#### Math Refresher for DS

Practical Session 3

## girafe

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How to find a reasonable approximate solution?

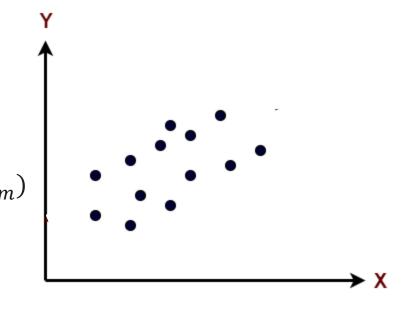


### Least Squares



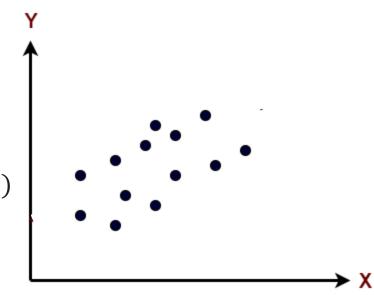
• Imagine that you have m observations:

$$(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$$



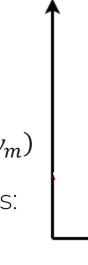
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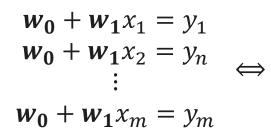
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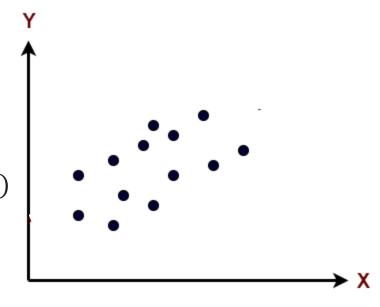
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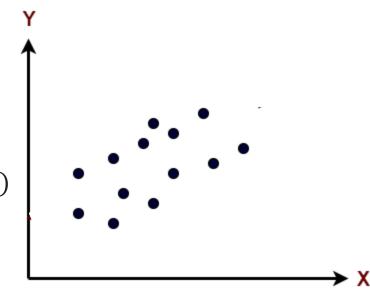


$$\begin{array}{c} w_0+w_1x_1=y_1\\ w_0+w_1x_2=y_n\\ \vdots\\ w_0+w_1x_m=y_m \end{array} \iff Xw=y, \text{ where } X=\begin{pmatrix} 1&x_1\\1&x_2\\ \vdots&\vdots\\1&m \end{pmatrix}, w=\begin{bmatrix} w_0\\w_1 \end{bmatrix}, y=\begin{bmatrix} y_1\\y_2\\ \vdots\\y_m \end{bmatrix}$$

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You want to draw a line through your observations:

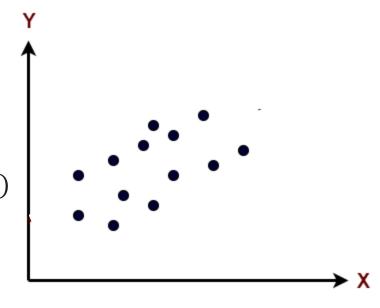


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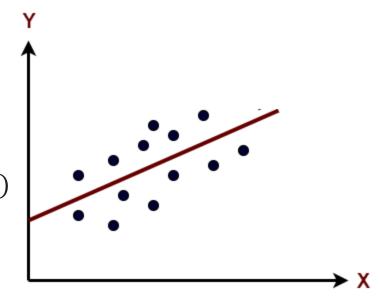


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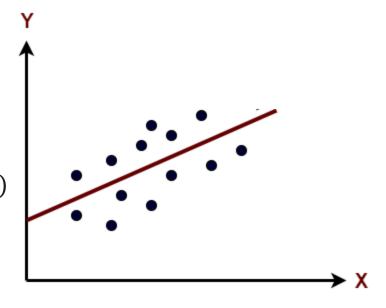


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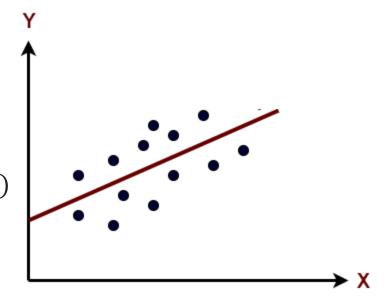


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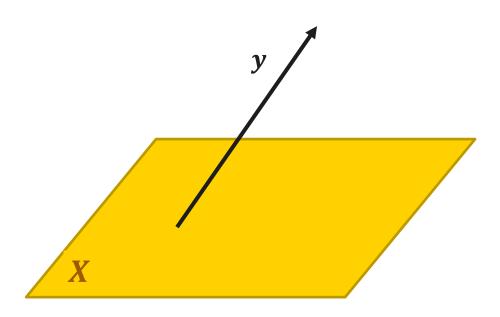


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- Let's look at it from the Linear Algebra perspective.

