# II - Linear and Logistic Regression

Formalism & Inference function

Loss function

Algorithms

## Regression Vs Classification



#### Regression

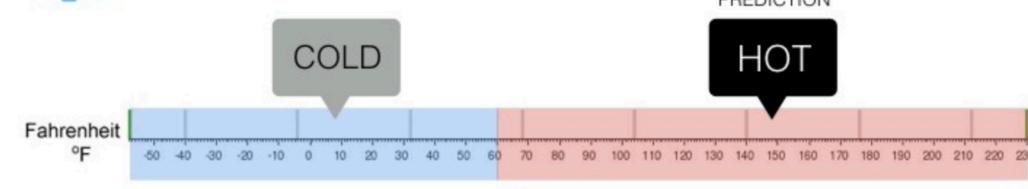
What is the temperature going to be tomorrow?



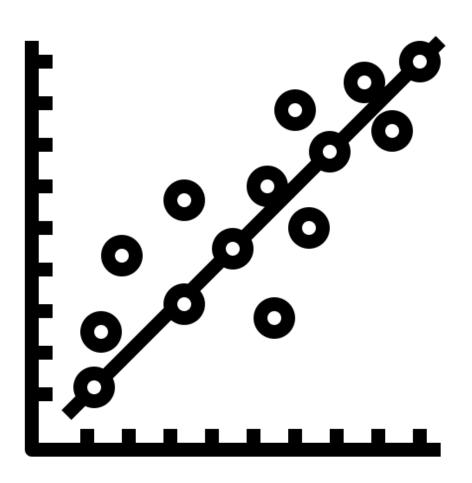


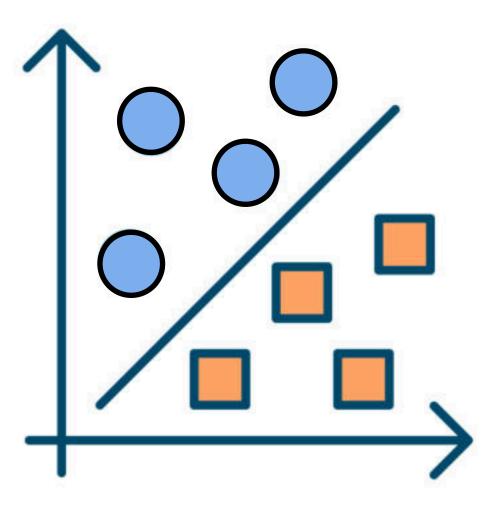
#### Classification

Will it be Cold or Hot tomorrow?



Source: Pintrest

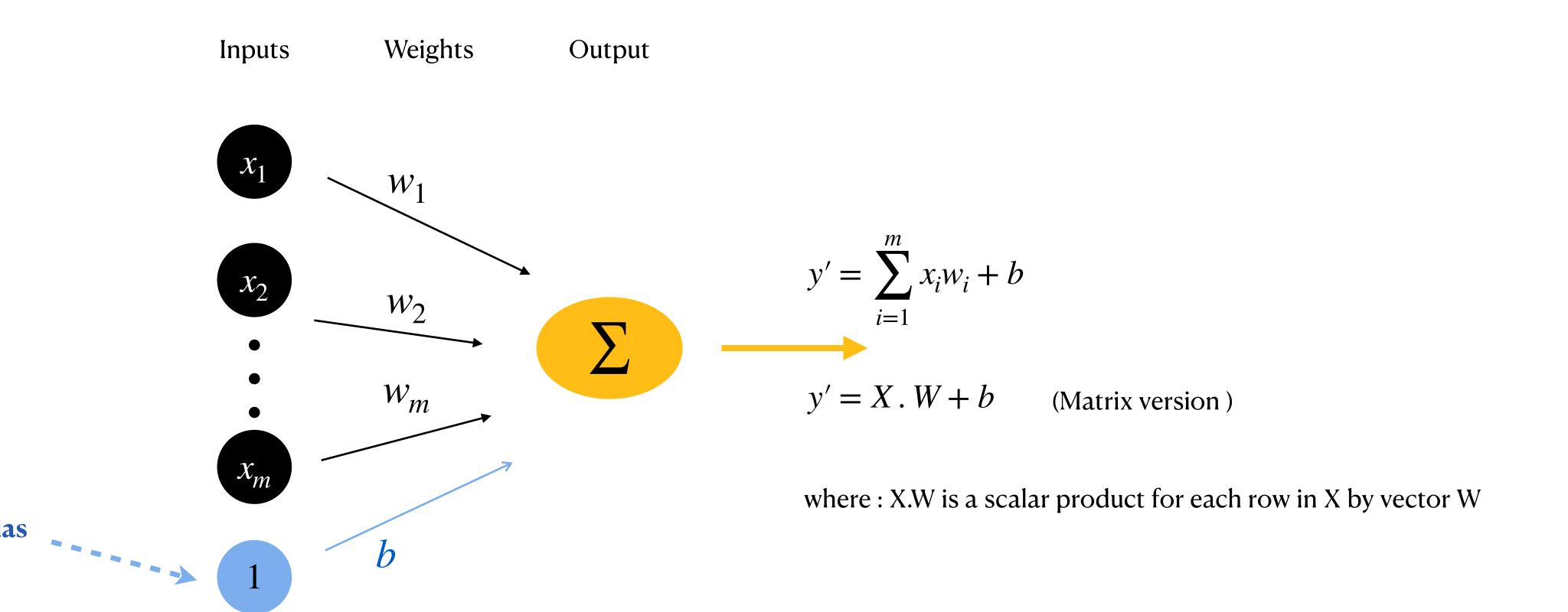




# Linear Regression Formalism

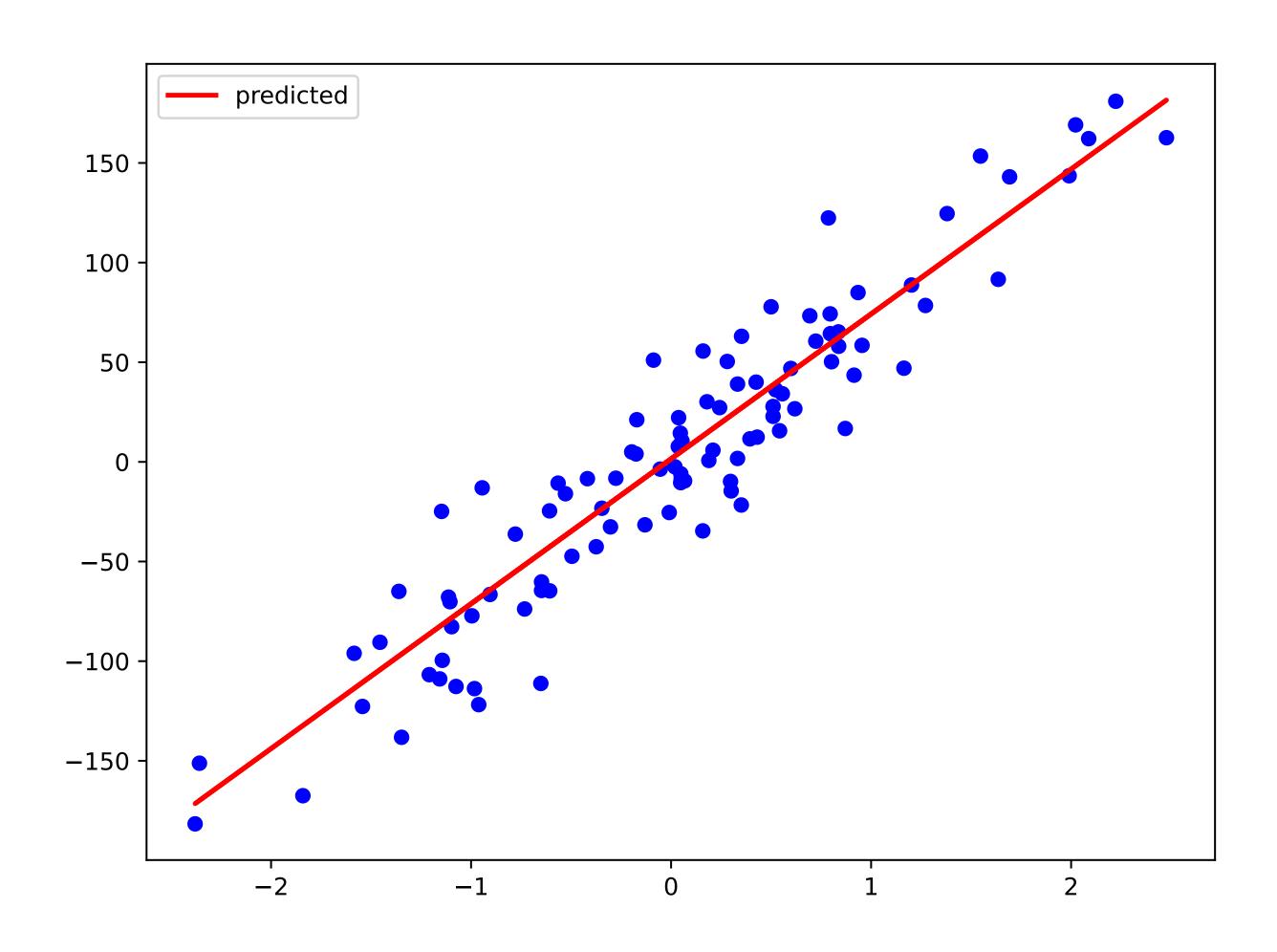
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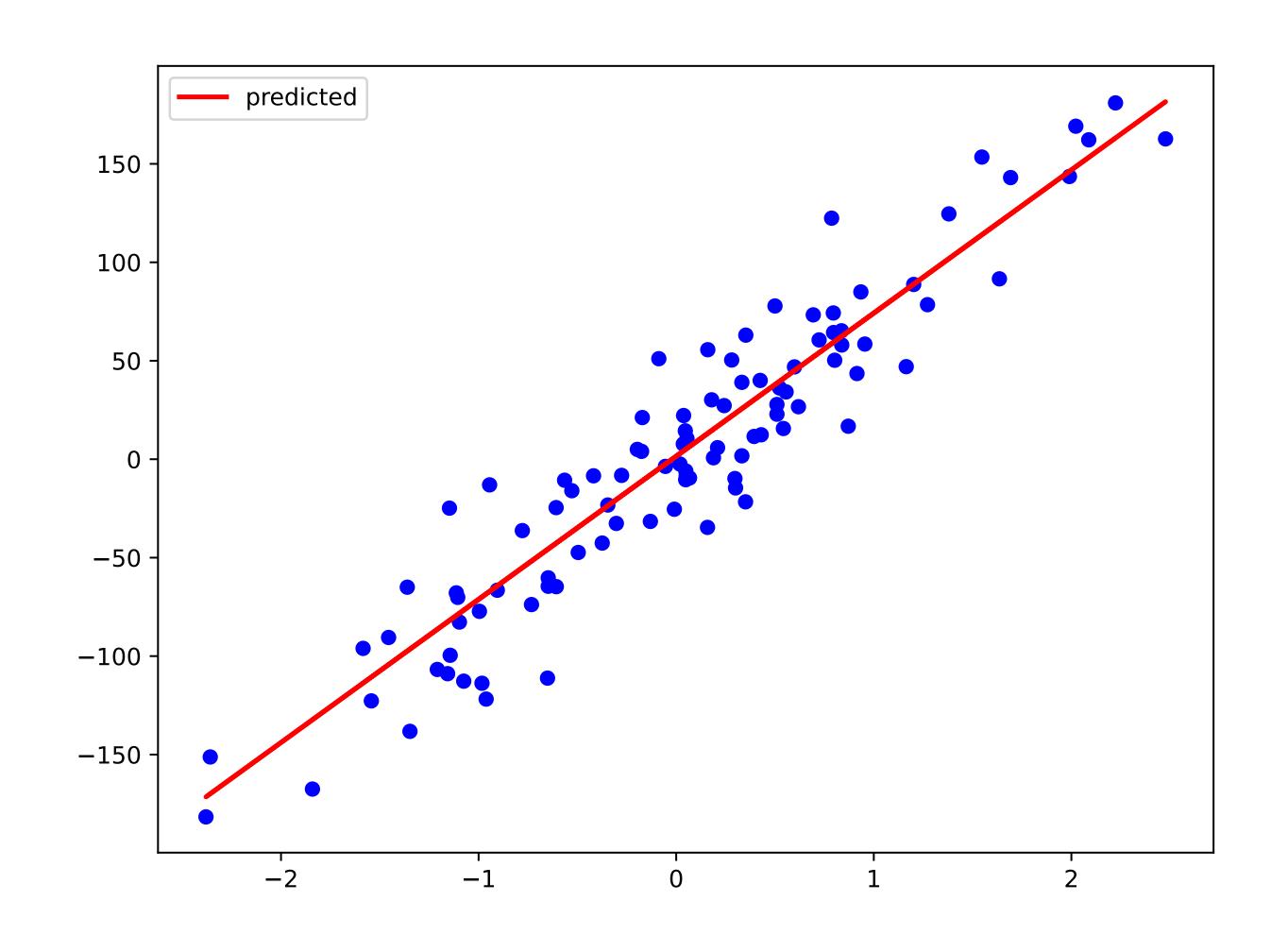


