Implementing Regression and Classification Using Neural Networks in scikit-learn

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Overview

Regression models using neural networks in scikit-learn

Mean square error (MSE) loss function

Using the MLPRegressor estimator to build regression models

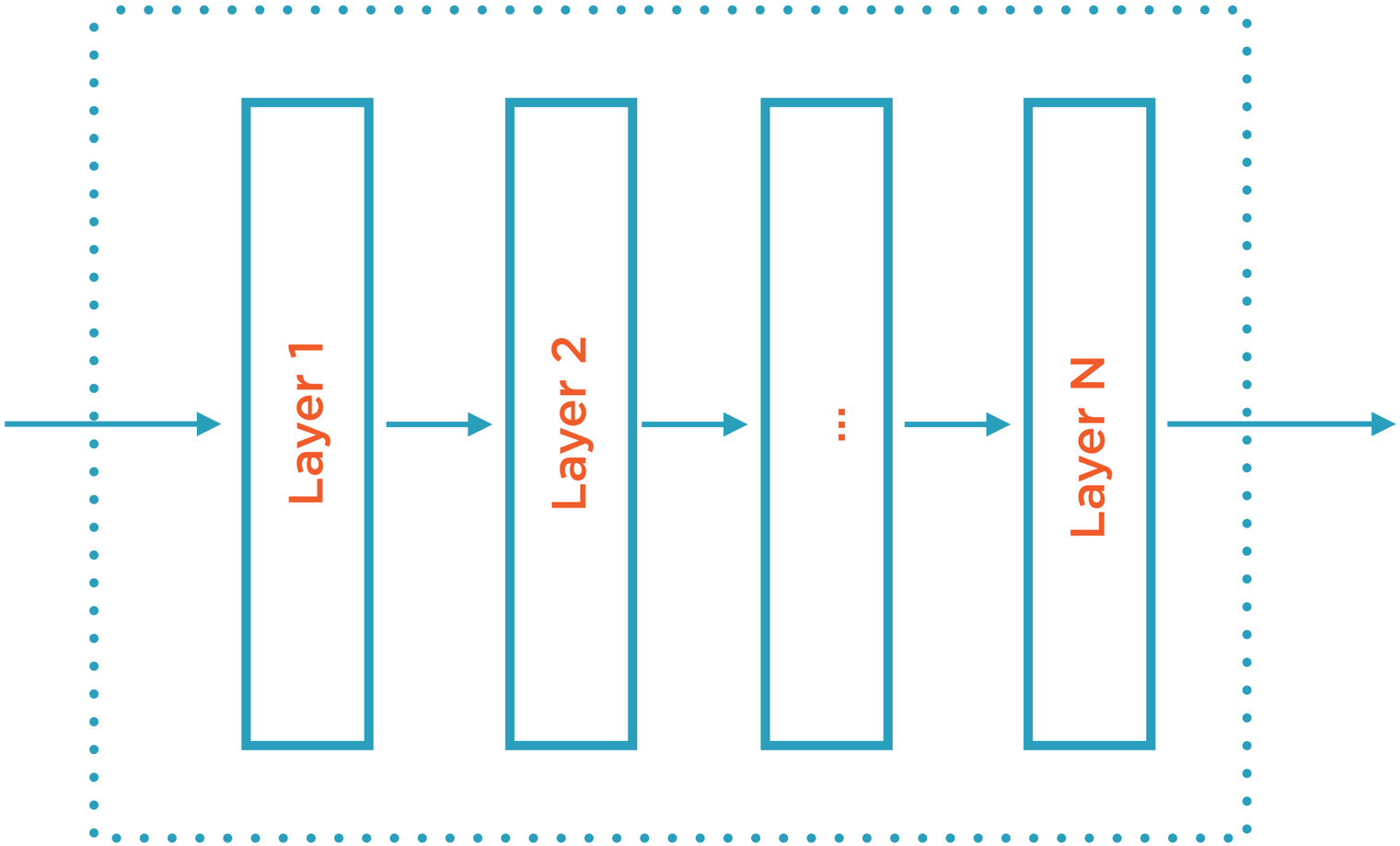
Classification models using neural networks in scikit-learn

Cross-entropy loss function

Using the MLPClassifier estimator to build classification models

Regression Using Neural Networks

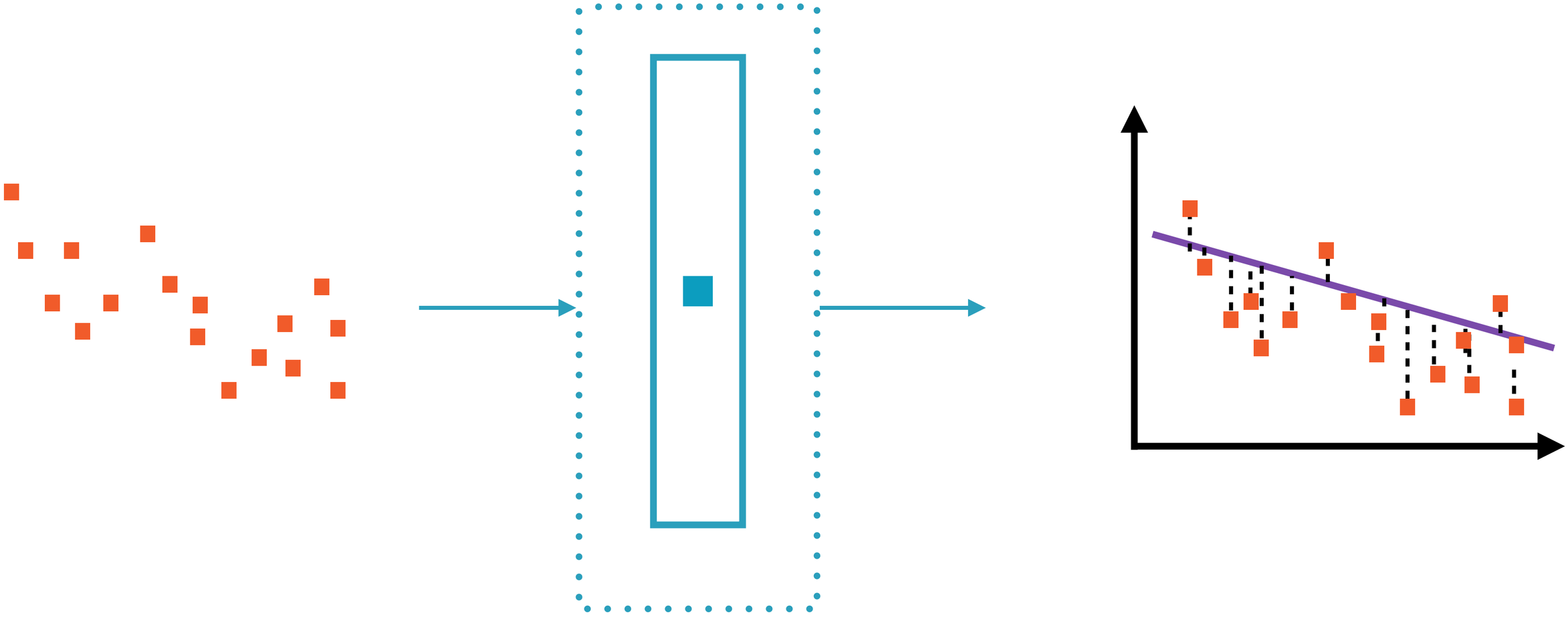
Neural Network Model



Network of interconnected layers

The **weights** and **biases** of individual neurons are determined during the **training** process

