Linear Regression

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IIT Gandhinagar

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Linear Regression

- Output is continuous in nature.

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- Examples of linear systems:

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  - $F = ma$

Linear Regression

- Output is continuous in nature.
- Examples of linear systems:
  - $F = ma$
  - $v = u + at$

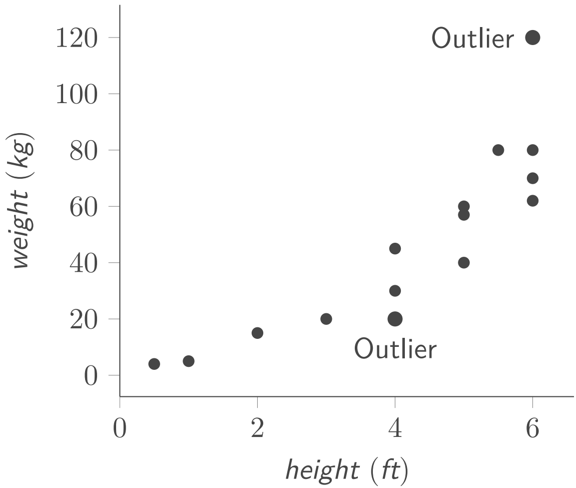
Task at hand

- 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 is the training points. The latter ones are testing points.

Scatter Plot



Matrix representation of the expression

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

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

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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$$\hat{\mathbf{y}}_{n\times 1} = \mathbf{X}_{n\times d}\boldsymbol{\theta}_{d\times 1}$$

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- θ_0 - Bias Term/Intercept Term

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- 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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- Mathematical representation:

$$\text{Demand} = f(\#\text{ occupants, Temperature})$$

Extension to multiple dimensions

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- Now consider examples in multiple dimensions
- Example: Predict the water demand of the IITGN campus
- Mathematical representation:

Demand = f(# occupants, Temperature)

- Linear form:

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

We can expect the following

- 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.

Normal Equation

Generalized Linear Regression Format

- Assuming N samples for training

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- Assuming N samples for training
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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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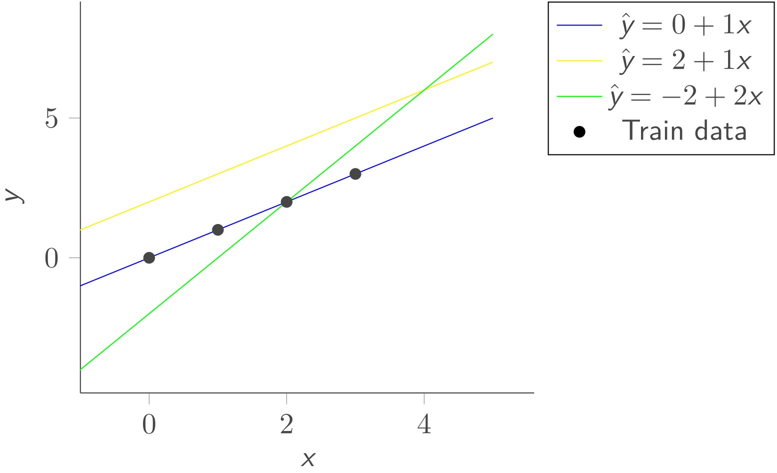
$$\boxed{\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}}$$

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

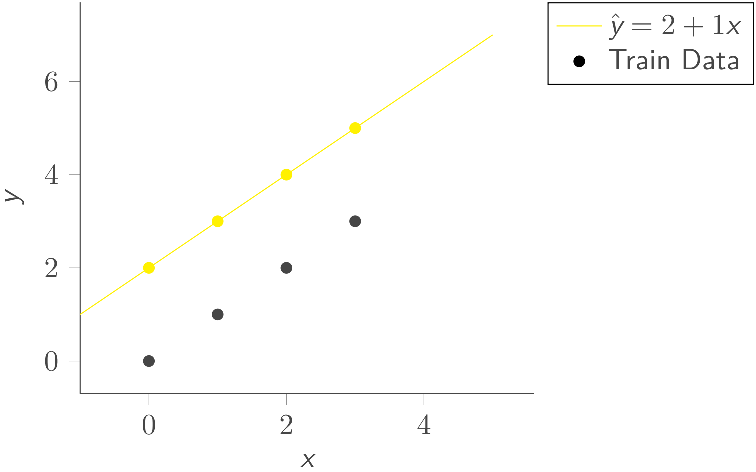
Relationships between feature and target variables

