

- Linear Regression
  - Theory of Linear Regression
  - Simple Implementation with Python
  - Scikit-Learn Overview
  - Linear Regression with Scikit-learn
  - Polynomial Regression
  - Regularization

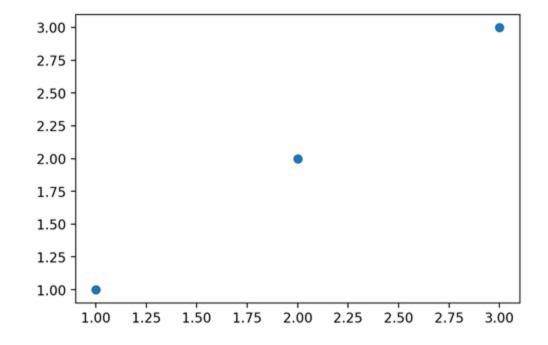
- This will include understanding:
  - Brief History
  - Linear Relationships
  - Ordinary Least Squares
  - Cost Functions
  - Gradient Descent
  - Vectorization

 1809 - Carl Friedrich Gauss publishes his methods of calculating orbits of celestial bodies.

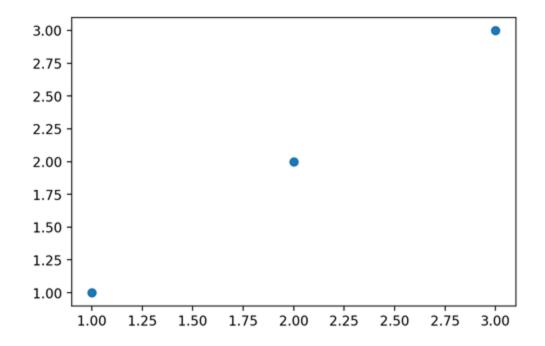
Claiming to have invented least-squares

back in 1795!

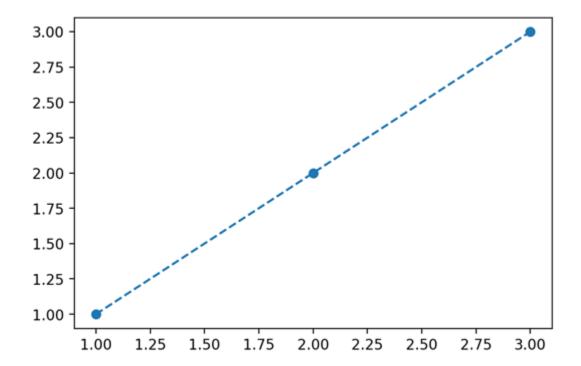
- Put simply, a linear relationship implies some constant straight line relationship.
- The simplest possible being y = x.



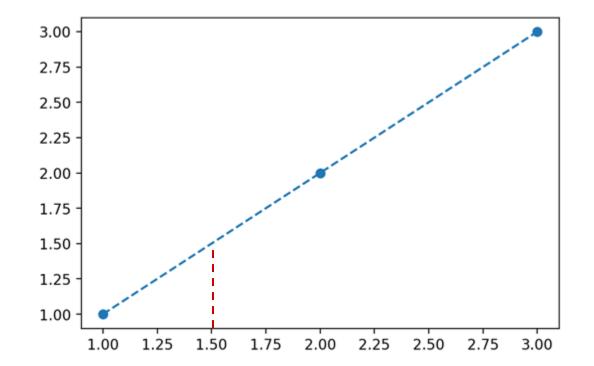
• Here we see x = [1,2,3] and y = [1,2,3]



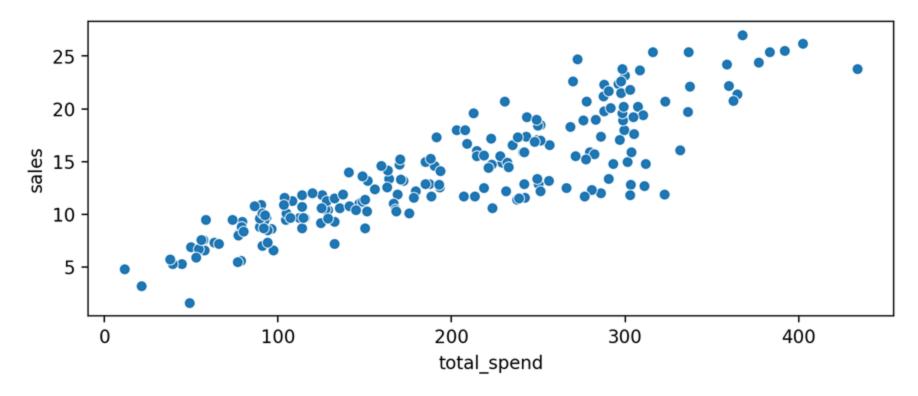
• We could then (based on the three real data points) build out the relationship y=x as our "fitted" line.



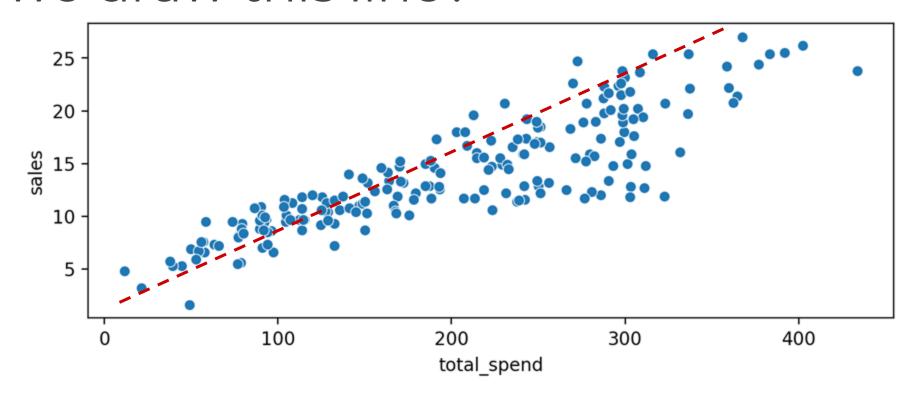
 This implies for some new x value I can predict its related y.



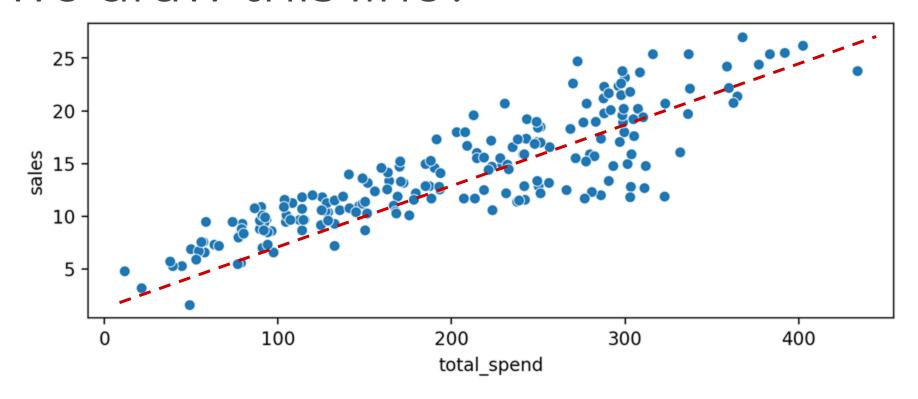
 But what happens with real data? Where do we draw this line?



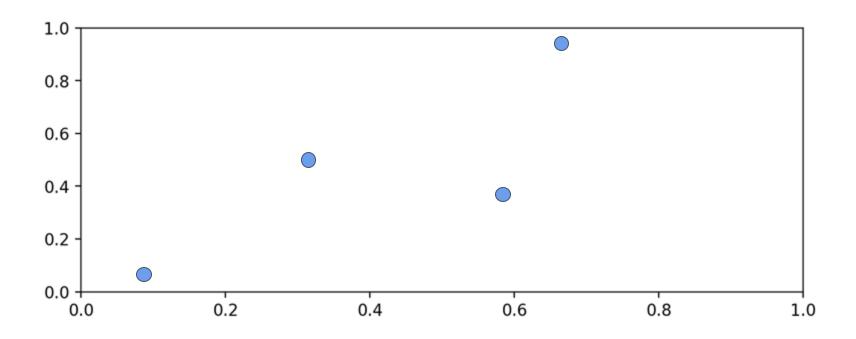
 But what happens with real data? Where do we draw this line?



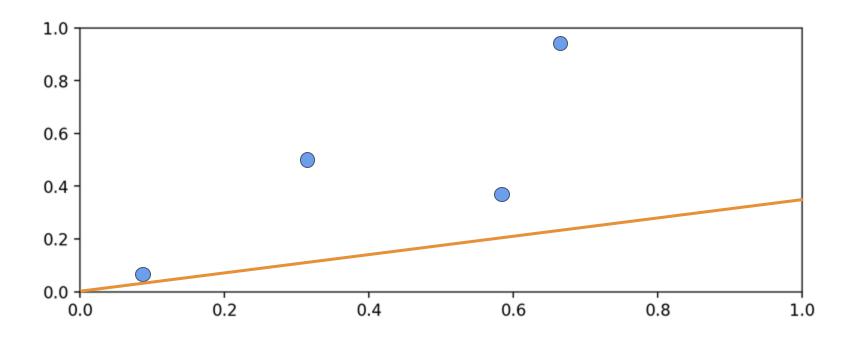
 But what happens with real data? Where do we draw this line?



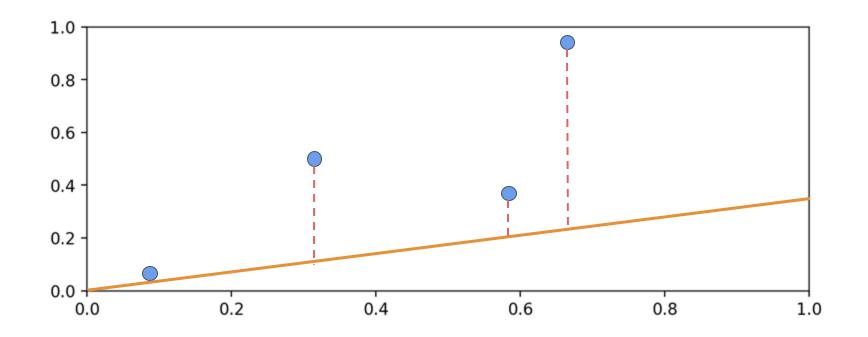
 Fundamentally, we understand we want to minimize the overall distance from the points to the line.



