Linear Regression

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IIT Gandhinagar

August 28, 2025

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Setup

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:
  - $F = ma$
  - $v = u + at$

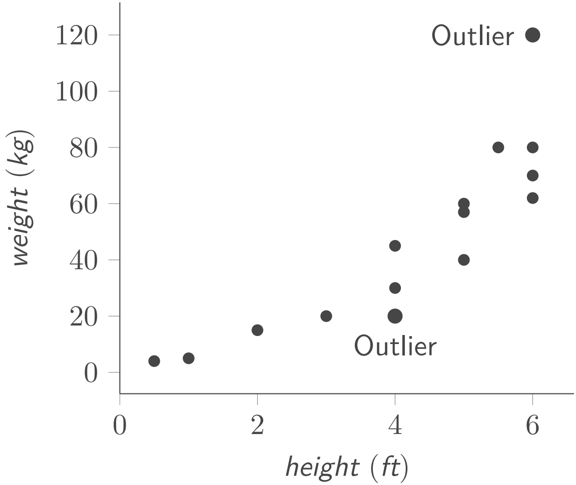
Task at hand

- 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

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

Matrix representation of the expression

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- $weight_N \approx \theta_0 + \theta_1 \cdot height_N$

$$\boxed{weight_i \approx \theta_0 + \theta_1 \cdot height_i}$$

Matrix representation of the expression

$$\begin{bmatrix} \mathit{weight}_1 \\ \mathit{weight}_2 \\ \dots \\ \mathit{weight}_N \end{bmatrix} = \begin{bmatrix} 1 & \mathit{height}_1 \\ 1 & \mathit{height}_2 \\ \dots & \dots \\ 1 & \mathit{height}_N \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

Matrix representation of the expression

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

- 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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- Mathematical representation:

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

Extension to multiple dimensions

- In the previous example $y = f(x)$, where x is one-dimensional
- 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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- where $\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$
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Linear Relationship

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  $\hat{demand}_i = \theta_0 + \theta_1 Temperature_i + \theta_2 Occupants_i$
- $\hat{demand}_i = x_i'^T \boldsymbol{\theta}$
- where $\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$
- 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 temperature increases, then θ_1 is likely to be positive

We can expect the following

- 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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- $\#$ Features $= M$

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Generalized Linear Regression Format

- Assuming N samples for training
- # Features = M

$$\begin{bmatrix} \hat{y_1} \\ \hat{y_2} \\ \vdots \\ \hat{y_N} \end{bmatrix}_{N\times 1} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,M} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,M} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{N,1} & x_{N,2} & \dots & x_{N,M} \end{bmatrix}_{N\times(M+1)} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_M \end{bmatrix}_{(M+1)\times 1}$$

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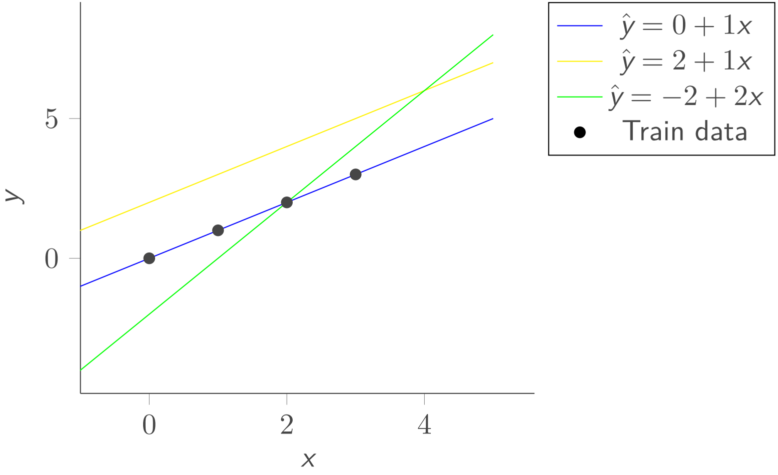
$$\boxed{\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}}$$

