# Multiple Regression Deriving the Matrix Form

Rahul Singh rsingh@arrsingh.com

$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1 + \beta_2 \hat{x}_2 + \beta_3 \hat{x}_3 + \dots + \beta_k \hat{x}_k$$

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- 1 dependent variable  $\hat{y}$
- k independent variables  $\hat{x}_1$ ,  $\hat{x}_2$ ,  $\hat{x}_3$  ...  $\hat{x}_k$  k+1 parameters  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ ,  $\beta_3$  ...  $\beta_k$

$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1 + \beta_2 \hat{x}_2 + \beta_3 \hat{x}_3 + \dots + \beta_k \hat{x}_k$$

$$\begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & \hat{x}_{10} & \hat{x}_{20} & \hat{x}_{30} & \dots & \hat{x}_{k0} \\ 1 & \hat{x}_{11} & \hat{x}_{21} & \hat{x}_{21} & \dots & \hat{x}_{k1} \\ 1 & \hat{x}_{12} & \hat{x}_{22} & \hat{x}_{22} & \dots & \hat{x}_{k2} \\ 1 & \hat{x}_{13} & \hat{x}_{23} & \hat{x}_{23} & \dots & \hat{x}_{k3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \hat{x}_{1n} & \hat{x}_{2n} & \hat{x}_{3n} & \dots & \hat{x}_{kn} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_k \end{bmatrix}$$

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$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1 + \beta_2 \hat{x}_2 + \beta_3 \hat{x}_3 + \dots + \beta_k \hat{x}_k$$

$$\hat{y}_n = 1 \times \beta_0 + \hat{x}_{1n} \times \beta_1 + \hat{x}_{2n} \times \beta_2 + \hat{x}_{3n} \times \beta_3 + \dots + \hat{x}_{kn} \times \beta_k$$

$$\begin{vmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{vmatrix} = \begin{vmatrix} 1 & \hat{x}_{10} & \hat{x}_{20} & \hat{x}_{30} & \dots & \hat{x}_{k0} \\ 1 & \hat{x}_{11} & \hat{x}_{21} & \hat{x}_{21} & \dots & \hat{x}_{k1} \\ 1 & \hat{x}_{12} & \hat{x}_{22} & \hat{x}_{22} & \dots & \hat{x}_{k2} \\ 1 & \hat{x}_{13} & \hat{x}_{23} & \hat{x}_{23} & \dots & \hat{x}_{k3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \hat{x}_{1n} & \hat{x}_{2n} & \hat{x}_{3n} & \dots & \hat{x}_{kn} \end{vmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_k \end{bmatrix}$$

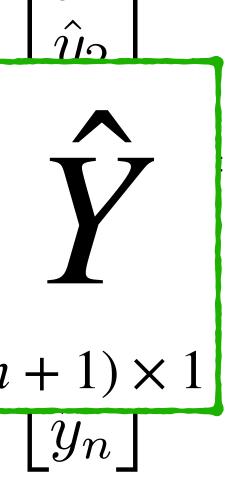
- 1 dependent variable  $\hat{y}$
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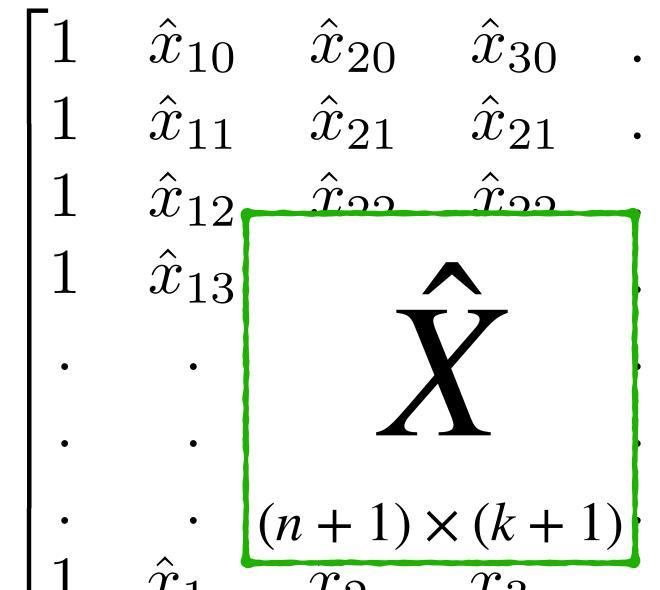
# Multiple Regression

