

Mathematical Concepts

Functions, Minimization, Gradient

Fundamentals of Artificial Intelligence

Fabien Cromieres

Kyoto University

bit.ly/2v6OjgT

What we are going to study/review

- Functions of one variable
- Functions of several variables
- Derivatives and Gradient
- Finding the minimum of a function with Gradient Descent

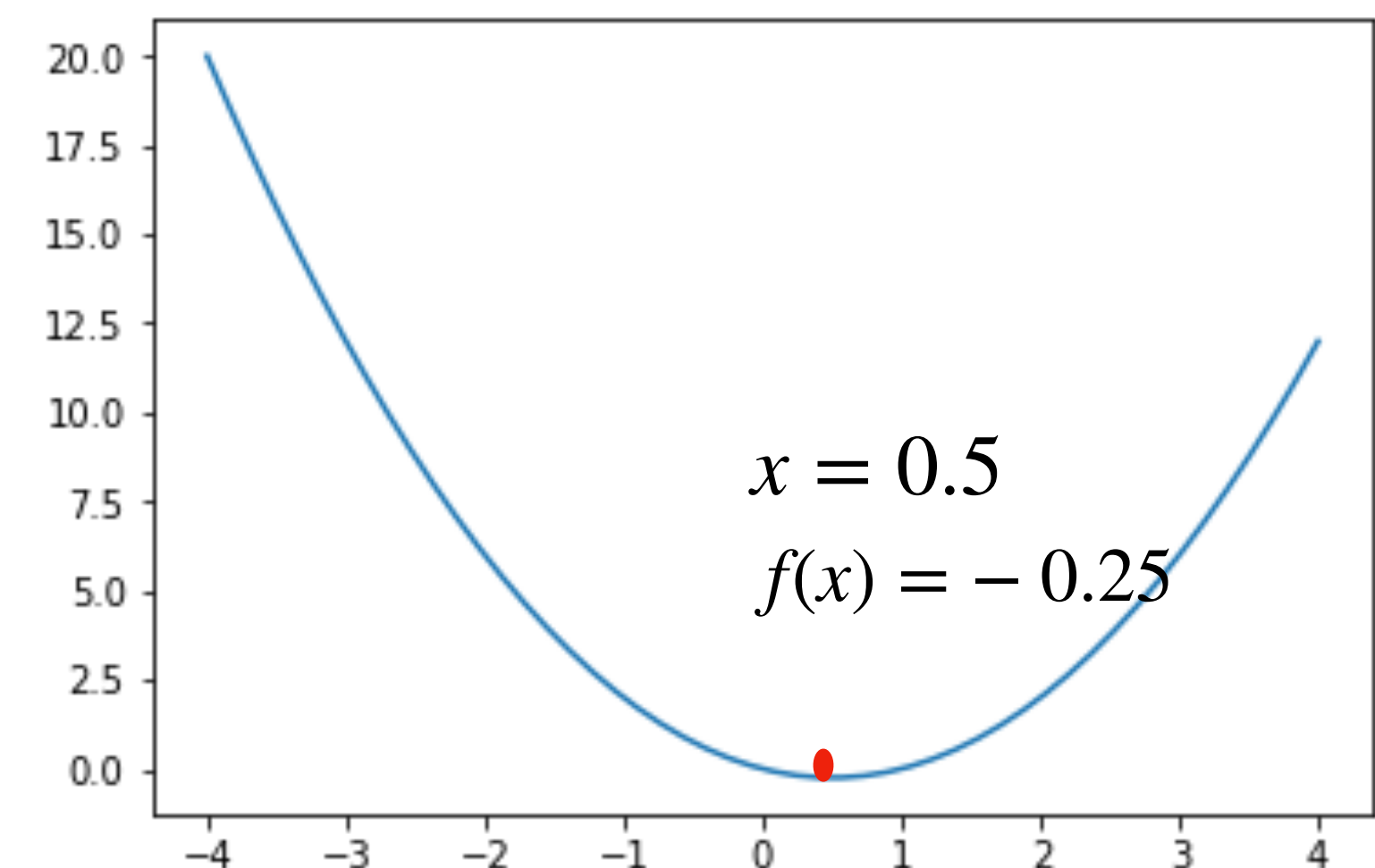
What we are going to study/review

- Given a function of **one variable**, find practically the value for which it is minimum
- a.k.a “univariate function”
- You should have seen how to do that for simple functions in High School