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

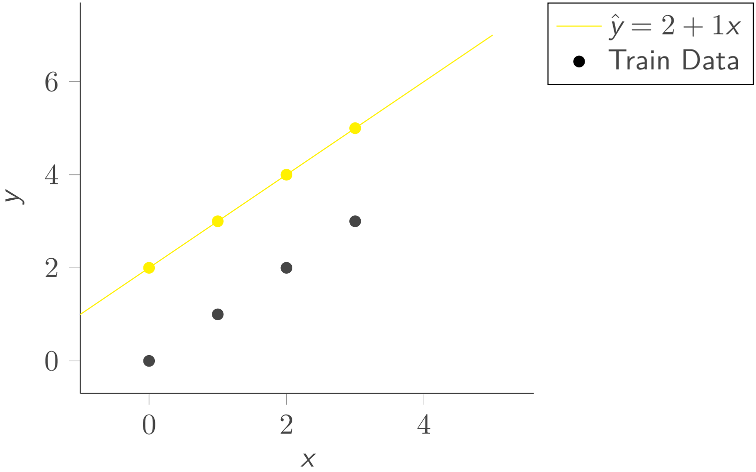
Relationships between feature and target variables

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



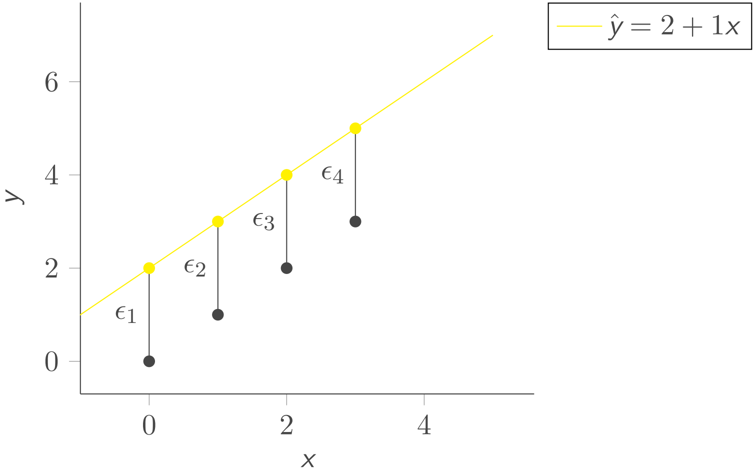
Relationships between feature and target variables

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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- Model specification:

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

- 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

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

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

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

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

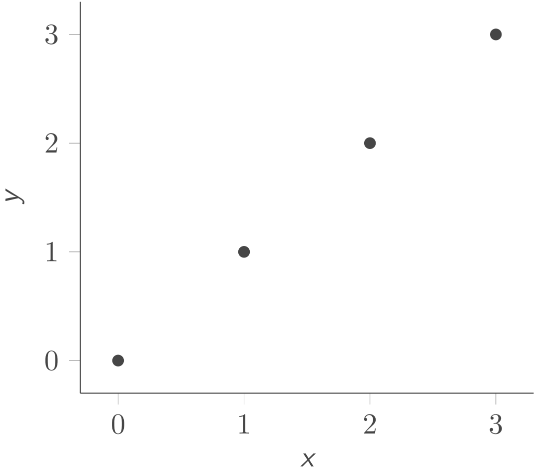
$$\boxed{\hat{\boldsymbol{\theta}}_{OLS} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}}$$

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

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

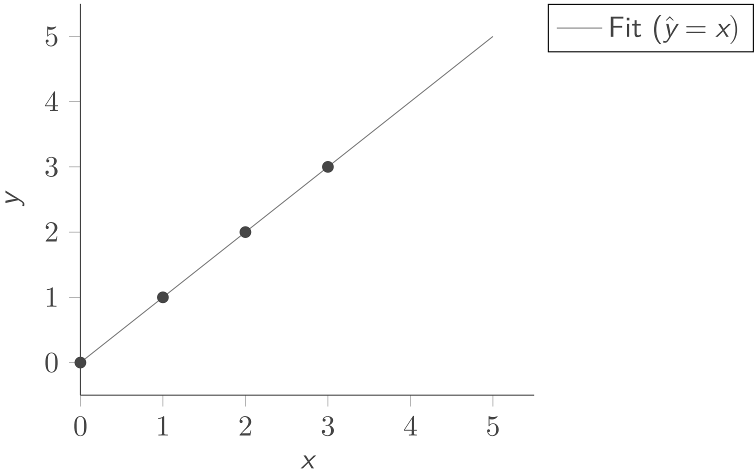
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

