

# Gradient Descent



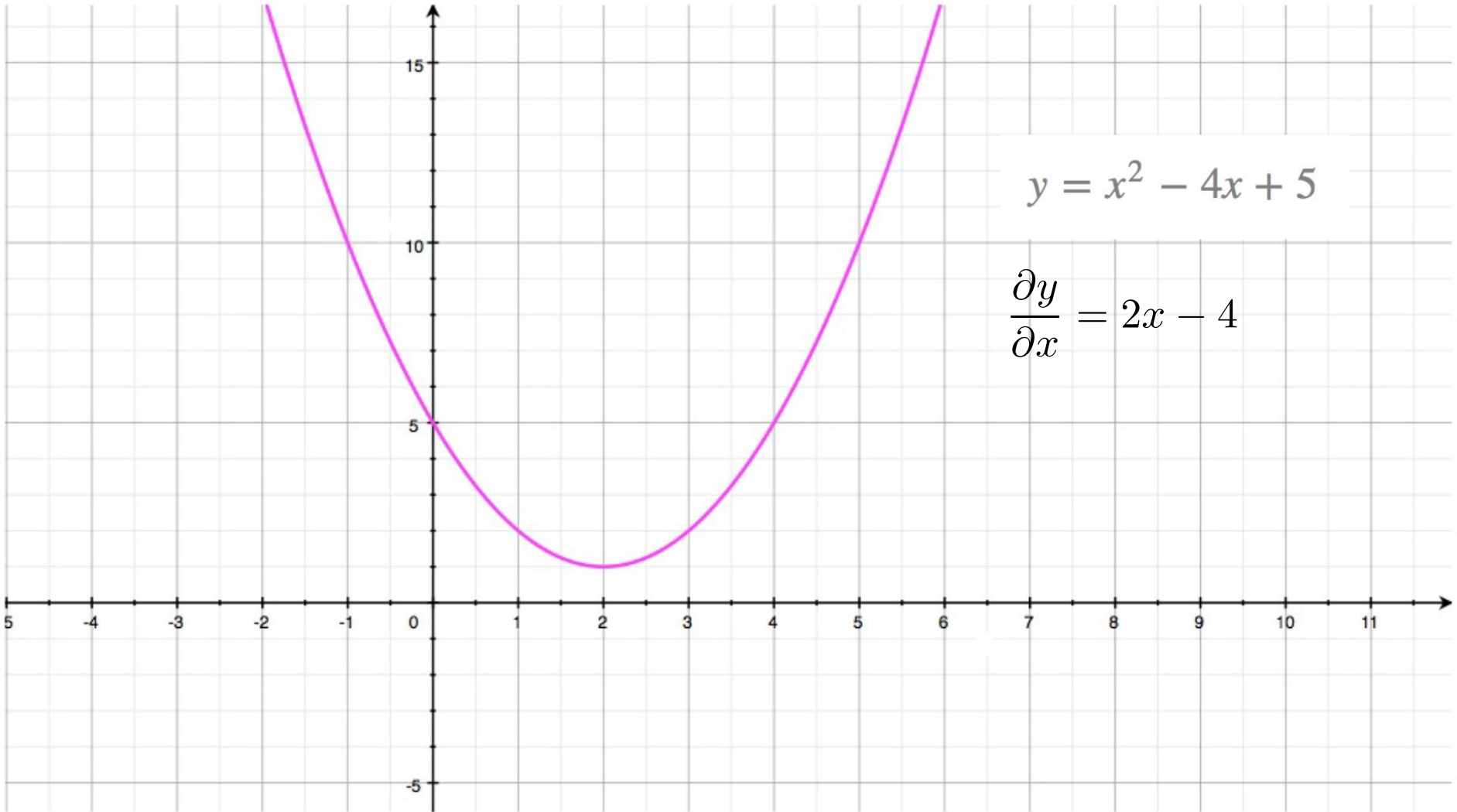
# Learning Objectives



- Explain the basics of gradient descent
- Discuss Batch Gradient Descent
- Describe the Stochastic Gradient Descent
- Explain the Mini-batch Gradient Descent



