

Multiple Regression

General Matrix form for Multiple Regression

Rahul Singh
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What is Simple Linear Regression

re·gres·sion

noun

A statistical method used to **predict** the relationship between a dependent variable and one or more independent variables

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in other words...

if we see some data (x, y) we can use linear regression to **predict** the y values for other values of x

What is Simple Linear Regression

re·gres·sion

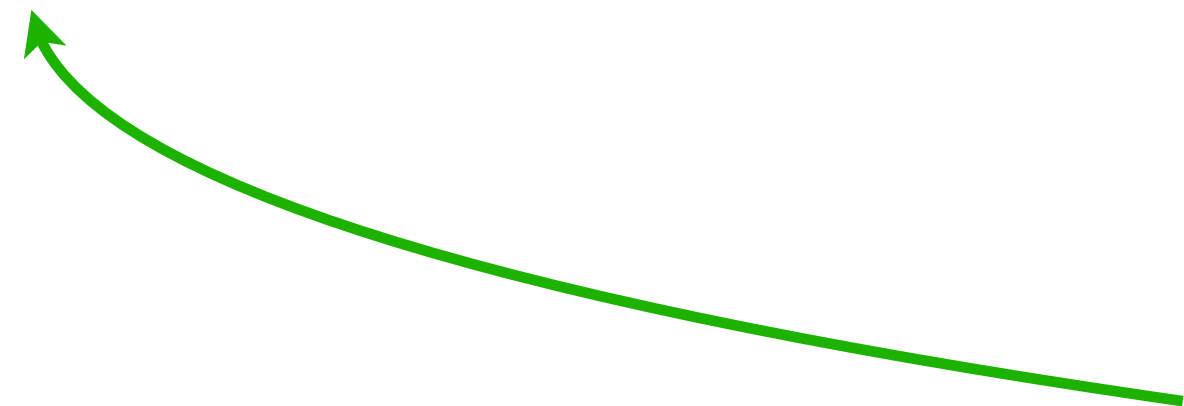
noun

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in other words...

if we see some data (x, y) we can use linear regression to **predict** the y values for other values of x

$$y = f(x)$$



y is the dependent variable

What is Simple Linear Regression

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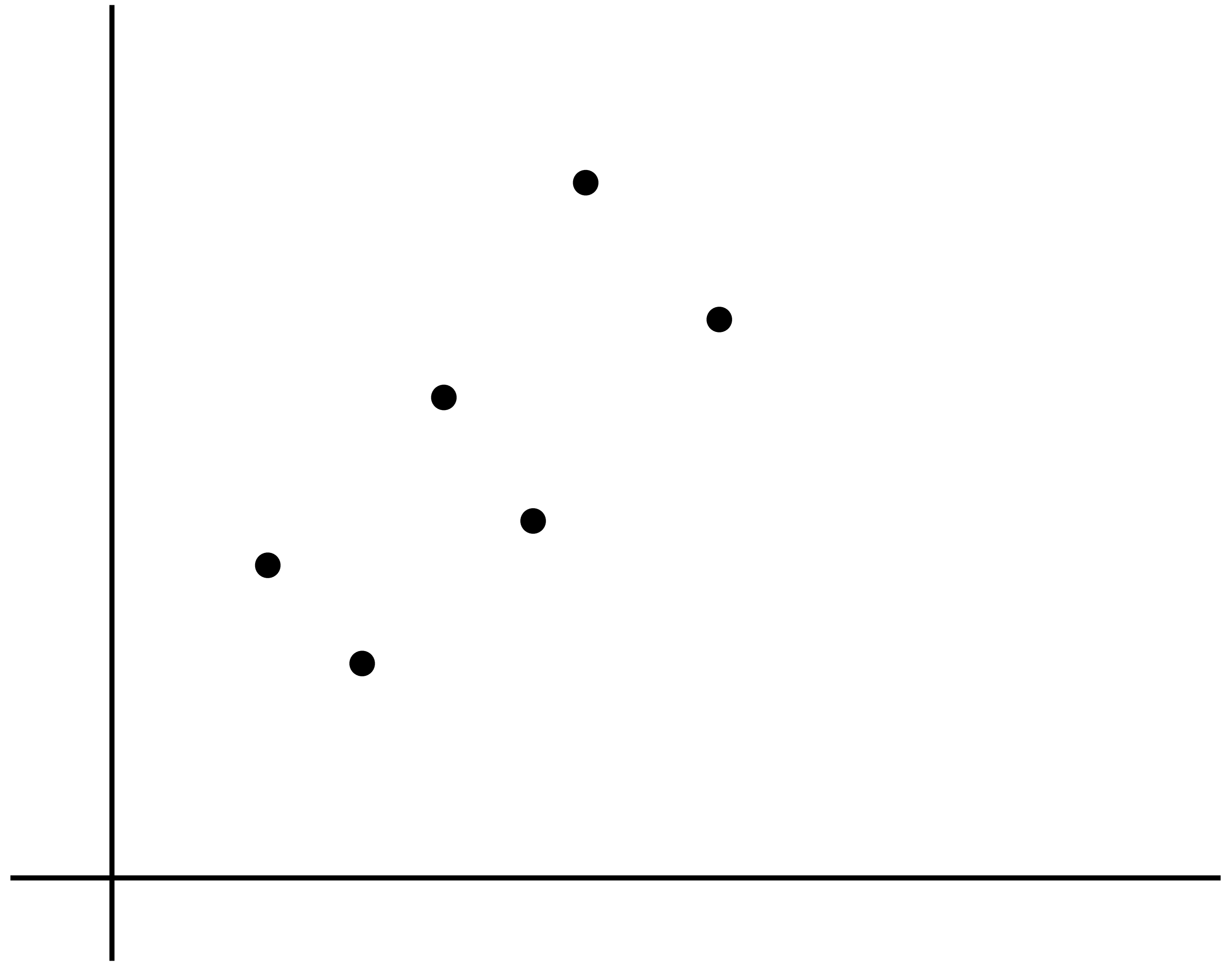
$$y = f(x)$$

x is the independent variable

y is the dependent variable

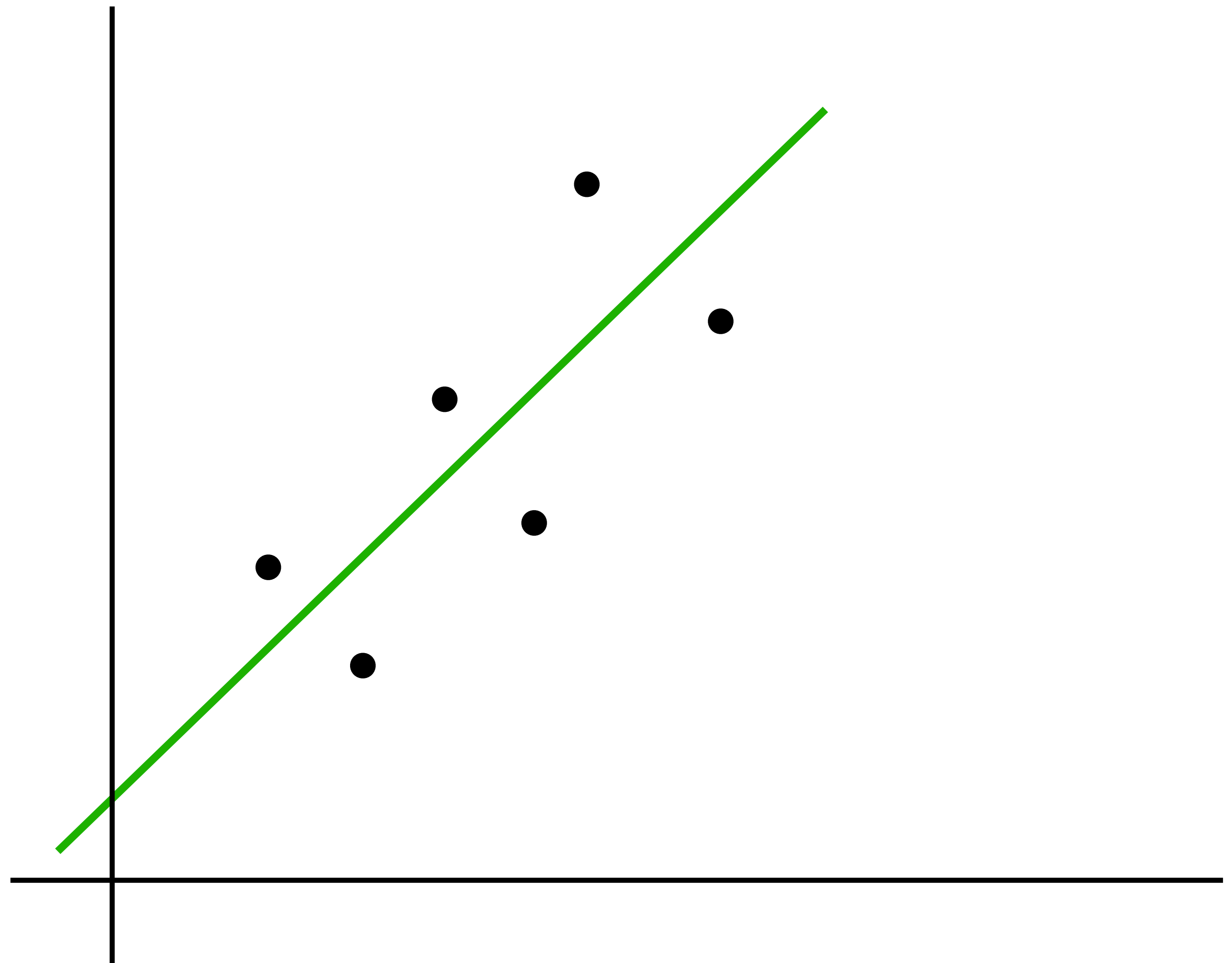
Fundamental Concept: Given a set of data (observations), find the values of β_0 and β_1 for the line that best fits the given data.

Simple Linear Regression



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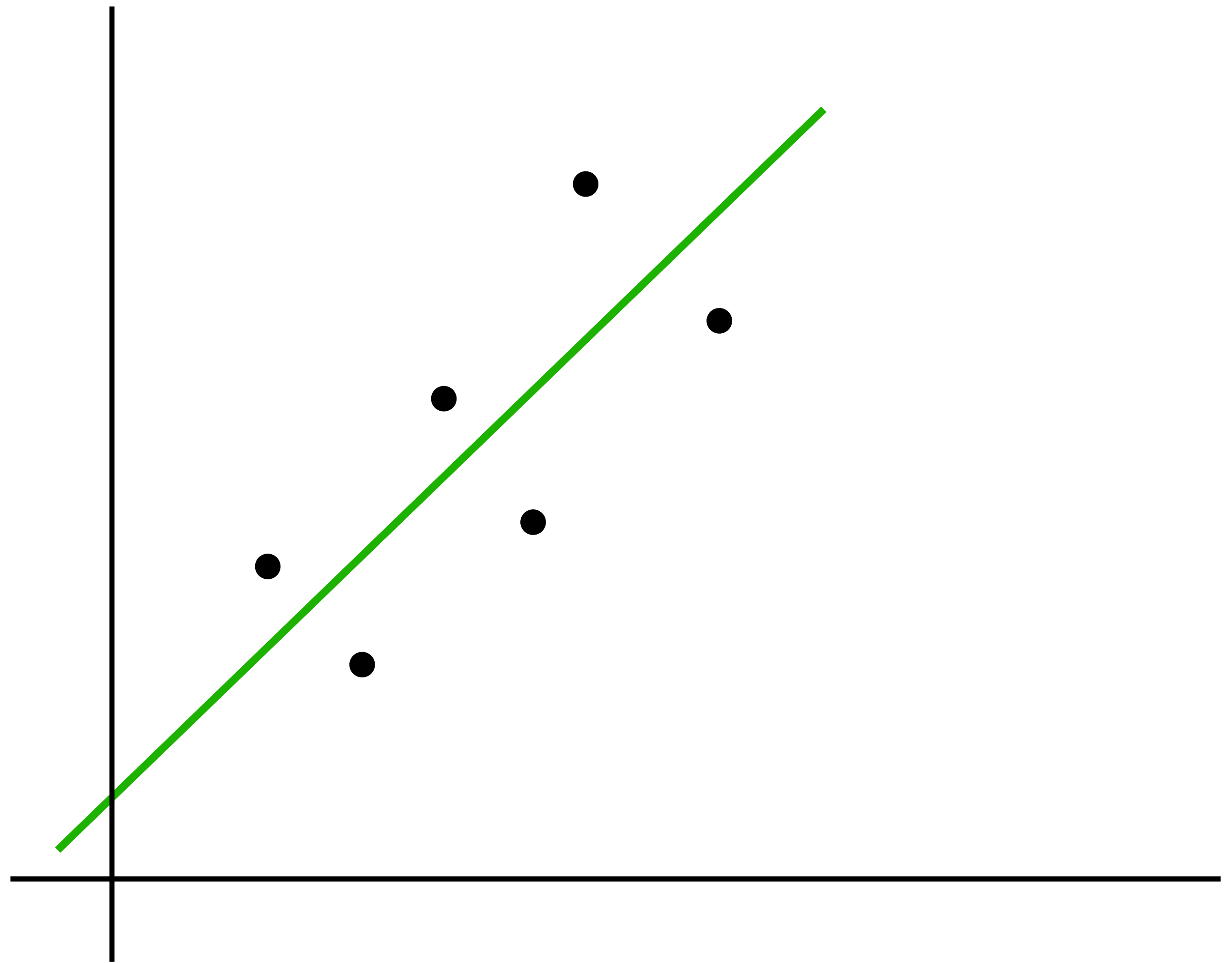
Simple Linear Regression



