Linear Regression

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IIT Gandhinagar

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Setup

- Output is continuous in nature.

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- Examples of linear systems:

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  - $F = ma$

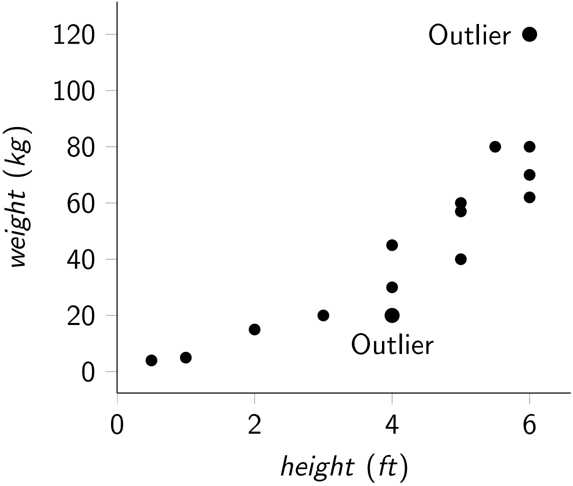
- Output is continuous in nature.
- Examples of linear systems:
    - $F = ma$
    - $v = u + at$

- 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

- $weight_1 \approx \theta_0 + \theta_1 \cdot height_1$

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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
- θ_1 - Slope

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

Extension to multiple dimensions

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> Demand = f(# occupants, Temperature)

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Examples in multiple dimensions.

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

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

$$\text{Demand} = \text{Base Demand} + K_1 * \#\ \text{occupants} + K_2 * \text{Temperature}$$

Intuition

We hope to:

- Learn f: $Demand = f(\#occupants, Temperature)$

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- To predict the condition for the testing set

We have

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

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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Generalized Linear Regression Format

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

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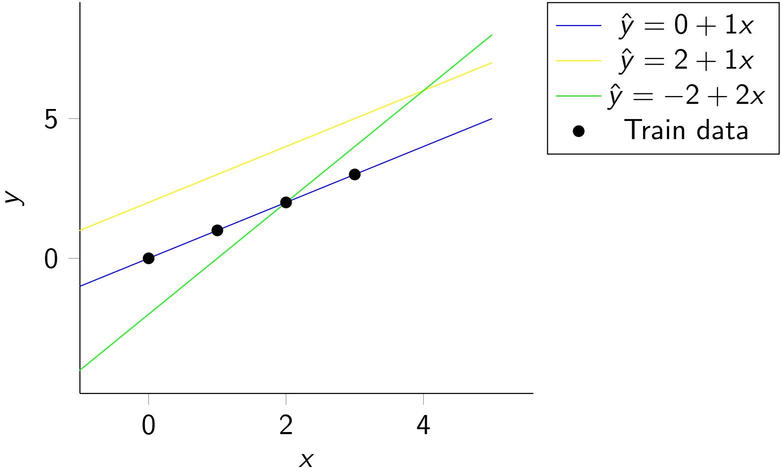
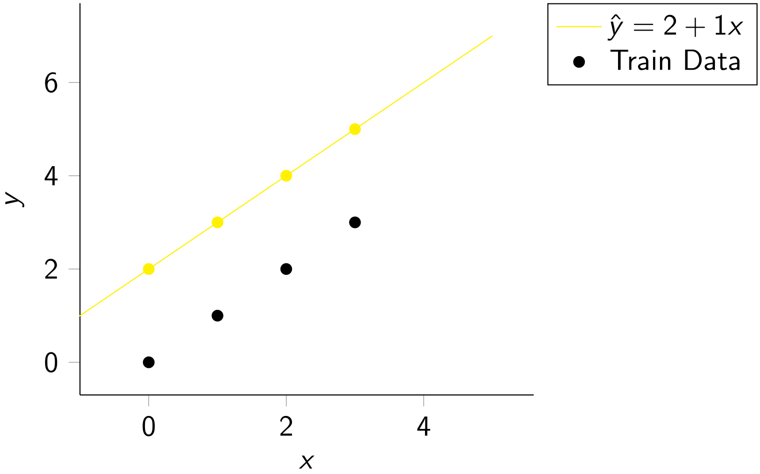
- Given multiples values of $\theta_0, \theta_1 \dots \theta_M$ how to choose which is the best?
- Let us consider an example in 2d

