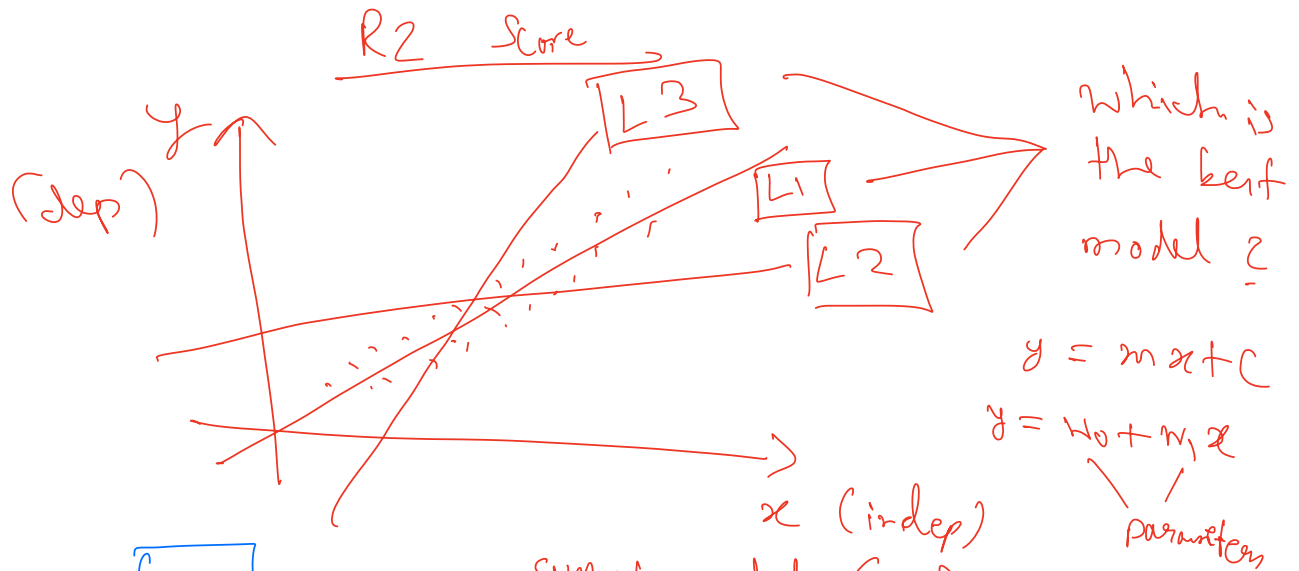


## Last Class - 25 May

- Linear Regression
- Single variable (Univariate) Prediction
- Gradient Descent (Batch GD)
- Mean Squared Error
- Derivatives & Gradients.
- Cars 24 price Prediction problem using single variable

## Today's class - May 27

- 1) Goodness of the Model (being trained or fit)
  - $R^2$  (Coefficient of Determination)
- 2) Univariate (single variable) analysis - review → features
- 3) Linear Regression Library from Python
- 4) Multivariate Regression (Multiple Variables) ↓
- 5) Adjusted  $R^2$  → features
- 6) Model Interpretability & Feature Importance