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- Used to *predict* continous values.
- Predict the value of a dependent variable based on the values of another independent variables.
- $\star$  General formulation, the inference function:  $y = X \cdot W + b$ 
  - y is the dependent variable: continous values we want to predict
  - X represent a data set of *n* samples and *m* features (independent variables).
  - W is a vector of weights (the unknown, we want to learn), of size (1,m).
  - b is a scalar value called the bias (unknown value, we want to learn).
- ★ The goal is to find vector of weights W and scalar term b

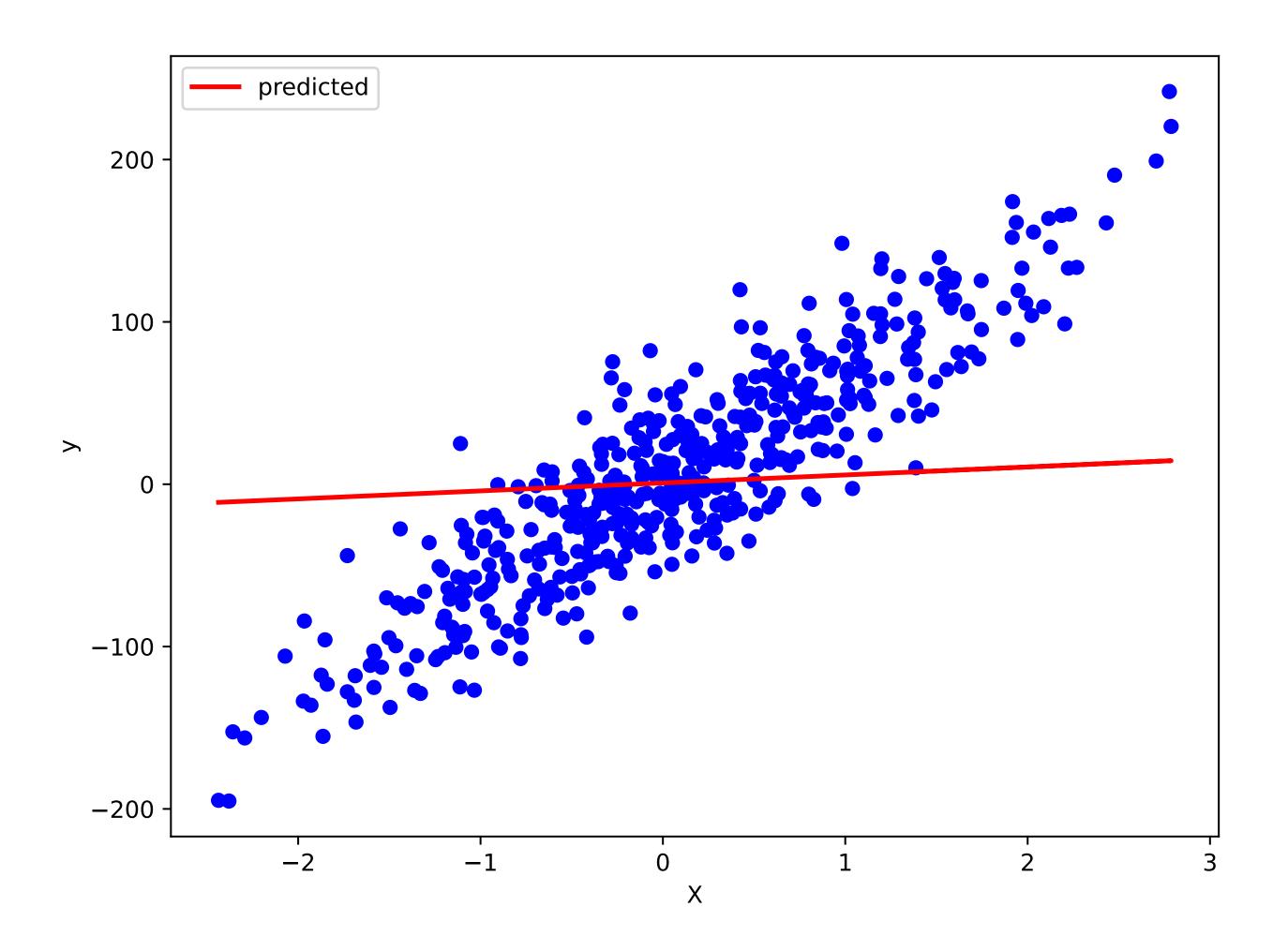
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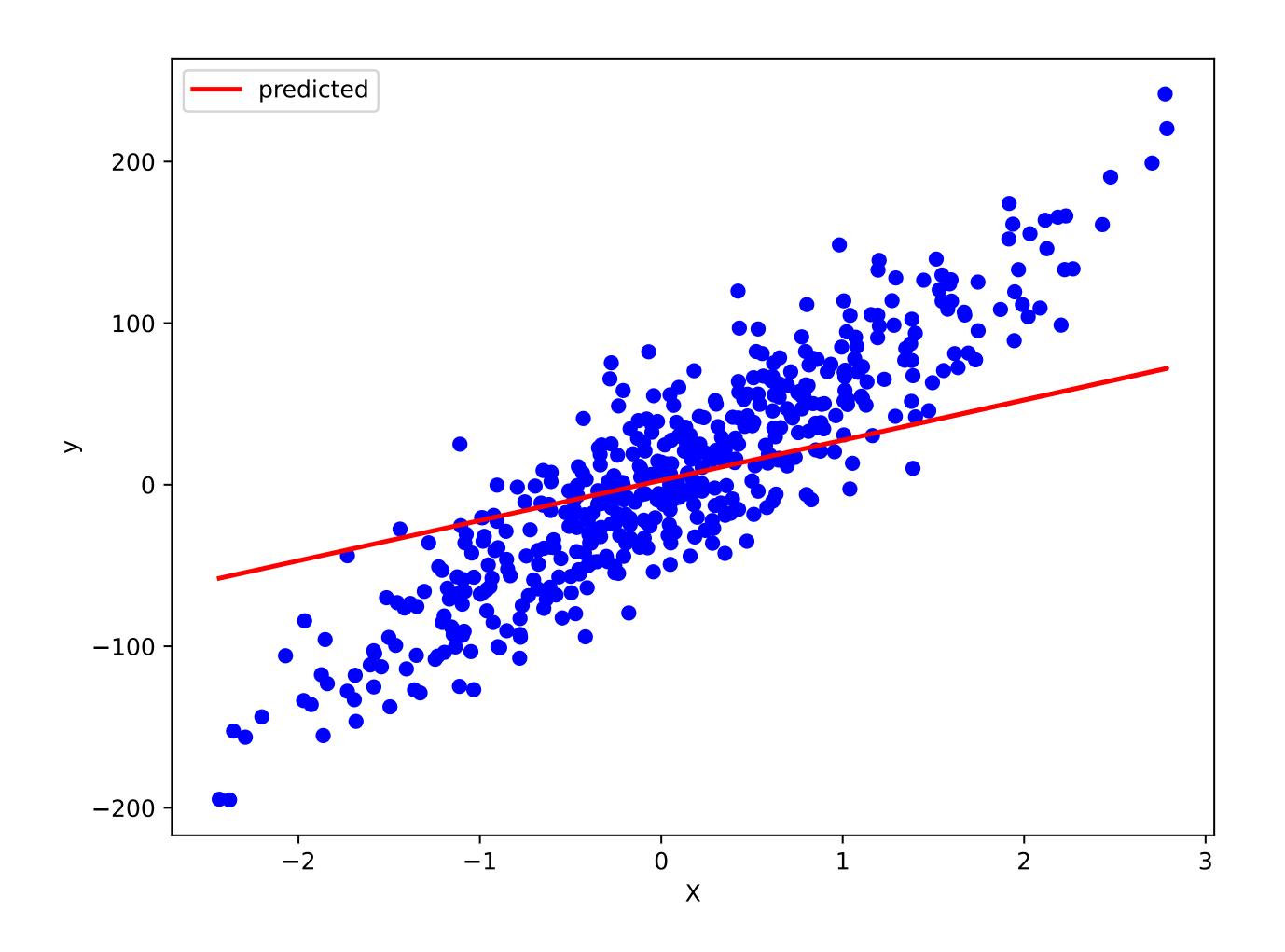
- We want to find the equation fiting the predicted line to the data.
- Example of data with only one weight (i.e. one feature 'w')
- Linear regression consists in finding this *infinite red line* (a line not a circle, arc, or other shape ... otherwise we need non-linear methods).
- We call this line a regression model.