# Getting Started

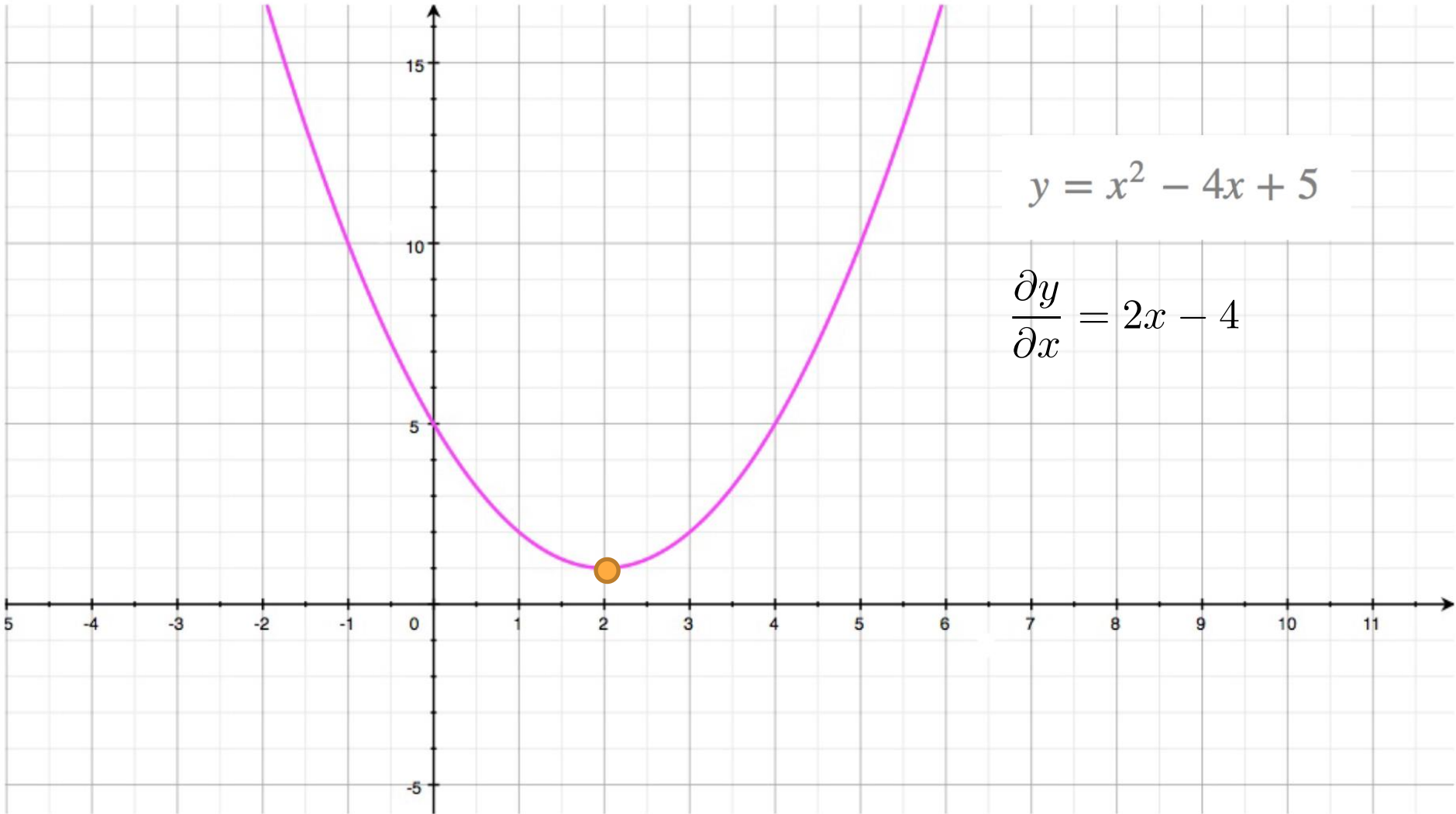


$$y = x^2 - 4x + 5$$

$$\frac{\partial y}{\partial x} = 2x - 4$$

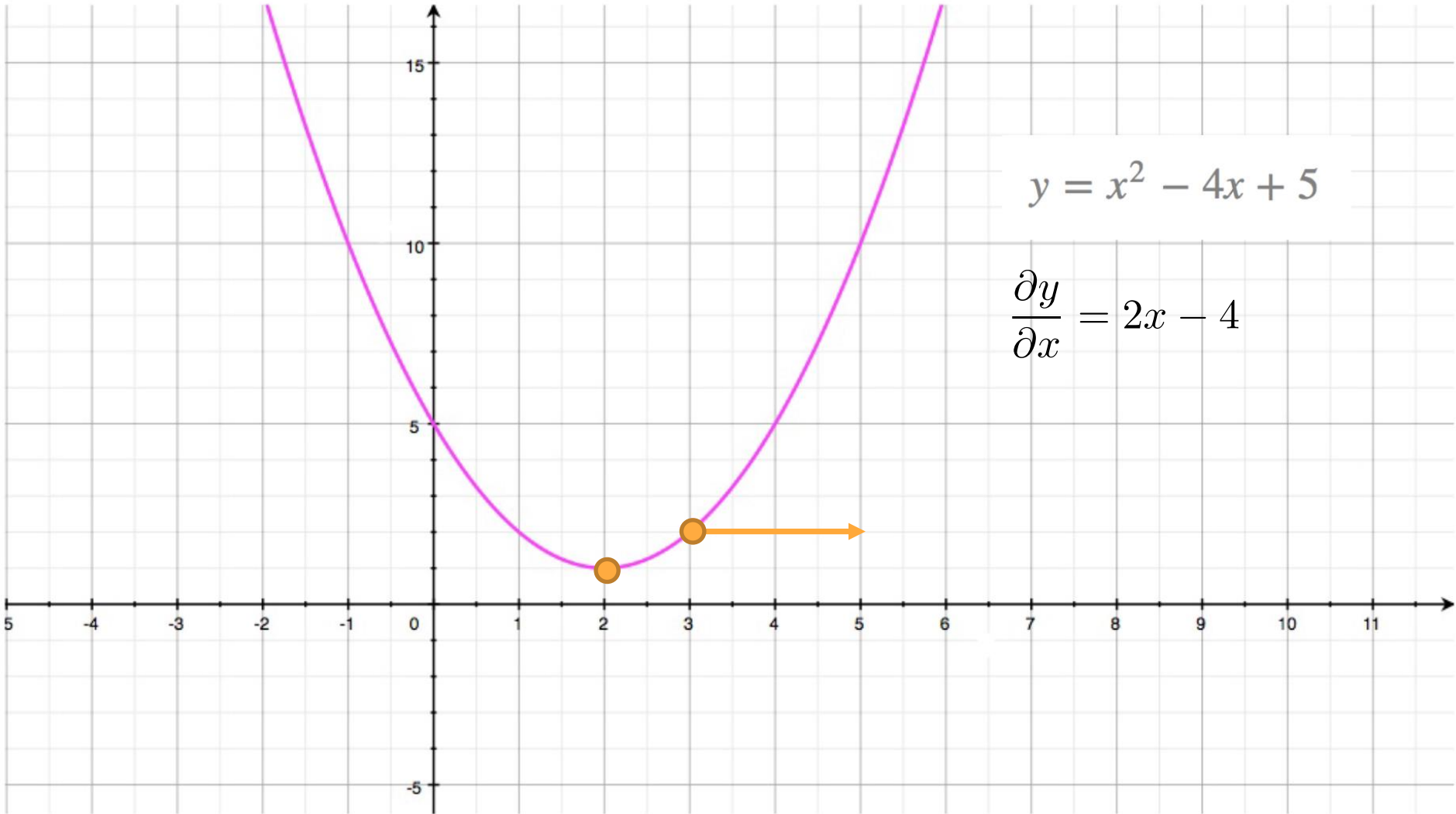
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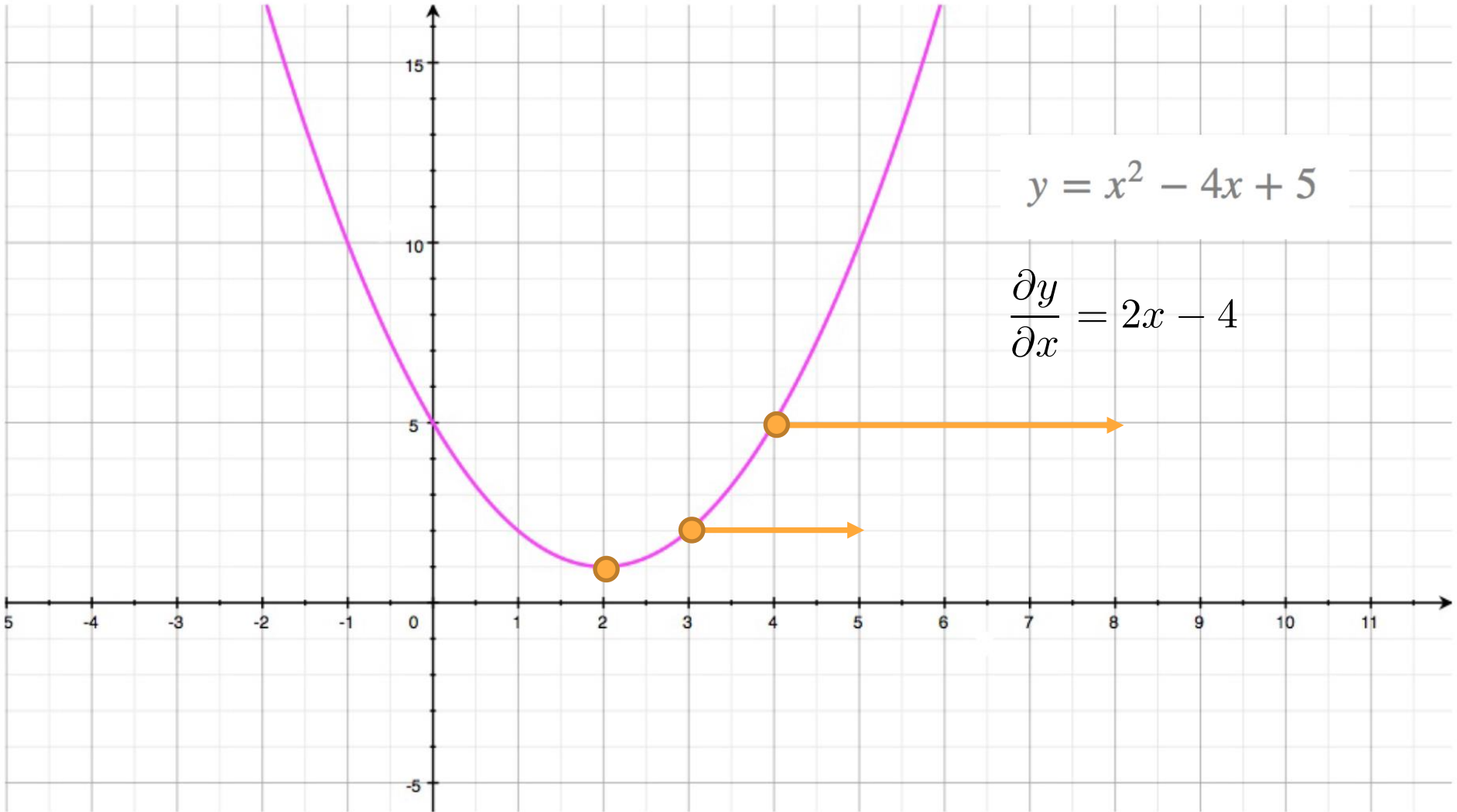
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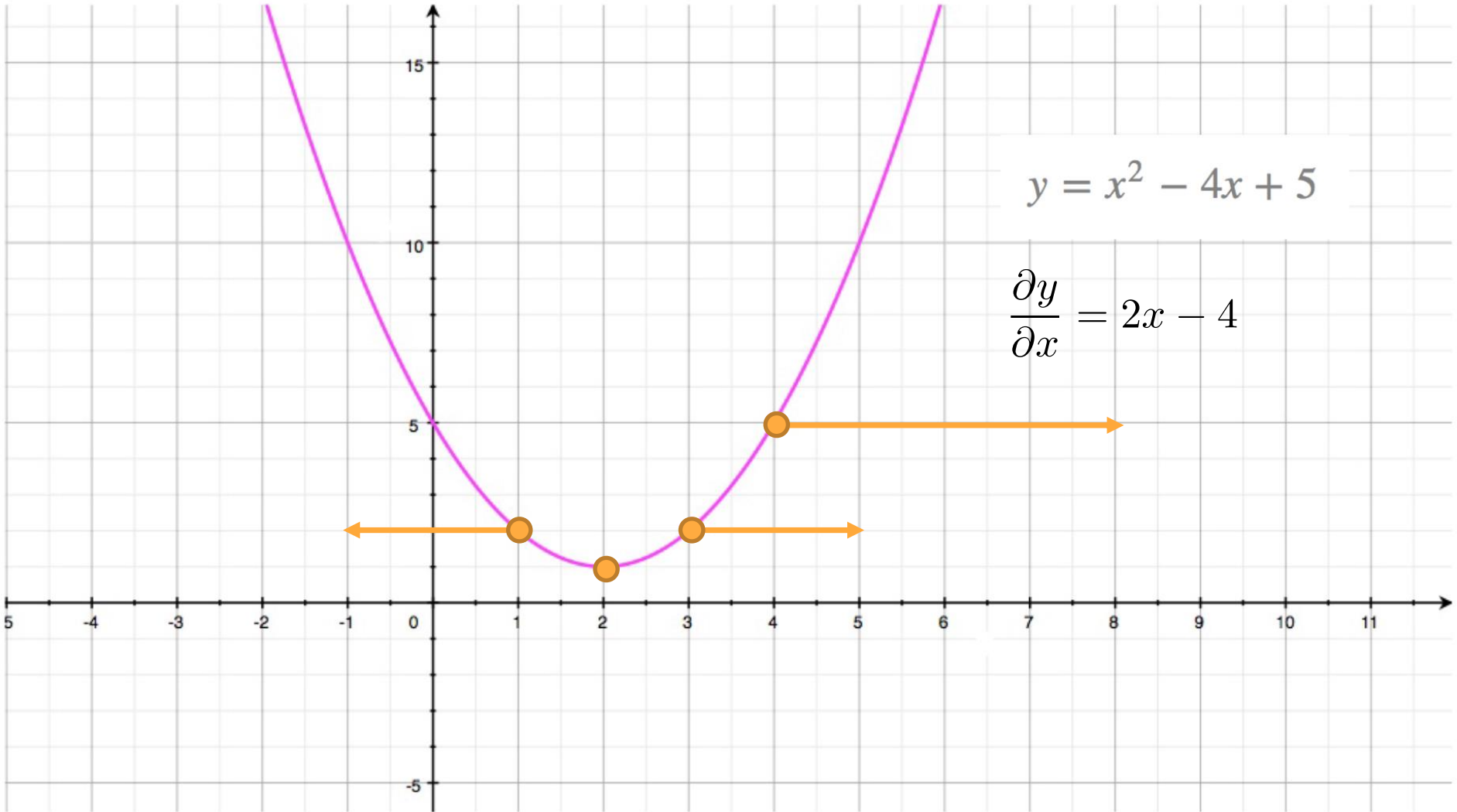
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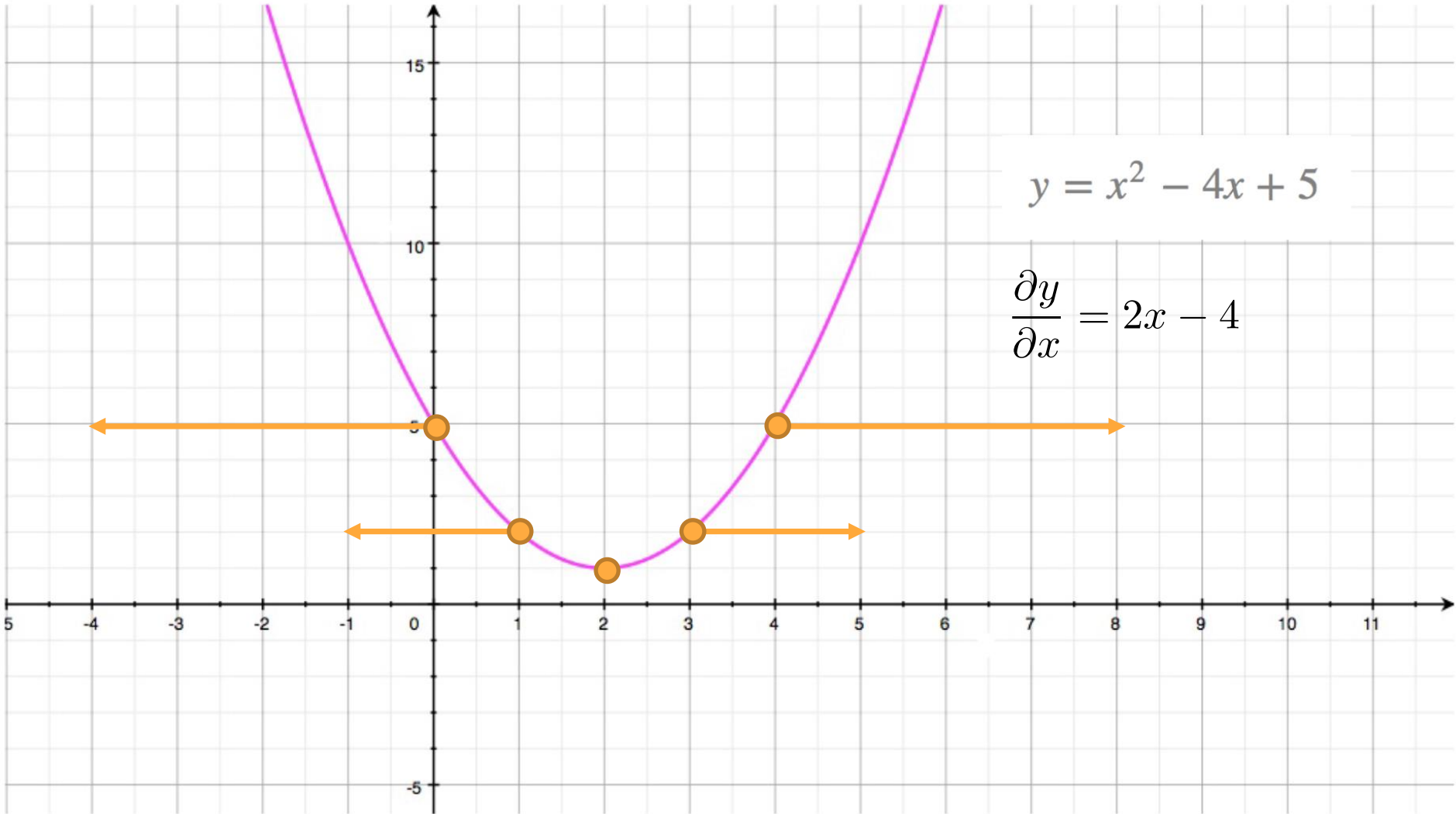
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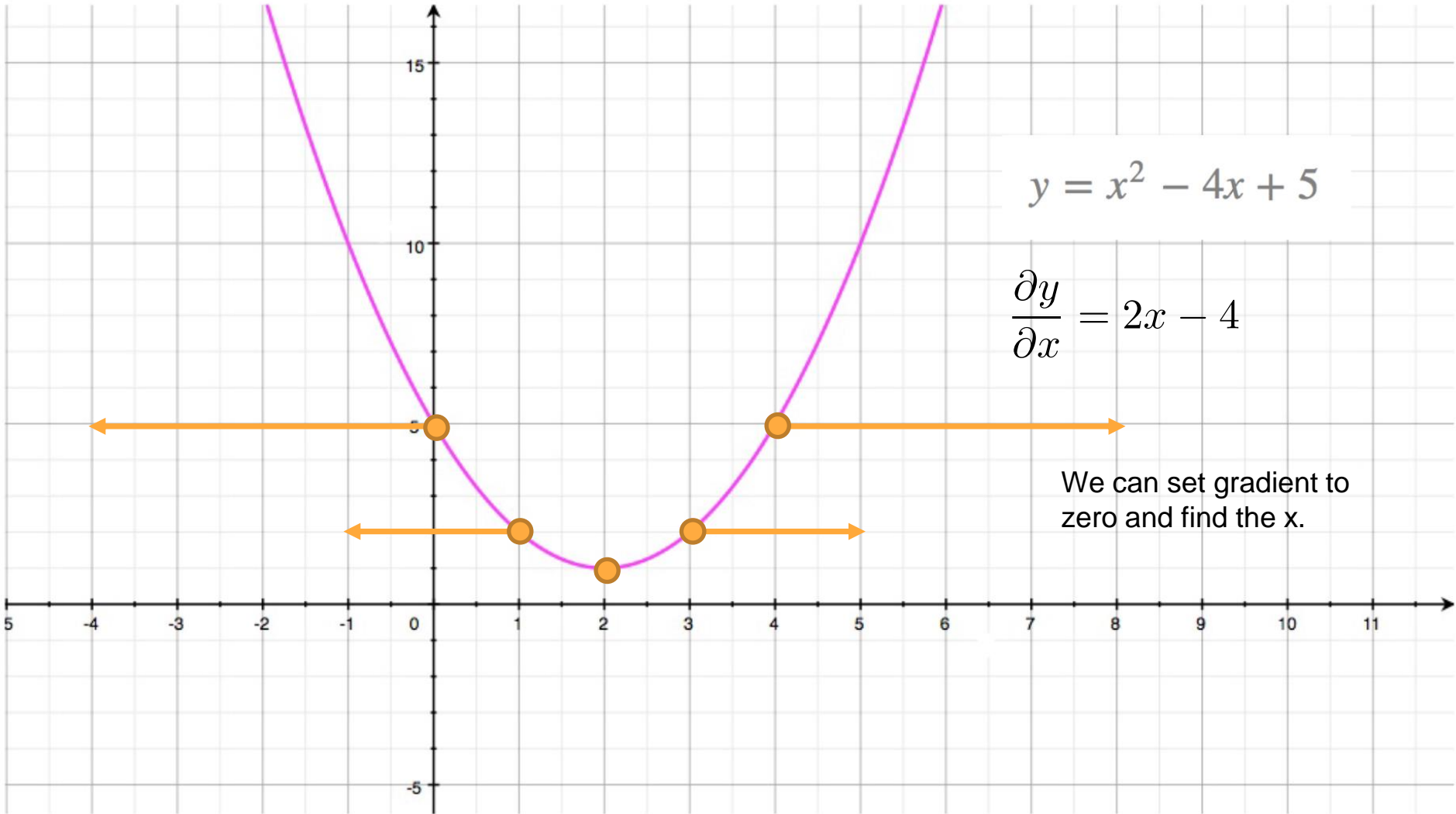
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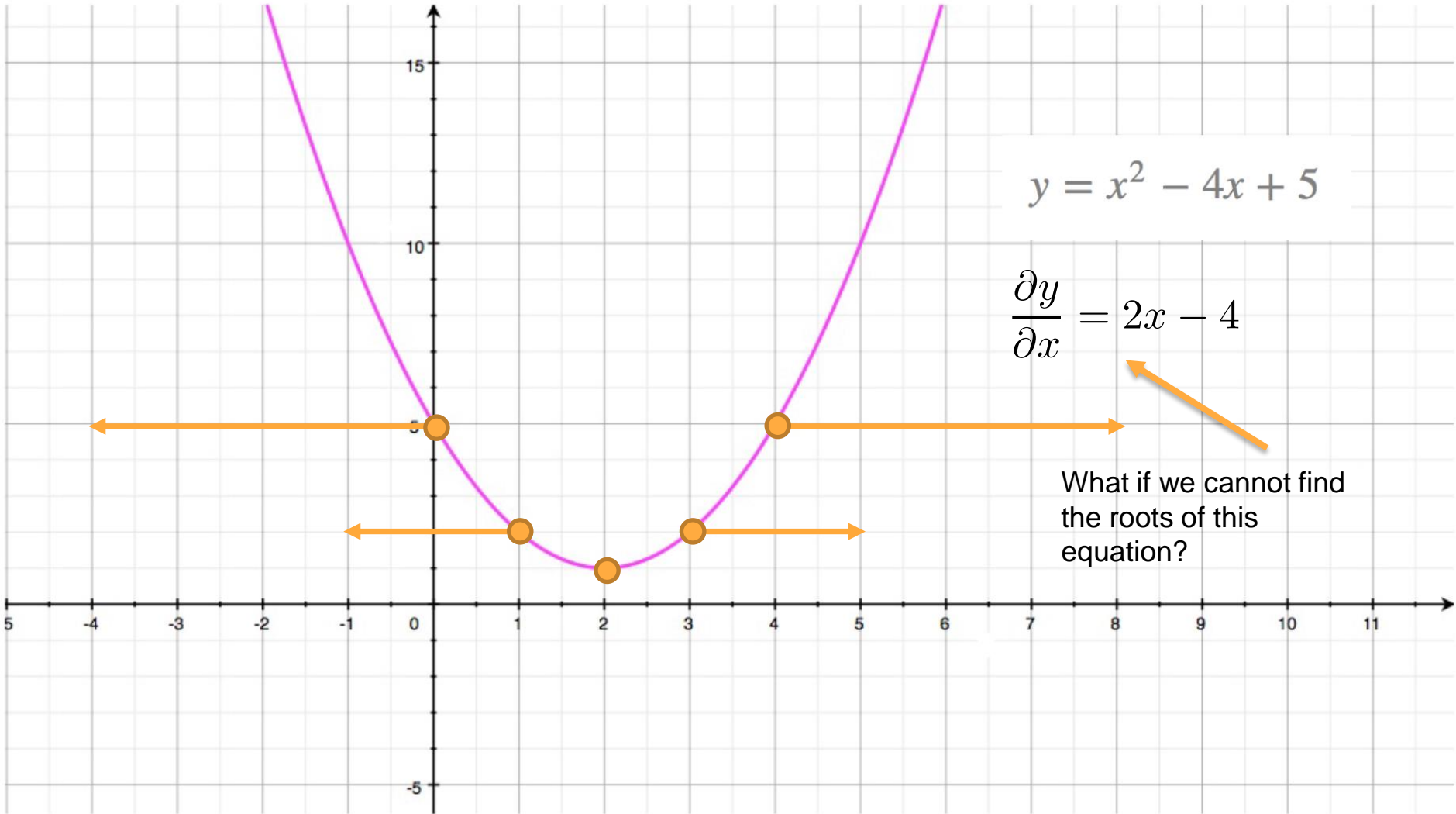
We can set gradient to zero and find the x.



