Linear Regression

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IIT Gandhinagar

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- Examples of linear systems:
  - $F = ma$
  - $v = u + at$

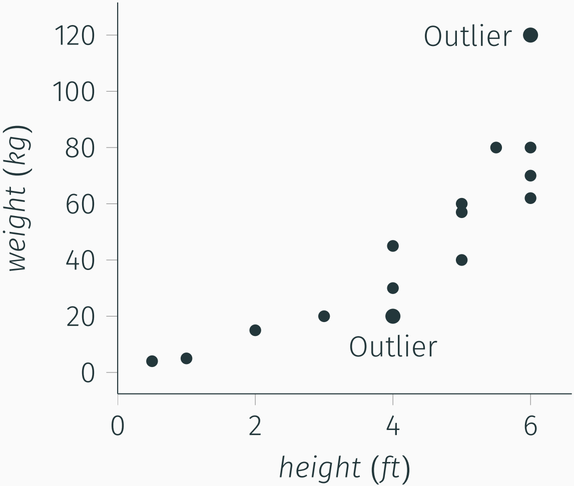
Task at hand

- TASK: Predict Weight = f(height)

Height	Weight
3	29
4	35
5	39
2	20
6	41
7	?
8	?
1	?

The first part of the dataset are the training points. The latter ones are testing points.

Scatter Plot



Matrix representation of the expression

- $weight_1 \approx \theta_0 + \theta_1 * height_1$
- $weight_2 \approx \theta_0 + \theta_1 * height_2$
- $weight_N \approx \theta_0 + \theta_1 * height_N$

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$$weight_i \approx \theta_0 + \theta_1 * height_i$$

Matrix representation of the expression

$$\begin{bmatrix} weight_1 \\ weight_2 \\ \dots \\ weight_N \end{bmatrix} = \begin{bmatrix} 1 & height_1 \\ 1 & height_2 \\ \dots & \dots \\ 1 & height_N \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

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$$W_{N\times 1} = X_{N\times 2}\theta_{2\times 1}$$

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- θ_0 - Bias Term/Intercept Term

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$$W_{N \times 1} = X_{N \times 2} \theta_{2 \times 1}$$

- θ_0 - Bias Term/Intercept Term
- θ_1 - Slope

Extension to multiple dimensions

In the previous example $y = f(x)$, where x is one-dimensional.

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Examples in multiple dimensions.

One example is to predict the water demand of the IITGN campus

Demand = f(# occupants, Temperature)

Demand = Base Demand + K_1 * # occupants + K_2 * Temperature

Intuition

We hope to:

- Learn f: $Demand = f(\#occupants, Temperature)$
- From training dataset
- To predict the condition for the testing set

Linear Relationship

We have

- $x_i = \begin{bmatrix} Temperature_i \\ \#Occupants_i \end{bmatrix}$

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- and $x_i' = \begin{bmatrix} 1 \\ Temperature_i \\ \#Occupants_i \end{bmatrix} = \begin{bmatrix} 1 \\ x_i \end{bmatrix}$
- Notice the transpose in the equation! This is because x_i is a column vector

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- Demand increases, if # occupants increases, then θ_2 is likely to be positive

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- Demand increases, if # occupants increases, then θ_2 is likely to be positive
- Demand increases, if temperature increases, then θ_1 is likely to be positive
- Base demand is independent of the temperature and the # occupants, but, likely positive, thus θ_0 is likely positive.

Generalized Linear Regression Format

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$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix}_{N\times 1} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,M} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,M} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{N,1} & x_{N,2} & \dots & x_{N,M} \end{bmatrix}_{N\times(M+1)} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_M \end{bmatrix}_{(M+1)\times 1}$$

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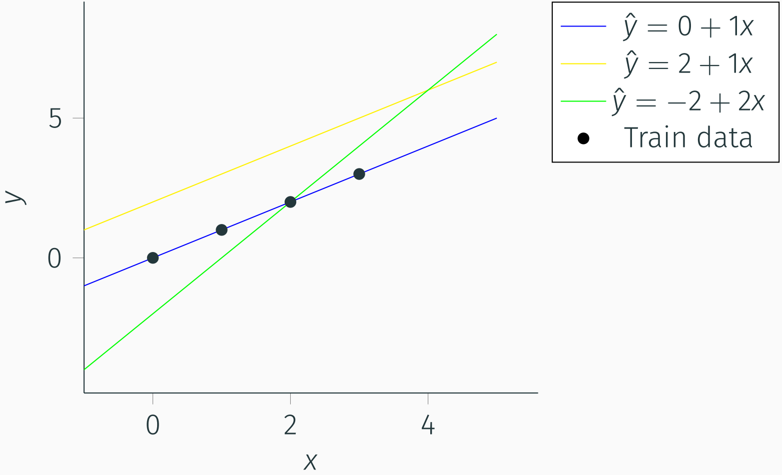
$$\hat{Y} = X\theta$$