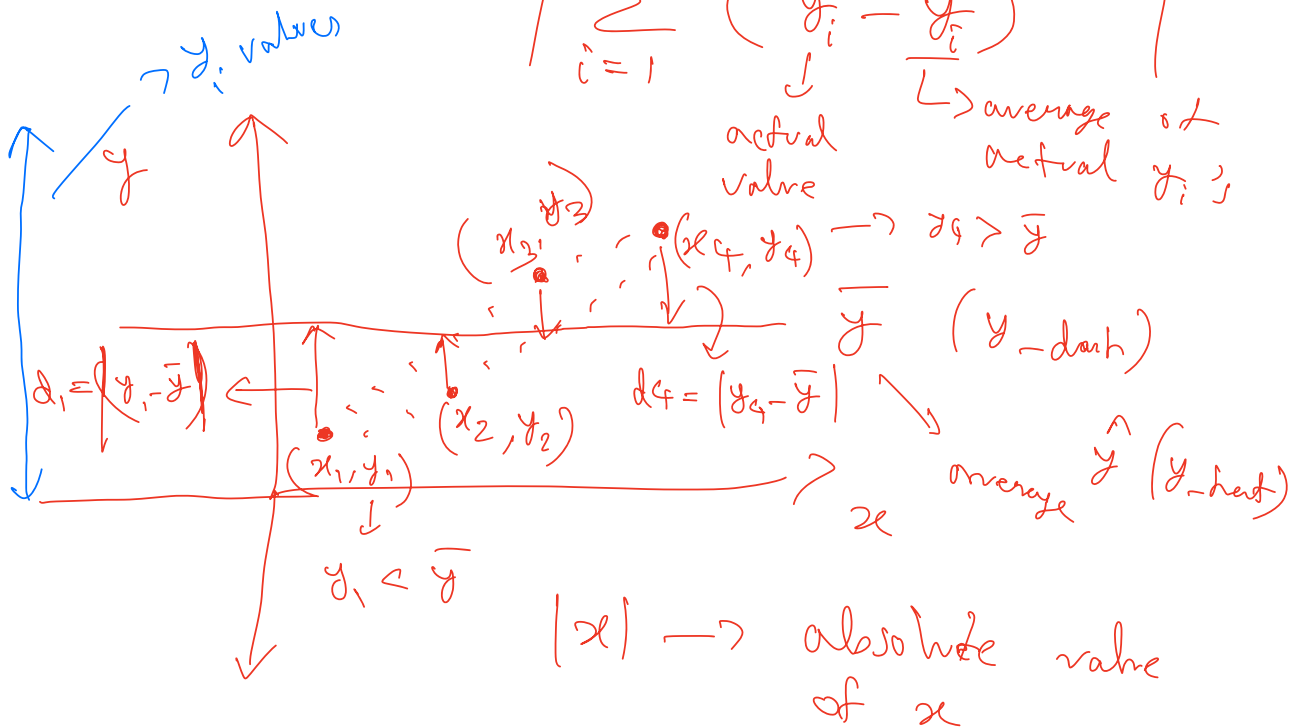
$$R^2 = 1 - \frac{\text{SUM of residuals (SR)}}{\text{Total Sum of Squares (TS)}}$$

$$\rightarrow \text{num} = SR = \sum_{i=1}^N (\hat{y}_i - y_i)^2$$

$\downarrow$  pred       $\downarrow$  actual

$$\rightarrow \text{den} = TS = \sum_{i=1}^N (y_i - \bar{y})^2$$

$\downarrow$  actual value       $\downarrow$  average of actual  $y_i$



$x^2 \rightarrow \text{true}$

$d_1 \rightarrow y_1 - \bar{y} < 0$

$d_k \rightarrow y_k - \bar{y} > 0$

$$R^2 = 1 - \frac{\sum_{i=1}^N (\hat{y}_i - y_i)^2 \rightarrow \text{num}}{\sum_{i=1}^N (y_i - \bar{y})^2 \rightarrow \text{den}}$$

Best Scenario

when all predictions ( $\hat{y}_i$ ) is equal to ground truth/ actual value ( $y_i$ ), i.e.  $\hat{y}_i = y_i$  for every  $i$

$$\hat{y}_i - y_i = 0 \text{ for every } i$$

$$\text{num} = 0$$

$$R^2 = 1 - \frac{0}{\text{something}} = 1$$

Worst Case Scenario

Say  $\text{num} > \text{den}$ , then  $\frac{\text{num}}{\text{den}} > 1$

$$\text{then } R^2 = 1 - \frac{\text{num}}{\text{den}} < 0 \quad \text{if } \frac{\text{num}}{\text{den}} = 2 \quad R^2 = 1 - 2 = -1$$

