

# Multiple Regression

## Deriving the Matrix Form

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# Multiple Regression

Linear Model in  $k$   
Dimensions

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \dots + \beta_{k-1} x_{k-1}$$

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{31} & \cdot & \cdot & \cdot & x_{(k-1)1} \\ 1 & x_{12} & x_{22} & x_{32} & \cdot & \cdot & \cdot & x_{(k-1)2} \\ 1 & x_{13} & x_{23} & x_{33} & \cdot & \cdot & \cdot & x_{(k-1)3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_{1n} & x_{2n} & x_{3n} & \cdot & \cdot & \cdot & x_{(k-1)n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_{k-1} \end{bmatrix}$$

- 1 dependent variable  $\hat{y}$
- $k - 1$  independent variables  $x_1, x_2, x_3 \dots x_{k-1}$
- $k$  parameters -  $\beta_0, \beta_1, \beta_2, \beta_3 \dots \beta_{k-1}$

# Multiple Regression

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$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \dots + \beta_{k-1} x_{k-1}$$

$$\hat{y}_n = 1 \times \beta_0 + \hat{x}_{1n} \times \beta_1 + \hat{x}_{2n} \times \beta_2 + \hat{x}_{3n} \times \beta_3 + \dots + \hat{x}_{kn} \times \beta_k$$
$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{31} & \cdot & \cdot & \cdot & x_{(k-1)1} \\ 1 & x_{12} & x_{22} & x_{32} & \cdot & \cdot & \cdot & x_{(k-1)2} \\ 1 & x_{13} & x_{23} & x_{33} & \cdot & \cdot & \cdot & x_{(k-1)3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_{1n} & x_{2n} & x_{3n} & \cdot & \cdot & \cdot & x_{(k-1)n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_{k-1} \end{bmatrix}$$

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# Multiple Regression

Linear Model in  $k$   
Dimensions

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \dots + \beta_{k-1} x_{k-1}$$

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

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

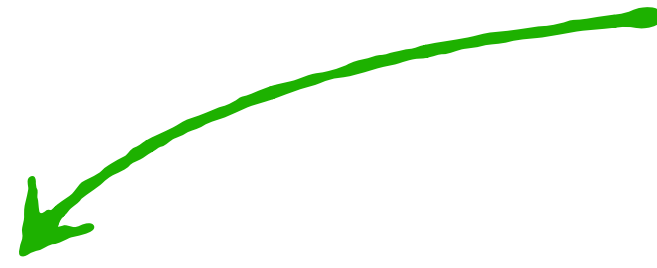
$$\begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix}_{n \times 1} = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{31} & \cdot & \cdot & \cdot & x_{(k-1)1} \\ 1 & x_{12} & x_{22} & \cdot & \cdot & \cdot & \cdot & x_{(k-1)2} \\ 1 & x_{13} & x_{23} & \cdot & \cdot & \cdot & \cdot & x_{(k-1)3} \\ \vdots & \vdots & \vdots & \cdot & \cdot & \cdot & \cdot & \vdots \\ \vdots & \vdots & \vdots & \cdot & \cdot & \cdot & \cdot & \vdots \\ 1 & x_{1n} & x_{2n} & x_{3n} & \cdot & \cdot & \cdot & x_{(k-1)n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{k-1} \end{bmatrix}_{k \times 1}$$

$X$   
 $n \times k$

- 1 dependent variable  $\hat{y}$
- $k - 1$  independent variables  $x_1, x_2, x_3 \dots x_{k-1}$
- $k$  parameters -  $\beta_0, \beta_1, \beta_2, \beta_3 \dots \beta_{k-1}$

# Simple Linear Regression

Linear Model in  
two Dimensions



$$\hat{y} = \beta_0 + \beta_1 x_1$$

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Linear Model in  
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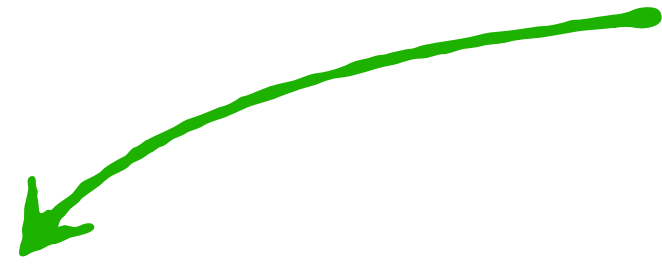
$$\hat{Y} = X\beta$$