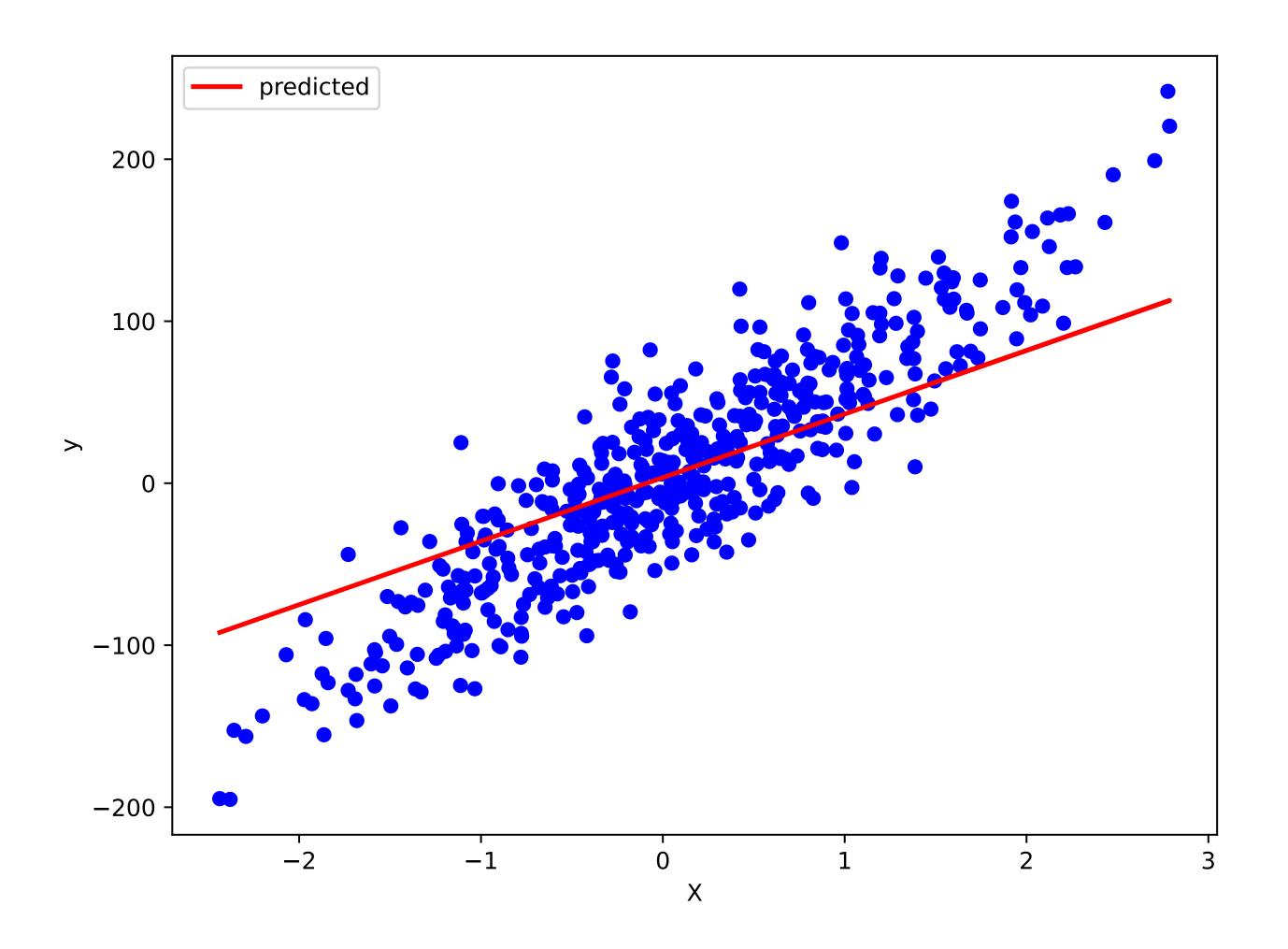
- Some value of weight 'w' and bias 'b'.
- These weights controls the shape of the line.