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



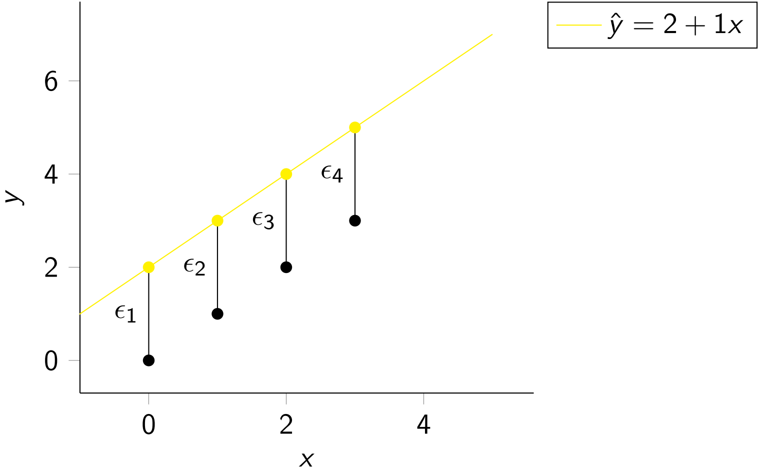
Relationships between feature and target variables

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

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

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- minimize $|\epsilon_1| + |\epsilon_2| + \cdots + |\epsilon_n|$ - L_1 Norm

Normal Equation

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To Learn: θ

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

To Learn: θ

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

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

Normal Equation

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Objective: Minimize $\epsilon^T \epsilon$

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

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

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

Substitute the values in the top equation

Minimizing the objective function

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

Substitute the values in the top equation

Normal Equation derivation

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

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

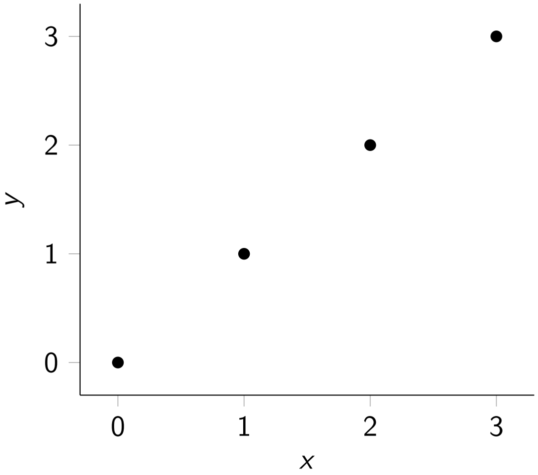
$$\hat{\theta}_{OLS} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}$$

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

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

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

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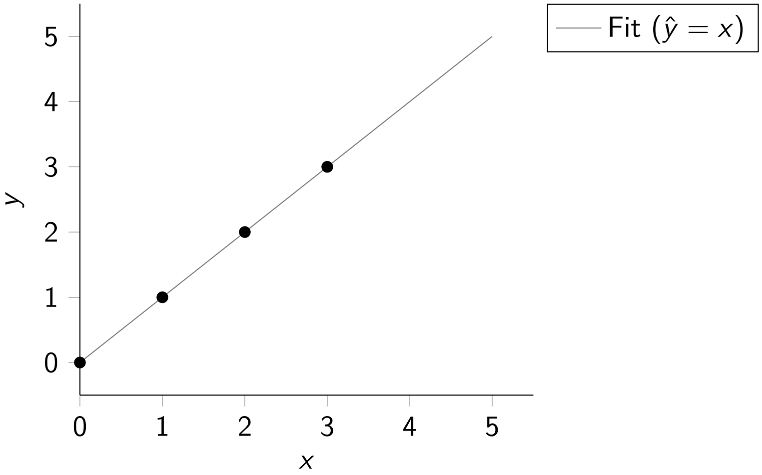
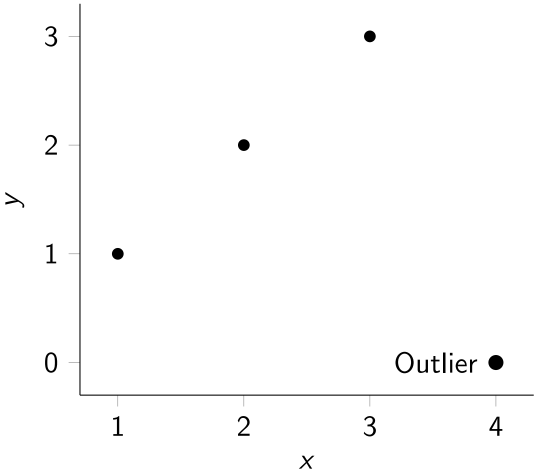