$$y = x^2 - 4x + 5$$

$$\frac{\partial y}{\partial x} = 2x - 4$$

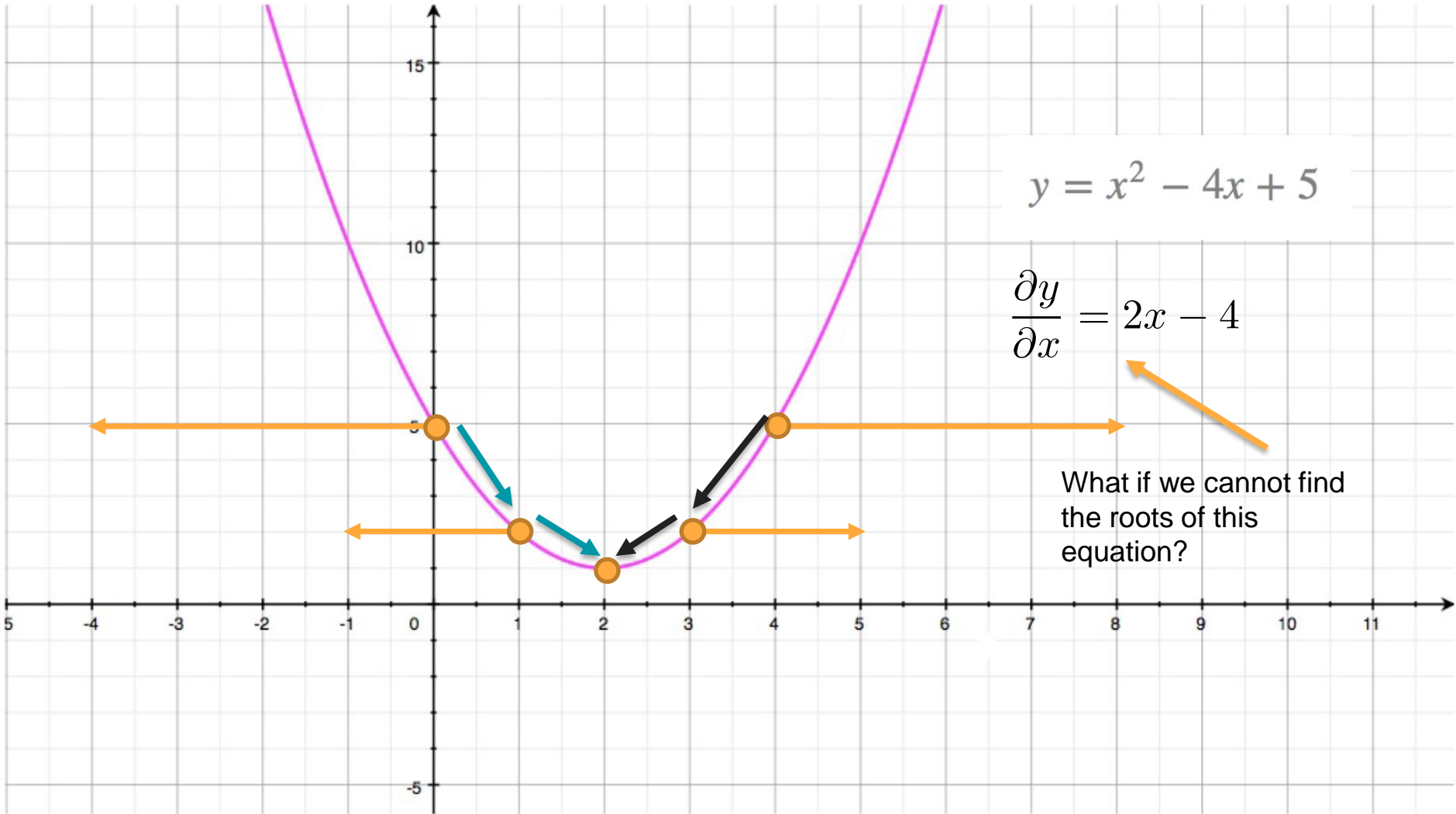
What if we cannot find  
the roots of this  
equation?



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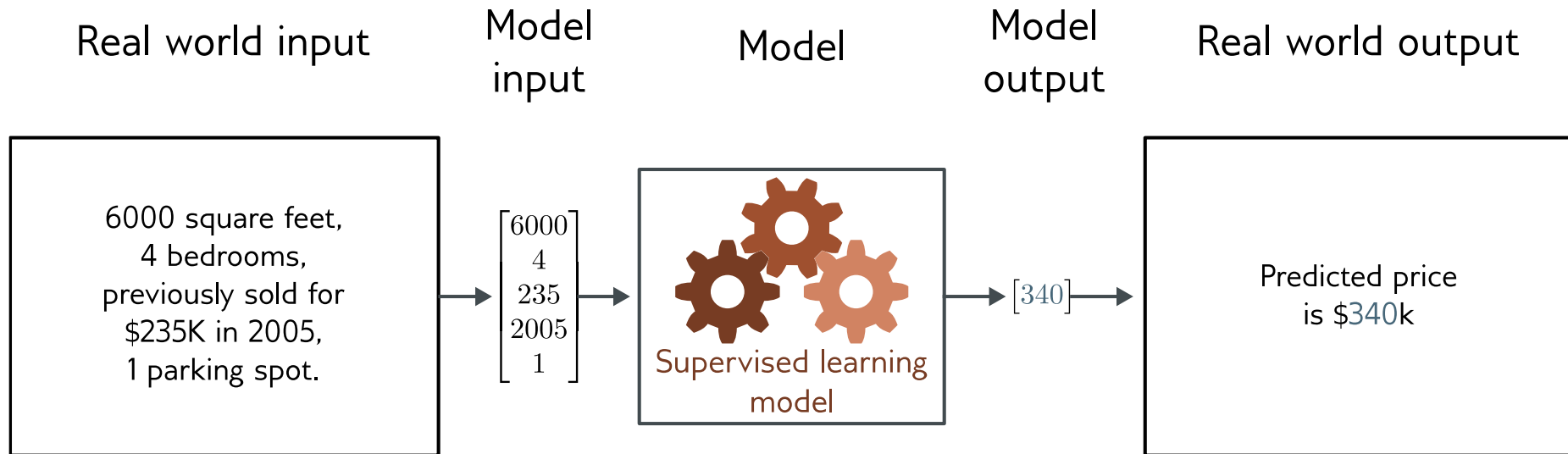
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What if we cannot find  
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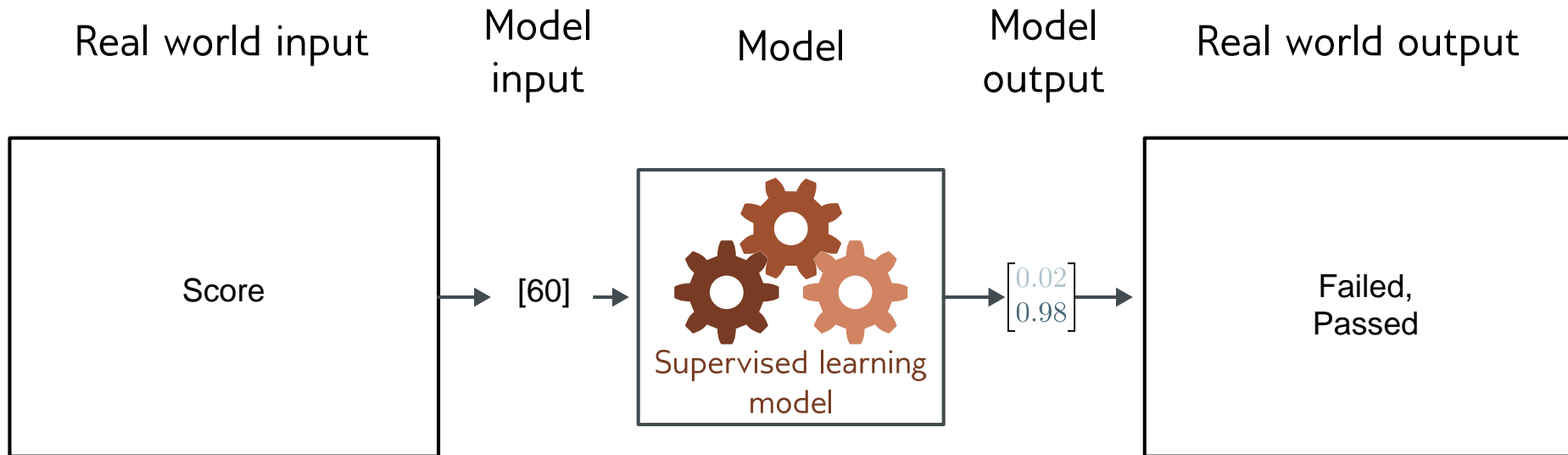
# ML Training vs. Finding the Minima of a Function ?

# Regression



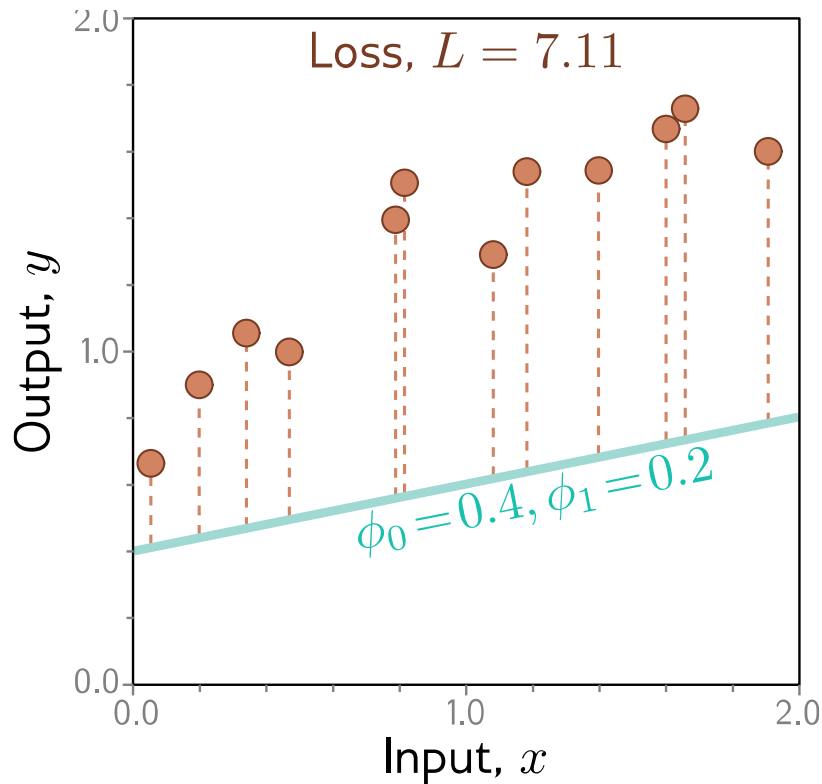
- Univariate regression problem (one output, real value)

# Text classification



- Binary classification problem (two discrete classes)

# 1D Linear Regression



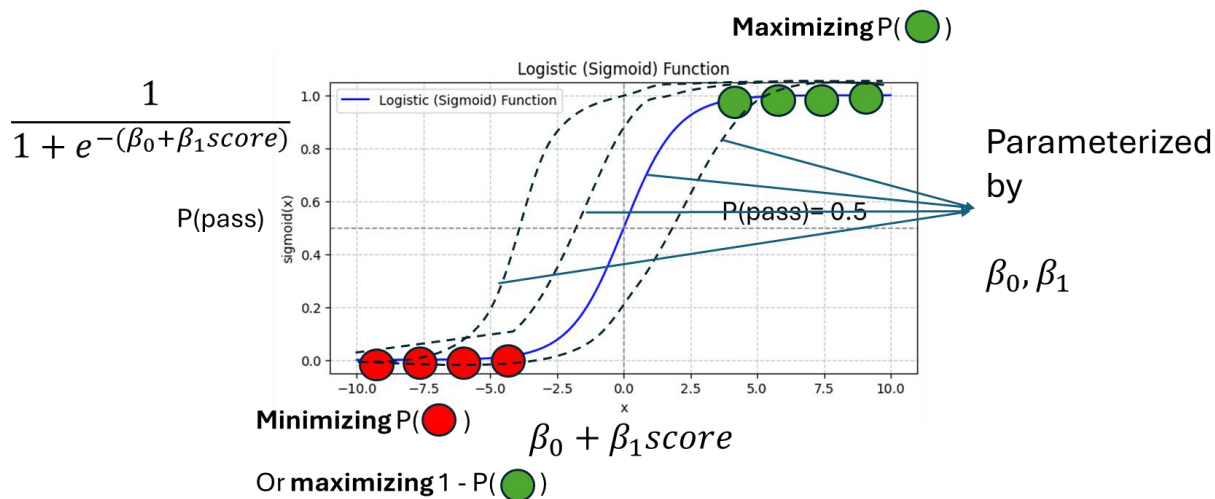
Loss function:

$$\begin{aligned} L[\phi] &= \sum_{i=1}^I (f[x_i, \phi] - y_i)^2 \\ &= \sum_{i=1}^I (\phi_0 + \phi_1 x_i - y_i)^2 \end{aligned}$$

“Least squares loss  
function”



# Logistic Regression



From maximization to minimization.

$$L(\beta) = - \prod_{s \text{ in } y_i = 1} p(x_i) * \prod_{s \text{ in } y_i = 0} (1 - p(x_i))$$

# Loss function

- Training dataset of  $I$  pairs of input/output examples:

$$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^I$$

- **Loss function** or **cost function** measures how bad model is:

or for short:

$$L[\phi, f[\mathbf{x}_i, \phi], \{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^I]$$

Learning  
parameters,  
 **$\beta, \theta$ , or  $\phi$**

$$L[\phi]$$

Returns a scalar that is smaller when  
model maps inputs to outputs better

Learning model: LR or LG ...