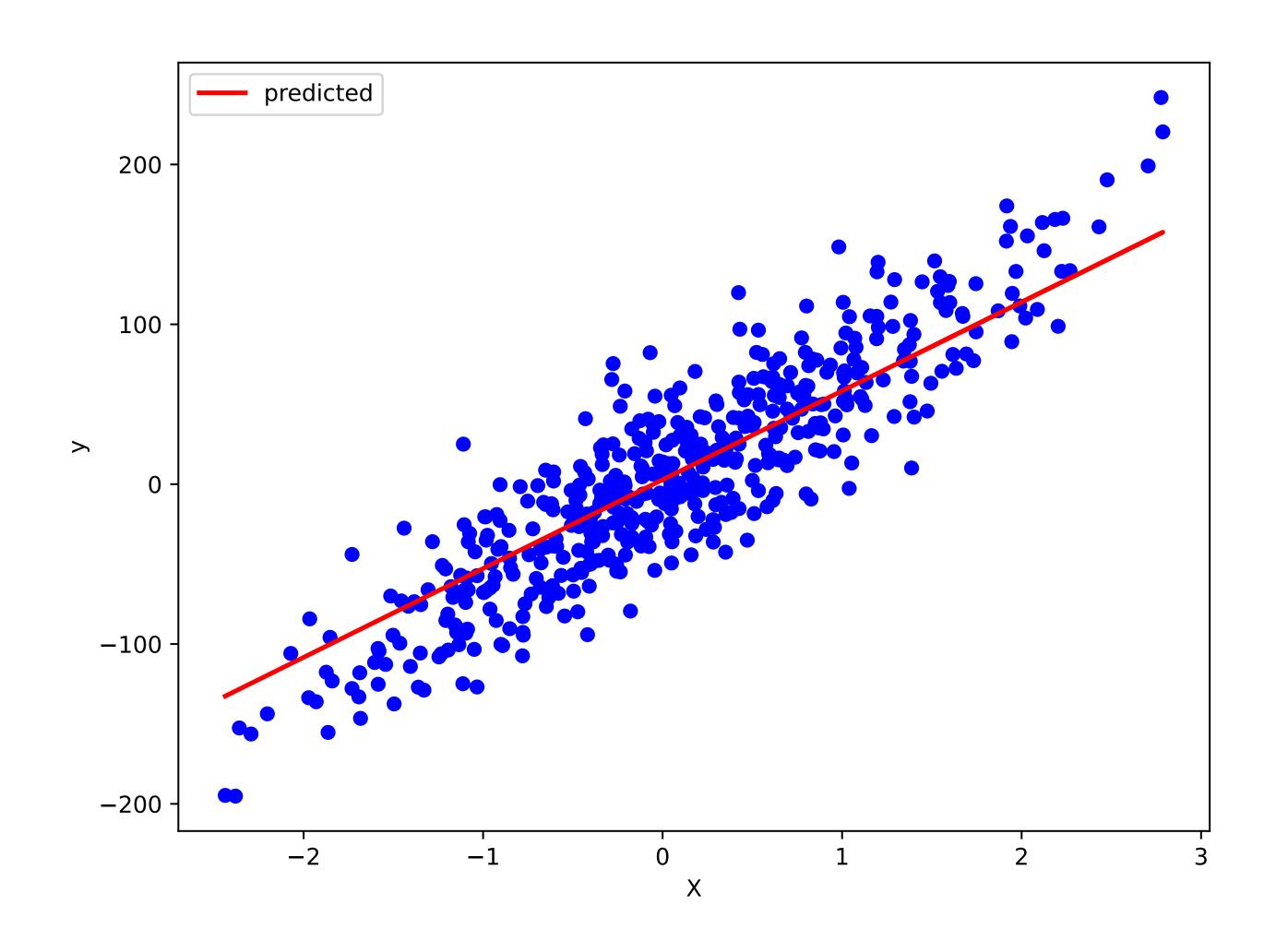
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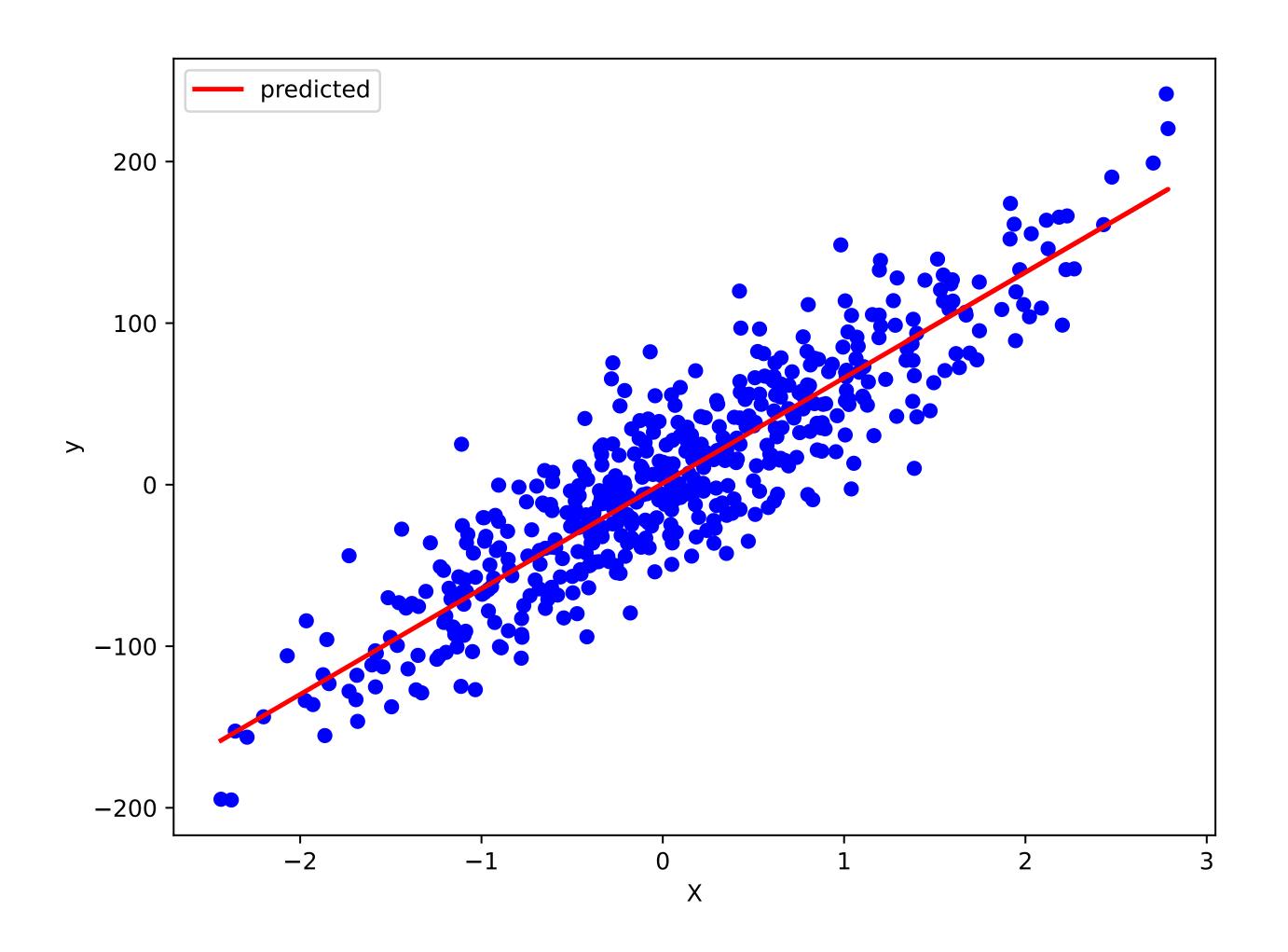
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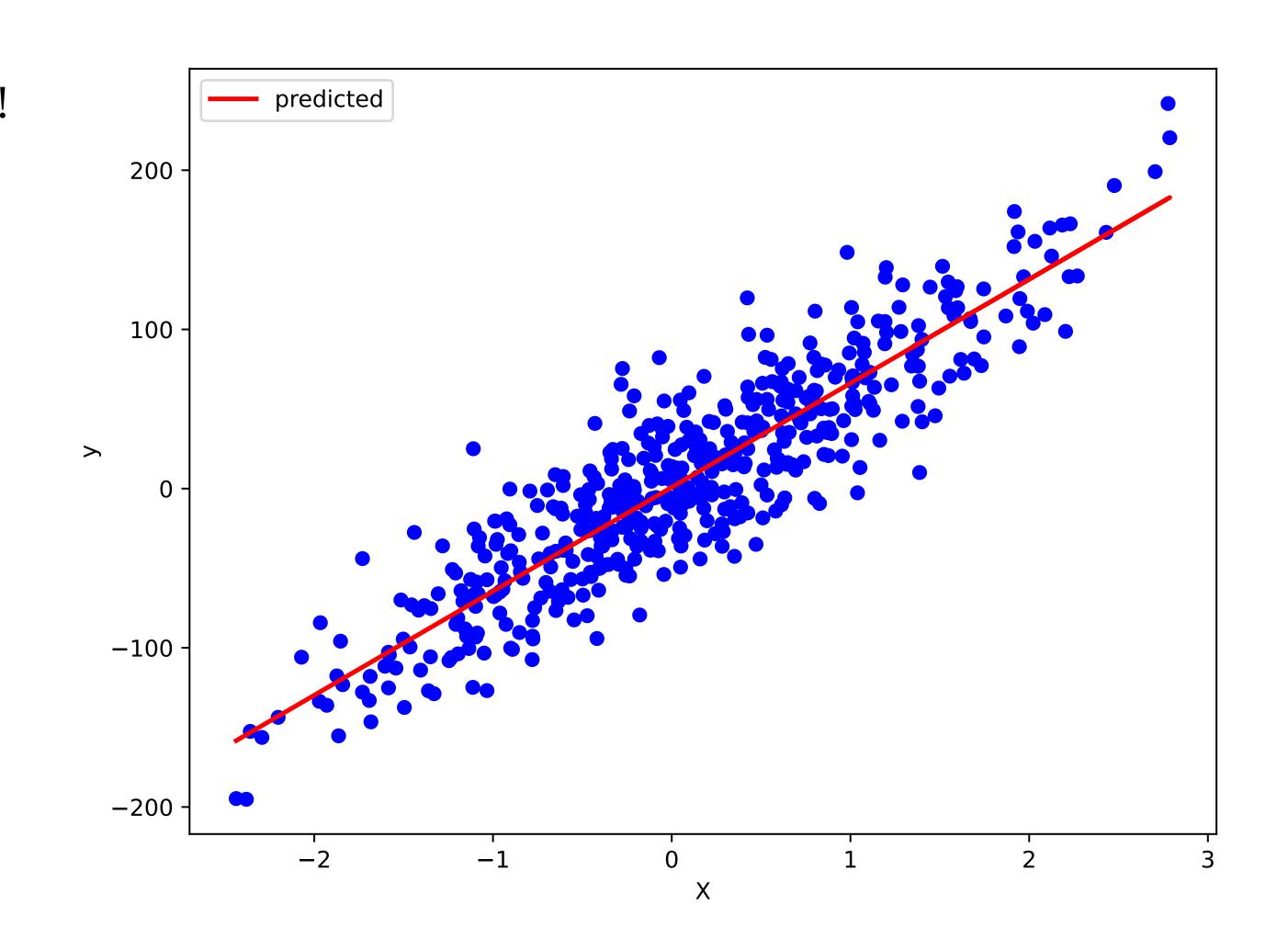
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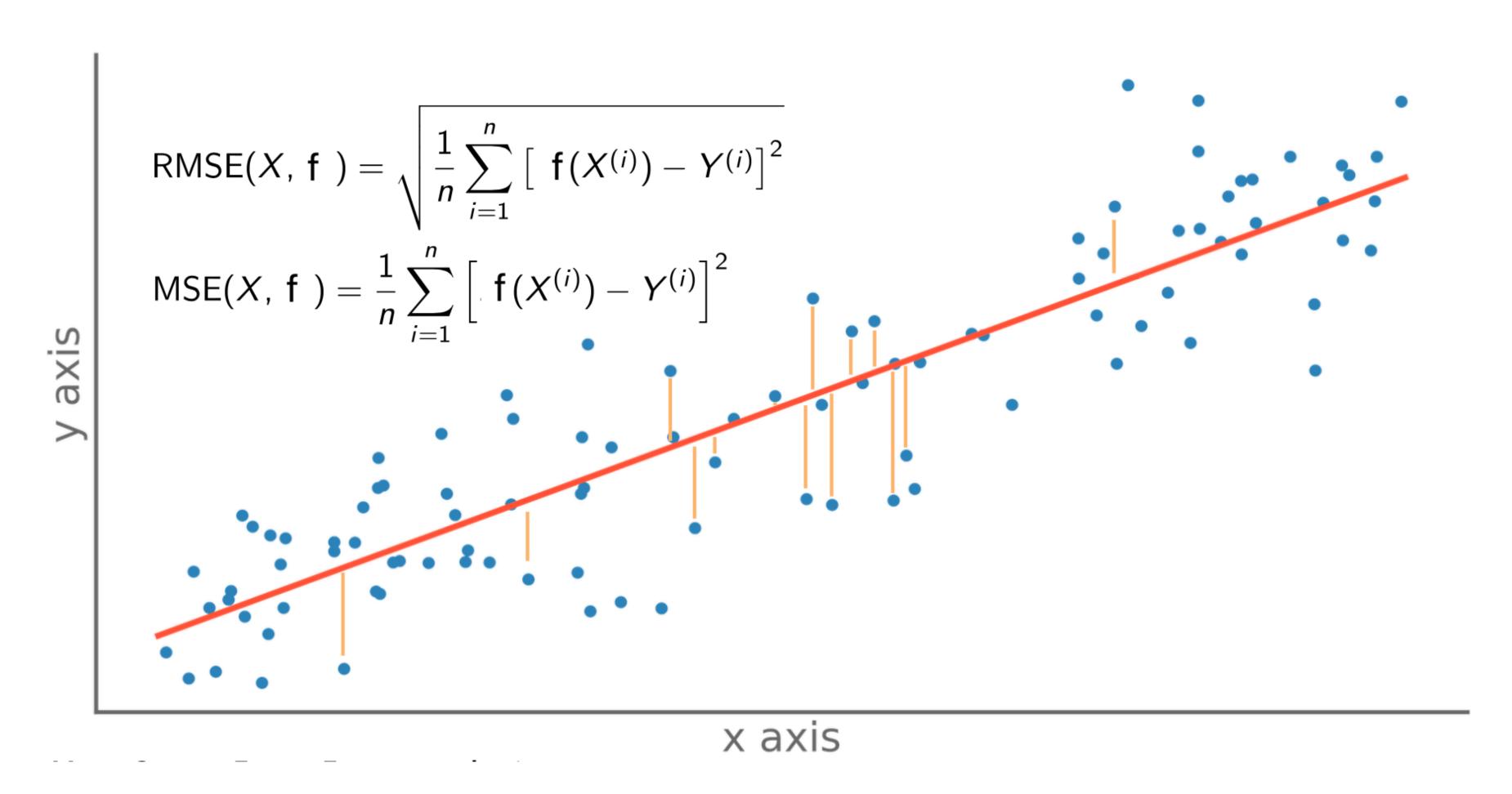
- Not easy to find the exact position of the line!
- We use an optimisation algorithm known as "Gradient Descent Algorithm".
- We can observe that the most fitting line is truly "close" to all the data points, especially when compared to the initial line (slide 6).