Fundamental Concept: Given a set of data (observations), find the values of β_0 and β_1 for the line that best fits the given data.

The line of best fit is $\hat{y} = \beta_0 + \beta_1 x$

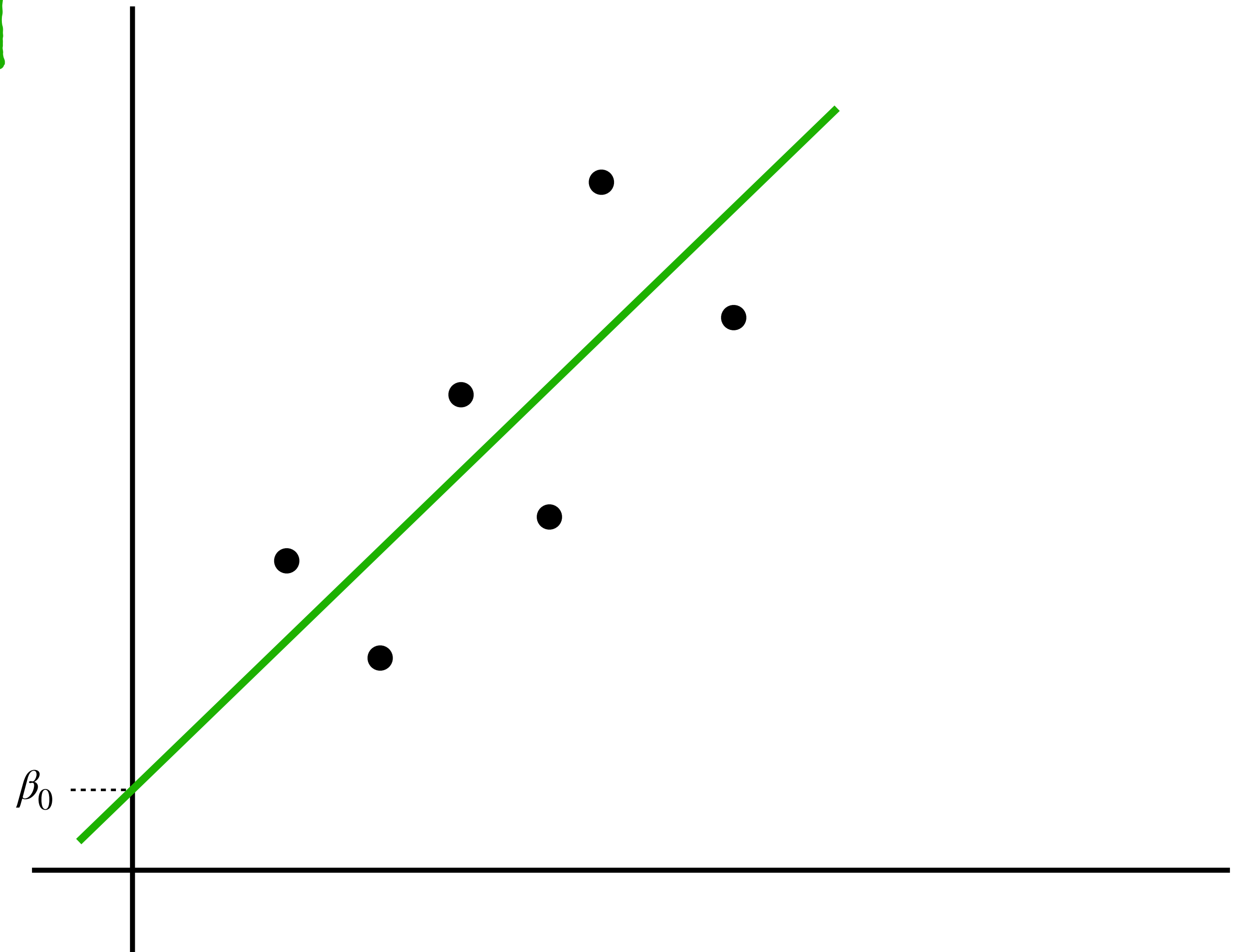
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β_0 Is the Y intercept



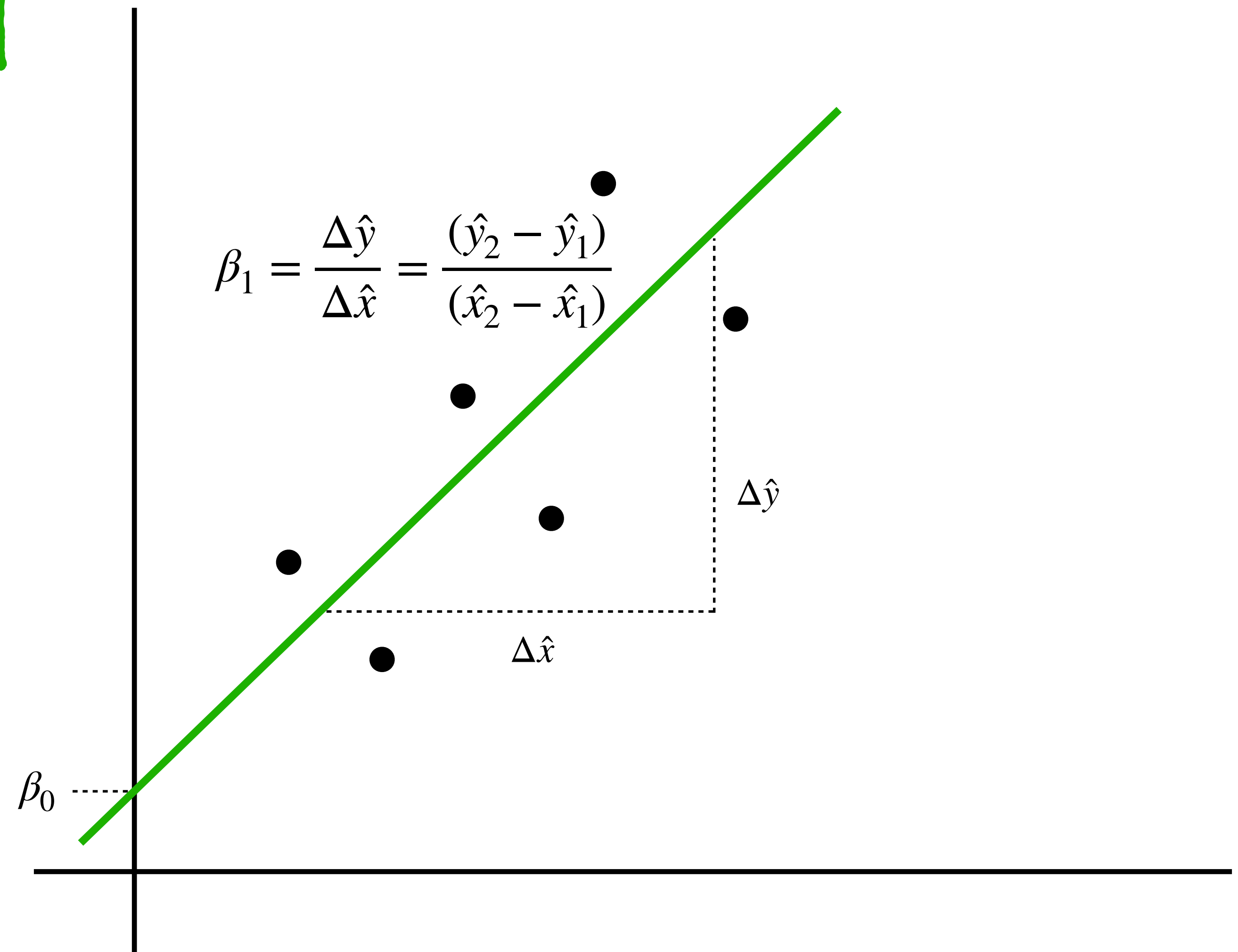
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The line of best fit is $\hat{y} = \beta_0 + \beta_1 \hat{x}$

β_0 Is the Y intercept

β_1 Is the slope of the line

Simple Linear Regression



Fundamental Concept: Given a set of data (observations), find the values of β_0 and β_1 for the line that best fits the given data.