Regression: The Simplest Neural Network

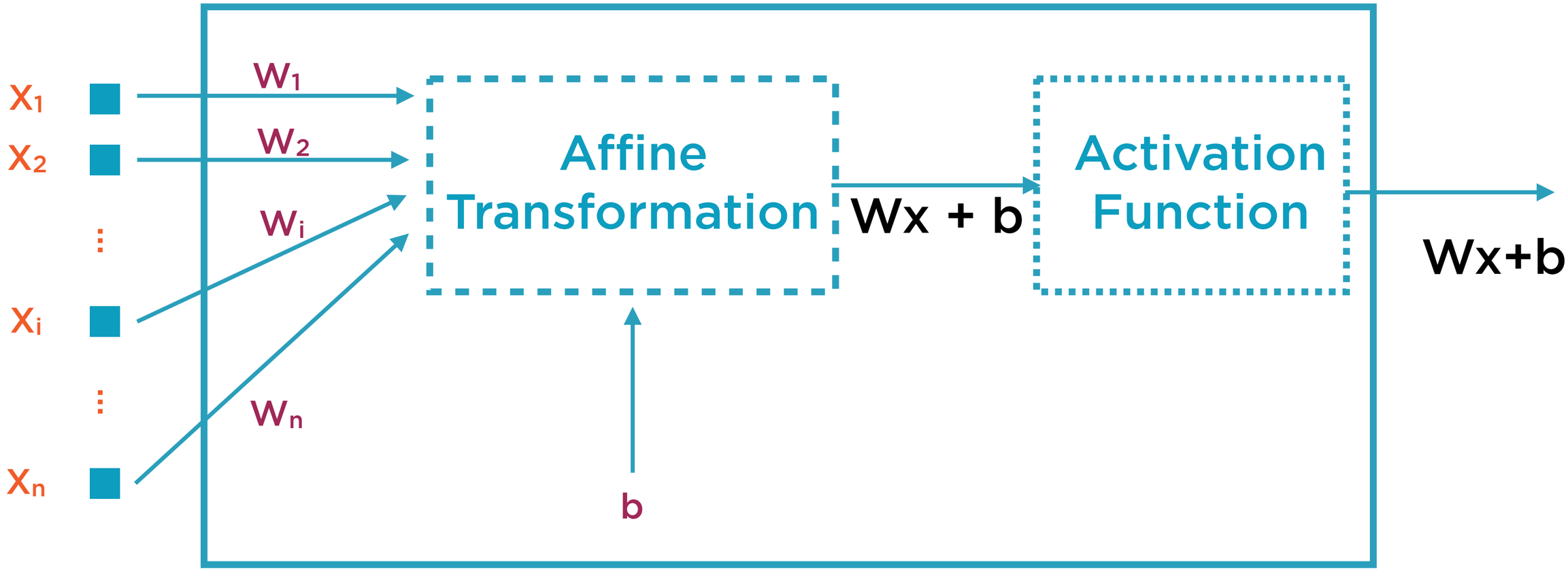


Set of Points

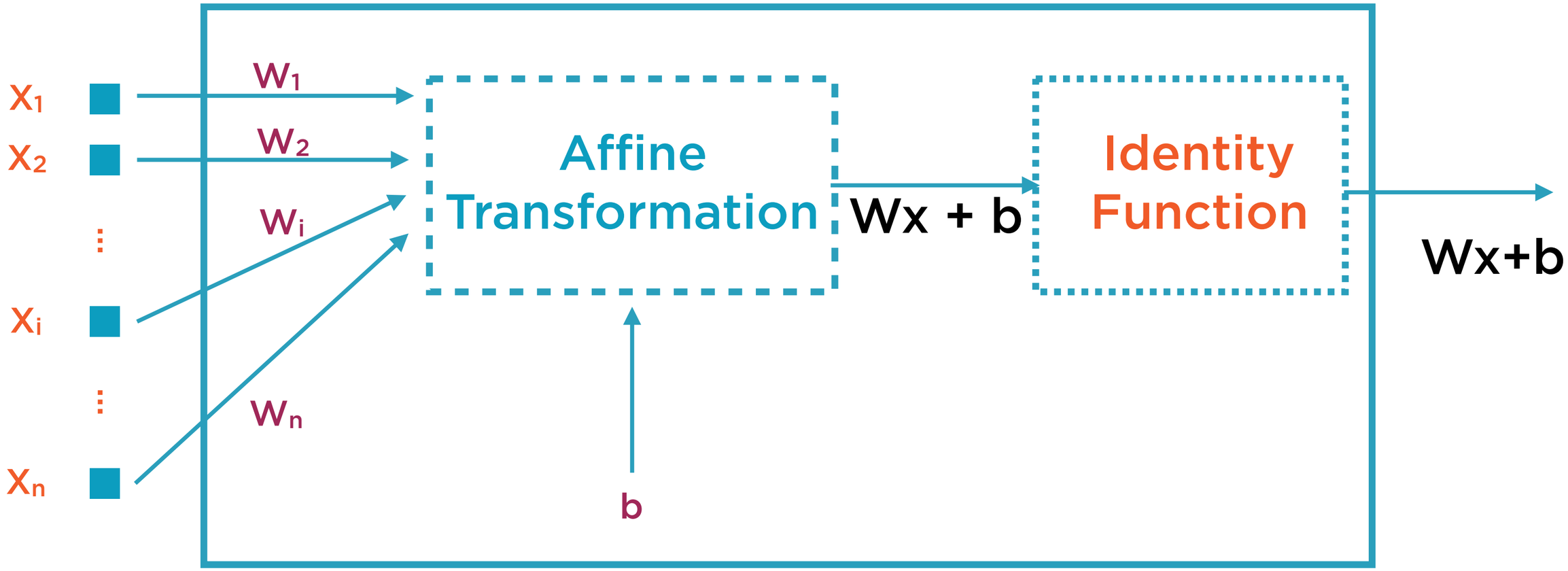
Single Neuron

Regression Line

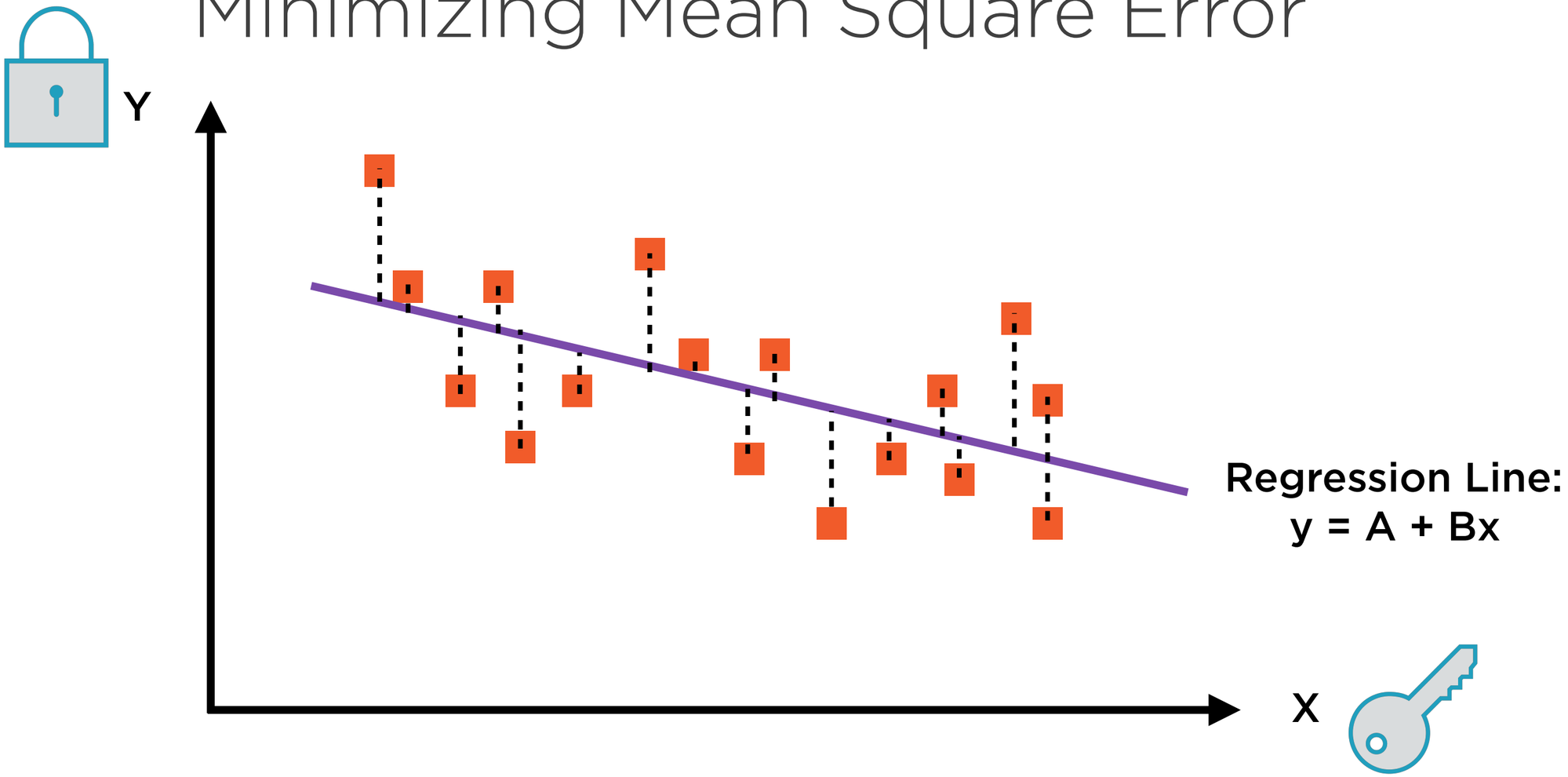
Regression: The Simplest Neural Network



Regression: The Simplest Neural Network



Minimizing Mean Square Error



The “best fit” line is called the regression line

The actual training of a neural network happens via Gradient Descent Optimization

Linear Regression as an Optimization Problem

Objective Function

Minimize variance of the residuals (MSE)

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Constraints

Express relationship as a straight line

$$y = Wx + b$$

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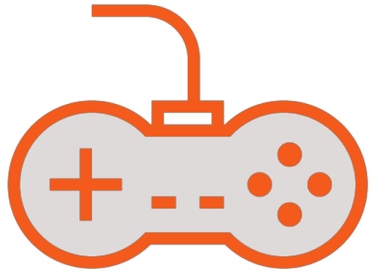
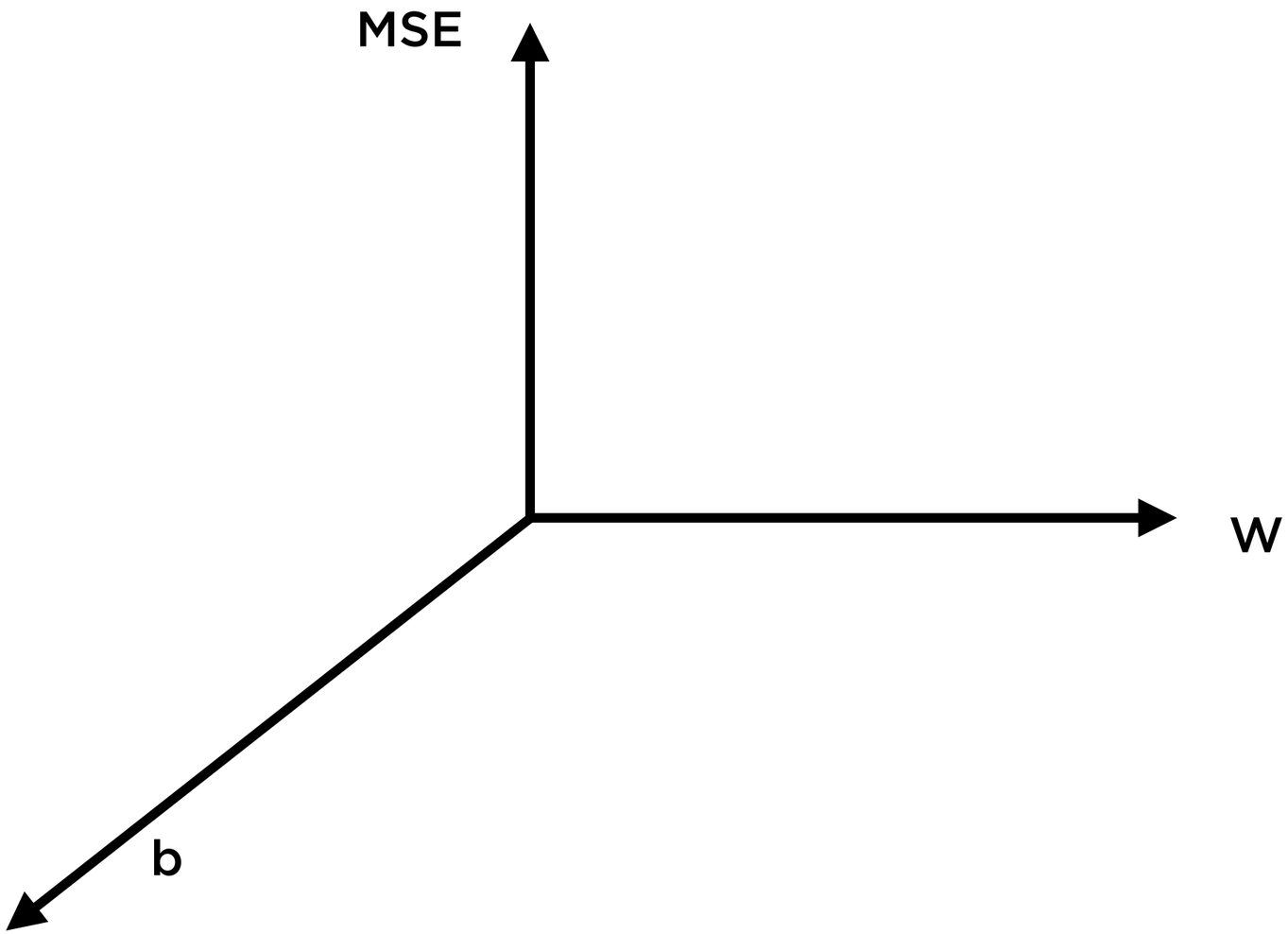


