Gradient DescentSimple Linear Regression using Gradient Descent

Rahul Singh rsingh@arrsingh.com

Problem Statement: Given a set of data points in \mathbb{R}^2 , $(x_1, y_1), (x_2, y_2), (x_0, y_0) \dots (x_n, y_n),$ find the line that best fits the data

Simple Linear Regression

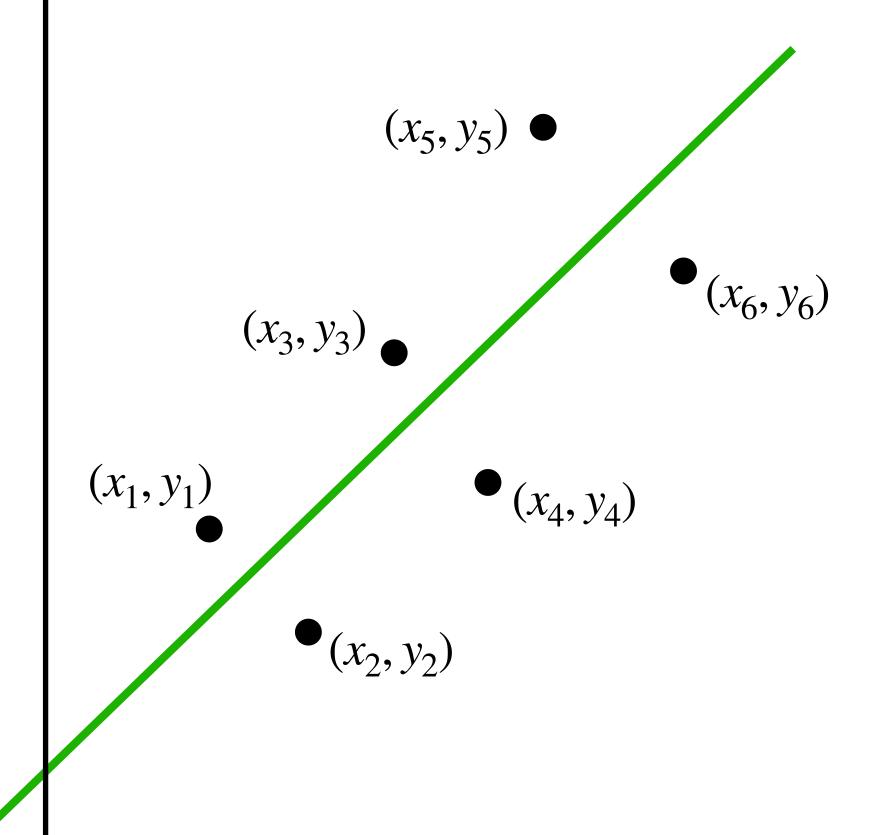
$$(x_{5}, y_{5}) \bullet$$
 $(x_{3}, y_{3}) \bullet$
 $(x_{1}, y_{1}) \bullet (x_{4}, y_{4})$
 $\bullet (x_{2}, y_{2})$

Height (inches)

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

Simple Linear Regression



Height (inches)

Problem Statement: Given a set of data points in ${\bf R}^2$,

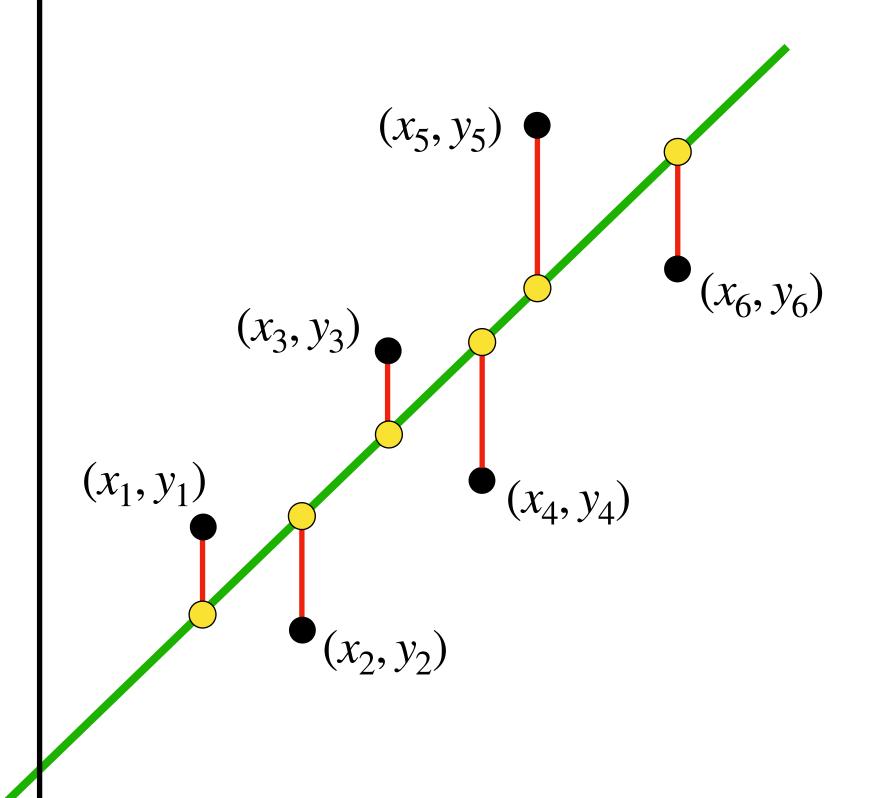
$$(x_1, y_1), (x_2, y_2), (x_0, y_0) \dots (x_n, y_n),$$
 find the line that minimizes the Mean Squared Error (MSE)

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

Mean Squared Error (MSE)

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

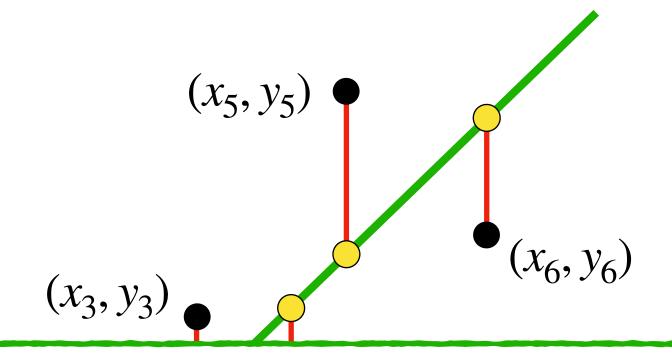
Simple Linear Regression



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$$(x_1, y_1), (x_2, y_2), (x_0, y_0) \dots (x_n, y_n),$$
 find the line that minimizes the

Mean Squared Error (MSE)



Here we divide the total squared error by 2n (rather than n) because it will make the first derivative simpler

 (x_2, y_2)

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

Mean Squared Error (MSE)

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

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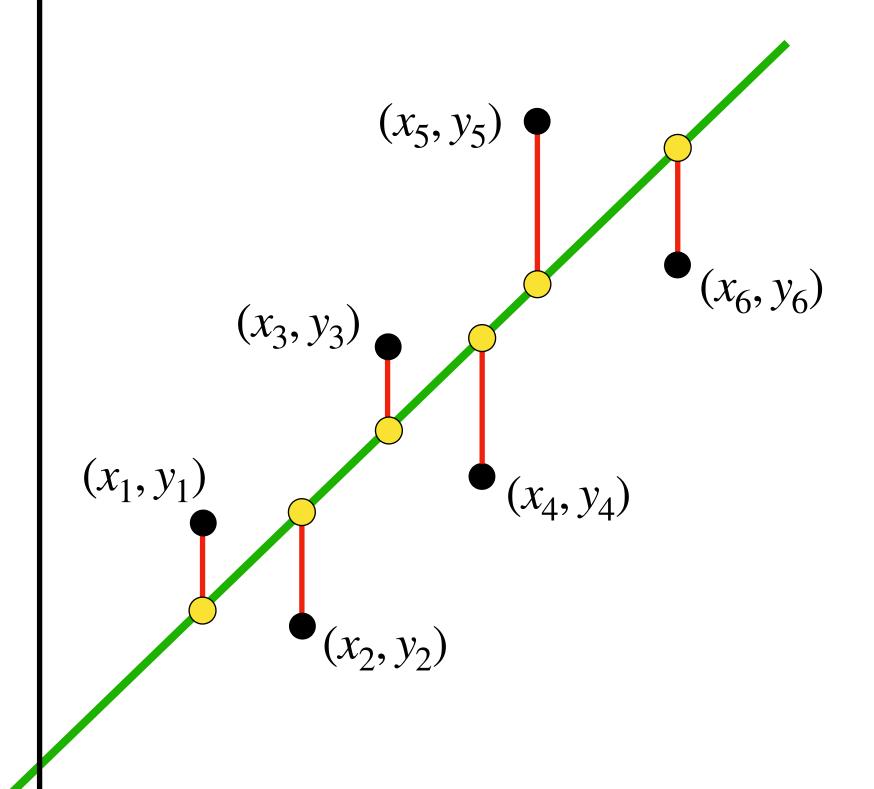
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Simple Linear Regression



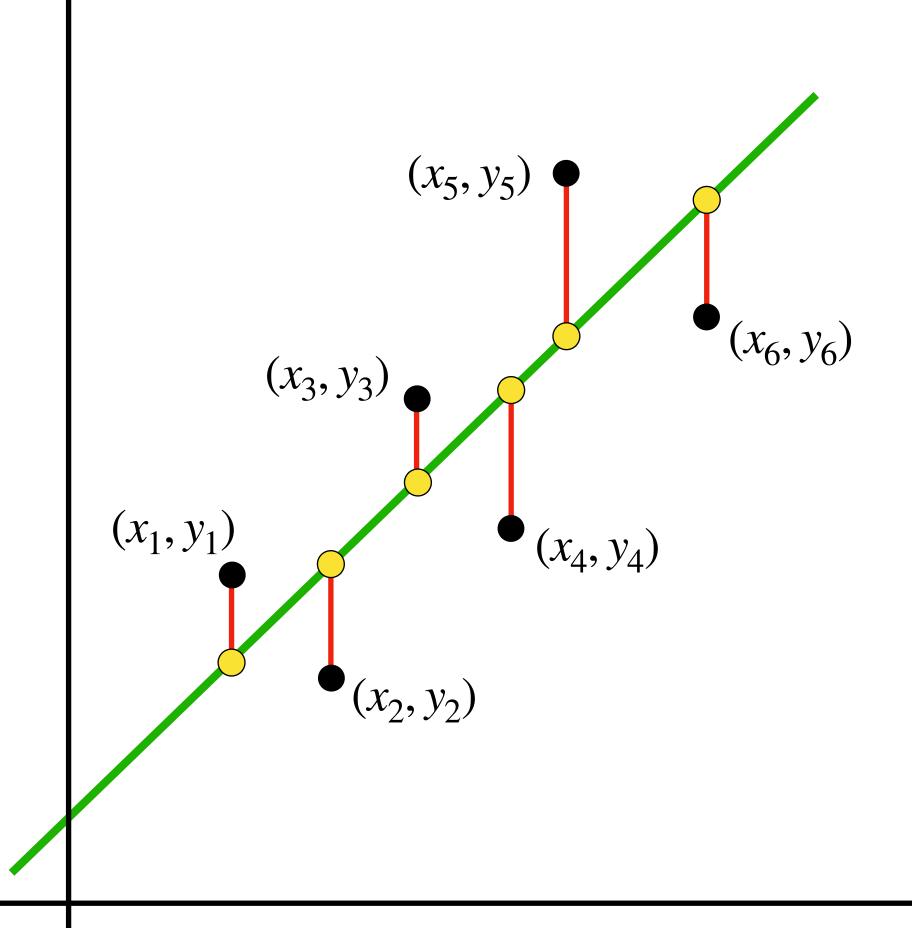
The Problem Statement:

Simple Linear Regression: Find the values of eta_0 and eta_1 such that the Mean Squared Error (MSE) is minimized.

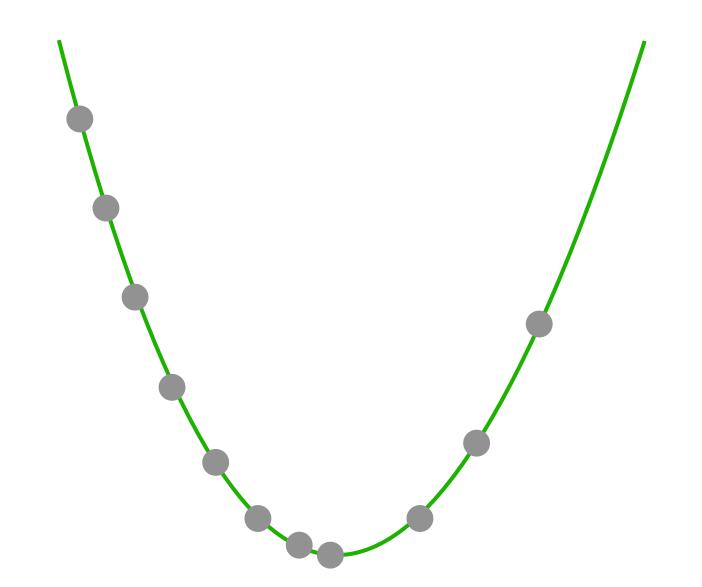
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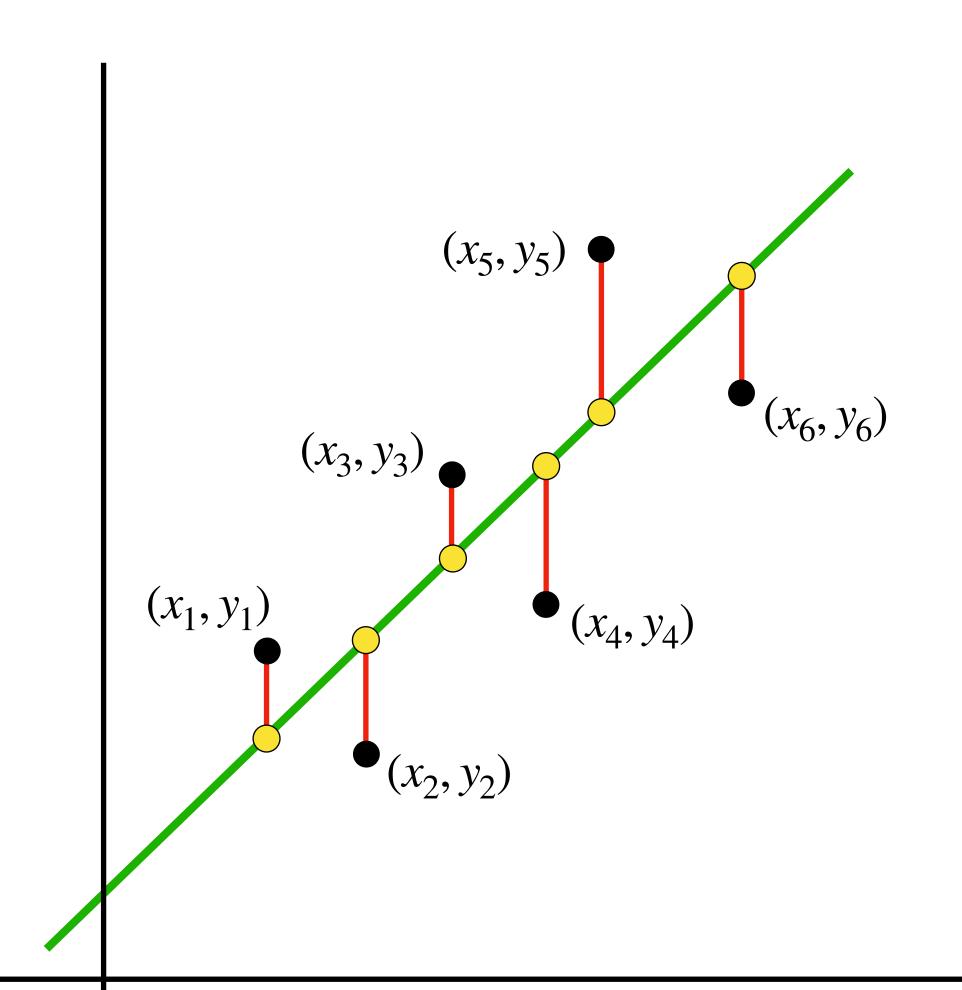