$$\frac{\text{num}}{\text{den}} \rightarrow \infty$$

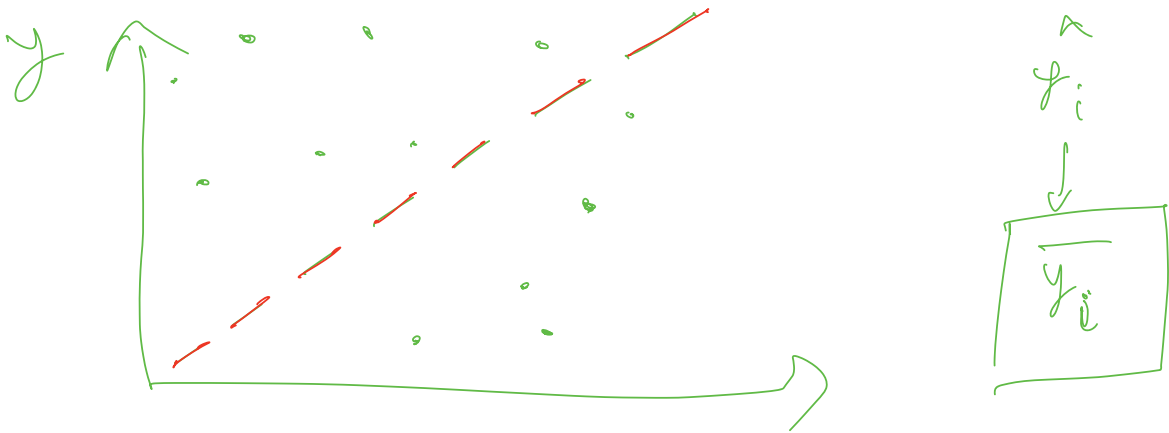
$$\rightarrow > 1$$

$$\text{which} \rightarrow R^2 \rightarrow -\infty$$

## Middle Case Scenario

$$\begin{aligned} \text{If } \text{num} < \text{den}, \quad \frac{\text{num}}{\text{den}} < 1 &\rightarrow 0.5 \\ &\Rightarrow R^2 = 1 - \frac{\text{num}}{\text{den}} \rightarrow 0 < R^2 < 1 \end{aligned}$$

$R^2 < 1 - 0.5 = 0.5$



Linear Regression Library:  $x$   
coeff\_  $\rightarrow w_1$   
intercept\_  $\rightarrow w_0$

$$\begin{aligned} X &\rightarrow (n\text{-samples}, n\text{-features}) \\ &\rightarrow (19820, 1) \end{aligned}$$

$$Y \rightarrow (n\text{-samples}, 1) \rightarrow (19820, 1)$$

$$x_i \rightarrow y_i = \boxed{w_0 + w_1 x_i}$$

$\downarrow$   
 $w_0, w_1$

100 samples  $\rightarrow$  50 , 50  
 $\downarrow$   $\downarrow$   
 class A class B

Random prediction  $\rightarrow$  50% correct

X ML model  $\rightarrow$  40% accuracy  
 $\downarrow$   
 bad job

✓ ML model2  $\rightarrow$  70% accuracy  
 $\downarrow$   
 might be useful better than random

Outliers cause denorm (Total Sum) in  
 $R^2$  score to be as large as possible,  
 And hamper the predictions as well.