Decision Variables

Values of W and b

Minimizing MSE



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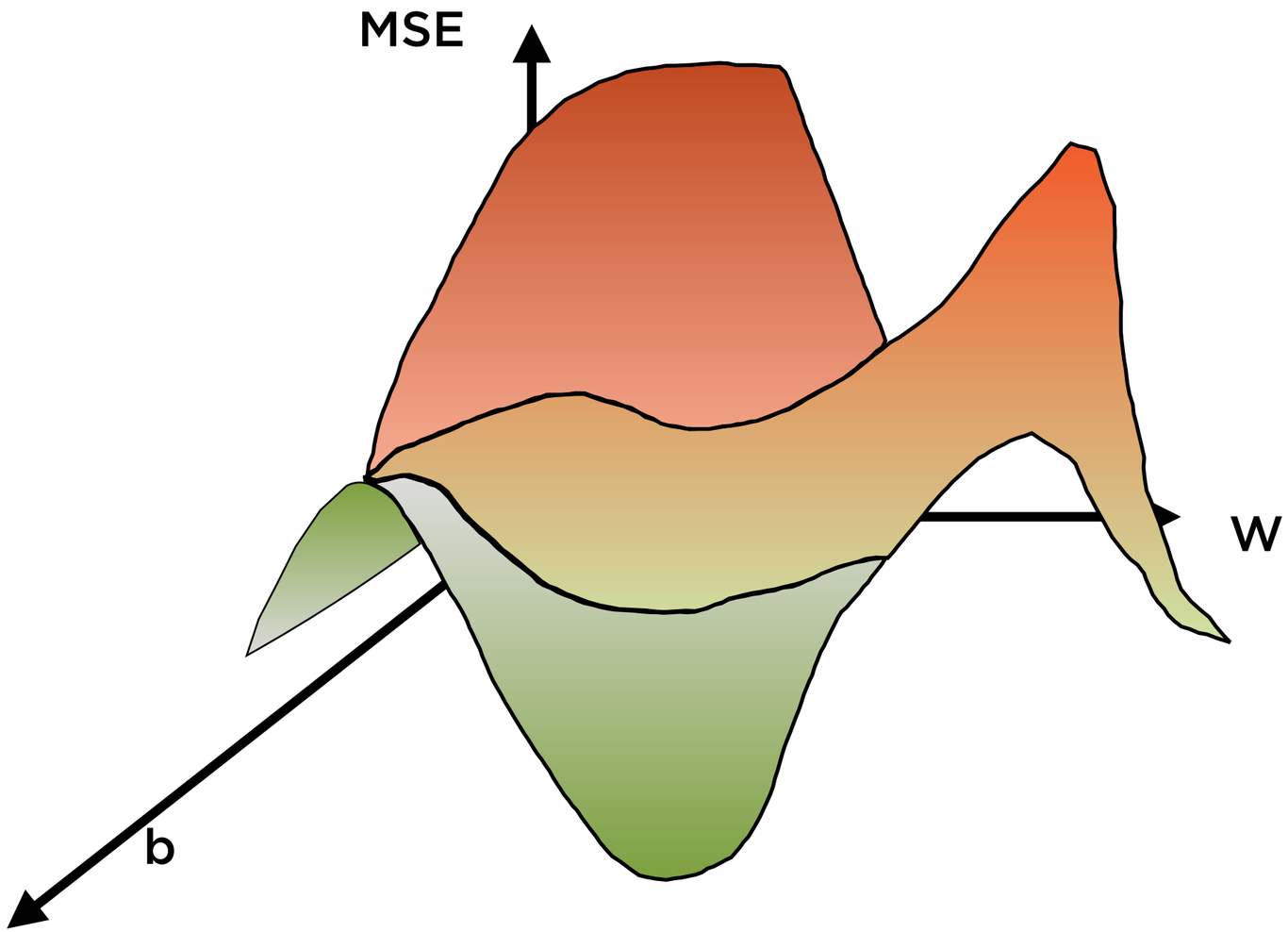

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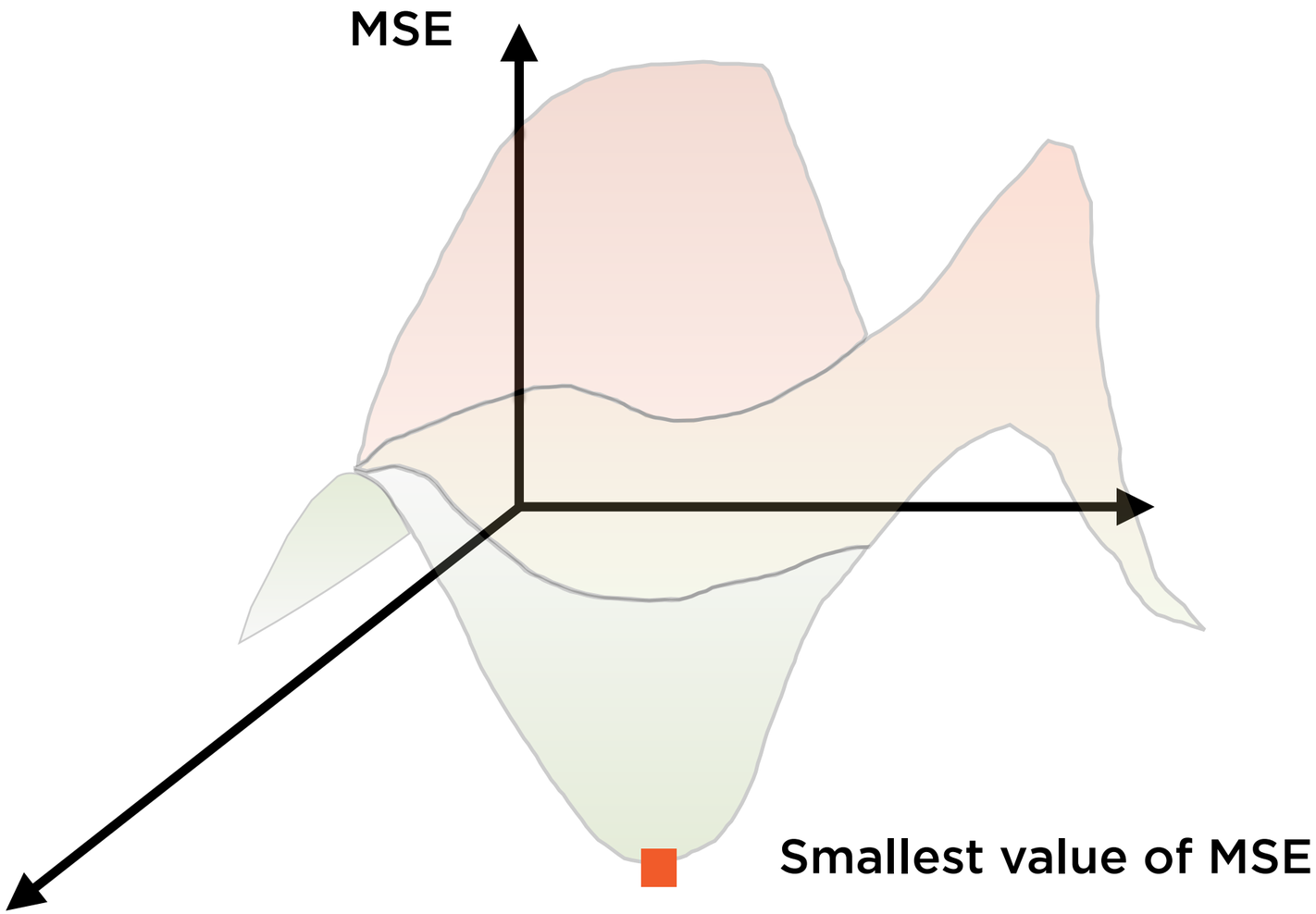

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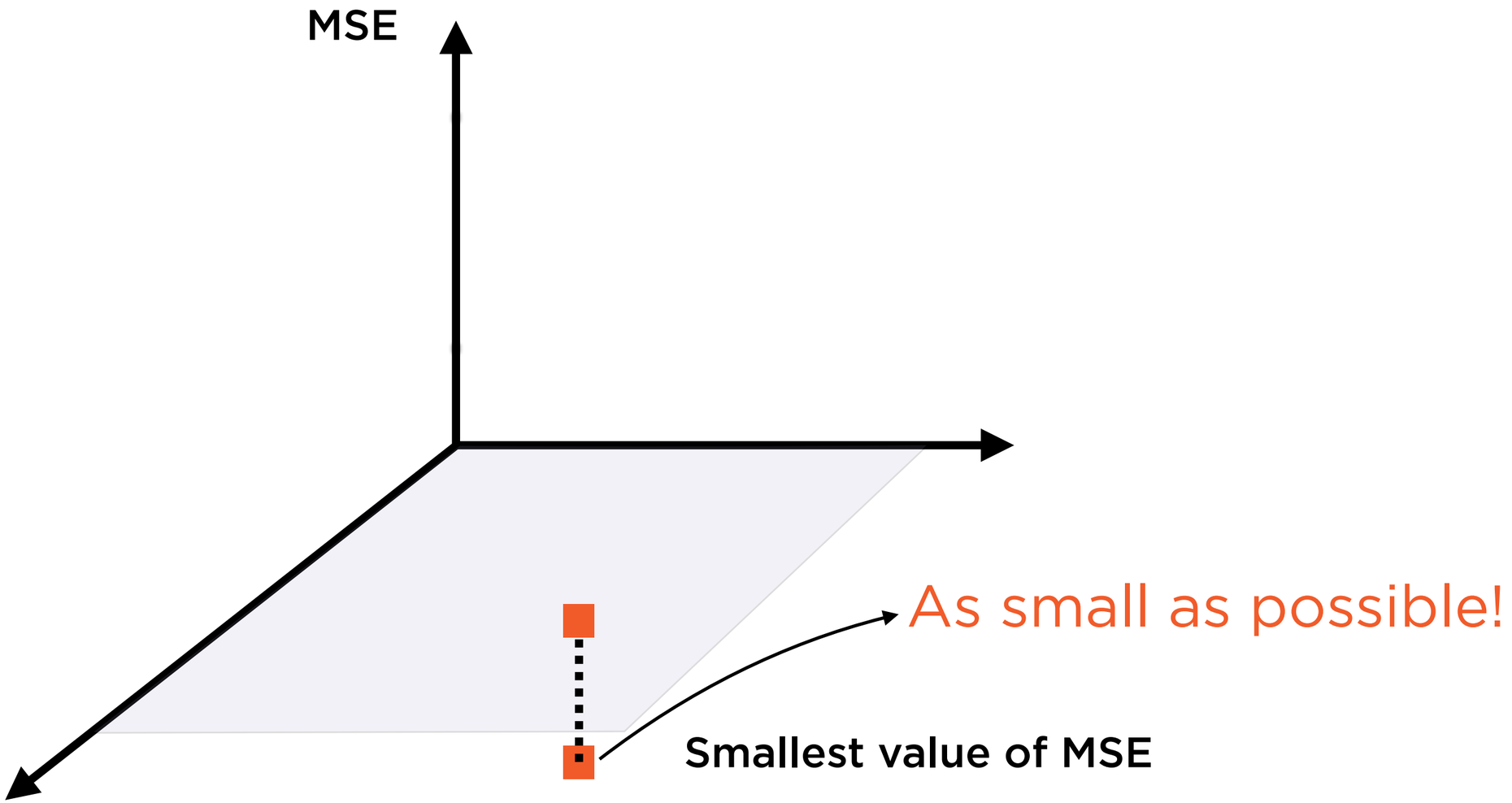