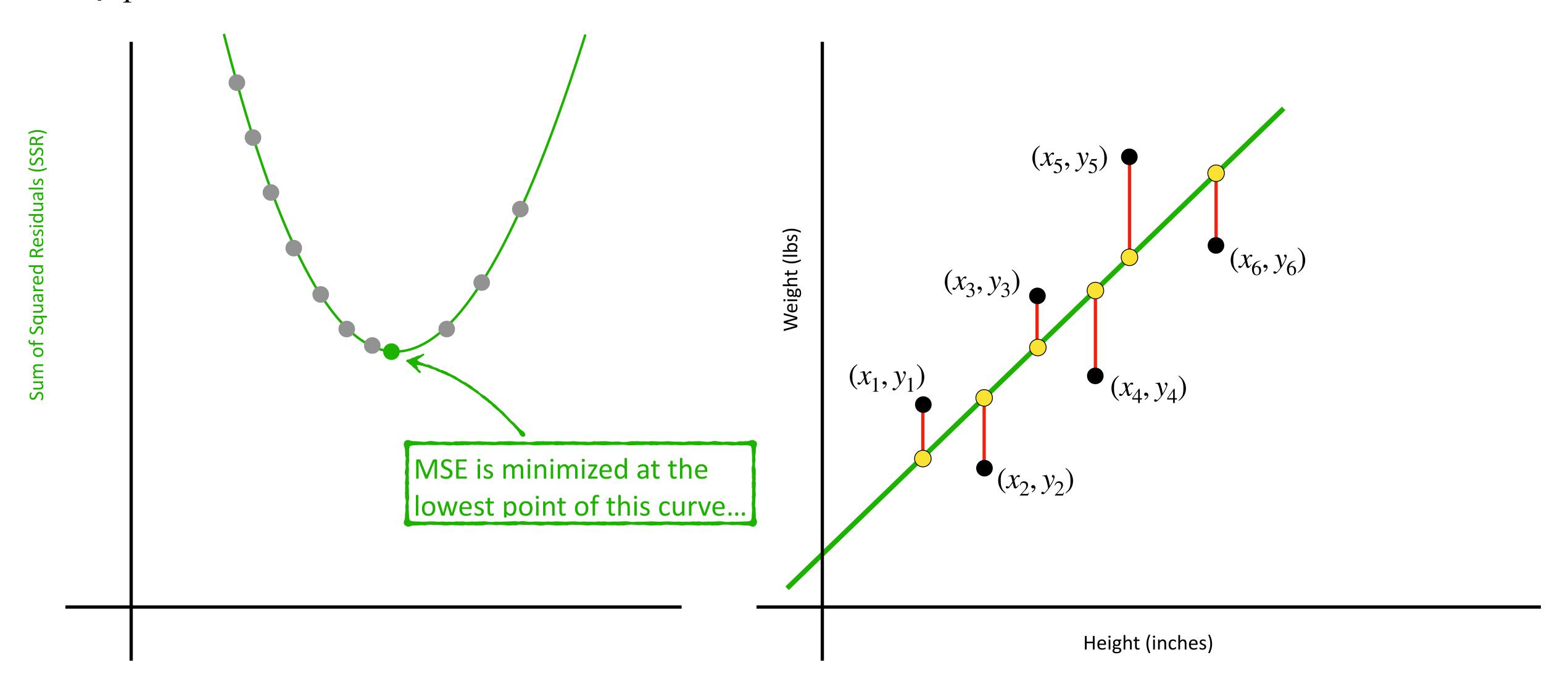
Simple Linear Regression

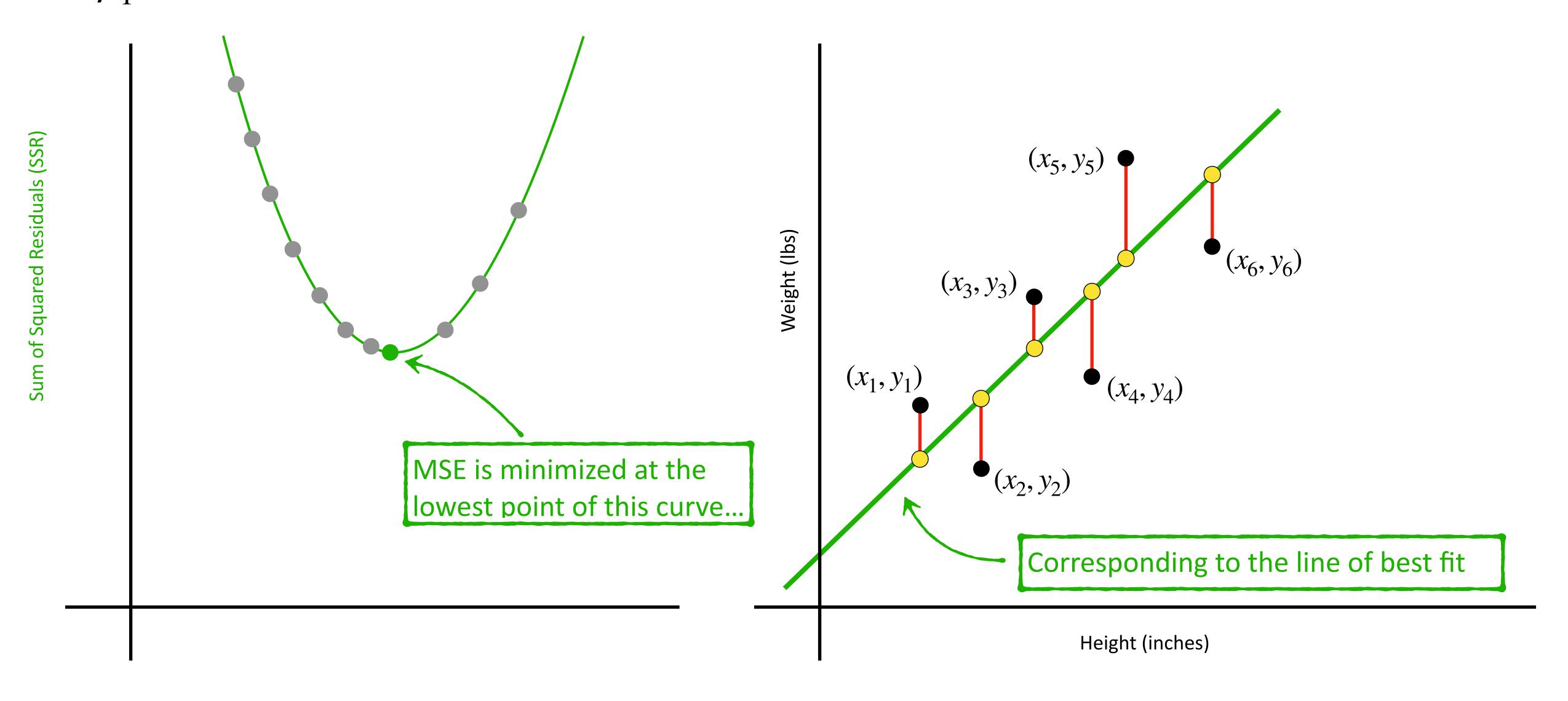


The Mean Squared Error (MSE) is

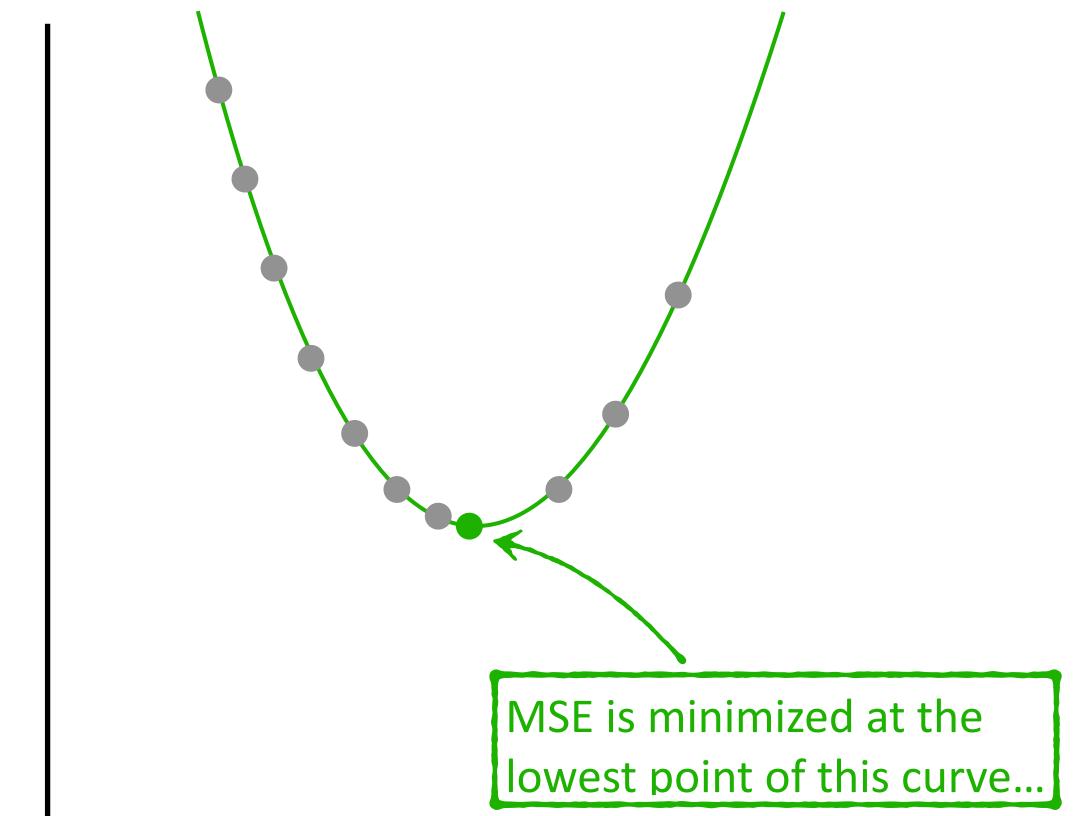
$$\frac{1}{2n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$







Residuals (SSR)



The Mean Squared Error (MSE) is...

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

The first derivative w.r.t β_0 and β_1 is...

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

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

... when the first derivative w.r.t β_0 and β_1 equals 0 See Tutorial on Differential Calculus

We can find the optimal values for eta_0 and eta_1 by solving these two equations...

... as we did in the tutorial on Simple Linear Regression

This time we will use **Gradient Descent** to find the optimal values of β_0 and β_1

The Mean Squared Error (MSE) is...

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

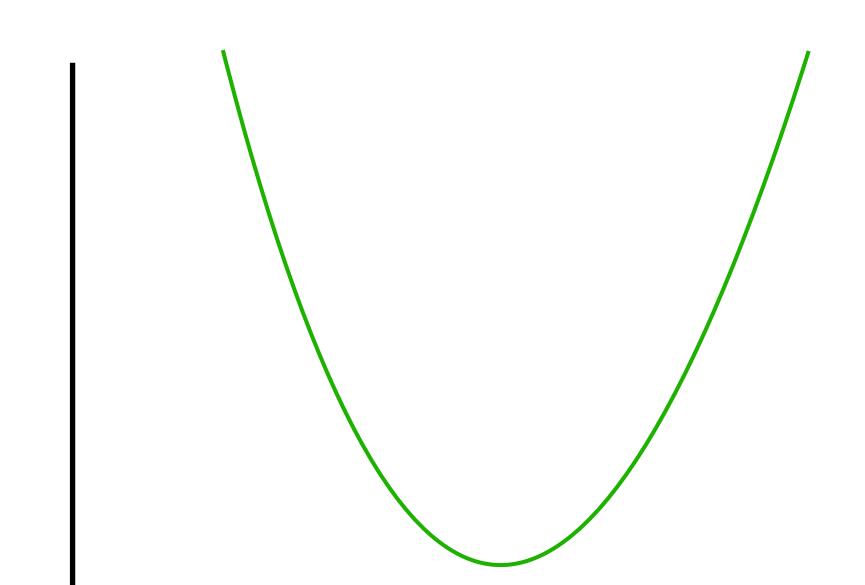
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Gradient Descent

Gradient Descent: Basic Concepts



The Mean Squared Error (MSE) is...

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

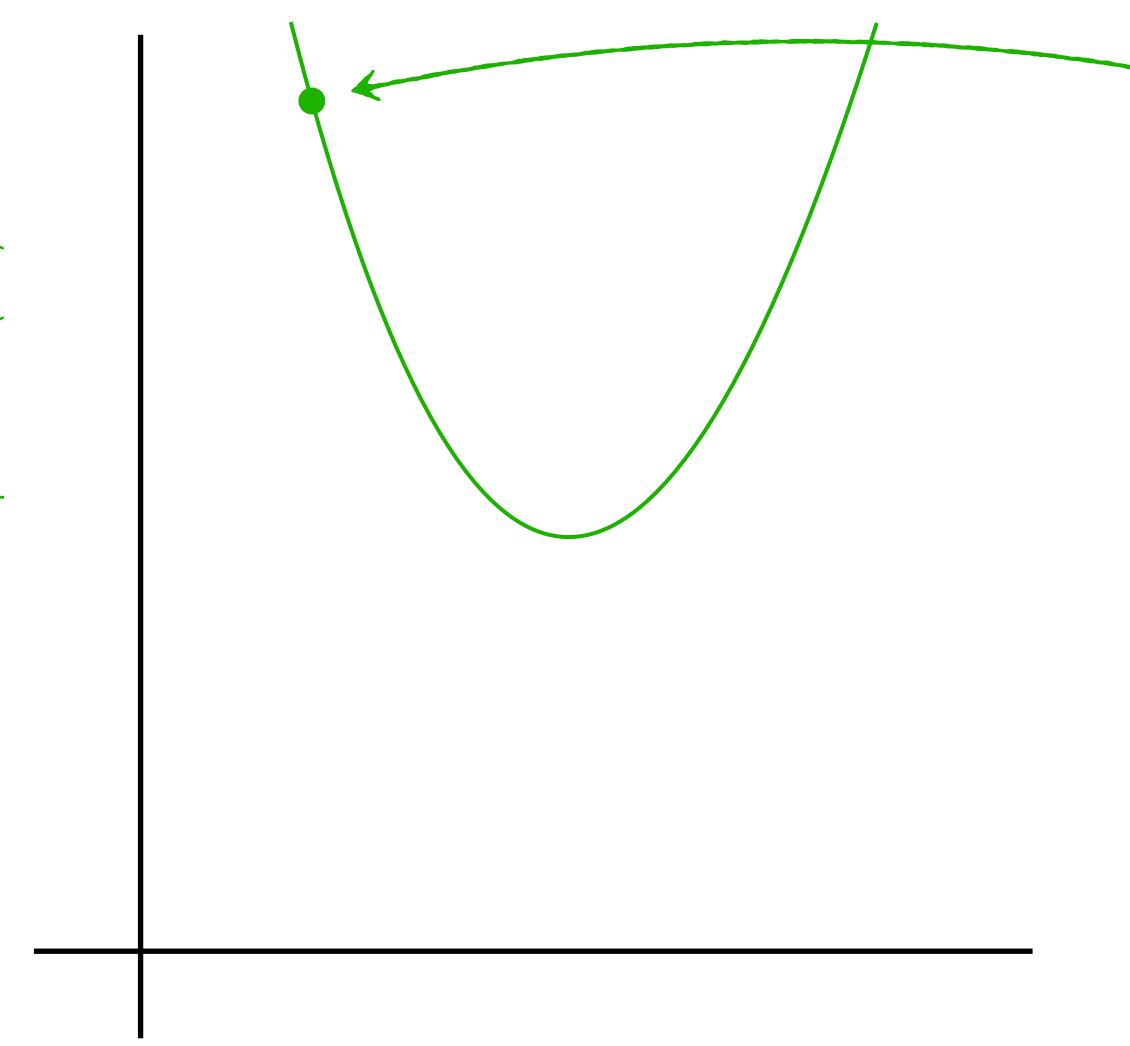
Observed Values

Gradient Descent

Every point on this curve is the MSE for different values of β_0 and β_1

For any given point on this curve, we can calculate the slope...

... the slope is the first derivative w.r.t eta_0 and eta_1



Gradient Descent

Gradient Descent: Basic Concept

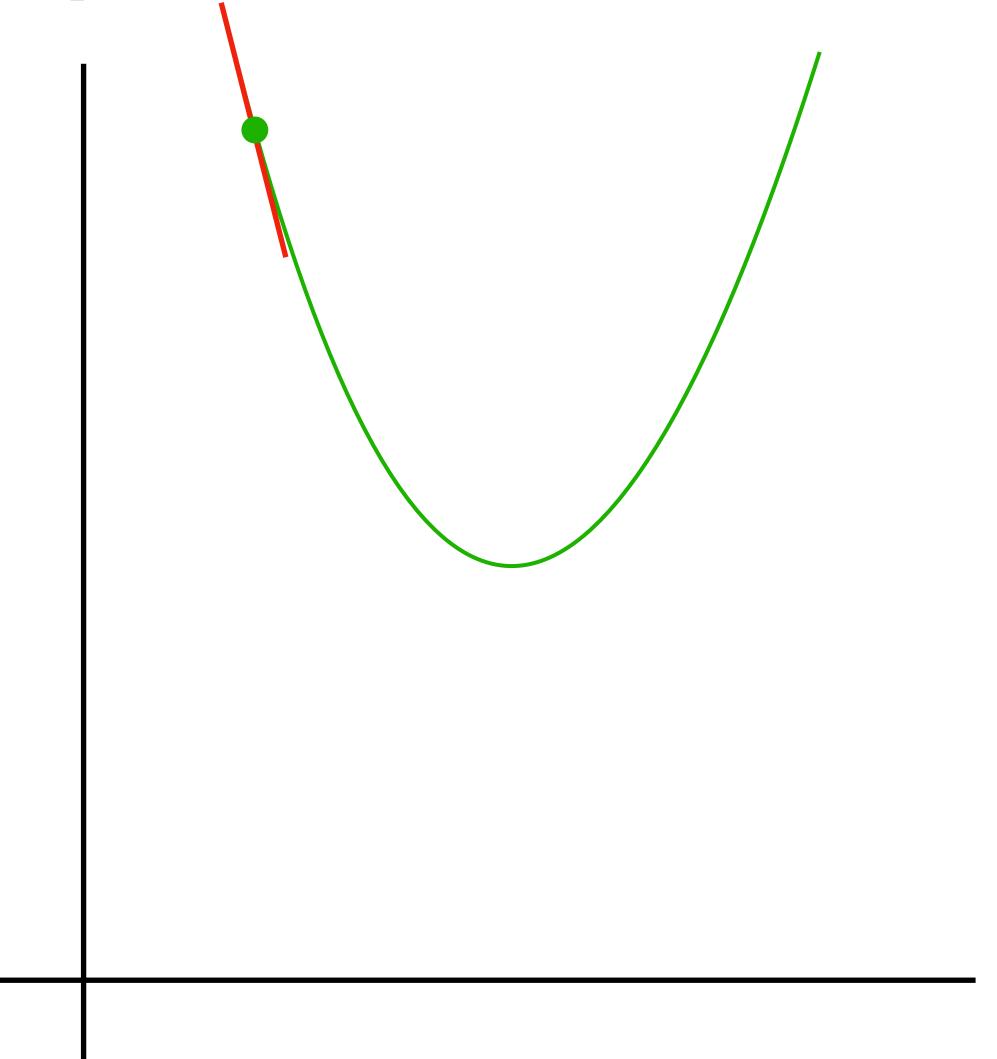
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Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