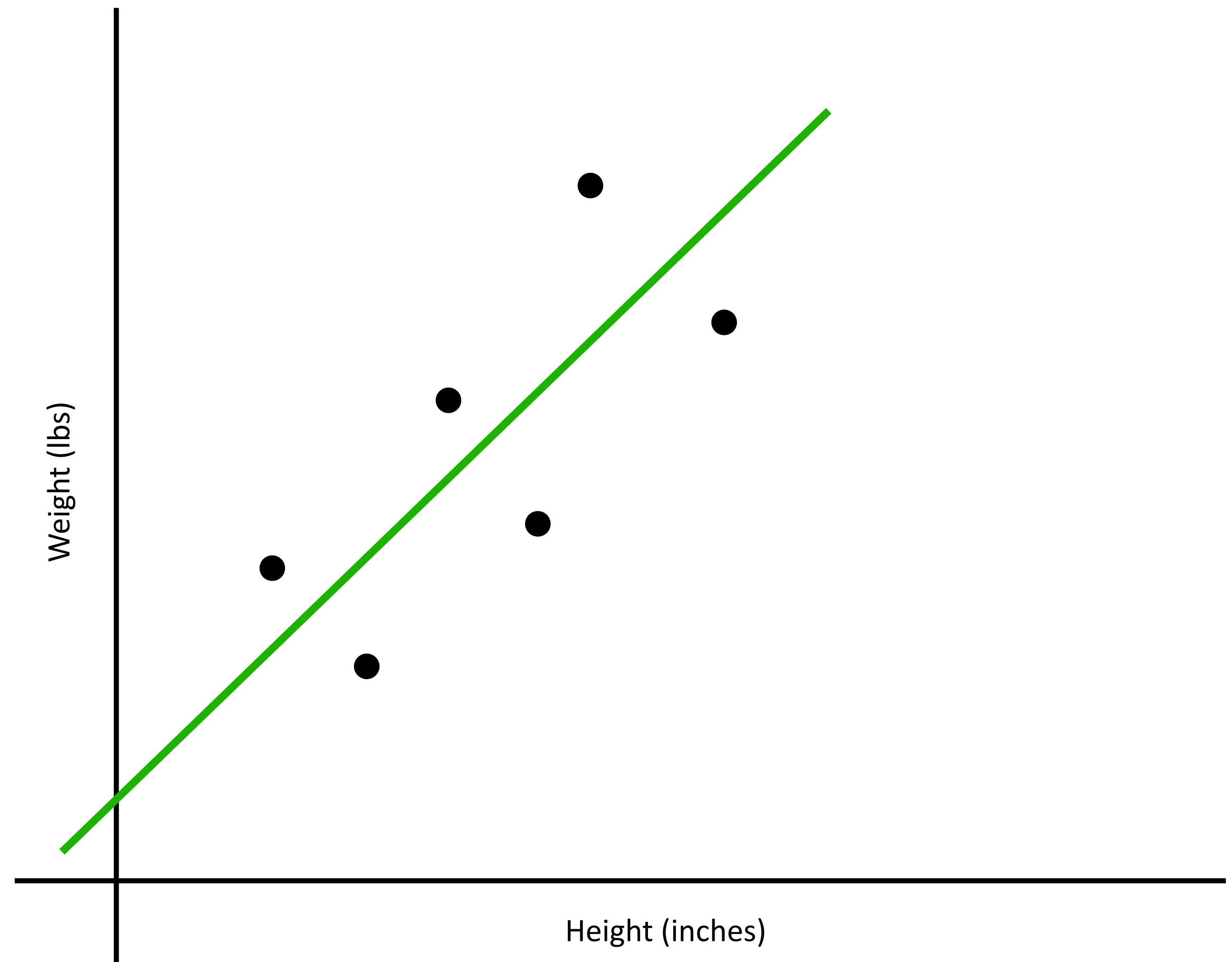
$$\hat{y} = \beta_0 + \beta_1 x$$

x is the independent variable

$\hat{y}$ is the dependent variable

Eg: Predict Weight ($\hat{y}$) given Height (x)

Simple Linear Regression



Fundamental Concept: Given a set of data (observations), find the values of β_0 and β_1 for the line that best fits the given data.

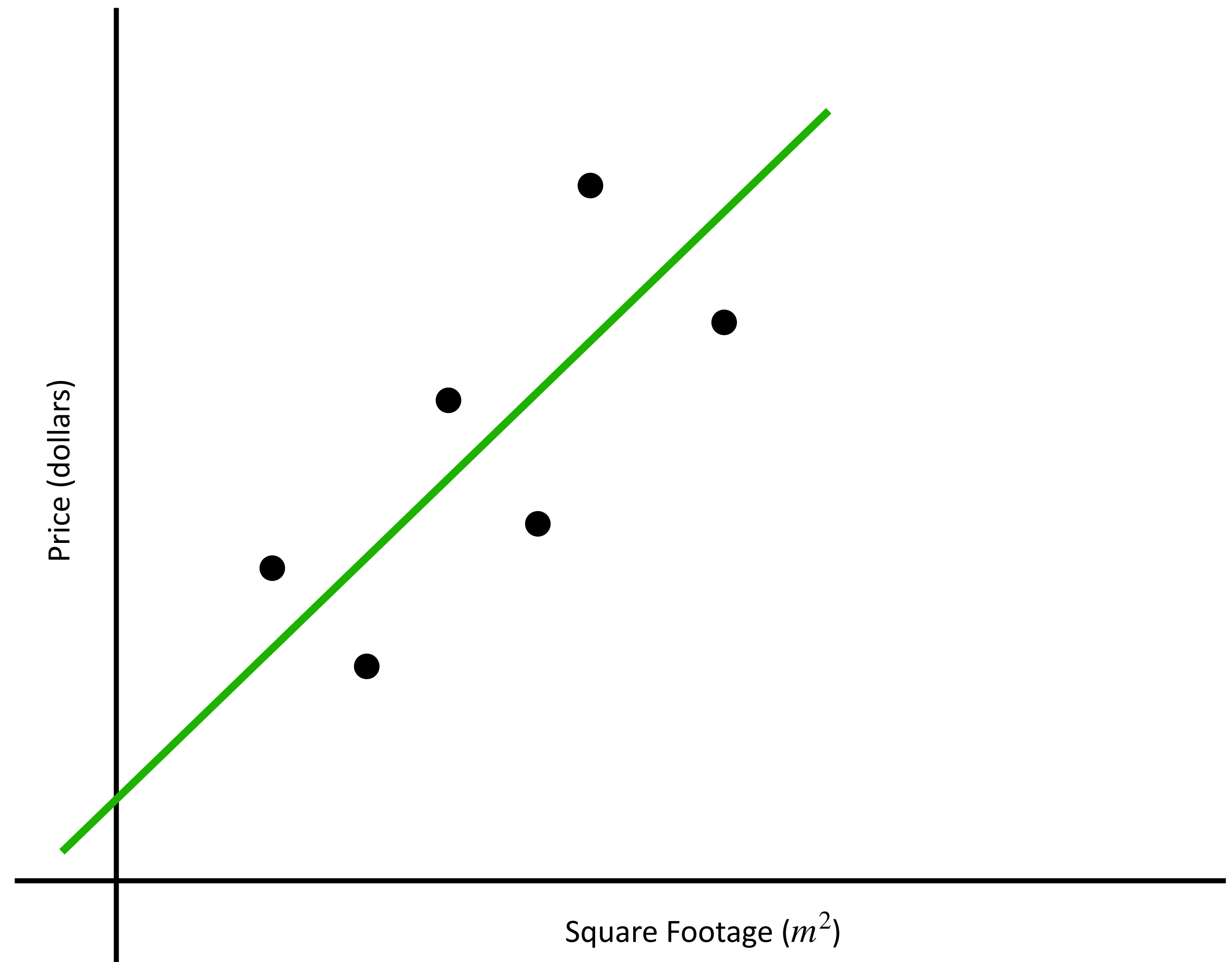
$$\hat{y} = \beta_0 + \beta_1 x$$

x represents
square
footage (m^2)

$\hat{y}$ represents
price (dollars)

Eg: Predict Price of a house ($\hat{y}$) given
Square Footage (x)

Simple Linear Regression



Fundamental Concept: Given a set of data (observations), find the values of β_0 and β_1 for the line that best fits the given data.

The line of best fit is $\hat{y} = \beta_0 + \beta_1 x$

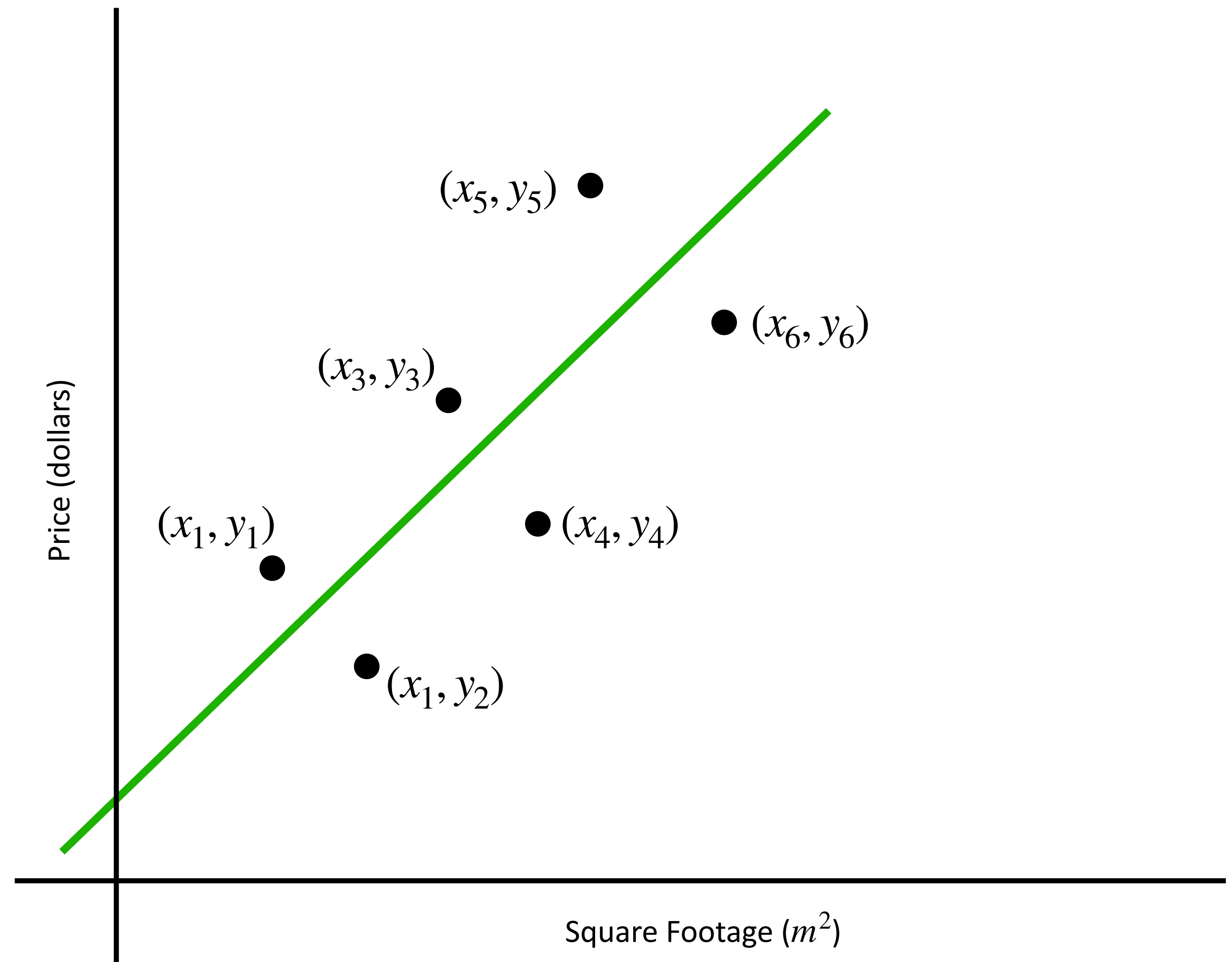
For each point calculate the squared distance to the line. Divide that by the number of data points.

$$\frac{(y_1 - \hat{y}_1)^2 + (y_2 - \hat{y}_2)^2 + (y_3 - \hat{y}_3)^2 + (y_4 - \hat{y}_4)^2 + (y_5 - \hat{y}_5)^2 + (y_6 - \hat{y}_6)^2}{n}$$