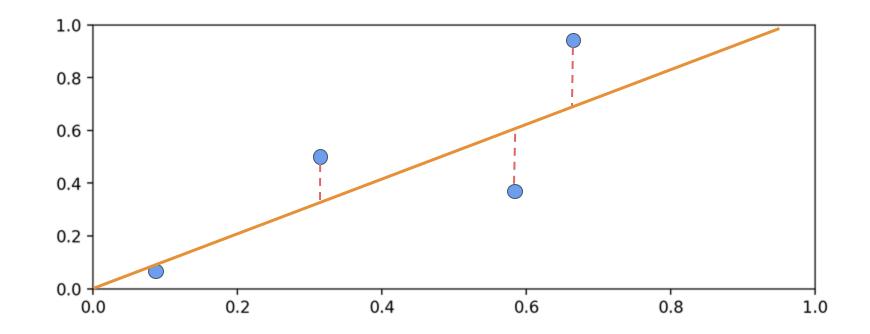
 Fundamentally, we understand we want to minimize the overall distance from the points to the line.



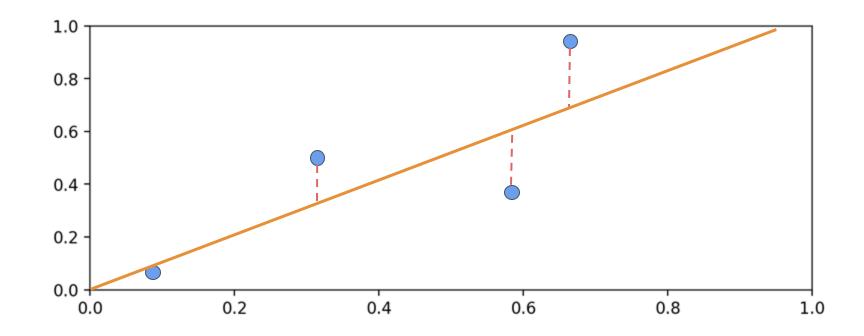
 We also know we can measure this error from the real data points to the line, known as the residual error.



 Some lines will clearly be better fits than others.

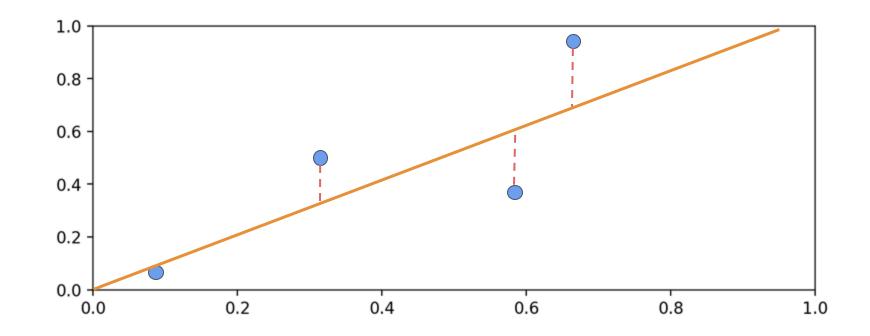


 We can also see the residuals can be both positive and negative.

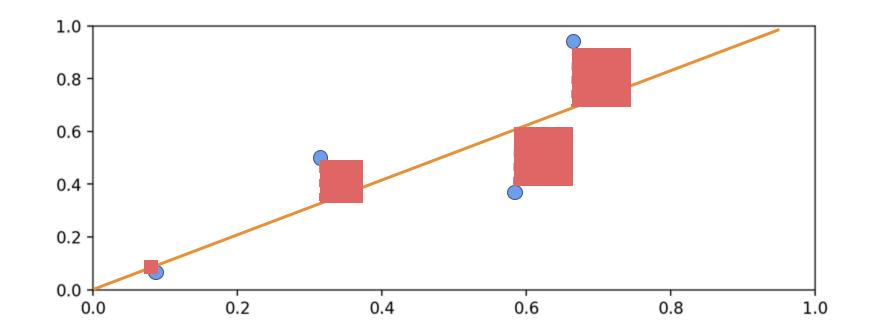


 Ordinary Least Squares (OLS) works by minimizing the sum of the squares of the differences between the observed dependent variable (values of the variable being observed) in the given dataset and those predicted by the linear function.

 We can visualize squared error to minimize:



 We can visualize squared error to minimize:



- Having a squared error will help us simplify our calculations later on when setting up a derivative.
- Let's continue exploring OLS by converting a real data set into mathematical notation, then working to solve a linear relationship between features and a variable!

# Introduction to Linear Regression

Algorithm Theory - Part Two OLS Equations

- Linear Regression OLS Theory
  - We know the equation of a simple straight line:
    - y = mx + b
      - m is slope
      - b is intercept with y-axis

- Linear Regression OLS Theory
  - We can see for y=mx+b there is only room for one possible feature x.
  - OLS will allow us to directly solve for the slope **m** and intercept **b**.
  - We will later see we'll need tools like gradient descent to scale this to multiple features.

• Linear Regression allows us to build a relationship between multiple **features** to estimate a **target output**.

Area m <sup>2</sup>	Bedrooms	Bathroom s	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

 We can translate this data into generalized mathematical notation...

X

Area m <sup>2</sup>	Bedrooms	Bathroom s	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

 We can translate this data into generalized mathematical notation...

	^		y
X <sub>1</sub>	X <sub>2</sub>	<b>X</b> <sub>3</sub>	У
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

 We can translate this data into generalized mathematical notation...

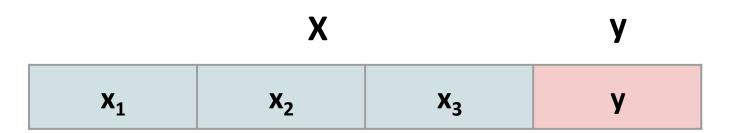
X

	<b>7</b>		•
X <sub>1</sub>	X <sub>2</sub>	<b>X</b> <sub>3</sub>	У
x <sup>1</sup> <sub>1</sub>	3	2	\$500,000
x <sup>2</sup> <sub>1</sub>	2	1	\$450,000
x <sup>3</sup> <sub>1</sub>	3	3	\$650,000
x <sup>4</sup> <sub>1</sub>	1	1	\$400,000
x <sup>5</sup> <sub>1</sub>	2	2	\$550,000

 Now let's build out a linear relationship between the features X and label y.

X		Y	
$X_1$	X <sub>2</sub>	<b>X</b> <sub>3</sub>	У
x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	<b>y</b> <sub>1</sub>
x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	<b>y</b> <sub>2</sub>
x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	<b>y</b> <sub>3</sub>
x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	У <sub>4</sub>
x <sup>5</sup> <sub>1</sub>	x <sup>5</sup> <sub>1</sub>	x <sup>5</sup> <sub>1</sub>	<b>y</b> <sub>5</sub>

 Now let's build out a linear relationship between the features X and label y.



Reformat for y = x equation



 Each feature should have some Beta coefficient associated with it.

y X 
$$\hat{y}$$
  $x_1$   $x_2$   $x_3$   $\hat{y}=eta_0x_0+\cdots+eta_nx_n$ 

 This is the same as the common notation for a simple line: y=mx+b

y X 
$$\hat{y}$$
  $x_1$   $x_2$   $x_3$   $\hat{y}=eta_0x_0+\cdots+eta_nx_n$ 

 This is stating there is some Beta coefficient for each feature to minimize error.

y X 
$$x_1$$
  $x_2$   $x_3$   $\hat{y}=eta_0x_0+\cdots+eta_nx_n$ 

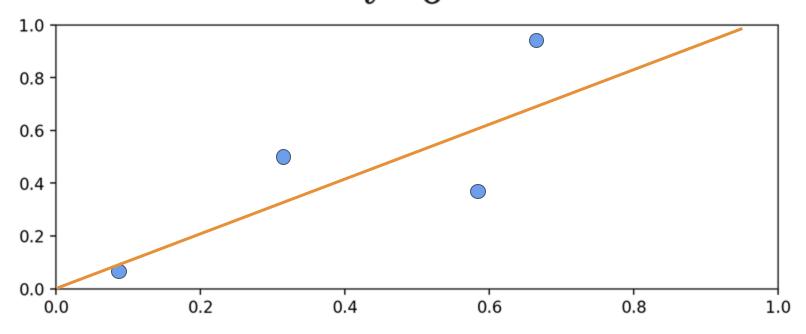
We can also express this equation as a sum:

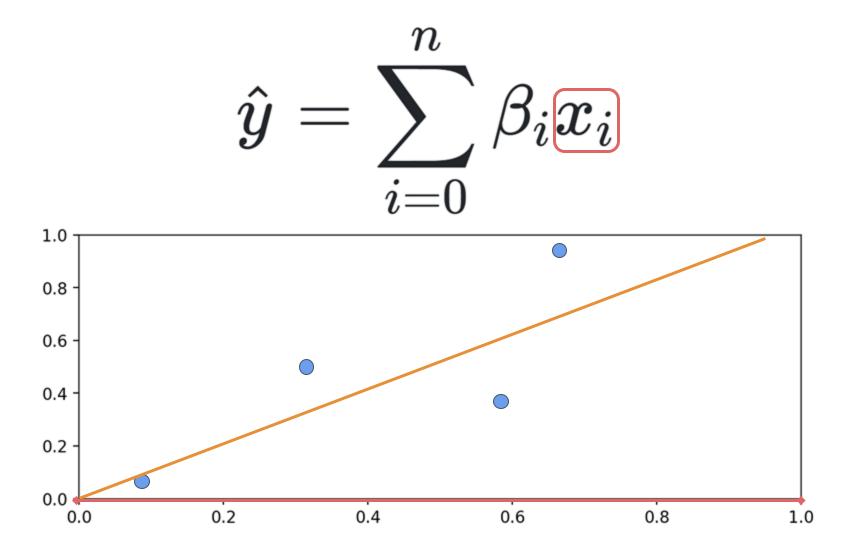
Note the y hat symbol displays a prediction.
 There is usually no set of Betas to create a perfect fit to y!