Step 3: Calculate a step size that is proportional to the slope

Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

and β_1 follows this curve



Gradient Descent

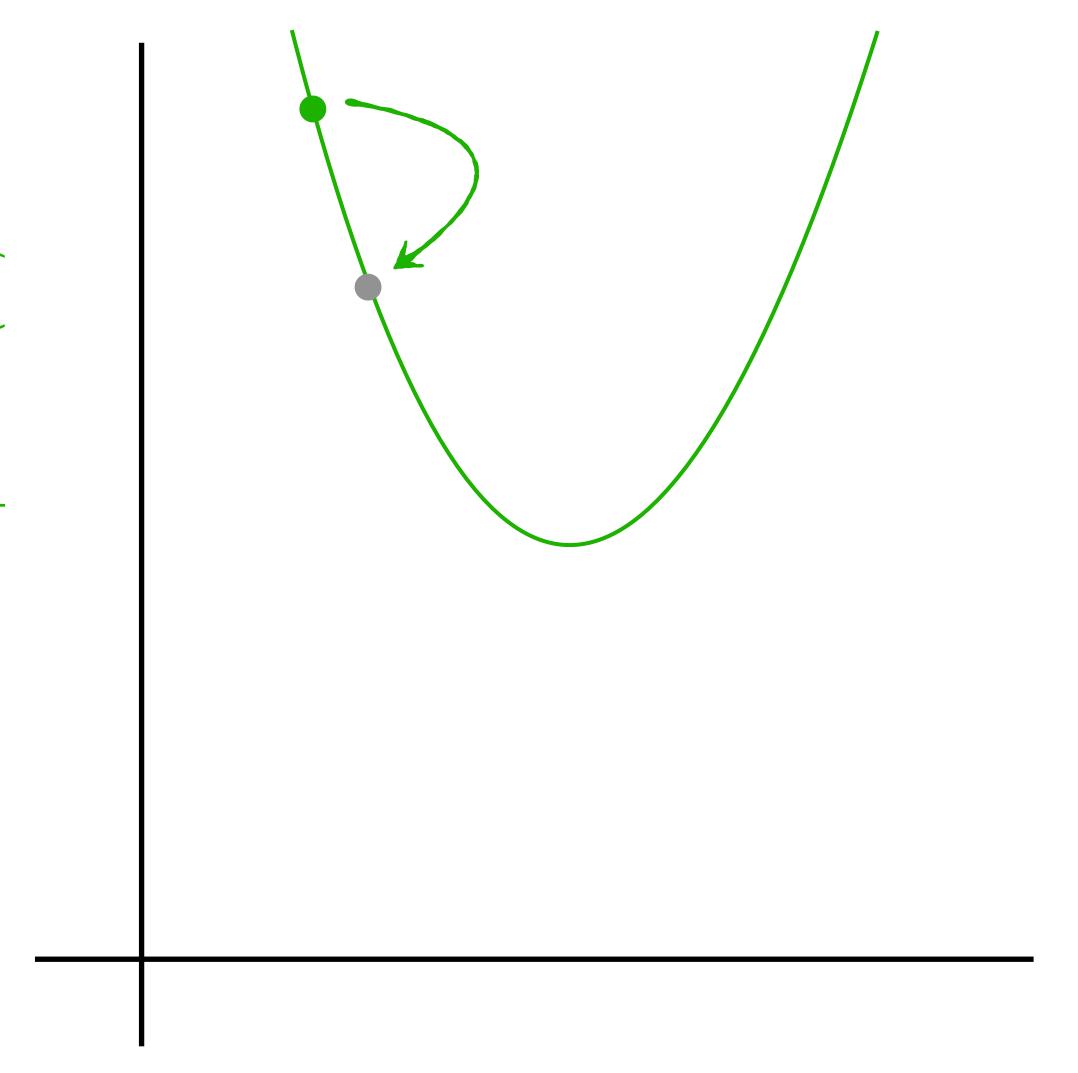
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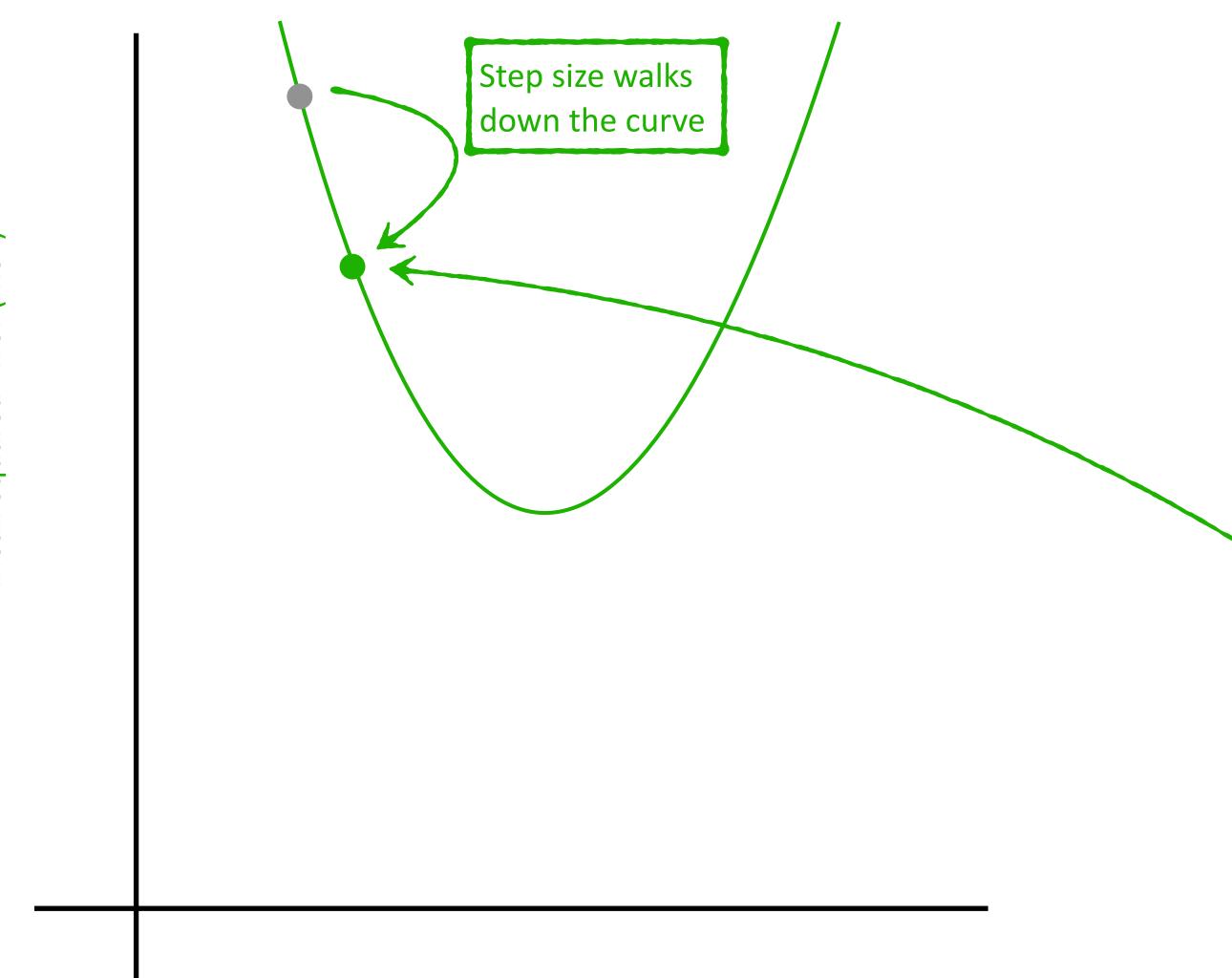
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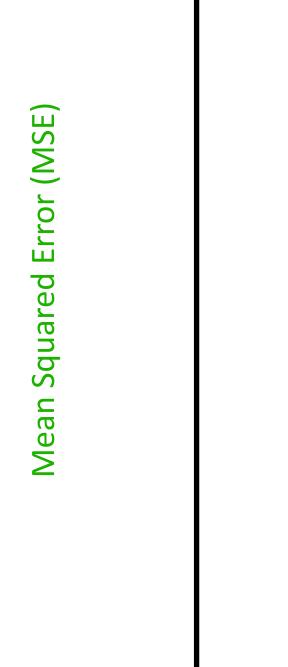
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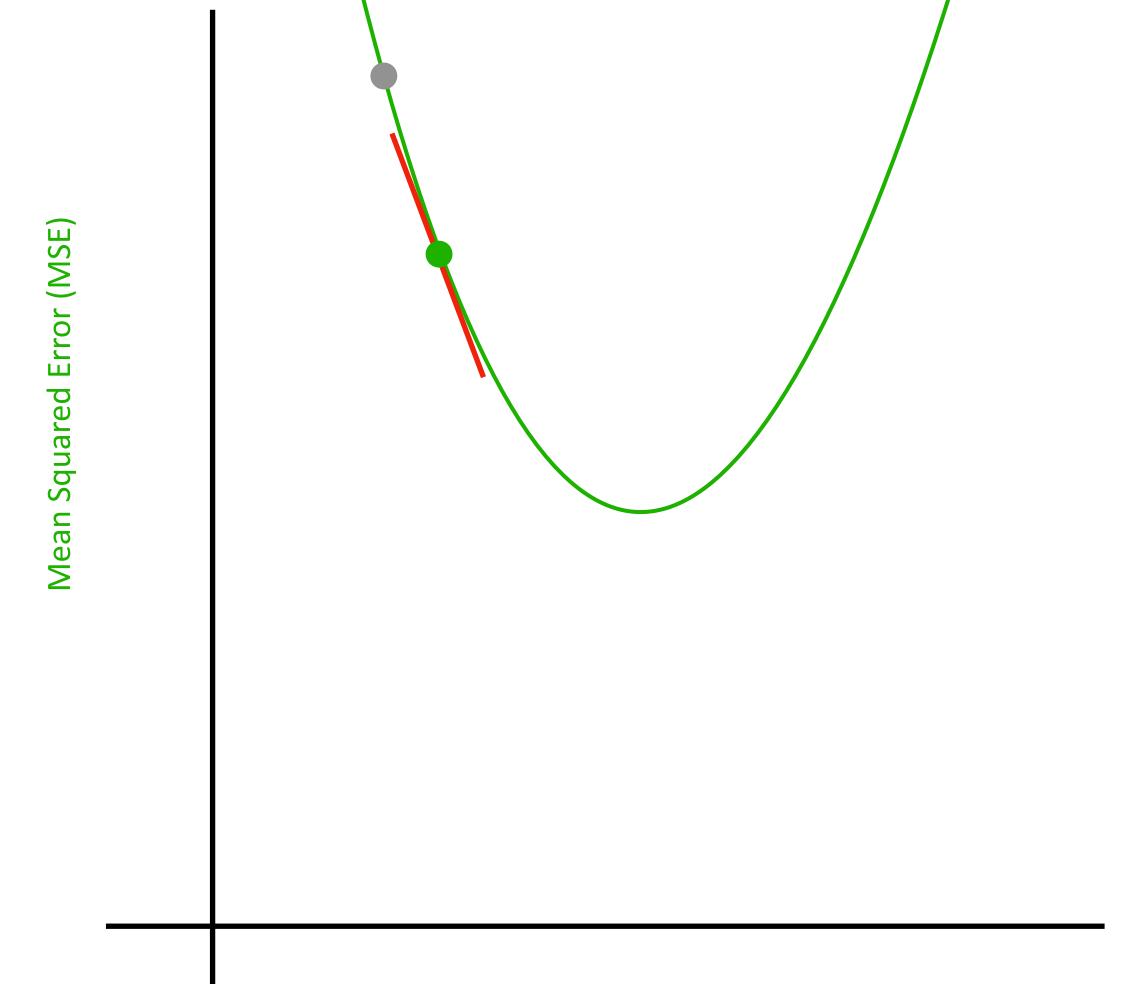
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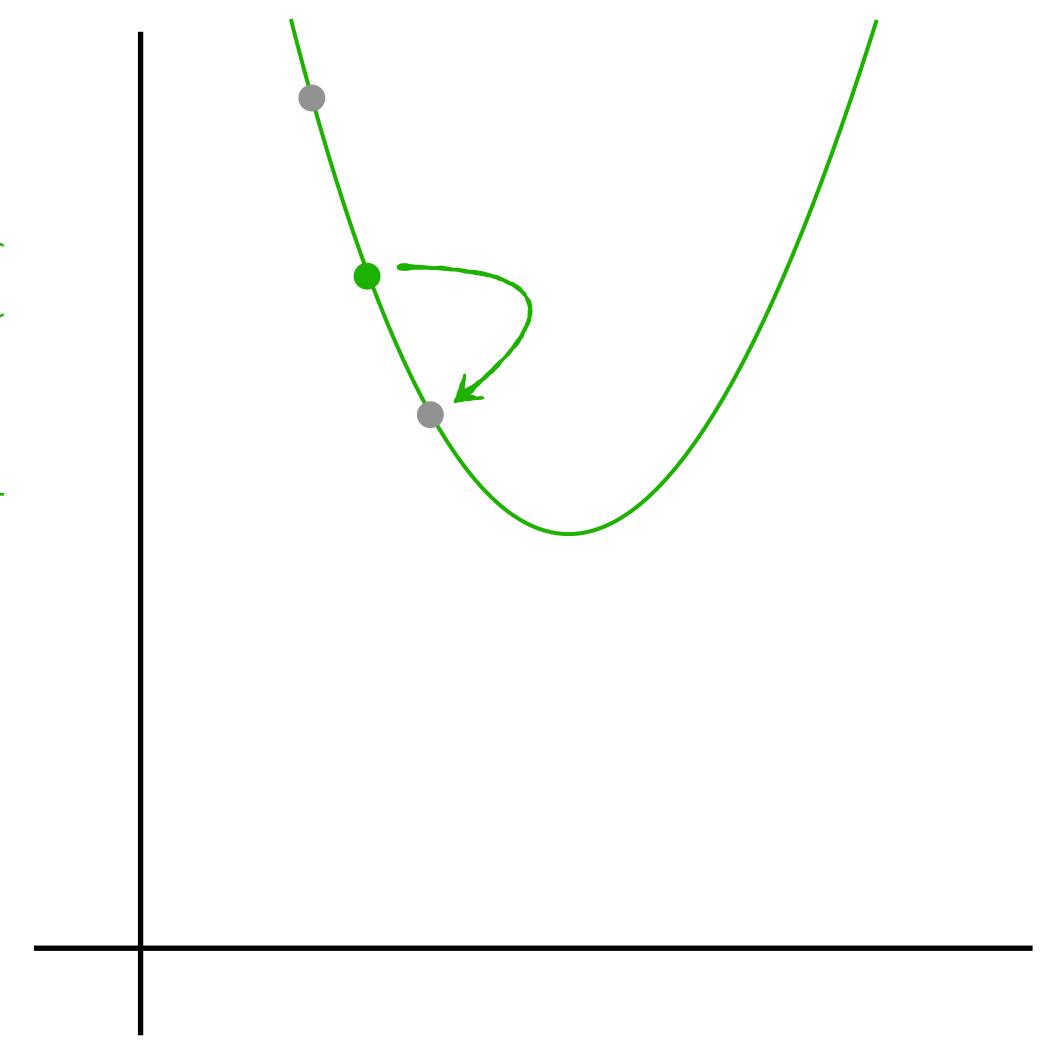
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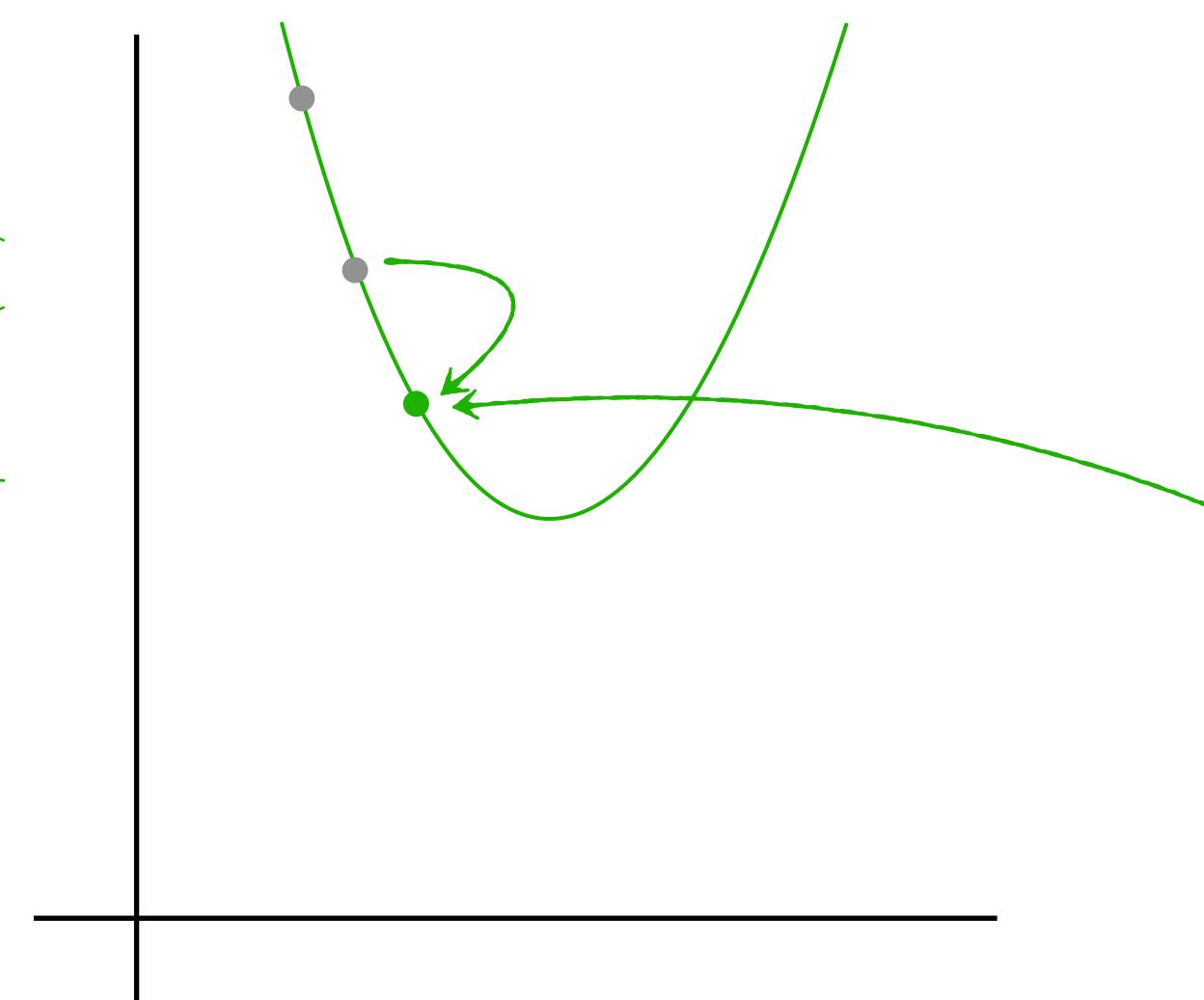
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Gradient Descent