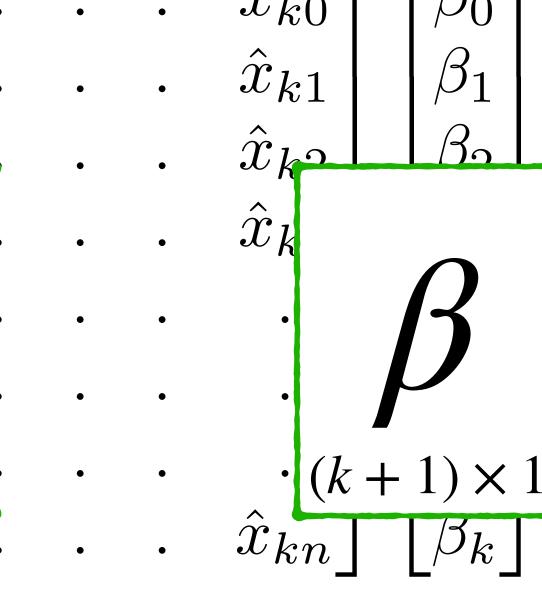
$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1 + \beta_2 \hat{x}_2 + \beta_3 \hat{x}_3 + \dots + \beta_k \hat{x}_k$$

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

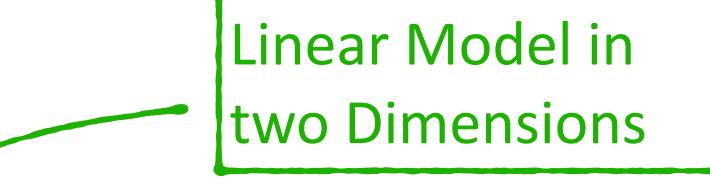
 $\hat{Y}$  &  $\beta$  are column vectors.  $\hat{X}$  is a matrix







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# Simple Linear Regression

$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1$$

$$\frac{1}{n} \| Y - \hat{Y} \|^2$$

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$$\frac{1}{n} \parallel Y - \hat{Y} \parallel^2$$