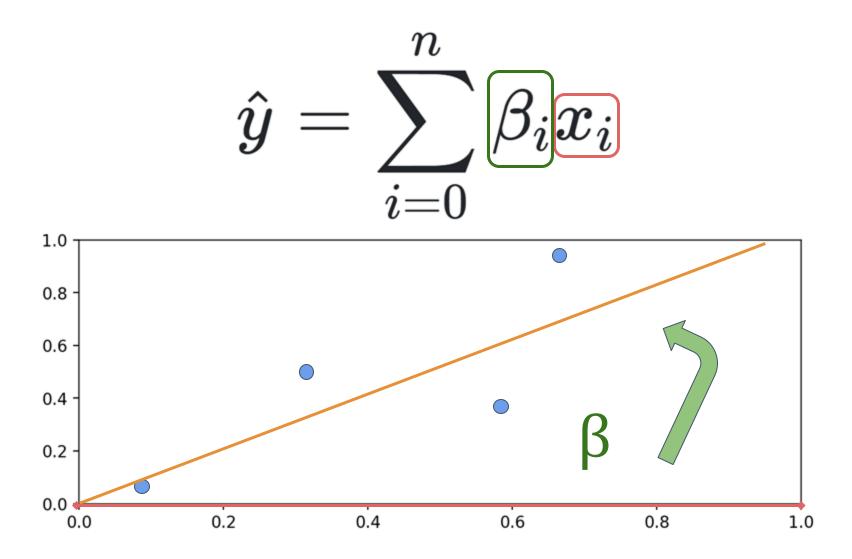
$$\hat{y} = \sum_{i=0}^n eta_i x_i$$

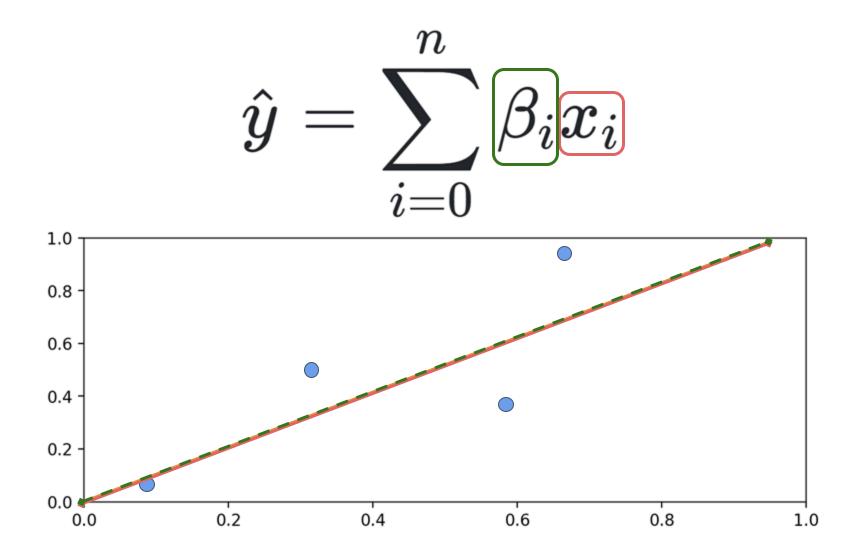
• Line equation:

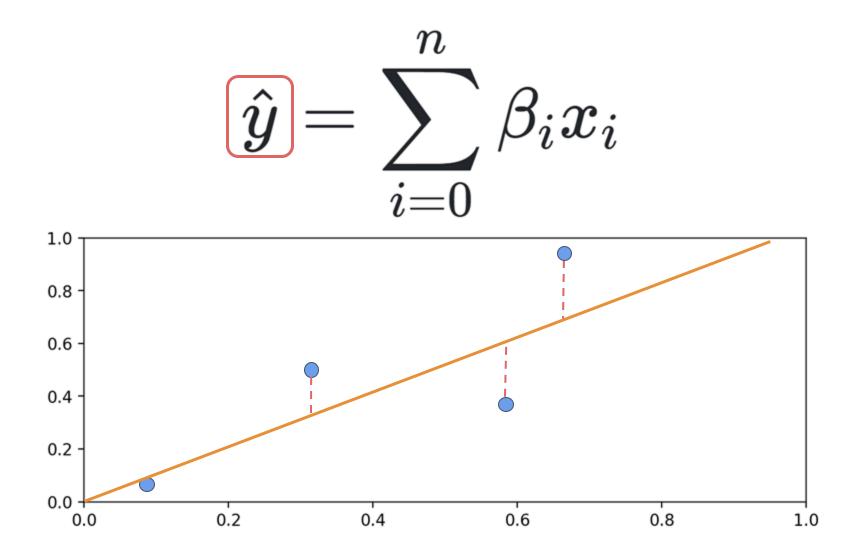
$$\hat{y} = \sum_{i=0}^{} eta_i x_i$$











- For simple problems with one X feature we can easily solve for Betas values with an analytical solution.
- Let's quickly solve a simple example problem, then later we will see that for multiple features we will need gradient descent.

- As we expand to more than a single feature however, an analytical solution quickly becomes unscalable.
- Instead we shift focus on minimizing a cost function with gradient descent.

 We can use gradient descent to solve a cost function to calculate Beta values!

$$\hat{y} = \sum_{i=0}^n eta_i x_i$$

### Introduction to Linear Regression

- What we know so far:
  - Linear Relationships
    - y = mx+b
  - OLS
    - Solve simple linear regression
  - Not scalable for multiple features
  - Translating real data to Matrix Notation
  - Generalized formula for Beta coefficients

 Recall we are searching for Beta values for a best-fit line.

$$\hat{y} = \sum_{i=0}^n eta_i x_i$$

 The equation below simply defines our line, but how to choose beta coefficients?

$$\hat{y} = \sum_{i=0}^n eta_i x_i$$

 We've decided to define a "best-fit" as minimizing the squared error.

$$\hat{y} = \sum_{i=0}^n eta_i x_i$$

• The residual error for some row j is:

$$y^j - \hat{y}^j$$

Squared Error for some row j is then:

$$\left(y^j - \hat{y}^j
ight)^2$$

Sum of squared errors for m rows is then:

$$\sum_{j=1}^m \left(y^j - \hat{y}^j
ight)^2$$

Average squared error for m rows is then:

$$-rac{1}{m}\sum_{j=1}^m \left(y^j-\hat{y}^j
ight)^2$$

 Our cost function can be defined by the squared error:

$$J(oldsymbol{eta}) = rac{1}{2m} \sum_{j=1}^m \left( y^j - \hat{y}^j 
ight)^2$$

It will be a function of Betas and Features!

$$egin{align} J(oldsymbol{eta}) &= rac{1}{2m} \sum_{j=1}^m \left( y^j - \hat{y}^j 
ight)^2 \ &= rac{1}{2m} \sum_{j=1}^m \left( y^j - \sum_{i=0}^n eta_i x_i^j 
ight)^2 \end{aligned}$$

 Recall from calculus to minimize a function we can take its derivative and set it equal to zero.

$$egin{align} rac{\partial J}{\partial eta_k}(oldsymbol{eta}) &= rac{\partial}{\partial eta_k} \Bigg(rac{1}{2m} \sum_{j=1}^m \Bigg(y^j - \sum_{i=0}^n eta_i x_i^j\Bigg)^2\Bigg) \ &= rac{1}{m} \sum_{j=1}^m \Bigg(y^j - \sum_{i=0}^n eta_i x_i^j\Bigg) (-x_k^j) \end{aligned}$$

 Recall from calculus to minimize a function we can take its derivative and set it equal to zero.

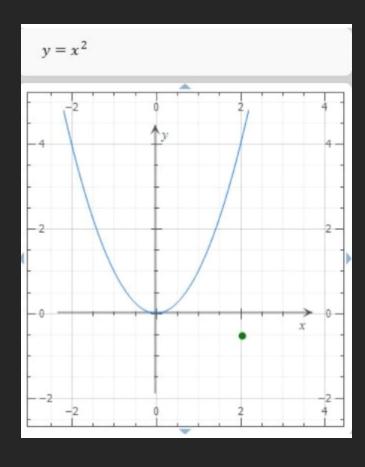
$$egin{align} rac{\partial J}{\partial eta_k}(oldsymbol{eta}) &= rac{\partial}{\partial eta_k} \Biggl(rac{1}{2m} \sum_{j=1}^m \Biggl(y^j - \sum_{i=0}^n eta_i x_i^j\Biggr)^{\!\!\!\!2}\Biggr) \ &= rac{1}{m} \sum_{j=1}^m \Biggl(y^j - \sum_{i=0}^n eta_i x_i^j\Biggr) (-x_k^j) \end{aligned}$$

- Unfortunately, it is not scalable to try to get an analytical solution to minimize this cost function.
- In the next lecture we will learn to use gradient descent to minimize this cost function.

## Introduction to Linear Regression

**Gradient Descent** 

#### **Gradient Descent**



Minimize 
$$f(x) = x^2$$

- Use calculus!
- df / dx = 2x = 0
- Solve for x: x = 0

# Gradient descent Linear Regression

- . Title: Linear Regression with Gradient Descent
- \* Content:
  - Linear regression aims to fit a line to a set of data points.
  - Equation:  $y=\beta_0+\beta_1x_1+\beta_2x_2+\ldots+\beta_nx_n$
  - Objective: Minimize the squared error between predicted values (from the linear model) and actual data points.
- **Title**: The Cost Function,  $J(\beta)$
- Content:
  - Defined as the Mean Squared Error (MSE):

$$J(eta) = rac{1}{2m} \sum_{i=1}^m (h_eta(x^{(i)}) - y^{(i)})^2$$

where:

$$h_\beta(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n$$

• Objective: Minimize  $J(\beta)$ .

#### Slide 3: Gradient Descent

- **Title**: Minimizing  $J(\beta)$  using Gradient Descent
- Content
- · Iteratively update each parameter:

$$eta_j := eta_j - lpha rac{\partial}{\partial eta_i} J(eta)$$

- Where
  - $\alpha$  is the learning rate.
- The partial derivative represents the gradient of the cost function with respect to the parameter β<sub>j</sub>.

- We just figured out a cost function to minimize!
- Taking the cost function derivative and then solving for zero to get the set of Beta coefficients will be too difficult to solve directly through an analytical solution.

 Instead we can describe this cost function through vectorized matrix notation and use gradient descent to have a computer figure out the set of Beta coefficient values that minimize the cost/loss function.