# Training

- Loss function:

$$L[\phi]$$

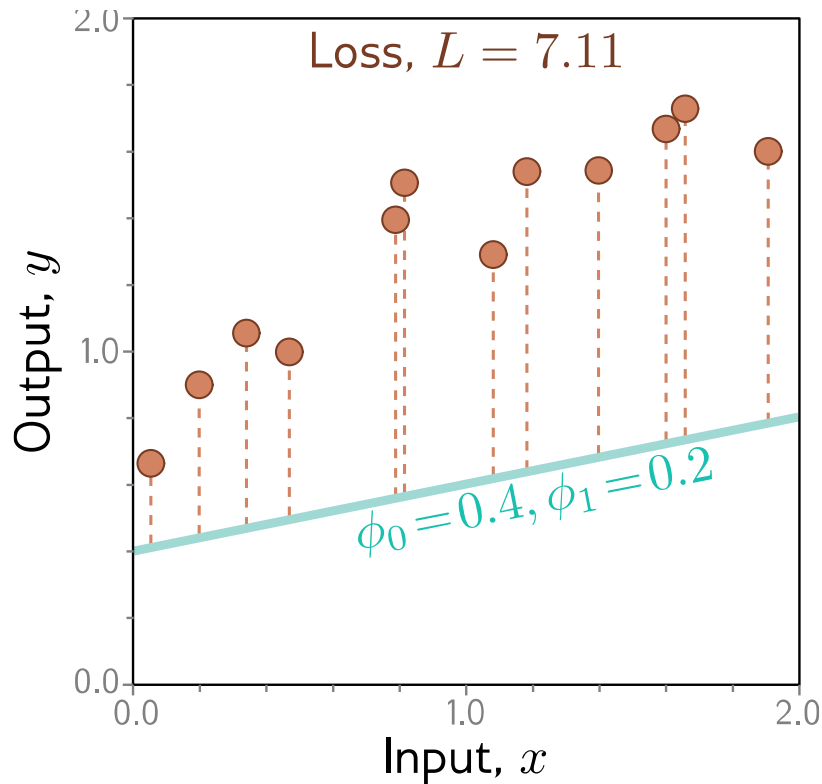


Returns a scalar that is smaller when model maps inputs to outputs better

- Find the parameters that minimize the loss:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}} [L[\phi]]$$

# Example: 1D Linear regression loss function



Loss function:

$$L[\phi] = \sum_{i=1}^I (f[x_i, \phi] - y_i)^2$$
$$= \sum_{i=1}^I (\phi_0 + \phi_1 x_i - y_i)^2$$

“Least squares loss function”

# Example: 1D Linear regression loss function

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}} [L[\phi]] \quad \text{minimize } \|y - X\phi\|_2^2$$

$$\frac{\partial L}{\partial \phi} = 0 \quad \text{solve for } \hat{\phi}$$

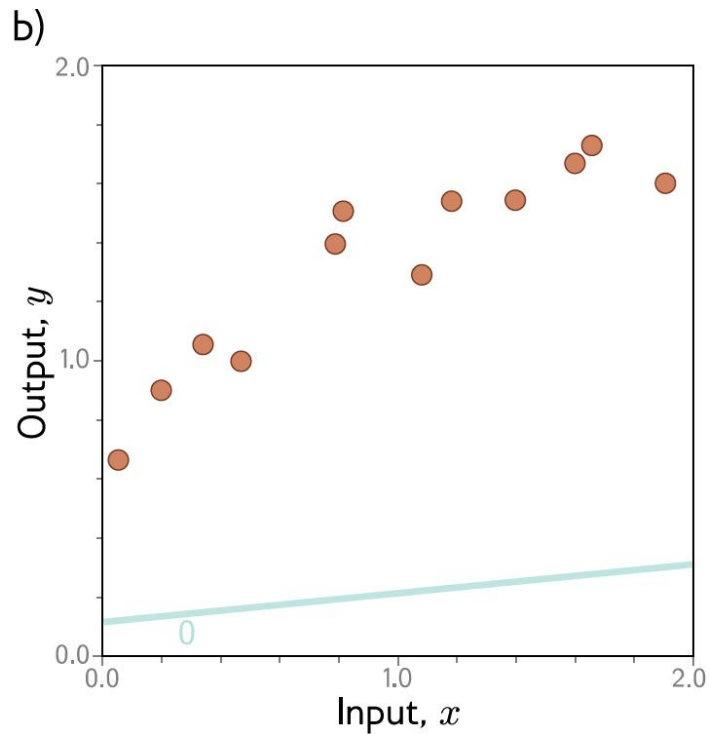
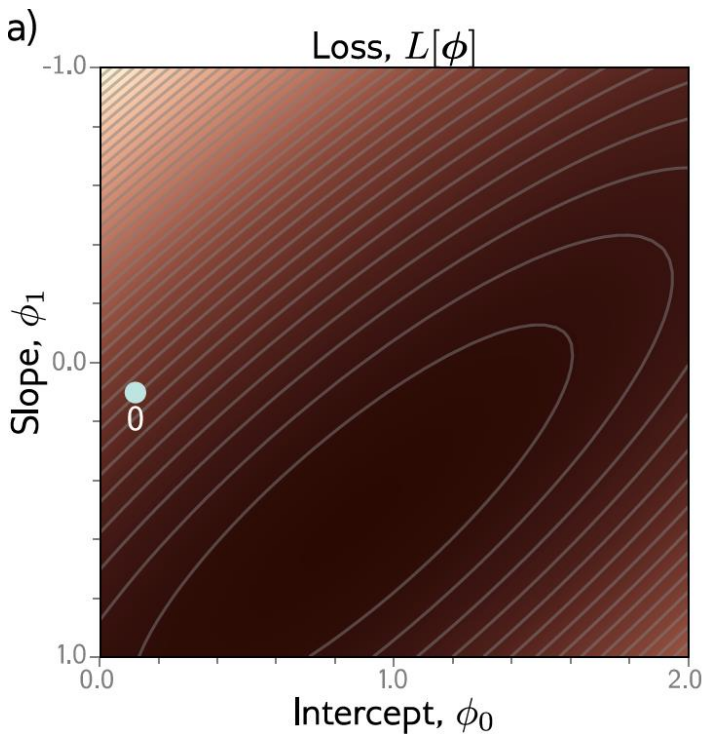


$$\phi = (X^T X)^{-1} X^T y \quad \longrightarrow \quad \text{Closed-form solution}$$

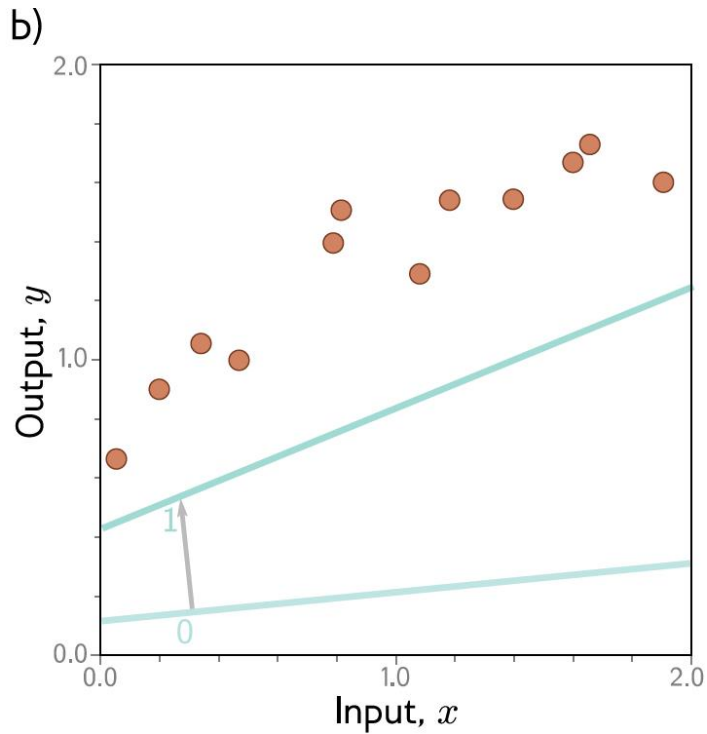
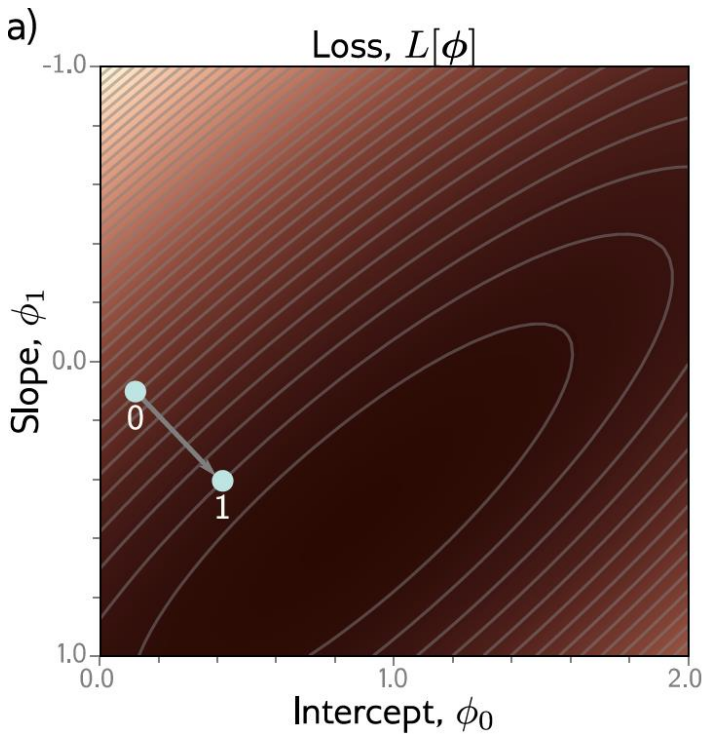
Where:

- $(X^T X)^{-1}$  is the inverse of the matrix product of the transpose of the design matrix  $X^T$  and  $X$ .
- $X^T$  is the transpose of the design matrix.
- $y$  is the vector of observed target values.

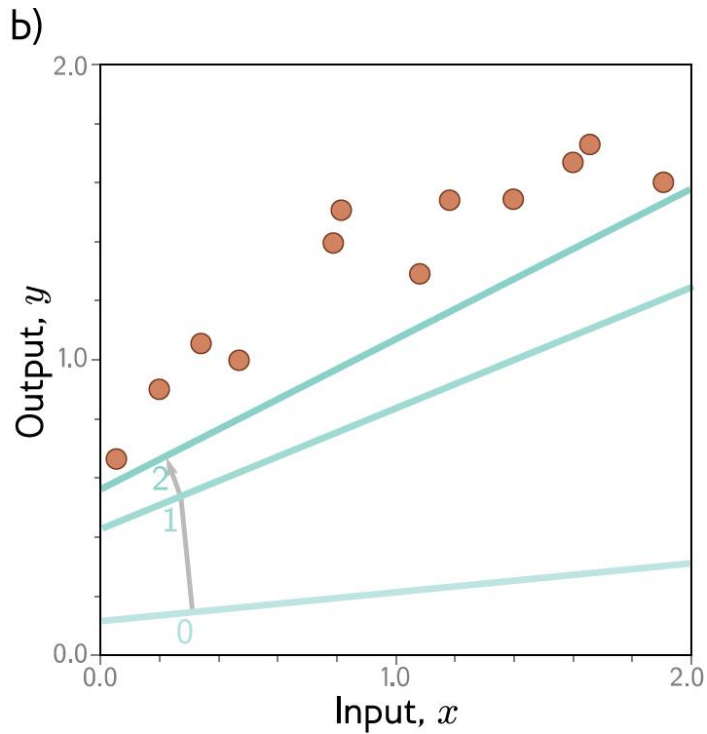
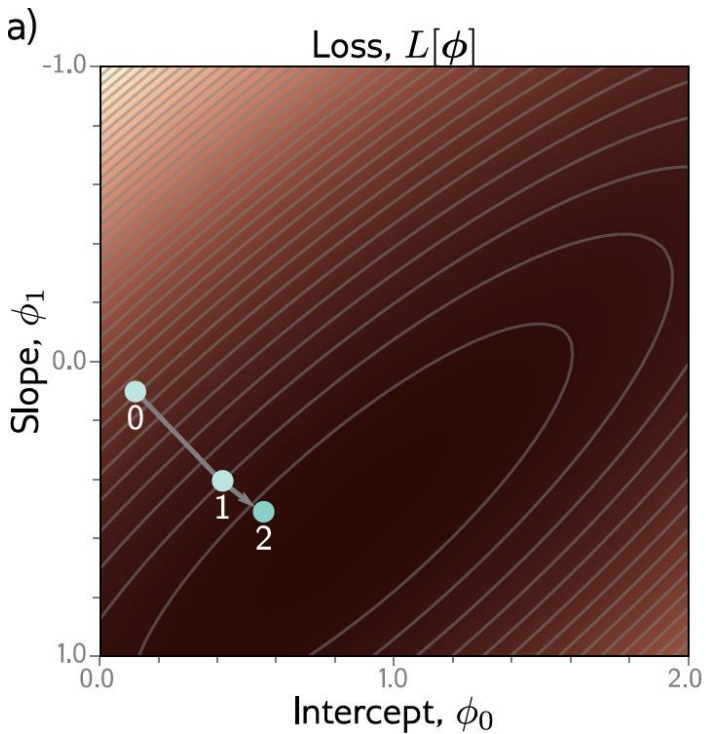
# What if there is no closed-form solution ?