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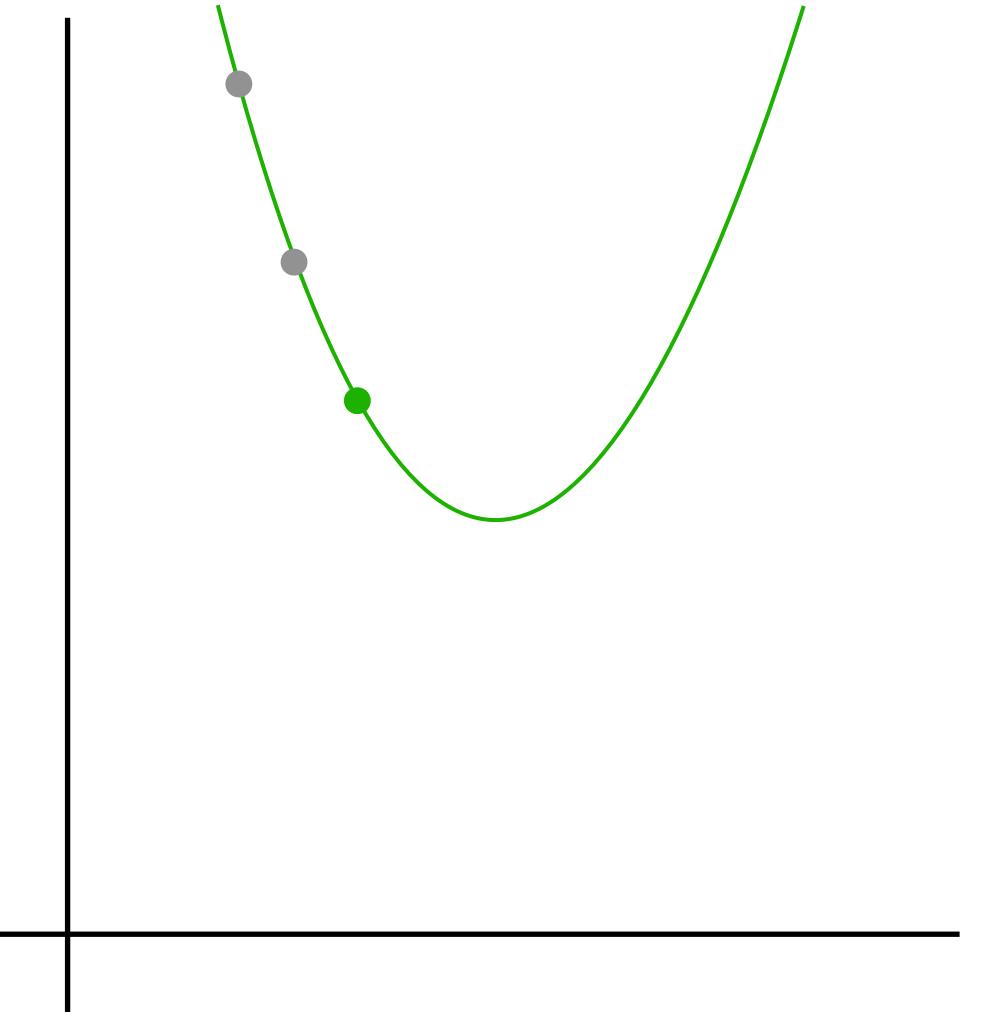
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Gradient Descent

Gradient Descent: Basic Concept

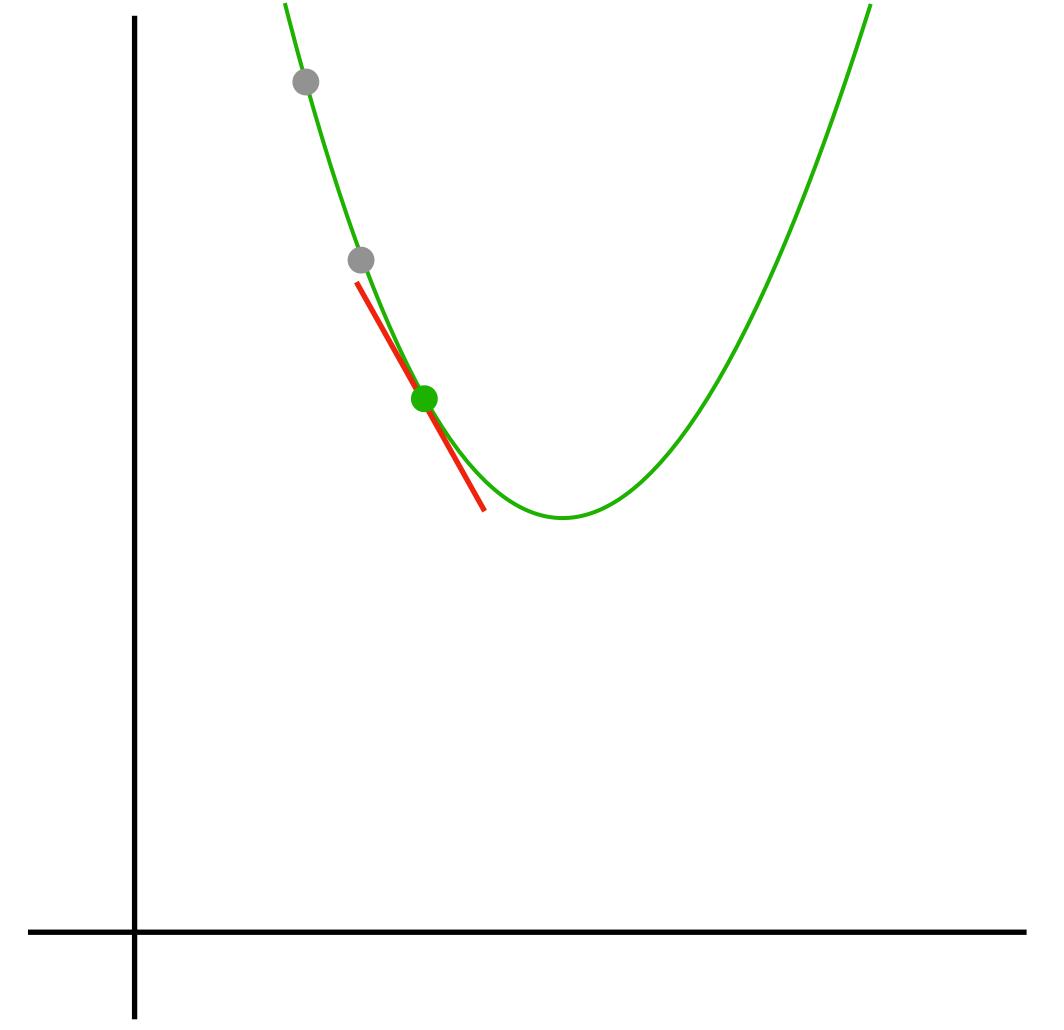
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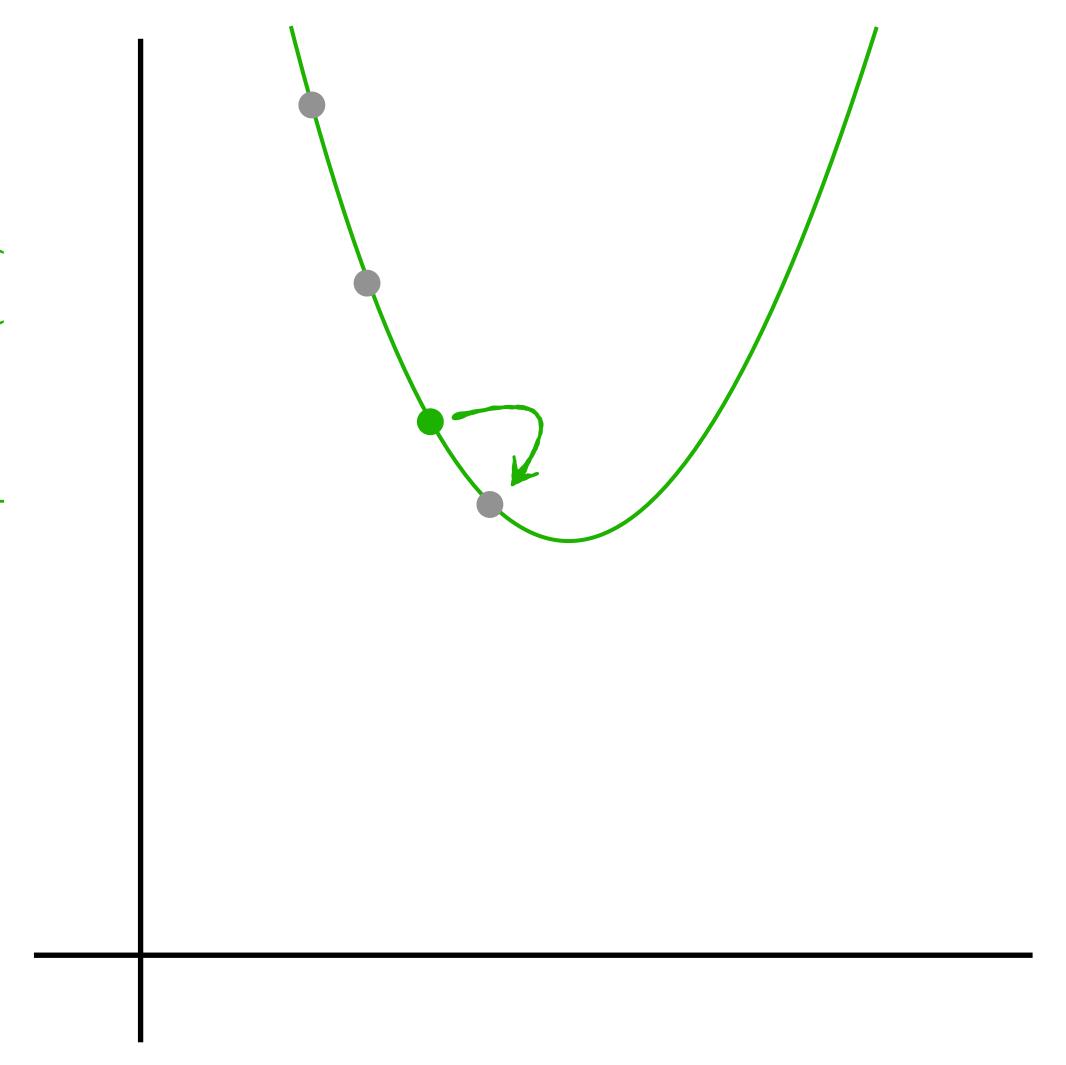
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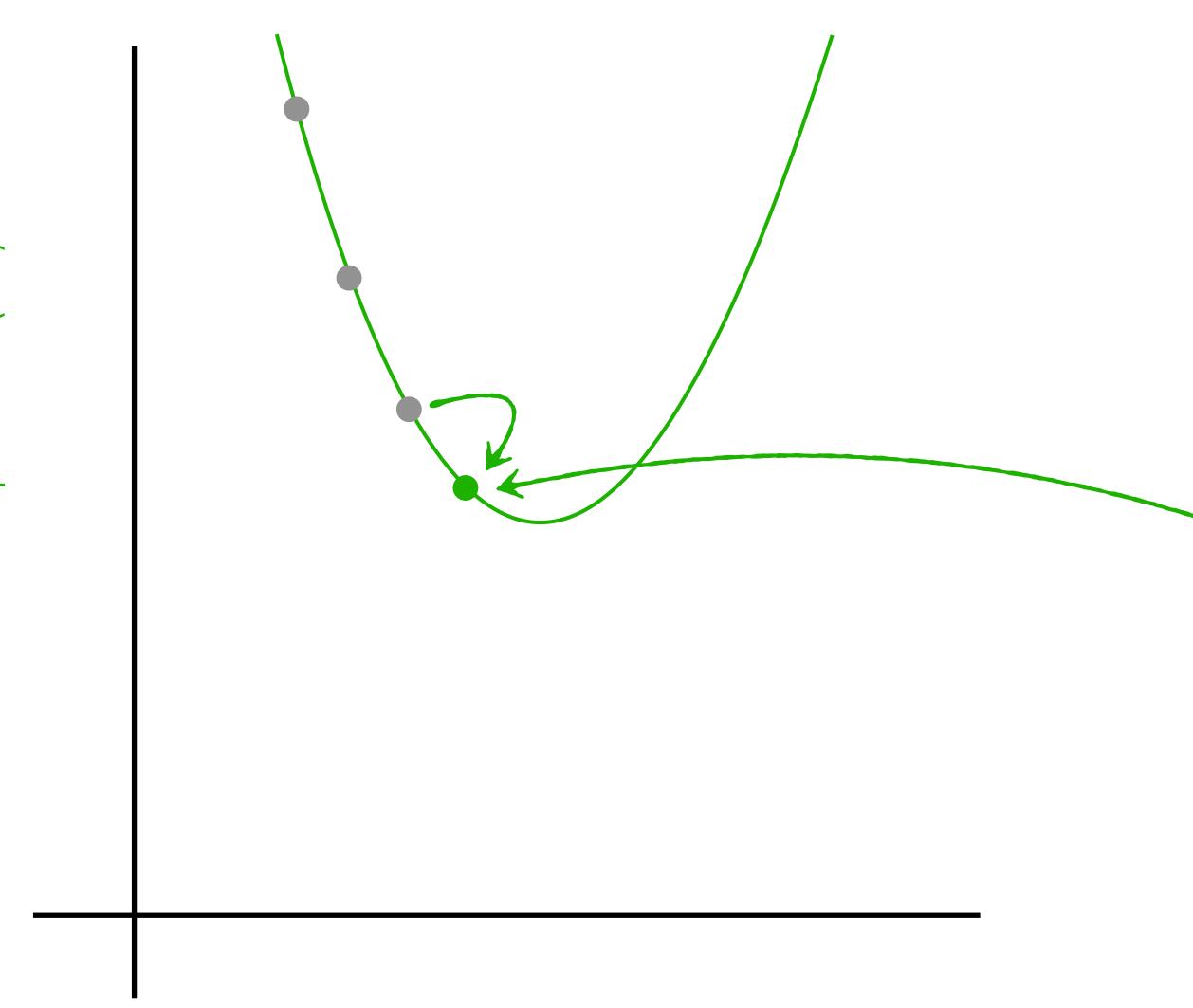
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Gradient Descent

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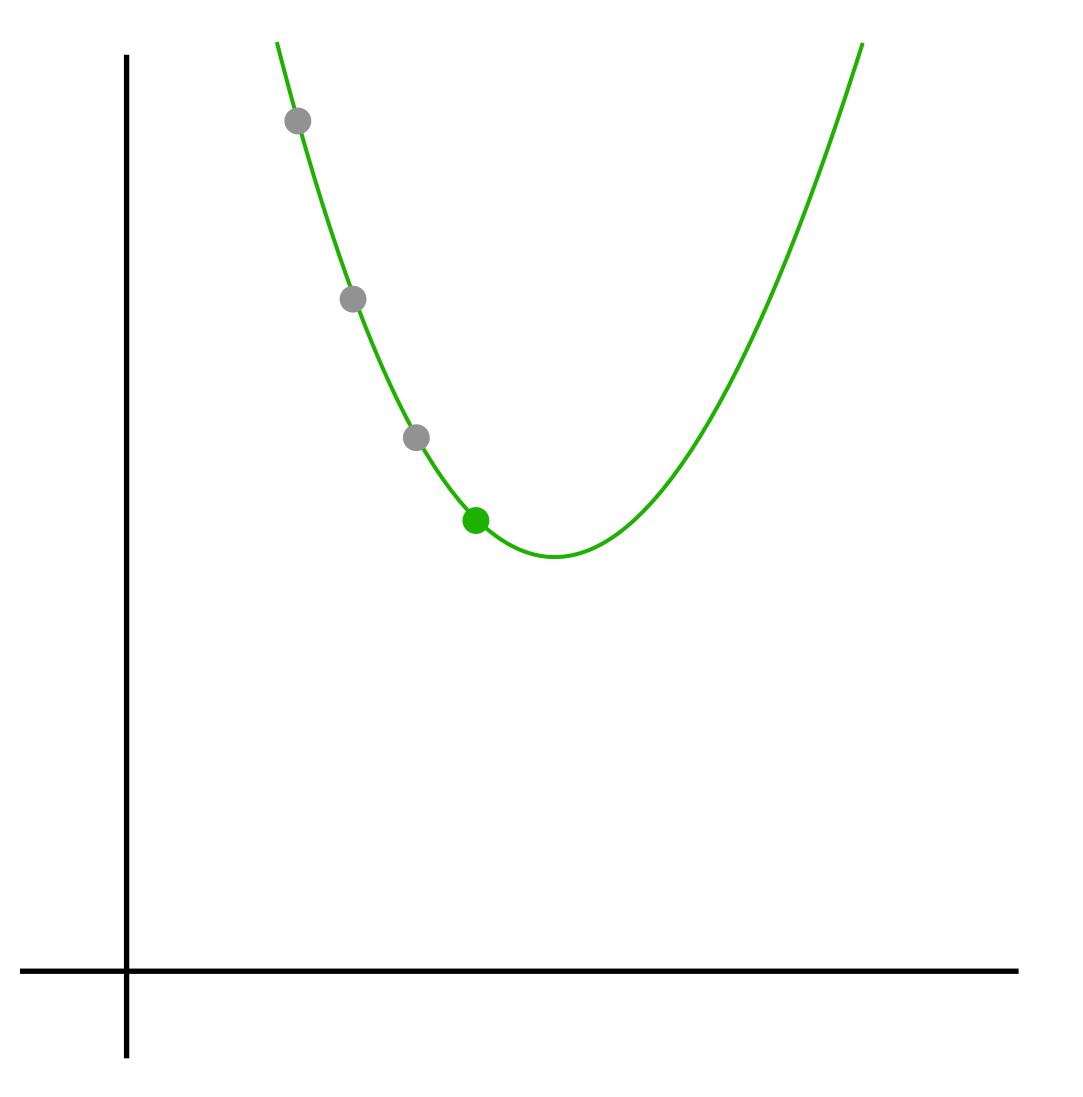
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Jean Squared Error (MSE)