$$f: \mathbb{R} \rightarrow \mathbb{R}$$

$$f(x) = x^2 - x$$

$$\arg \min_x f(x)$$



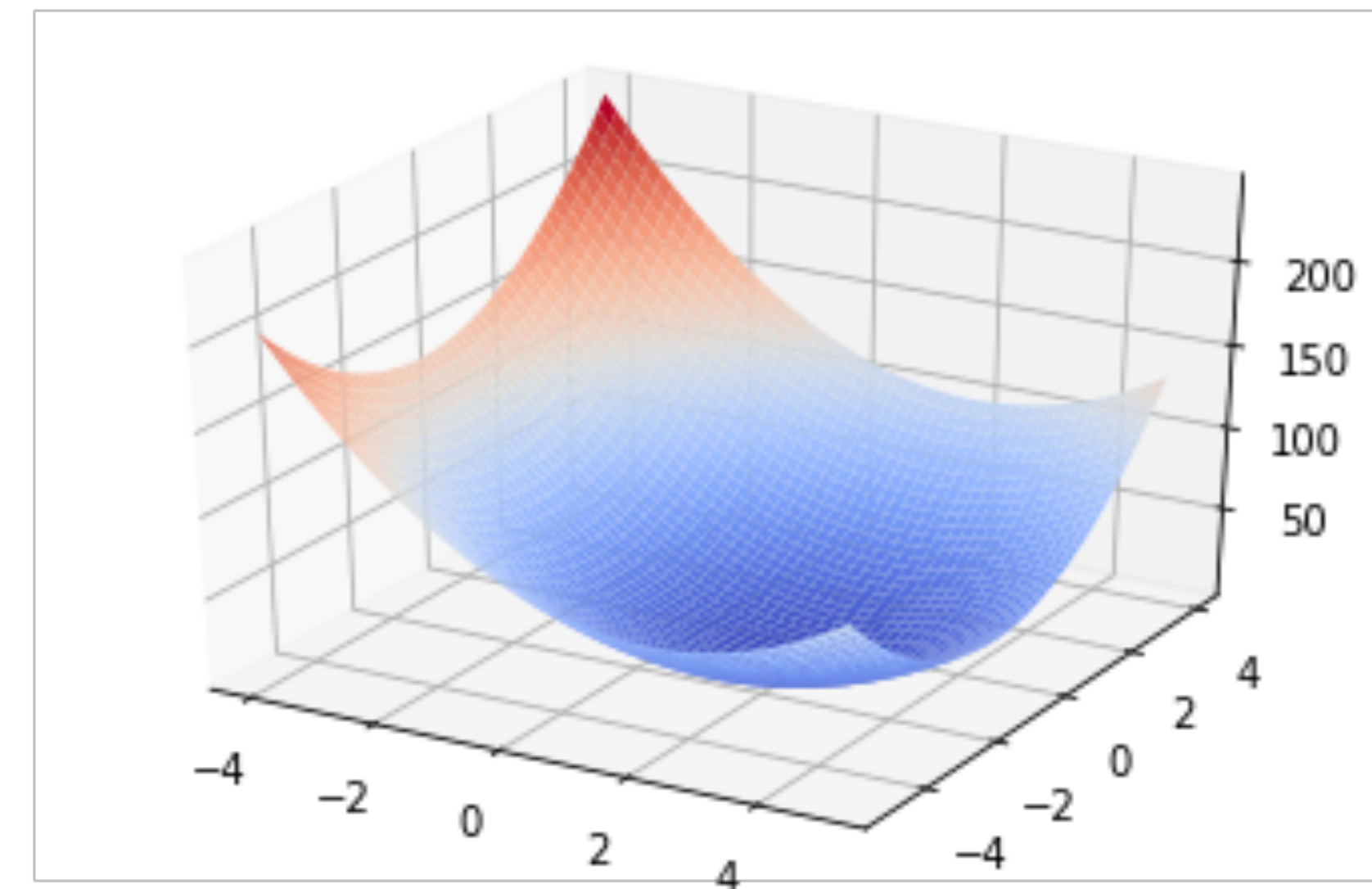
What we are going to study/review

$$f: \mathbb{R}^2 \rightarrow \mathbb{R}$$

$$f(x, y) = (x + y)^2 + 1$$

$$\arg \min_{x, y} f(x, y)$$

- Given a function of **several variables**, find the value for which it is minimum
- a.k.a “multivariate function”

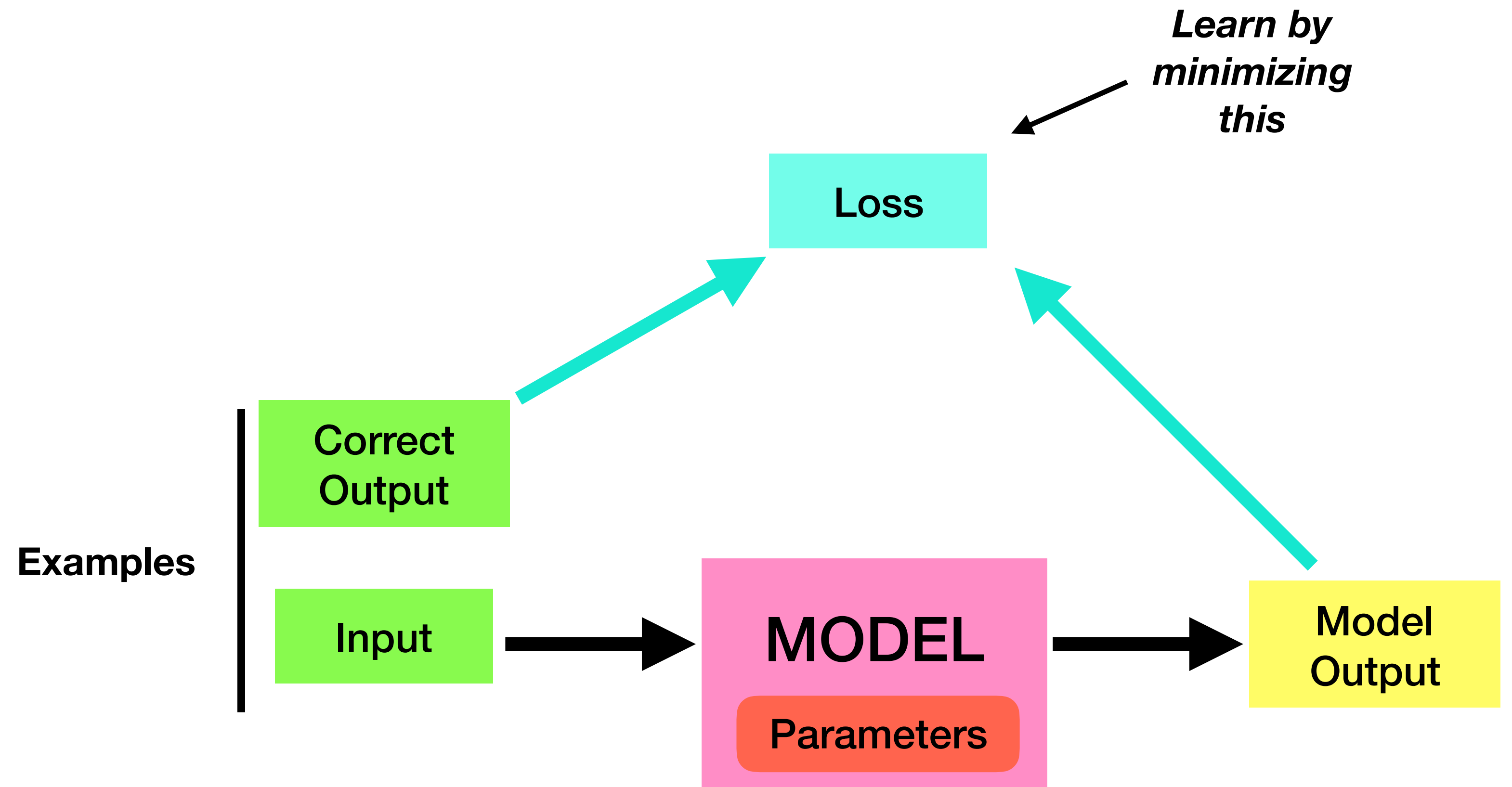


Why we do it?

- Actually, almost all algorithms of supervised machine learning consist in finding the **minimum** of a **function of several variable**