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

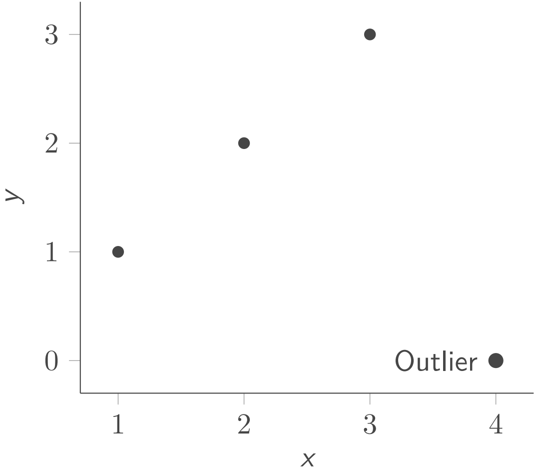


Effect of outlier

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

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

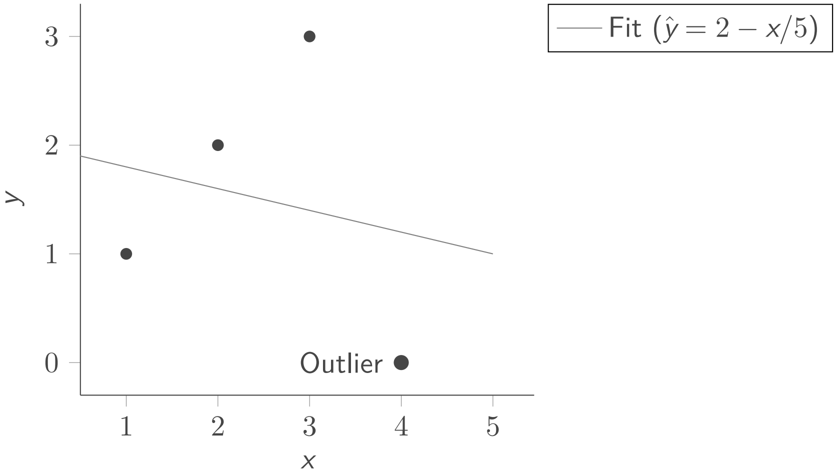
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

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

Variable Transformation

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

Variable Transformation

Add the higher degree features to the previous table

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

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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!

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

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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

Span of vectors

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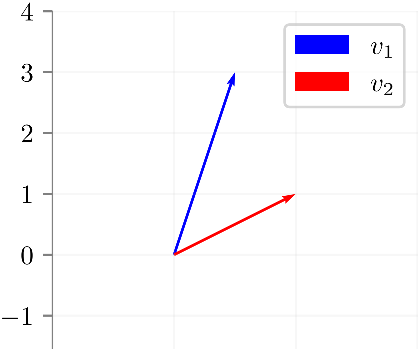
Example

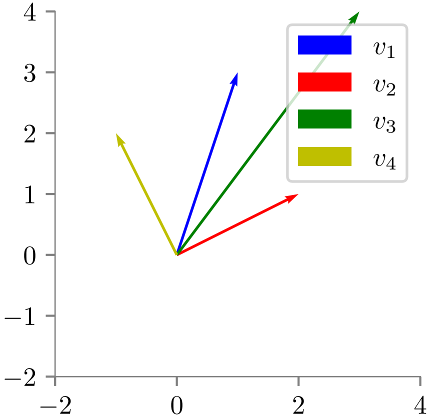
Find the span of $\left(\begin{bmatrix}1\\3\end{bmatrix}, \begin{bmatrix}2\\1\end{bmatrix}\right)$

Notebook: geometric-linear-regression.html

Interactive geometric visualization of vector spans and linear regression



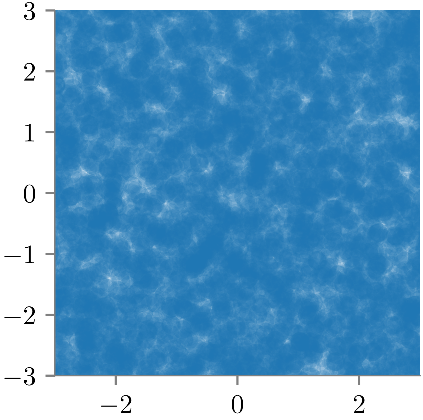
Example



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

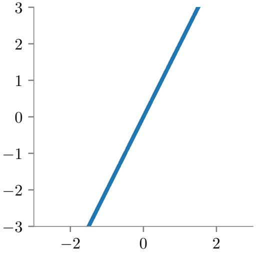


$\text{Span}((v_1, v_2)) \in \mathcal{R}^2$

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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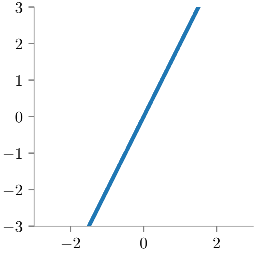