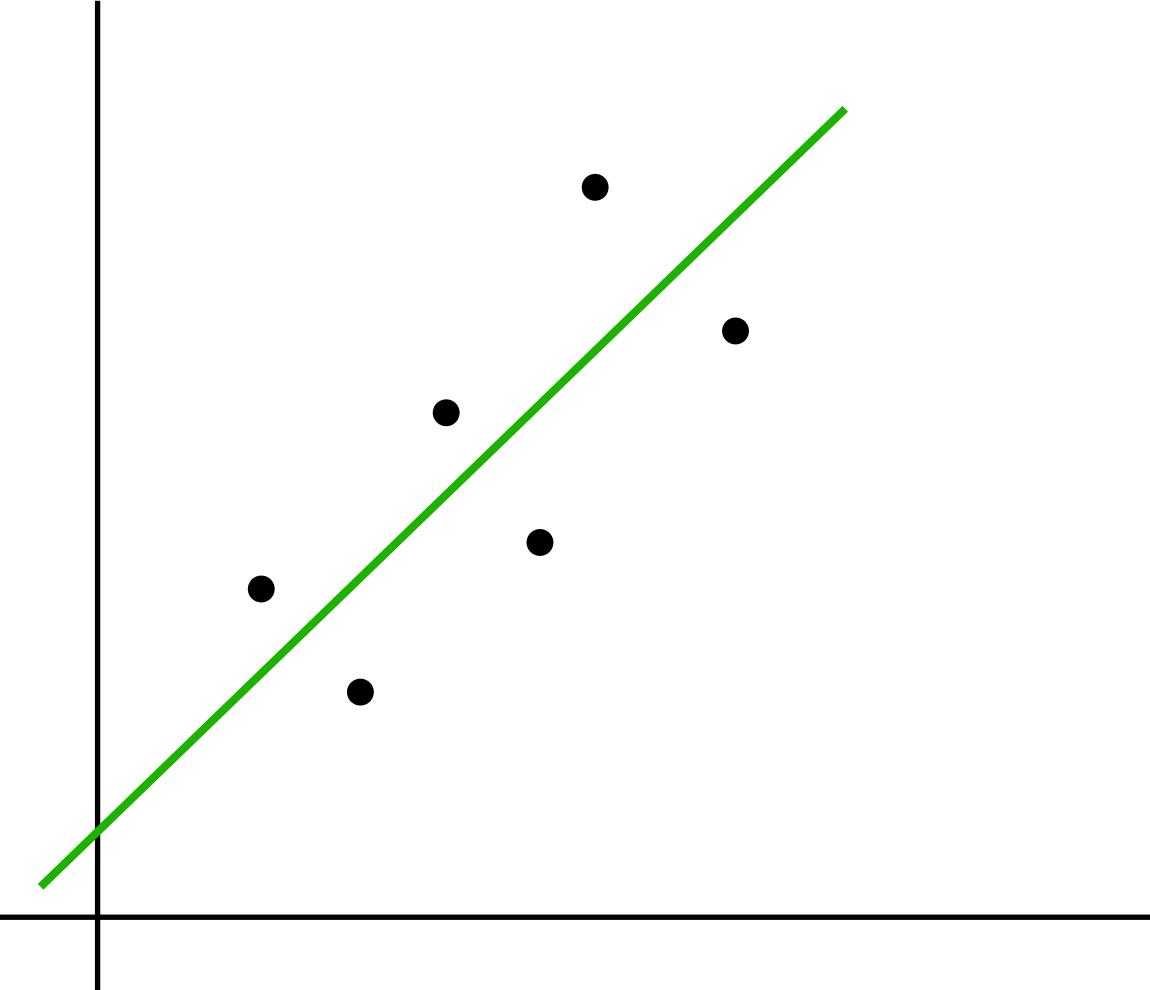
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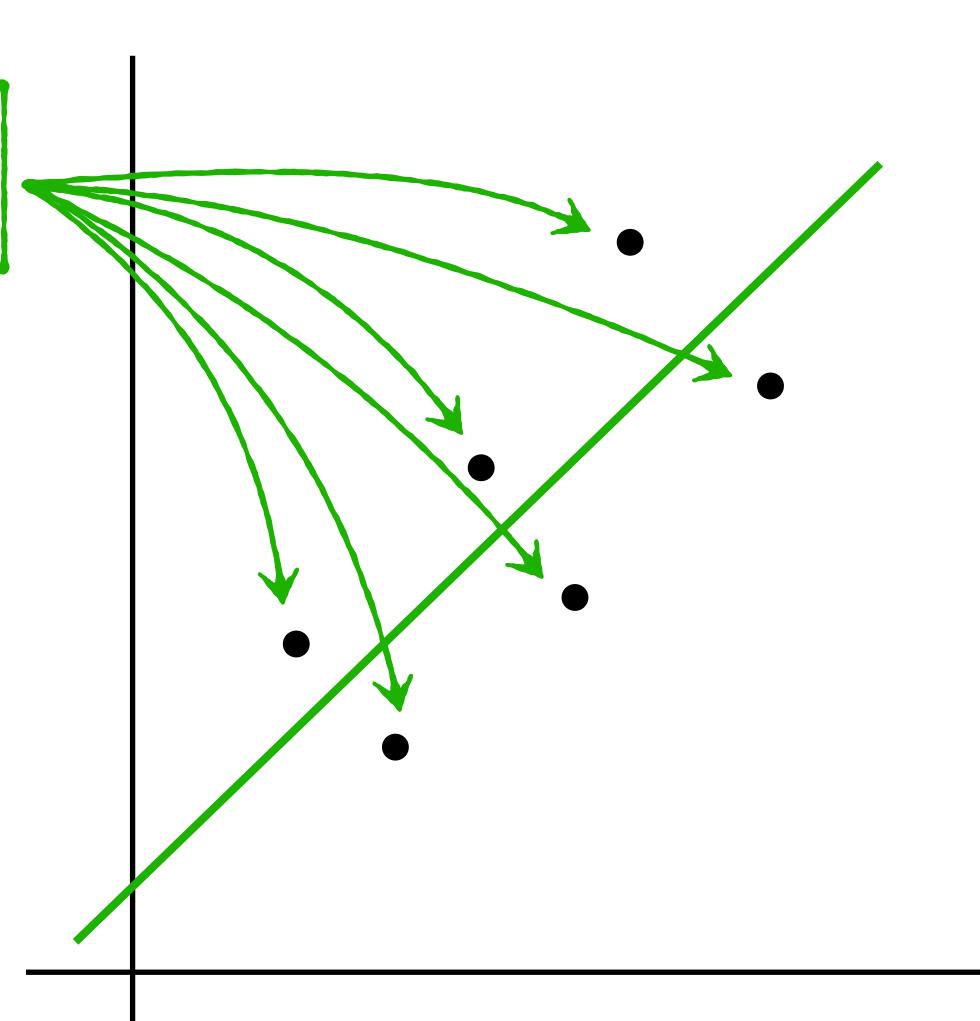
$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1$$