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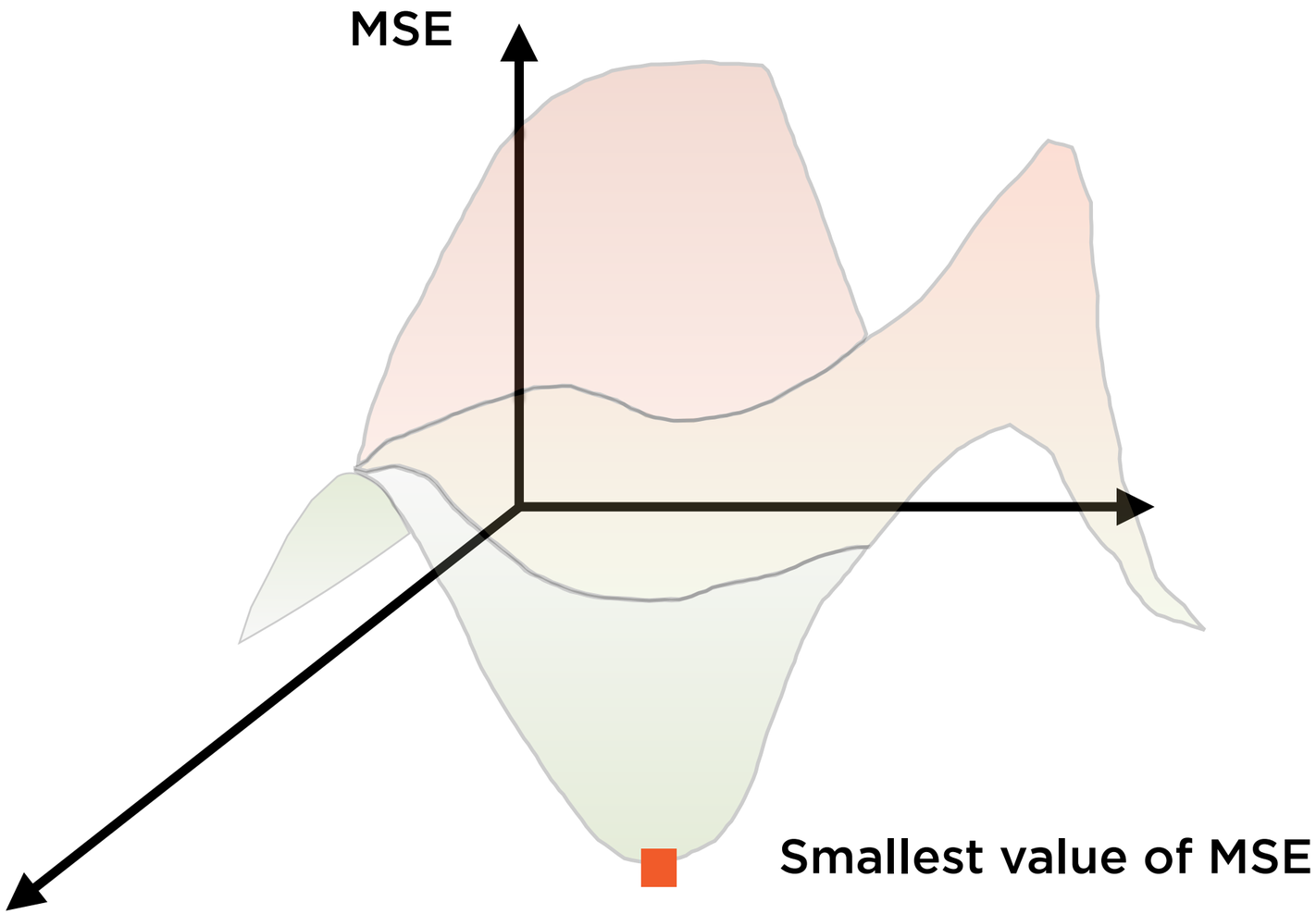

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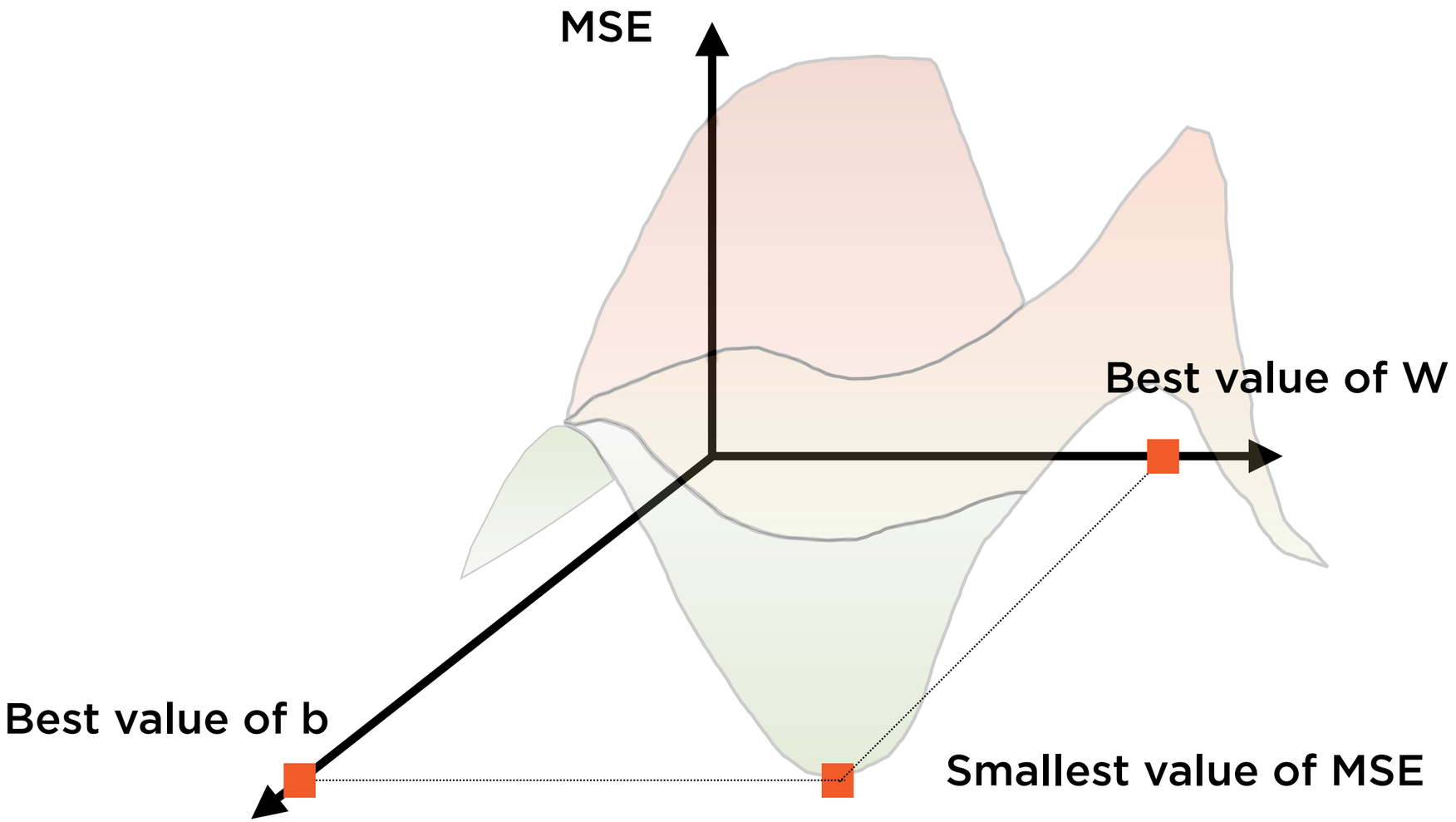
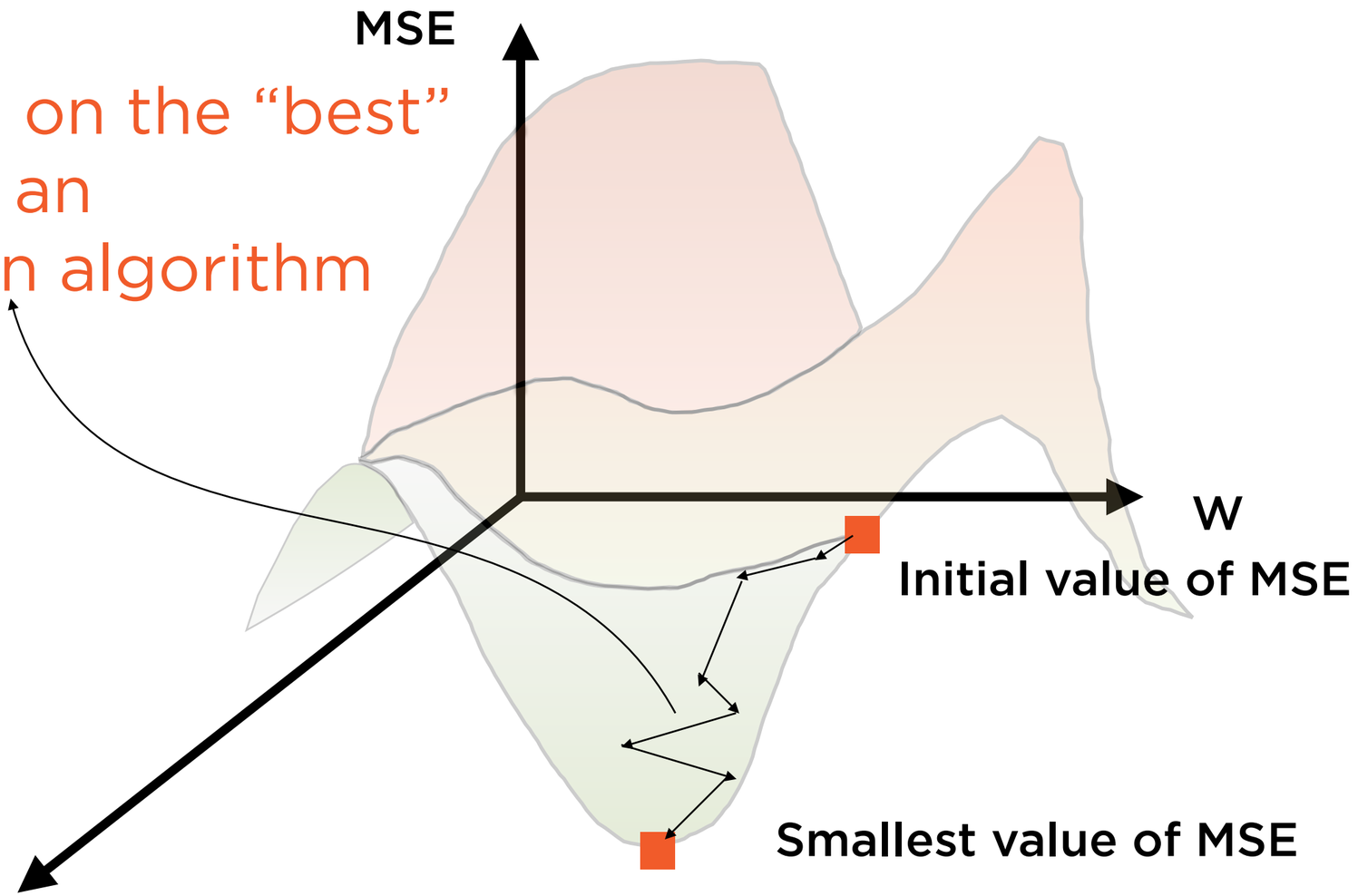