Matrix form



# Simple Linear Regression

Linear Model in  
two Dimensions

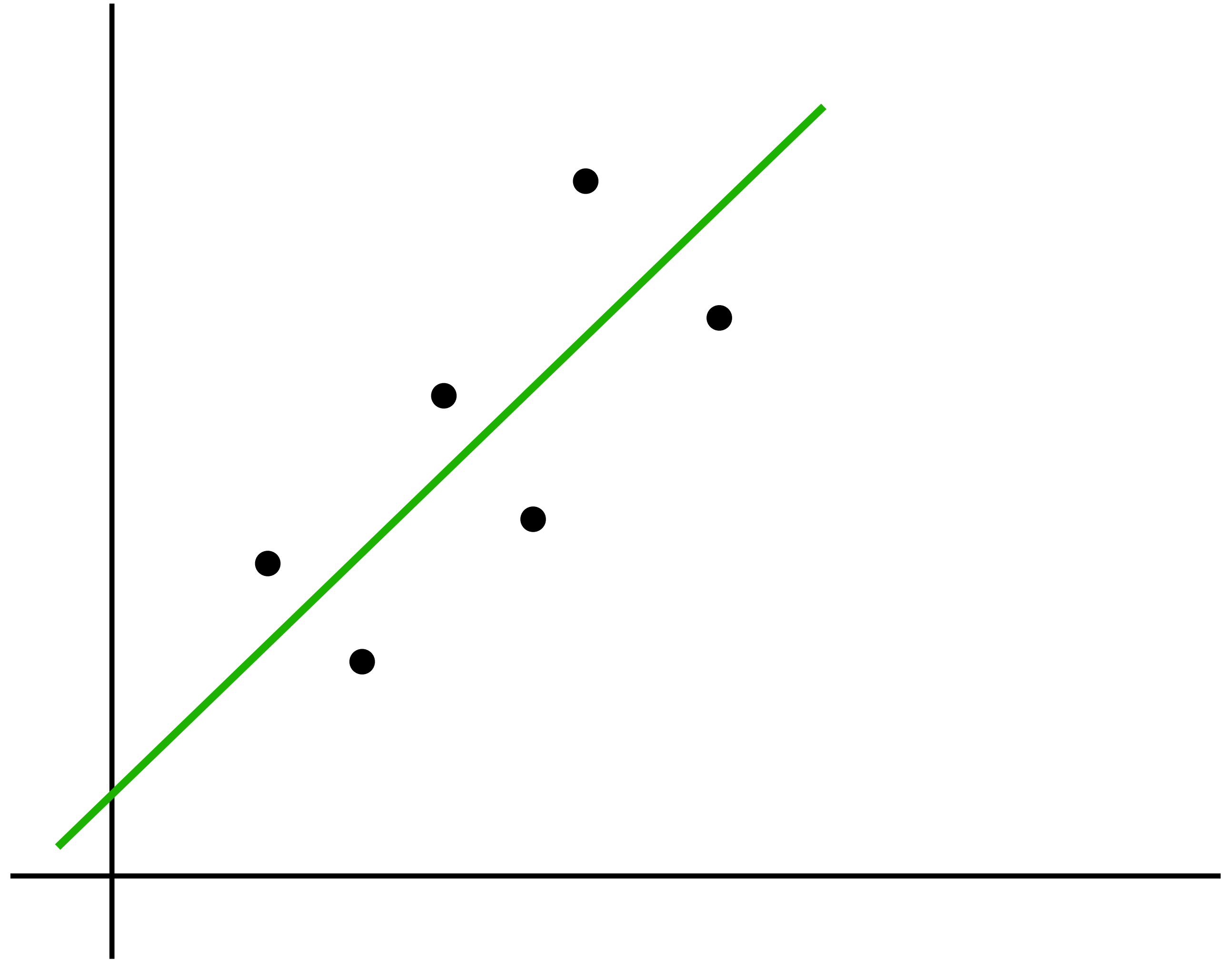


$$\hat{y} = \beta_0 + \beta_1 x_1$$

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



Matrix form