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



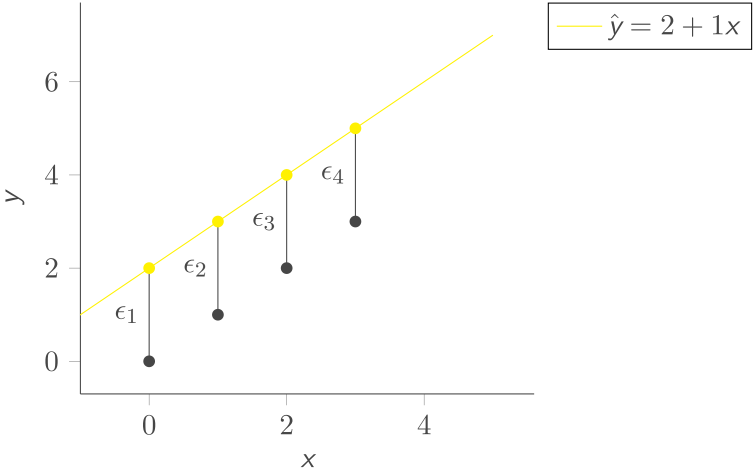
Relationships between feature and target variables

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

- $y_i = \hat{y}_i + \epsilon_i$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$

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- ϵ_i denotes the error/residual for i^{th} sample
- θ_0, θ_1: The parameters of the linear regression
- $\epsilon_i = y_i - \hat{y}_i$
- $\epsilon_i = y_i - (\theta_0 + x_i \cdot \theta_1)$

Good fit

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

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

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

Normal Equation

- Model specification:

$$\boxed{\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon}}$$

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- To Learn: $\boldsymbol{\theta}$

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- Model specification:

$$\boxed{\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon}}$$

- To Learn: $\boldsymbol{\theta}$
- Objective: minimize $\epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_N^2$

Normal Equation

$$\boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_N \end{bmatrix}$$

Normal Equation

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Objective: Minimize $\boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}$

Derivation of Normal Equation

$$\boldsymbol{\epsilon} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}$$

$$\boldsymbol{\epsilon}^\top \boldsymbol{\epsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$

$$= \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

This is what we wish to minimize

Minimizing the objective function

$$\frac{\partial \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}}{\partial \boldsymbol{\theta}} = \mathbf{0}$$

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

Substitute the values in the top equation

Normal Equation derivation

$$\mathbf{0} = -2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

$$\mathbf{X}^\top \mathbf{y} = \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

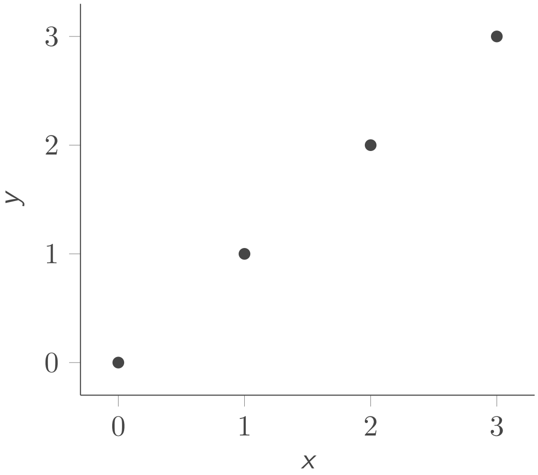
$$\boxed{\hat{\boldsymbol{\theta}}_{OLS} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}}$$

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

$$\mathbf{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}$$

$$\mathbf{X}^\top = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix}$$

$$\mathbf{X}^\top \mathbf{X} = \begin{bmatrix} 4 & 6 \\ 6 & 14 \end{bmatrix}$$

Given the data above, find θ_0 and θ_1.