 Recall we now have the derivative of the cost function:

$$egin{aligned} rac{\partial J}{\partial eta_k}(oldsymbol{eta}) &= rac{1}{m} \sum_{j=1}^m \Bigg( y^j - \sum_{i=0}^n eta_i x_i^j \Bigg) (-x_k^j) \end{aligned}$$

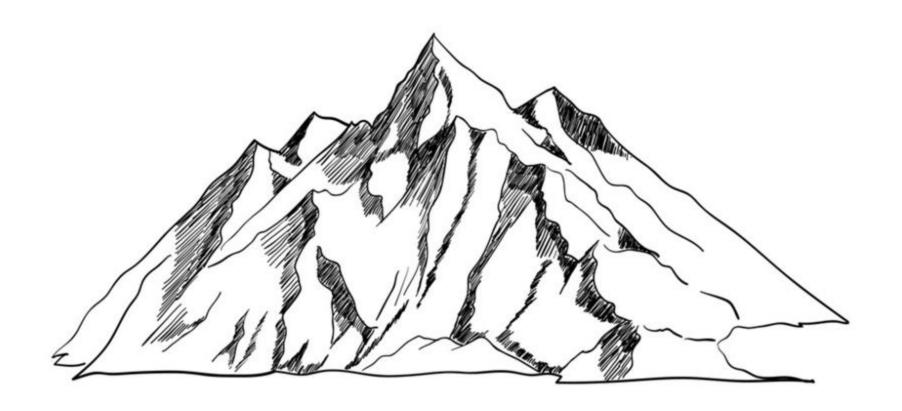
• Use a **gradient** to express the derivative of the cost function with respect to each  $\beta$ 

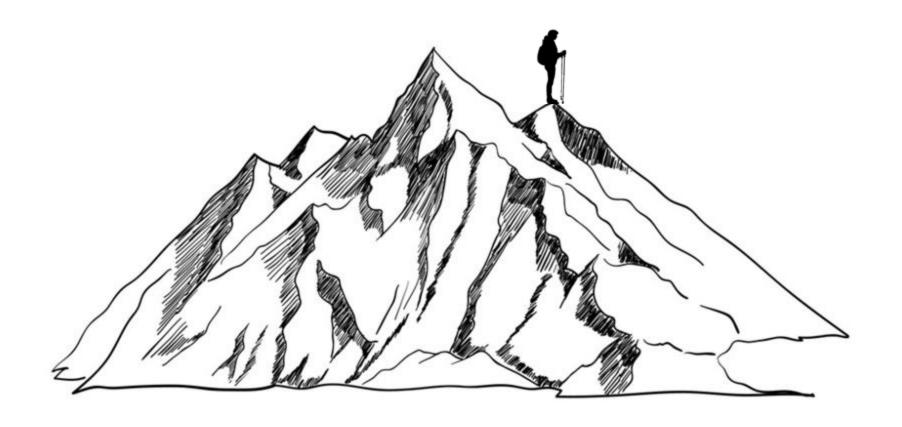
$$abla_{oldsymbol{eta}J} = egin{bmatrix} rac{\partial J}{\partial eta_0} \ dots \ rac{\partial J}{\partial eta_n} \end{bmatrix}$$

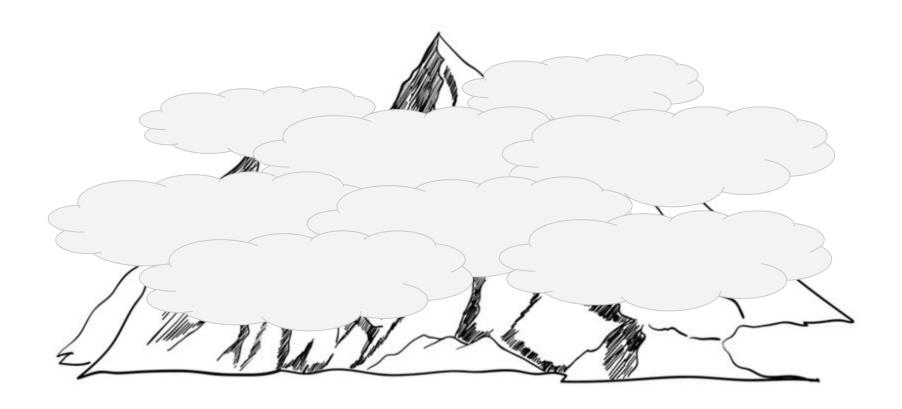
 We also already know what this cost function derivative is equal to:

$$abla_{oldsymbol{eta}} J = egin{bmatrix} -rac{1}{m} \sum_{j=1}^m \left(y^j - \sum_{i=0}^n eta_i x_i^j
ight) x_0^j \ dots \ -rac{1}{m} \sum_{j=1}^m \left(y^j - \sum_{i=0}^n eta_i x_i^j
ight) x_n^j \end{bmatrix} = egin{bmatrix} rac{\partial J}{\partial eta_0} \ dots \ rac{\partial J}{\partial eta_n} \end{bmatrix}$$

- We can use gradient descent to computationally search for the coefficients that minimize this gradient.
- Let's visually explore what this looks like in the case of a single Beta value.