Given a matrix 
$$(Y)$$
 of observations

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

Matrix form

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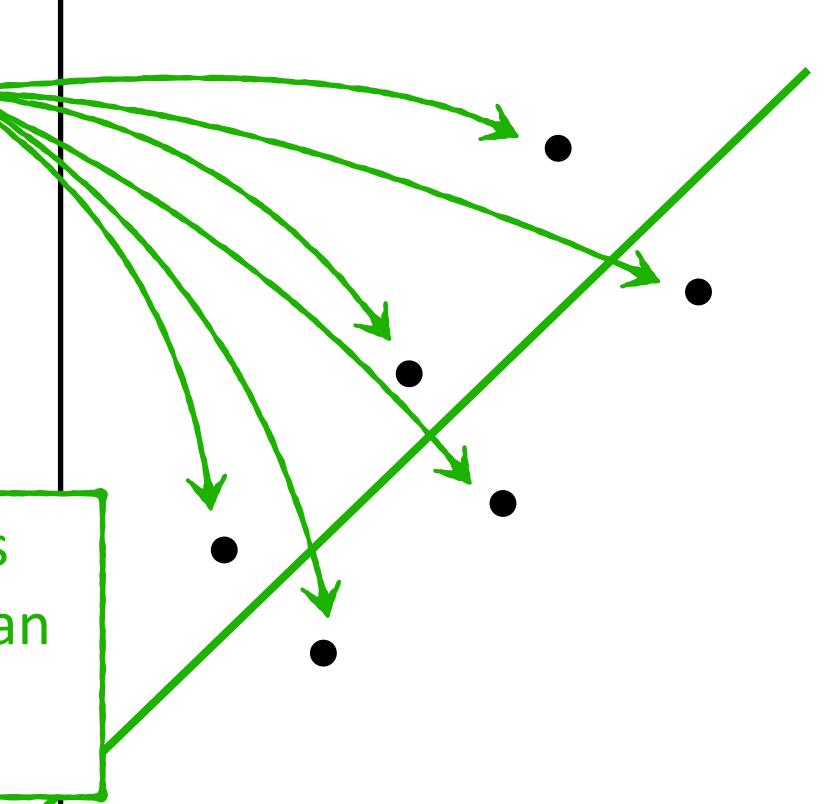
Matrix form

#### The Mean Squared Error (MSE)

$$\frac{1}{n} \parallel Y - \hat{Y} \parallel^2$$

The two parallel vertical lines mean that this is the Euclidean Norm of the matrix