# Simple Linear Regression

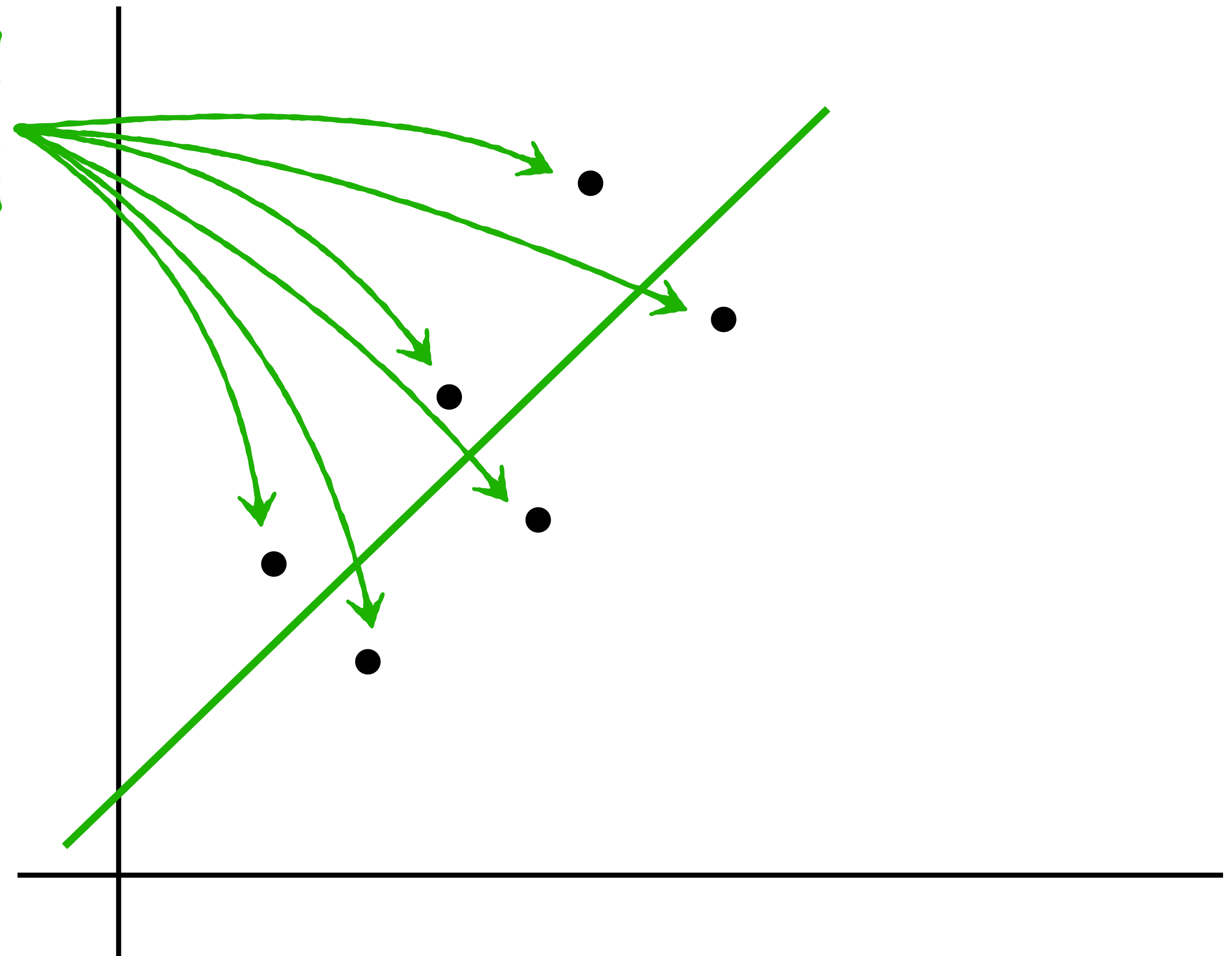
Linear Model in  
two Dimensions

$$\hat{y} = \beta_0 + \beta_1 x_1$$

Given a matrix ( $Y$ )  
of observations

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

Matrix form