Effect of outlier

x	y
1	1
2	2
3	3
4	0

Compute the θ_0 and θ_1.

Scatter Plot



Worked out example

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

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

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

Given the data above, find θ_0 and θ_1.

Worked out example

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

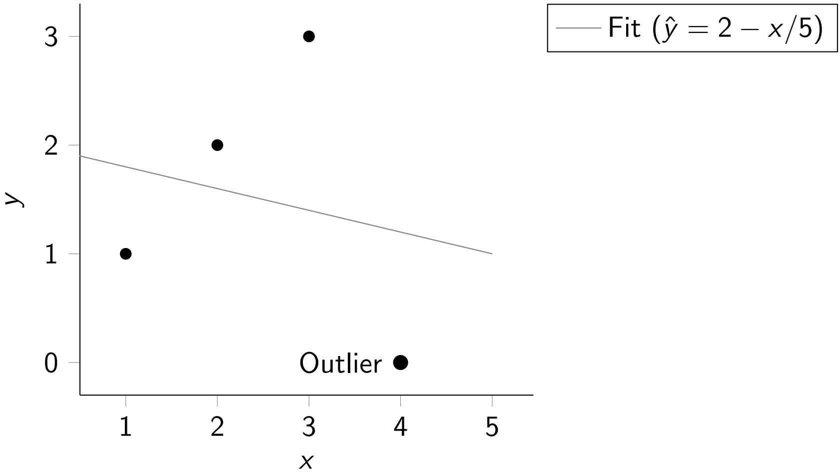
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

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

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

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

Variable Transformation

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

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- 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: $\phi(x) = \{1, x, x^2, x^3, \dots\}$

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- Fourier basis: $\phi(x) = \{1, \sin(x), \cos(x), \sin(2x), \cos(2x), \dots\}$

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- 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: $\phi(x) = \{1, \exp(-\frac{(x-\mu_1)^2}{2\sigma^2}), \exp(-\frac{(x-\mu_2)^2}{2\sigma^2}), \dots\}$

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- Sigmoid basis: $\phi(x) = \{1, \sigma(x-\mu_1), \sigma(x-\mu_2), \dots\}$ where $\sigma(x) = \frac{1}{1+e^{-x}}$

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.

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

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

Span of vectors

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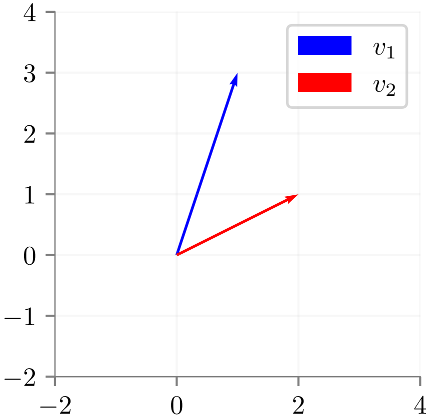
If we stack the vectors $v_1, v_2, \ldots, v_i$ as columns of a matrix V, then the span of $v_1, v_2, \ldots, v_i$ is given as $V\alpha$ where $\alpha \in \mathbb{R}^i$