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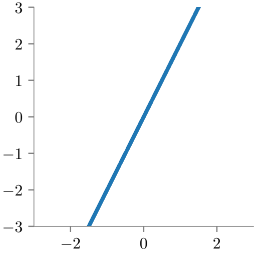
- No
- Span of the above set is along the line $y = 2x$



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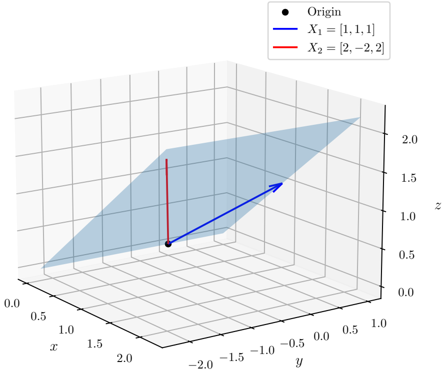
- Visualization:



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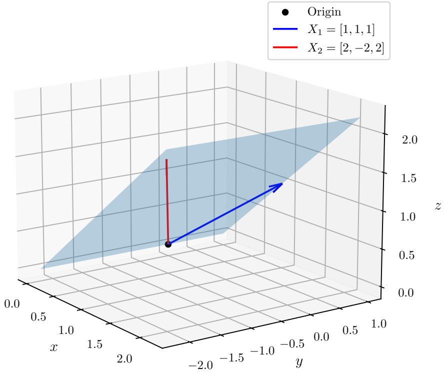

- The span is the plane $z = x$ or $x_3 = x_1$

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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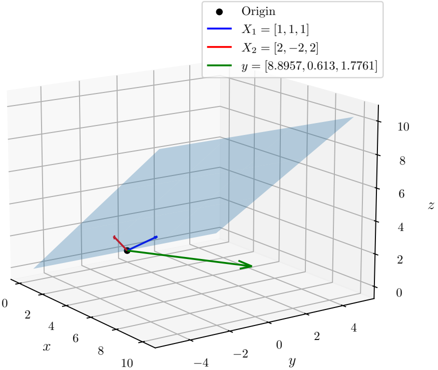

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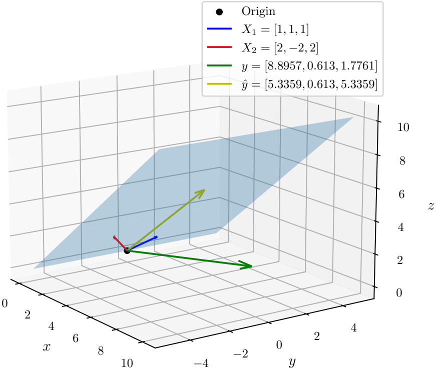
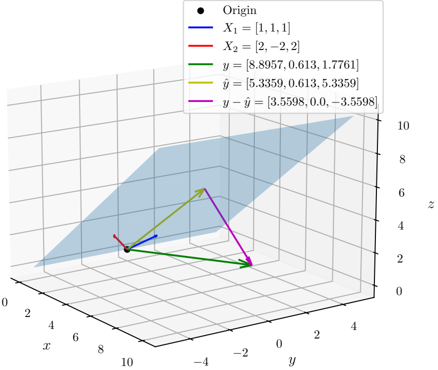


- We seek a $\hat{\mathbf{y}}$ in the span of the columns of $\mathbf{X}$ such that it is closest to $\mathbf{y}$

Geometric Interpretation



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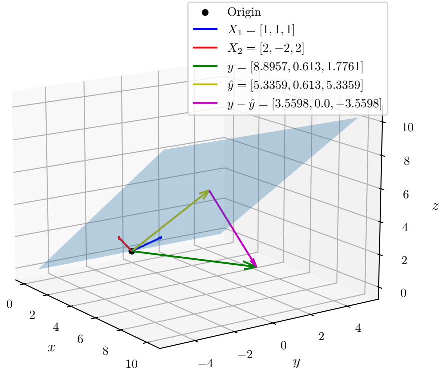