See Tutorial on Matrices & Differential Calculus



# Simple Linear Regression

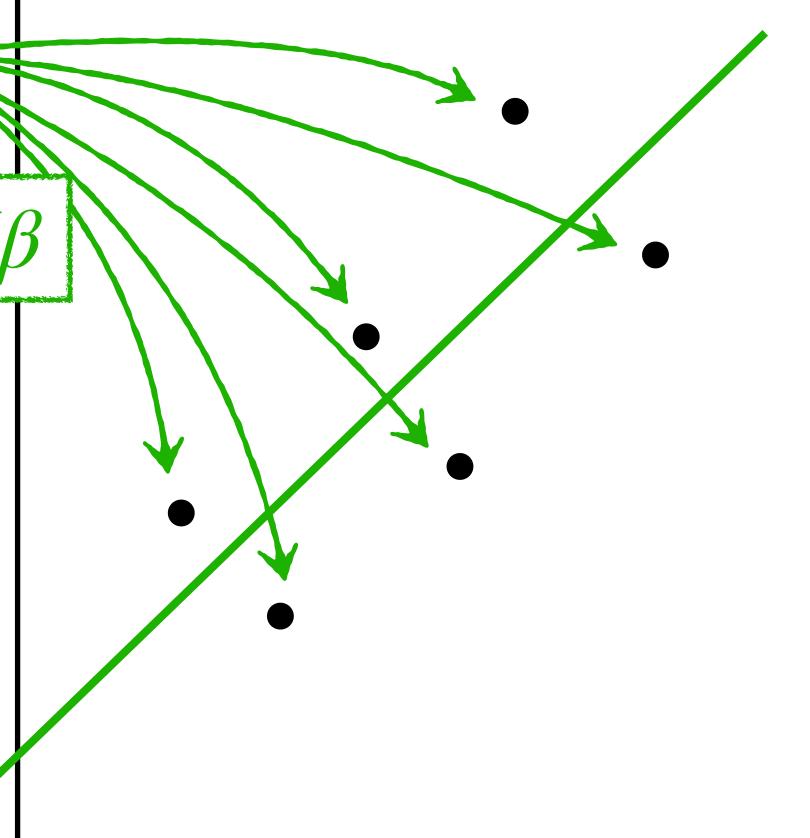
$$\hat{y} = \beta_0 + \beta_1 \hat{x}_1$$

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

Given a matrix (Y)of observations

Substituting  $\hat{Y} = \hat{X}\beta$ 

$$\frac{1}{n} \| Y - \hat{Y} \|^2 = \frac{1}{n} \| Y - \hat{X}\beta \|^2$$



## Simple Linear Regression

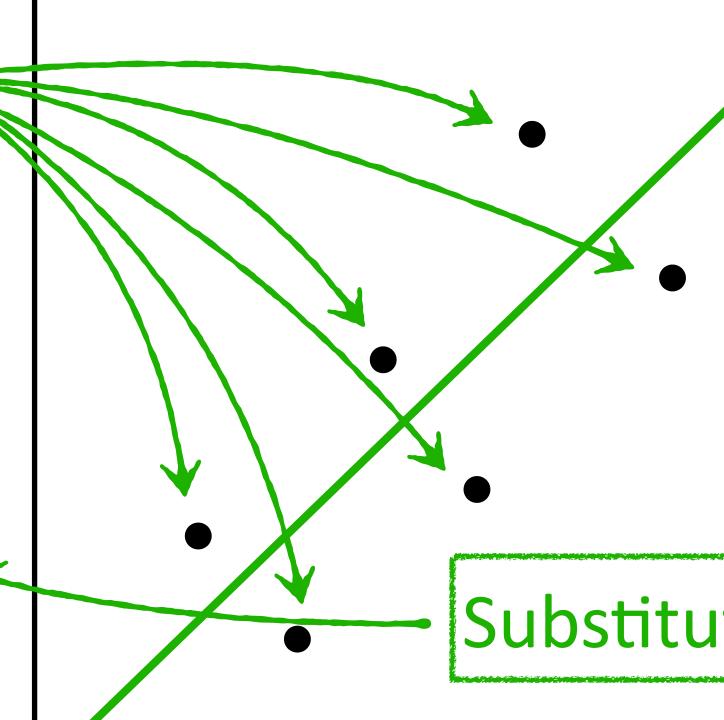
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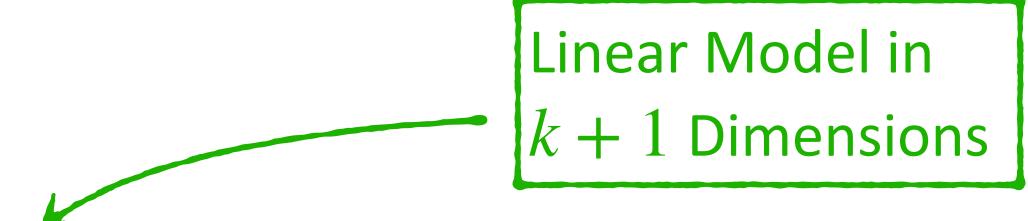
$$\hat{Y} = \hat{X}\beta$$