# Simple Linear Regression

Linear Model in  
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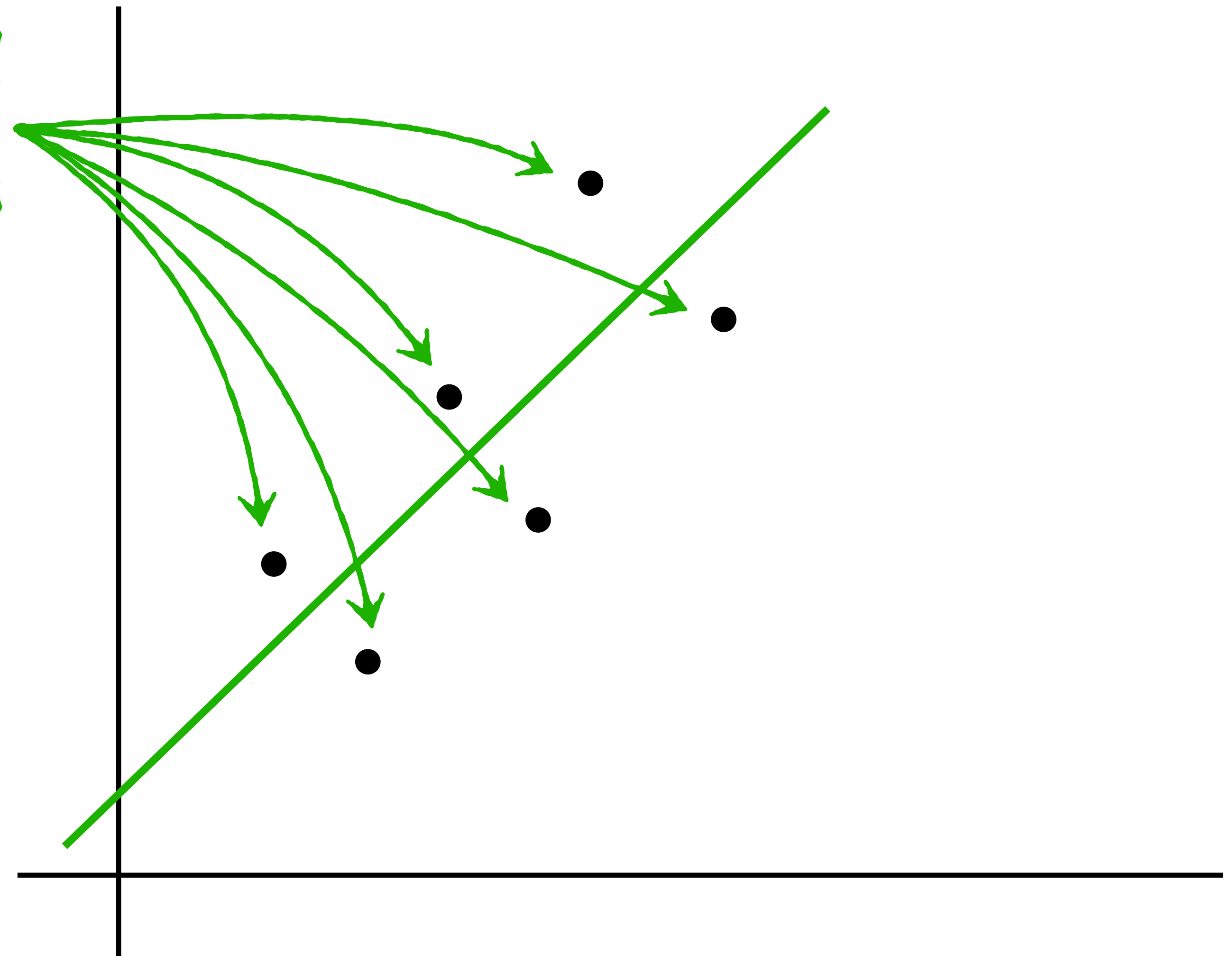
Given a matrix ( $Y$ )  
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Matrix form