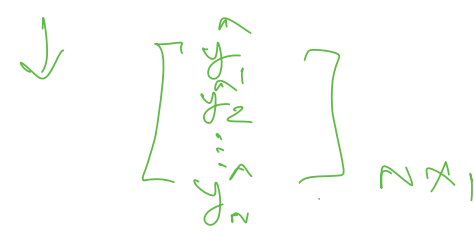
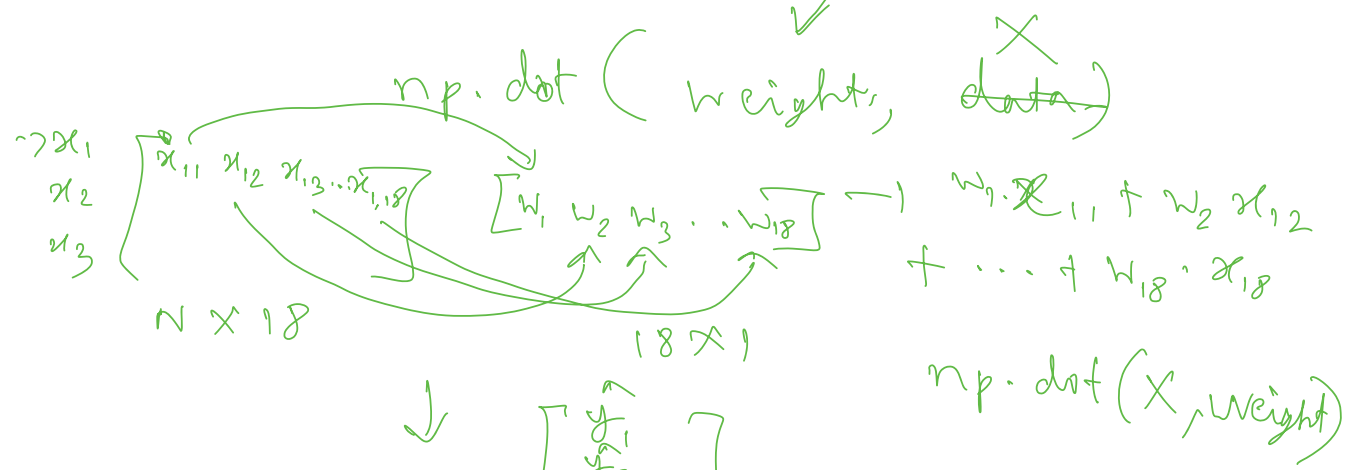
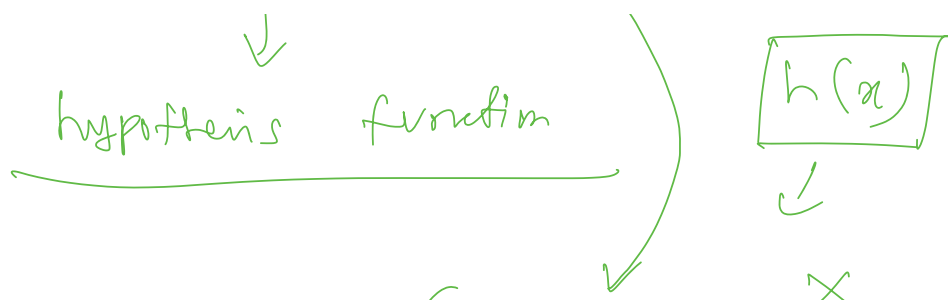
$$X = (x_1, x_2, \dots, x_{17})$$

$$\begin{pmatrix} 1, & x_1, & x_2, & \dots, & x_{17} \end{pmatrix}$$

$$\downarrow \quad \downarrow \quad \downarrow \quad \quad \downarrow$$

$$\boxed{w_0} \quad w_1 \quad w_2 \quad \quad w_{17}$$

$$f(x_i) = w_0 + w_1 x_{i1} + w_2 x_{i2} + \dots + w_n x_{in}$$



$w_0 \cdot 1 + w_1 \cdot x_1 + w_2 \cdot x_2 + \dots + w_d \cdot x_d$

$\boxed{w_0, w_1}$

$L(w_0, w_1) = (y - (w_0 + w_1 x))^2$   
 $\downarrow$   
 $(x, y)$

$L(w_0, w_1) = (y_i - (w_0 + w_1 x_i))^2$   
 $\downarrow$   
 $(x_i, y_i)$

$\left. \frac{\partial L}{\partial w_1} \right|_{x=x_i} = -2 (y - \hat{y}_i) \cdot x_i$