“Gradient Descent”

Converging on the “best” value using an optimization algorithm



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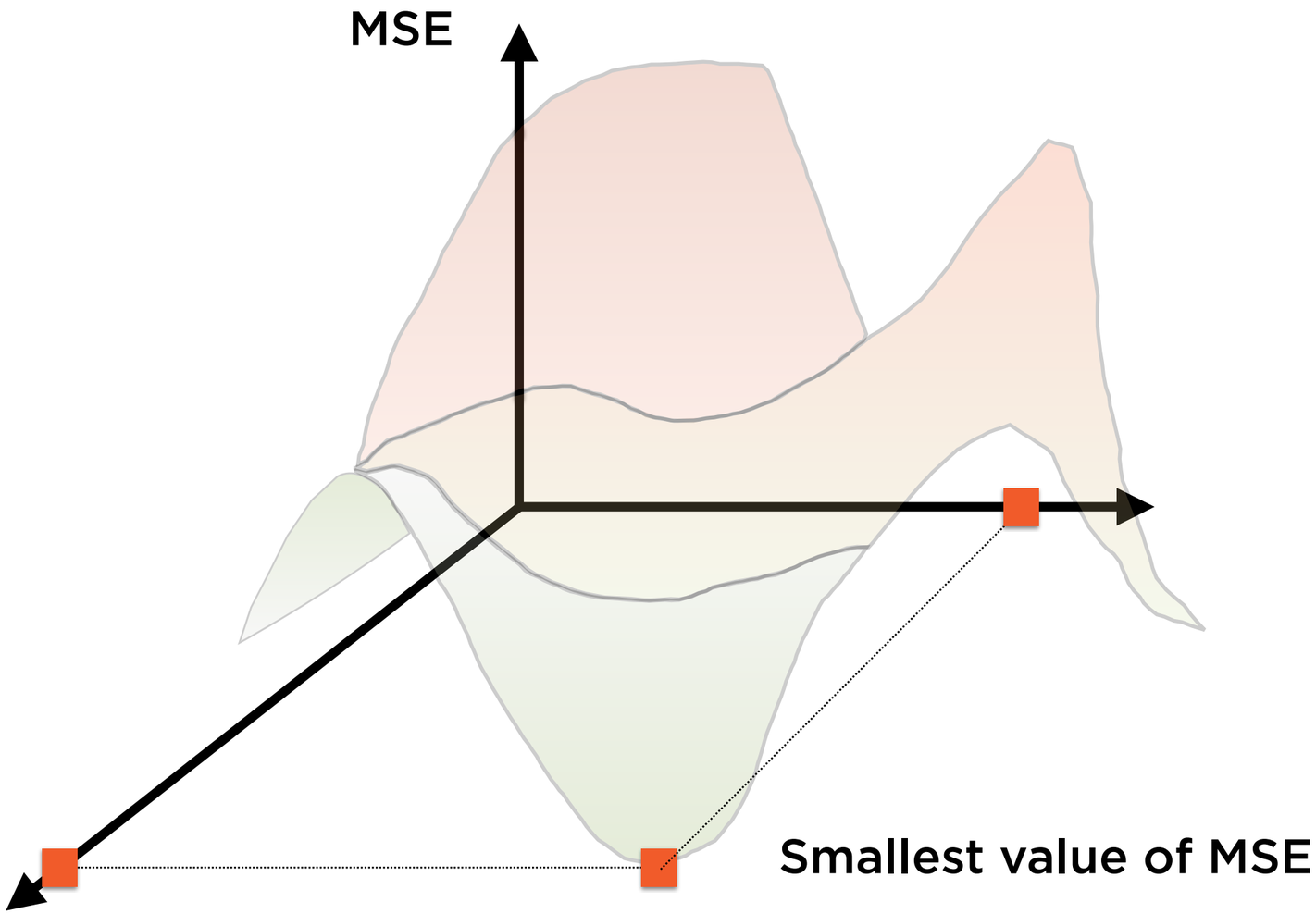
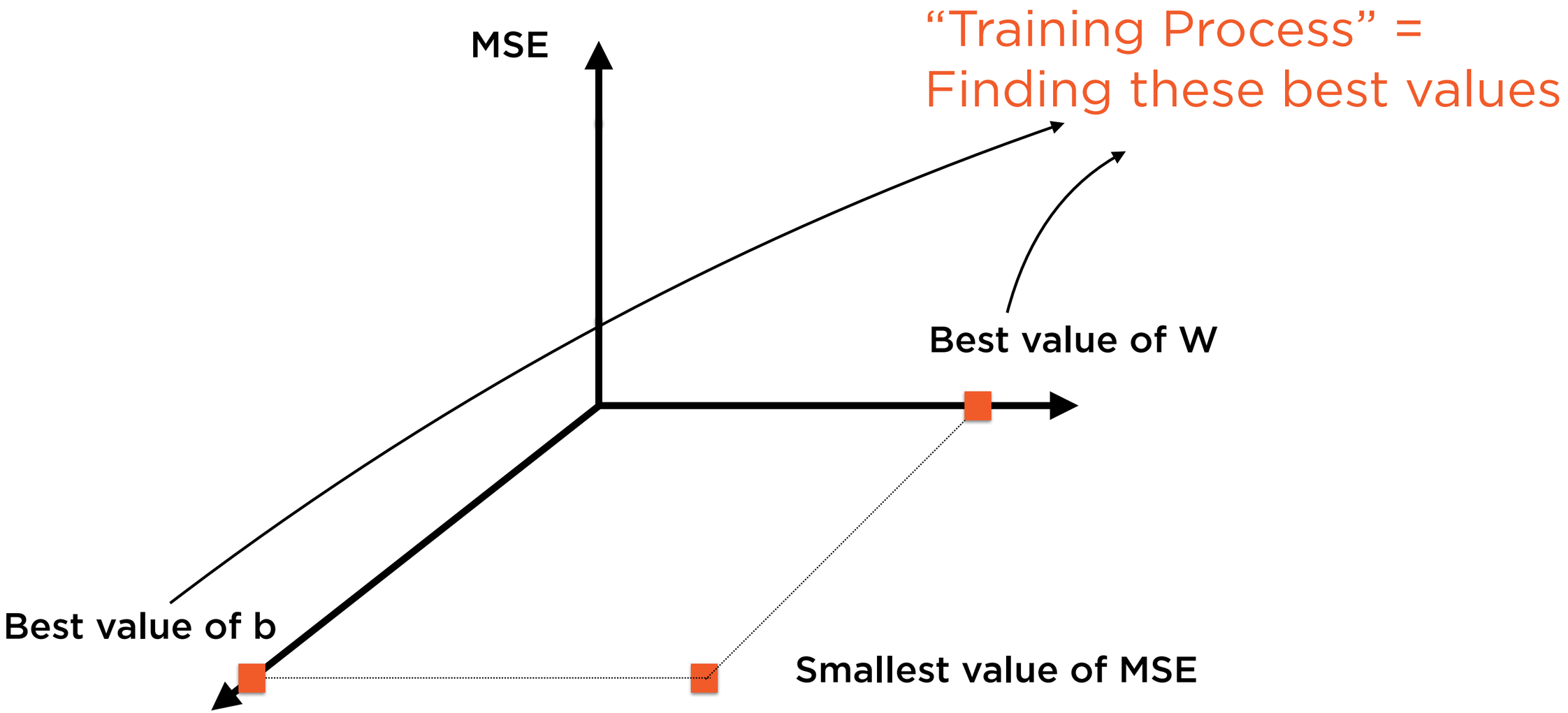


“Training” the Algorithm



$$Parameters^{t+1} = Parameters^{t} - learning\_rate \times Gradient(\theta^{t})$$

Basic SGD Optimizer

Move each parameter value in the direction of reducing gradient

$$Parameters^{t+1} = Parameters^{t} - \mathbf{learning\_rate} \times Gradient(\theta^{t})$$

Basic SGD Optimizer

The size of the step in the direction of reducing gradients

$$momentum\_vec^{t} = momentum\_coeff + learning\_rate \times Gradient(\theta)^{t}$$

$$Parameters^{t+1} = Parameters^{t} - momentum\_vec$$

Momentum-based Optimizer

Momentum vector helps accelerate in the direction where gradient is decreasing

$$momentum\_vec^{t} = momentum\_coeff + learning\_rate \times Gradient(\theta)^{t}$$

$$Parameters^{t+1} = Parameters^{t} - momentum\_vec$$

Momentum-based Optimizer

Gradients at each step weighted by those in previous step

Benefit: Faster convergence

$$momentum\_vec^{t} = momentum\_coeff + learning\_rate \times Gradient(\theta)^{t}$$

$$Parameters^{t+1} = Parameters^{t} - momentum\_vec$$

Momentum-based Optimizer

Need a momentum coefficient, between 0 and 1 to prevent overshooting

scikit-learn Optimizers

Relatively small number of optimizers supported

Plain-vanilla SGD optimizer

Adam optimizer

L-BFGS optimizer

Neural Networks in scikit-learn

Multi-layer Perceptrons (MLP)

Restricted Boltzmann Machines (RBM)

Neural Networks in scikit-learn

Multi-layer Perceptrons (MLP)

Restricted Boltzmann Machines (RBM)