Example

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



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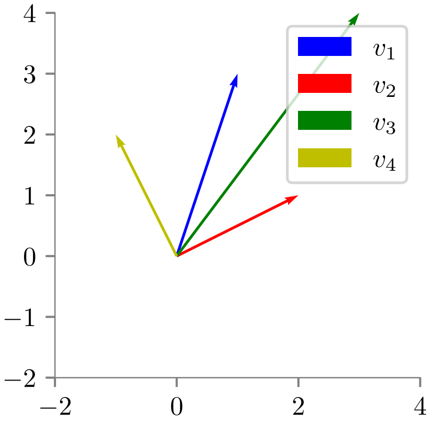
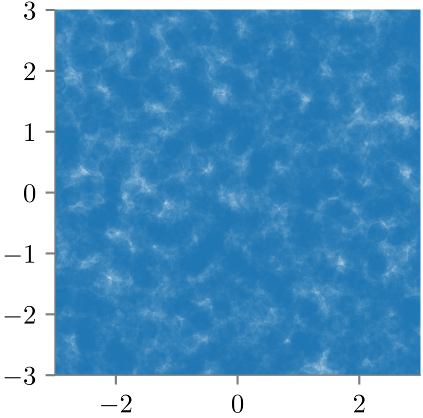


We have $v_3 = v_1 + v_2$

We have $v_4 = v_1 - v_2$

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



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

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

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

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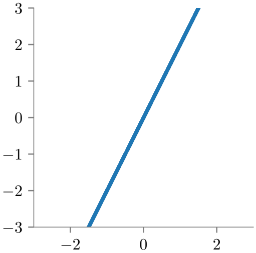
Span of the above set is along the line $y = 2x$



Example

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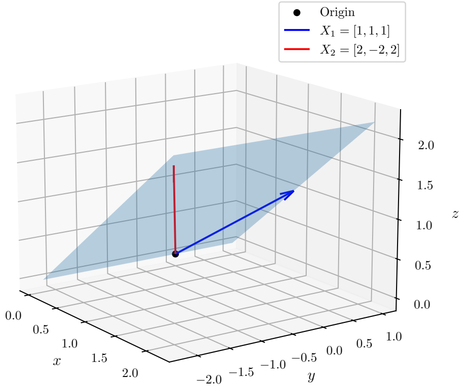

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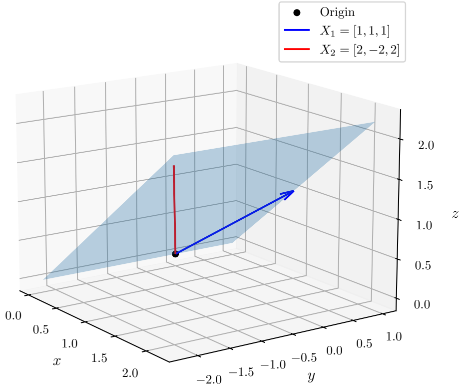

The span is the plane $z = x$ or $x_3 = x_1$

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

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

- We are trying to learn $\boldsymbol{\theta}$ for $\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$ such that $||\mathbf{y} - \hat{\mathbf{y}}||_2$ is minimised

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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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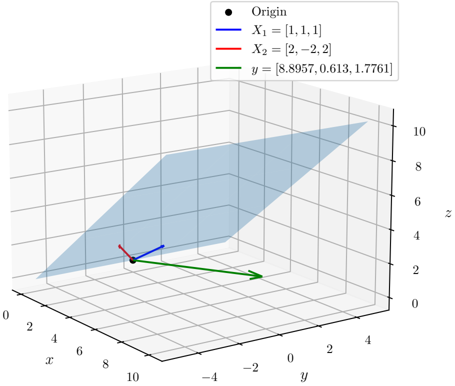
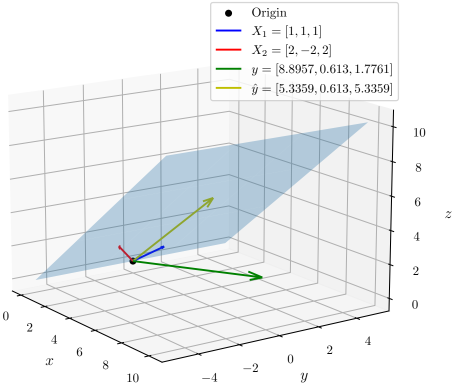
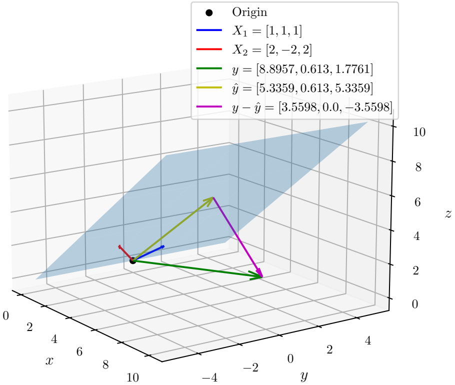