Gradient Descent

Gradient Descent: Basic Concept

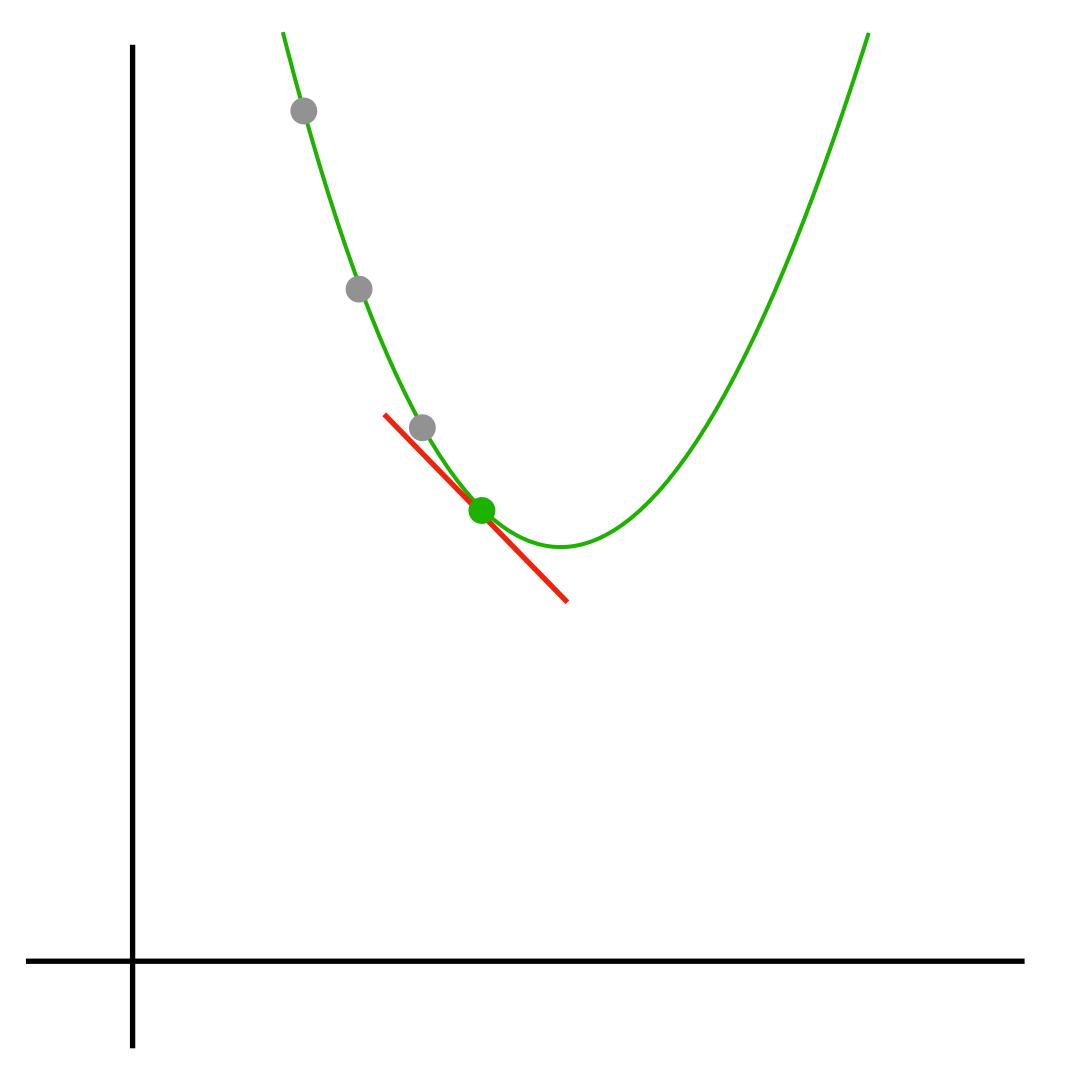
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Gradient Descent

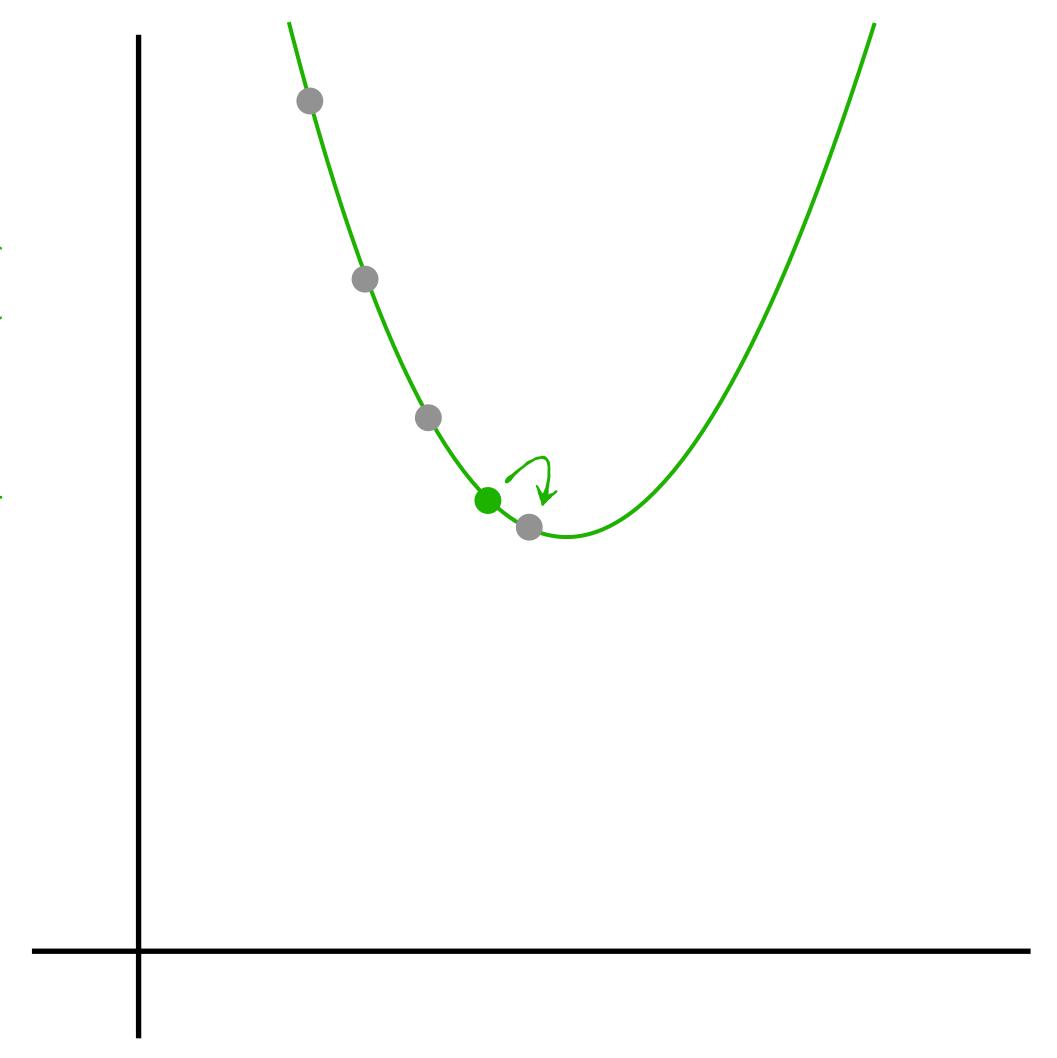
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Gradient Descent

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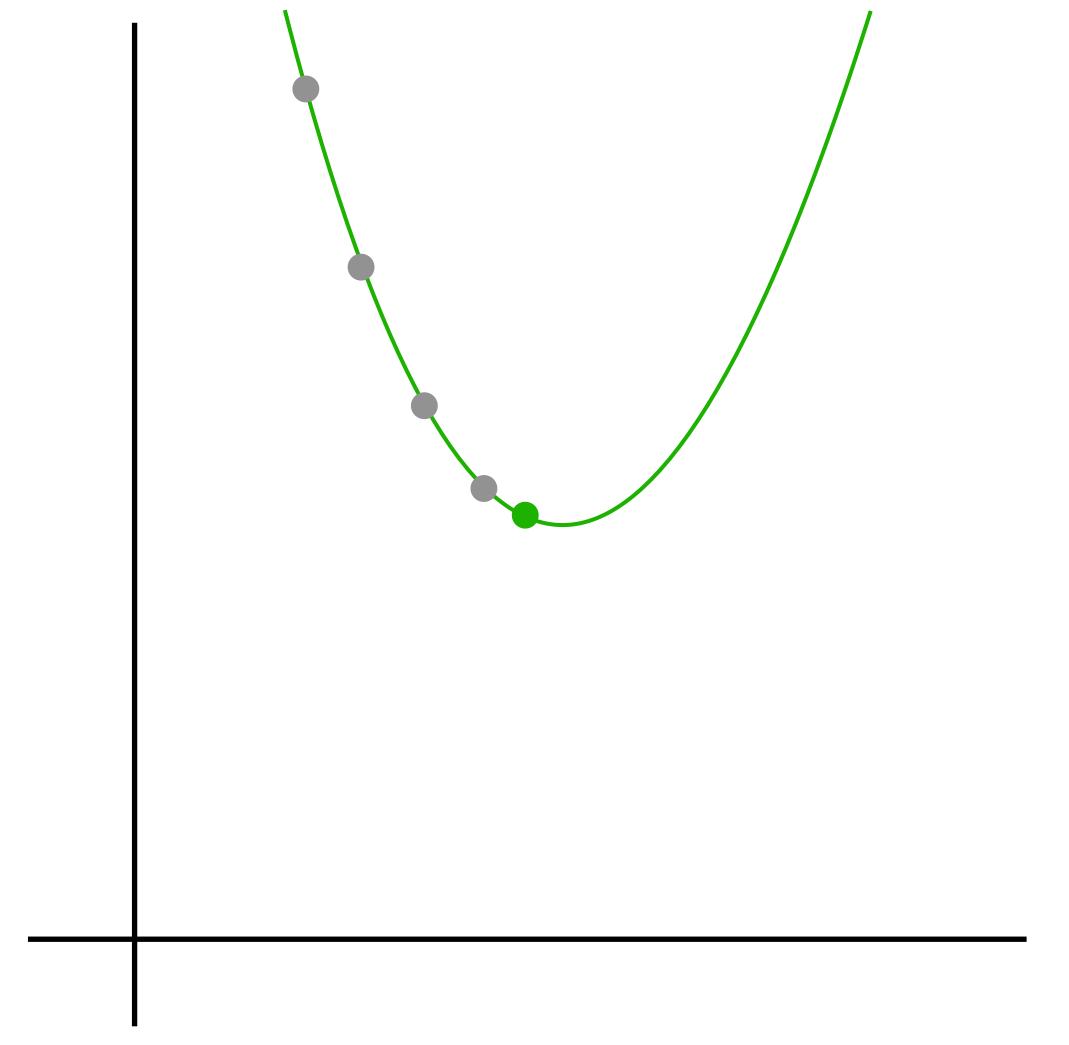
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Gradient Descent

Gradient Descent: Basic Concept

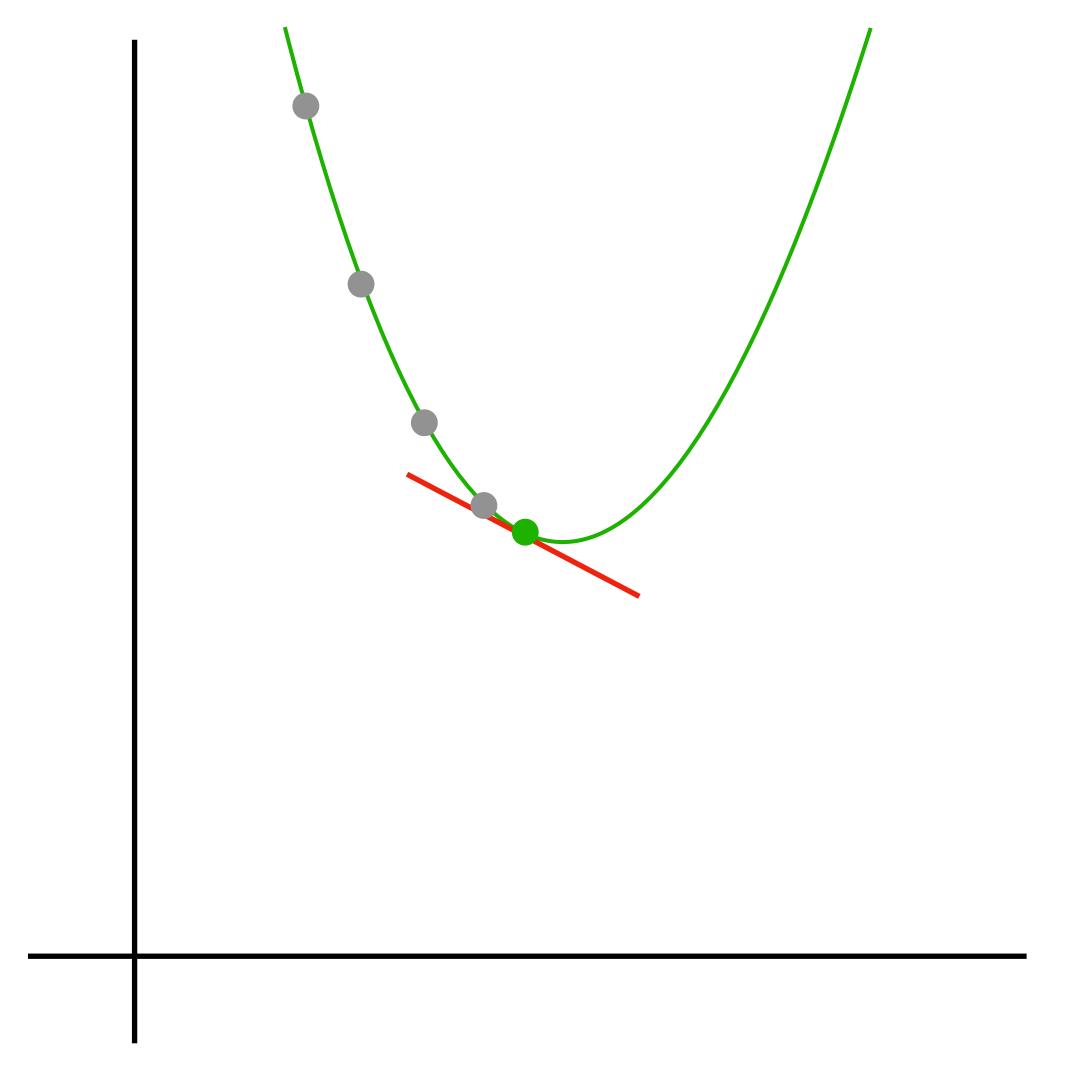
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Gradient Descent