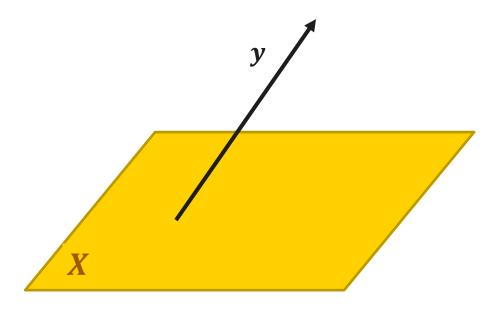


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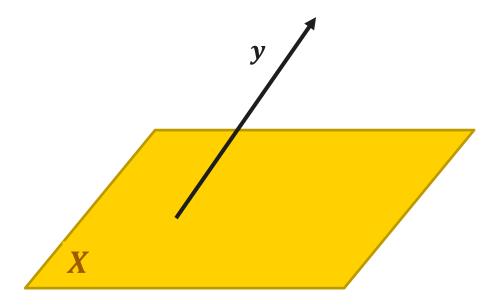
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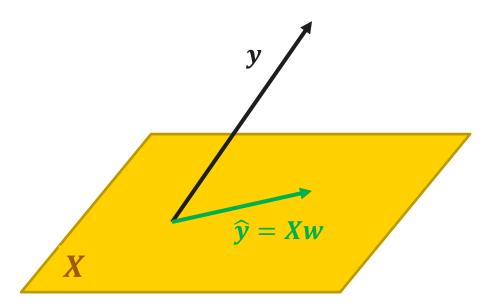


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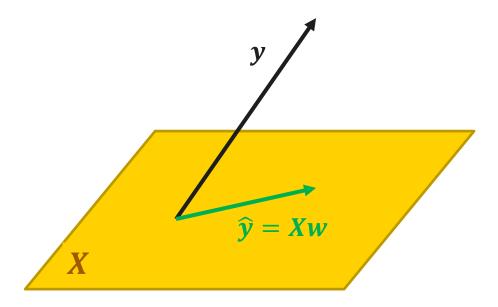
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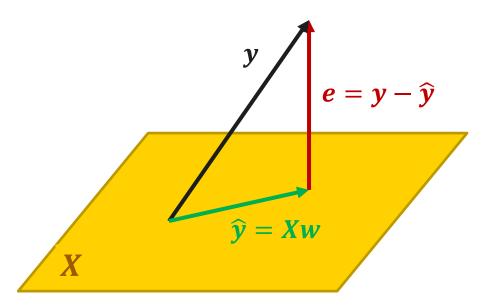
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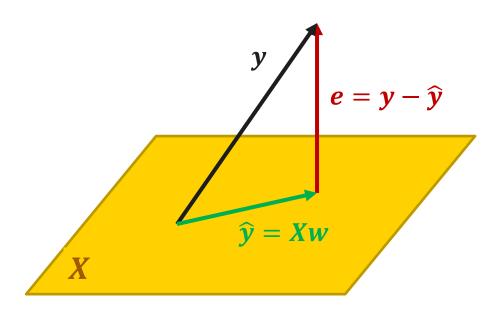
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• What do  $\hat{y}$  and e look like?



# Orthogonal Projections



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- Example:

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \perp span \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$$



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$$W = span \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}, \qquad W_{\perp} = span \left\{ \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$



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- $x_W$  orthogonal projection of x onto W.
- $x_W$  is the closest vector to x in W.