The **Mean Squared Error (MSE)**

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



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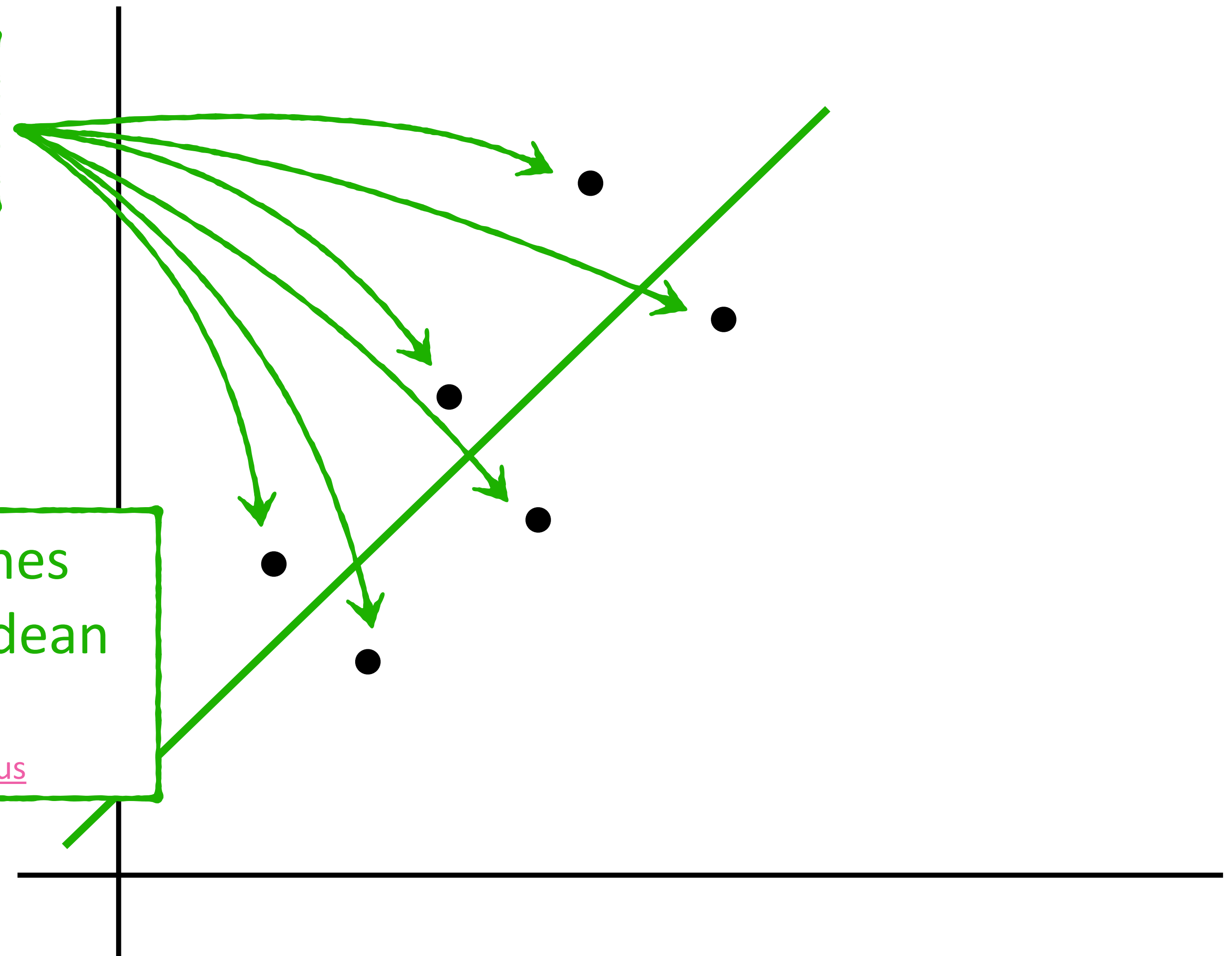
Matrix form

The **Mean Squared Error (MSE)**

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

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

[See Tutorial on Matrices & Differential Calculus](#)