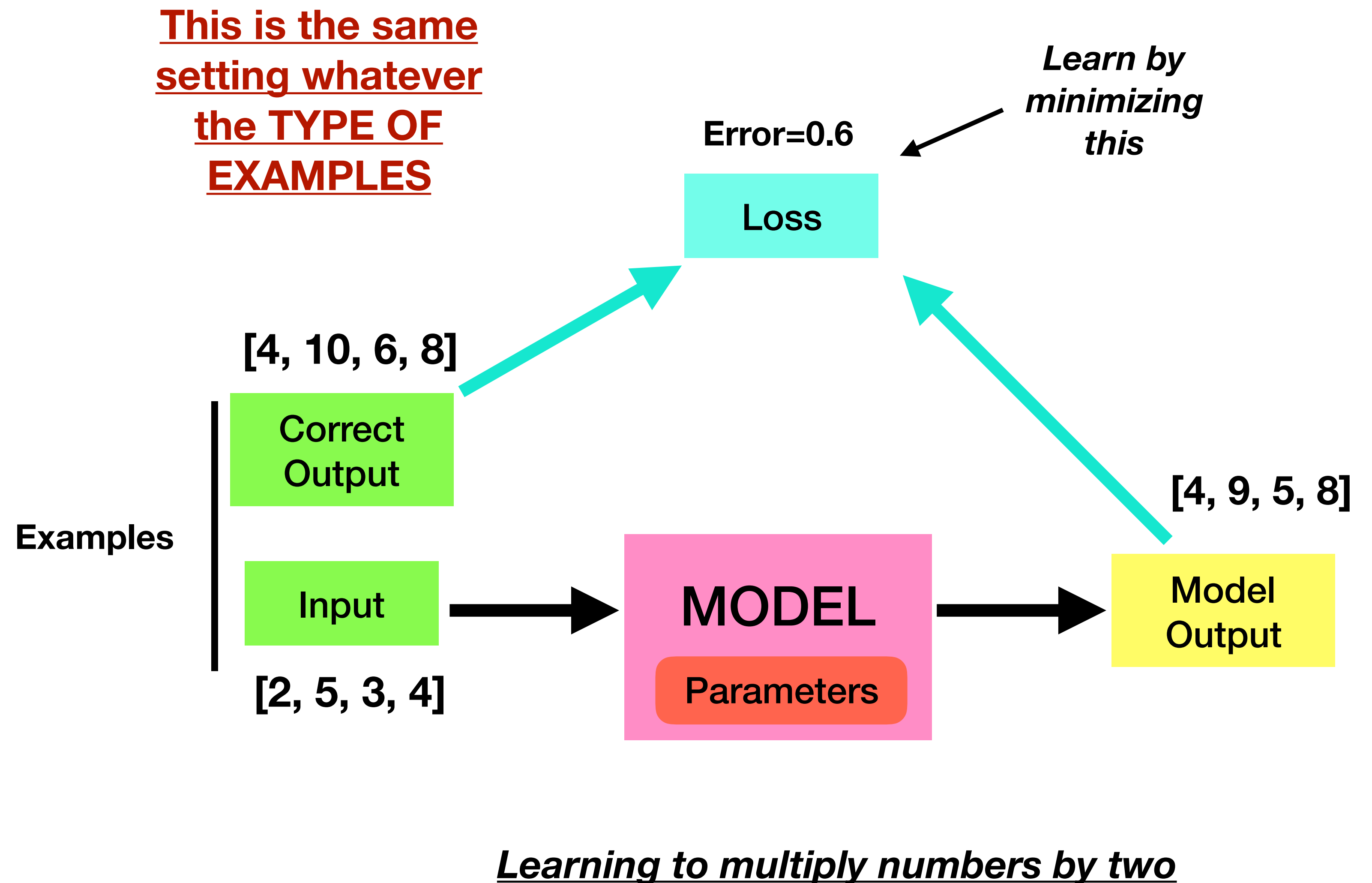
Supervised Learning

- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



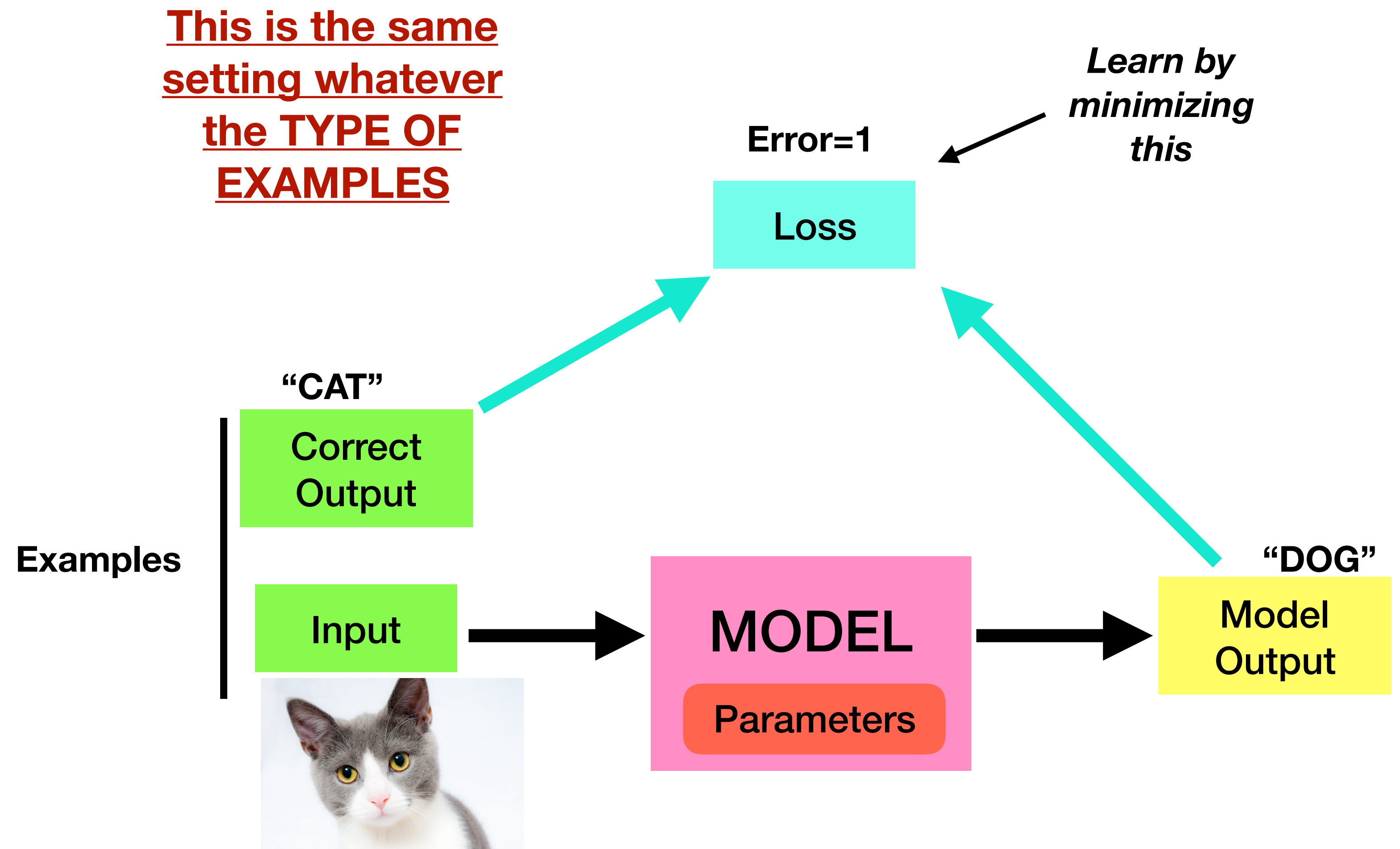
Supervised Learning

- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



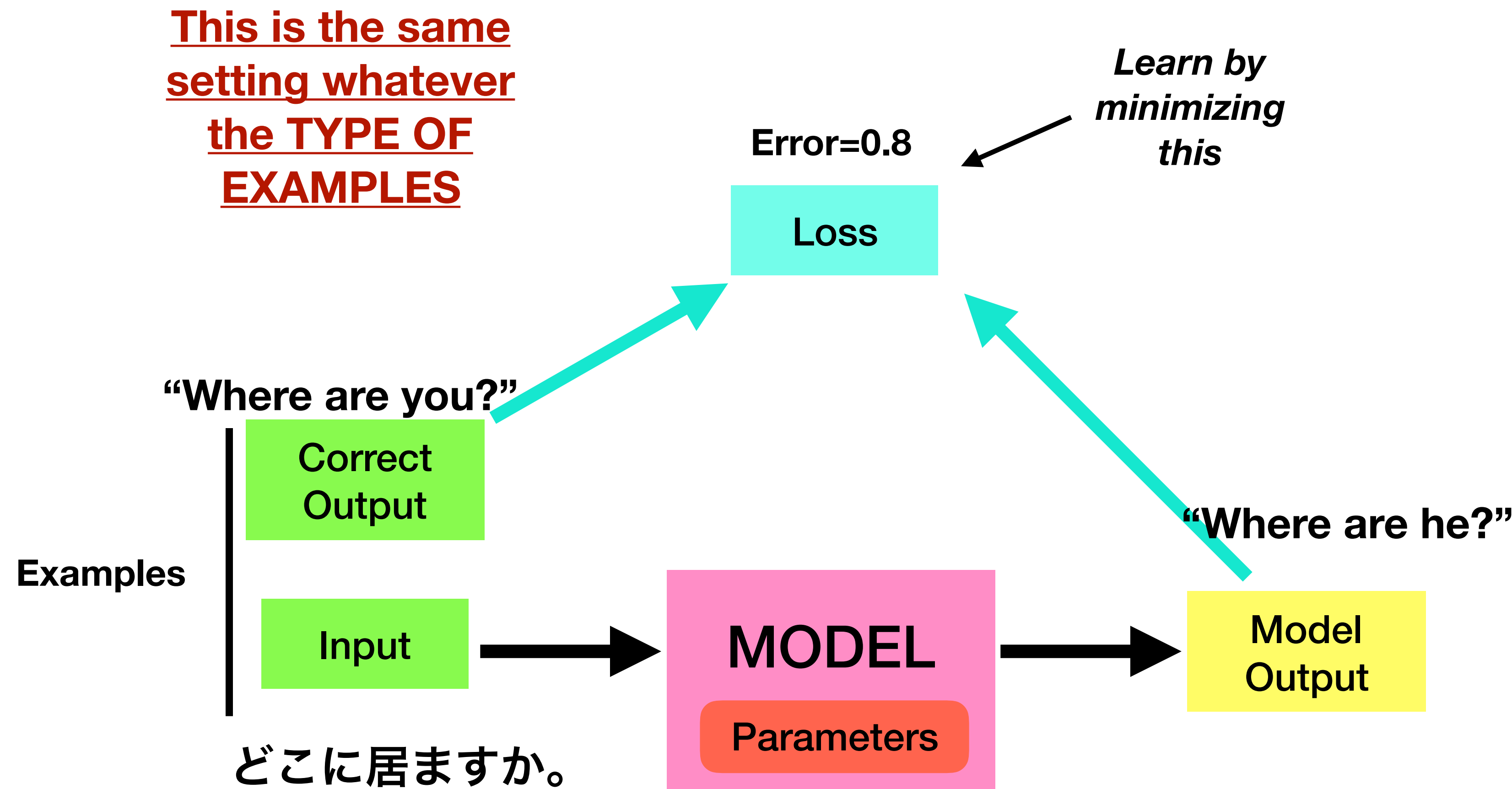
Supervised Learning

- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



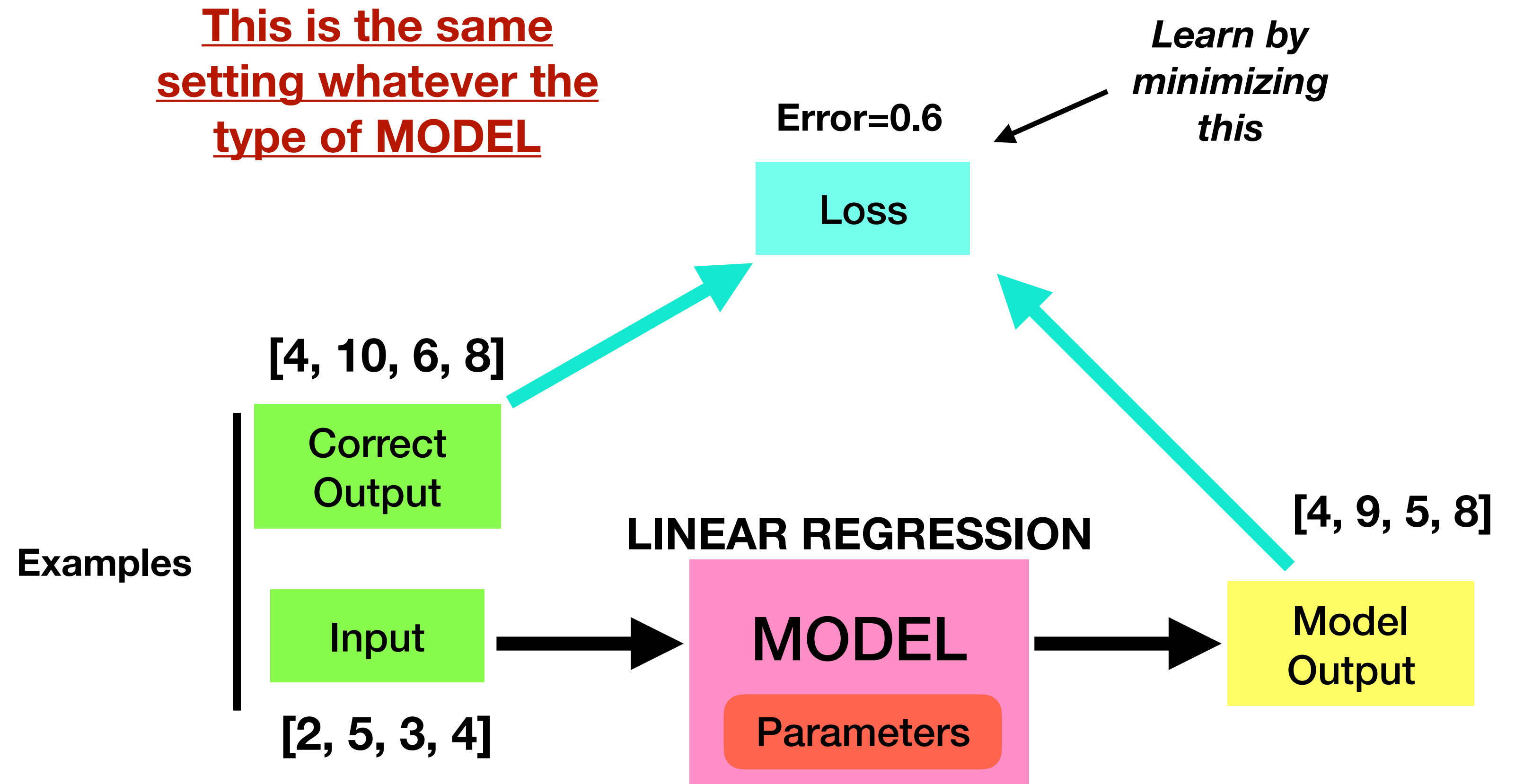
Supervised Learning

- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



Supervised Learning

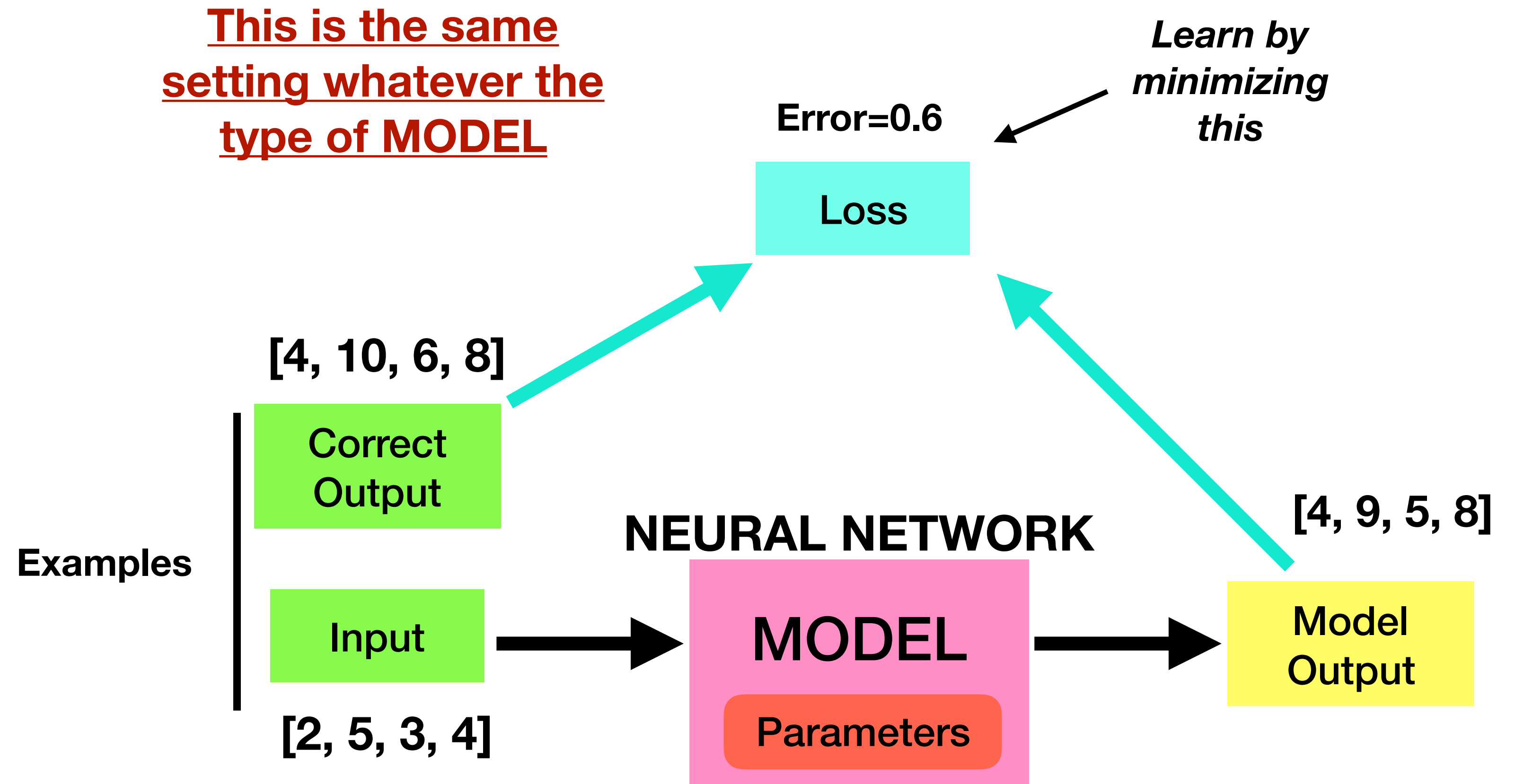
- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



Learning to multiply numbers by two with a Linear Regression Model

Supervised Learning

- In supervised learning, we usually have:
 - A **MODEL**: a “parameterized” function that takes input and produce output
 - A **Loss**: A function that compute how different the model output is from the correct output
 - **Examples** of input and correct output



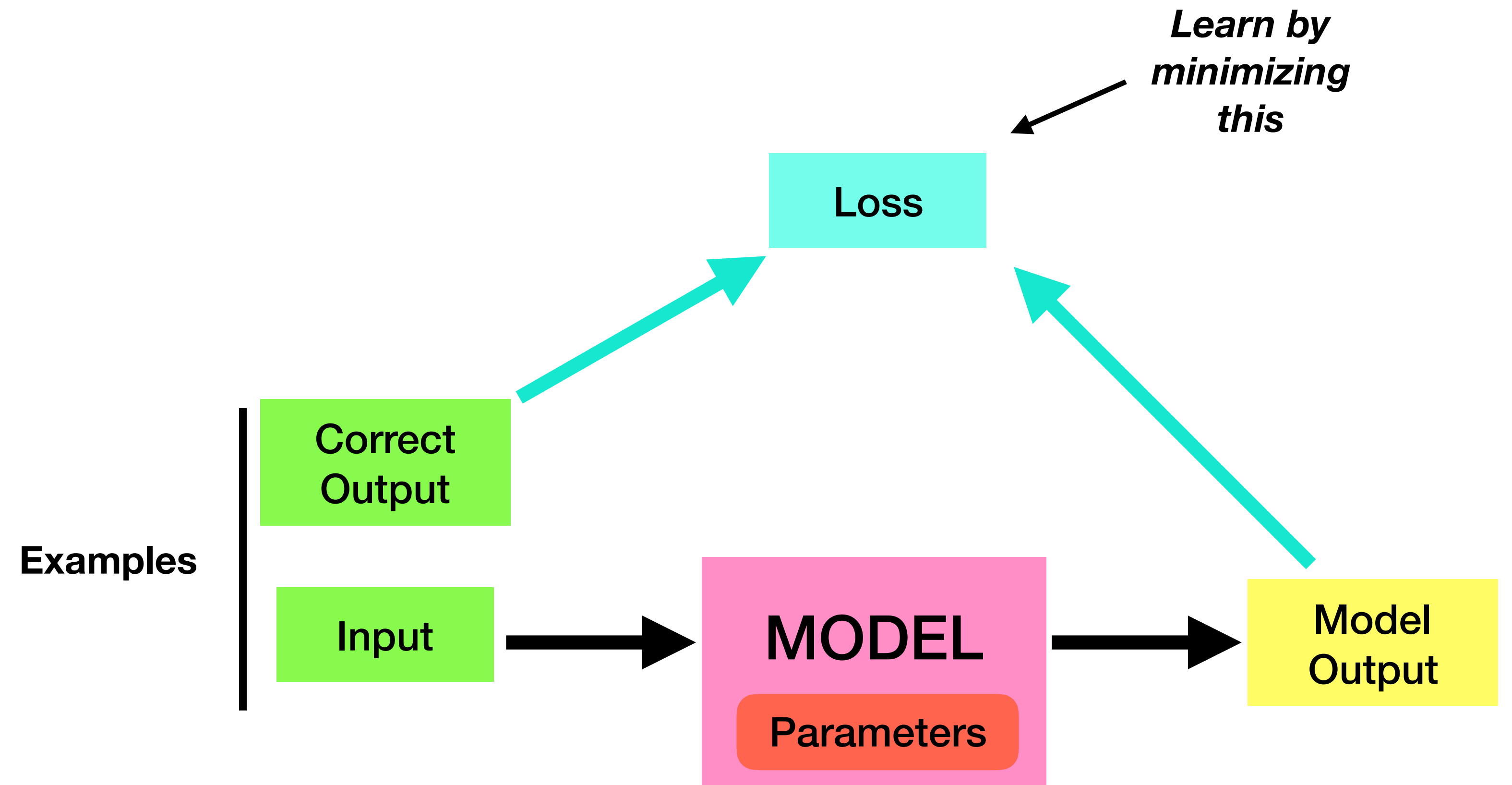
Learning to multiply numbers by two with a Neural Network

Terminology

- Because minimizing a loss is the main way for “learning”, for us, the following expressions have all the same meaning:
 - **Minimizing** the Loss of a Model for some examples
 - **Training** a Model on some examples
 - Having a Model **learn** from some examples

Supervised Learning

- We will go back to these concepts later in the semester
- For now, let us focus on methods for minimizing a function



Minimizing a function of one
variable

Functions of one variable

- Hopefully, you are all familiar with the concept of “*functions of one variable*”
- Terminology: also called “*Univariate function*”
- Take a single number as input, give a single number as output

$$f: \mathbb{R} \rightarrow \mathbb{R}$$

$$f(x) = x^2 - x$$

$$f(-1) = 2$$

$$f(0) = 0$$

$$f(0.1) = -0.99$$

Minimizing a function of one variable

- Given a function of one variable $f(x)$, what is the input number x that gives the smallest output number?
- We note this number $\arg \min_x f(x)$
- What is $\arg \min_x f(x)$ for $f(x) = x^2 + 3$?
- What is $\arg \min_x f(x)$ for $f(x) = x$?
- What is $\arg \min_x f(x)$ for $f(x) = x^2 - x$?