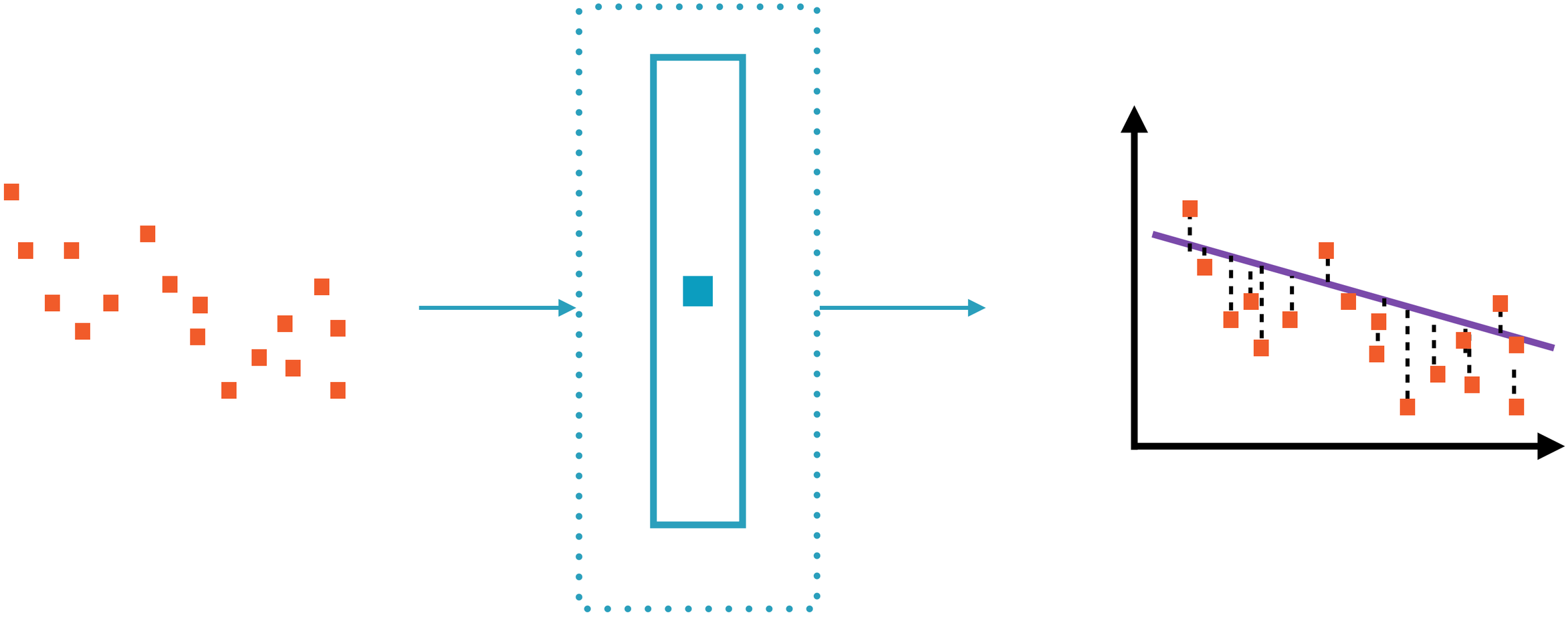
MLPRegressor estimator object to build regression models

Demo

Build and train a regression model using neural networks in scikit-learn using the MLPRegressor estimator

Classification Using Neural Networks

Linear Regression with One Neuron



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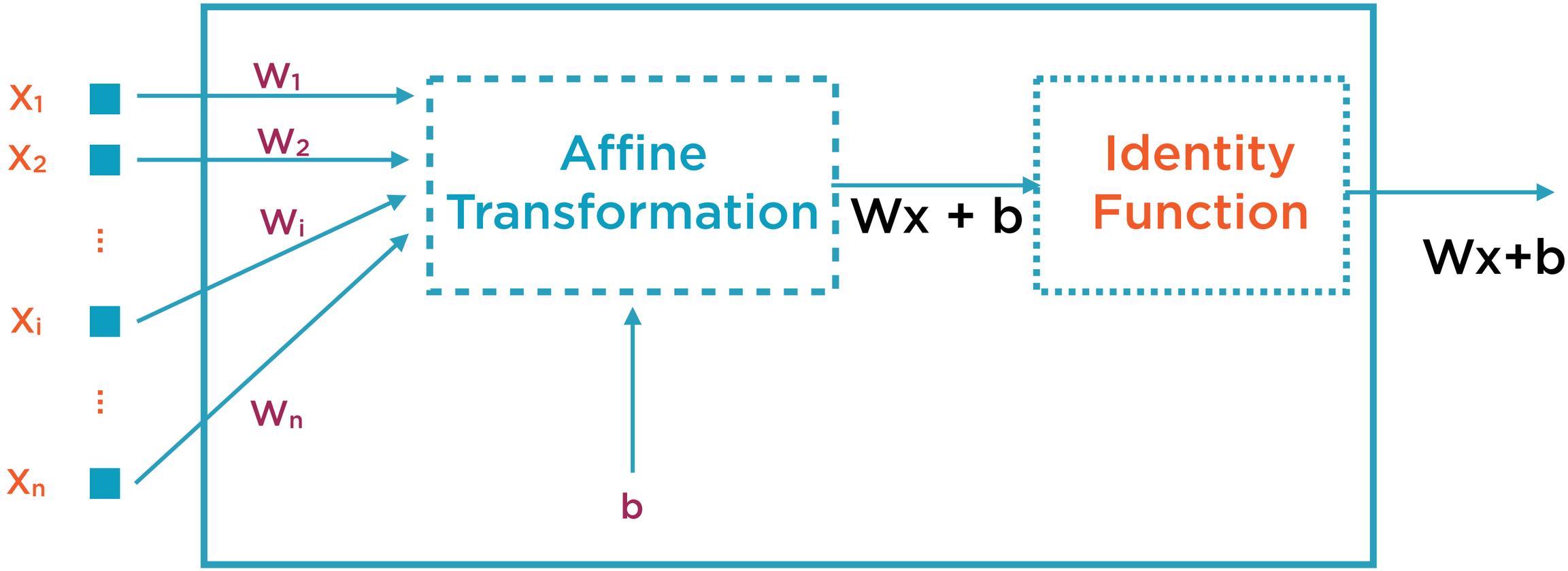
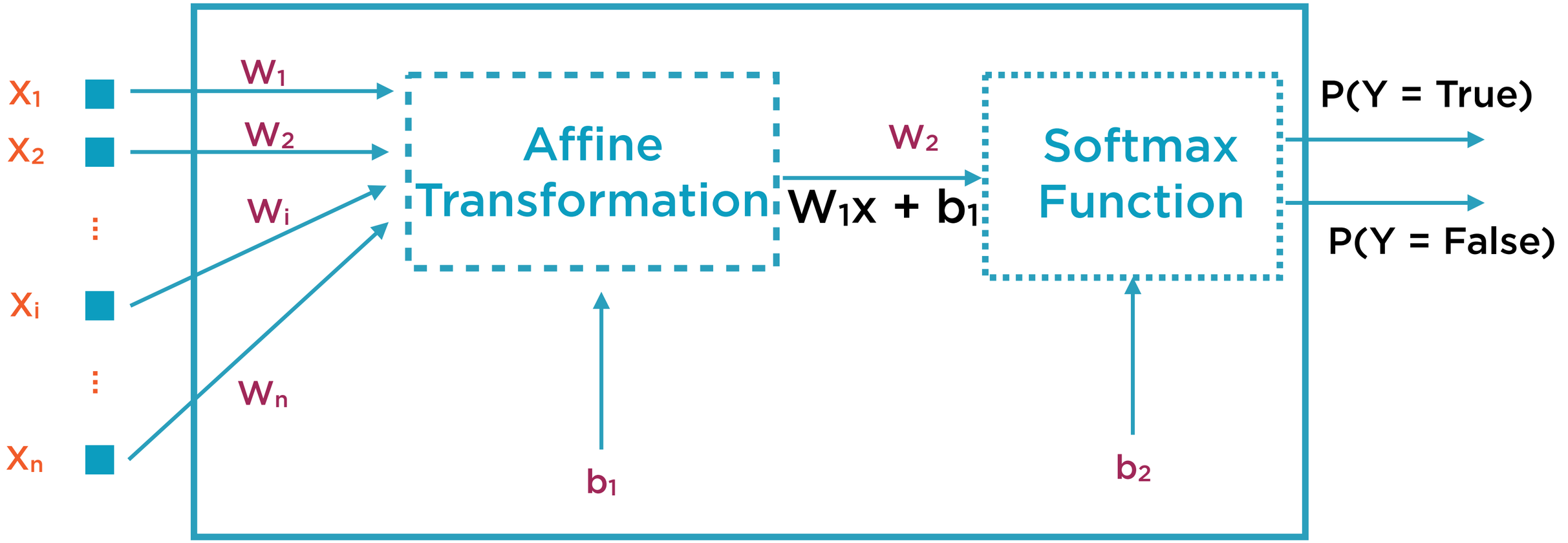