Worked out example

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{20} \begin{bmatrix} 14 & -6 \\ -6 & 4 \end{bmatrix}$$

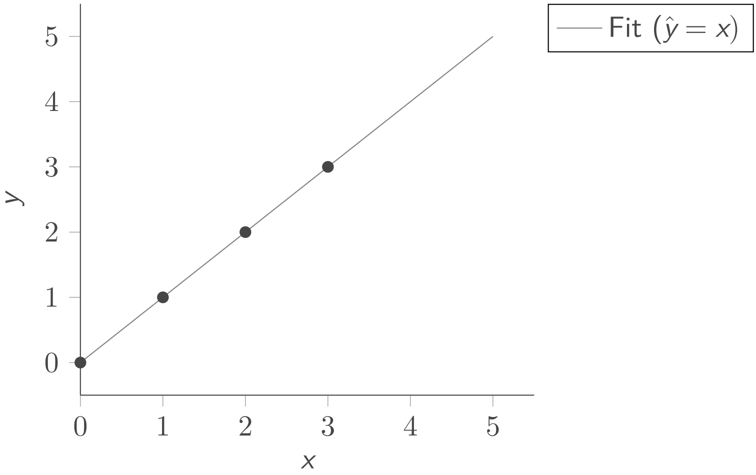
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked out example

$$\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1}(\mathbf{X}^\top \mathbf{y})$$

$$\begin{bmatrix}\theta_0 \\ \theta_1\end{bmatrix} = \frac{1}{20}\begin{bmatrix}14 & -6 \\ -6 & 4\end{bmatrix}\begin{bmatrix}6 \\ 14\end{bmatrix} = \begin{bmatrix}0 \\ 1\end{bmatrix}$$

Scatter Plot

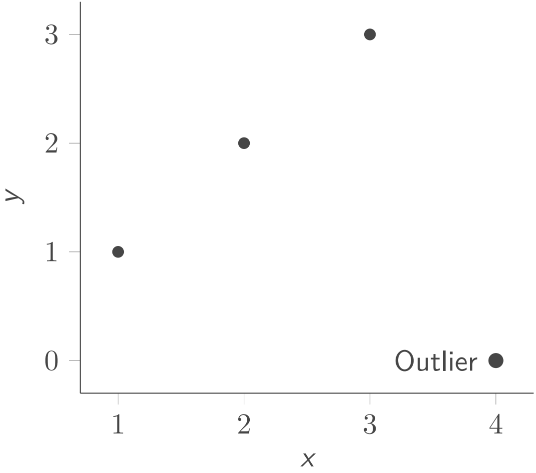


Effect of outlier

x	y
1	1
2	2
3	3
4	0

Compute the θ_0 and θ_1.

Scatter Plot



Worked out example

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}$$

$$\mathbf{X}^\top = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$\mathbf{X}^\top \mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

Given the data above, find θ_0 and θ_1.

Worked out example

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{20} \begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}$$

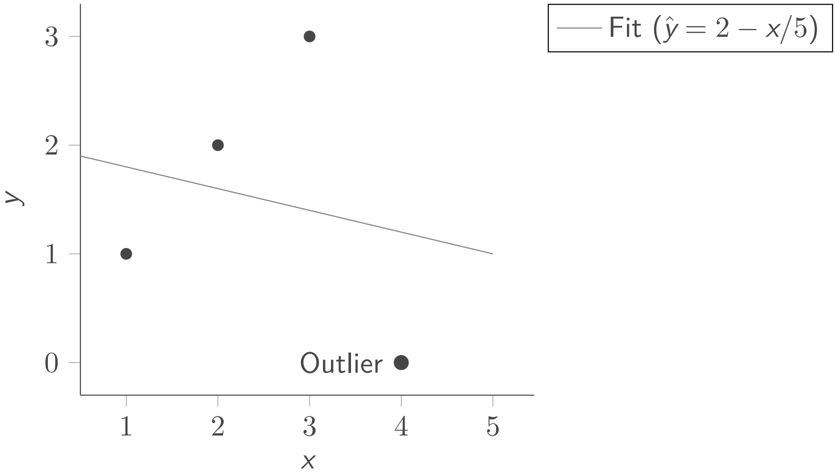
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked out example

$$\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1}(\mathbf{X}^\top \mathbf{y})$$

$$\begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} 2 \\ (-1/5) \end{bmatrix}$$

Scatter Plot



Basis Expansion

Variable Transformation

Transform the data, by including the higher power terms in the feature space.