- We seek a $\hat{\mathbf{y}}$ in the span of the columns of $\mathbf{X}$ such that it is closest to $\mathbf{y}$

Geometric Interpretation



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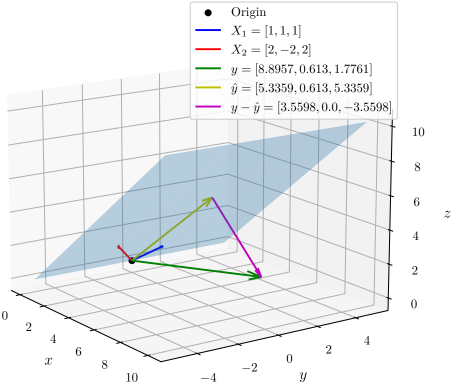

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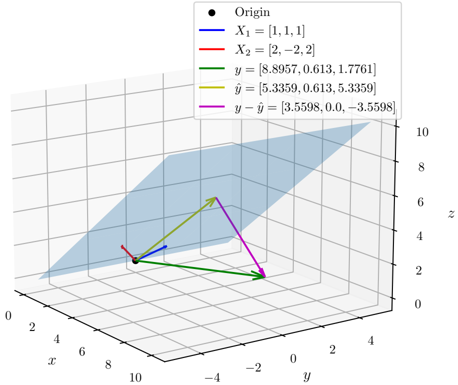

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- $\mathbf{X}^\top\mathbf{y} = \mathbf{X}^\top\mathbf{X}\boldsymbol{\theta}$ or $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$

Regularization

The Problem: Overfitting

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- This prevents coefficients from becoming too large

Ridge Regression (L2 Regularization)

Objective Function:

$$J(\boldsymbol{\theta}) = \mathrm{MSE} + \lambda \sum_{j=1}^{n} \theta_j^2$$

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- Note: $(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})$ is always invertible for $\lambda > 0$

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- **Use Case**: When you suspect many features are irrelevant

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Dummy Variables and Multicollinearity

Multi-collinearity

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

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This condition arises when the $|X^TX| = 0$.

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

The matrix X is not full rank.

Multi-collinearity

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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- Drop variables
- Avoid dummy variable trap

Dummy variables

Say Pollution in Delhi = P

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But, wind direction is a categorical variable.
It is denoted as follows {N:0, E:1, W:2, S:3 }

Can we use the direct encoding?
Then this implies that S>W>E>N

N-1 Variable encoding

	Is it N?	Is it E?	Is it W?
N	1	0	0
E	0	1	0
W	0	0	1
S	0	0	0

N Variable encoding

	Is it N?	Is it E?	Is it W?	Is it S?
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Is it S = 1 - (Is it N + Is it W + Is it E)

Binary Encoding

N	00
E	01
W	10
S	11

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W and S are related by one bit.

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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	...

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

Encoding

Interpreting Dummy variables

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

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

Interpreting Dummy Variables

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Is Female	height
1	5
1	5.2
1	5.4
0	5.8
0	6

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$height_i = \theta_0 + \theta_1 * (\text{Is Female}) + \epsilon_i$

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We get $\theta_0 = 5.9$ and $\theta_1 =$ -0.7
$\theta_0 =$ Avg height of Male $= 5.9$
$\theta_0 + \theta_1$ is chosen based (equal to) on 5, 5.2, 5.4 (for three records).

Interpreting Dummy Variables

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$height_i = \theta_0 + \theta_1$ * (Is Female) $+ \epsilon_i$

We get $\theta_0 = 5.9$ and $\theta_1 =$ -0.7

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Now, θ_0 can be interpreted as average person height. θ_1 as the amount that female height is above average and male height is below average.

Practice and Review

Pop Quiz: Linear Regression

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4. What are the assumptions behind linear regression?

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