# Simple Linear Regression

Linear Model in  
two Dimensions

$$\hat{y} = \beta_0 + \beta_1 x_1$$

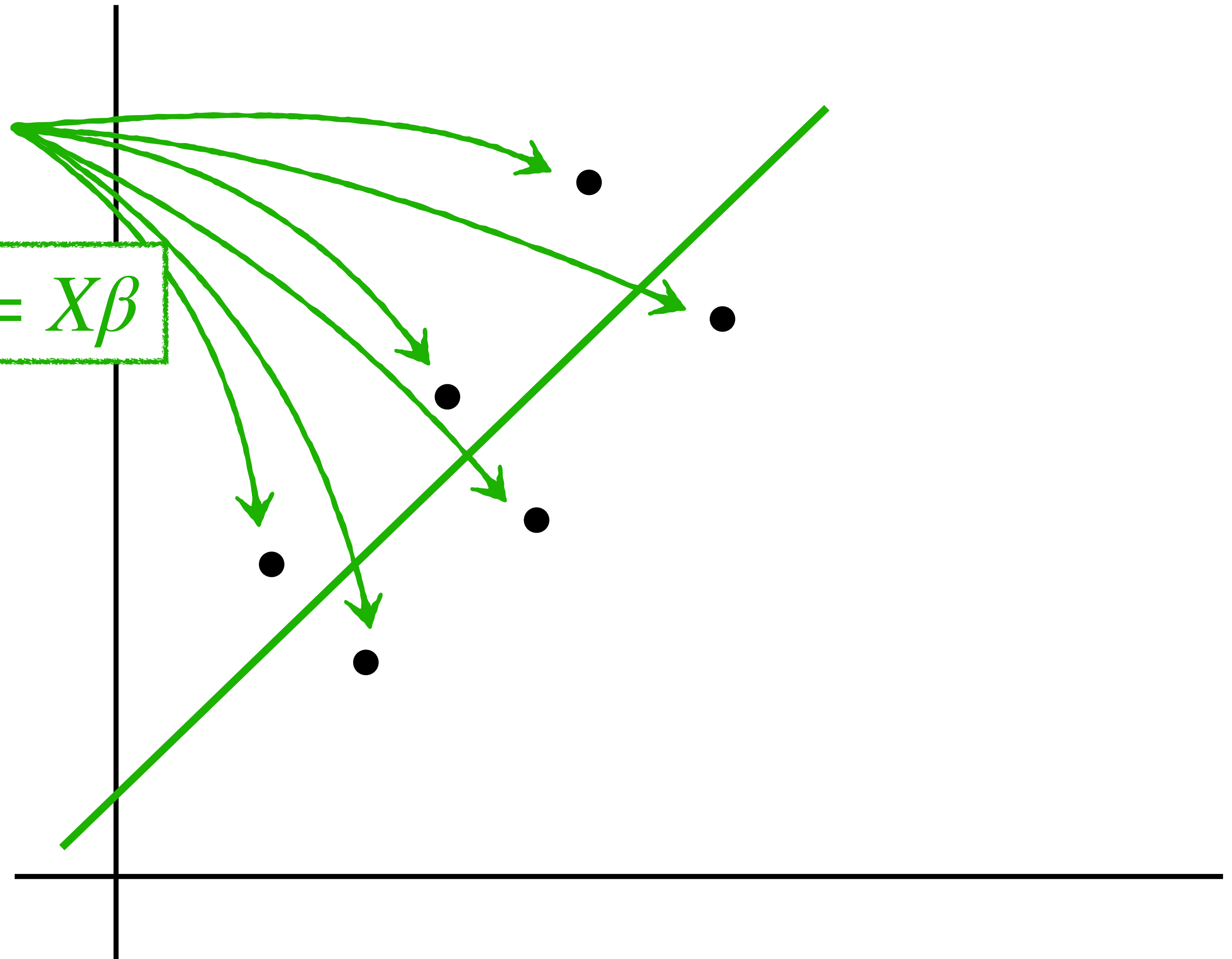
Given a matrix ( $Y$ )  
of observations

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

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

The **Mean Squared Error (MSE)**

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



# Multiple Regression

Linear Model in  $k$   
Dimensions



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

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

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# Multiple Regression

Linear Model in  $k$   
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$$\hat{Y} = X\beta$$

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

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**The Problem Statement:**

**Multiple Regression:** Compute the matrix  $\beta$  such that the Mean Squared Error (MSE) is minimized.

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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  $\beta$

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

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

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Euclidean norm of a matrix:

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

[See the Tutorial on Vectors & Matrices](#)

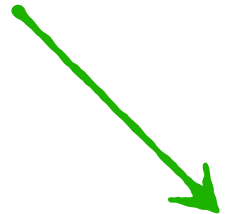


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$$\frac{\partial}{\partial \beta} \frac{1}{n} \| Y - X\beta \|^2 = 0$$


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

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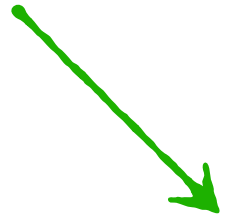
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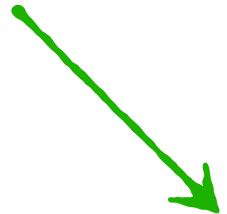
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Expanding the first parenthesis

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Expanding the first parenthesis

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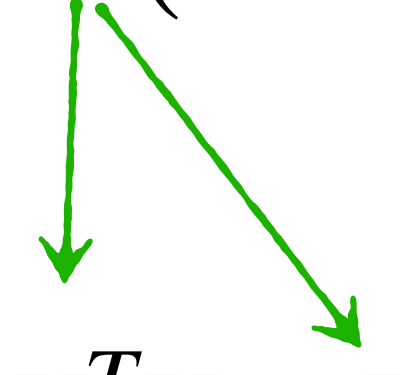
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Expanding the second parenthesis  
 $(AB)^T = B^T A^T$