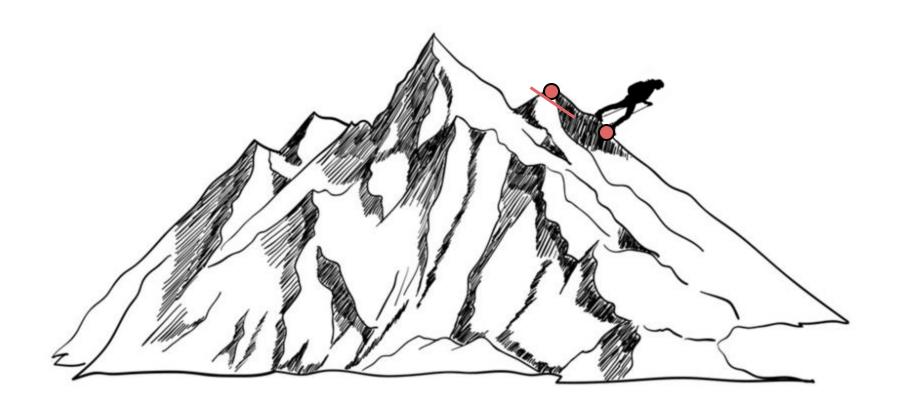


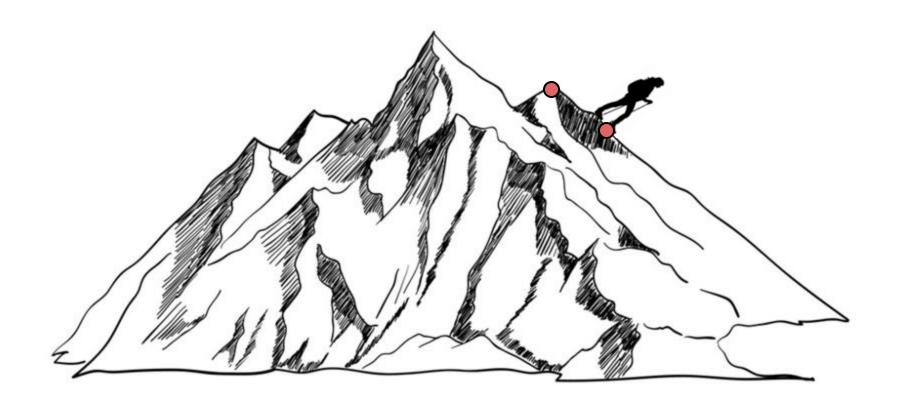


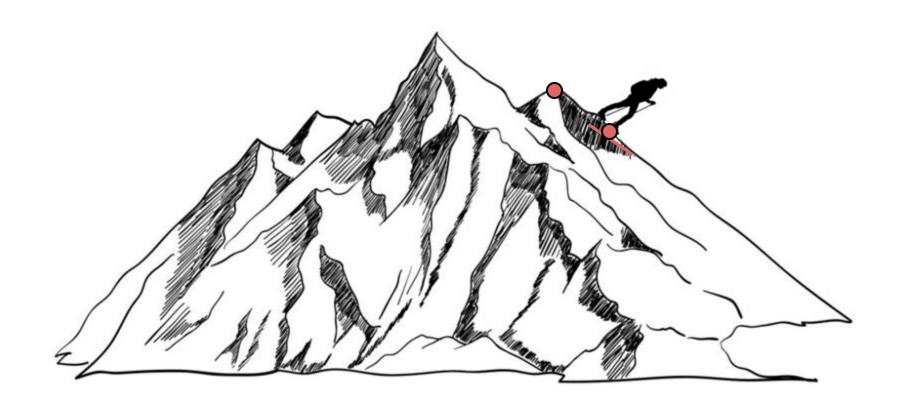


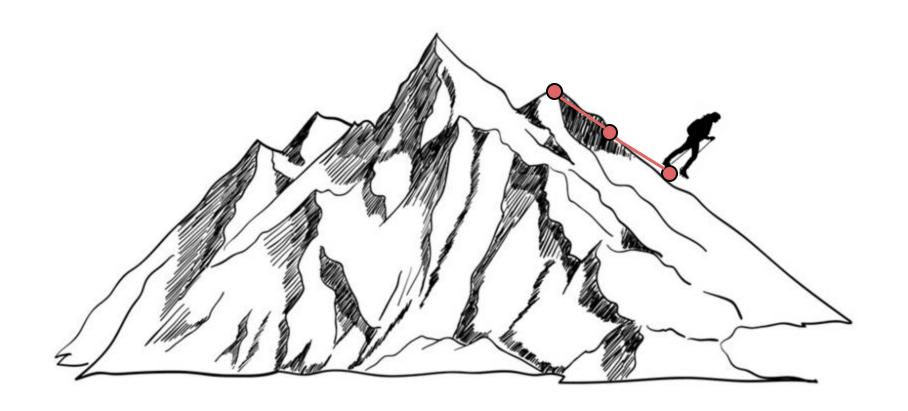


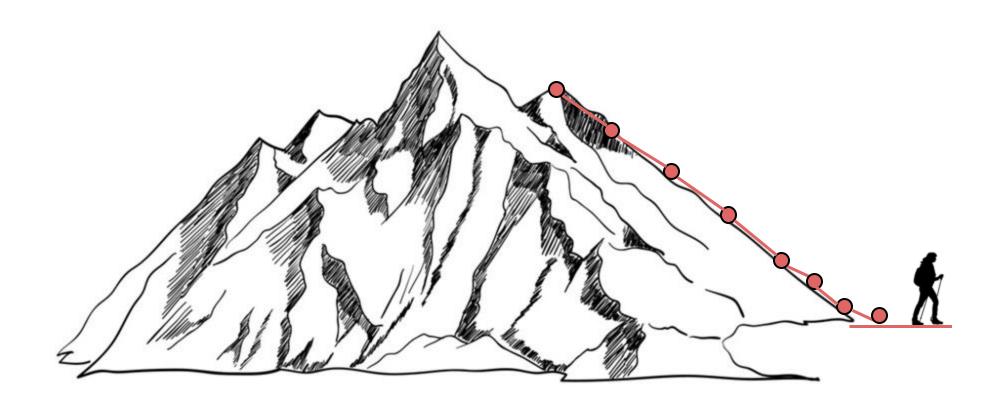






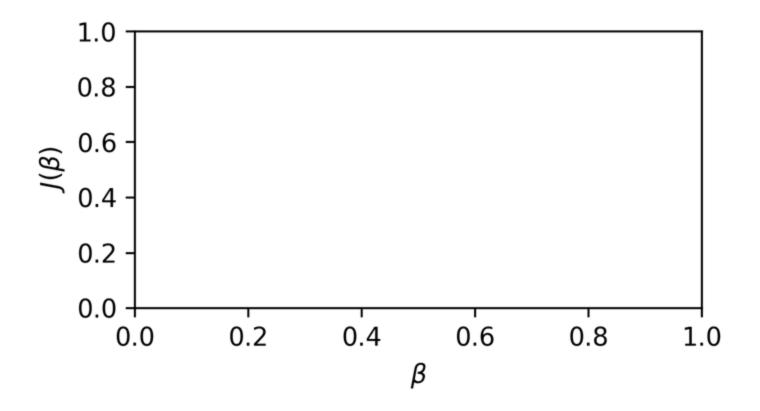




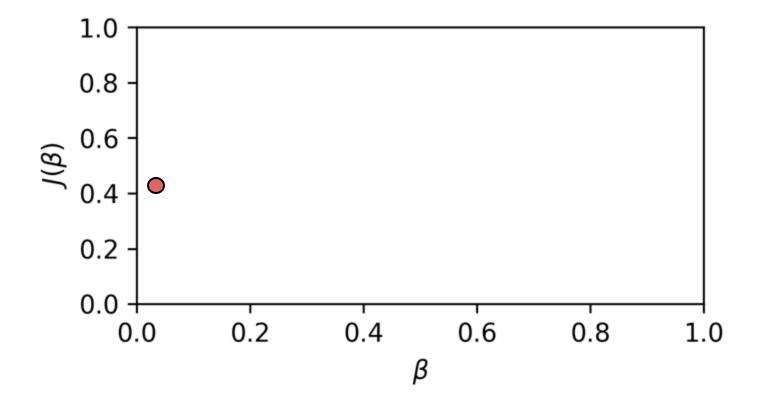


- This is exactly what gradient descent does!
- It even looks similar for the case of a single coefficient search.

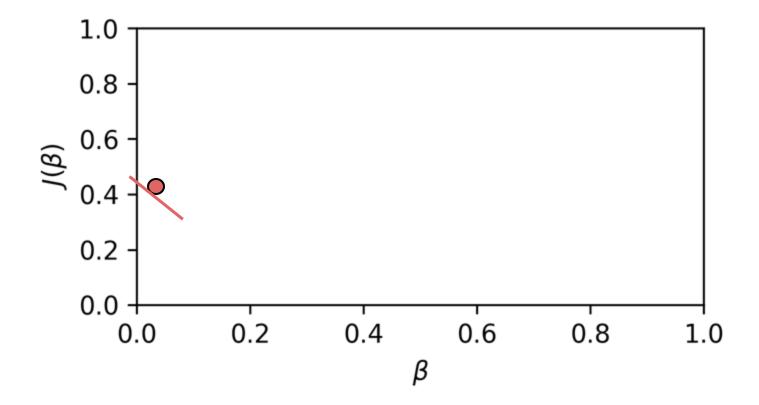
• 1 dimensional cost function (single Beta)



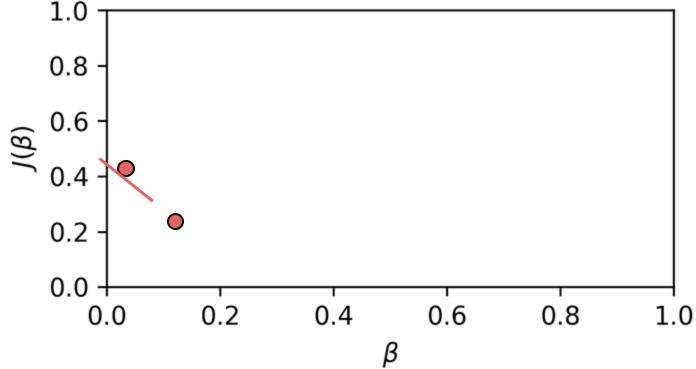
Choose a starting point



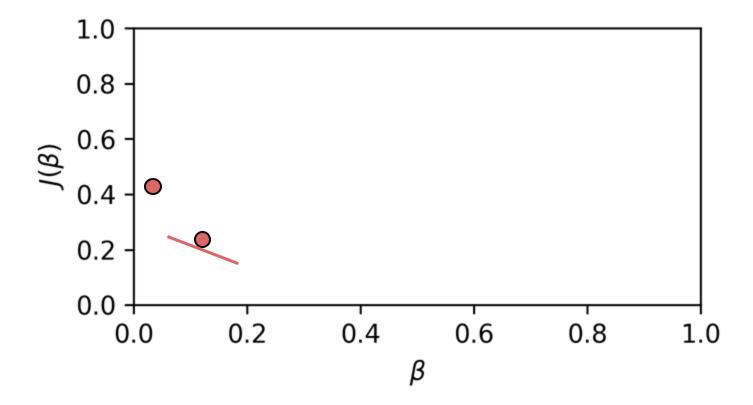
Calculate gradient at that point



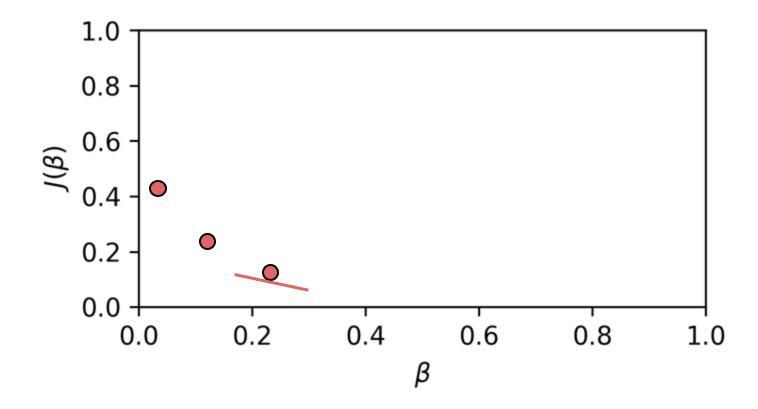
Step forward proportional to negative gradient



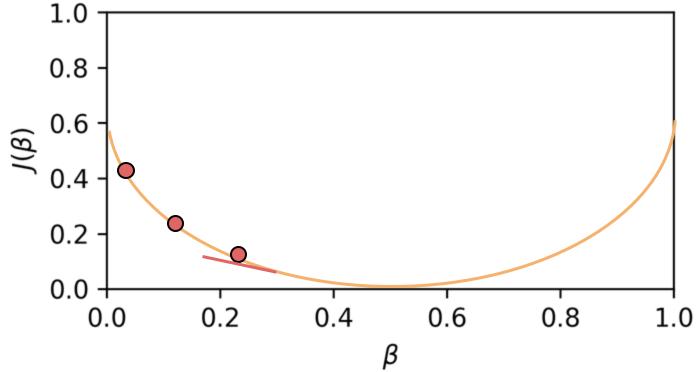
Repeat the steps



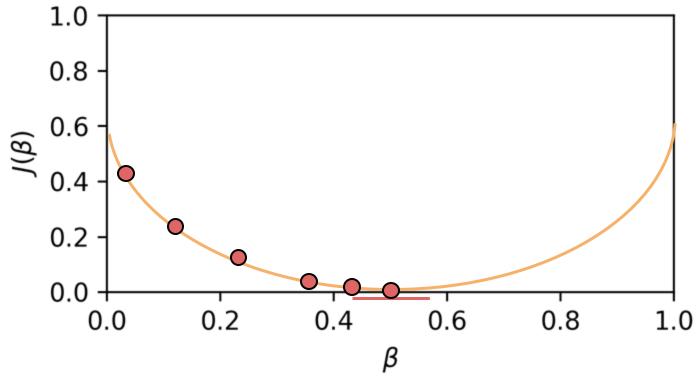
Repeat the steps



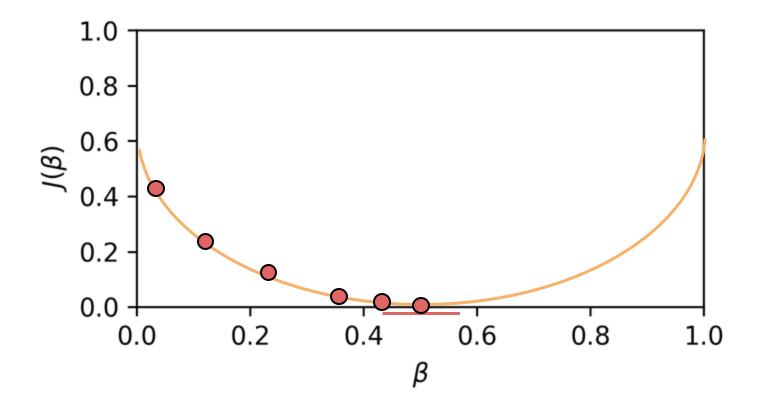
Note how we are essentially mapping the gradient!



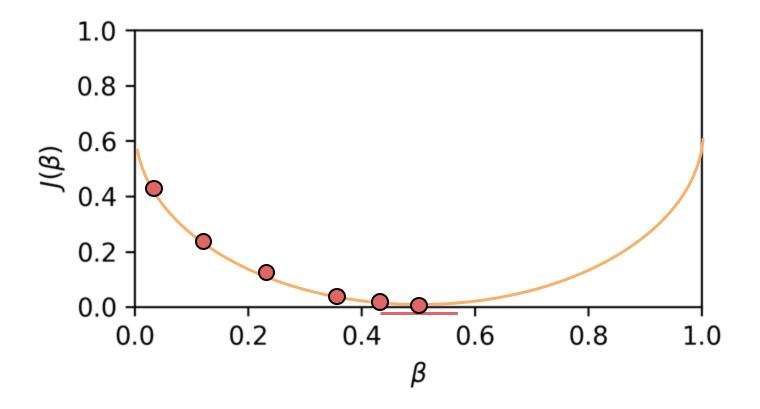
 Eventually we will find the Beta that minimizes the cost function!