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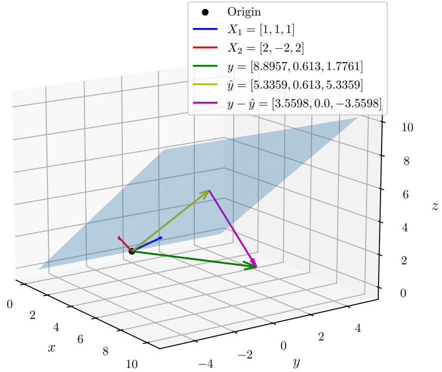

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- $\mathbf{X}^\top\mathbf{y} = \mathbf{X}^\top\mathbf{X}\boldsymbol{\theta}$ or $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$

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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- Cannot uniquely solve for $\boldsymbol{\theta}$!

Multi-collinearity: Definition and Problems

Definition: Multicollinearity

Arises when predictor variables/features in $\mathbf{X}$ can be expressed as a linear combination of others

Types:

- **Perfect**: Exact linear relationship (determinant $= 0$)

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- Can't interpret individual feature importance

Why Multicollinearity Causes Instability

The core problem: Multiple parameter combinations give identical results

Example: Simple Example

If $x_2 = 2x_1$ exactly, then:
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- Result: Wildly different coefficients for same data

Numerical Example: Why Coefficients Go Wild

Dataset: House prices with sq_ft and sq_m (perfectly correlated)

Price ($k)	sq_ft	sq_m
200	2000	186
300	3000	279
400	4000	372

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Key Points:

Solutions: Drop one variable, or use regularization (Ridge/Lasso)

Dummy Variables: The Problem

Example: Pollution in Delhi = P

- Model specification:

  P $= \theta_0 + \theta_1$*#Vehicles $+ \theta_2$* *Wind speed* $+ \theta_3$ * *Wind Direction*

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- Model assumes: S is "3 times better" than N for reducing pollution

One-Hot Encoding (N-1 Variables)

Correct approach: Use binary indicators for each category

N-1 encoding (recommended)

Wind Direction	Is North?	Is East?	Is West?
North	1	0	0
East	0	1	0
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Key Points:

South is the **reference category** - all others are compared to it

Why Not N Variables?

Full encoding (problematic):

Wind	Is N?	Is E?	Is W?	Is S?
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Important: Multicollinearity Problem!

Notice: Is_N + Is_E + Is_W + Is_S = 1 (always!)
One column is perfectly predictable from the others

N-1 vs N Encoding: The Dummy Variable Trap

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Example: The Dummy Variable Trap

Always use N-1 dummy variables for N categories.
The omitted category becomes the **baseline/reference**.

Binary Encoding

N	00
E	01
W	10
S	11

- W and S are related by one bit

Binary Encoding

N	00
E	01
W	10
S	11

- W and S are related by one bit
- This introduces dependencies between them, and this can cause confusion in classifiers

Interpreting Dummy variables

Gender	height
F	...
F	...
F	...
M	...
M	...

Interpreting Dummy variables

Gender	height
F	...
F	...
F	...
M	...
M	...

Encoding

Interpreting Dummy variables

Gender	height
F	...
F	...
F	...
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M	...

Encoding

Is Female	height
1	...
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1	...
0	...
0	...

Interpreting Dummy Variables

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Is Female	height
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1	5.2
1	5.4
0	5.8
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- **Male height** $= \theta_0 = 5.9$
- So θ_1 = Avg(female) - Avg(male) = 5.2 - 5.9 = -0.7

Alternative Encoding: +1/-1 Scheme

Instead of 0/1, we could use +1/-1:

Example: +1/-1 Encoding

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Key Points: Interpretation

- $\theta_0 =$ overall average height across all people
- $\theta_1 =$ half the difference between female and male heights

Summary: Categorical Variable Encodings

Method	**Good?**	**Variables**	**Issue**
Ordinal (0,1,2,3)	No	1	Implies fake ordering
Full One-Hot	No	N	Multicollinearity
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Definition: Best Practice

Use **N-1 one-hot encoding** for categorical variables.
Choose the most common category as reference.

Practice and Review

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4. What are the assumptions behind linear regression?

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- **Foundation**: Building block for more complex models