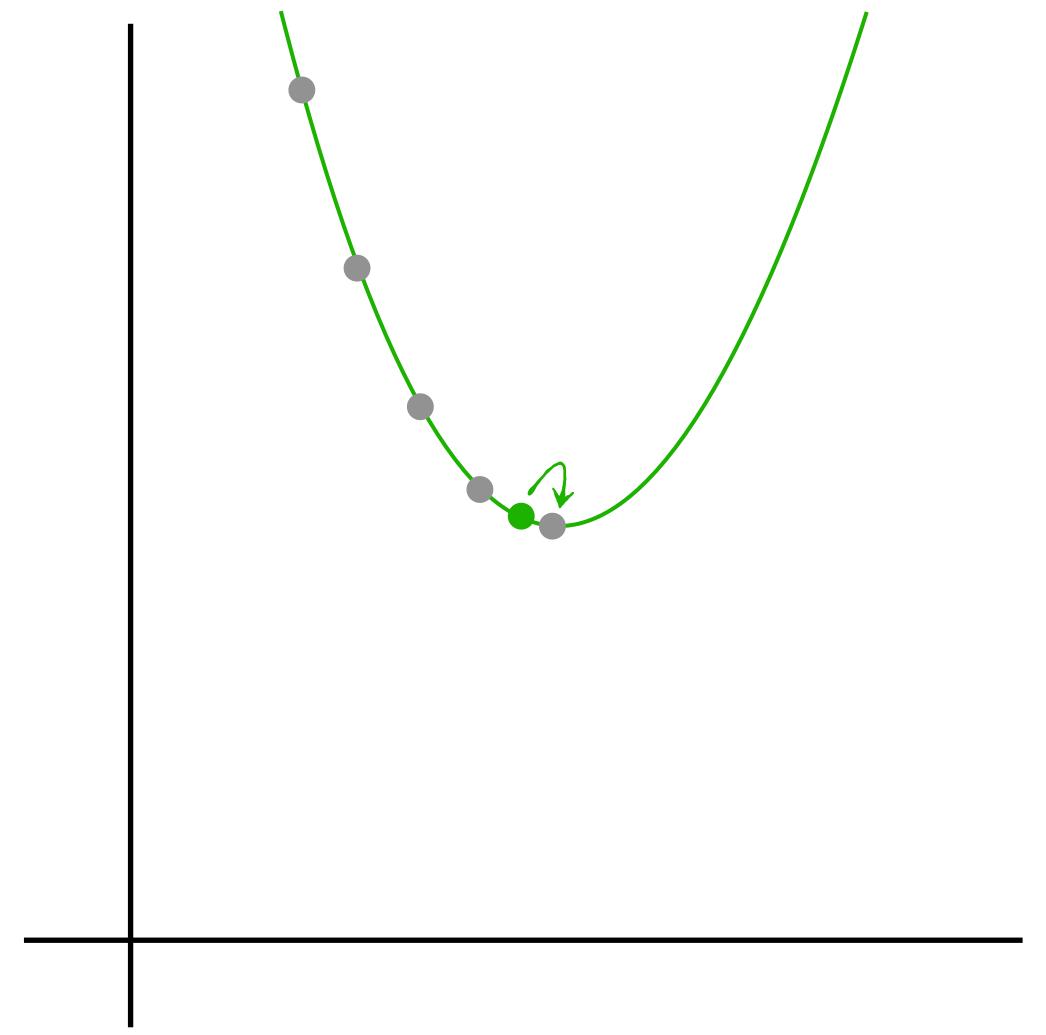
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Gradient Descent

Gradient Descent: Basic Concept

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Gradient Descent

Gradient Descent: Basic Concept

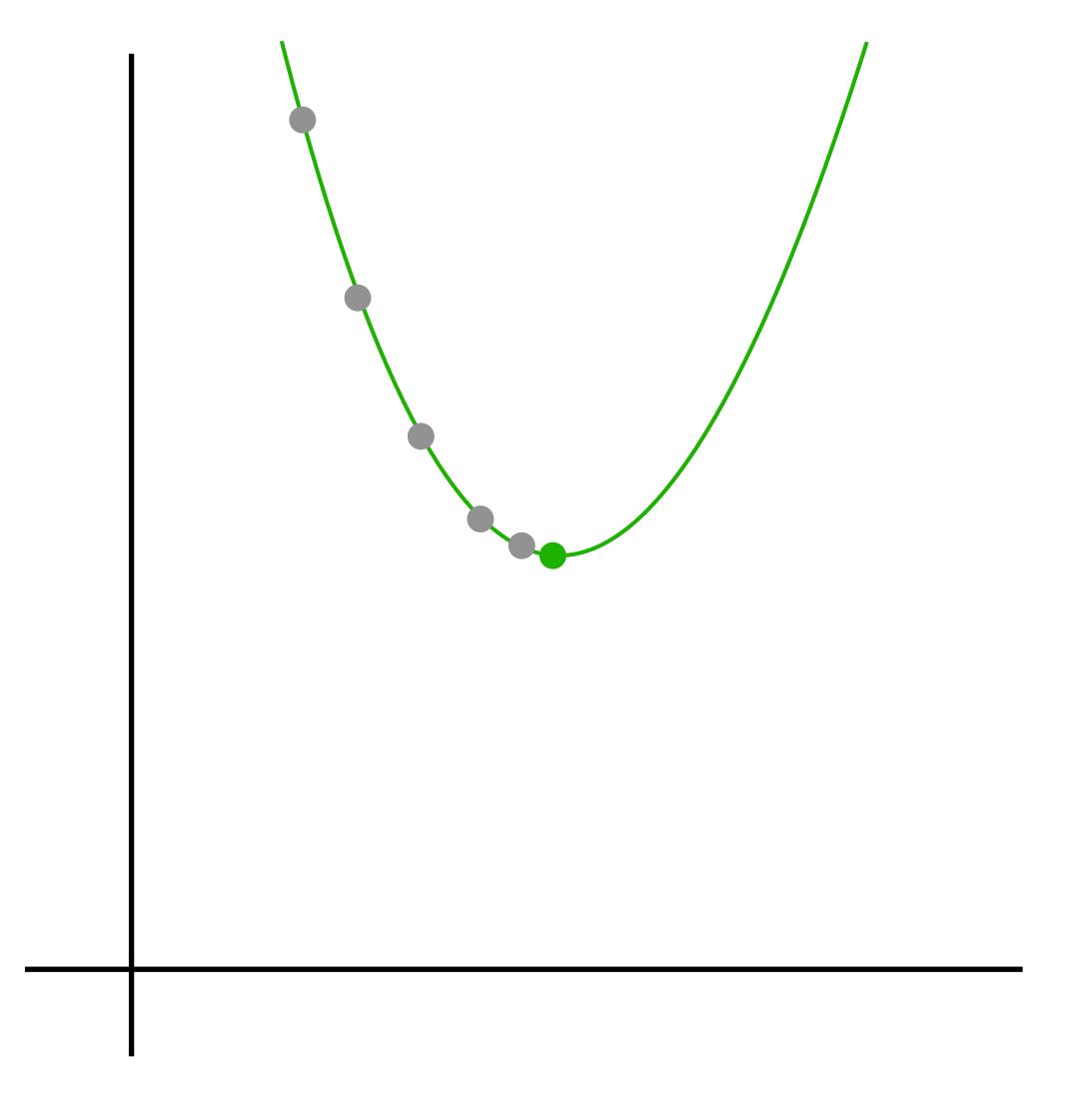
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Gradient Descent

Gradient Descent: Basic Concept

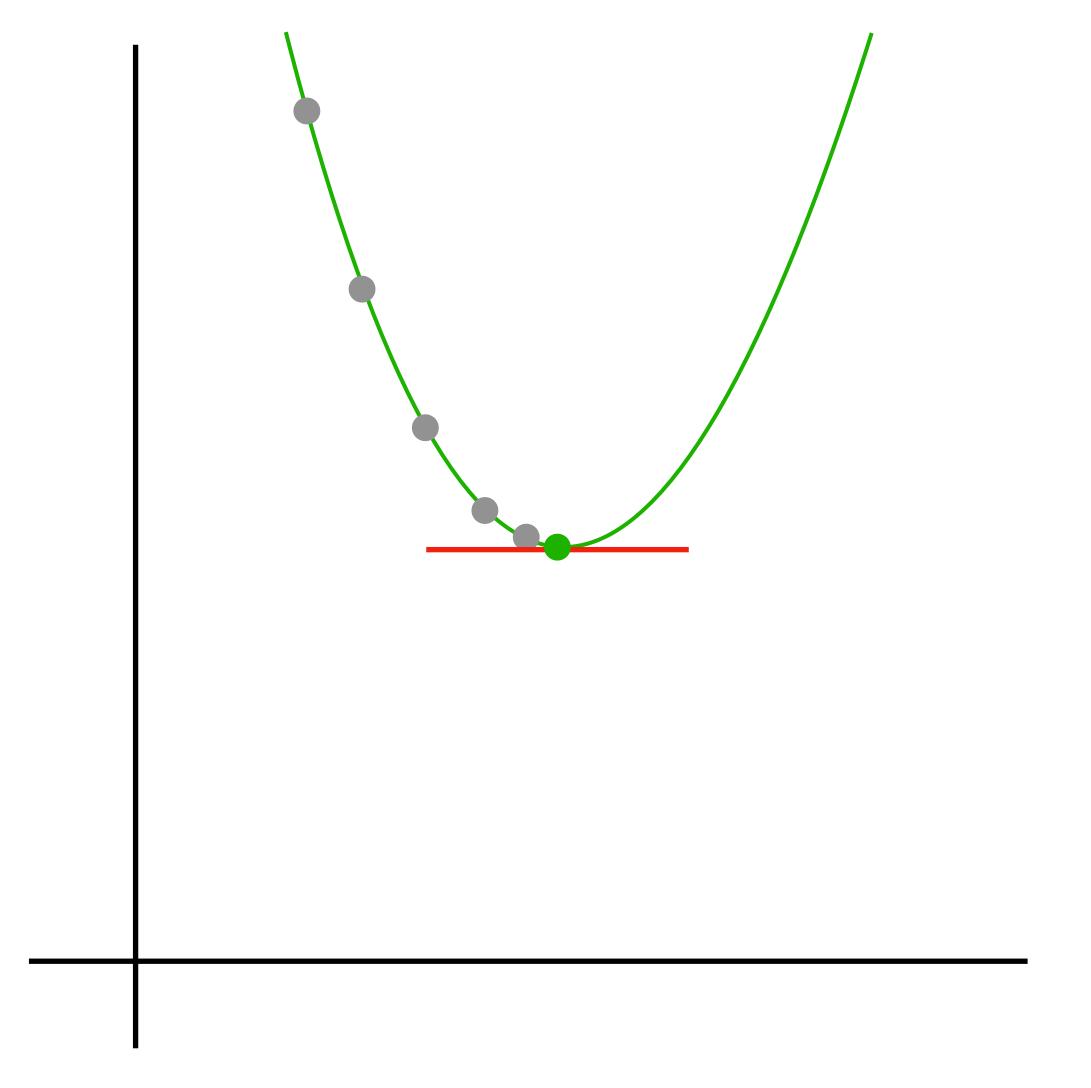
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Gradient Descent

Gradient Descent: Basic Concept

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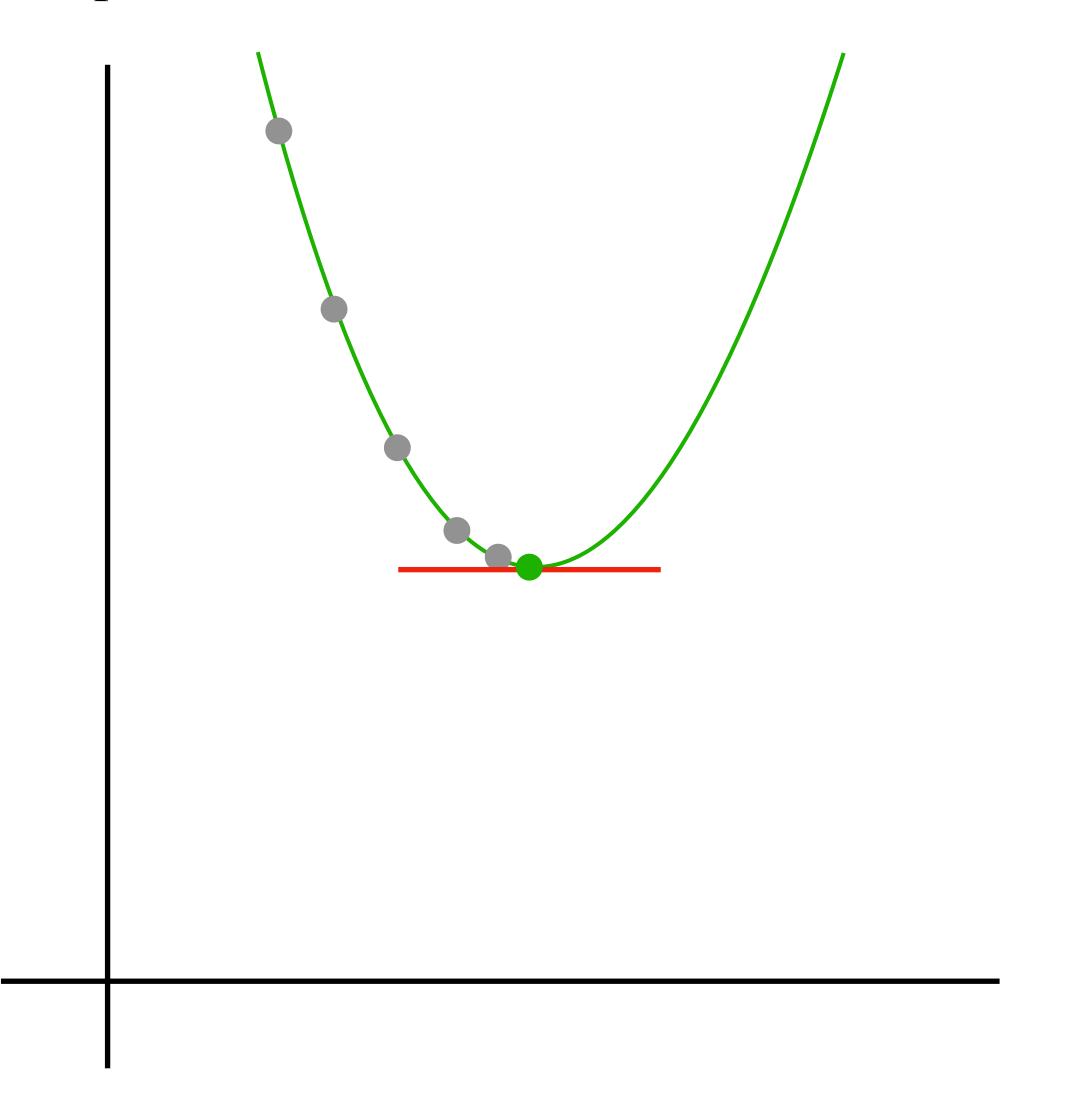
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Gradient Descent

and β_1 follows this curve

Gradient Descent: Basic Concept



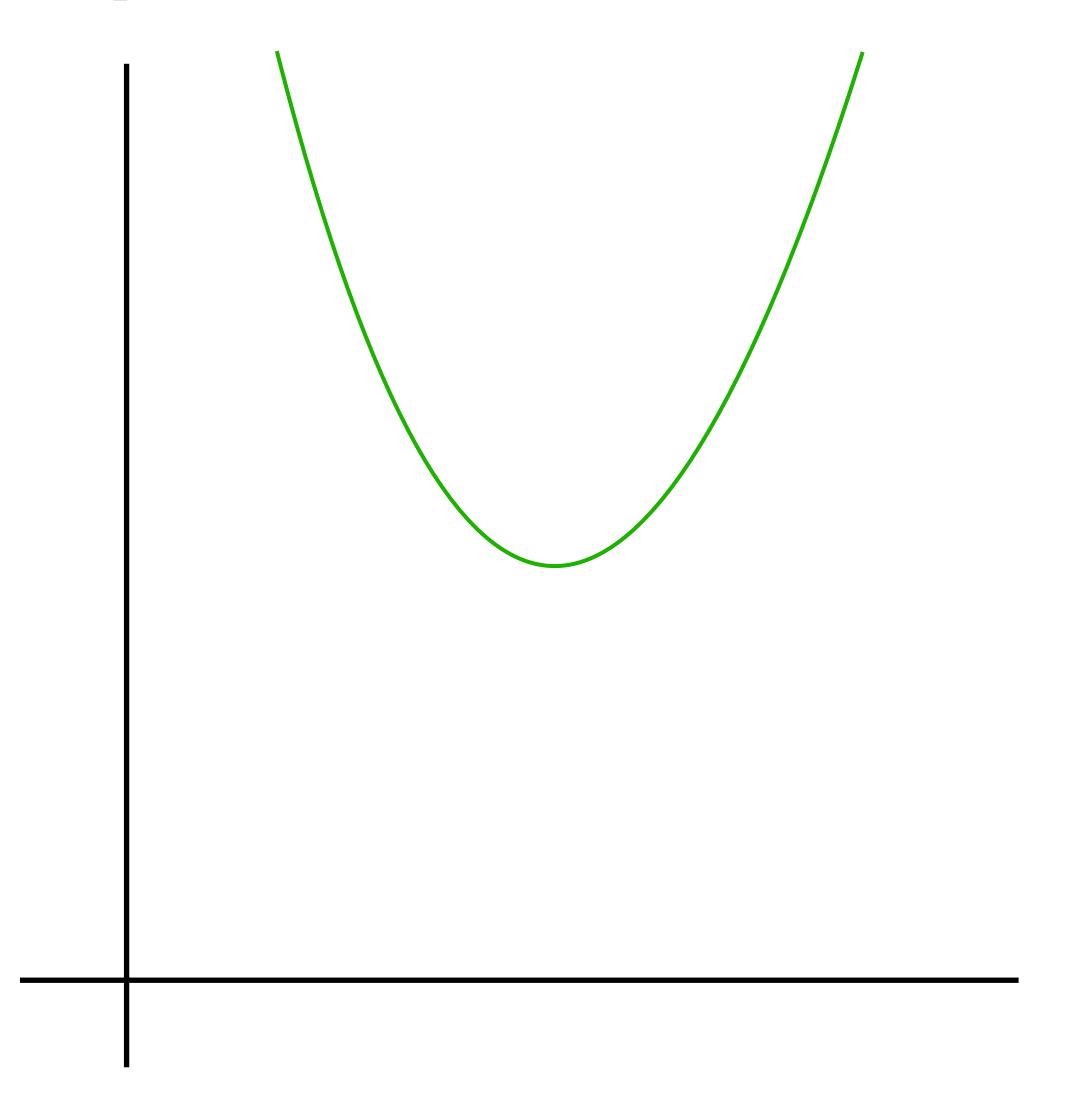
Gradient Descent continues in this manner until the step size is close to zero or a fixed number of iterations

Gradient Descent

Gradient Descent: Lets walk through the algorithm

Gradient Descent

and β_1 follows this curve



Gradient Descent: Basic Concept

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

Mean Squared Error (MSE)

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

The first derivative w.r.t β_0 and β_1 is...