t	s
0	0
1	6
3	24
4	36

The above table represents the data before transformation

Variable Transformation

Add the higher degree features to the previous table

t	t^2	s
0	0	0
1	1	6
3	9	24
4	16	36

- The above table represents the data after transformation

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- Now, we can write $\hat{s} = f(t, t^2)$

Variable Transformation

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- The above table represents the data after transformation
- Now, we can write $\hat{s} = f(t, t^2)$
- Other transformations: $\log(x), x_1 \times x_2$

A big caveat: Linear in what?![1]

1. $\hat{s} = \theta_0 + \theta_1 * t$ is linear

[1] https://stats.stackexchange.com/questions/8689/what-does-linear-stand-for-in-linear-regression

A big caveat: Linear in what?![1]

1. $\hat{s} = \theta_0 + \theta_1 * t$ is linear
2. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2$ linear?

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2. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2$ linear?
3. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2 + \theta_3 * \cos(t^3)$ linear?

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4. Is $\hat{s} = \theta_0 + \theta_1 * t + \mathrm{e}^{\theta_2} * t$ linear?

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5. All except #4 are linear models!

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4. Is $\hat{s} = \theta_0 + \theta_1 * t + \mathrm{e}^{\theta_2} * t$ linear?
5. All except #4 are linear models!
6. Linear refers to the relationship between the parameters that you are estimating ($\boldsymbol{\theta}$) and the outcome

[1] https://stats.stackexchange.com/questions/8689/what-does-linear-stand-for-in-linear-regression

Basis Functions

- Linear regression only refers to linear in the parameters
- We can perform an arbitrary nonlinear transformation $\phi(x)$ of the inputs x and then linearly combine the components of this transformation.
- $\phi : \mathbb{R}^D \to \mathbb{R}^K$ is called the basis function

Basis Functions

Some examples of basis functions:

- Polynomial basis: $\phi(x) = \{1, x, x^2, x^3, \dots\}$
- Fourier basis: $\phi(x) = \{1, \sin(x), \cos(x), \sin(2x), \cos(2x), \dots\}$
- Gaussian basis: $\phi(x) = \{1, \exp(-\frac{(x-\mu_1)^2}{2\sigma^2}), \exp(-\frac{(x-\mu_2)^2}{2\sigma^2}), \dots\}$
- Sigmoid basis: $\phi(x) = \{1, \sigma(x-\mu_1), \sigma(x-\mu_2), \dots\}$ where $\sigma(x) = \frac{1}{1+e^{-x}}$

Notebook: basis.html

Interactive examples and visualizations of different basis functions

Geometric Interpretation

Linear Combination of Vectors

- Let $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \ldots, \mathbf{v}_i$ be vectors in $\mathbb{R}^D$, where D denotes the dimensions

where $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_i \in \mathbb{R}$

Linear Combination of Vectors

- Let $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \ldots, \mathbf{v}_i$ be vectors in $\mathbb{R}^D$, where D denotes the dimensions
- A linear combination of $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \ldots, \mathbf{v}_i$ is of the following form:

$$\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \alpha_3 \mathbf{v}_3 + \cdots + \alpha_i \mathbf{v}_i$$

where $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_i \in \mathbb{R}$

Span of vectors

- Let $v_1, v_2, \ldots, v_i$ be vectors in $\mathbb{R}^D$, with D dimensions

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- Let $v_1, v_2, \ldots, v_i$ be vectors in $\mathbb{R}^D$, with D dimensions
- The span of $v_1, v_2, \ldots, v_i$ is denoted by SPAN$\{v_1, v_2, \ldots, v_i\}$:

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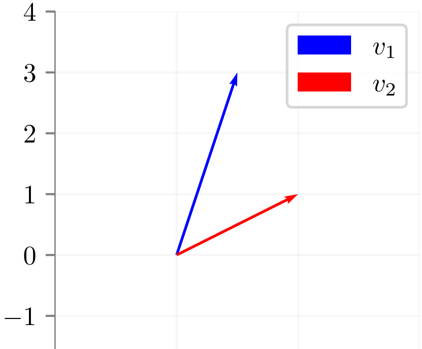
Example