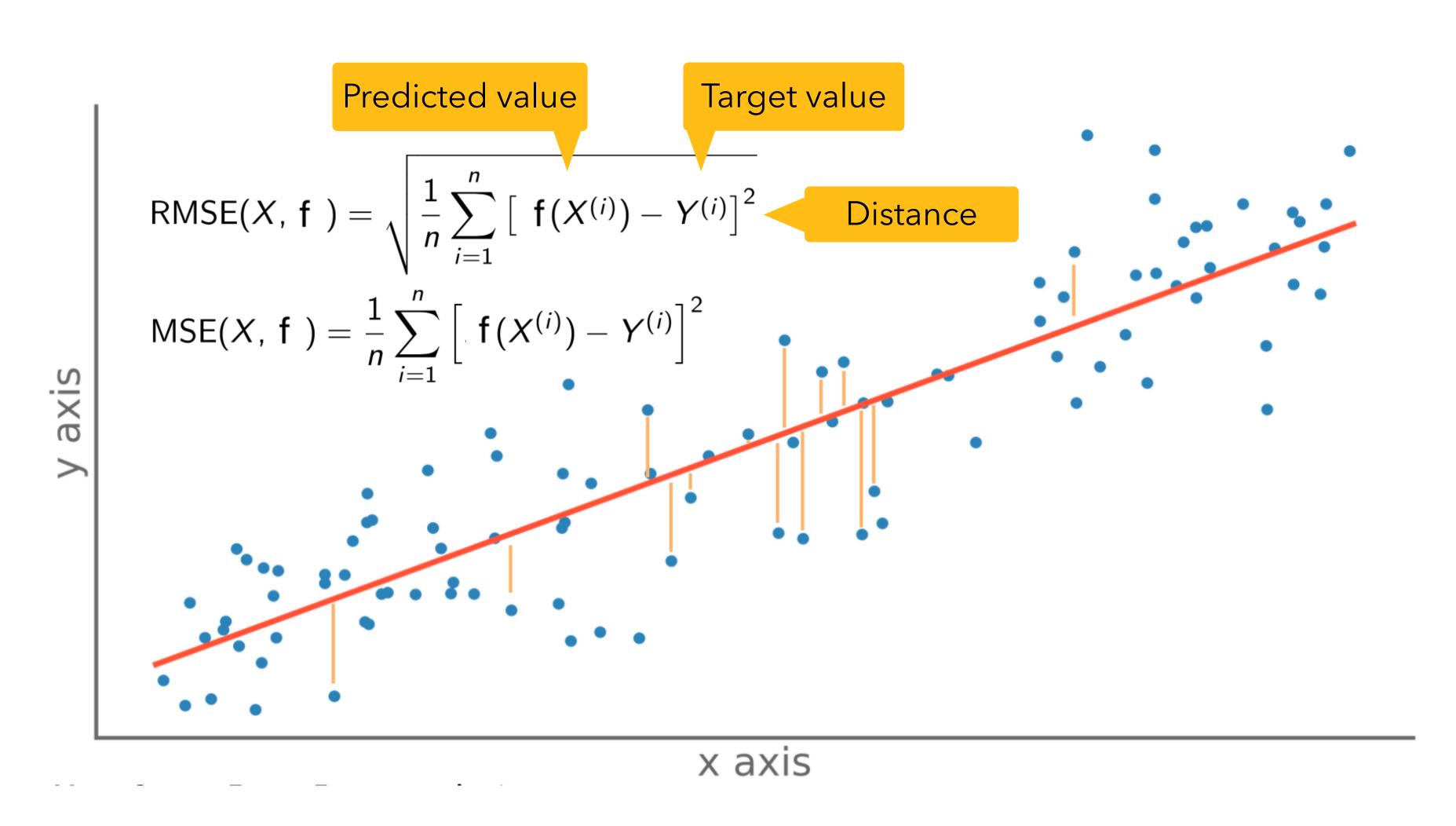
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- We can observe that the most fitting line is truly "close" to all the data points, especially when compared to the initial line (slide 6).
- This closeness is mathematically quantified by *a loss (or error) function*.
- The objective of GDA algorithm is to *minimize* this specified loss function.



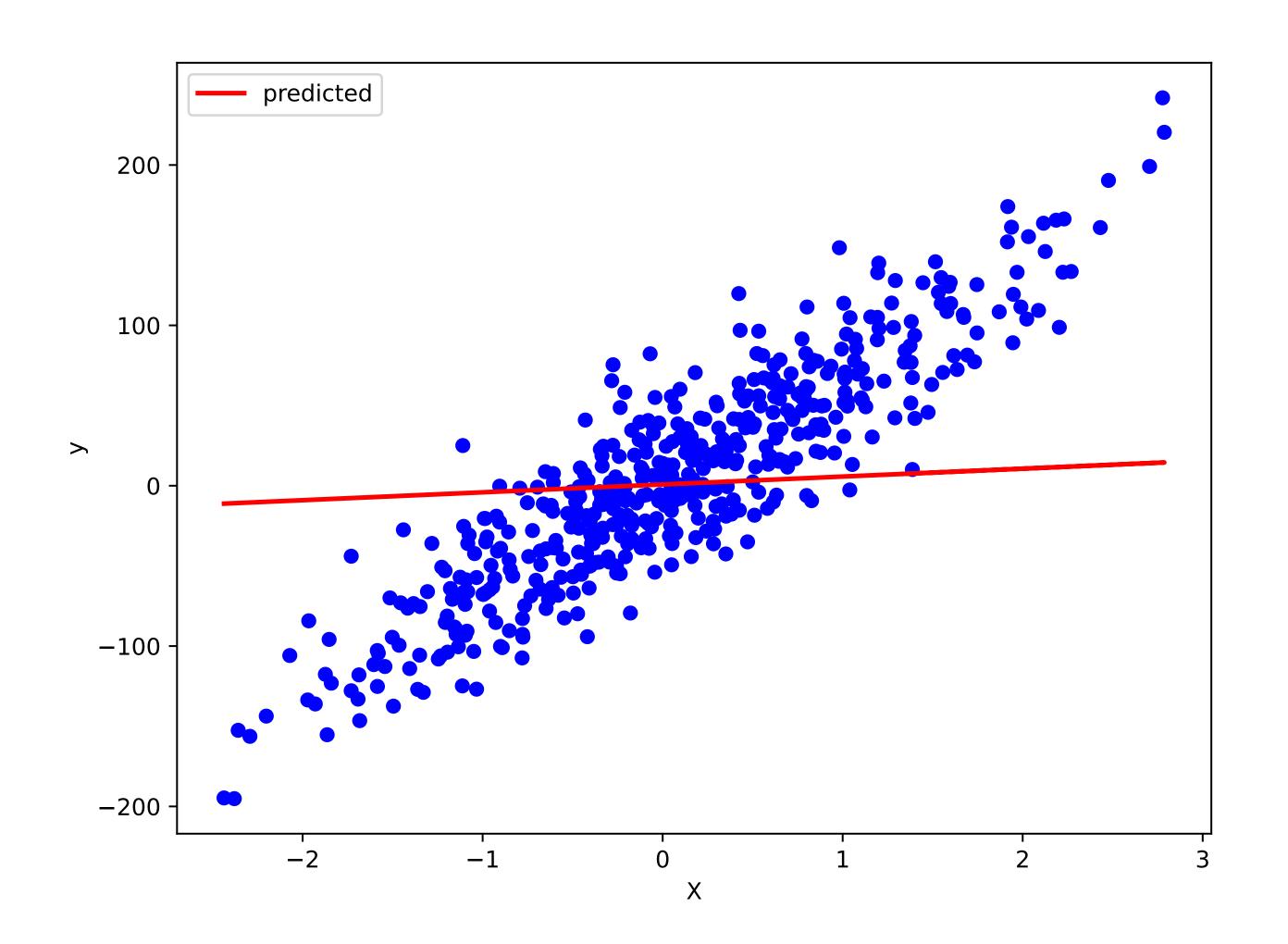
- Some of the most used error functions in LR:
- \* MSE: Mean Square Error function.
- \* RMSE: Root Mean Square Error function.