# Example: 1D Linear regression training

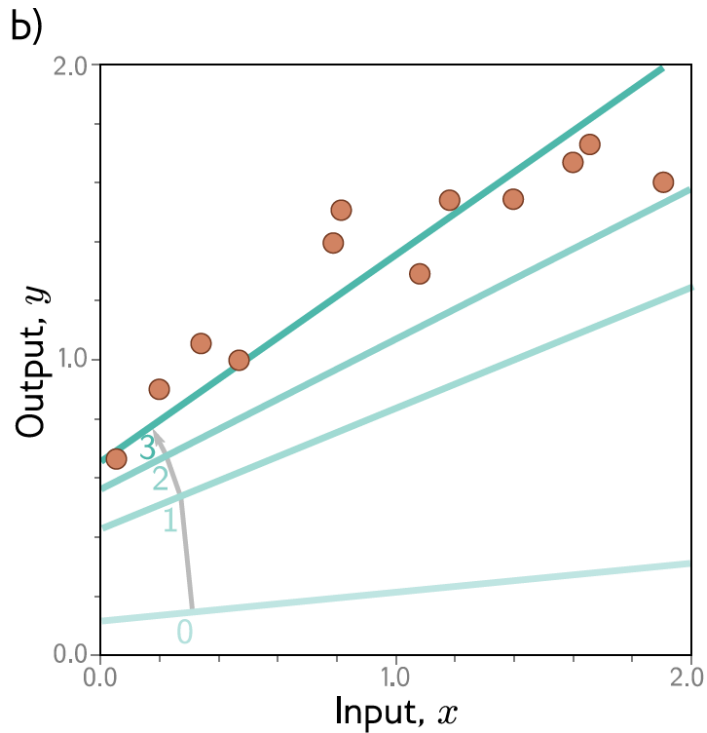
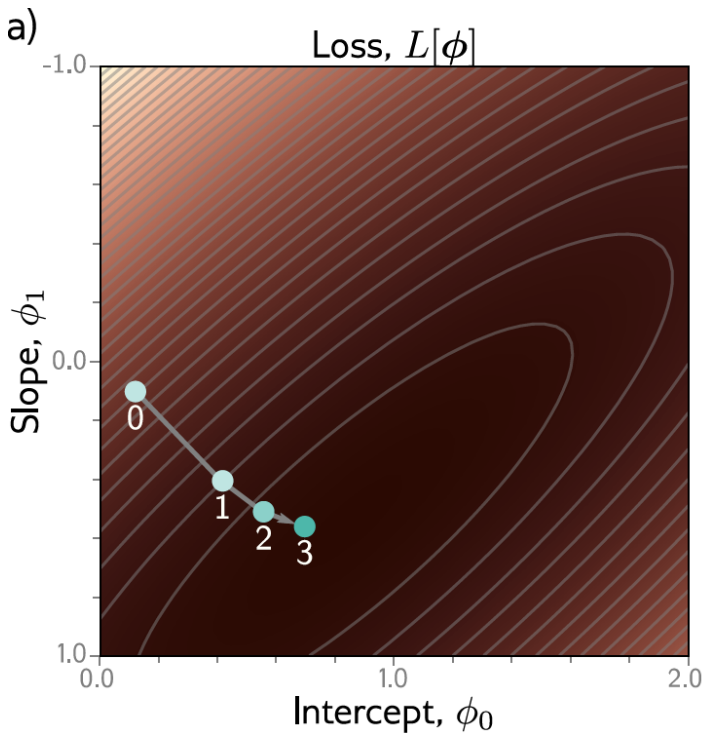


# Example: 1D Linear regression training

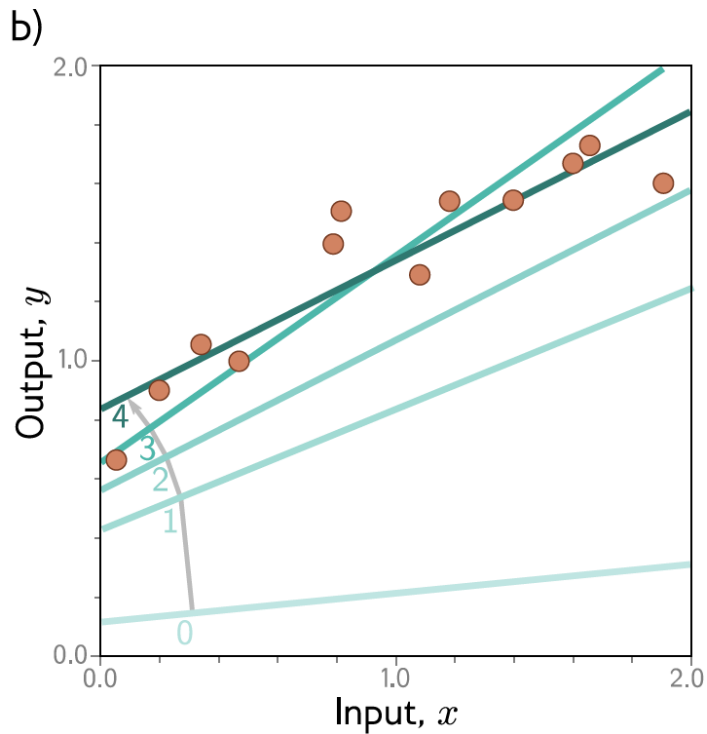
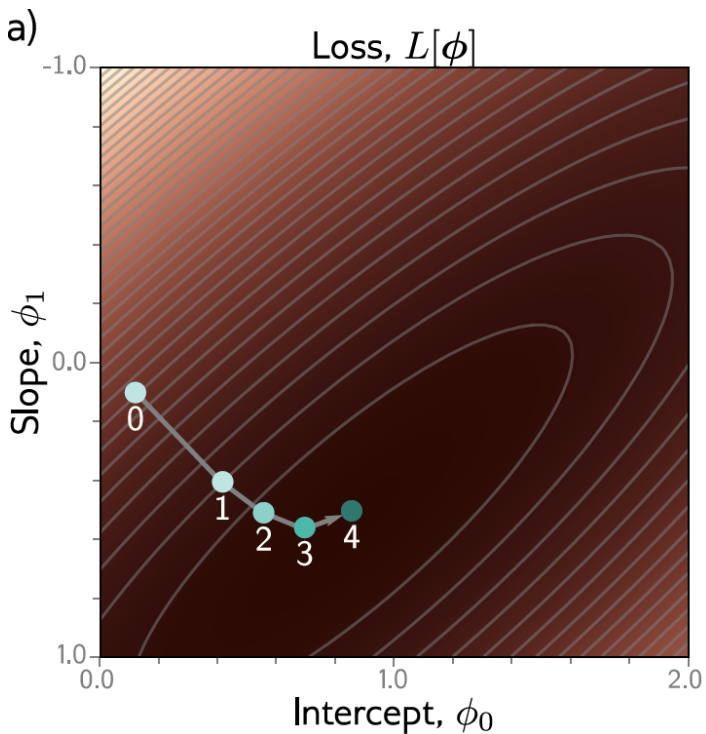




# Example: 1D Linear regression training



# Example: 1D Linear regression training



This technique is known as **gradient descent**

# Introduction to Gradient Descent

# Gradient descent algorithm

**Step 1.** Compute the derivatives of the loss with respect to the parameters:

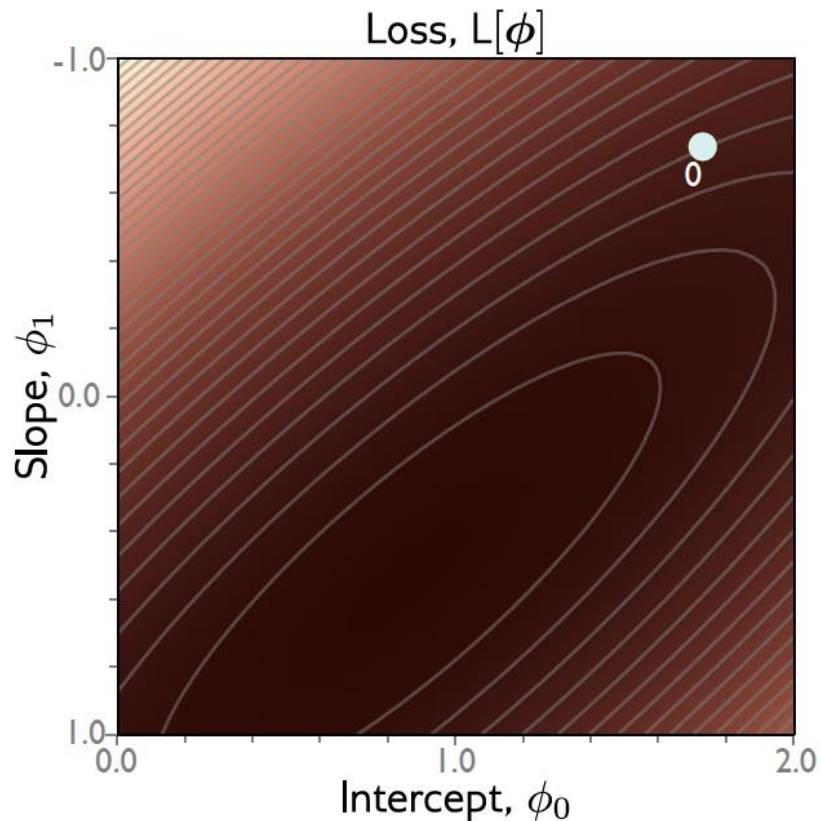
$$\frac{\partial L}{\partial \phi} = \begin{bmatrix} \frac{\partial L}{\partial \phi_0} \\ \frac{\partial L}{\partial \phi_1} \\ \vdots \\ \frac{\partial L}{\partial \phi_N} \end{bmatrix}.$$

**Step 2.** Update the parameters according to the rule:

$$\phi \longleftarrow \phi - \alpha \frac{\partial L}{\partial \phi},$$

where the positive scalar  $\alpha$  determines the magnitude of the change.

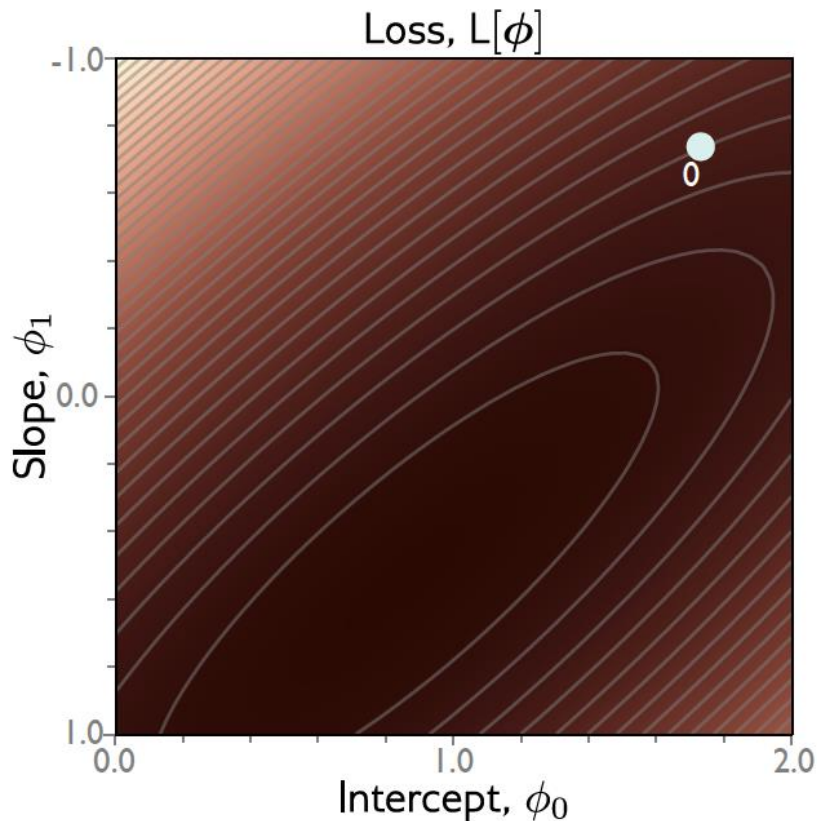
# Gradient descent



Step 1: Compute derivatives (slopes of function) with Respect to the parameters

$$\begin{aligned} L[\phi] &= \sum_{i=1}^I \ell_i = \sum_{i=1}^I (f[x_i, \phi] - y_i)^2 \\ &= \sum_{i=1}^I (\phi_0 + \phi_1 x_i - y_i)^2 \end{aligned}$$

# Gradient descent

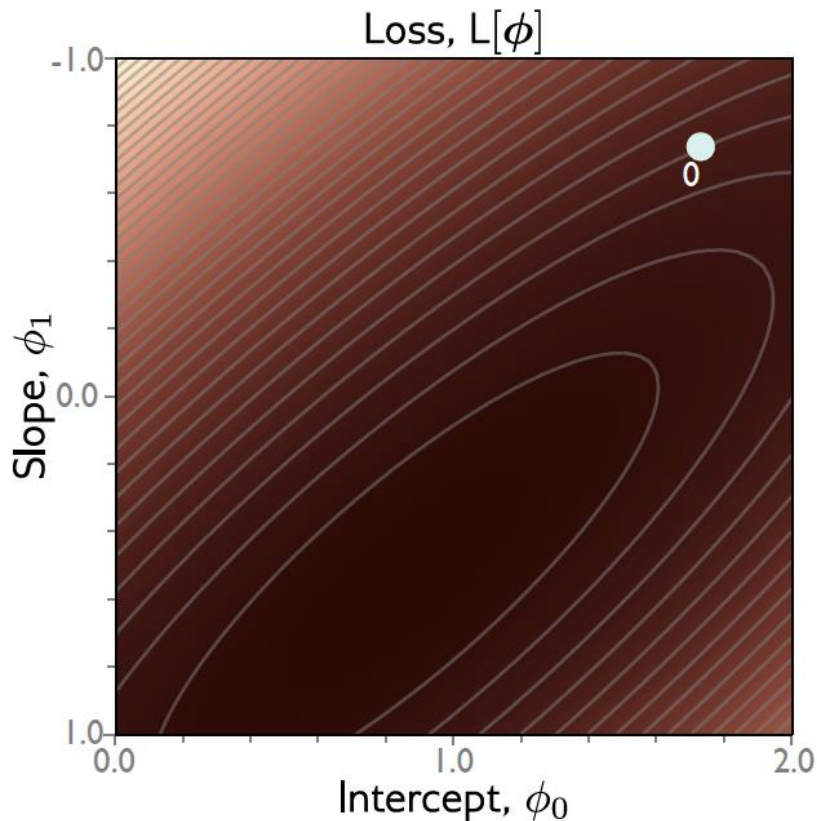


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# Gradient descent



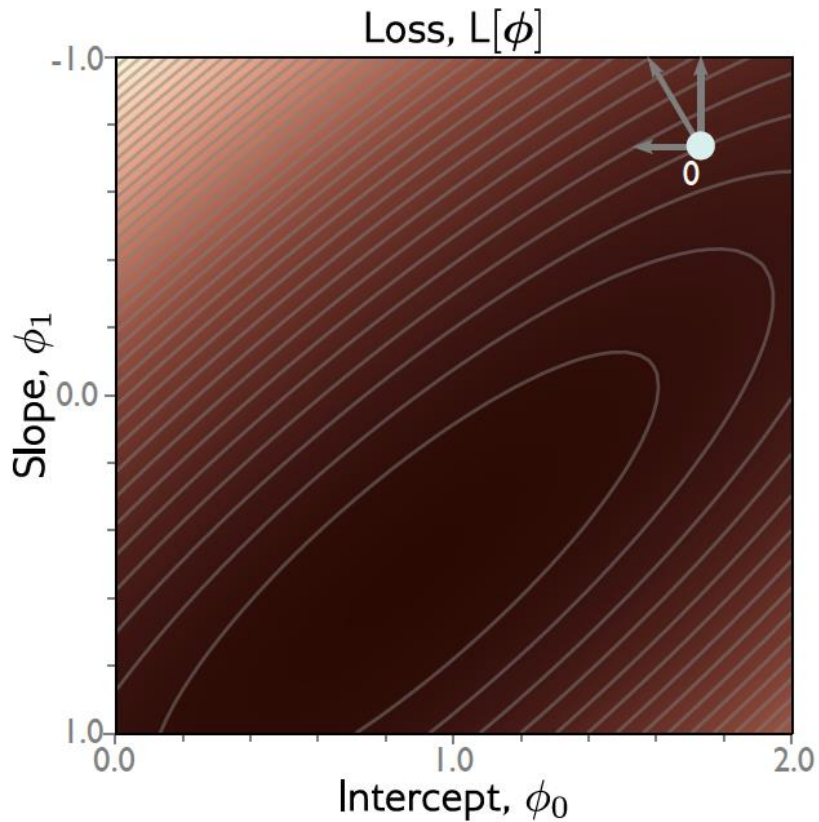
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# Gradient descent