Minimizing a function of one variable

pollev.com/fabiencromie576

- Given a function of one variable $f(x)$, what is the input number x that gives the smallest output number?
- We note this number $\arg \min_x f(x)$
- What is $\arg \min_x f(x)$ for $f(x) = x^2 + 3$?
- What is $\arg \min_x f(x)$ for $f(x) = x$?
- What is $\arg \min_x f(x)$ for $f(x) = x^2 - x$?

The “High School” view of minimization

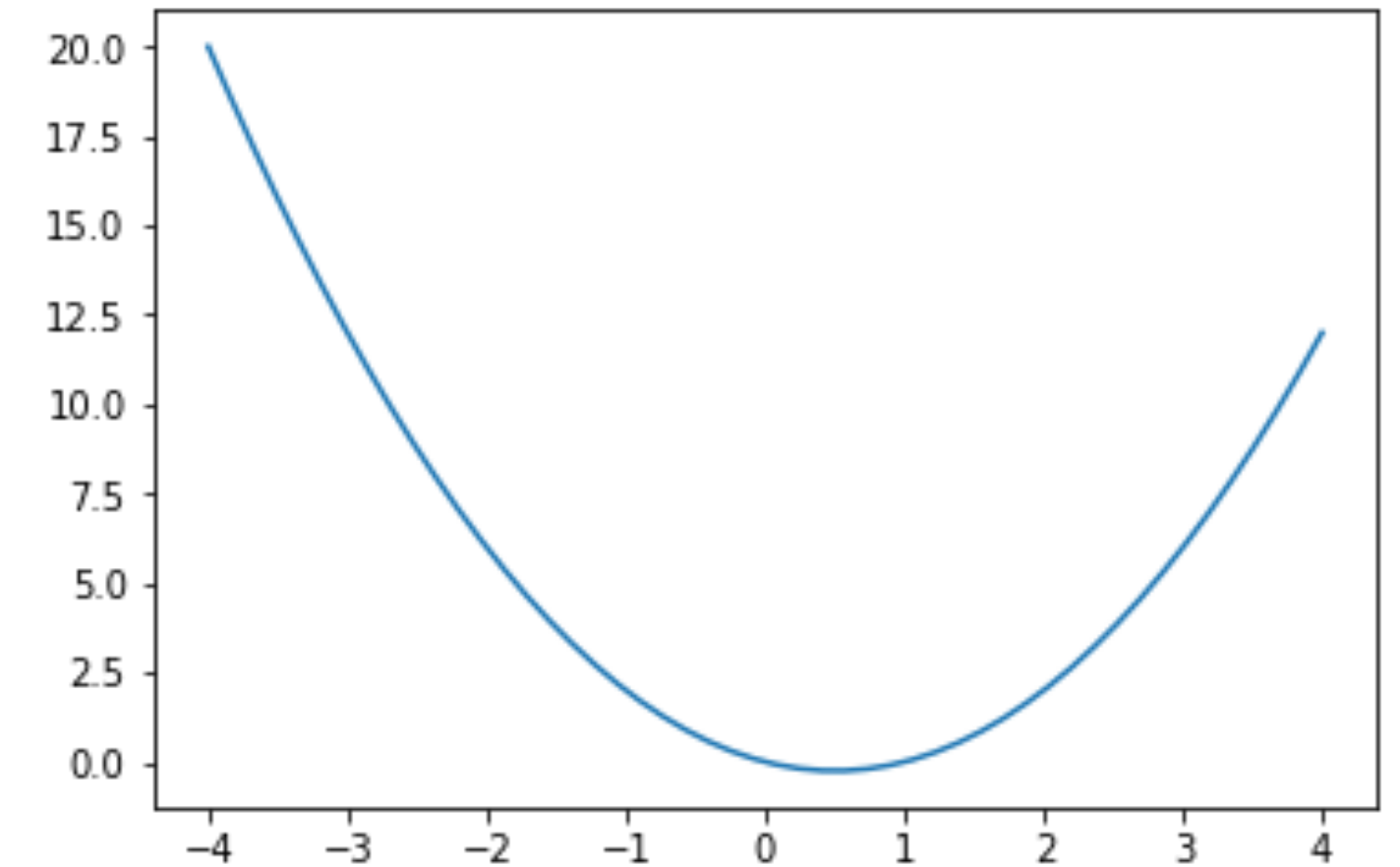
- Let us start by recalling what we learn in high school

The “High School” view of minimization

- Let us start by recalling what we learn in high school

To minimize $f(x)$:

1. Compute first derivative $f'(x)$
3. Compute second derivative $f''(x)$
5. Find x_0 such that $f'(x_0) = 0$
6. If $f''(x_0) > 0$ then x_0 is a local minimum of f



$$f: \mathbb{R} \rightarrow \mathbb{R}$$
$$f(x) = x^2 - x$$

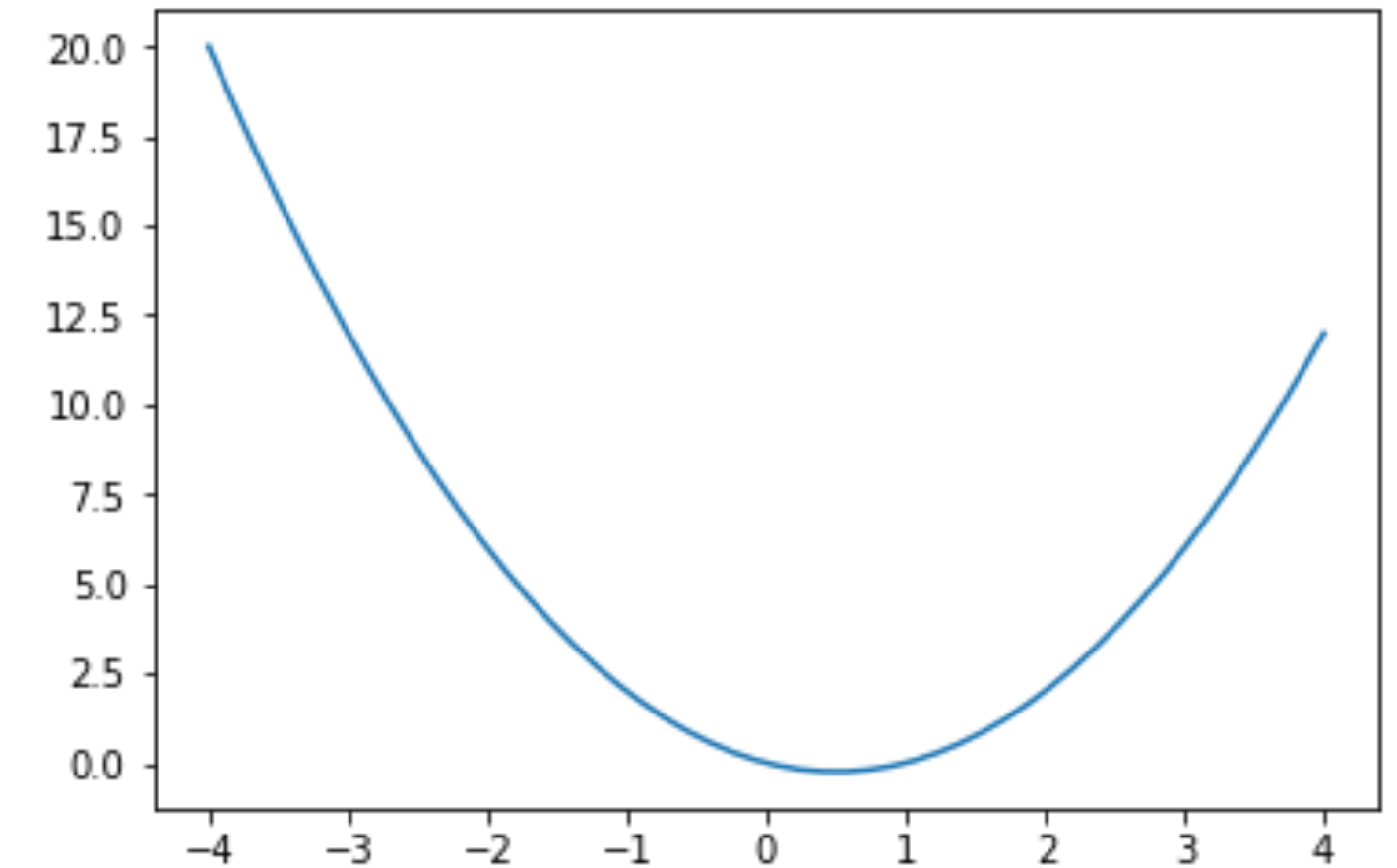
Note: It is not how we will minimize functions in practice