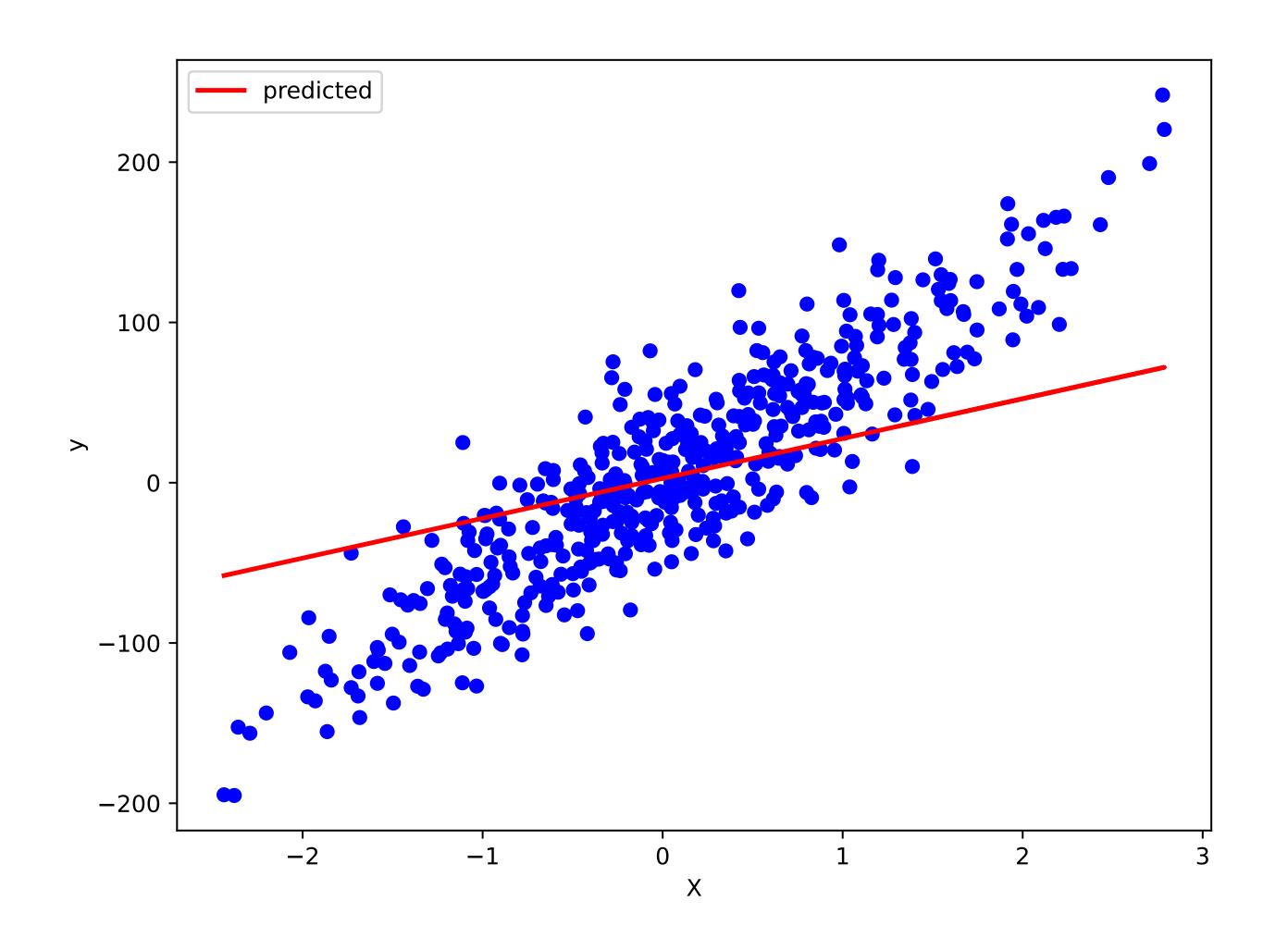
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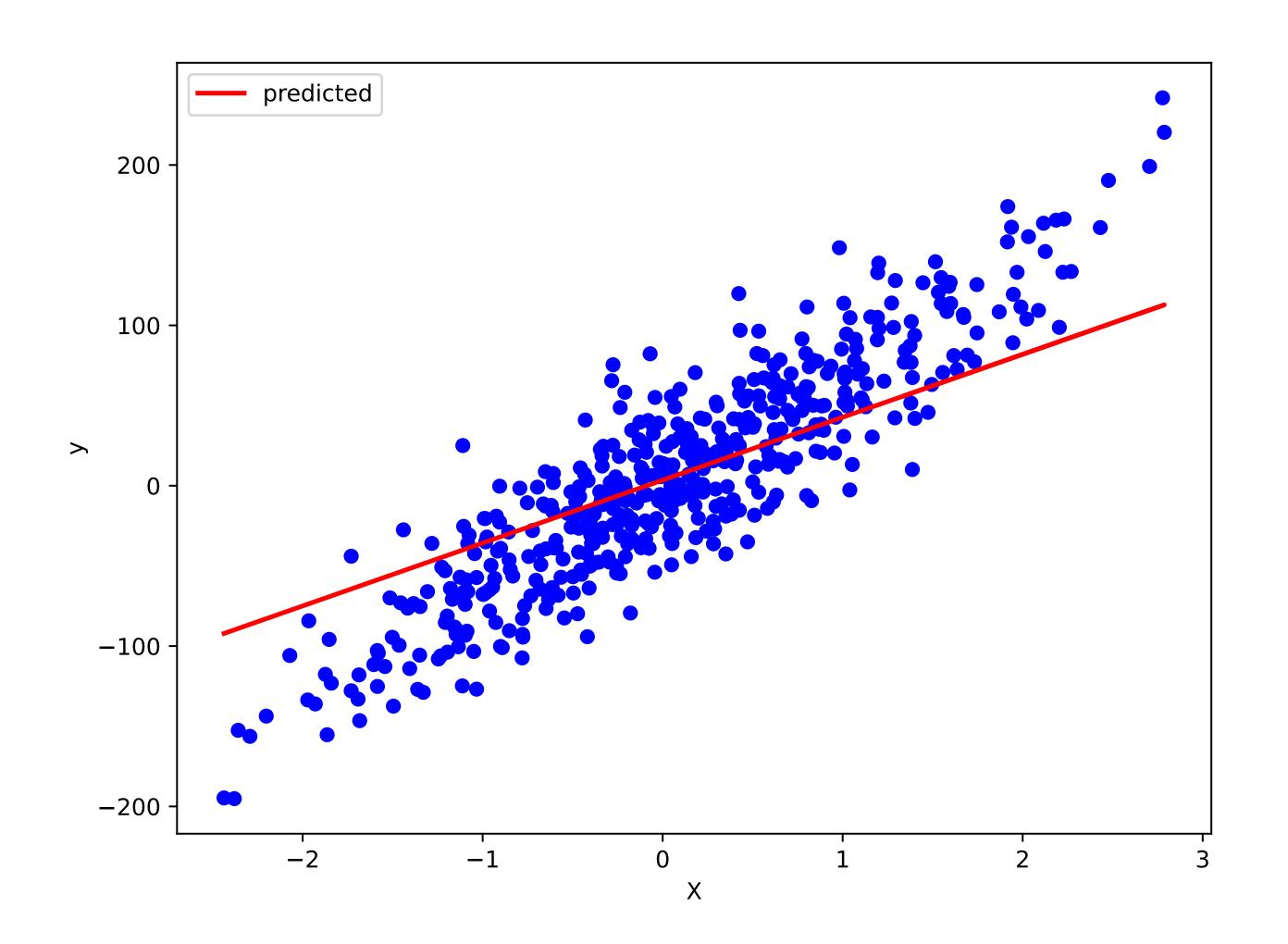
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- These weights controls the shape of the line.
- MSE = 4600



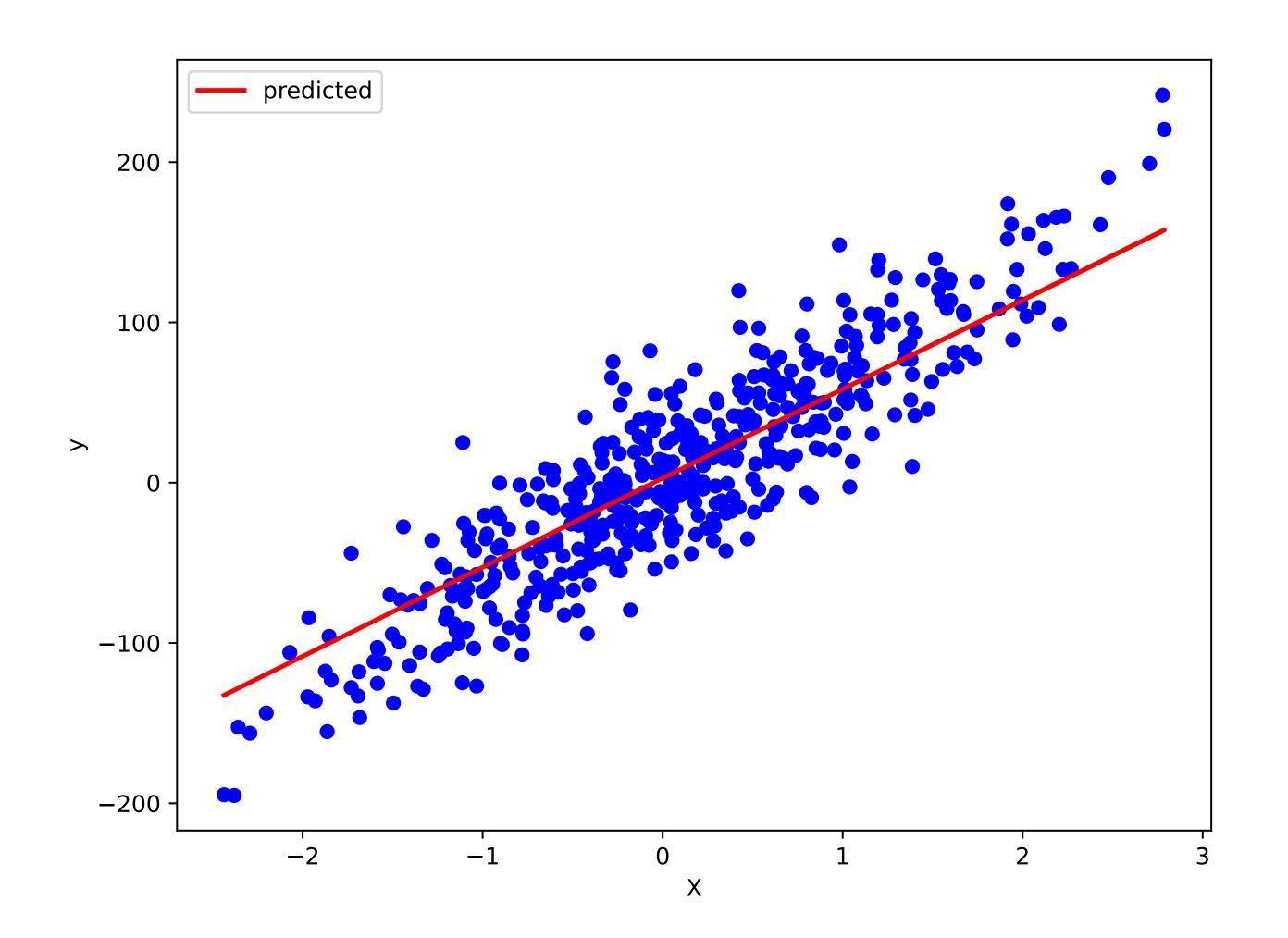
- Some value of weight 'w' and bias 'b'.
- These weights controls the shape of the line.
- $MSE = 2495 \downarrow$