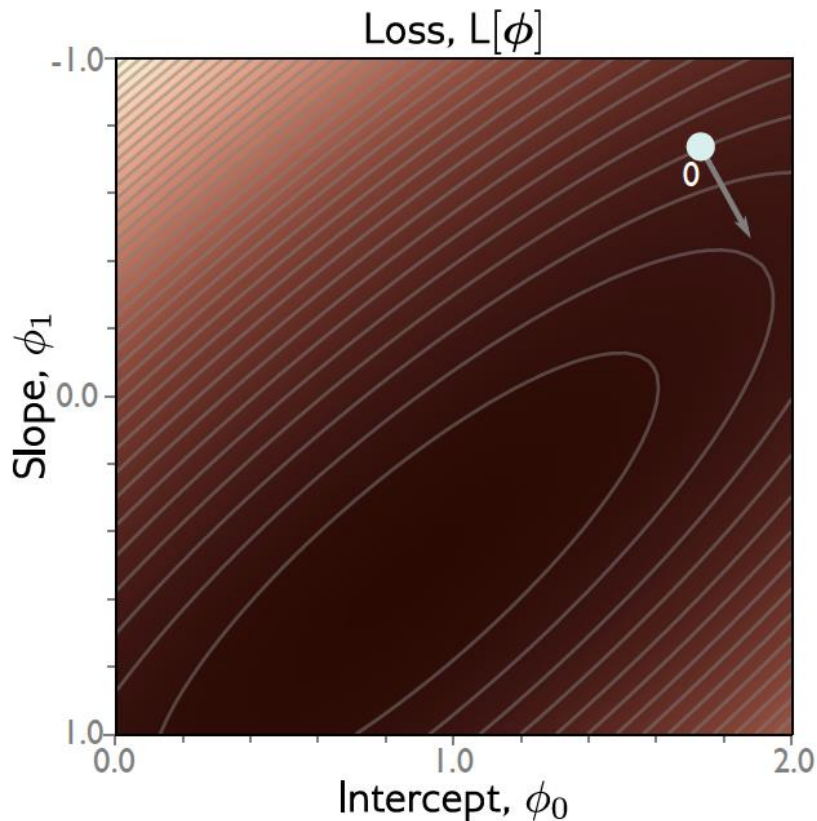
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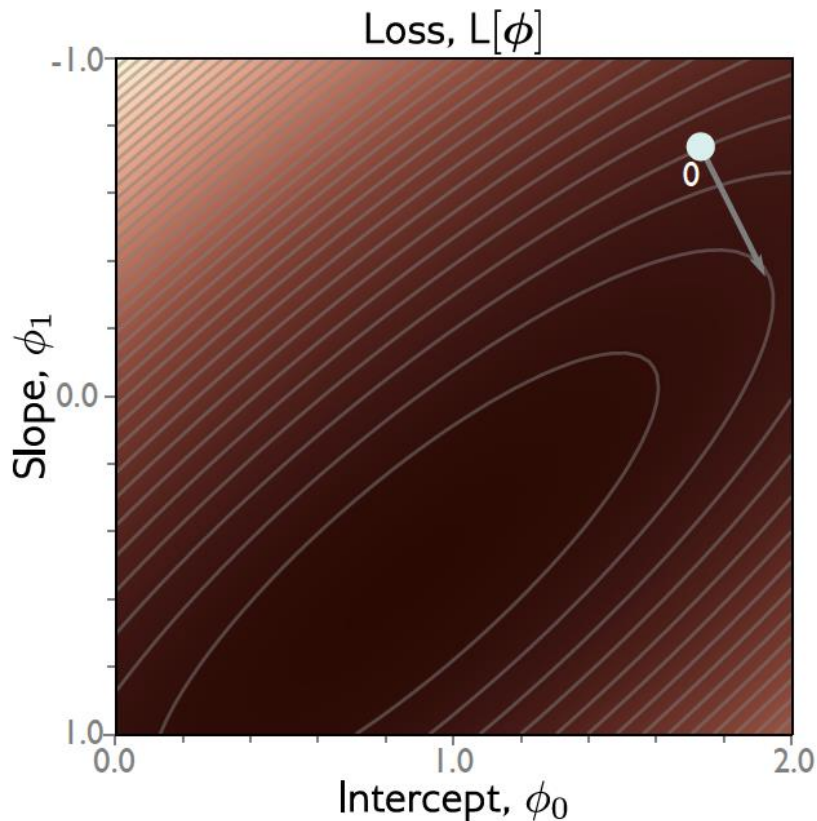
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Step 2: Update parameters according to rule

$$\phi \longleftarrow \phi - \alpha \frac{\partial L}{\partial \phi}$$

$\alpha$  = step size or **learning rate** if fixed

# Gradient descent



Step 1: Compute derivatives (slopes of function) with Respect to the parameters

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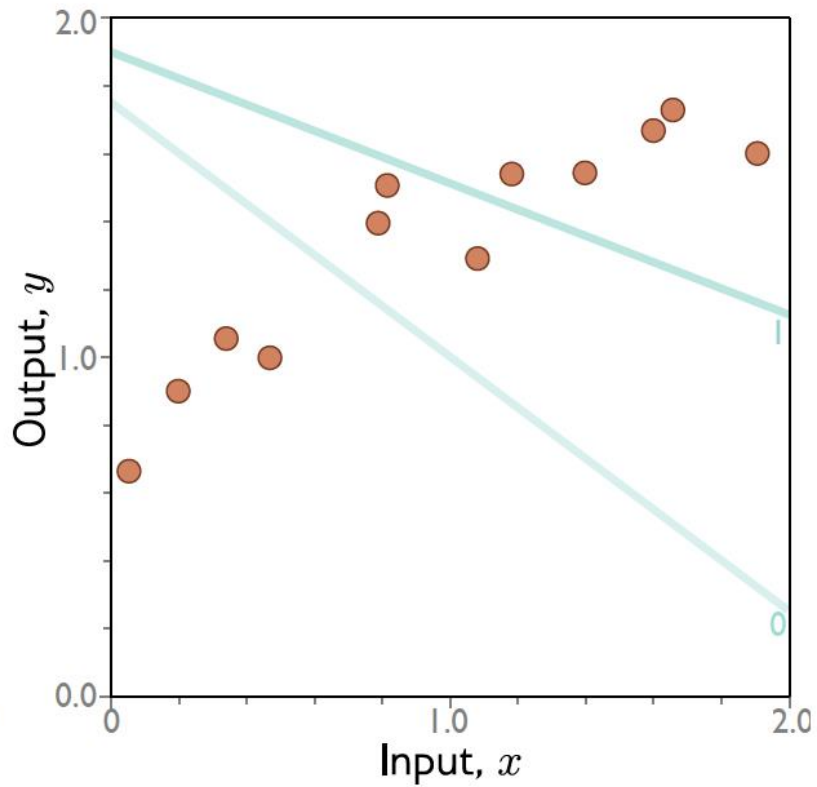
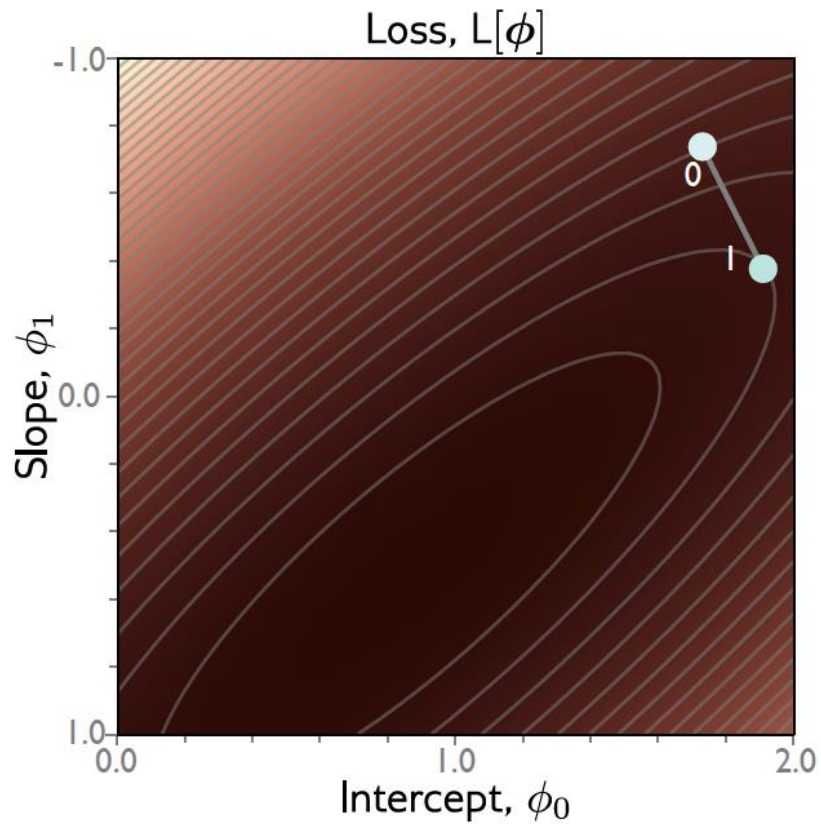
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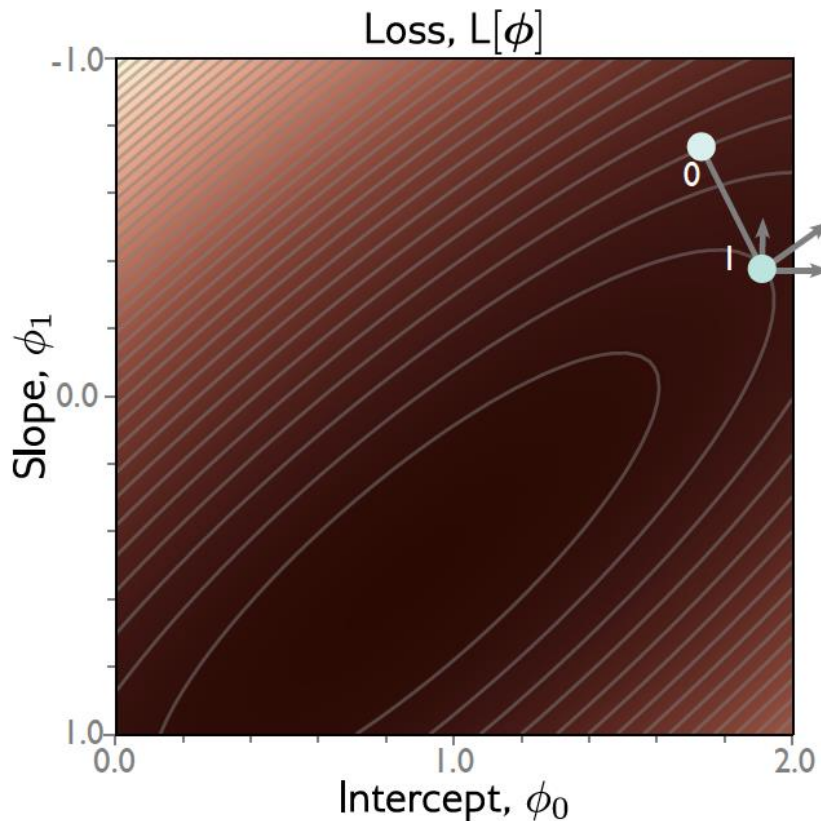
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# Gradient descent