This is the **Mean Squared Error (MSE)**

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

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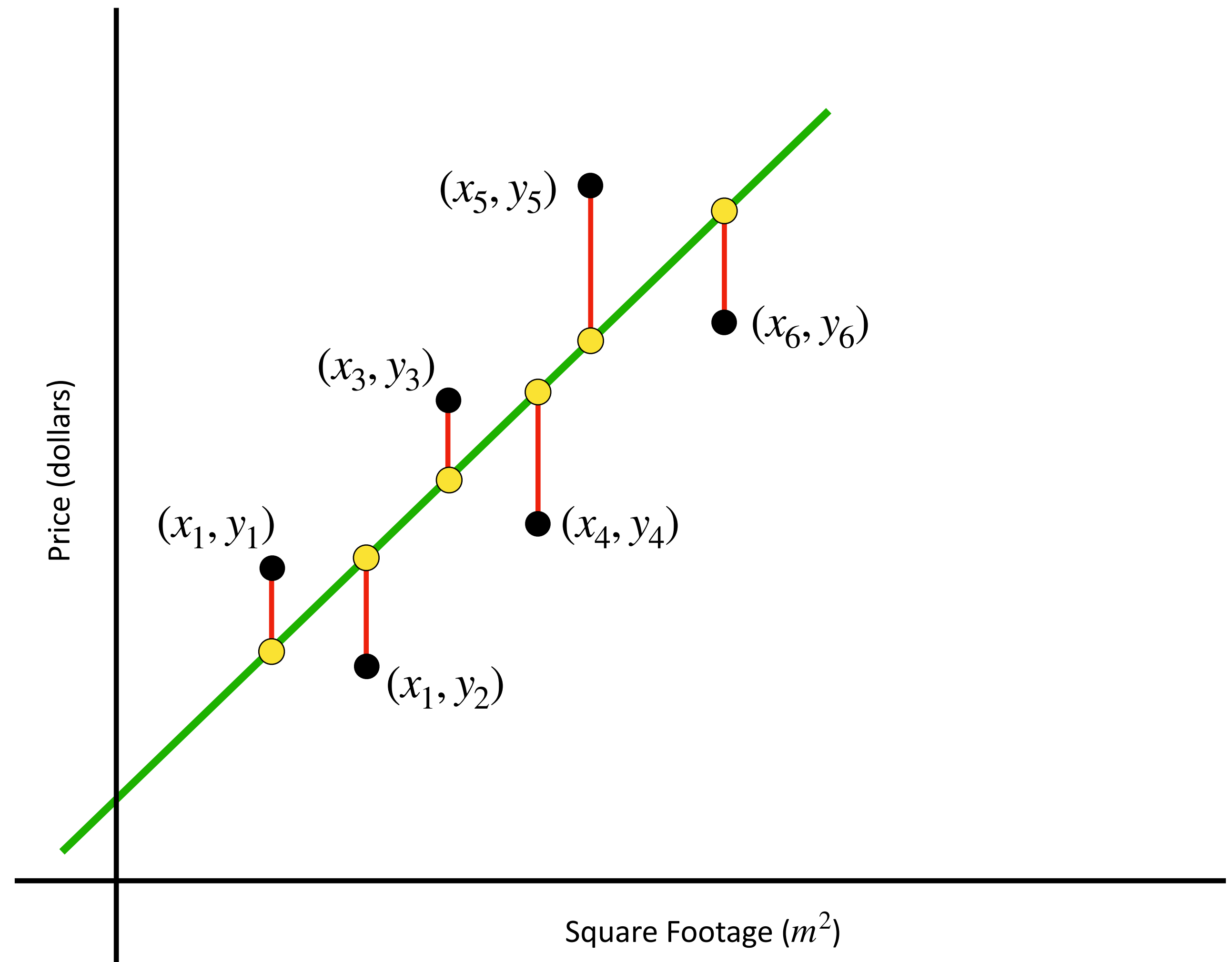
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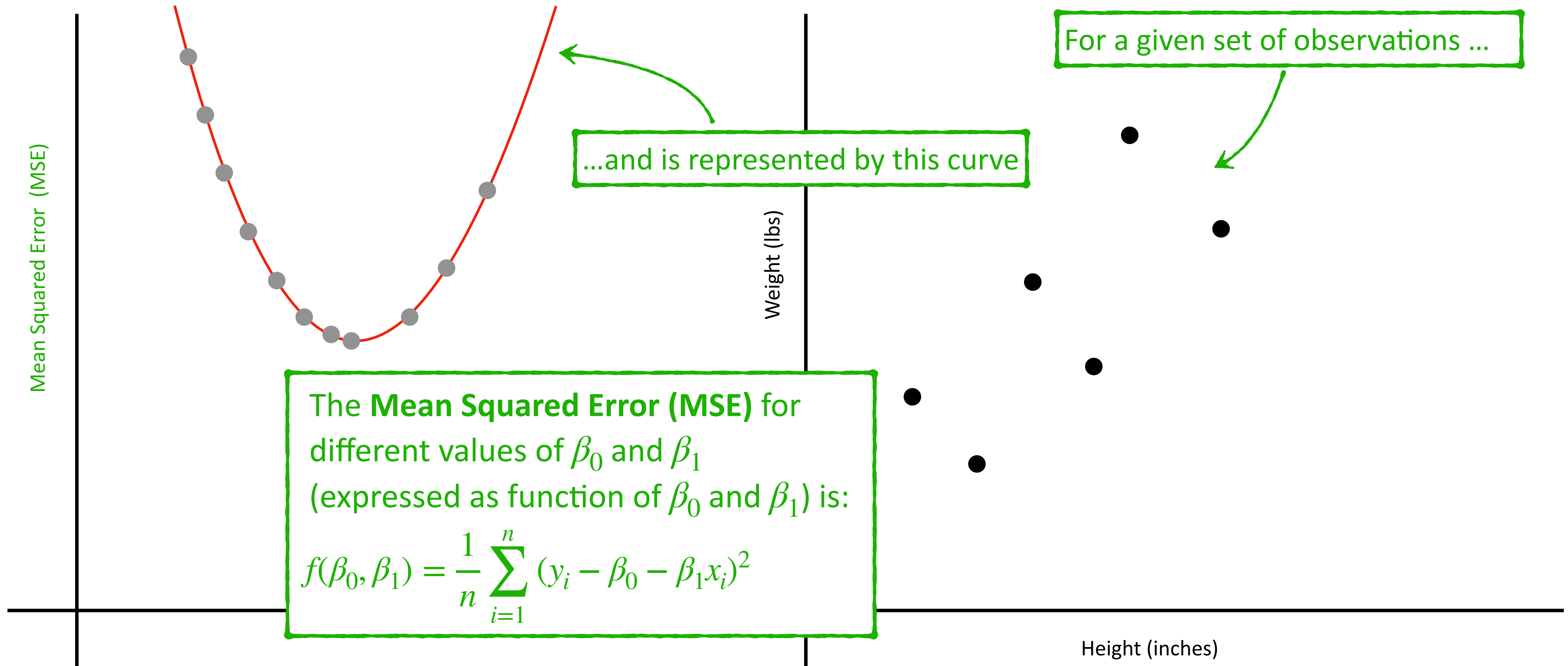
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Simple Linear Regression



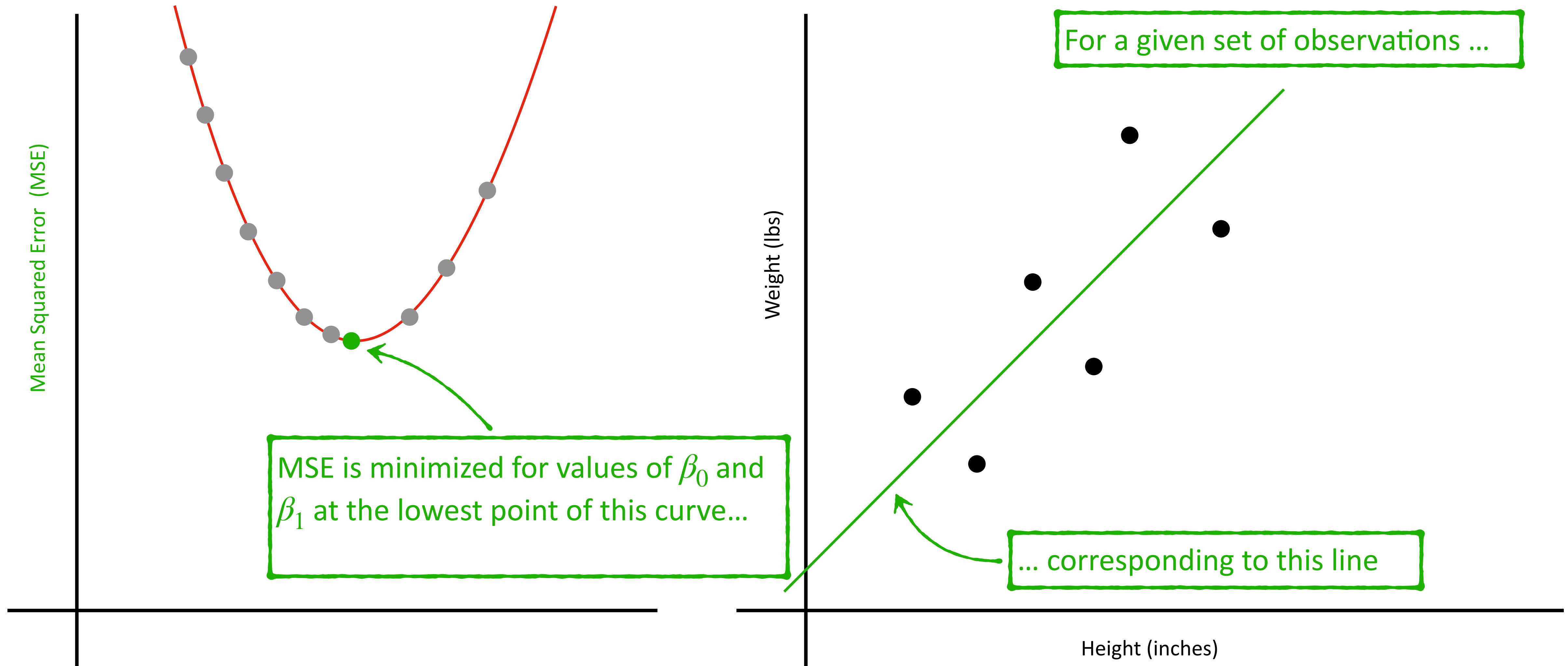
Mean Squared Error (MSE) for various values of β_0 and β_1