The “High School” view of minimization

- Let us start by recalling what we learn in high school

To minimize $f(x)$:

1. Compute first derivative $f'(x)$
3. Compute second derivative $f''(x)$
5. Find x_0 such that $f'(x_0) = 0$
6. If $f''(x_0) > 0$ then x_0 is a local minimum of f

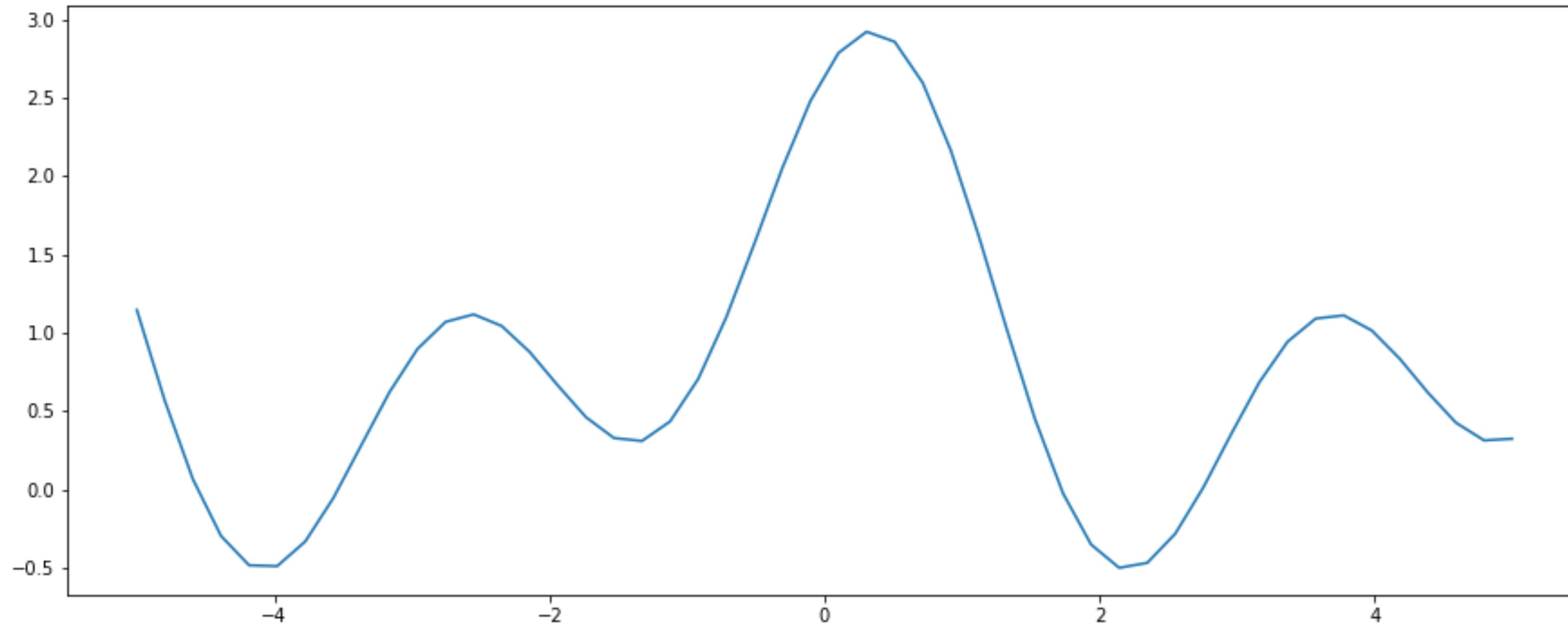


$$\begin{aligned} f &: \mathbb{R} \rightarrow \mathbb{R} \\ f(x) &= x^2 - x \\ f'(x) &= 2x - 1 \rightarrow x_0 = 0.5 \\ f''(x) &= 2 \end{aligned}$$

Note: It is not how we will minimize functions in practice

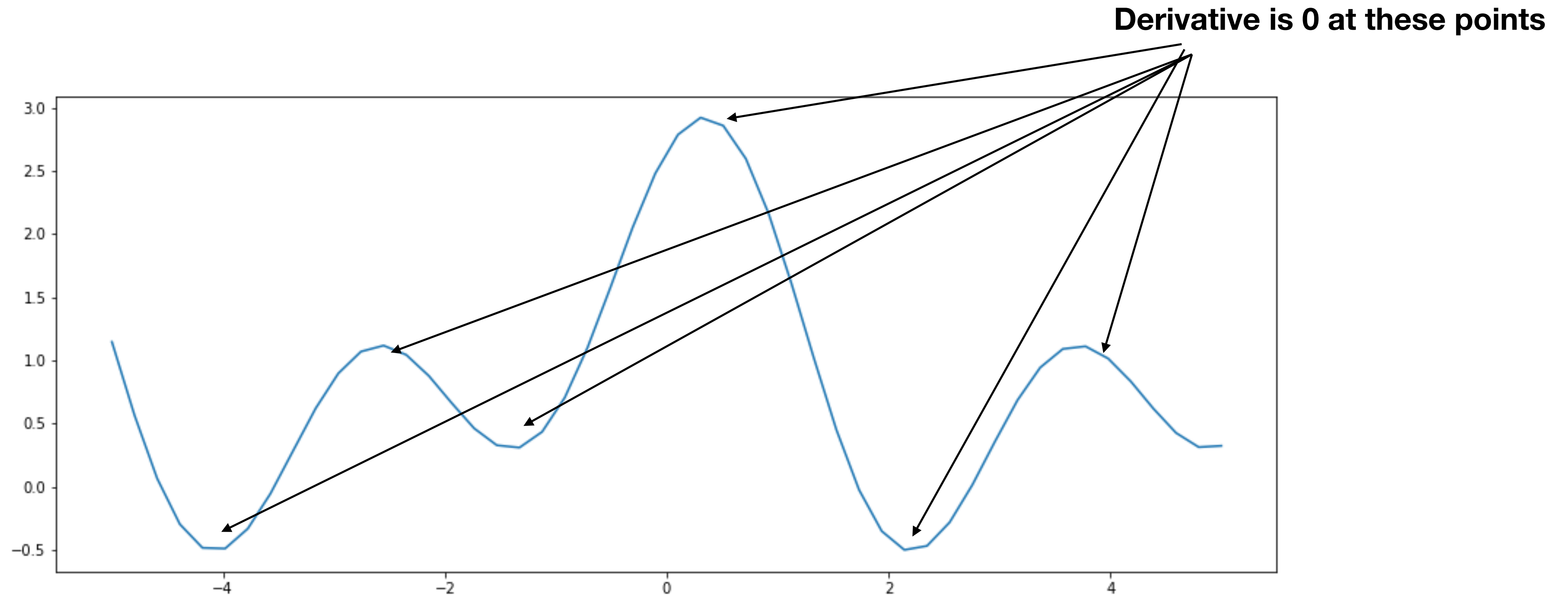
Local minimum, local maximum

- Note that the condition on the second derivative is important to distinguish **minimums** from **maximum**