# Gradient descent



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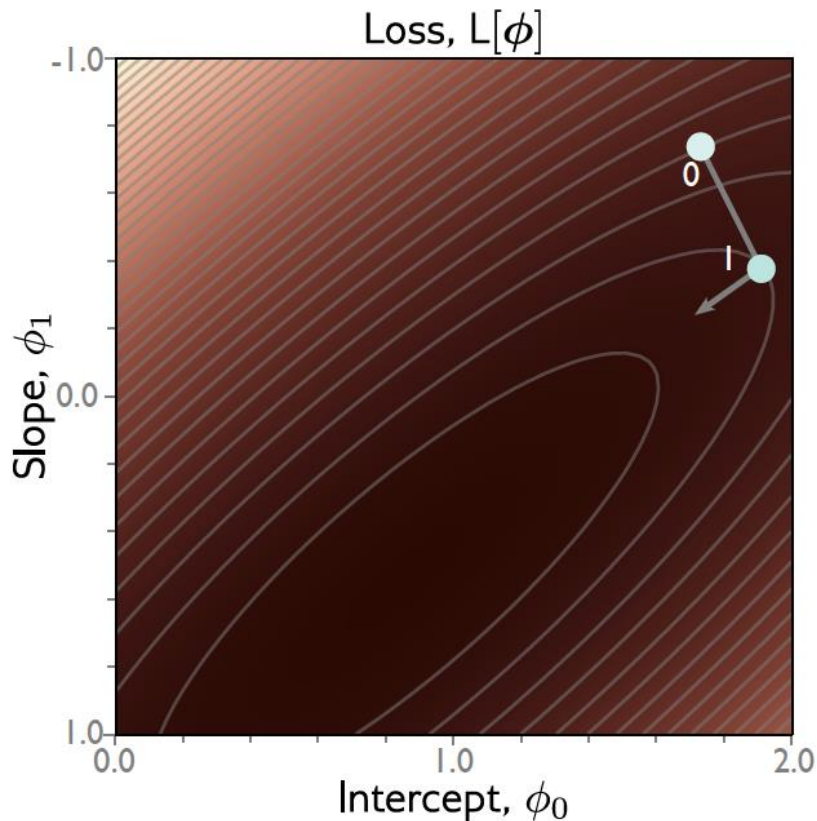
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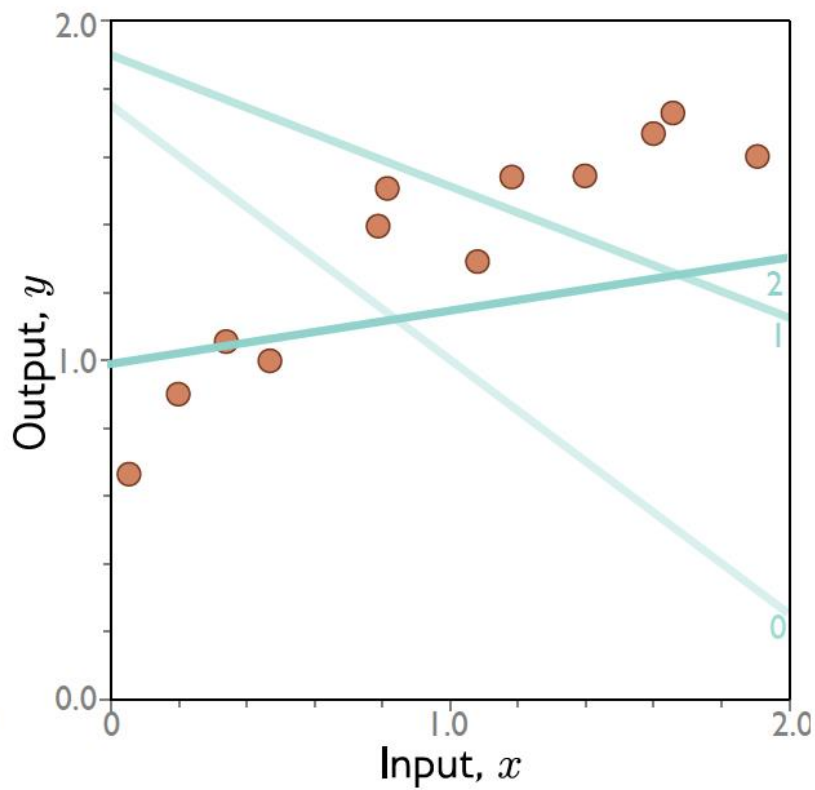
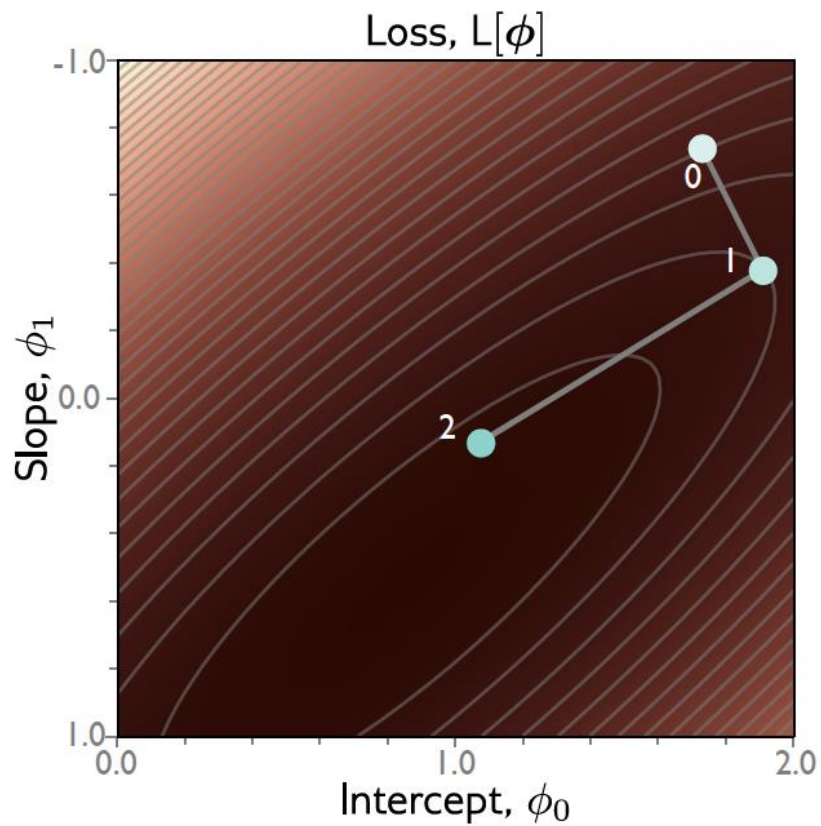
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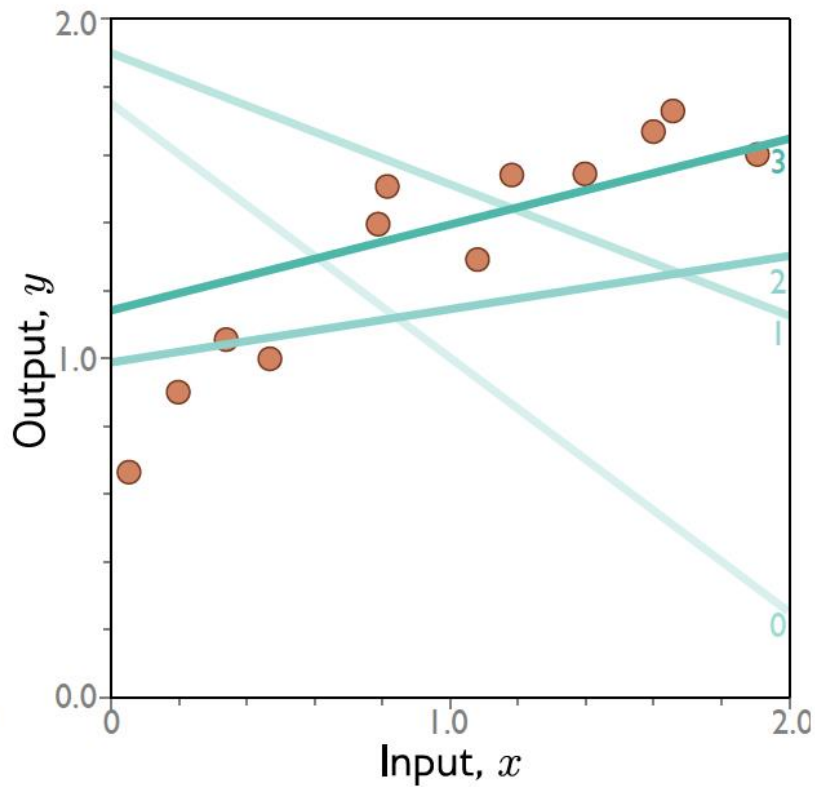
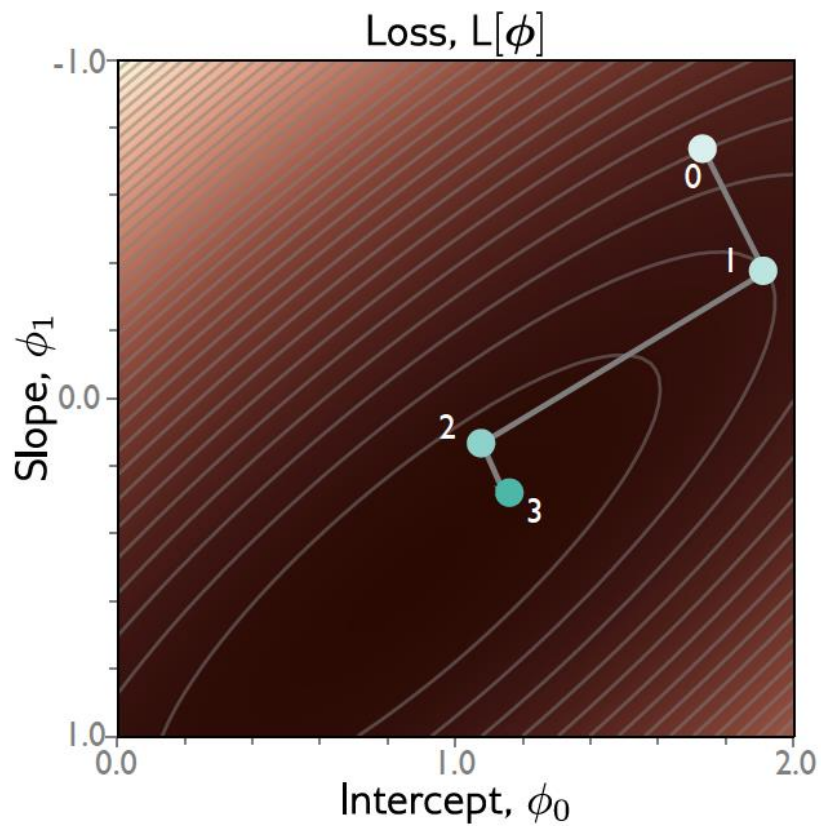
$\alpha$  = step size

# Gradient descent

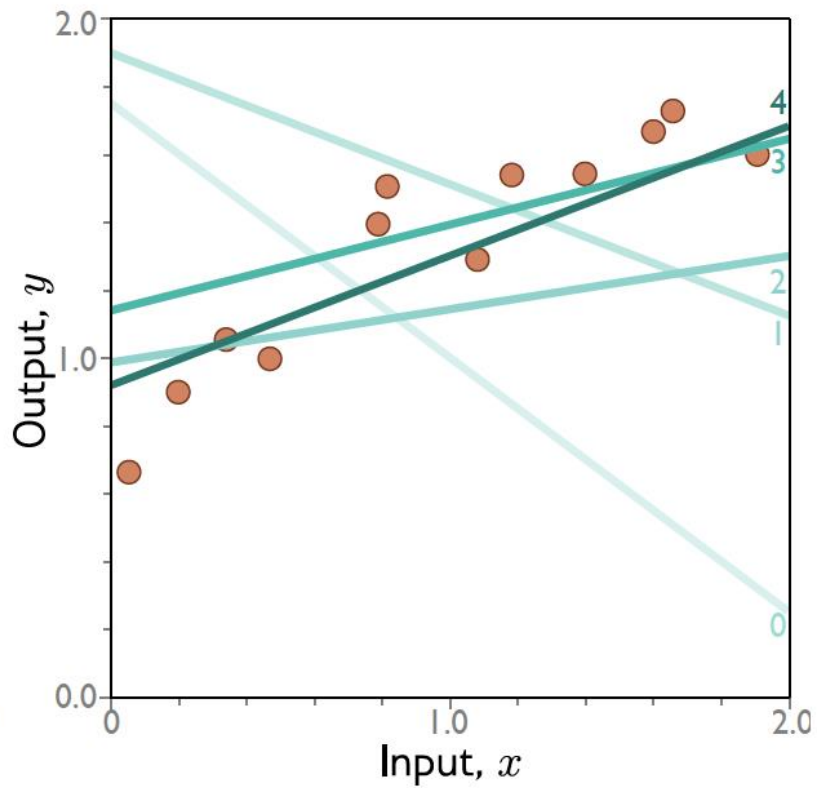
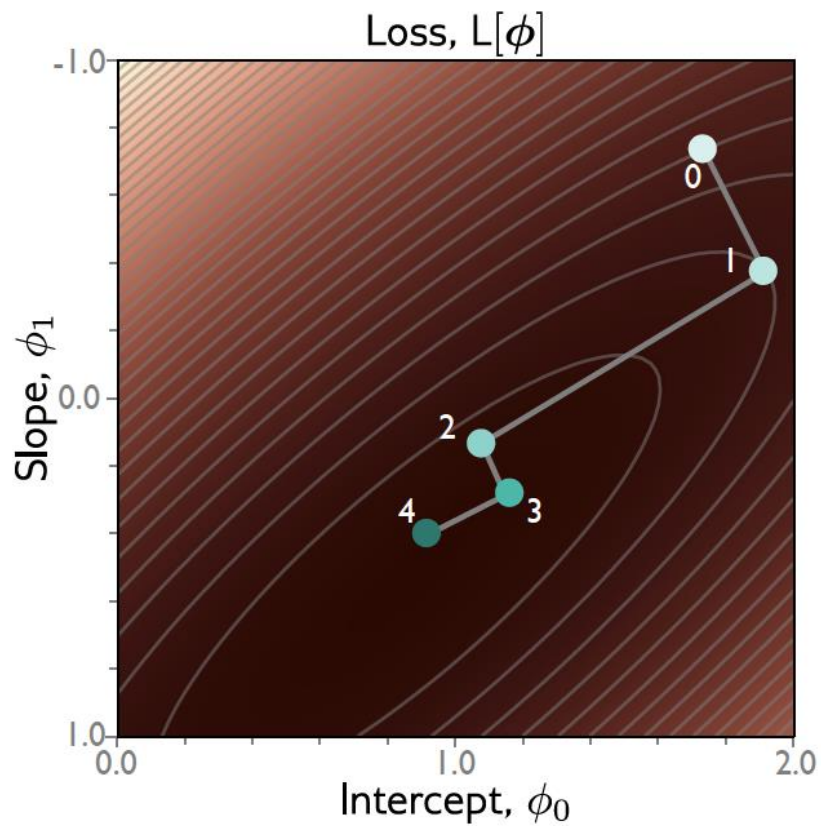