#### The Mean Squared Error (MSE)

$$\frac{1}{n} \| Y - \hat{Y} \|^2 = \frac{1}{n} \| Y - \hat{X}\beta \|^2 = \frac{1}{n} \| Y - X\beta \|^2$$



Substituting  $\hat{X}\beta = X\beta$ 



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

#### The Mean Squared Error (MSE):

$$\frac{1}{n} \| Y - X\beta \|^2$$



# Multiple Regression

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

The Mean Squared Error (MSE):

$$\frac{1}{m} \| Y - X\beta \|^2$$

#### **The Problem Statement:**

**Multiple Regression:** Compute the matrix etasuch that the Mean Squared Error (MSE) is minimized.

To derive value of the matrix  $\beta$  we calculate the partial derivative of the Mean Squared Error (MSE) w.r.t  $\beta$  and solve for  $\beta$ 

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Euclidean norm of a matrix:

$$||A|| = \sqrt{A^T A}$$

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$$\frac{\partial}{\partial \beta} \frac{1}{n} \| Y - X\beta \|^{2} = 0$$

$$\Rightarrow \frac{1}{n} \frac{\partial}{\partial \beta} \left( \sqrt{(Y - X\beta)^{T} (Y - X\beta)} \right)^{2} = 0$$

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$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow \frac{\partial}{\partial \beta} (Y - X\beta)^T (Y - X\beta) = 0$$

Expanding the first parenthesis

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\frac{\partial}{\partial \beta} A = 0$$

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$$\downarrow \qquad \qquad \frac{\partial}{\partial \beta} A = 0$$

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$$\frac{\partial}{\partial \beta} A \beta = A$$

Proof:  $\beta^T X^T Y = (X^T Y)\beta$ 

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• X is a  $(n + 1) \times (k + 1)$  matrix

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- $\beta$  is a  $(k + 1) \times 1$  column vector
- $\Rightarrow X\beta$  is a  $(n+1) \times 1$  column vector
- $\Rightarrow (X\beta)^T$  is  $1 \times (n+1)$  row vector

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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- $\beta$  is a  $(k + 1) \times 1$  column vector
- $\Rightarrow X\beta$  is a  $(n+1) \times 1$  column vector
- $\Rightarrow (X\beta)^T$  is  $1 \times (n+1)$  row vector
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$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} (X^T Y)^T \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

Proof: 
$$\beta^T X^T Y = (X^T Y)\beta$$

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- if A is symmetric then  $A = A^T$

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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- therefore...