Simple Linear Regression



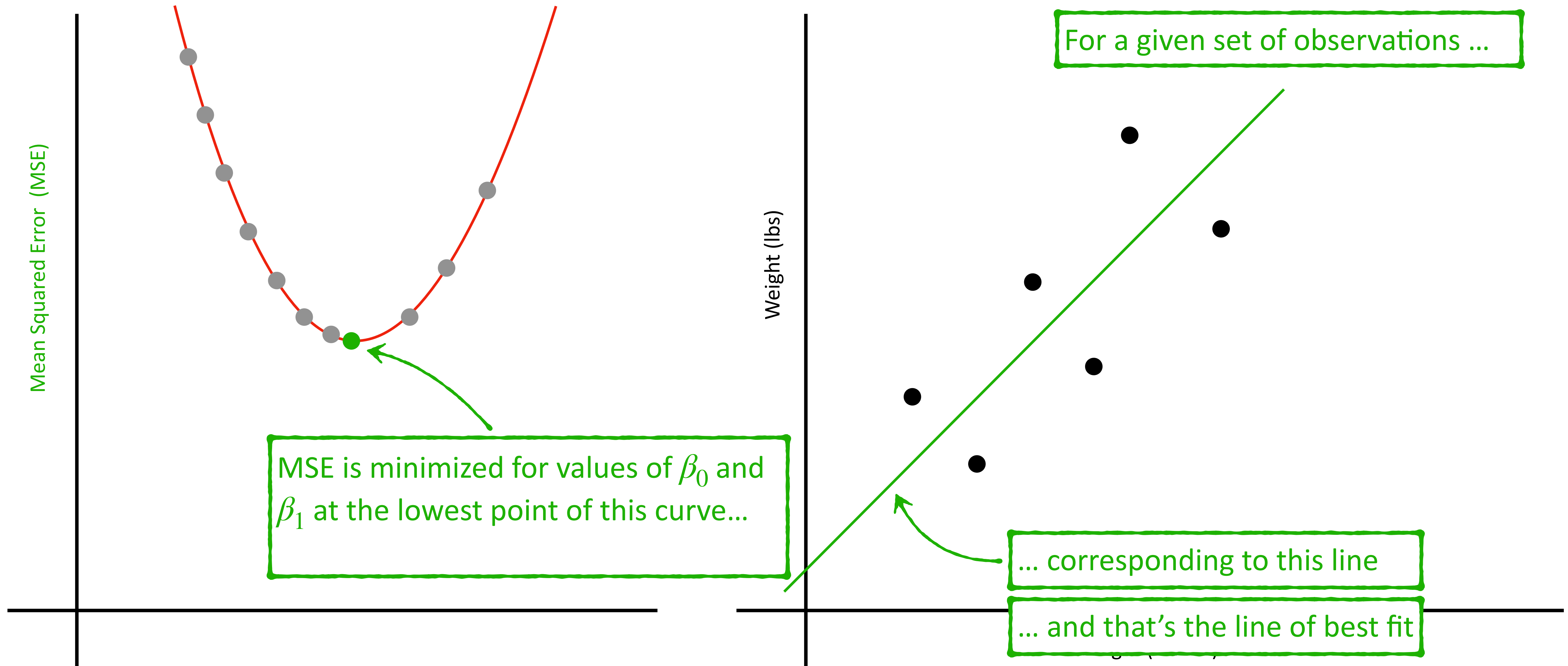
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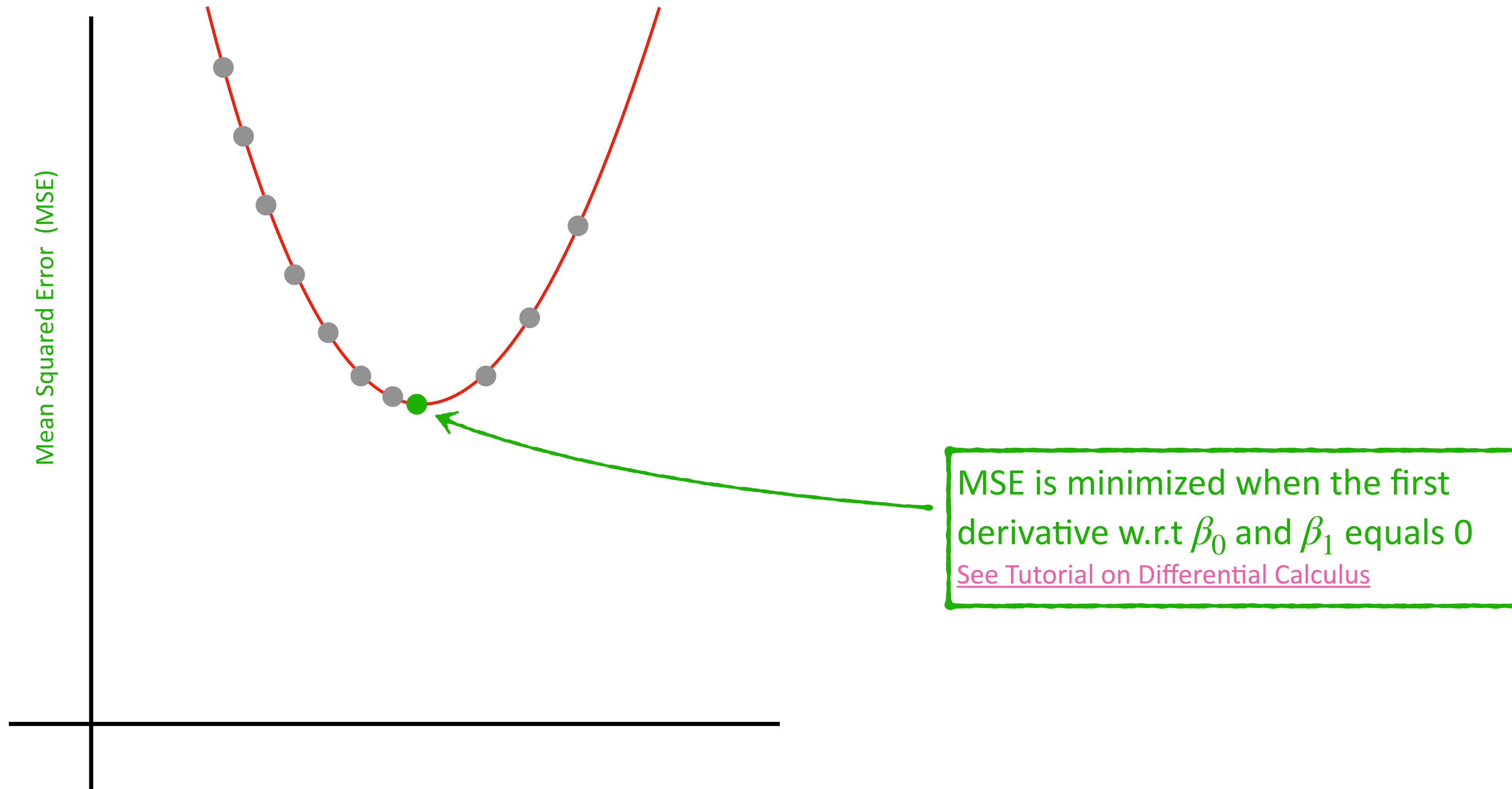
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The **Mean Squared Error (MSE)** is

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

Partial Derivatives w.r.t β_0 and β_1

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 = 0 \quad \cdots \quad eq(1)$$

$$\frac{\partial}{\partial \beta_1} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 = 0 \quad \cdots \quad eq(2)$$

MSE is minimized when the first derivative w.r.t β_0 and β_1 equals 0

[See Tutorial on Differential Calculus](#)

Mean Squared Error (MSE) for various values of β_0 and β_1

Simple Linear Regression

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Solving both equations for β_0 and β_1
we get...

MSE is minimized when the first derivative w.r.t β_0 and β_1 equals 0

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Simple Linear Regression

$$\beta_0 = \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}$$

$$\beta_1 = \frac{n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2}$$

This is known as the **Closed Form Solution** for Simple Linear Regression

For the details on how the two equations are solved see [Proof of the Closed Form Solution](#)

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Simple Linear Regression

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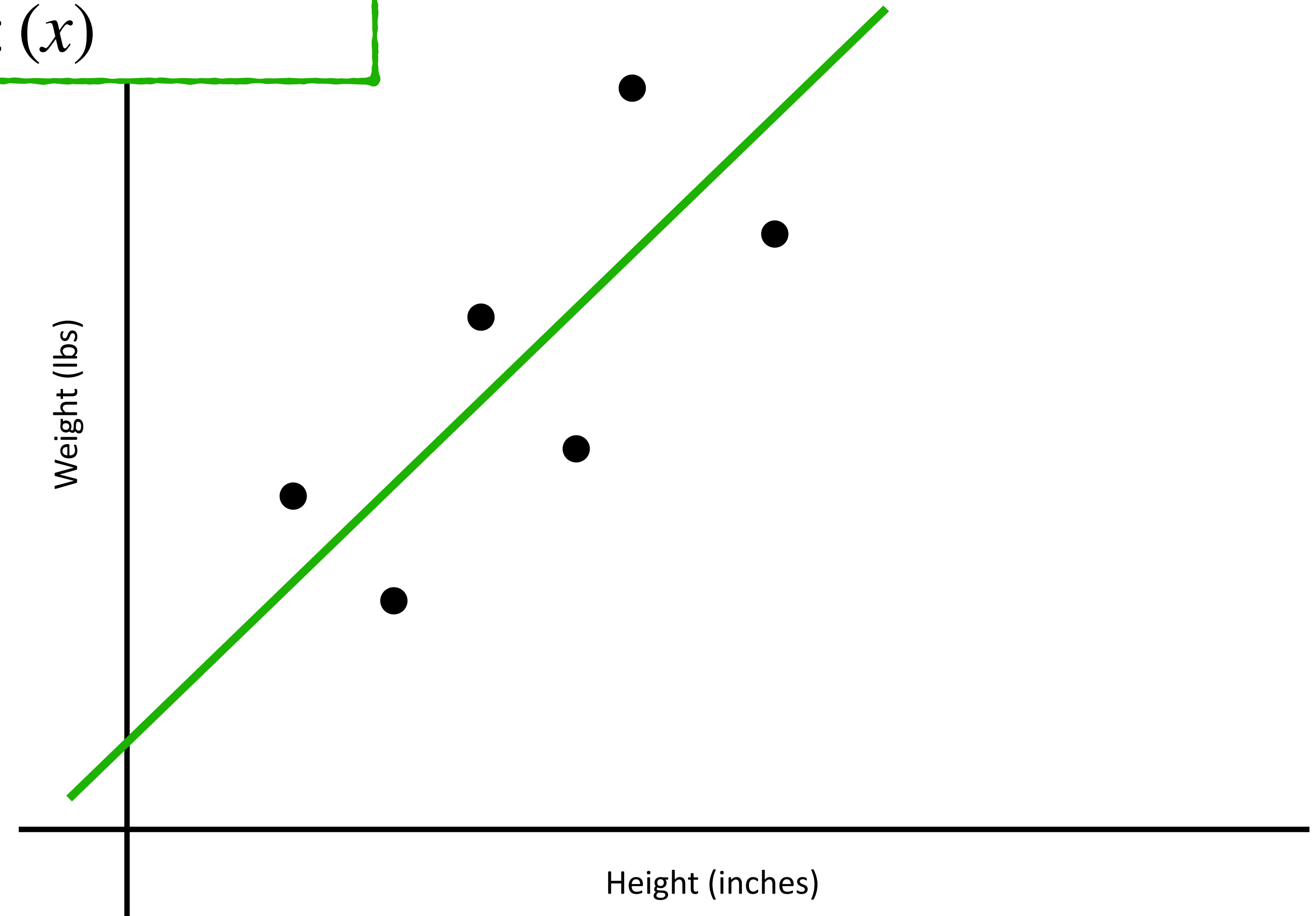
Simple Linear Regression

1 dependent variable

1 independent variable

Eg: Predict Weight ($\hat{y}$) of a person given Height (x)

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



Simple Linear Regression

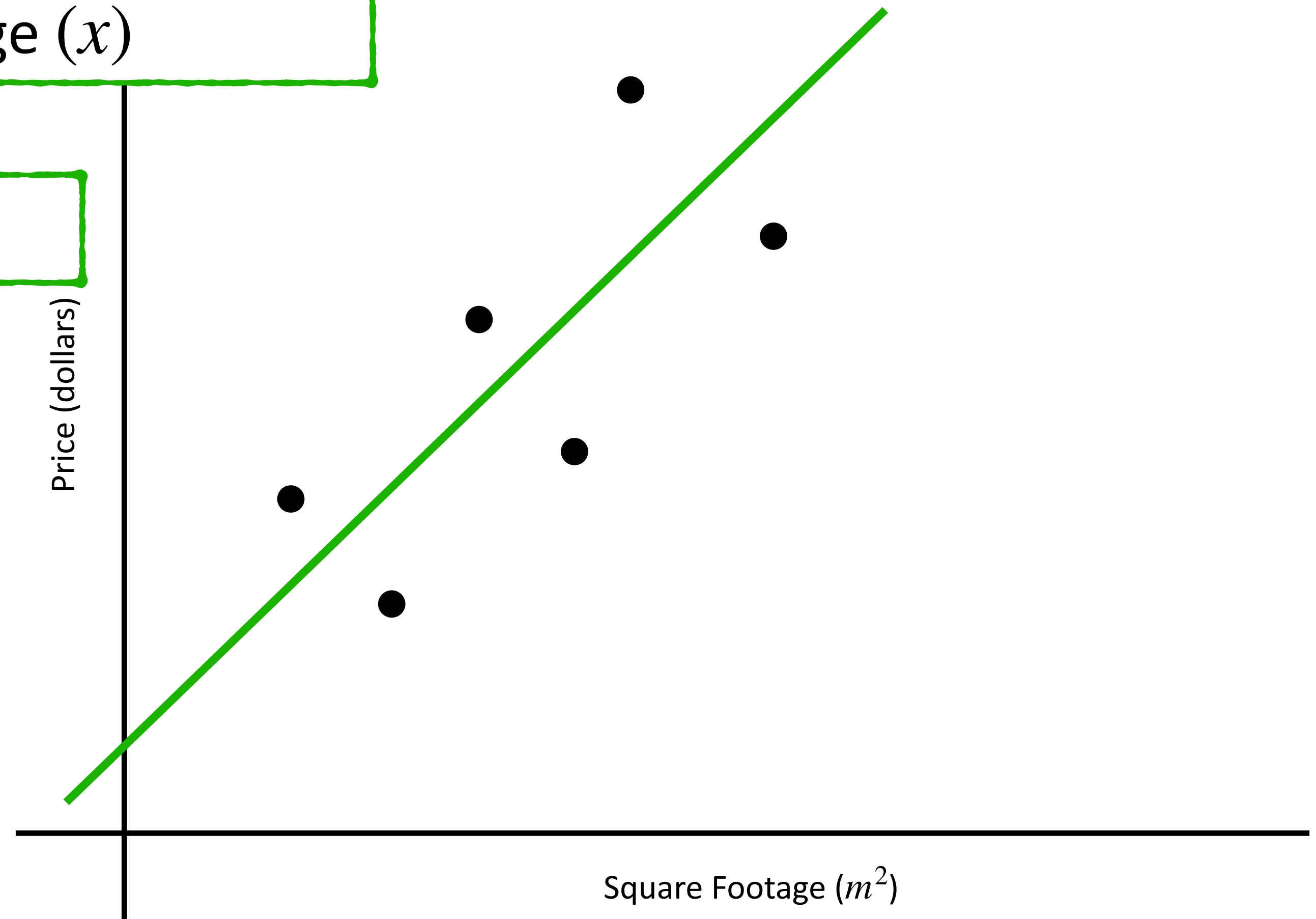
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Eg: Predict Price of a house ($\hat{y}$)
given Square Footage (x)