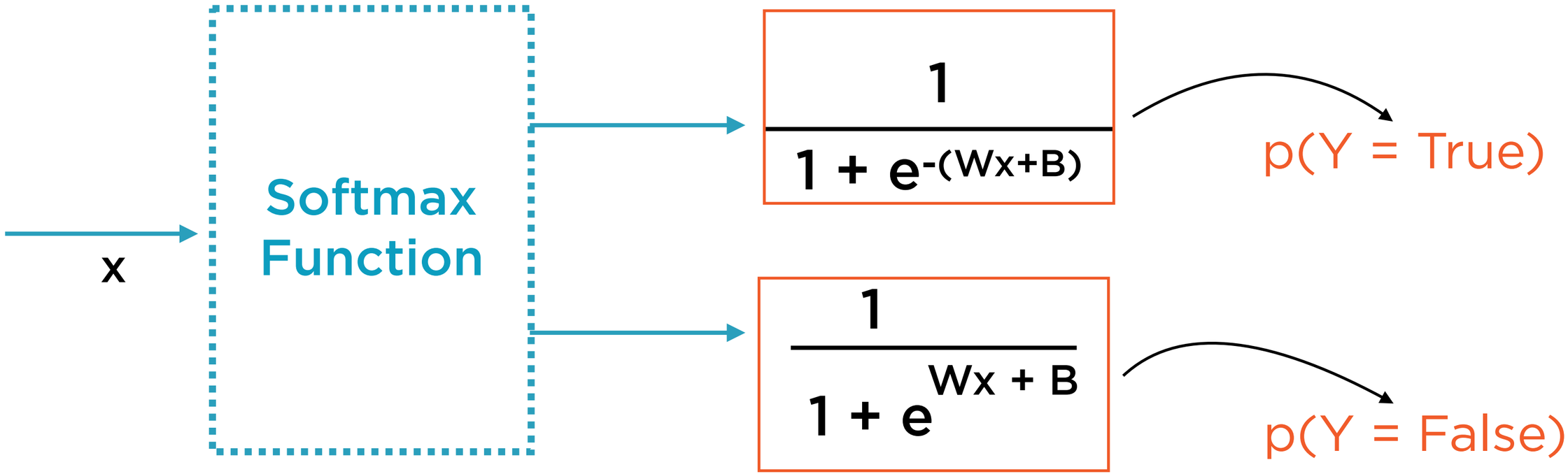
Linear Regression with One Neuron

Linear Classification with One Neuron

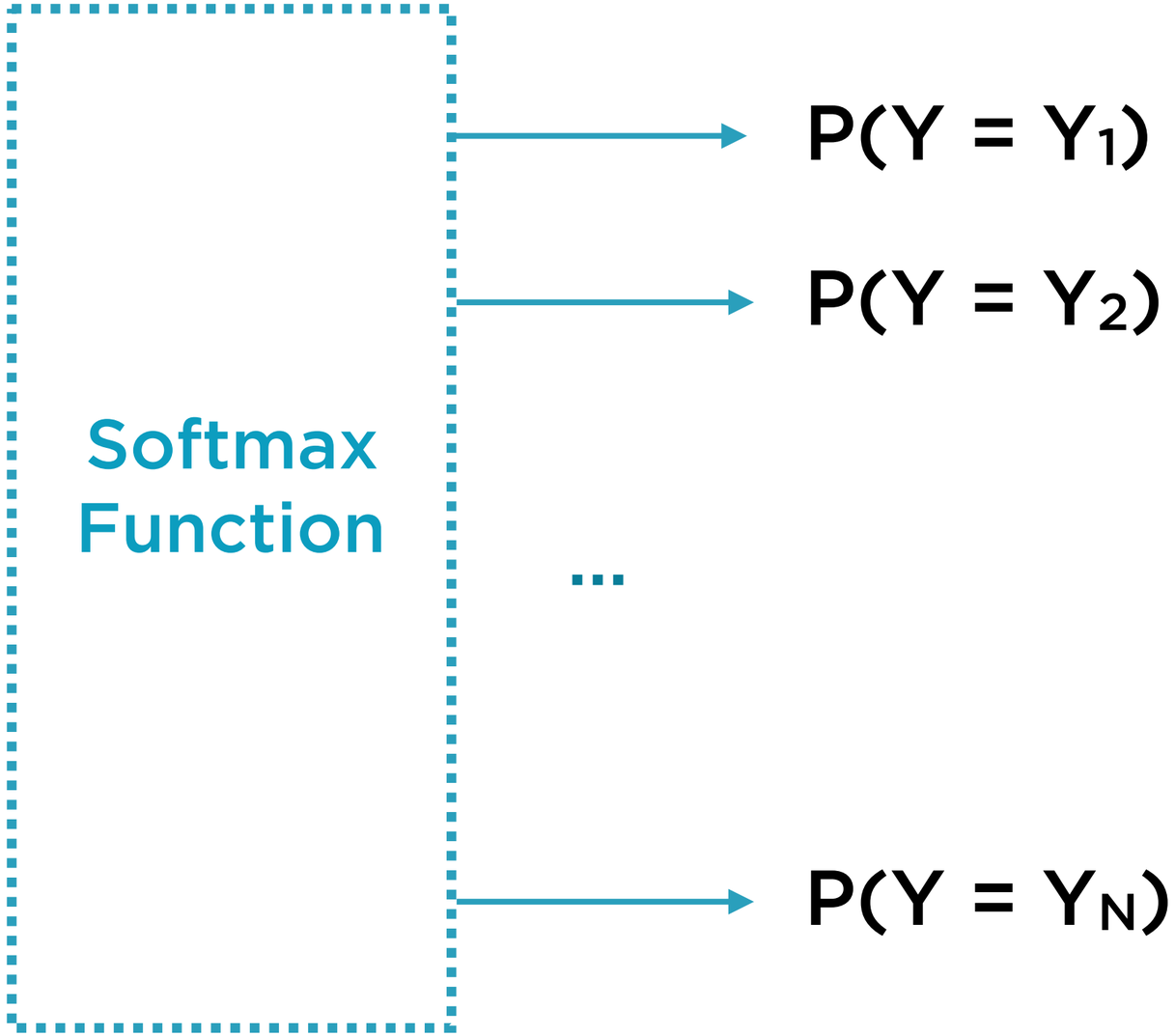
Linear Classification with One Neuron



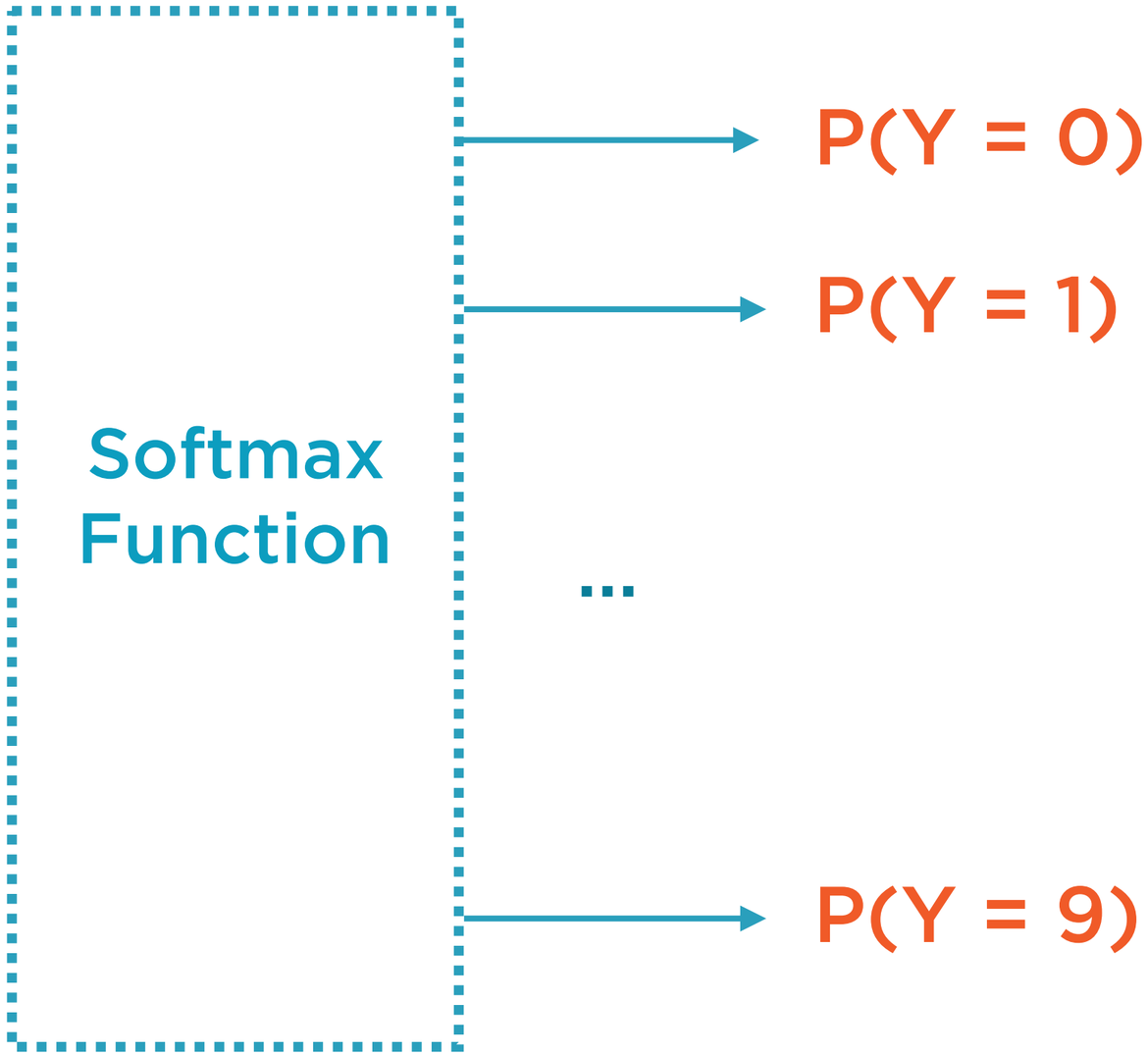
SoftMax for True/False Classification



SoftMax N-category Classification

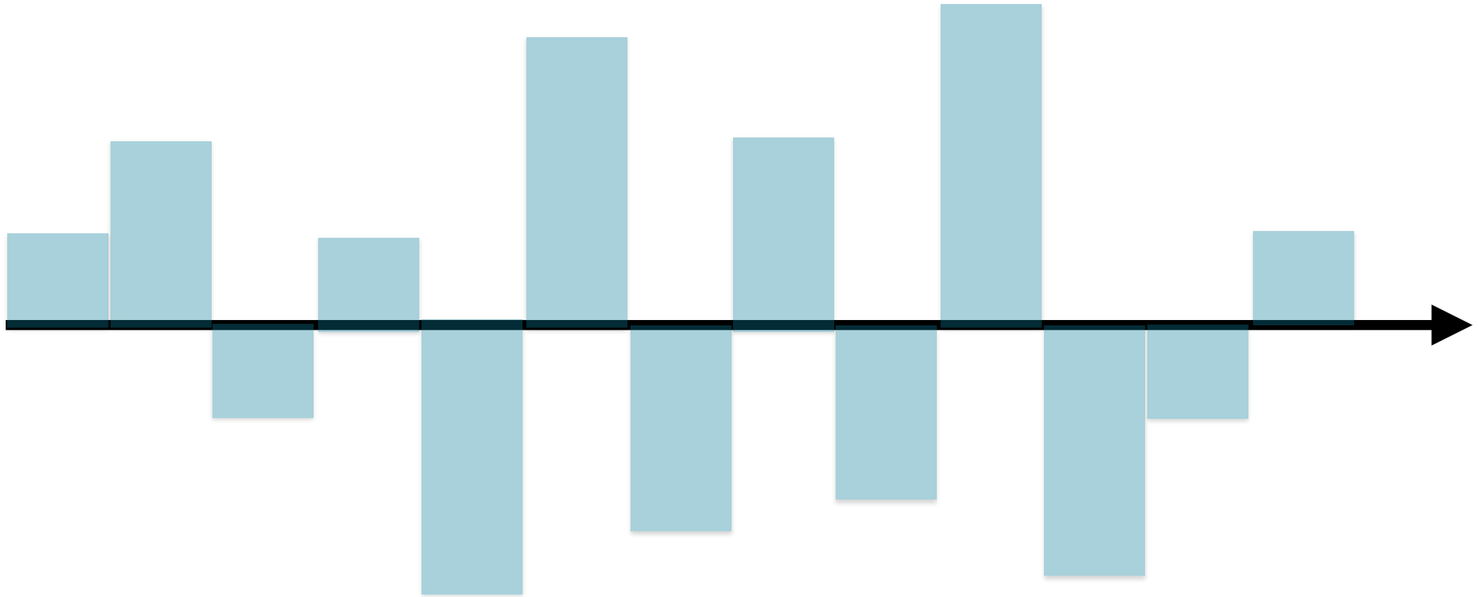


SoftMax for Digit Classification

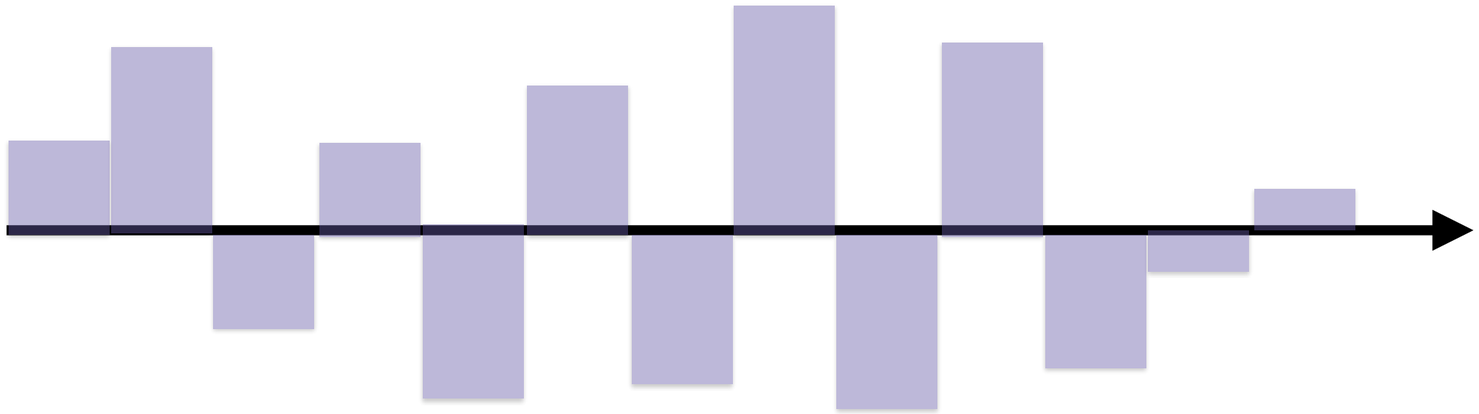


Intuition: Low Cross Entropy

Y_{actual}



$Y_{predicted}$



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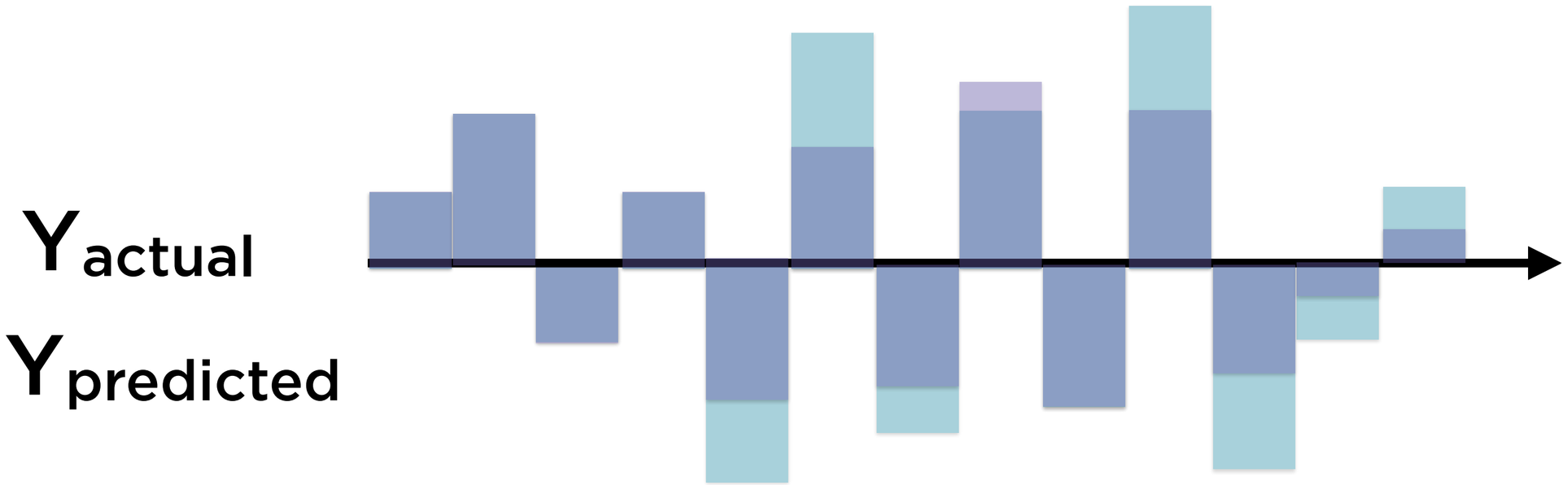

The labels of the two series are in-synch