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

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

Gradient Descent

Gradient Descent: Algorithm

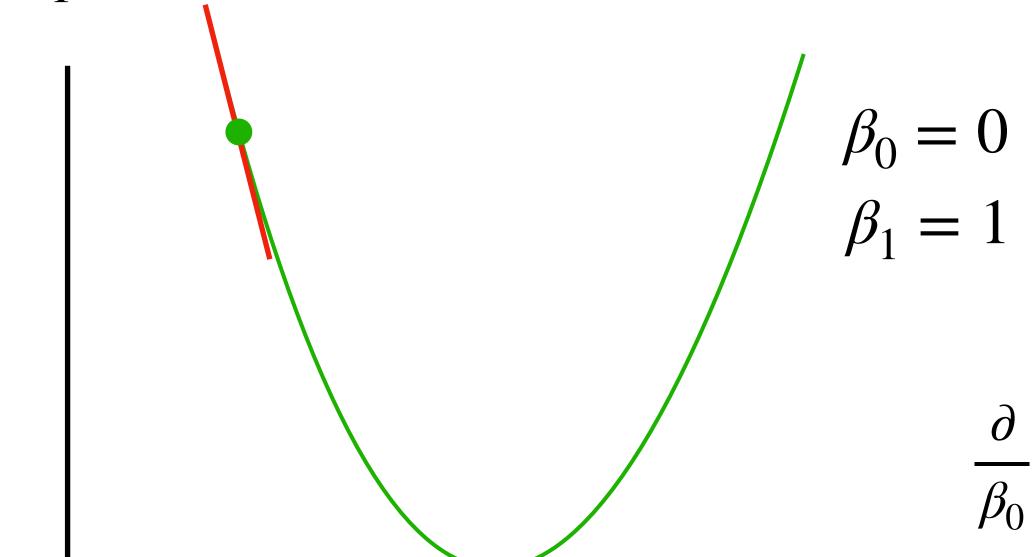
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Step 3: Calculate a step size that is proportional to the slope

Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

and β_1 follows this curve



$$\beta_0 = 0$$

$$\beta_1 = 1$$

Gradient Descent: Basic Concept

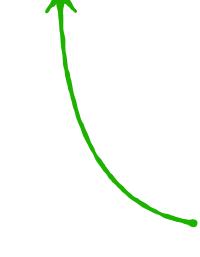
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$$\frac{\partial}{\beta_0} MSE = \frac{\partial}{\partial \beta_0} \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 = -\frac{1}{n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)$$

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

Plugin the values of x_i and y_i from the observations and the values of eta_0 and eta_1



i	Height (in)	Weight (lbs)
1	62	138
2	55	178
3	44	123
4	75	200
5	65	229
6	50	102

$\beta_0 = 0$ $\beta_1 = 1$

Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

Step 3: Calculate a step size that is proportional to the slope

$$step_size_{\beta_0} = \frac{\partial}{\partial \beta_0} MSE \times learning_rate$$

$$step_size_{\beta_1} = \frac{\partial}{\partial \beta_1} MSE \times learning_rate$$

learning_rate is a small value that determines how the algorithm adjusts the parameters on each iteration. Too large and it will take big steps and fail to converge. Too small and it will take many small steps and take too long to converge.

Step size walks $\beta_0 = 1.2$ $\beta_1 = 2.3$ down the curve

Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

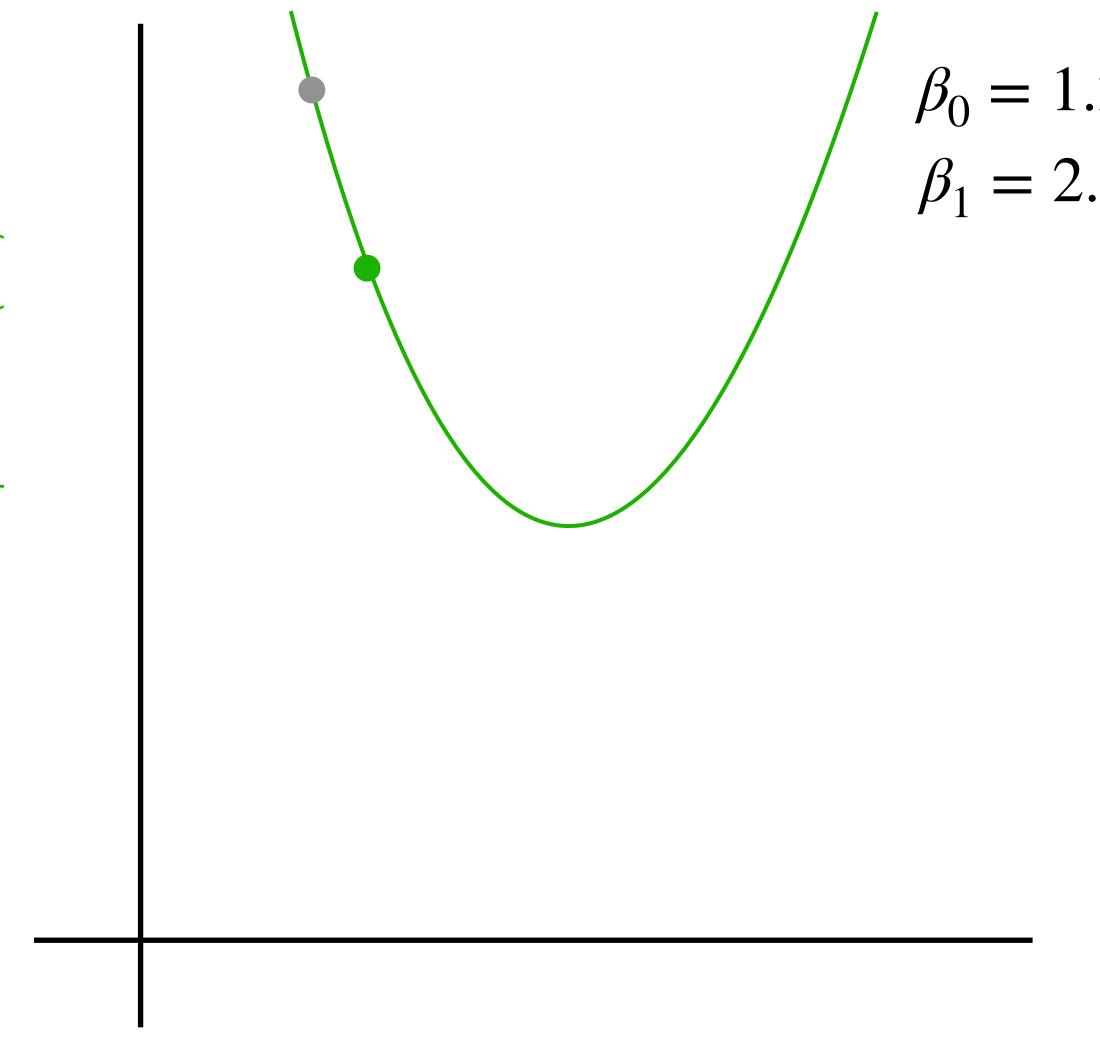
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Step 3: Calculate a step size that is proportional to the slope

Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

$$\beta_0 = \beta_0 - step_size_{\beta_0}$$

$$\beta_1 = \beta_1 - step_size_{\beta_1}$$



Gradient Descent

Gradient Descent: Basic Concept

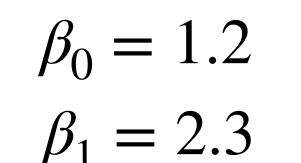
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and β_1 follows this curve



$$\beta_1 = 2.3$$

Gradient Descent

Gradient Descent: Basic Concept

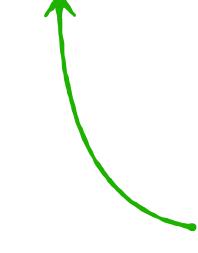
Step 1: Start with random values for β_0 and β_1

Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

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

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

Plugin the values of x_i and y_i from the observations and the values of β_0 and β_1



i	Height (in)	Weight (lbs)
1	62	138
2	55	178
3	44	123
4	75	200
5	65	229
6	50	102

$\beta_0 = 1.2$ $\beta_1 = 2.3$

$$\beta_1 = 2.3$$

Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

Step 3: Calculate a step size that is proportional to the slope

$$step_size_{\beta_0} = \frac{\partial}{\partial \beta_0} MSE \times learning_rate$$

$$step_size_{\beta_1} = \frac{\partial}{\partial \beta_1} MSE \times learning_rate$$

 $learning_rate$ is a small value that determines how the algorithm adjusts the parameters on each iteration. Too large and it will take big steps and fail to converge. Too small and it will take many small steps and take too long to converge.

Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

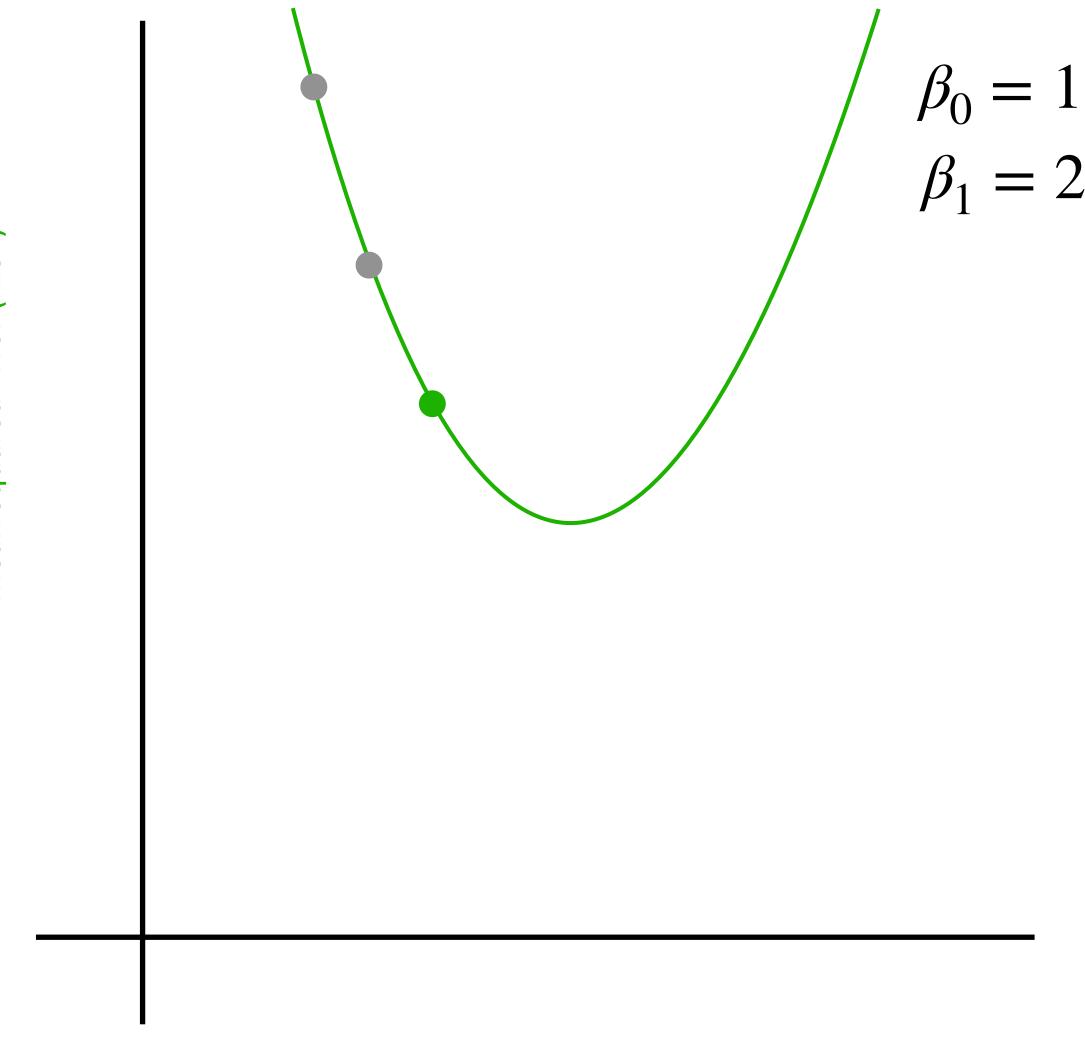
Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

Step 3: Calculate a step size that is proportional to the slope

Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

$$\beta_0 = \beta_0 - step_size_{\beta_0}$$

$$\beta_1 = \beta_1 - step_size_{\beta_1}$$



Gradient Descent

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Step 1: Start with random values for β_0 and β_1

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Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

Mean Squared Error (MSE) for various values of β_0

and β_1 follows this curve

$$\beta_0 = 1.5$$
 $\beta_1 = 2.8$

$$\beta_1 = 2.8$$

Gradient Descent

Gradient Descent: Basic Concept

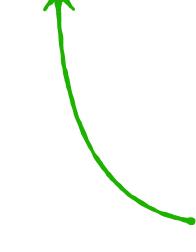
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Plugin the values of x_i and y_i from the observations and the values of eta_0 and eta_1



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$$\beta_0 = 1.5$$
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Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

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Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

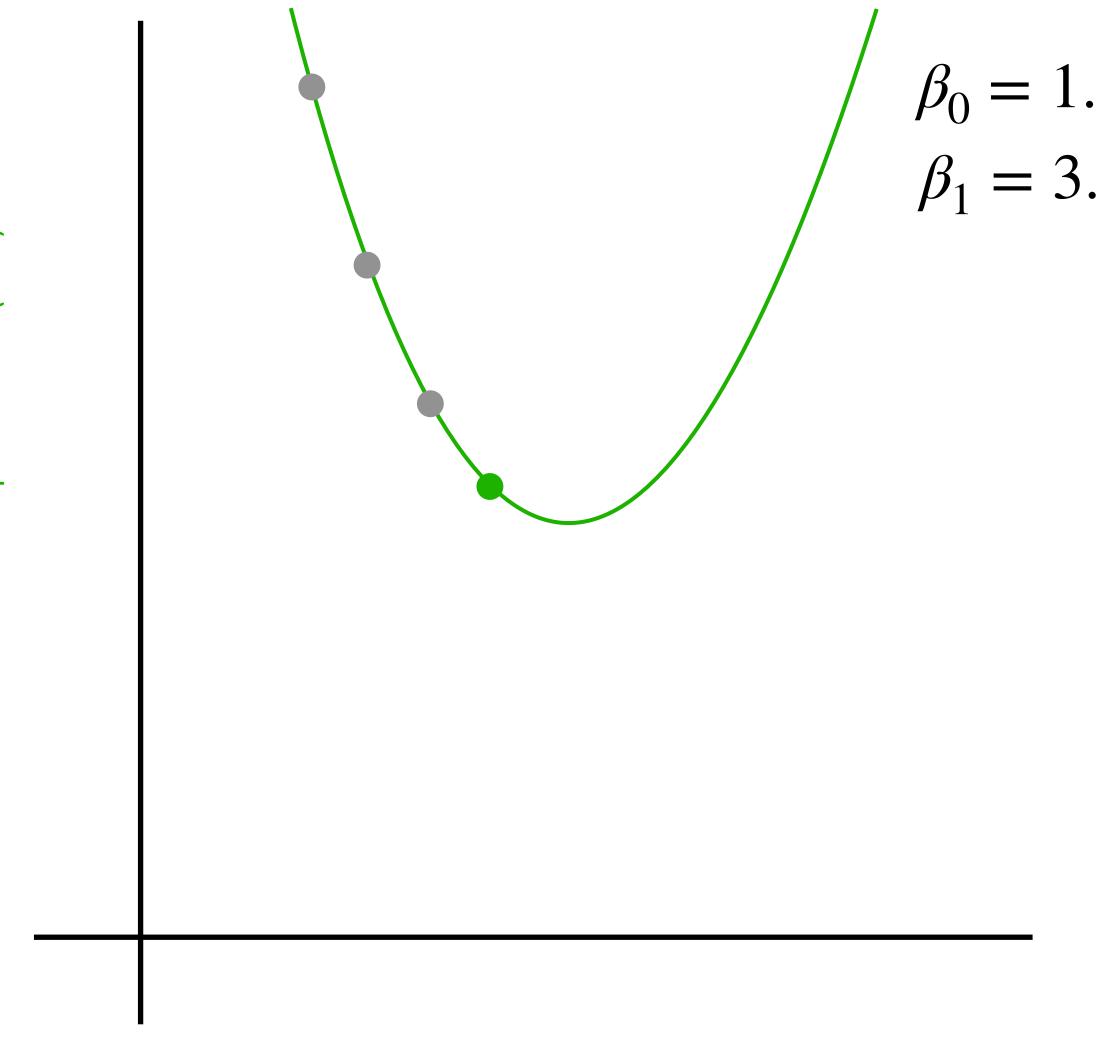
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Step 4: Calculate new values for β_0 and β_1 by subtracting the step size

$$\beta_0 = \beta_0 - step_size_{\beta_0}$$

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Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

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Mean Squared Error (MSE) for various values of β_0

and β_1 follows this curve

$$\beta_0 = 1.8$$
 $\beta_1 = 3.1$

$$\beta_1 = 3.1$$

Gradient Descent

Gradient Descent: Basic Concept

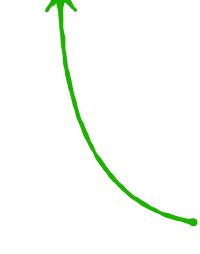
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Plugin the values of x_i and y_i from the observations and the values of eta_0 and eta_1



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$\beta_0 = 1.8$ $\beta_1 = 3.1$