2 Parameters - β_0 and β_1

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Simple Linear Regression

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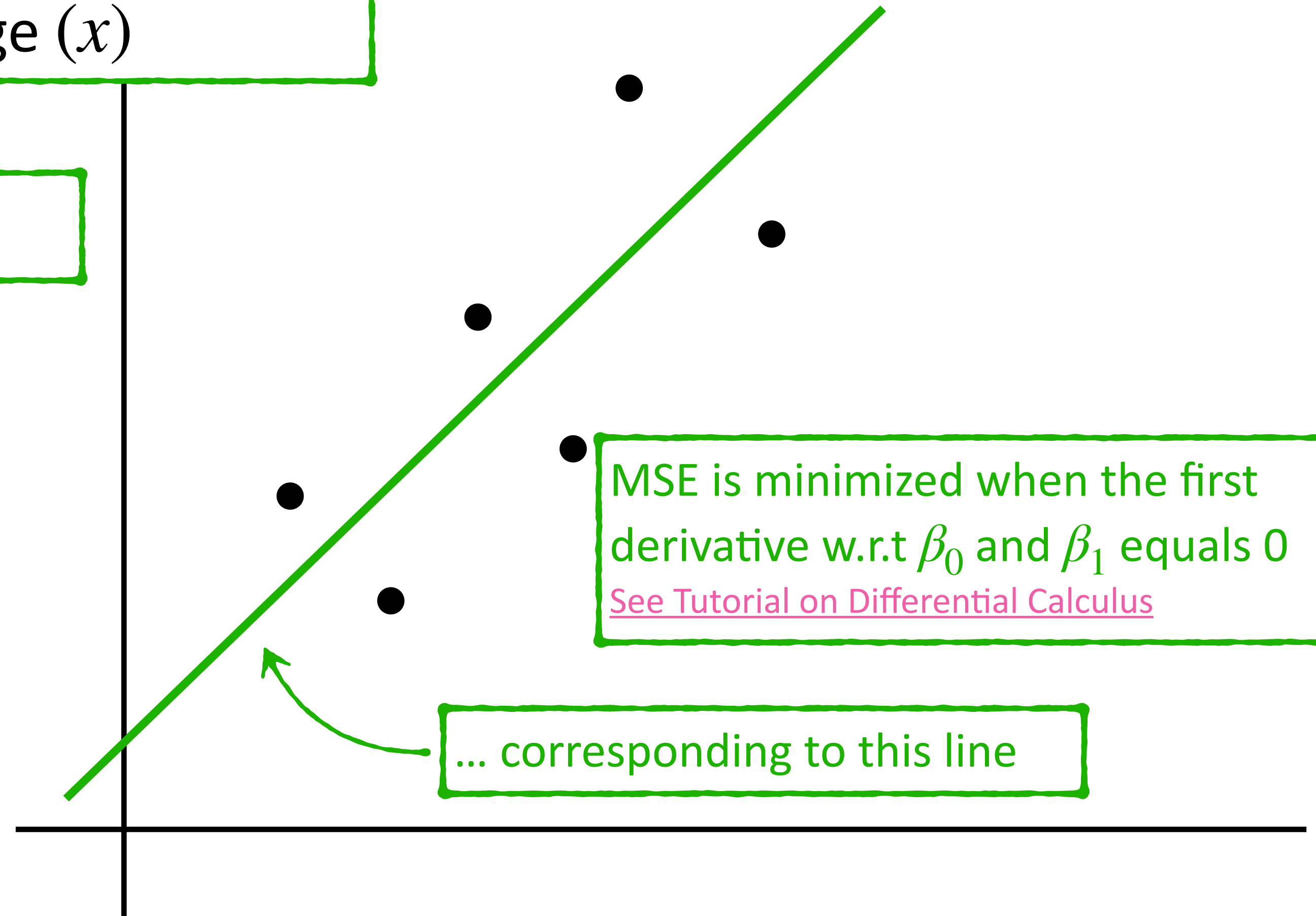
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Goal: Find the values of β_0 and β_1 that minimizes the Mean Squared Error (MSE)

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

MSE is minimized when the first derivative w.r.t β_0 and β_1 equals 0
[See Tutorial on Differential Calculus](#)

... corresponding to this line



Simple Linear Regression

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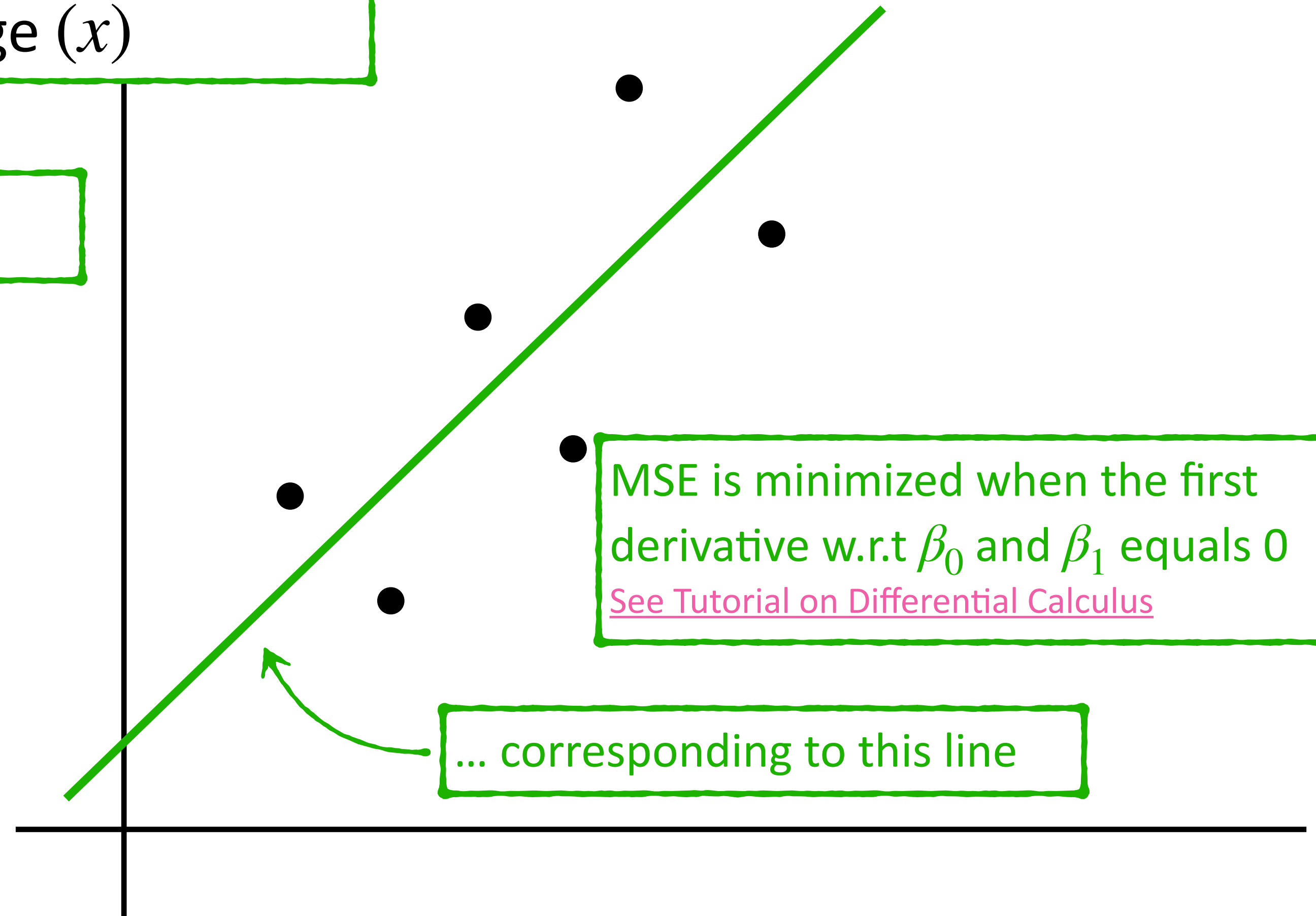
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... corresponding to this line

... and that's the line of best fit

1 dependent variable

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

$$\beta_0 = \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}$$

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Simple Linear Regression

We solve for **two** Parameters - β_0 and β_1
- by solving **two** equations...

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 = 0 \quad \cdots \quad eq(1)$$

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Simple Linear Regression

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

Predict Price ($\hat{y}$) of a house given
Square Footage (x)

Simple Linear Regression

- 1 dependent variable $\hat{y}$
- 1 independent variable x
- 2 Parameters - β_0 and β_1
- We solve 2 equations to find the values of β_0 and β_1

Multiple Regression

What if we wanted to predict price of a house, given Square Footage **and** Number of bedrooms?

Multiple Regression

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

1 dependent variable $\hat{y}$

2 independent variables

x_1 represents the square footage

x_2 represents the number of bedrooms

What if we wanted to predict price of a house, given Square Footage **and** Number of bedrooms?

Multiple Regression

1 dependent variable $\hat{y}$

2 independent variables

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$\hat{x}_1$ represents the square footage

$\hat{x}_2$ represents the number of bedrooms

Goal: Find the values of β_0 , β_1 and β_2 that minimizes the Sum of Squared Residuals (SSR)

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

MSE is minimized when the first derivative w.r.t β_0 , β_1 and β_2 equals 0

[See Tutorial on Differential Calculus](#)

We solve for **three** Parameters - β_0 , β_1 and β_2 - by solving **three** equations...

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 = 0$$

$$\frac{\partial}{\partial \beta_1} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 = 0$$

$$\frac{\partial}{\partial \beta_2} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 = 0$$

Multiple Regression

1 dependent variable $\hat{y}$

2 independent variables

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Multiple Regression

Lets generalize this...

A linear model with...

1 dependent variable $\hat{y}$

Multiple Regression

2 independent variables

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

Has 3 parameters

And a cost function...

$$\frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2$$

That can be minimized by solving 3 equations

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 = 0$$

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$$\frac{\partial}{\partial \beta_2} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 = 0$$

A linear model with...

1 dependent variable $\hat{y}$

Multiple Regression

3 independent variables

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

Has 4 parameters

And a cost function...

$$\frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - \beta_3 x_{3i})^2$$

That can be minimized by solving 4 equations

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - \beta_3 x_{3i})^2 = 0$$

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A linear model with...