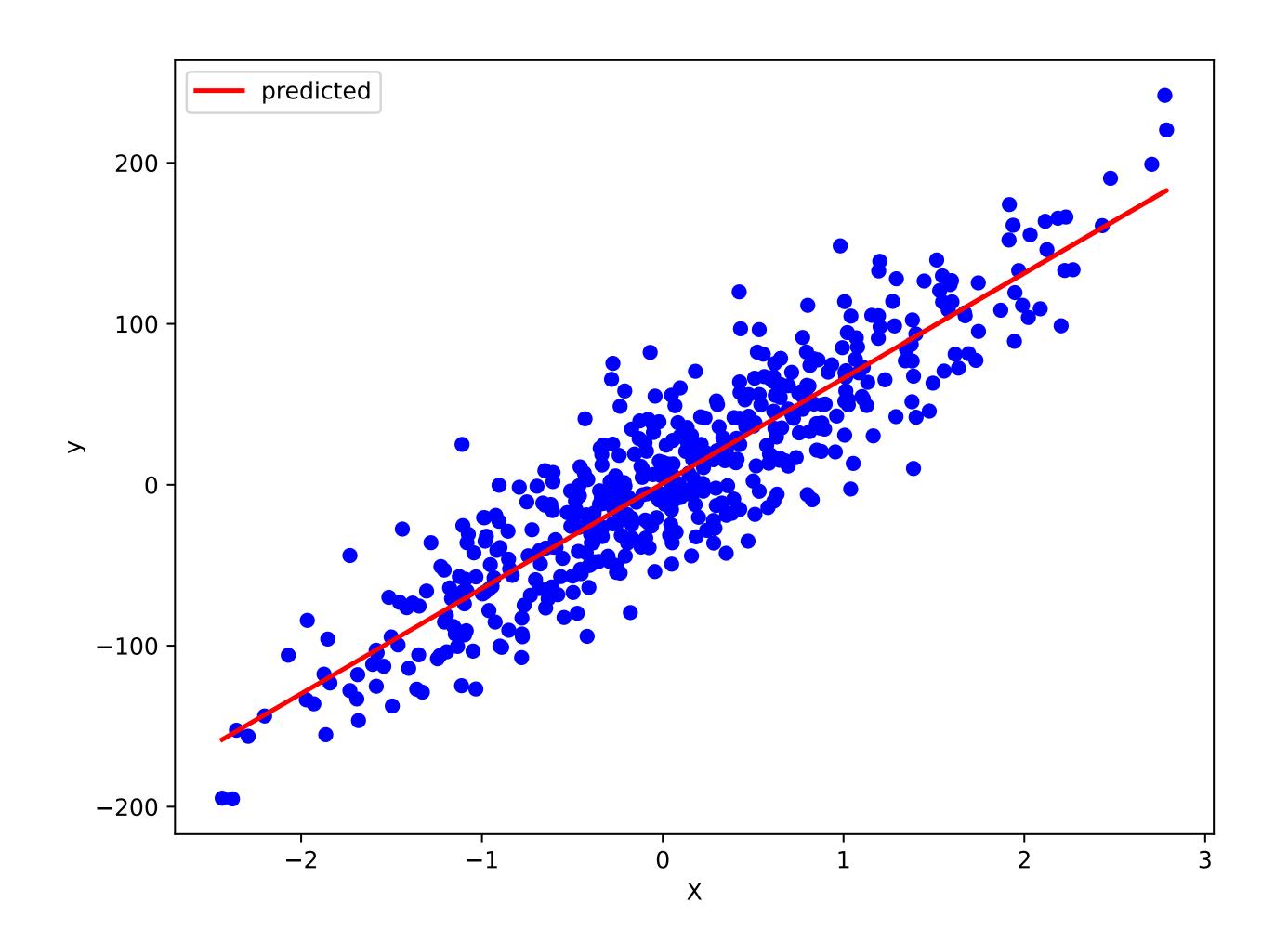
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- These weights controls the shape of the line.
- $MSE = 1520 \downarrow$



- Some value of weight 'w' and bias 'b'.
- These weights controls the shape of the line.
- MSE = 956
- Almost!



- Optimal value of weight 'w' and bias 'b'.
- We can observe, that most fited line is realy "close" to the whole data points, compared to the first line (in slide 6).
- MSE = 903



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• We first define 
$$J(W) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, y_i') = \frac{1}{n} \sum_{i=1}^{n} [y_i - y_i']^2$$
 (i.e. MSE equation)

• In matrix form : 
$$J(W) = \frac{1}{n} \sum_{i=1}^{n} [Y - (X.W + b)]^2$$

- We want to find weights W (and bias b ) that minimizes J(W), how ?
- ▶ Randomly ... but we can find a better and direct way : **gradient calculation**

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- The gradient of a function at a given point shows the direction of the fastest increase in the function's value.
- Gradient descent uses this property to find the function's minimum by systematically moving to the *opposite direction*.

### Gradient Descent Algorithm

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#### Gradient of weights:

$$\frac{\delta J(W)}{\delta W} = \frac{\delta}{\delta W} \left[ \frac{1}{n} \sum_{i=1}^{n} \left[ y_i - (x_i, W + b) \right]^2 \right]$$

$$= \frac{2}{n} \sum_{i=1}^{n} -x_i [y_i - (x_i, W + b)]$$

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#### ► Gradient of **bias** :

$$\frac{\delta J(W)}{\delta b} = \frac{\delta}{db} \left[ \frac{1}{n} \sum_{i=1}^{n} \left[ y_i - (x_i \cdot W + b) \right]^2 \right]$$

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$$= \frac{2}{n} \sum_{i=1}^{n} - \left[ y_i - y_i' \right]$$

$$= -\frac{2}{n} \left( Y - Y' \right) \quad \text{(matrix form)}$$

- $\rightarrow$  Entry: Data input values X of size (*n* samples, *m* features), data target values Y of size (*n*, 1) MaxIterations, learning rate  $\alpha$
- $\rightarrow$  Output: Weights W of size (1, m), and bias b

#### \* Training (Learning weights)

- **Initialisation**: random values for vector W, and bias b
- While termination condition:

#### For each sample $(x_i, y_i)$ :

- Calculate predicted value  $y_i' = x_i \cdot W + b$
- Compute gradient  $\frac{\delta J(W)}{\delta W}$  and  $\frac{\delta J(W)}{\delta b}$
- Updating weights :  $W = W \alpha \frac{\delta J(W)}{\delta W}$  Updating bias :  $b = b \alpha \frac{\delta J(W)}{\delta b}$
- (3) Return W, b

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#### \* Learning rate $\alpha \in [0,1]$

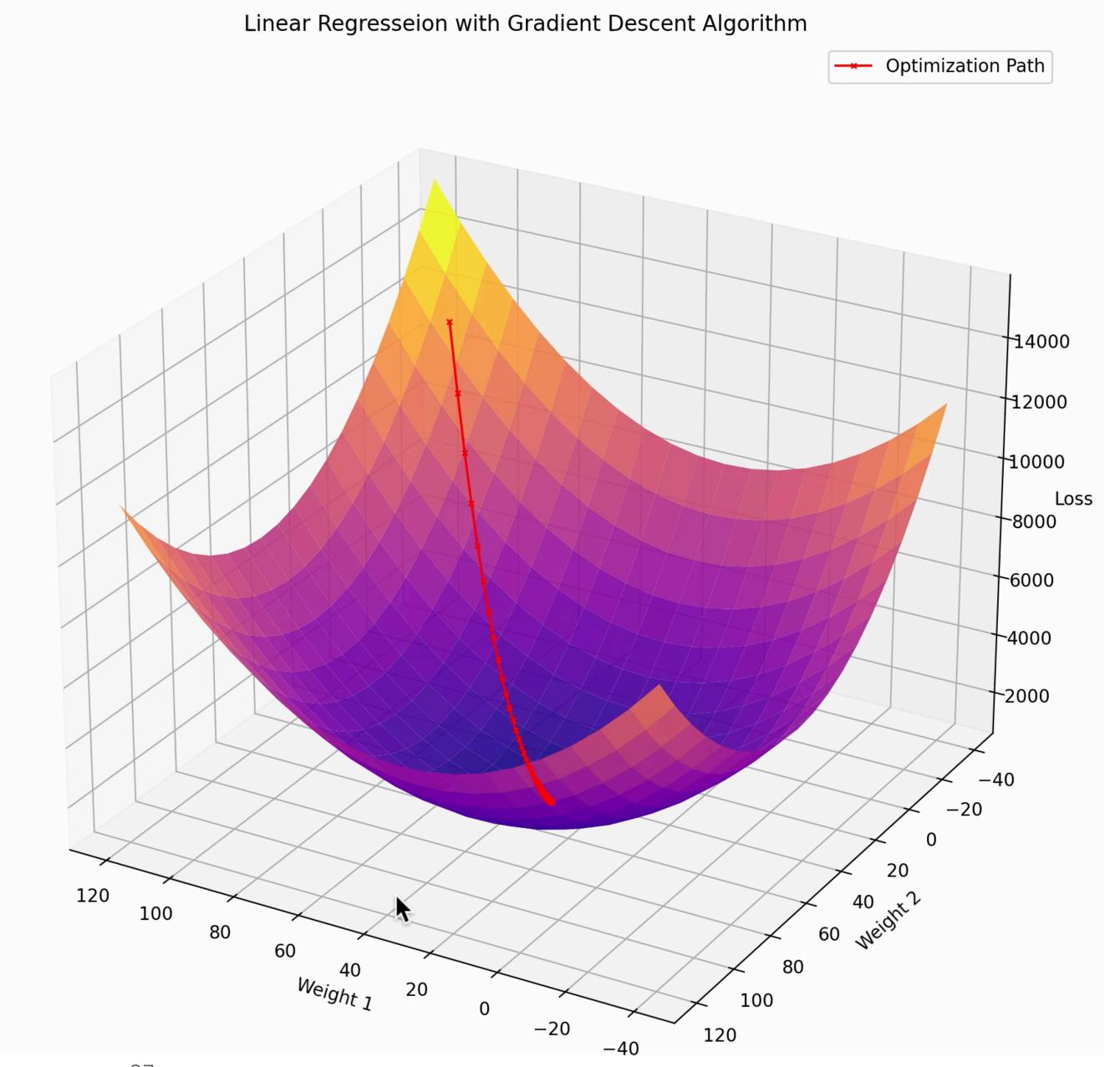
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- Big value => Big updating steps
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#### **★** Prediction (Testing model)

Simply calculate  $y_i' = x_i$ . W + b

### Linear Regression GDA & Loss landscape

- Observe here, a model with two weights (not a single weight as in the former example!).
- For each paire (weight1, weight 2), MSE value (third axis) is calculated. Obtaining MSE landscape.
- So the GDA algorithm: starts from some value of weights, then minimize progressively MSE error until arriving to optimal value.
- The GDA algorithm trajectory is ploted in red.
- MSE is a convex function!



