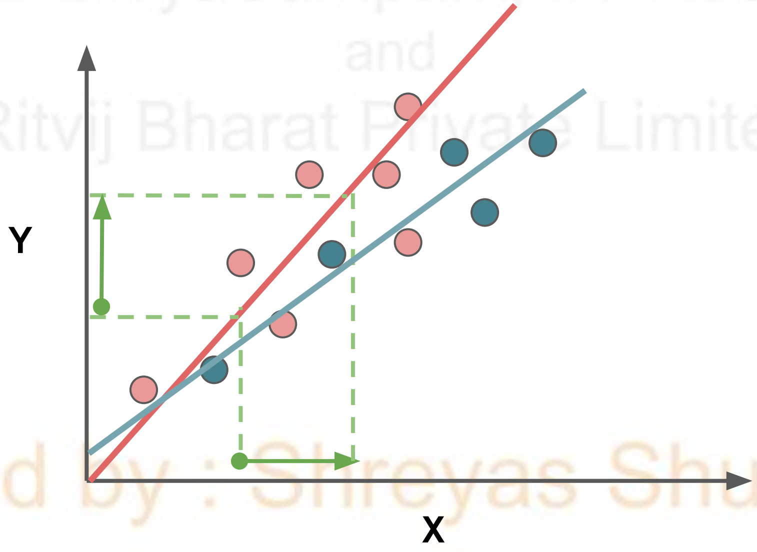
Generalize better to unseen data

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \boxed{\lambda \sum_{j=1}^{p}\beta_j^2}$$

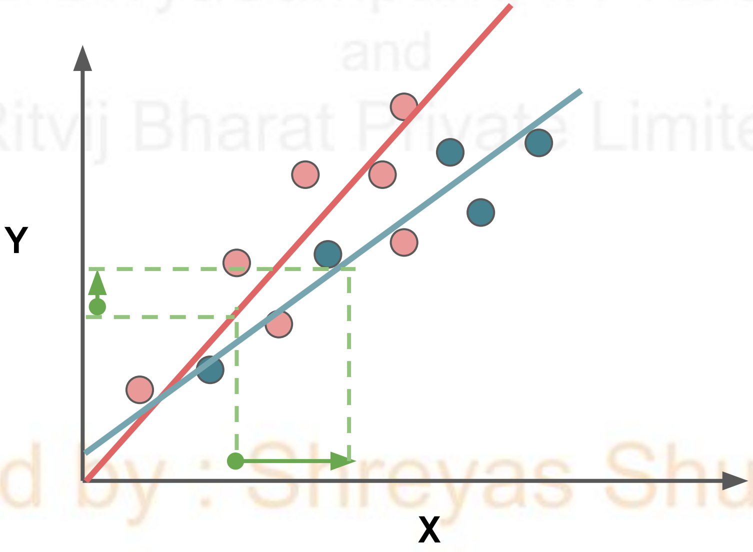


- Consider overfitting to training set
- An increase in X results in a greater y response:

- Compare to a more generalized model that used Ridge Regression
- Same feature change does not produce as much y response:

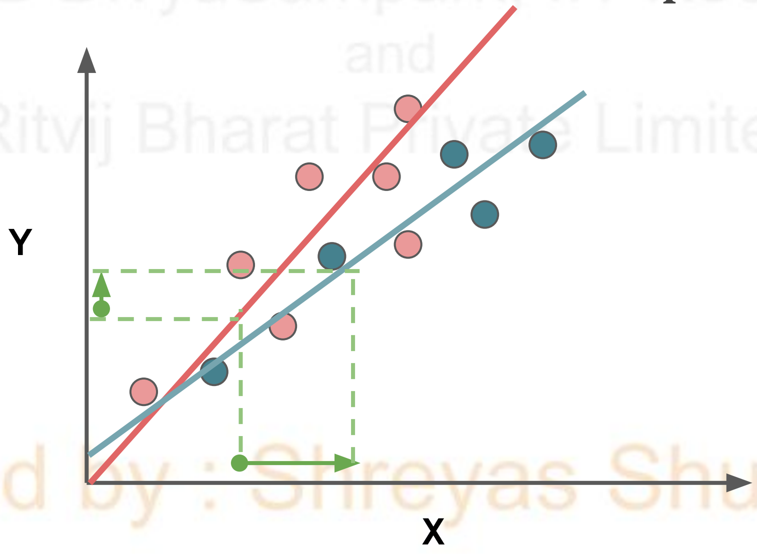


Same feature change does not produce as much y response



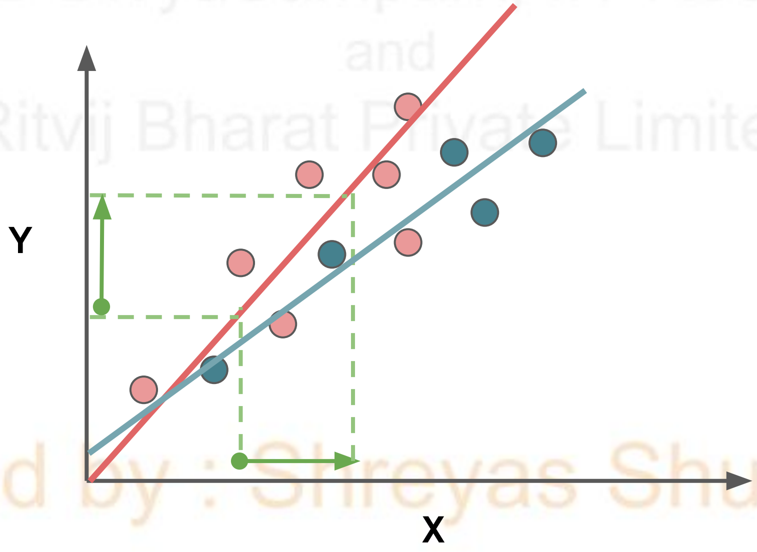
Ridge Regression

- Trying to minimize a squared Beta term leads us to punish larger coefficients.
- In the case of a single feature, a larger Beta means a steeper sloped line.
- A steeper sloped line would mean more response per increase in X value.