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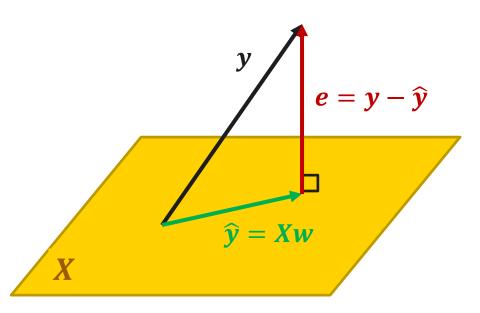
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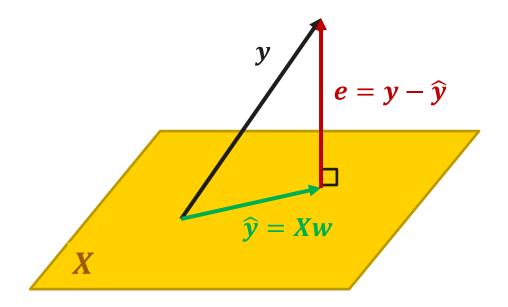
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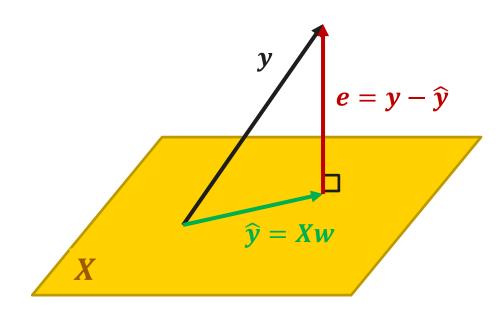
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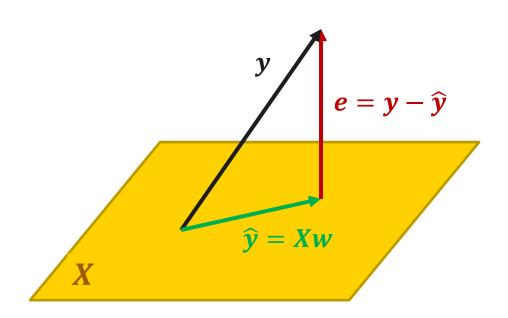


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  - $\hat{y}$  is the orthogonal projection of y onto the column space of X! e is orthogonal onto the column space of X.



$$Xw^* = \hat{y} = y - e$$

 $\hat{y}$  - orthogonal projection of y onto col(X) $w^* = ?$  - optimal weights

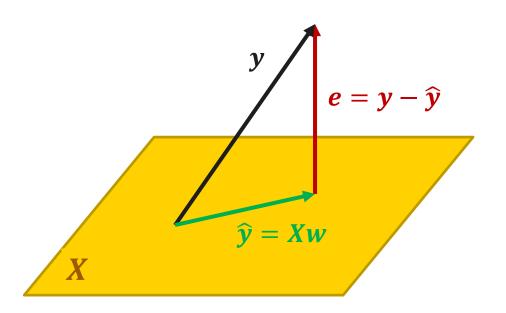




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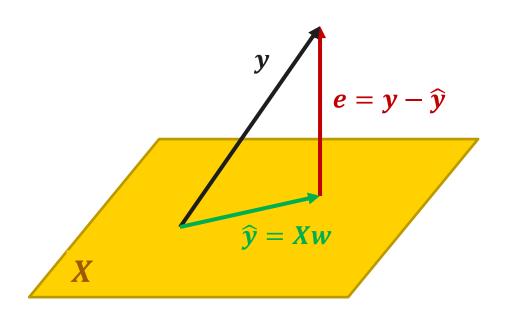