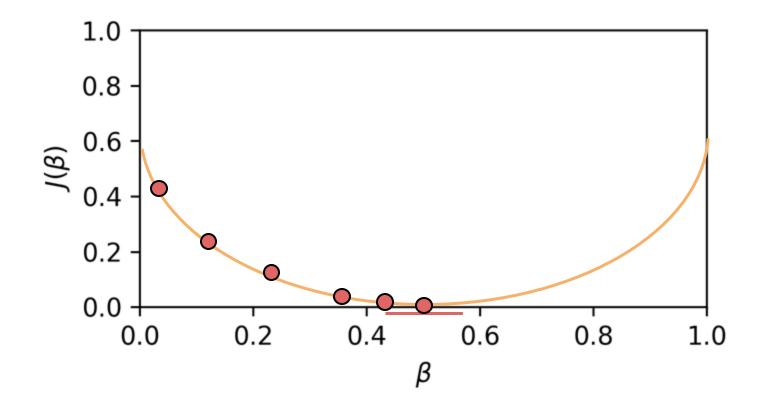
Steps are proportional to negative gradient!



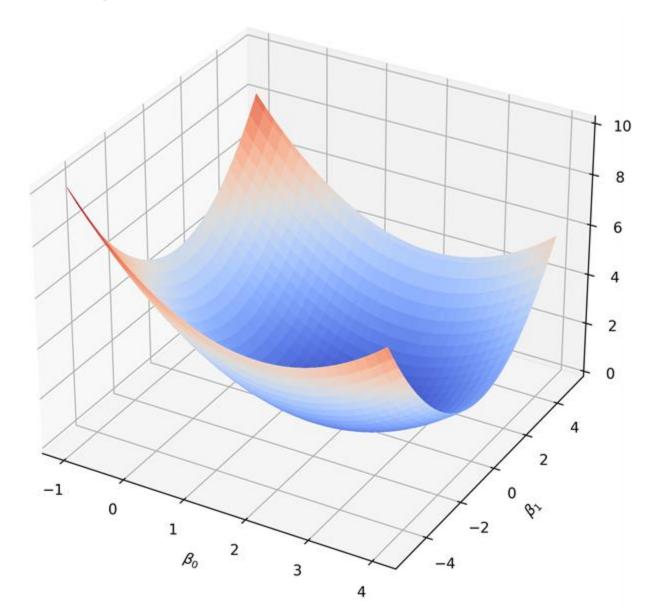
Steeper gradient at start gives larger steps.

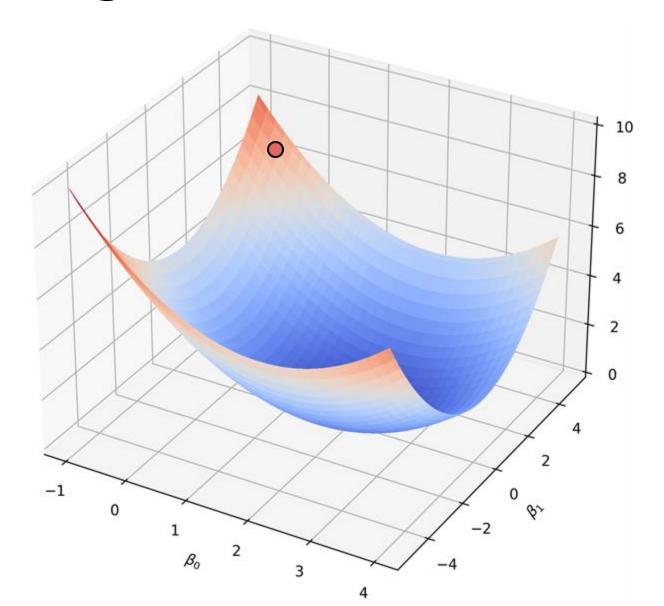


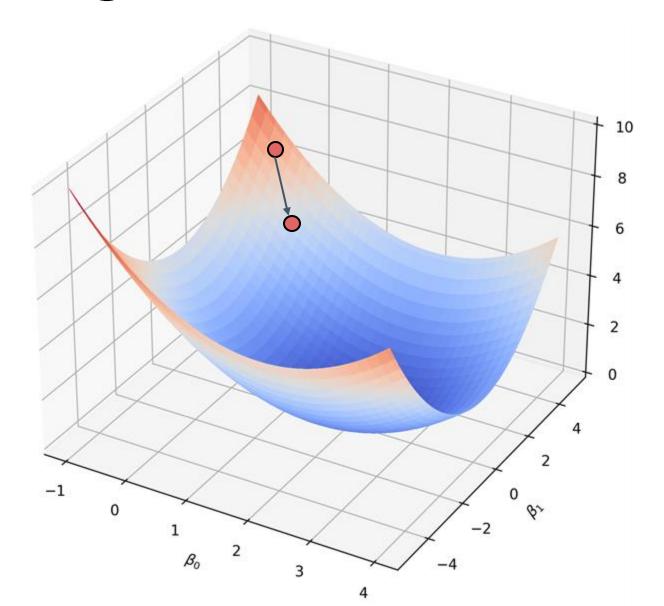
Smaller gradient at end gives smaller steps.

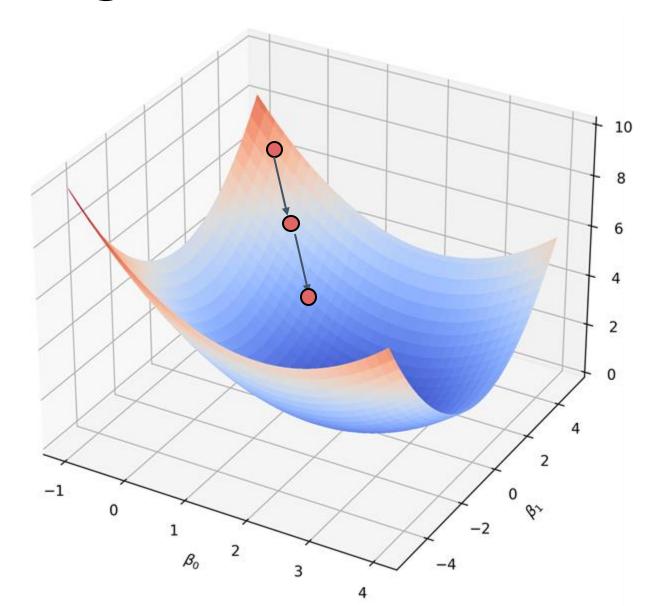


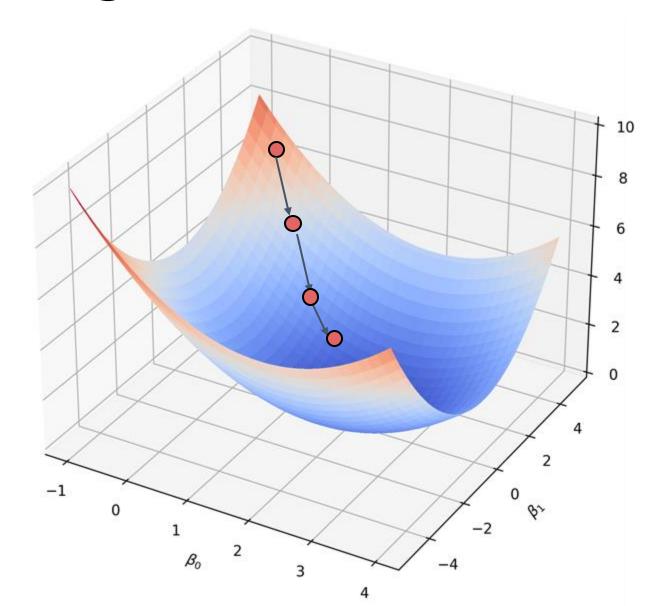
- To further understand this, let's visualize this gradient descent search for two Beta values.
- Process is still the same:
  - Calculate gradient at point.
  - Move in a step size proportional to negative gradient.
  - Repeat until minimum is found.

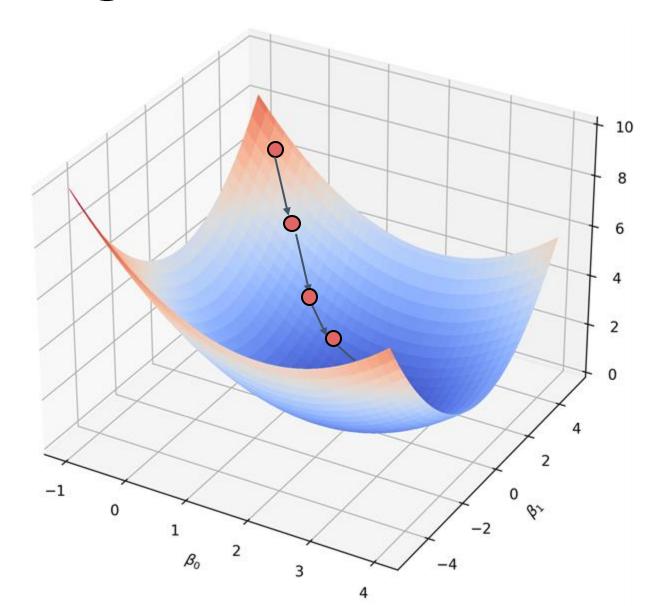


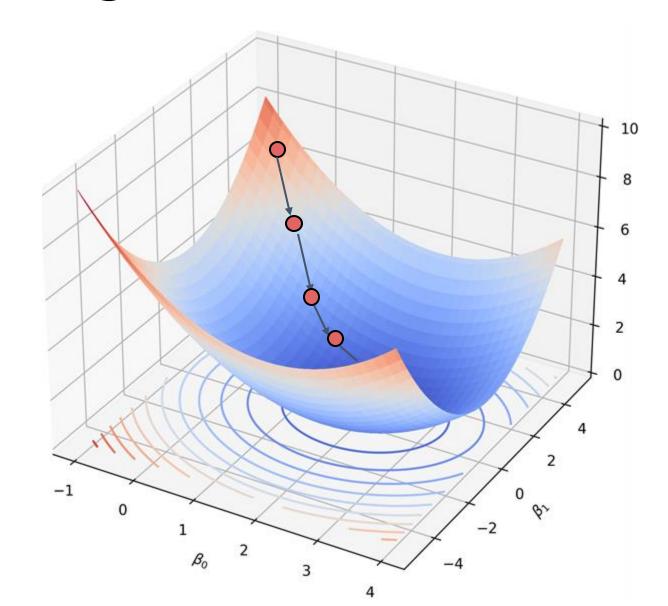


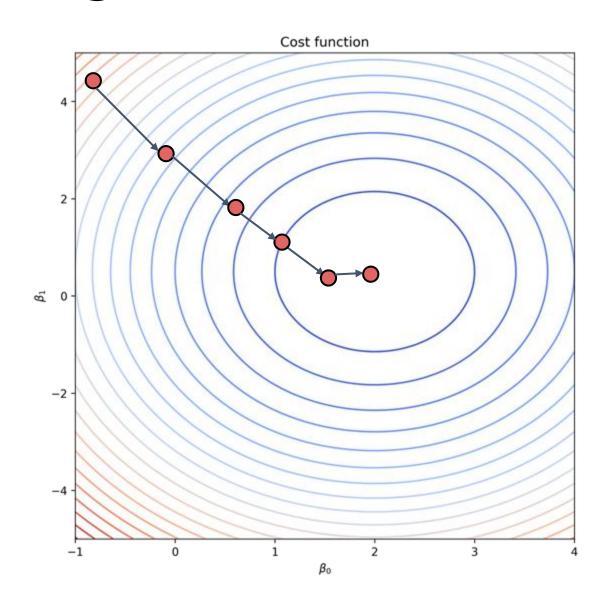












- Finally! We can now leverage all our computational power to find optimal Beta coefficients that minimize the cost function producing the line of best fit!
- We are now ready to code out Linear Regression!