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Expanding to the derivatives of  
the individual terms

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Expanding to the derivatives of  
the individual terms

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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**


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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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


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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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



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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

$$\begin{aligned} \beta^T X^T Y &= (\beta^T X^T) Y & A^T B^T &= (BA)^T \\ &= (X \beta)^T Y \end{aligned}$$

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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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$$\begin{aligned} \beta^T X^T Y &= (\beta^T X^T) Y \\ &= (X \beta)^T Y \end{aligned}$$

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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

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- $X$  is a  $(n + 1) \times (k + 1)$  matrix
- $\beta$  is a  $(k + 1) \times 1$  column vector

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

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- $\beta$  is a  $(k + 1) \times 1$  column vector
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**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

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Scalars are always symmetric

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- therefore...



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$$\begin{aligned} \beta^T X^T Y &= (\beta^T X^T Y)^T \\ &= (X^T Y)^T \beta \end{aligned} \quad \boxed{\text{Q.E.D.}}$$

**Multiple Regression: Compute the matrix  $\beta$  such that the SSR is minimized.**

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

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$$\begin{aligned} (AB)^T &= B^T A^T \\ (A^T)^T &= A \end{aligned}$$



**Multiple Regression: Compute the matrix  $\beta$  such that the SSR is minimized.**

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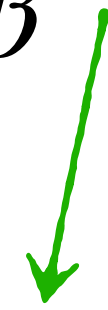
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$$\Rightarrow 0 - Y^T X - \frac{\partial}{\partial \beta} Y^T X \beta + \frac{\partial}{\partial \beta} \beta^T X^T X \beta = 0$$

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

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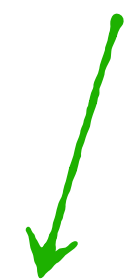


$$\Rightarrow 0 - Y^T X - Y^T X + 2\beta^T(X^T X) = 0$$

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

if  $A$  is symmetric...

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

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

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

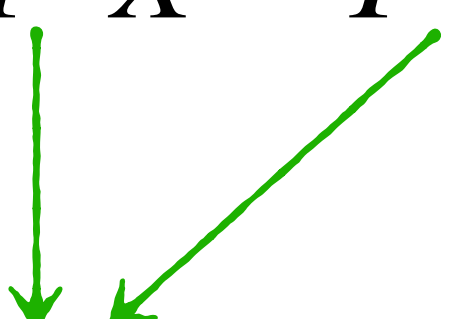
Combining the two terms

**Multiple Regression: Compute the matrix  $\beta$  such that the SSR is minimized.**

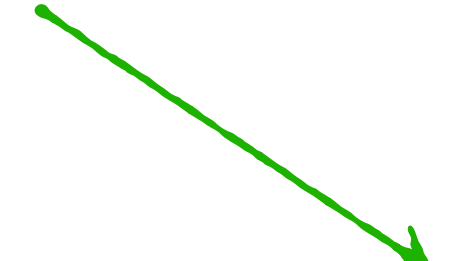
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Combining the two terms


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

Adding  $2Y^T X$  to both sides



**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

Divide both sides by 2

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Divide both sides by 2

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

Divide both sides by 2

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

Transpose both sides

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

Divide both sides by 2

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

Transpose both sides

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

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



**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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Transpose both sides

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

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

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

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

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

**Multiple Regression: Compute the matrix  $\beta$  such that the MSE is minimized.**

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

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  $(X^T X)^{-1}$

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

**Q.E.D**

# 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.

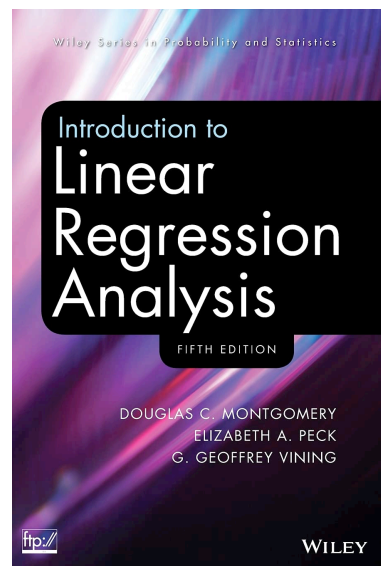
## Multiple Regression ↗

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>