$$\lambda \sum_{j=1}^{p} \beta_j^2$$

Again, in the case of a single feature that larger beta means a steeper sloped line and that would would mean more response per increase in X value.



- What about the lambda term?
- We simply use cross-validation to explore multiple lambda options and then choose the best one!

$$\text{Error} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

Ridge Regression

Important Notes

- Sklearn refers to lambda as alpha
- For cross validation metrics, sklearn uses a “scorer object”. All scorer objects follow the convention that **higher** return values are **better** than lower return values.
- For example, obviously higher accuracy is better.
- But higher RMSE is actually worse!
- So Scikit-Learn fixes this by using a negative RMSE as its scorer metric.

$$\text{Error} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \boxed{\lambda} \sum_{j=1}^{p} \beta_j^2$$

- This allows for uniformity across **all** scorer metrics, even across different tasks types.
- The same idea of uniformity across model classes applies to referring to the penalty strength parameter as **alpha**.

Lasso Regression
L1 Regularization

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \text{RSS} + \boxed{\lambda\sum_{j=1}^{p}|\beta_j|}$$

L1 adds a penalty which is equal to the **absolute value** of the magnitude of coefficients.

How is it different from L2 ?

- Limits the size of the coefficients.
- Can yield sparse models where some coefficients can become zero.

- LASSO can make some of the coefficients to be zero when the tuning parameter λ is sufficiently large.
- As a result, Models generated from the LASSO are generally much easier to interpret.

- LassoCV operates on checking a number of alphas within a range, instead of providing the alphas directly.
- Let’s explore the results of LASSO in Python and Scikit-Learn!

Elastic Net

L1 and L2 Regularization

- We know Lasso is able to shrink coefficients to zero, but we haven't taken a deeper dive into how or why that is.
- This ability becomes more clear when learning about **elastic net**
- Elastic net combines L1 and L2

There is some sum **s** which allows to rewrite the penalty as a requirement:

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad \boxed{\text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \le s}$$

and

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad \boxed{\text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \le s,}$$

- Simple thought experiment:
  - A simple equation:
    - $\hat{y} = \beta_1 x_1 + \beta_2 x_2$
  - We know that regularization can be expressed as an additional requirement that RSS is subject to.

- Thought experiment:
  - A simple equation:
    - $\hat{\mathbf{y}} = \boldsymbol{\beta}_1\mathbf{x}_1 + \boldsymbol{\beta}_2\mathbf{x}_2$
  - L1 constrains the sum of absolute values. $\sum|\boldsymbol{\beta}|$
  - L2 constrains the sum of squared values. $\sum\boldsymbol{\beta}^2$
- There is some sum **s** that the penalty is less than.

- For two features: $\hat{\mathbf{y}} = \boldsymbol{\beta}_1\mathbf{x}_1 + \boldsymbol{\beta}_2\mathbf{x}_2$
- Lasso Regression Penalty:

$$|\boldsymbol{\beta}_1| + |\boldsymbol{\beta}_2| \leq \boldsymbol{s}$$

- Ridge Regression Penalty:

$$\boldsymbol{\beta}_1^2 + \boldsymbol{\beta}_2^2 \leq \boldsymbol{s}$$

- Elastic Net seeks to improve on both L1 and L2 Regularization by combining them
- Here we seek to minimize RSS and **both** the squared and absolute value terms
- Notice there are **two** distinct lambda values for each penalty:

$$\text{Error} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda_1\sum_{j=1}^{p}\beta_j^2 + \lambda_2\sum_{j=1}^{p}|\beta_j|$$

We can express this as a ratio between L1 and L2:

$$\frac{\sum_{i=1}^{n}(y_i - x_i^J \hat{\beta})^2}{2n} + \lambda \left(\frac{1-\alpha}{2} \sum_{j=1}^{m} \hat{\beta}_j^2 + \alpha \sum_{j=1}^{m} |\hat{\beta}_j| \right)$$

Simplified notation:

$$\hat{\beta} \equiv \underset{\beta}{\operatorname{argmin}}(\|y - X\beta\|^2 + \lambda_2 \|\beta\|^2 + \lambda_1 \|\beta\|_1)$$

Let’s explore how to perform Elastic Net with Python and Scikit-learn!

$$\frac{\sum_{i=1}^{n}(y_i - x_i^J \hat{\beta})^2}{2n} + \lambda \left(\frac{1-\alpha}{2} \sum_{j=1}^{m} \hat{\beta}_j^2 + \alpha \sum_{j=1}^{m} |\hat{\beta}_j| \right)$$