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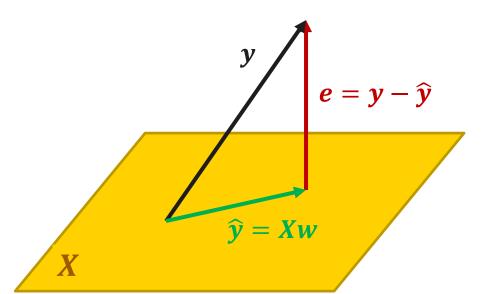
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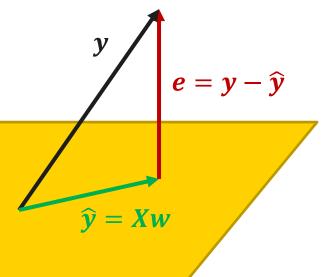
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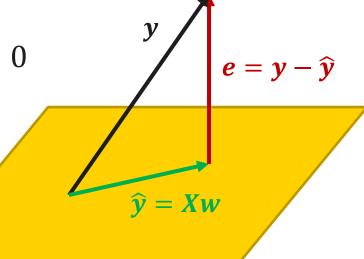
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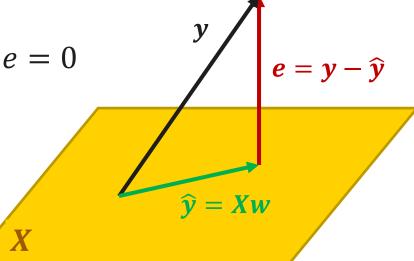
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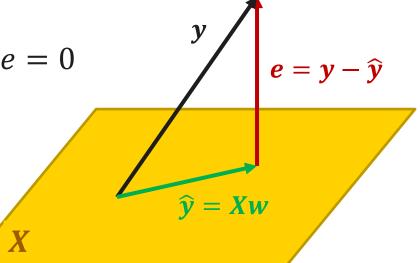
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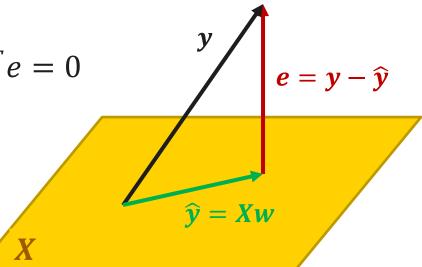
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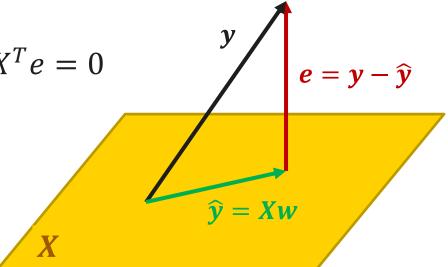
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$$\widehat{\boldsymbol{y}} = \boldsymbol{X} \boldsymbol{w}^* = \boldsymbol{X} (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$





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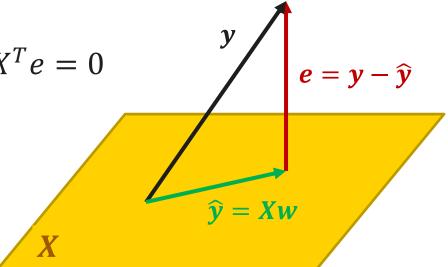
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$$\widehat{y} = Xw^* = X(X^TX)^{-1}X^Ty$$
projection matrix



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But  $v \neq 0$  and rank(X) = n (no linearly dependent columns)

 $\Rightarrow$  contradiction.



- We derived that  $w = (X^T X)^{-1} X^T y$ . But can we be sure  $(X^T X)^{-1}$  exists?
- Suppose it doesn't.

$$\Rightarrow \exists v \neq 0: \ X^T X v = 0:$$

$$X^T X v = 0$$

$$v^T X^T X v = 0$$

$$(Xv)^T (Xv) = 0$$

$$(Xv, Xv) = ||Xv||^2 = 0 \iff Xv = 0$$

But  $v \neq 0$  and rank(X) = n (no linearly dependent columns)

 $\Rightarrow$  contradiction.

So,  $(X^TX)^{-1}$  exists.



• Observations  $(x_i, y_i)$ :

• With least squares, fit a line  $y = w_0 + w_1 x$  through these points.

Reminder:  $w^* = (X^T X)^{-1} X^T y$ 

• Observations  $(x_i, y_i)$ :

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$$X^T X = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix}, \qquad (X^T X)^{-1} = \qquad , \qquad (X^T X)^{-1} X^T =$$



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$$X^{T}X = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix}, \qquad (X^{T}X)^{-1} = \begin{bmatrix} 7/3 & -1 \\ -3/2 & 1 \end{bmatrix}, \qquad (X^{T}X)^{-1}X^{T} = \begin{bmatrix} 7/3 & -1 \\ -3/2 & 1 \end{bmatrix}$$



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$$w = (X^T X)^{-1} X^T y = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix} \rightarrow \text{regression line}$$

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$$w = (X^T X)^{-1} X^T y = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix} \rightarrow \text{regression line } y = 1 + 0.5 x.$$