$\rightarrow \boxed{\frac{\partial L}{\partial w_p}} = \frac{1}{N} \sum_{i=1}^N -2 (y - \hat{y}_i) \cdot x_i \rightarrow x_{i,p}$   
 $\downarrow$   
 $x_i$

$\left. \frac{\partial L}{\partial w_0} \right|_{x=x_i} = -2 (y - \hat{y}_i)$

$\frac{\partial L}{\partial w_0} = \frac{1}{N} \sum_{i=1}^N -2 (y - \hat{y}_i) \rightarrow x_{i,0}$   
 $\downarrow$   
 $1$

$$\frac{\partial L}{\partial w_j} \Big|_{j=0,1,2,\dots,D} = \frac{1}{N} \sum_{i=1}^N (y_i - \underset{\substack{\downarrow \\ f(x_i)}}{h(x_i)}) \left( \underset{\substack{\downarrow \\ \text{for } w_j, \\ x_{ij}}}{-x_{ij}} \right)$$

$w_0, w_1$

$w_0, w_1, w_2, \dots$

$x_0, x_1, x_2, \dots$

$$\frac{\partial L}{\partial w_3} = \frac{1}{N} \sum_{i=1}^N 2(y_i - \hat{y}_i) (-x_{i3})$$

$\downarrow \quad \downarrow \quad \downarrow$

$$h(x_i) = w_0 + w_1 x_{i1} + w_2 x_{i2} + \dots + w_d x_{id}$$

gradient  $\rightarrow$  vector  $\left[ \frac{\partial L}{\partial w_0}, \frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, \dots, \frac{\partial L}{\partial w_d} \right]$

$(8 \times 1) \rightarrow$  vector

$$w_0 \leftarrow w_0 - \eta \cdot \frac{\partial L}{\partial w_0}$$

$$w_j \leftarrow w_j - \underset{\substack{\downarrow \\ \text{learning rate}}}{\eta} \cdot \frac{\partial L}{\partial w_j}$$

R2 score

Adjusted R2 score

Adjusted  $R^2 \rightarrow \left[ 1 - \frac{(1-R^2)(n-1)}{n-d-1} \right]$

$\downarrow$        $\downarrow$        $\rightarrow$  number of dim / features  
 not samples / data points

Case 1:  $\frac{d \text{ increases}}{d \uparrow}$ , not significant change in  $R^2$   
 $R^2 \xrightarrow{\text{constant}} R^2$ ,  $d \uparrow$ ,  $n-d-1 \downarrow$  dec

adj  $R^2$

$\downarrow$  dec

$\frac{(1-R^2)(n-1)}{n-d-1 \downarrow} \uparrow$  inc

$\text{adj } R^2 = 1 - \left( \frac{(1-R^2)(n-1)}{n-d-1} \right) \downarrow$

$\downarrow$  dec

Case 2:  $\frac{d \text{ increases}}{d \uparrow}$ , AND  $\frac{R^2 \uparrow \text{ increases}}{R^2 \uparrow}$  significantly

$d \uparrow, n-d-1 \downarrow \Rightarrow \frac{(1-R^2)(n-1)}{(n-d-1) \downarrow} \uparrow \times$

$R^2 \uparrow$

$R^2 \text{ increase} \gg d \uparrow$

$\times$

$0 < R^2 < 1$

$R^2 \text{ increase} < d \text{ increase}$

$d \uparrow, n-d-1 \downarrow$

$R^2 \uparrow, 1-R^2 \downarrow$

$\frac{\downarrow (1-R^2)(n-1)}{(n-d-1) \downarrow}$

$\downarrow$

$\text{adj } R^2 = \left[ 1 - \frac{(1-R^2)(n-1)}{(n-d-1)} \right] \uparrow$



## Feature Importance

$$y = w_0 + w_1 x_1 + \overset{18 \text{ features}}{\underset{\substack{\nearrow w_2 \\ \nearrow w_3}}{\textcircled{2}}} x_2 + \textcircled{10} x_3 + w_4 x_4 + \dots + w_{18} x_{18}$$