Relationships between feature and target variables

- There could be different $\theta_0, \theta_1 \ldots \theta_M$. Each of them can represents a relationship.
- Given multiples values of $\theta_0, \theta_1 \ldots \theta_M$ how to choose which is the best?
- Let us consider an example in 2d

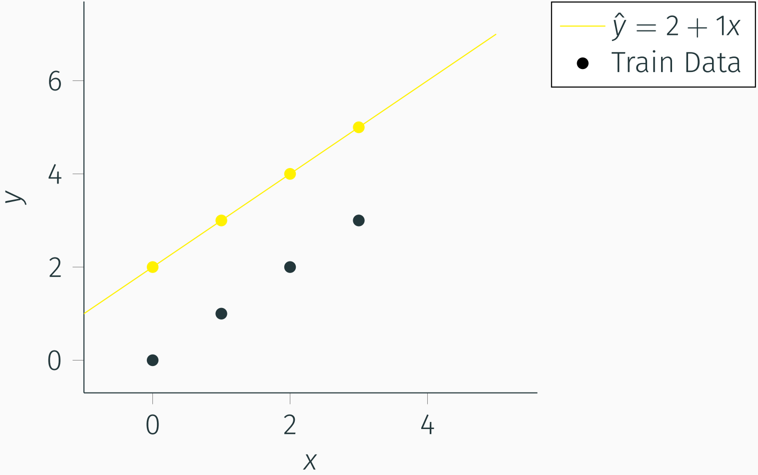
Relationships between feature and target variables

Out of the three fits, which one do we choose?



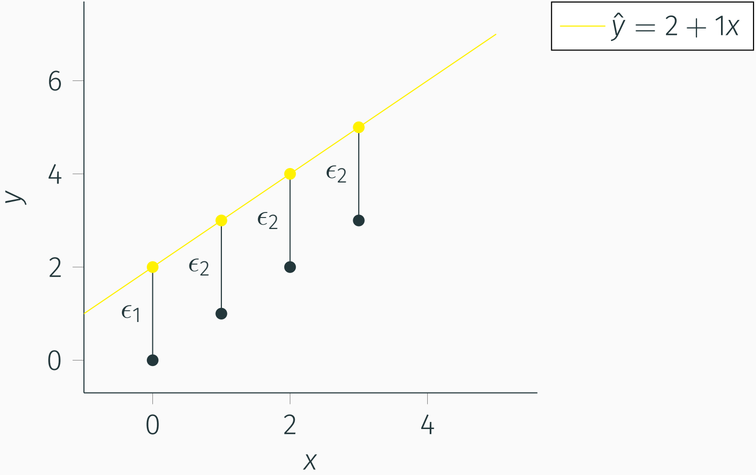
Relationships between feature and target variables

We have $\hat{y} = 2 + 1x$ as one relationship.



Relationships between feature and target variables

How far is our estimated $\hat{y}$ from ground truth y?



Error terms

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- θ_0, θ_1: The parameters of the linear regression
- $\epsilon_i = y_i - \hat{y}_i$
- $\epsilon_i = y_i - (\theta_0 + x_i \times \theta_1)$

Good fit

- $|\epsilon_1|, |\epsilon_2|, |\epsilon_3|, \ldots$ should be small.

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- minimize $\epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_N^2$ - L_2 Norm
- minimize $|\epsilon_1| + |\epsilon_1| + \cdots + |\epsilon_1|$ - L_1 Norm

Normal Equation

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$$Y = X\theta + \epsilon$$

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To Learn: θ

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Objective: minimize $\epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_N^2$

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$$\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_1 \\ \vdots \\ \epsilon_N \end{bmatrix}$$

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Objective: Minimize $\epsilon^T \epsilon$

Derivation of Normal Equation

$$
\begin{aligned}
\epsilon &= y - X\theta \\
\epsilon^T &= (y - X\theta)^T = y^T - \theta^T X^T \\
\epsilon^T \epsilon &= (y^T - \theta^T X^T)(y - X\theta) \\
&= y^T y - \theta^T X^T y - y^T X\theta + \theta^T X^T X\theta \\
&= y^T y - 2y^T X\theta + \theta^T X^T X\theta
\end{aligned}
$$

This is what we wish to minimize

Minimizing the objective function

$$\frac{\partial \epsilon^T \epsilon}{\partial \theta} = 0 \tag{1}$$

- $\frac{\partial}{\partial \theta} y^T y = 0$
- $\frac{\partial}{\partial \theta}(-2y^T X\theta) = (-2y^T X)^T = -2X^T y$
- $\frac{\partial}{\partial \theta}(\theta^T X^T X\theta) = 2X^T X\theta$