## Practical Activity 1 (part I)

**Linear Regression** 

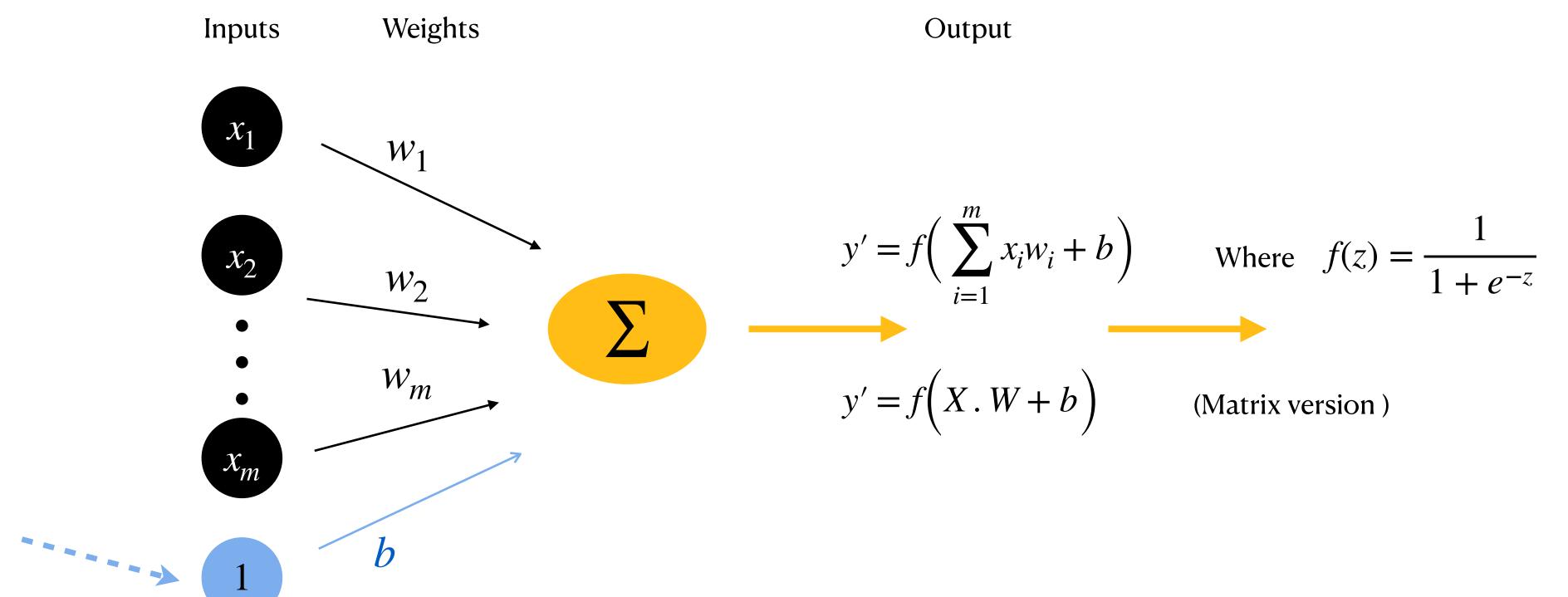
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- LABs comprise groups of up to 2 students.
- Bonuses can be attributed! if the teacher considers the results to be relevant.

# Logistic Regression Formalism

- One of fundamental methods in *superviserd Machine Learning*.
- Used for binary classification tasks!
- Outcome variable is categorical with two possible outcomes (e.g., 0 or 1)
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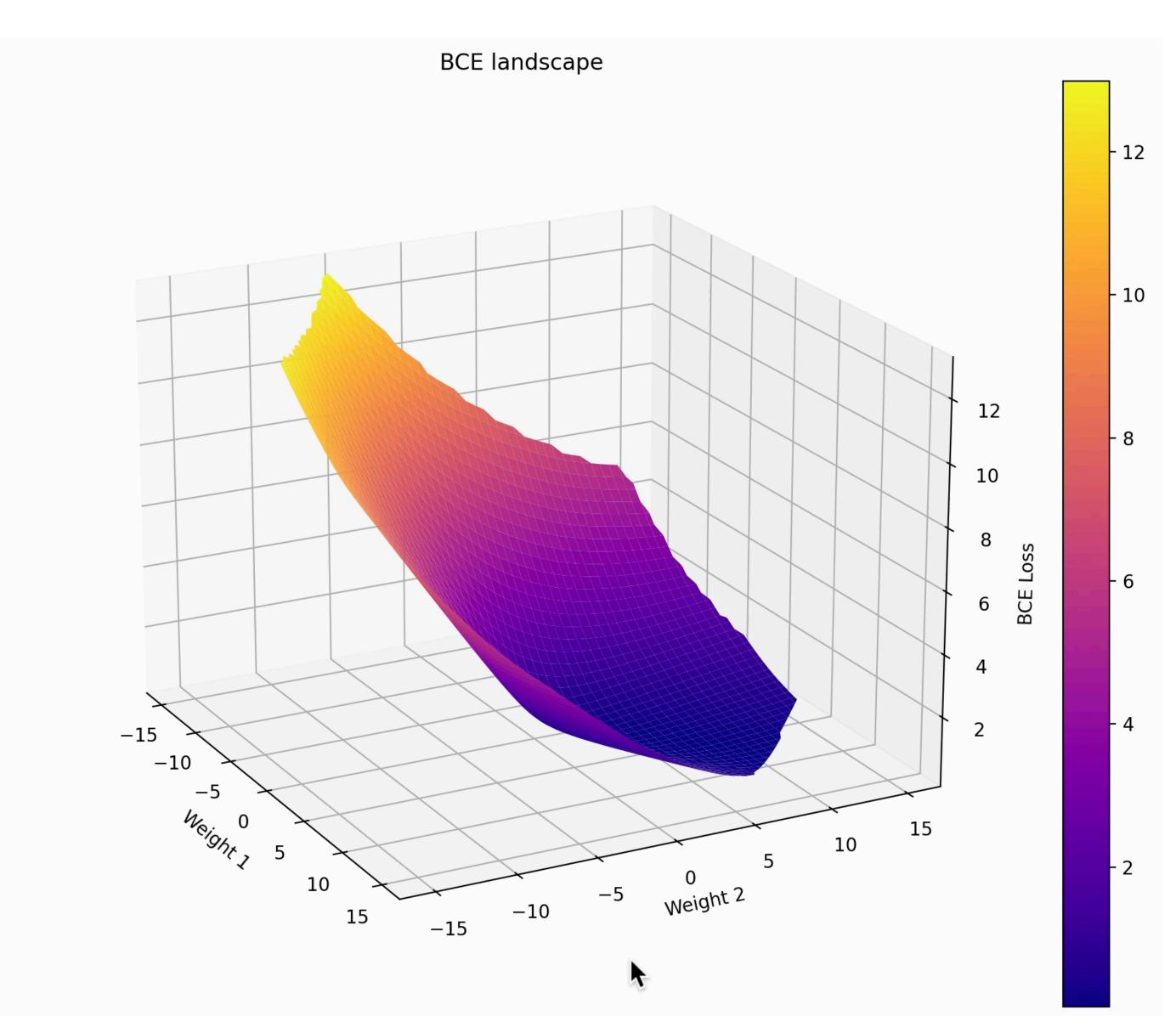


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- ★ General formulation, the inference function: y = f(X.W + b) where  $f(z) = \frac{1}{1 + e^{-z}}$ 
  - y is the dependent variable: continous values we want to predict
  - X represent a data set of *n* samples and *m* features (independent variables).
  - W is a vector of weights (the unknown, we want to learn), of size (1,m).
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- ★ The goal is to find vector of weights W and scalar term b

# Logistic Regression Loss function

- Logistic regression does not use MSE because its output is probabilistic bounded between 0 and 1.
- It uses a loss function known as the log loss (or *Binary* Cross-Entropy loss) for binary classification.
- It measures the penalty for a given class prediction in terms of the distance from the actual label.
- $J(W) = -\frac{1}{n} \sum_{i=1}^{n} \left[ y_i log(y_i') + (1 y_i) log(1 y_i') \right]$
- → *BCE* is a convex function, for simple LR case!



# Logistic Regression Gradient Descent Algorithm

- As for MSE error, BCE is also convex which ensures that Gradient Descent Algorithm has a global minimum
- Before introducing this algorithm, let's first discuss the underlying intuition.

► We first define : 
$$J(W) = -\frac{1}{n} \sum_{i=1}^{n} \left[ y_i log(y_i') + (1 - y_i) log(1 - y_i') \right]$$
 (i.e. BCE equation)

- Where :  $y'_i = \frac{1}{1 + e^{-(X.W+b)}}$  (i.e. the sigmoid function)
- We want to find weights W (and bias b ) that **minimizes** J(W), we calculat gradients :

► Gradient of weights : 
$$\frac{\delta J(W)}{\delta W} = -\frac{1}{n}X^T(Y - Y')$$

► Gradient of bias : 
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## Logistic Regression

### Gradient Descent Algorithm

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#### Training (Learning weights)

- (1) **Initialisation**: random values for vector W, and bias b
- (2) While termination condition:

#### For each random sample $(x_i, y_i)$ :

- Calculate predicted value  $y'_i = \left[1 + e^{-(x_i \cdot W + b)}\right]^{-1}$
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- (3) **Return** *W*, b

#### **\*Learning rate** $\alpha \in [0,1]$

- needs to be adjusted carrefully
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#### **★**Prediction (Testing model)

- Simply calculate  $y'_i = \left[1 + e^{-(x_i \cdot W + b)}\right]^{-1} \in [0,1]$
- if  $(y_i' \ge Threshold)$  then  $x_i$  is a cat else  $x_i$  is a dog

#### **★**Accuracy

An accuracy function may be used to verify the accuracy of the model: predicted classes Vs target classes for each  $x_i$ .

### Summary: Distinctions

	Linear Regression	Logistic Regression
The purpose	<b>Prediction</b> of continuous values	Binary <b>Classification</b>
The model form	X.W+b	$\left[1 + e^{-(X.W+b)}\right]^{-1}$
The loss function	Mean Squared Error (MSE)	Binary Cross-Entropy (BCE)
The algorithm	GDA	GDA
Limitation	Data landscape must be linear	Linear separation of data

For more complicated data landscapes => Polynomial Regression or use of Neural Networks.

### Summary: Use cases

Linear Regression	Logistic Regression
Prediction of <i>adult characteristics</i> based on parent's characteristics	Fraud detection: can help teams identify anomalies in data that may predict fraud
Predicting <i>product sales</i> volume as a function of price, time of year and store location	Disease prediction: Predicting whether a person will develop heart disease based on IMC, smoking habits and genetic predisposition
Predict the <i>price of an airline ticket</i> as a function of origin, destination, time of year and airline company	Attrition prediction: it could be useful for HR and management to know whether high-performing employees are at risk of leaving the organization

## Practical Activity 1 (part II)

**Logistic Regression** 

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