$$w_2 = 2, \quad w_3 = 10$$

~~$x_3$~~

Let's say  $x_2 \xrightarrow{\text{inc}} 1 \text{ unit}$

$$y \xrightarrow{\text{inc}} 2 \text{ units} \rightarrow (w_0 + w_1 x_1 + w_3 x_3 + \dots + w_{18} x_{18})$$

$$y = \boxed{1} + 2 x_2$$

$$x_2 = 3$$

$$\left. \begin{array}{l} y = 1 + 2 \times 3 \\ x_2 = 4 \\ y = 1 + 2 \times 4 \end{array} \right\} \rightarrow y \xrightarrow{\text{inc}} 2 \text{ units}$$

$$x_3 \xrightarrow{\text{inc}} 1 \text{ unit}, \quad y \xrightarrow{\text{inc}} 10 \text{ units}$$

$$\left[ \begin{array}{l} y = w_0 + w_1 x_1 + (-5) \cdot x_2 + (-4) \cdot x_3 + \\ w_4 x_4 + \dots + w_{18} x_{18} \\ x_2 \xrightarrow{\text{inc}} 1 \text{ unit}, \quad y \xrightarrow{\text{dec}} 5 \text{ units} \quad \checkmark \text{ more change} \end{array} \right.$$

$x_3 \xrightarrow{\text{inc}} 1 \text{ unit}, y \xrightarrow{\text{dec}} 4 \text{ units}$

feature imp of  $x_i \rightarrow |w_i|$

$$y = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_{18} x_{18}$$

$$y (\text{resale price}) = w_0 + w_1 (\text{age}) + w_2 (\text{km-driven})$$

$\downarrow$  10,000  $\downarrow$   
100

age  $\rightarrow$  0 to 50 years

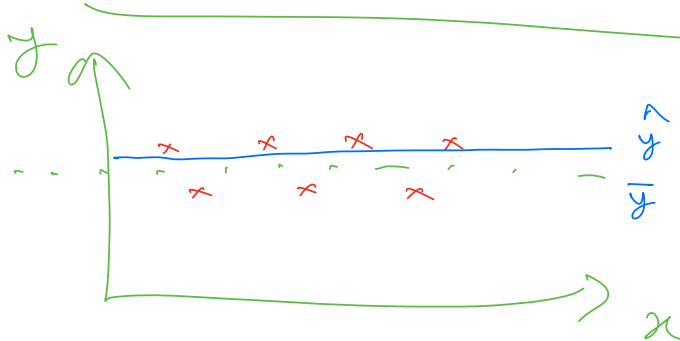
km-driven  $\rightarrow$  0 to 1,00,000 km

Scaling  $\rightarrow$  zero mean, unit std

Standard scaler

min-max scaler

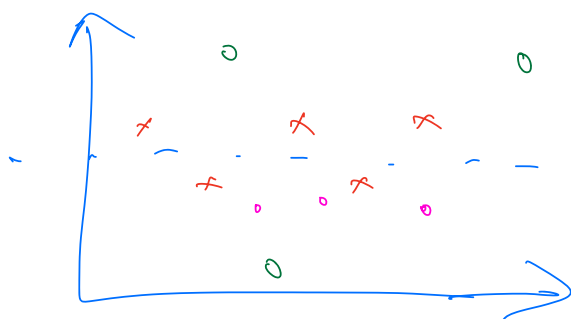
model interpretability



$$\boxed{\text{MSE} \rightarrow 0.5}$$

$$\boxed{\text{RMSE} \rightarrow 0.43}$$

$$\boxed{\begin{matrix} 0.5 & 0.6 \\ 0.7 & - \end{matrix}}$$



$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$$

with outliers  $\rightarrow 0.5, 100$   
 w/o outliers  $\rightarrow 0.5$