# Gradient descent

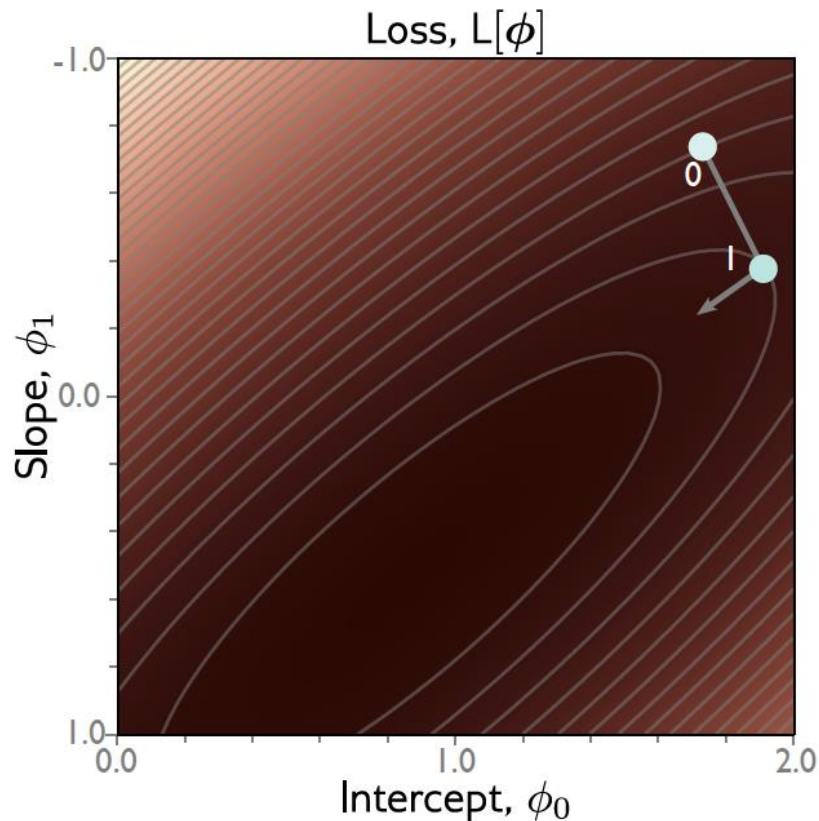


# Gradient descent





# Line Search



Step 1: Compute derivatives (slopes of function) with Respect to the parameters

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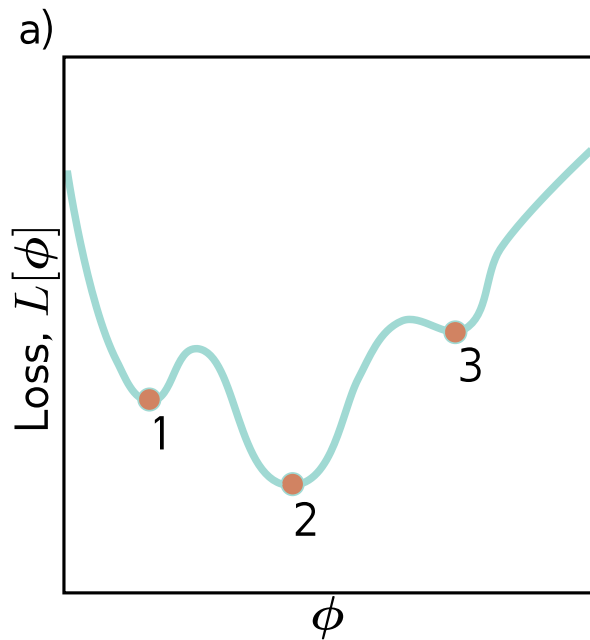
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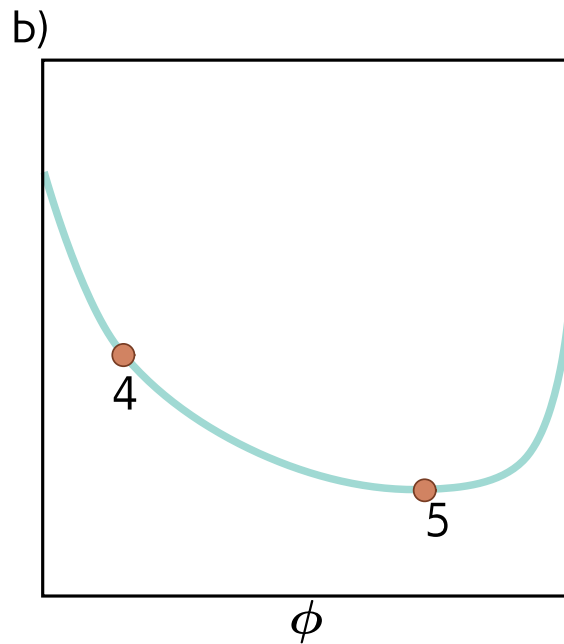
$$\phi \leftarrow \phi - \alpha \frac{\partial L}{\partial \phi}$$

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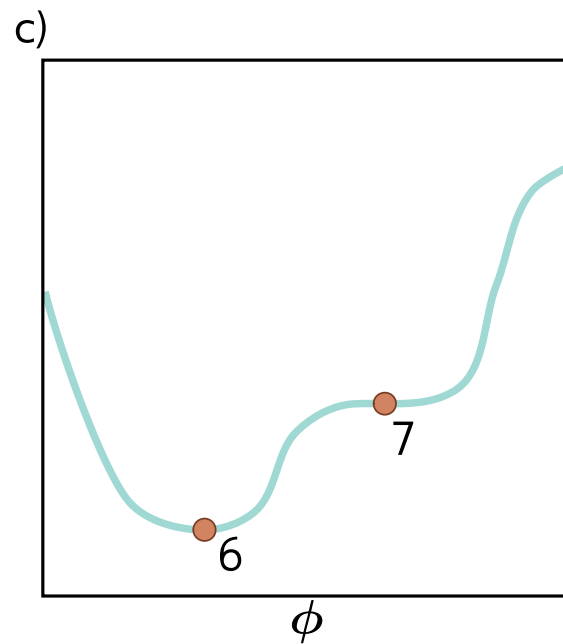
# Convex problems



Non convex

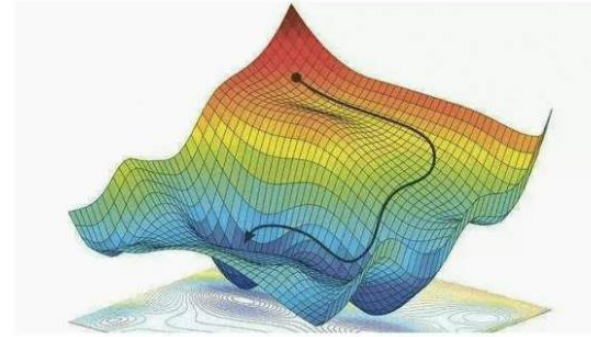
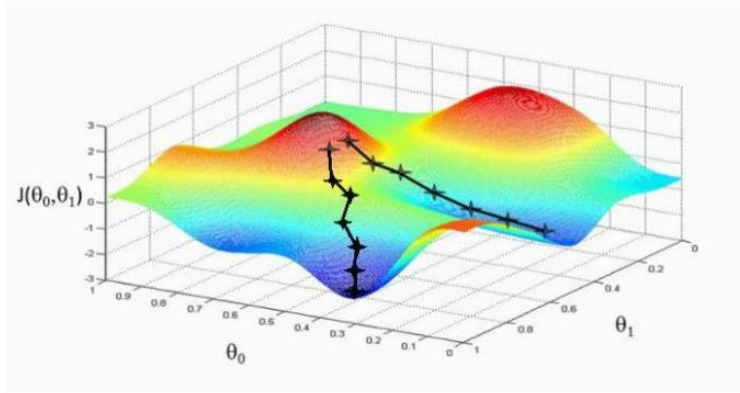


Convex



Non-Convex

# How Does Gradient Descent Work?

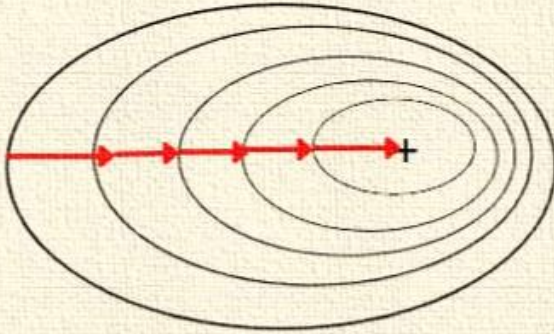


[https://en.wikipedia.org/wiki/Gradient\\_descent](https://en.wikipedia.org/wiki/Gradient_descent)

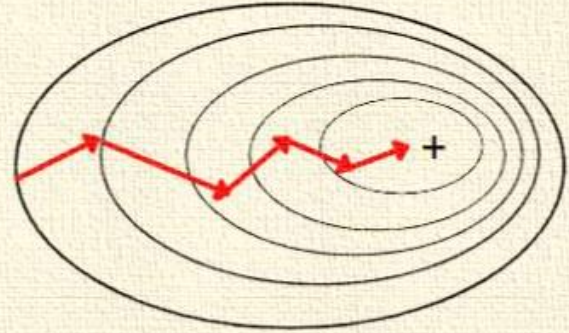
- Having more than one input variable or a more complex function than the Squared Loss, one might get Loss Functions that look like landscapes.
- Gradient Descent will help find the minimum of these functions by cleverly combining different combinations of parameters.

# Gradient Descent Types

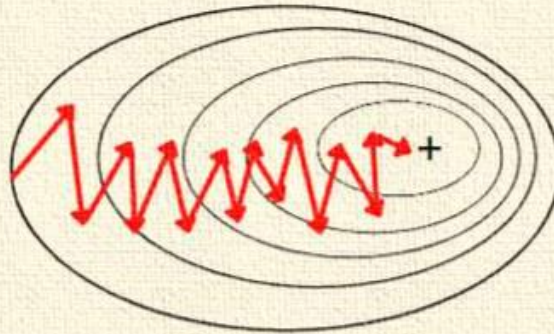
**Batch Gradient Descent**

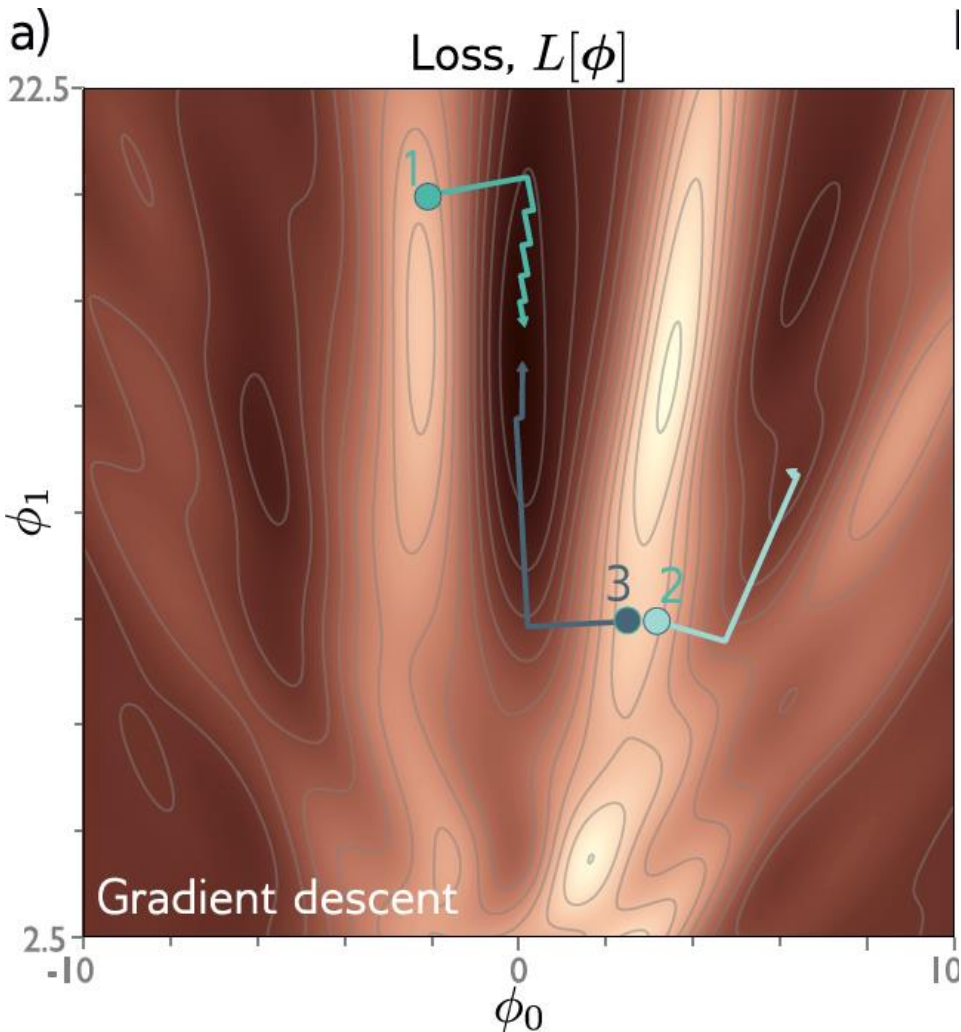


**Mini-Batch Gradient Descent**



**Stochastic Gradient Descent**





Batch Gradient Descent

$$\phi_{t+1} \leftarrow \phi_t - \alpha \sum_{i=1}^I \frac{\partial \ell_i[\phi_t]}{\partial \phi},$$

Mini-Batch Gradient Descent

$$\phi_{t+1} \leftarrow \phi_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\phi_t]}{\partial \phi},$$

Stochastic Gradient Descent

Batch size is 1.

Fixed learning rate  $\alpha$

# Batch Gradient Descent

# Batch Gradient Descent

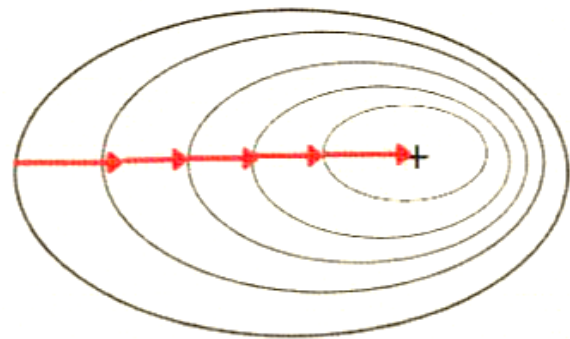
Batch Gradient Descent is also called Vanilla Gradient Descent because of its pure, unmodified version of a vanilla version.

## Pros

- Produces a stable error gradient and a stable convergence
- Deterministic (given the same data)

## Cons

- This can be problematic for very large datasets
- Can converge in a way that is not optimal (get stuck in local minimum)





# Stochastic Gradient Descent



# Stochastic Gradient Descent

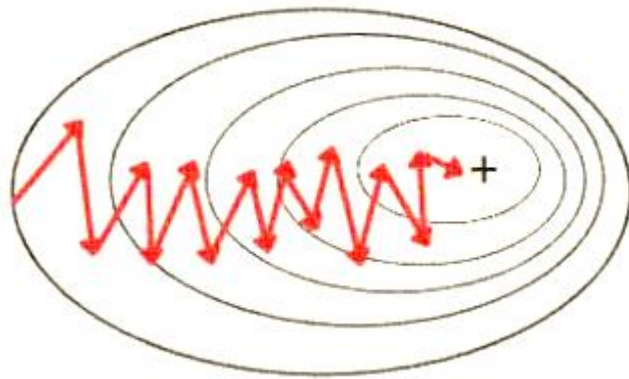
The algorithm will update the weights after each training example. To make this method work, the dataset needs to be shuffled, and the algorithm needs to take random training samples.

## Pros

- Works for very large datasets
- Can potentially converge faster than Batch Gradient Descent
- Chances of being trapped in local minimum are lower

## Cons

- Path to a minimum can be noisy
- Non-deterministic



# Mini-batch Gradient Descent

# Mini-batch Gradient Descent (Standard Practice)

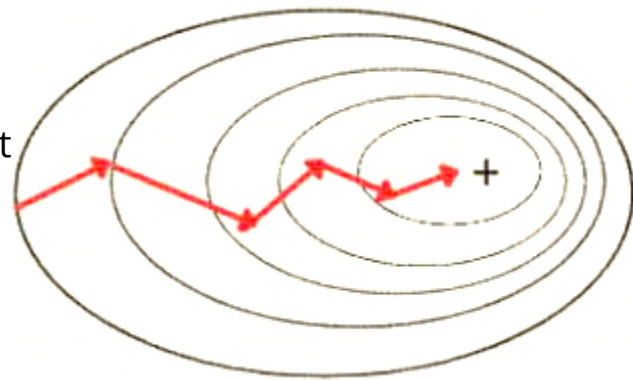
The algorithm will update the weights after the  $n$  training example. This dataset is usually shuffled as well as in Stochastic Gradient Descent.

## Pros

- Compromise between Batch and Stochastic Gradient descent
- Batch size can be adapted depending on the dataset
- Works for very large datasets
- Chances of being trapped in local minimum are lower

## Cons

- Batch size is another hyper-parameter





# Thank you