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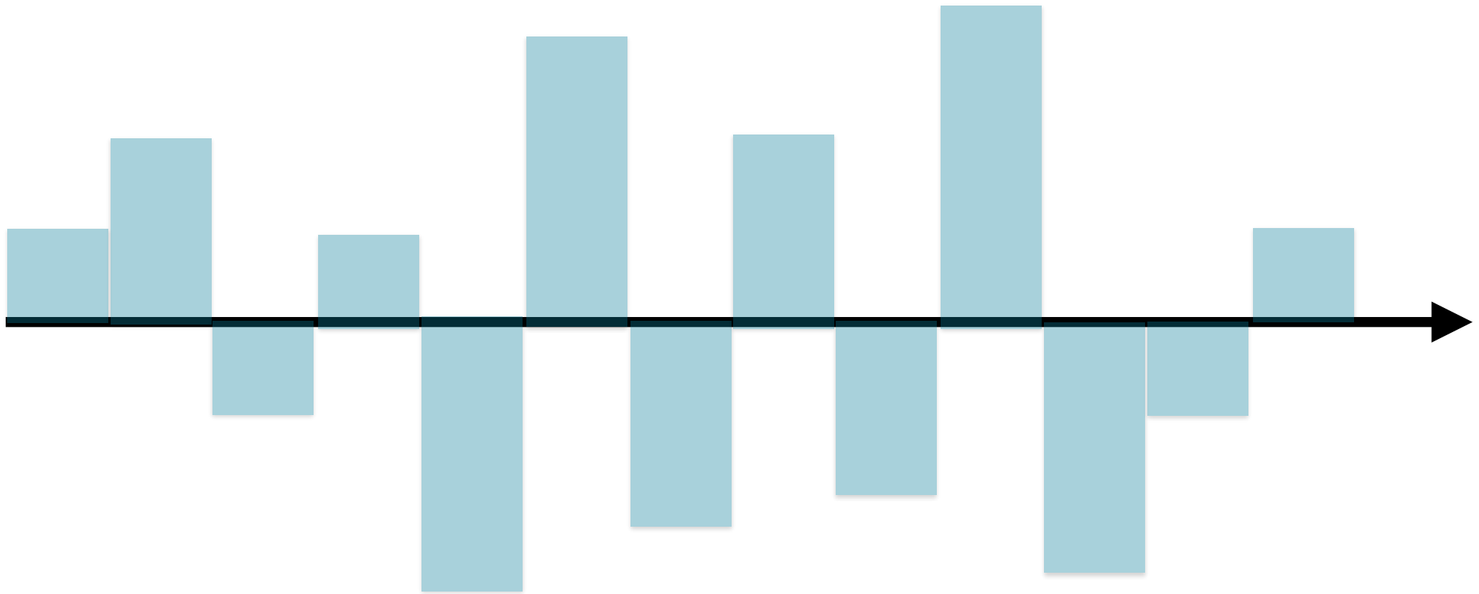

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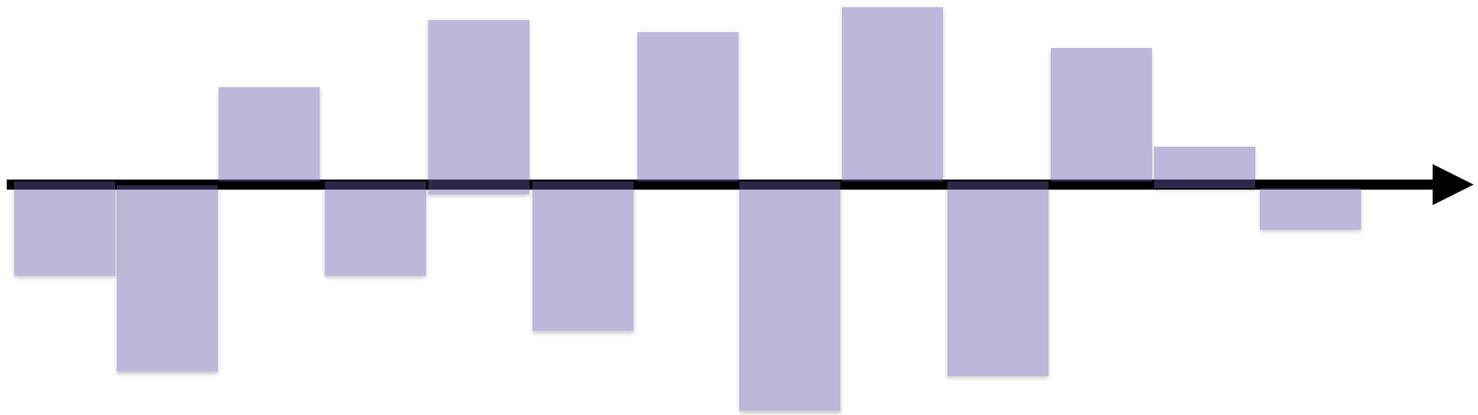

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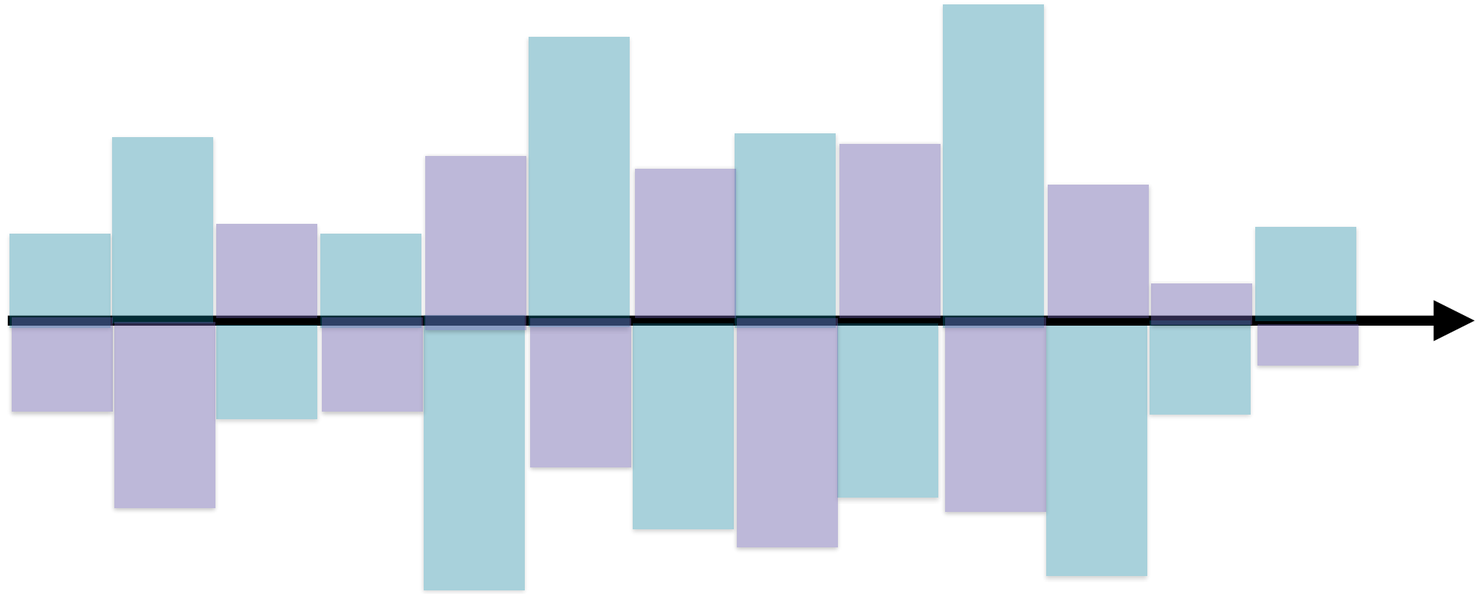

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Demo

Build and train a classification model using neural networks in scikit-learn using the MLPClassifier estimator

Summary

Regression models using neural networks in scikit-learn

Mean square error (MSE) loss function

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Cross-entropy loss function

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