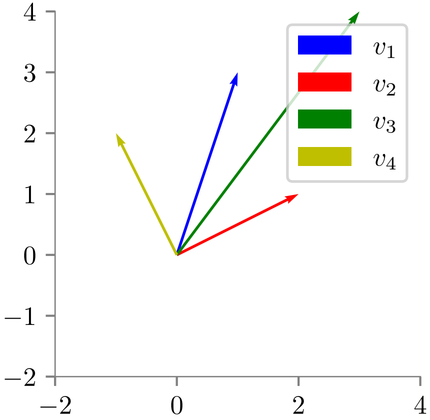
Find the span of $\left(\begin{bmatrix}1\\3\end{bmatrix}, \begin{bmatrix}2\\1\end{bmatrix}\right)$

Notebook: geometric-linear-regression.html

Interactive geometric visualization of vector spans and linear regression



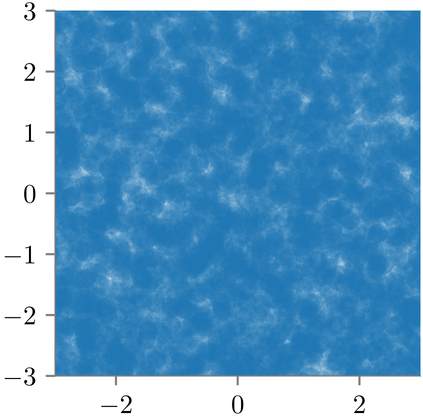
Example



We have $v_3 = v_1 + v_2$
We have $v_4 = v_1 - v_2$

Example

Simulating the above example in python using different values of α_1 and α_2

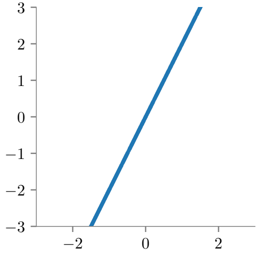


$\text{Span}((v_1, v_2)) \in \mathcal{R}^2$

Example

Find the span of $\left(\begin{bmatrix}1\\2\end{bmatrix}, \begin{bmatrix}2\\4\end{bmatrix}\right)$

- Can we obtain a point (x, y) s.t. $x = 3y$?



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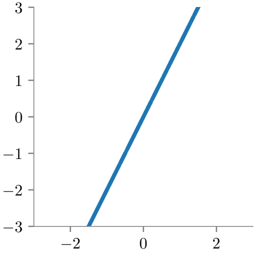

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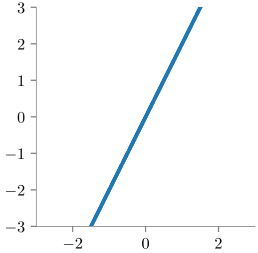
- No
- Span of the above set is along the line $y = 2x$



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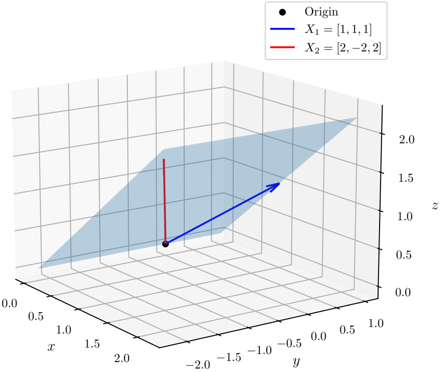
- Visualization:



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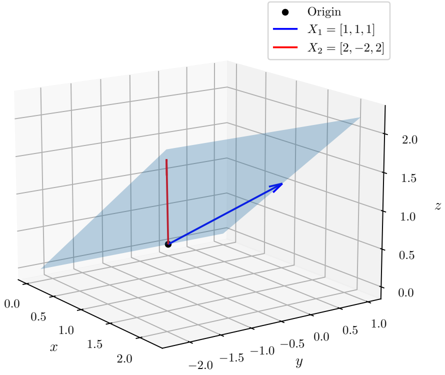

- The span is the plane $z = x$ or $x_3 = x_1$

Geometric Interpretation

Consider $\mathbf{X}$ and $\mathbf{y}$ as follows.

$$\mathbf{X} = \begin{pmatrix} 1 & 2 \\ 1 & -2 \\ 1 & 2 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 8.8957 \\ 0.6130 \\ 1.7761 \end{pmatrix}$$

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- We wish to find $\hat{\mathbf{y}}$ such that

$$\underset{\hat{\mathbf{y}} \in SPAN\{\bar{x_1}, \bar{x_2}, \ldots, \bar{x_D}\}}{\arg\min} ||\mathbf{y} - \hat{\mathbf{y}}||_2$$