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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Proof: 
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- $\Rightarrow \beta^T X^T Y$  is symmetric
- if A is symmetric then  $A = A^T$
- therefore...

$$\beta^T X^T Y = (\beta^T X^T Y)^T$$
$$= (X^T Y)^T \beta$$

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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- therefore...

$$\beta^T X^T Y = (\beta^T X^T Y)^T$$

$$= (X^T Y)^T \beta \quad Q.E.D$$

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} (X^T Y)^T \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow \frac{\partial}{\partial \beta} Y^T Y - \frac{\partial}{\partial \beta} Y^T X \beta - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} \beta^T X^T Y + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\frac{\partial}{\partial \beta} A \beta = A$$

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\frac{\partial}{\partial \beta} A\beta = A$$

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + 2\beta^T (X^T X) = 0$$

$$\frac{\partial}{\partial \beta} A\beta = A$$

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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$$\Rightarrow 0 - Y^T X - Y^T X + 2\beta^T (X^T X) = 0$$

$$\frac{\partial}{\partial \beta} A \beta = A$$

$$\frac{\partial}{\partial \beta} \beta^T A \beta = \beta^T (A^T + A)$$

if A is symmetric...

$$\frac{\partial}{\partial \beta} \beta^T A \beta = \beta^T (A + A)$$
$$\frac{\partial}{\partial \beta} \beta^T A \beta = 2\beta^T A$$
$$\frac{\partial}{\partial \beta} \beta^T A \beta = 2\beta^T A$$

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + 2\beta^T (X^T X) = 0$$

$$\Rightarrow -2Y^T X + 2\beta^T (X^T X) = 0$$
 Combining the two terms

$$\Rightarrow -2Y^TX + 2\beta^T(X^TX) = 0$$

 $\frac{\partial}{\partial \beta} A \beta = A$ 

$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\frac{\partial \beta}{\partial \beta} A \beta = A$$

$$\Rightarrow 0 - Y^T X - Y^T X + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

$$\Rightarrow 0 - Y^T X - Y^T X + 2\beta^T (X^T X) = 0$$

$$\Rightarrow -2Y^TX + 2\beta^T(X^TX) = 0$$

Combining the two terms

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Adding  $2Y^TX$  to both sides

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

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$$\Rightarrow \beta^T X^T X = Y^T X$$

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Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow X^T X \beta = X^T Y$$

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

Transpose both sides

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow X^T X \beta = X^T Y$$

Multiply both sides by  $(X^TX)^{-1}$ 

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

Transpose both sides

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow X^T X \beta = X^T Y$$

$$\Rightarrow \beta = (X^T X)^{-1} (X^T Y)$$

Multiply both sides by  $(X^TX)^{-1}$ 

$$\Rightarrow 2\beta^T X^T X = 2Y^T X$$

Divide both sides by 2

$$\Rightarrow \beta^T X^T X = Y^T X$$

Transpose both sides

$$\Rightarrow (\beta^T X^T X)^T = (Y^T X)^T$$

$$(AB)^T = B^T A^T$$

$$(A^T)^T = A$$

$$\Rightarrow X^T X \beta = X^T Y$$

$$\Rightarrow \beta = (X^T X)^{-1} (X^T Y)$$

Multiply both sides by  $(X^TX)^{-1}$ 



# Related Tutorials & Textbooks

#### Simple Linear Regression

A statistical technique of making predictions from data. The tutorial introduces a linear model in two dimensions and uses that model to predict the value of one dependent variable given one independent variable.

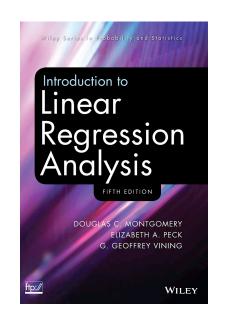
#### Multiple Regression []

Multiple regression extends the two dimensional linear model introduced in Simple Linear Regression to k+1 dimensions with one dependent variable, k independent variables and k+1 parameters.

#### **Gradient Descent for Multiple Regression**

Gradient Descent algorithm for multiple regression and how it can be used to optimize k + 1 parameters for a Linear model in multiple dimensions.

#### **Recommended Textbooks**



#### **Introduction to Linear Regression Analysis**

by Douglas C. Montgomery, Elizabeth A. Peck, G. Geoffrey Vining

For a complete list of tutorials see:

https://arrsingh.com/ai-tutorials