## Scikit-Learn Overview

#### Supervised Machine Learning Process

 Scikit-Learn easily does this split (as well as more advanced cross-validation)



**TRAIN** 

**TEST** 

Area m <sup>2</sup>	Bedrooms	Bathroom	Price
		S	
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

from sklearn.model\_selection import train\_test\_split
X\_train, X\_test, y\_train, y\_test = train\_test\_split(X, y)

```
from sklearn.model_family import ModelAlgo
mymodel = ModelAlgo(param1,param2)
```

```
from sklearn.model_family import ModelAlgo
mymodel = ModelAlgo(param1,param2)
mymodel.fit(X_train,y_train)
```

```
from sklearn.model_family import ModelAlgo
mymodel = ModelAlgo(param1,param2)
mymodel.fit(X_train,y_train)
predictions = mymodel.predict(X_test)
```

```
from sklearn.model_family import ModelAlgo
mymodel = ModelAlgo(param1,param2)
mymodel.fit(X_train,y_train)
predictions = mymodel.predict(X_test)
```

from sklearn.metrics import error\_metric

```
from sklearn.model_family import ModelAlgo
mymodel = ModelAlgo(param1,param2)
mymodel.fit(X_train,y_train)
predictions = mymodel.predict(X_test)
```

from sklearn.metrics import error\_metric
performance = error\_metric(y\_test,predictions)

# Performance Evaluation

**Regression Metrics** 

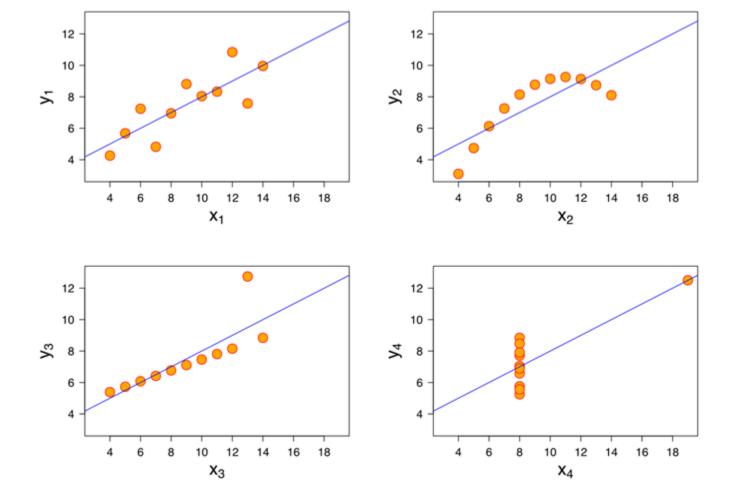
## Evaluating Regression

- Let's discuss some of the most common evaluation metrics for regression:
  - Mean Absolute Error
  - Mean Squared Error
  - Root Mean Square Error

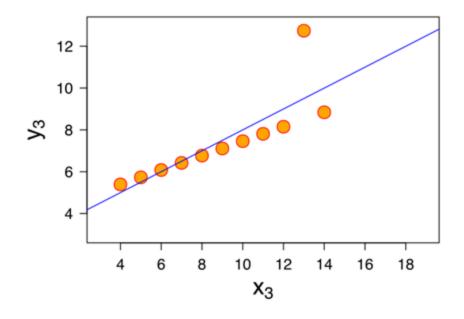
- Mean Absolute Error (MAE)
  - This is the mean of the absolute value of errors.
  - Easy to understand

$$\frac{1}{n}\sum_{i=1}^{n}|y_{i}-\mathring{y}_{i}|$$

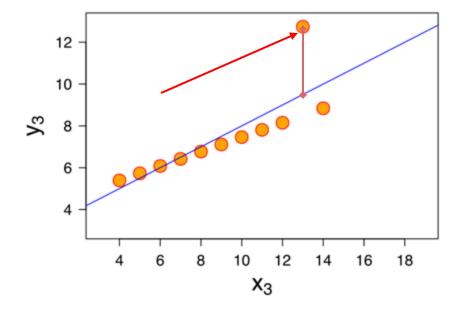
MAE won't punish large errors however.



MAE won't punish large errors however.



 We want our error metrics to account for these!



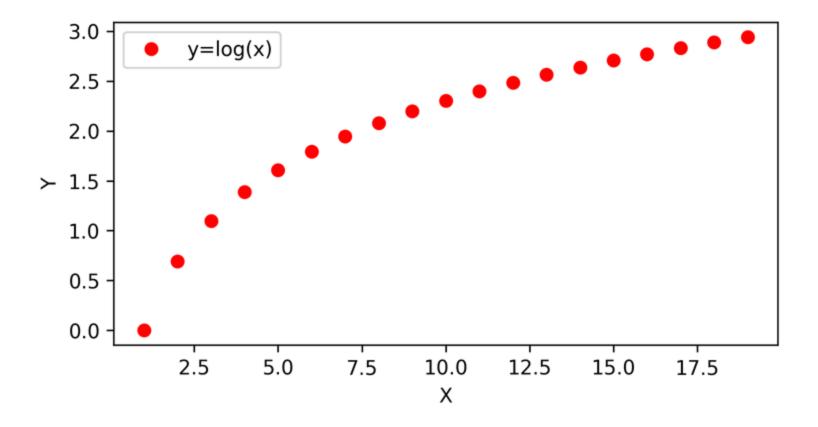
- Mean Squared Error (MSE)
  - Issue with MSE:
    - Different units than y.
    - It reports units of y squared!

$$\frac{1}{n}\sum_{i=1}^{n}(y_{i}-\hat{y}_{i})^{2}$$

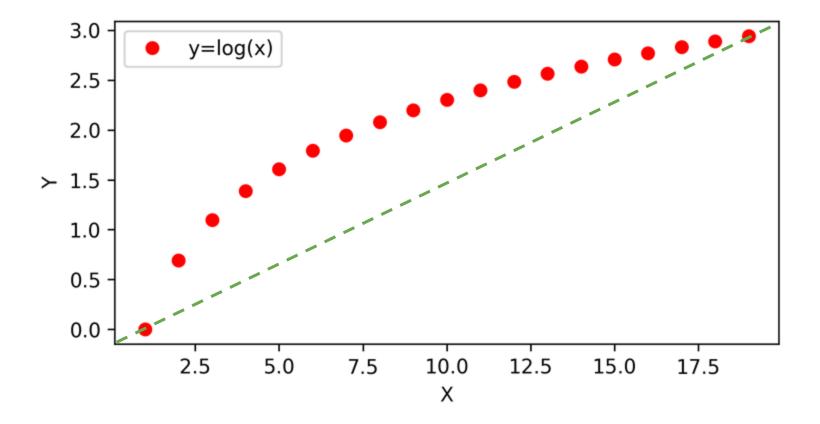
- Root Mean Square Error (RMSE)
  - This is the root of the mean of the squared errors.
  - Most popular (has same units as y)

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i-\mathring{y}_i)^2}$$

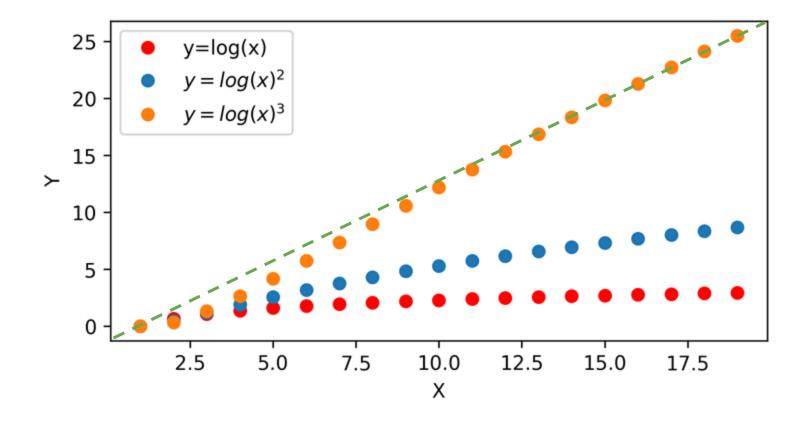
• Imagine a feature that is not linear:



• Will be difficult to find a linear relationship

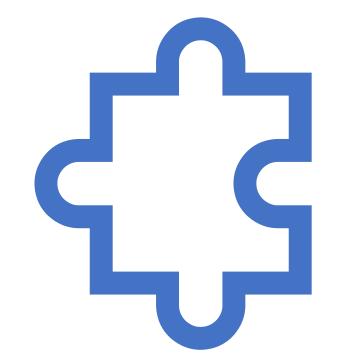


Even more so for higher orders!



- Converting Two Features A and B
  - o 1, A, B, A<sup>2</sup>, AB, B<sup>2</sup>

- Converting Two Features A and B
  - o 1, A, B, A<sup>2</sup>, AB, B<sup>2</sup>
- Generalized terms of features  $X_1$  and  $X_2$ 
  - $\circ$  1, X<sub>1</sub>, X<sub>2</sub>, X<sub>1</sub><sup>2</sup>, X<sub>1</sub>X<sub>2</sub>, X<sub>2</sub><sup>2</sup>



- Regularization seeks to solve a few common model issues by:
  - Minimizing model complexity
  - Penalizing the loss function
  - Reducing model overfitting (add more bias to reduce model variance)

- In general, we can think of regularization as a way to reduce model overfitting and variance.
  - Requires some additional bias
  - Requires a search for optimal penalty hyperparameter.

- Three main types of Regularization:
  - L1 Regularization
    - LASSO Regression
  - L2 Regularization
    - Ridge Regression
  - Combining L1 and L2
    - Elastic Net

- L1 regularization adds a penalty equal to the absolute value of the magnitude of coefficients.
  - Limits the size of the coefficients.
  - Can yield sparse models where some coefficients can become zero.