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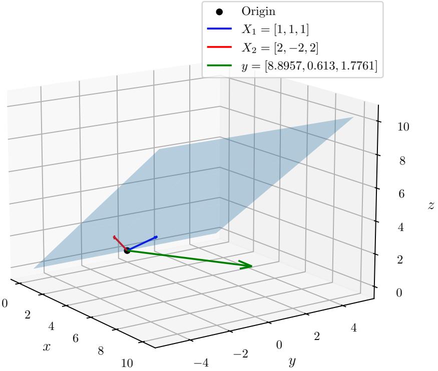

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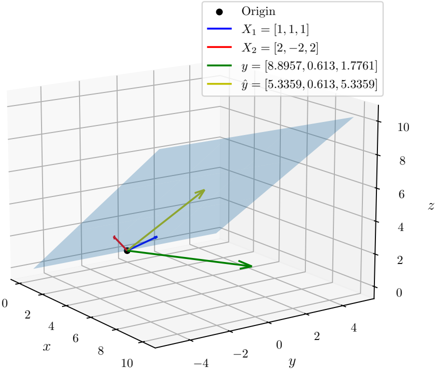

- We seek a $\hat{\mathbf{y}}$ in the span of the columns of $\mathbf{X}$ such that it is closest to $\mathbf{y}$

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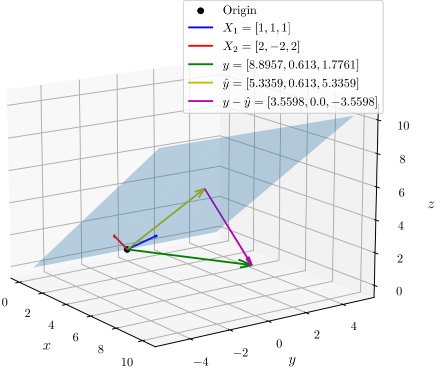

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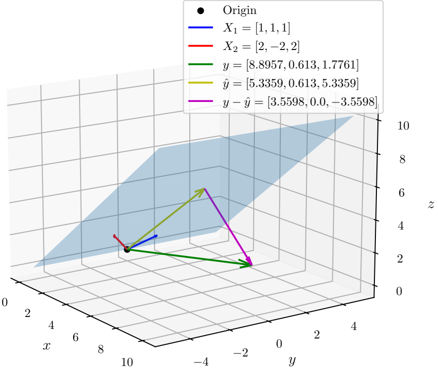

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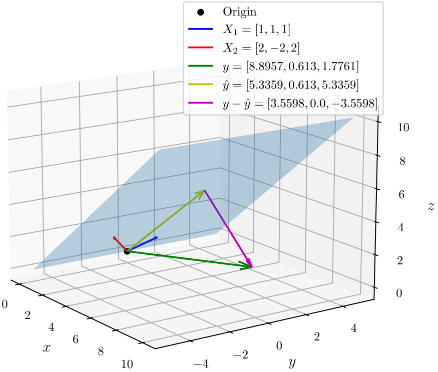

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- $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = 0$
- $\mathbf{X}^\top\mathbf{y} = \mathbf{X}^\top\mathbf{X}\boldsymbol{\theta}$ or $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$

Dummy Variables and Multicollinearity

Multi-collinearity

- There can be situations where inverse of $\mathbf{X}^\top\mathbf{X}$ is not computable

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 3 & 6 \end{bmatrix} \tag{1}$$

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- The matrix X is not full rank

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It arises when one or more predictor variables/features in X can be expressed as a linear combination of others

How to tackle it?

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- Avoid dummy variable trap

Dummy variables

Say Pollution in Delhi = P

- Model specification:

  P $= \theta_0 + \theta_1$*#Vehicles $+ \theta_1$* *Wind speed* $+ \theta_3$ * *Wind Direction*

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- This incorrectly implies that S>W>E>N (a meaningless ordering)

Dummy Variables

N-1 Variable encoding

	Is it N?	Is it E?	Is it W?
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Dummy Variables

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- W and S are related by one bit
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- $\theta_1 =$ Avg. female height (5+5.2+5.4)/3 - Avg. male height(5.9)

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Practice and Review

Pop Quiz: Linear Regression

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