1 dependent variable $\hat{y}$

Multiple Regression

$k - 1$ independent variables $x_1 \dots x_{k-1}$

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

Has k parameters

And a cost function...

$$\frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - \beta_3 x_{3i} - \dots - \beta_{k-1} x_{k-1i})^2$$

That can be minimized by solving k equations

$$\frac{\partial}{\partial \beta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - \beta_3 x_{3i} - \dots - \beta_{k-1} x_{k-1i})^2 = 0$$

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$\vdots$

$$\frac{\partial}{\partial \beta_{k-1}} \frac{1}{n} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - \beta_3 x_{3i} - \dots - \beta_{k-1} x_{k-1i})^2 = 0$$

Multiple Regression

k independent variables $x_1 \dots x_k$

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

Has $k + 1$ parameters

And a cost function

Solving k linear equations isn't practical

$$\sum_{i=0}^n (y_i - \beta_0 - \beta_1 \hat{x}_{1i} - \beta_2 \hat{x}_{2i} - \beta_3 \hat{x}_{3i} - \dots - \beta_k \hat{x}_{ki})^2$$

That can be minimized by solving $k + 1$ equations

$$\frac{\partial}{\partial \beta_n} \sum_{i=0}^n (y_i - \beta_0 - \beta_1 \hat{x}_{1i} - \beta_2 \hat{x}_{2i} - \beta_3 \hat{x}_{3i} - \dots - \beta_k \hat{x}_{ki})^2 = 0$$

$$- \beta_k \hat{x}_{ki})^2 = 0$$

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Lets use a Matrix

Simple Linear Regression

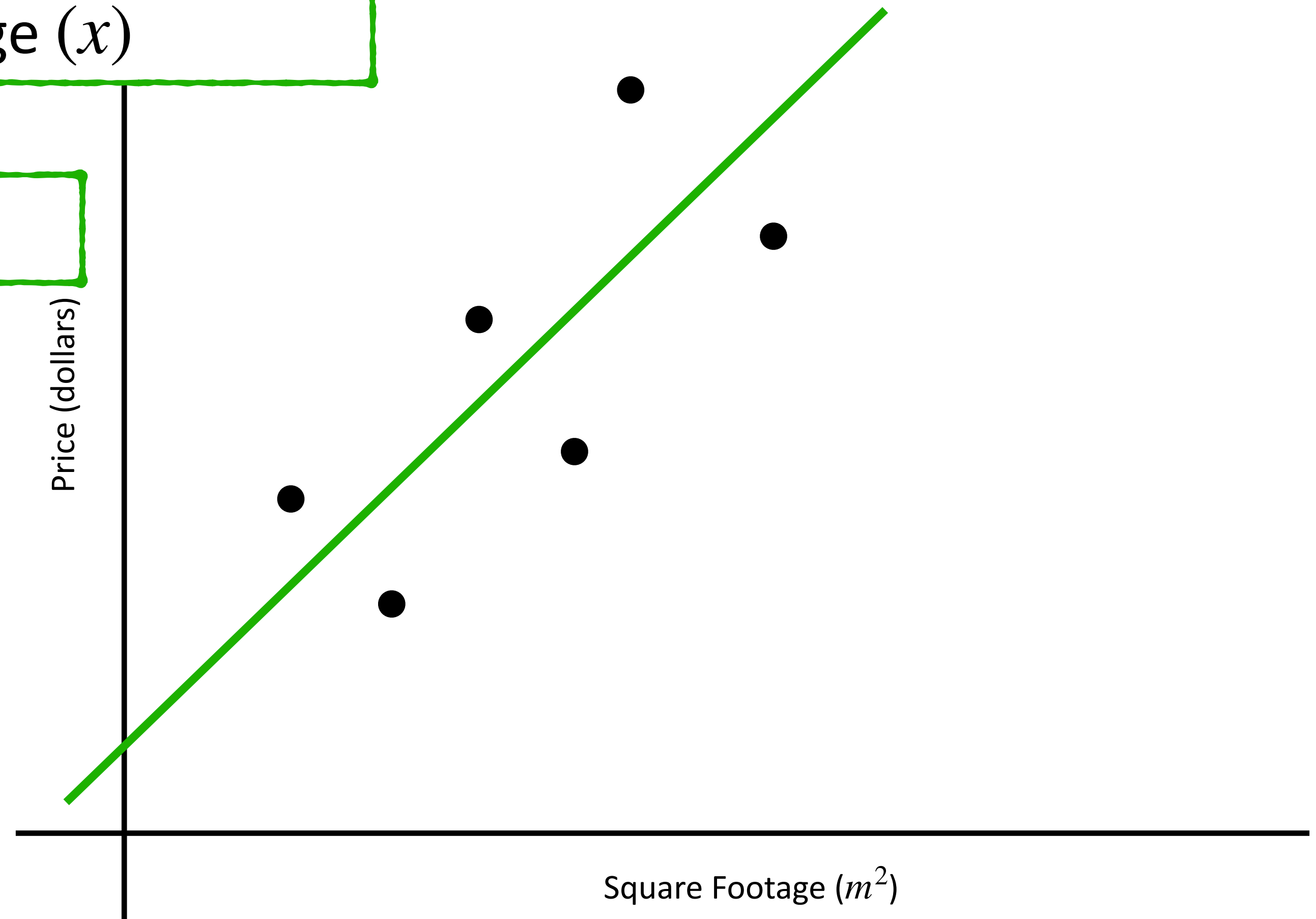
1 dependent variable

1 independent variable

Eg: Predict Price of a house ($\hat{y}$)
given Square Footage (x)

2 Parameters - β_0 and β_1

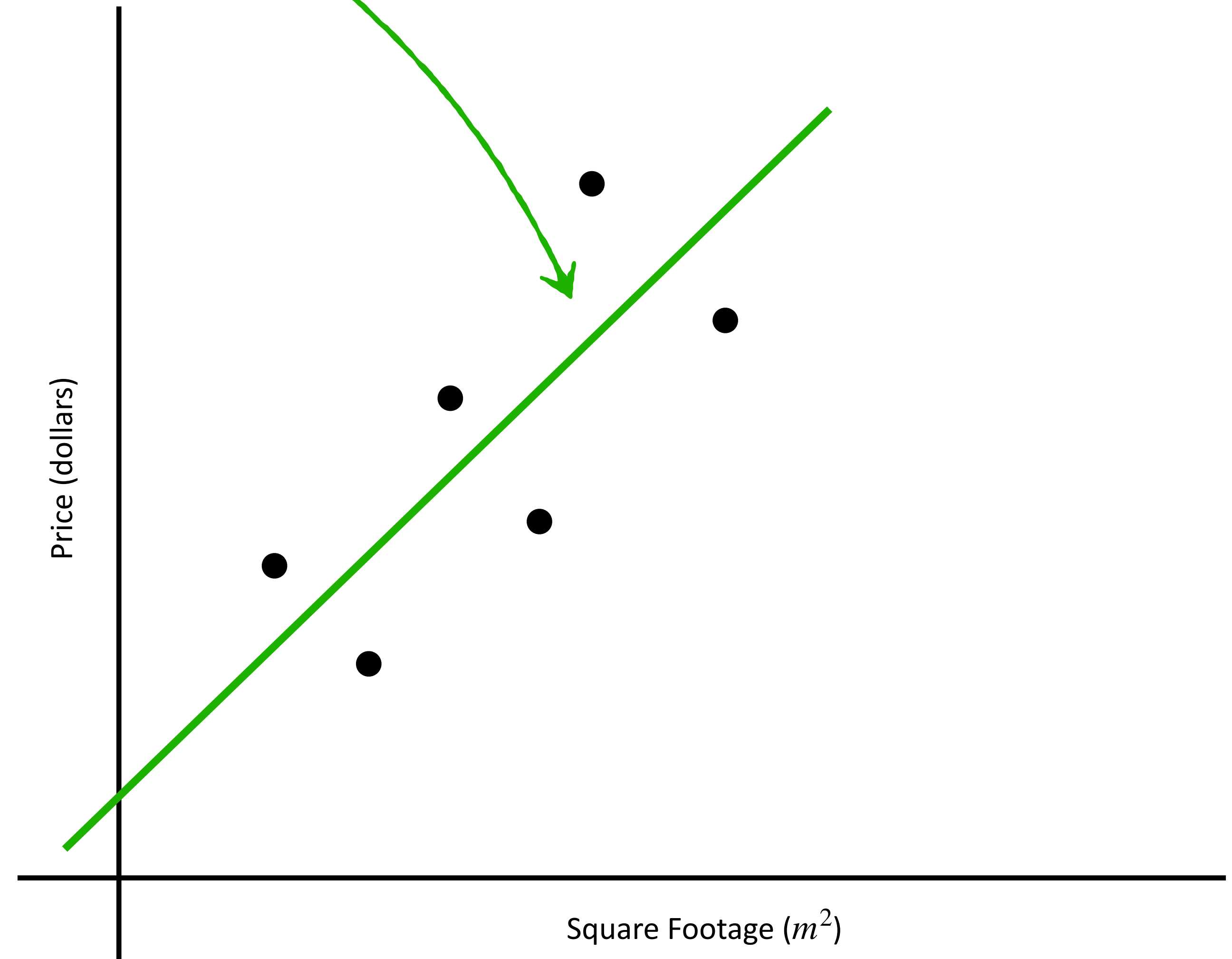
$$\hat{y} = \beta_0 + \beta_1 x$$



Simple Linear Regression

Line of Best Fit...

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



Simple Linear Regression

Line of Best Fit...

...can be represented as a matrix

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

$$\hat{y}_1 = 1 \times \beta_0 + x_1 \times \beta_1$$

$$\hat{y}_2 = 1 \times \beta_0 + x_2 \times \beta_1$$

$$\hat{y}_3 = 1 \times \beta_0 + x_3 \times \beta_1$$

⋮

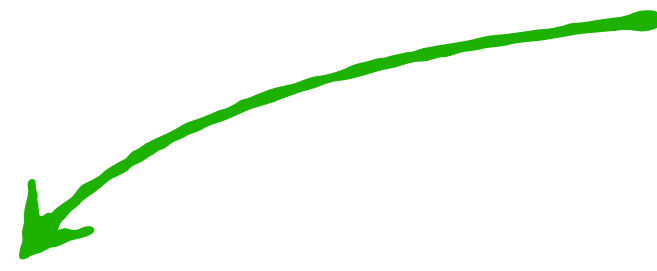
$$\hat{y}_n = 1 \times \beta_0 + x_n \times \beta_1$$

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

- 1 dependent variable $\hat{y}$
- 1 independent variables x
- 2 parameters - β_0 and β_1

Simple Linear Regression

Linear Model in 2 Dimensions



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

$$\hat{y}_1 = 1 \times \beta_0 + x_1 \times \beta_1$$

$$\hat{y}_2 = 1 \times \beta_0 + x_2 \times \beta_1$$

$$\hat{y}_3 = 1 \times \beta_0 + x_3 \times \beta_1$$

$\vdots$

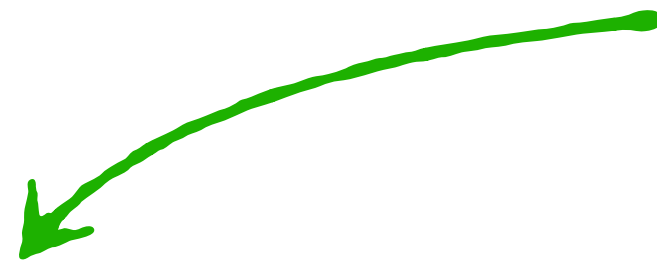
$$\hat{y}_n = 1 \times \beta_0 + x_n \times \beta_1$$

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

- 1 dependent variable $\hat{y}$
- 1 independent variables x
- 2 parameters - β_0 and β_1