 L1 regularization adds a penalty equal to the absolute value of the magnitude of coefficients.

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

- L2 regularization adds a penalty equal to the square of the magnitude of coefficients.
  - All coefficients are shrunk by the same factor.
  - Does not necessarily eliminate coefficients.

 L2 regularization adds a penalty equal to the square of the magnitude of coefficients.

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

 Elastic net combines L1 and L2 with the addition of an alpha parameter deciding the ratio between them:

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

# Feature Scaling

## Feature Scaling

- Standardization:
  - Rescales data to have a mean ( $\mu$ ) of 0 and standard deviation ( $\sigma$ ) of 1 (unit variance).

$$X_{changed} = \frac{X - \mu}{\sigma}$$

## Feature Scaling

- Normalization:
  - Scales all data values to be between 0 and 1.

$$X_{changed} = rac{X - X_{min}}{X_{max} - X_{min}}$$

#### Feature Scaling

- Feature scaling process:
  - Perform train test split
  - Fit to training feature data
  - Transform training feature data
  - Transform test feature data

 Let's convert this data into colored blocks for cross-validation

X y

Area m <sup>2</sup>	Bedrooms	Bathroom s	Price
200	3	2	\$500,000
190 230	3	1	\$450,000
		3	\$650,000
180	1	1	\$400,000
210	2	2	\$550,000

Convert to generalized form

X <sub>1</sub>	X <sub>2</sub>	<b>X</b> <sub>3</sub>	У
x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	<b>y</b> <sub>1</sub>
x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	<b>y</b> <sub>2</sub>
x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	<b>У</b> 3
x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	У <sub>4</sub>
x <sup>5</sup> <sub>1</sub>	x <sup>5</sup> <sub>1</sub>	x <sup>5</sup> <sub>1</sub>	<b>y</b> <sub>5</sub>

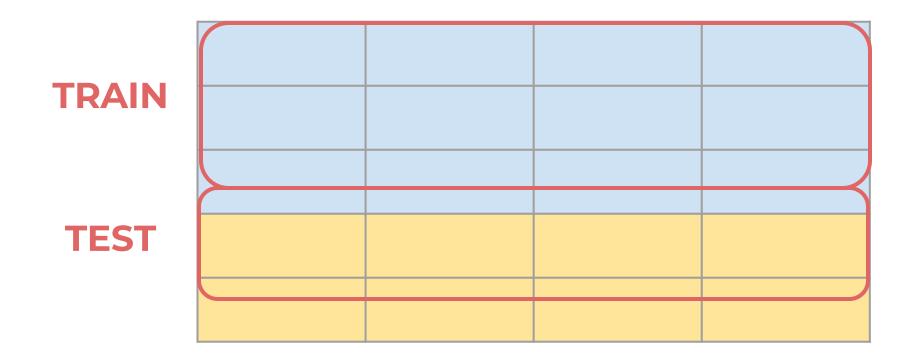
**TRAIN** 

**TEST** 

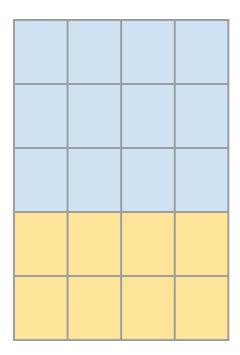
Color based off train vs. test set.

	X		Y
X <sub>1</sub>	X <sub>2</sub>	<b>X</b> <sub>3</sub>	У
x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	x <sup>1</sup> <sub>1</sub>	<b>y</b> <sub>1</sub>
x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	x <sup>2</sup> <sub>1</sub>	<b>y</b> <sub>2</sub>
x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	x <sup>3</sup> <sub>1</sub>	<b>y</b> <sub>3</sub>
x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	x <sup>4</sup> <sub>1</sub>	<b>y</b> <sub>4</sub>
x <sup>5</sup> 1	X <sup>5</sup> <sub>1</sub>	x <sup>5</sup> 1	V <sub>5</sub>

 Now we have all data, colored by training set versus test set.

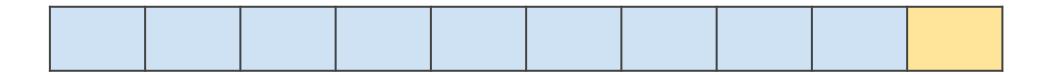


Rotate and resize:

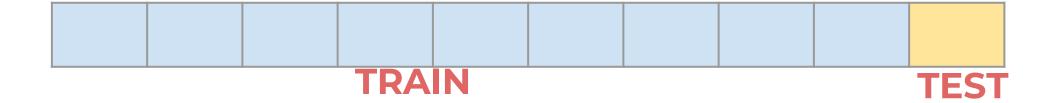


• Rotate and resize:

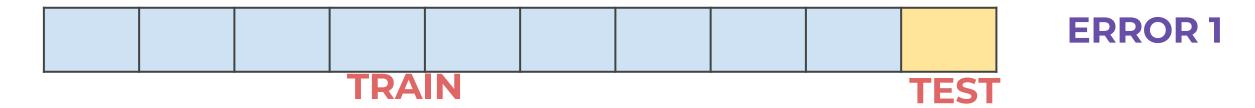
• 1/K left as test set



Now we can represent full data and splits:



Train model and get error metric for split:



Repeat for another 1/K split

ERROR 1					
ERROR 2					

Keep repeating for all possible splits

ERROR					
ERROR					
ERROR					

Keep repeating for all possible K splits

ERROR 1						
ERROR 2						
ERROR 3						
•••			••	•		
ERROR K						

Get average error

ERR						
ERR						
ERR						
••			• •	•		
ERR						

ERROR 1

ERROR 2

ERROR 3

•••

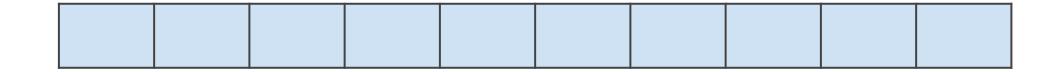
ERROR K

MEAN ERROR

- We were able to train on all data and evaluate on all data!
- We get a better sense of true performance across multiple potential splits.
- What is the cost of this?
  - We have to repeat computations K number of times!

- This is known as K-fold cross-validation.
- 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.
  - Computationally expensive!

Start with entire data set:



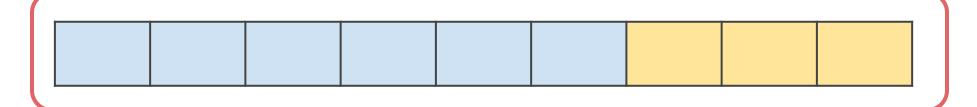
Remove a hold out test set



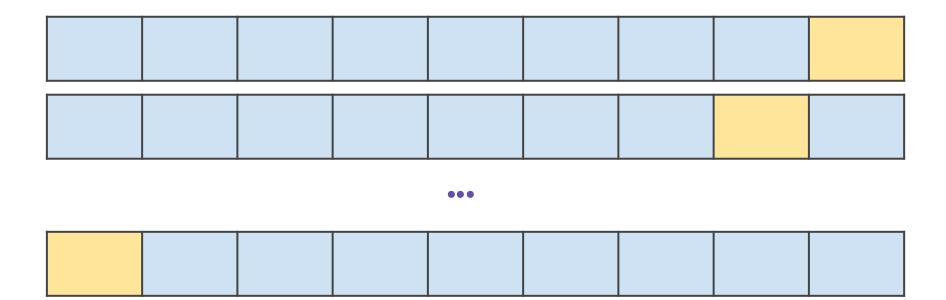
• Perform "classic" train test split:



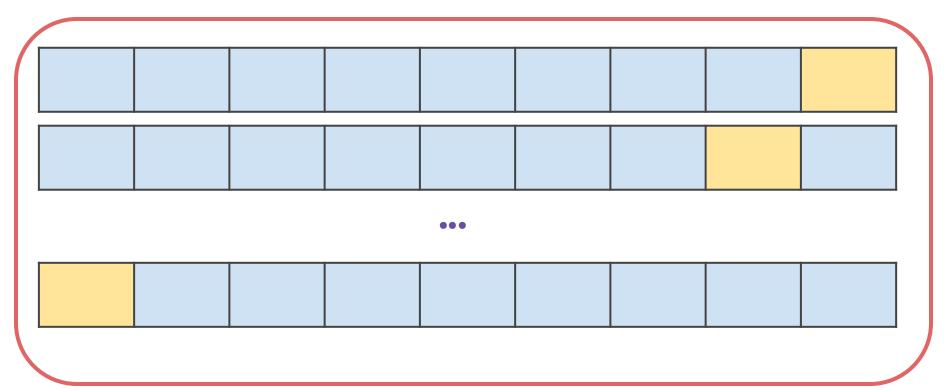
Train and tune on this data:



Or K-Fold cross validation



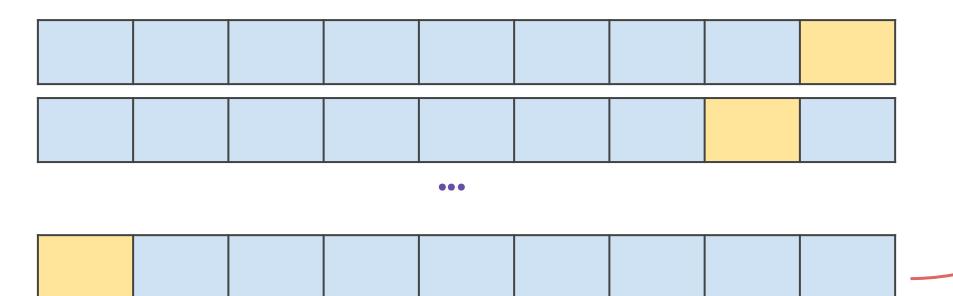
Train and tune on this data:



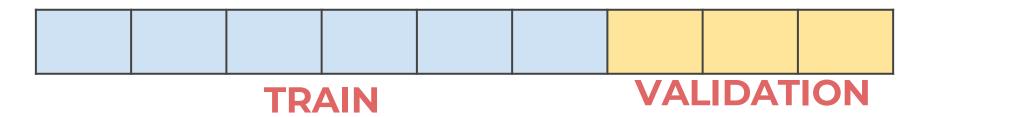
 After training and tuning perform final evaluation hold out test set.

	1		1	ı		
	•	•••				

• Can **not** tune after this **final** test evaluation!



Train | Validation | Test Split





- Allows us to get a true final performance metric to report.
- No editing model after this!