Substitute the values in the top equation

Normal Equation derivation

$$0 = -2X^T y + 2X^T X\theta$$

$$X^T y = X^T X\theta$$

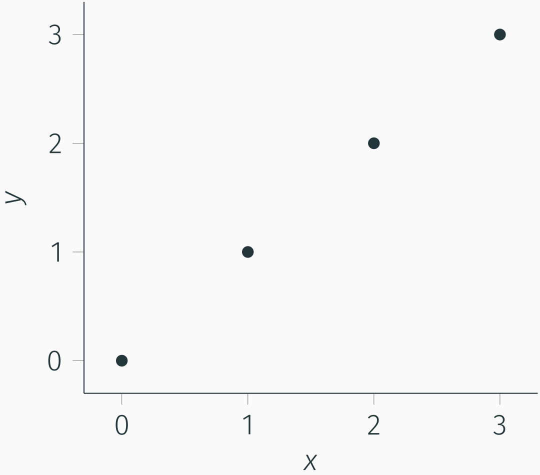
$$\hat{\theta}_{OLS} = (X^T X)^{-1} X^T y$$

Worked out example

x	y
0	0
1	1
2	2
3	3

Given the data above, find θ_0 and θ_1.

Scatter Plot



Worked out example

$$
\begin{aligned}
X &= \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \\
X^T &= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \\
X^T X &= \begin{bmatrix} 4 & 6 \\ 6 & 14 \end{bmatrix}
\end{aligned} \tag{2}
$$

Given the data above, find θ_0 and θ_1.

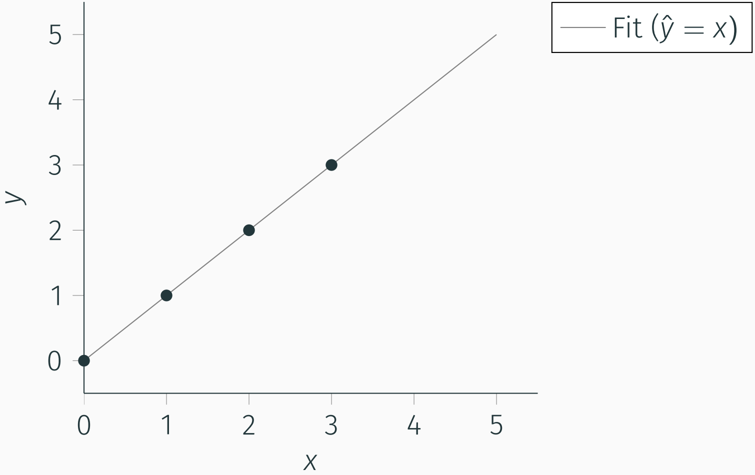
Worked out example

$$
\begin{aligned}
(X^T X)^{-1} &= \frac{1}{20}\begin{bmatrix} 14 & -6 \\ -6 & 4 \end{bmatrix} \\
X^T y &= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}
\end{aligned} \tag{3}
$$

Worked out example

$$\theta = (X^T X)^{-1}(X^T y)$$
$$\begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \frac{1}{20}\begin{bmatrix} 14 & -6 \\ -6 & 4 \end{bmatrix}\begin{bmatrix} 6 \\ 14 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{4}$$

Scatter Plot

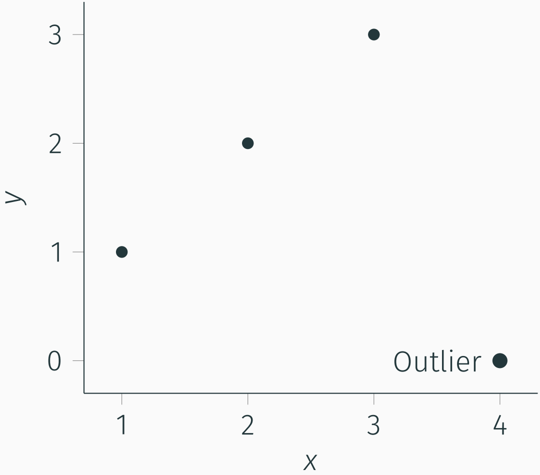


Effect of outlier

x	y
1	1
2	2
3	3
4	0

Compute the θ_0 and θ_1.

Scatter Plot



Worked out example

$$
\begin{aligned}
X &= \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \\
X^T &= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \end{bmatrix} \\
X^T X &= \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}
\end{aligned} \tag{5}
$$

Given the data above, find θ_0 and θ_1.

Worked out example

$$
\begin{aligned}
(X^T X)^{-1} &= \frac{1}{20}\begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix} \\
X^T y &= \begin{bmatrix} 6 \\ 14 \end{bmatrix}
\end{aligned} \tag{6}
$$

Worked out example

$$\theta = (X^T X)^{-1}(X^T y)$$
$$\begin{bmatrix}\theta_0 \\ \theta_1\end{bmatrix} = \begin{bmatrix} 2 \\ (-1/5)\end{bmatrix} \tag{7}$$

Scatter Plot