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

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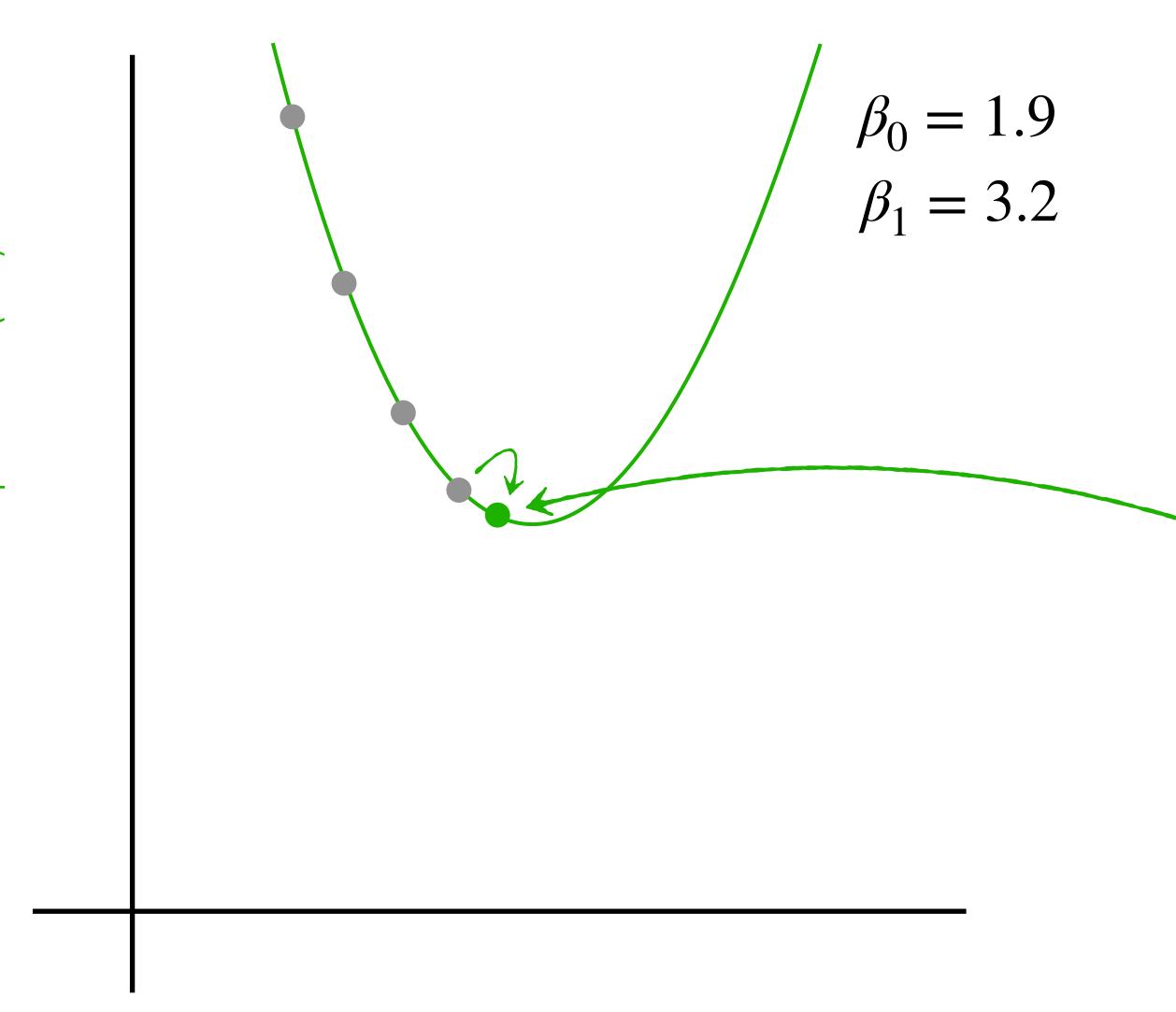
Gradient Descent

Step 3: Calculate a step size that is proportional to the slope

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Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

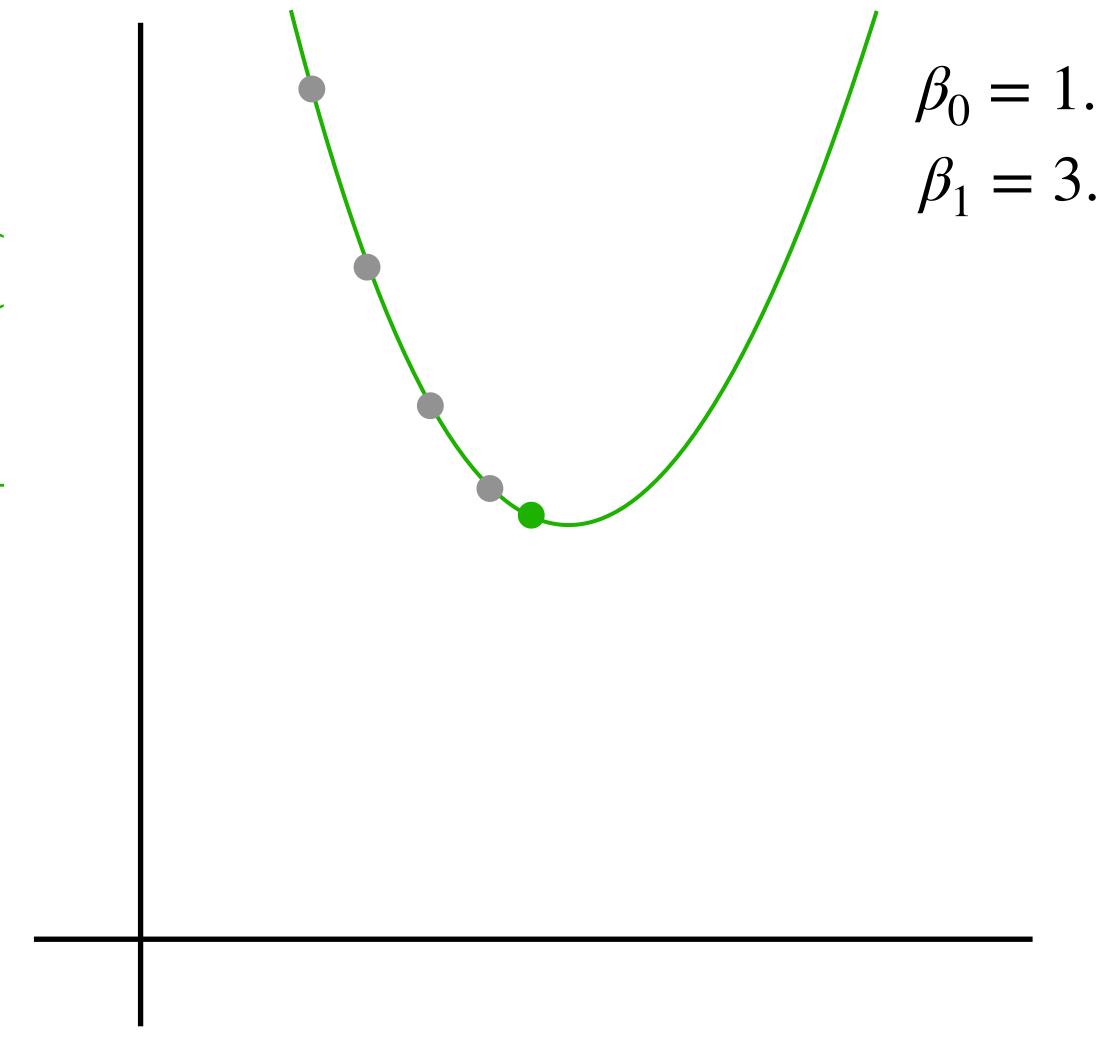
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$$\beta_0 = \beta_0 - step_size_{\beta_0}$$

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Gradient Descent

Gradient Descent: Basic Concept

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Step 2: Compute the partial derivative of the MSE w.r.t β_0 and β_1 - this is the slope at that point

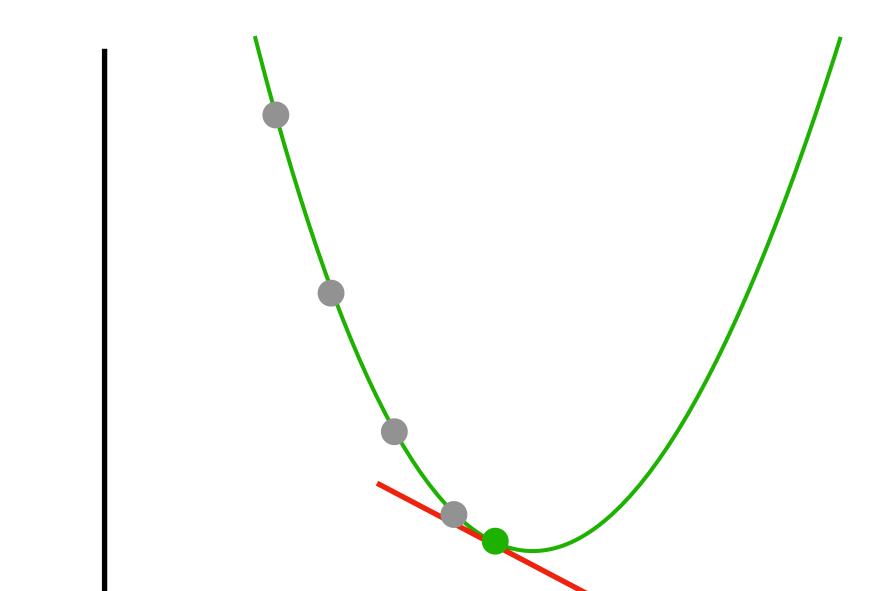
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Mean Squared Error (MSE) for various values of β_0

Gradient Descent

and β_1 follows this curve



$$\beta_0 = 1.9$$
 $\beta_1 = 3.2$

$$\beta_1 = 3.2$$

Gradient Descent: Basic Concept

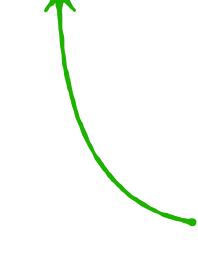
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$\beta_0 = 1.9$ $\beta_1 = 3.2$

Gradient Descent

Gradient Descent: Basic Concept

Step 1: Start with random values for β_0 and β_1

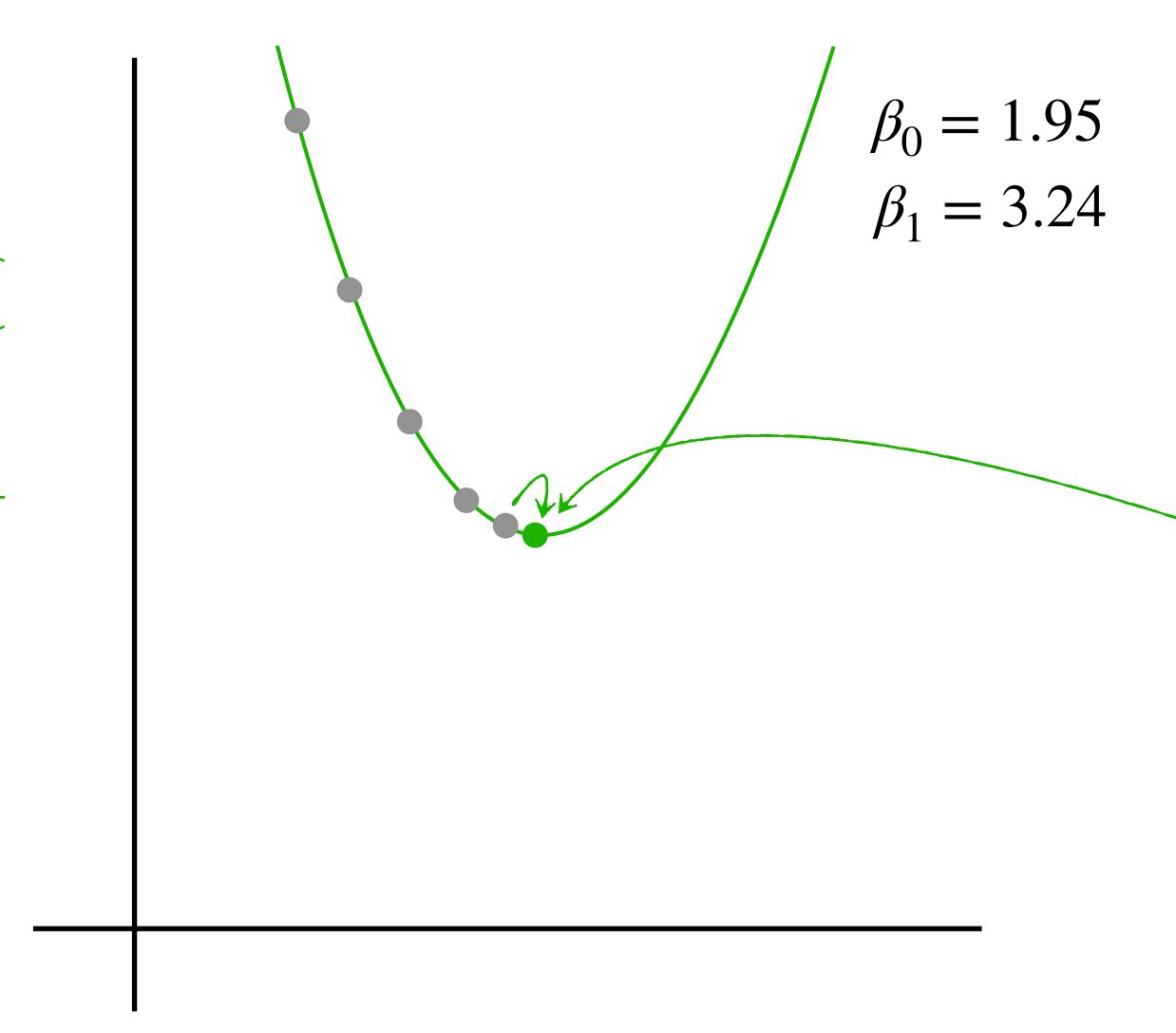
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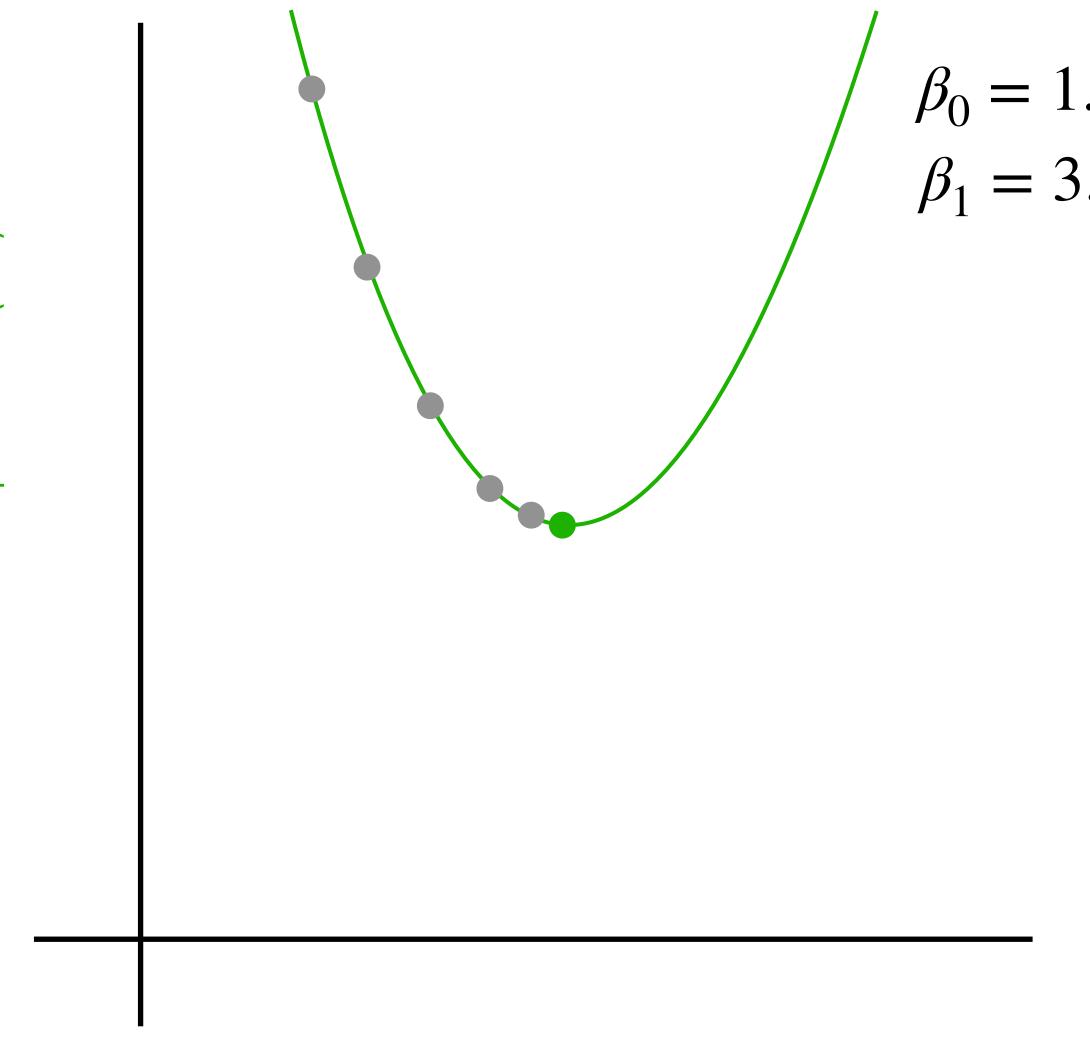
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Mean Squared Error (MSE) for various values of β_0

Gradient Descent

and β_1 follows this curve

$$\beta_0 = 1.95$$

$$\beta_0 = 1.95$$
 $\beta_1 = 3.24$

Gradient Descent: Basic Concept

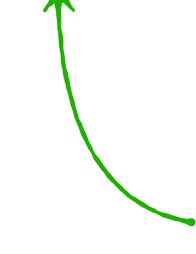
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If step_size < 0.0001 then stop

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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.

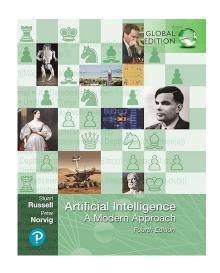
Multiple Regression []

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



<u>Artificial Intelligence: A Modern Approach</u>

by Peter Norvig, Stuart Russell

For a complete list of tutorials see:

https://arrsingh.com/ai-tutorials