Multiple Regression

Linear Model in 3 Dimensions



$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\hat{y}_1 = 1 \times \beta_0 + x_{11} \times \beta_1 + x_{21} \times \beta_2$$

$$\hat{y}_2 = 1 \times \beta_0 + x_{12} \times \beta_1 + x_{22} \times \beta_2$$

$$\hat{y}_3 = 1 \times \beta_0 + x_{13} \times \beta_1 + x_{23} \times \beta_2$$

$\vdots$

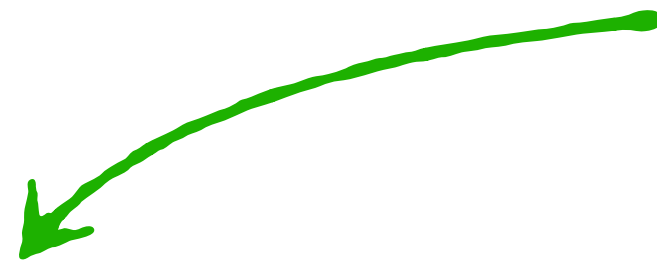
$$\hat{y}_n = 1 \times \beta_0 + x_{1n} \times \beta_1 + x_{2n} \times \beta_2$$

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ 1 & x_{13} & x_{23} \\ \vdots & & \\ 1 & x_{1n} & x_{2n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

- 1 dependent variable $\hat{y}$
- 2 independent variables x_1 and x_2
- 3 parameters - β_0 , β_1 and β_2

Multiple Regression

Linear Model in 4
Dimensions



$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

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

- 1 dependent variable $\hat{y}$
- 3 independent variables x_1, x_2 and x_3
- 4 parameters - $\beta_0, \beta_1, \beta_2$ and β_3

Multiple Regression

Linear Model in k
Dimensions

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

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

- 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

Linear Model in k
Dimensions

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

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

$\hat{Y}$ is a column vector
and X is a matrix

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

- 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

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

Given a matrix (Y)
of observations

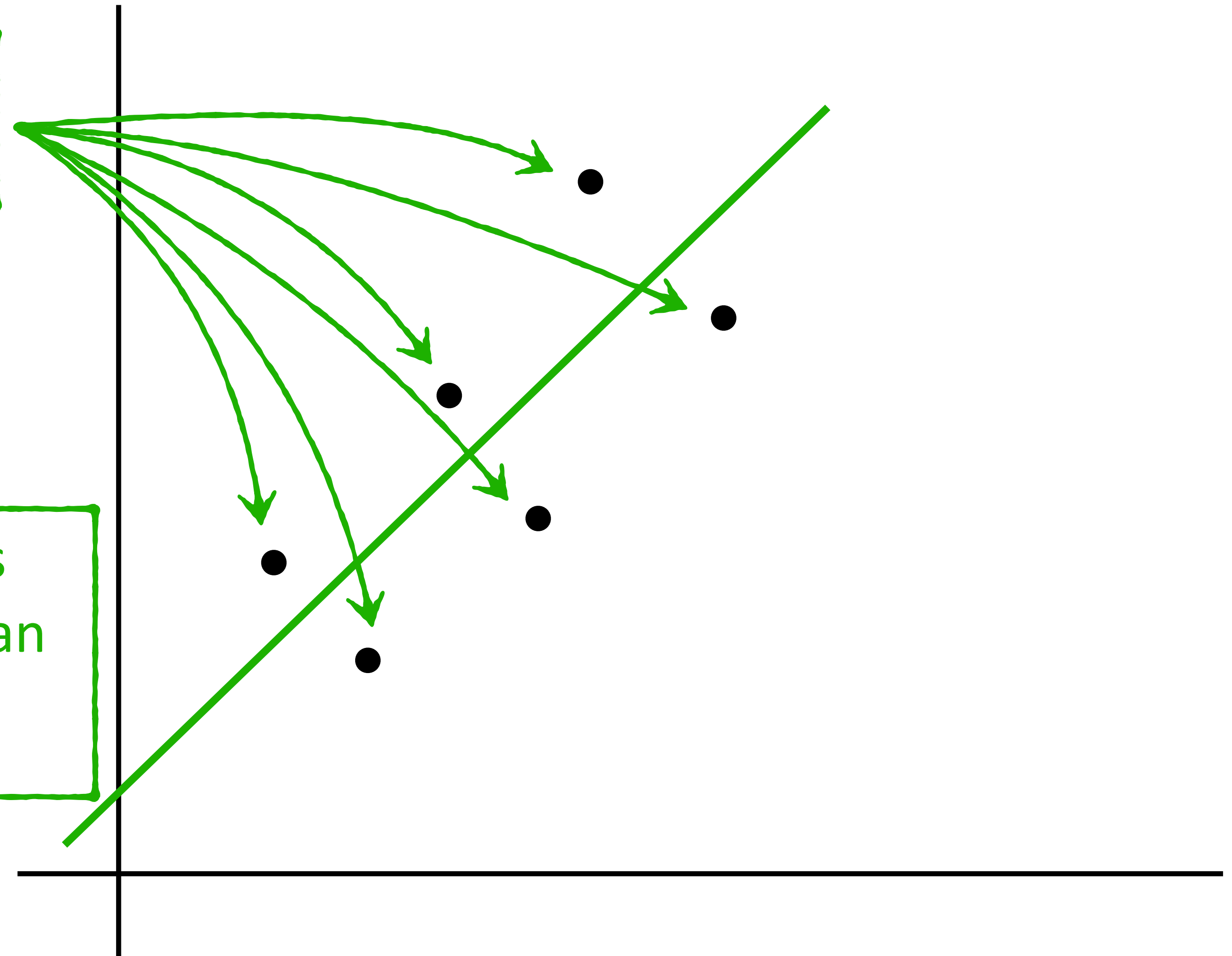
$$\hat{Y} = X\beta$$

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 Vectors & Matrices](#)



Multiple Regression

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

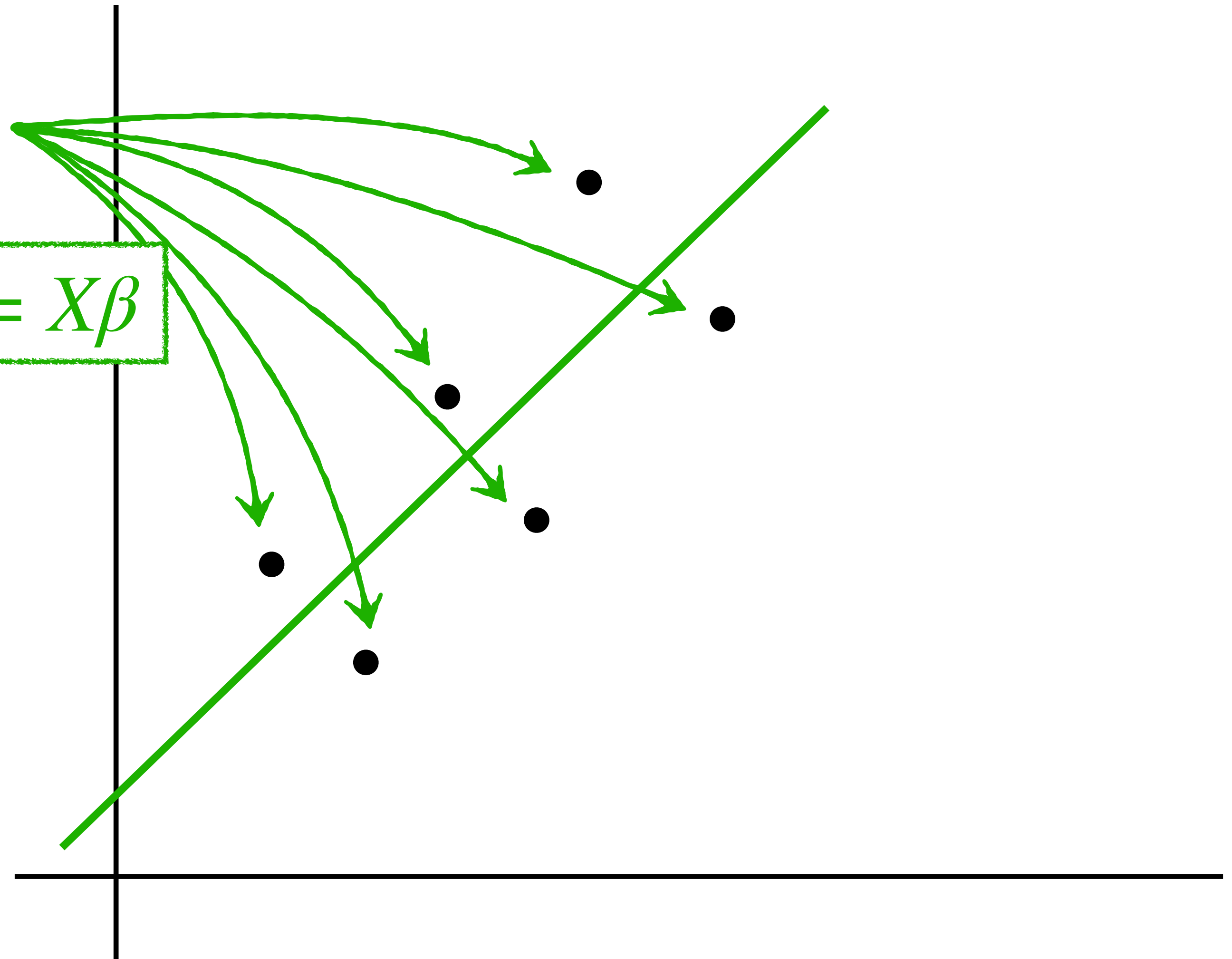
$$\hat{Y} = X\beta$$

The **Mean Squared Error (MSE)**

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

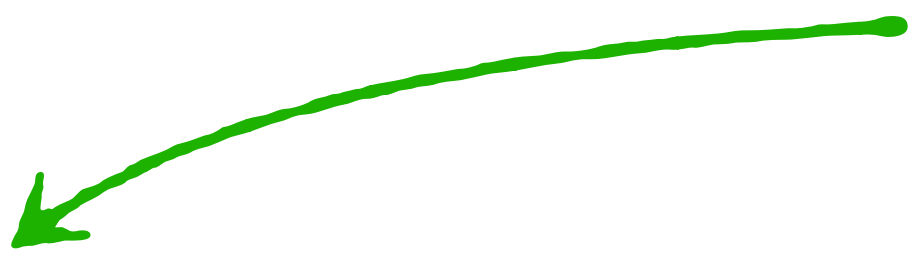
Given a matrix (Y)
of observations

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



Multiple Regression

Linear Model in k
Dimensions



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

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

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

The Problem Statement:

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

Multiple Regression

The Problem Statement:

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

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

This is the cost function (aka loss function) that we must minimize.

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

We take the partial derivative and set it = 0

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

Solving for β

For the details of the derivation see the tutorial on [Derivation of the Matrix Form for Multiple Regression](#)

The Problem Statement:

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

Solution:

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

This is the **Closed form solution** for **Multiple Regression**. However this requires inverting a matrix which is not always possible.

For more details on the reasons why see the [tutorial on Vectors & Matrices](#)

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.

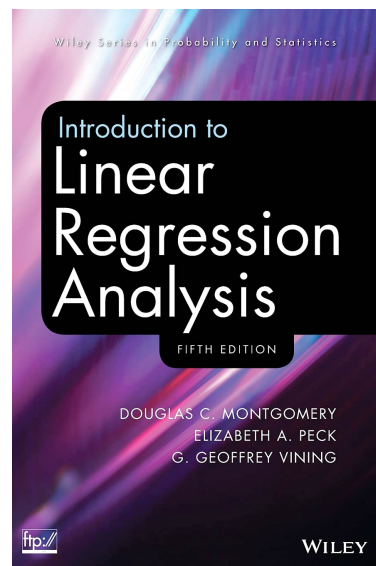
Multiple Regression: Deriving the Matrix Form ↗

A proof of the closed form matrix representation of the multiple regression model. This closed form represents a linear model with $k + 1$ parameters and solves for the matrix β . This requires a matrix inverse that is not always possible.

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>