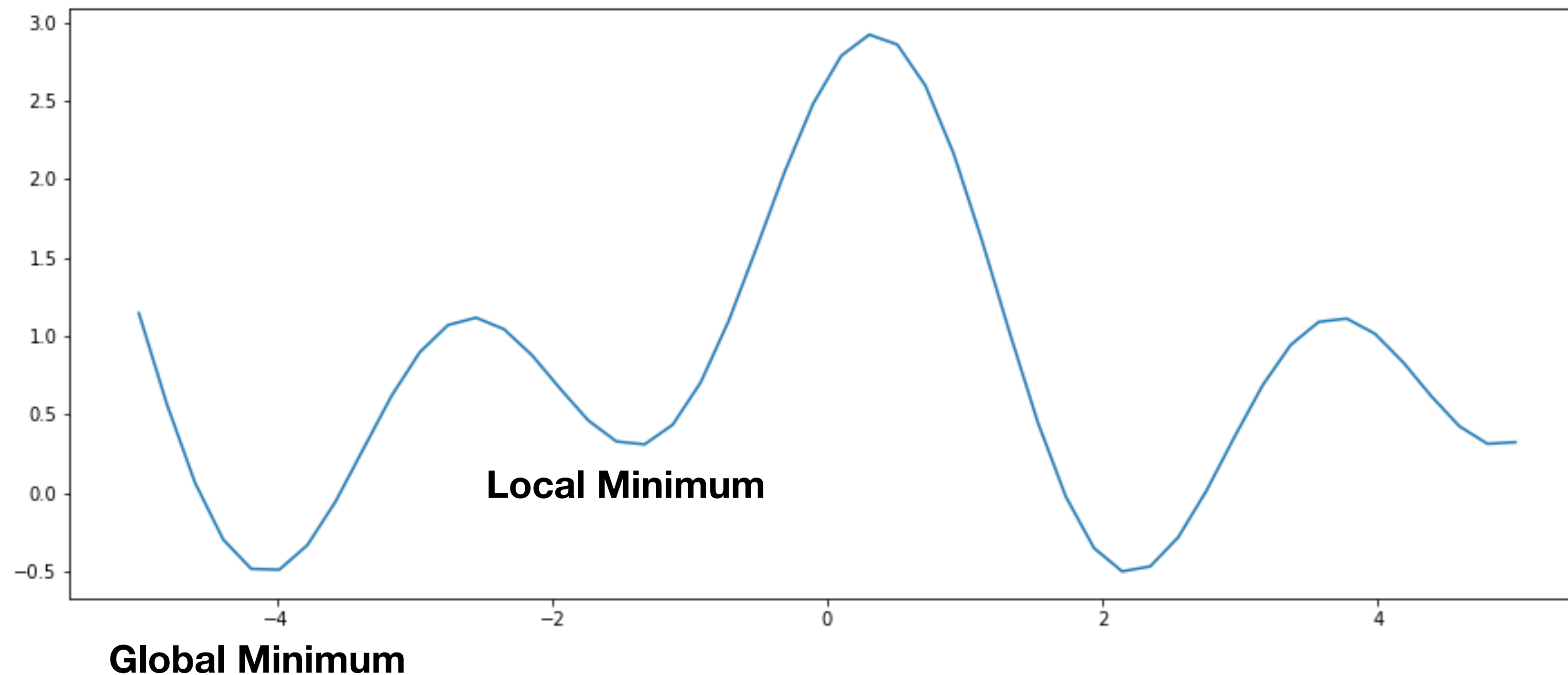
Local minimum, local maximum

- Note that the condition on the second derivative is important to distinguish **minimums** from **maximums**



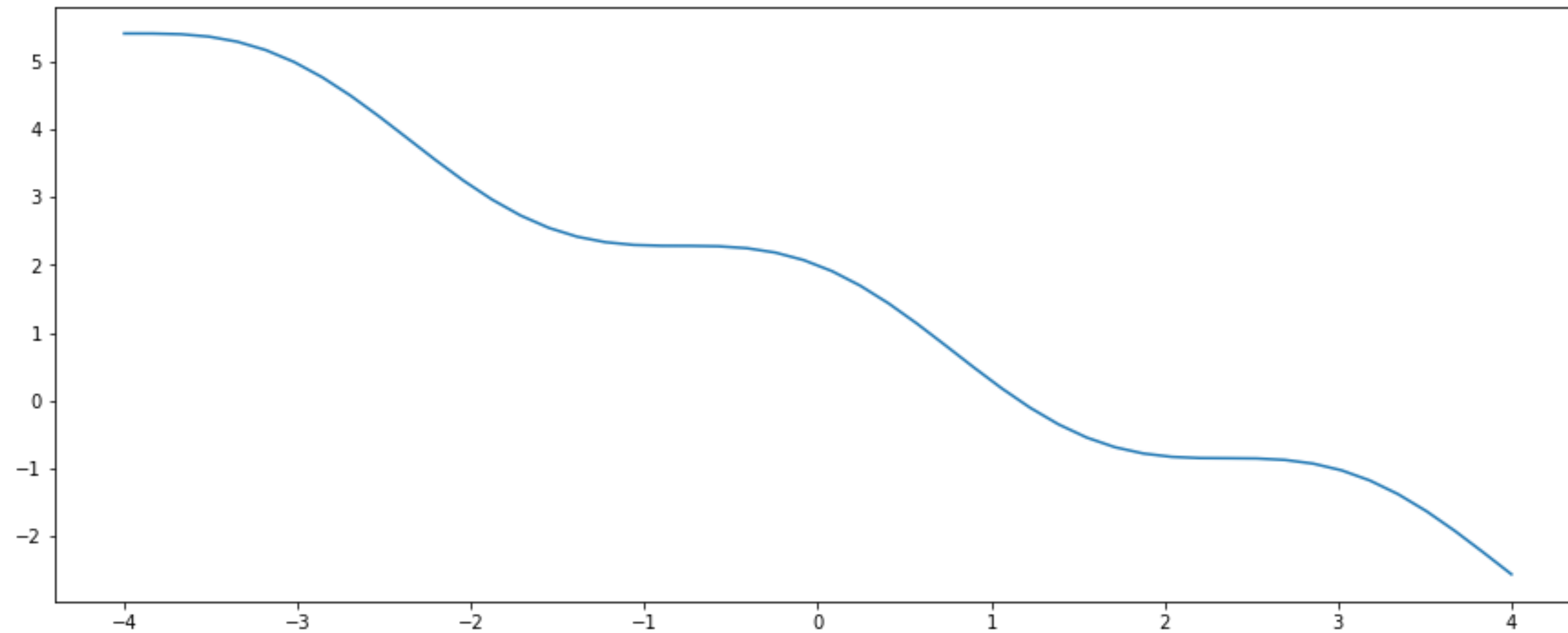
Local minimum, local maximum

- Note that the condition on the second derivative is important to distinguish **minimums** from **maximum**
- Also, the solution could be only a **local minimum**



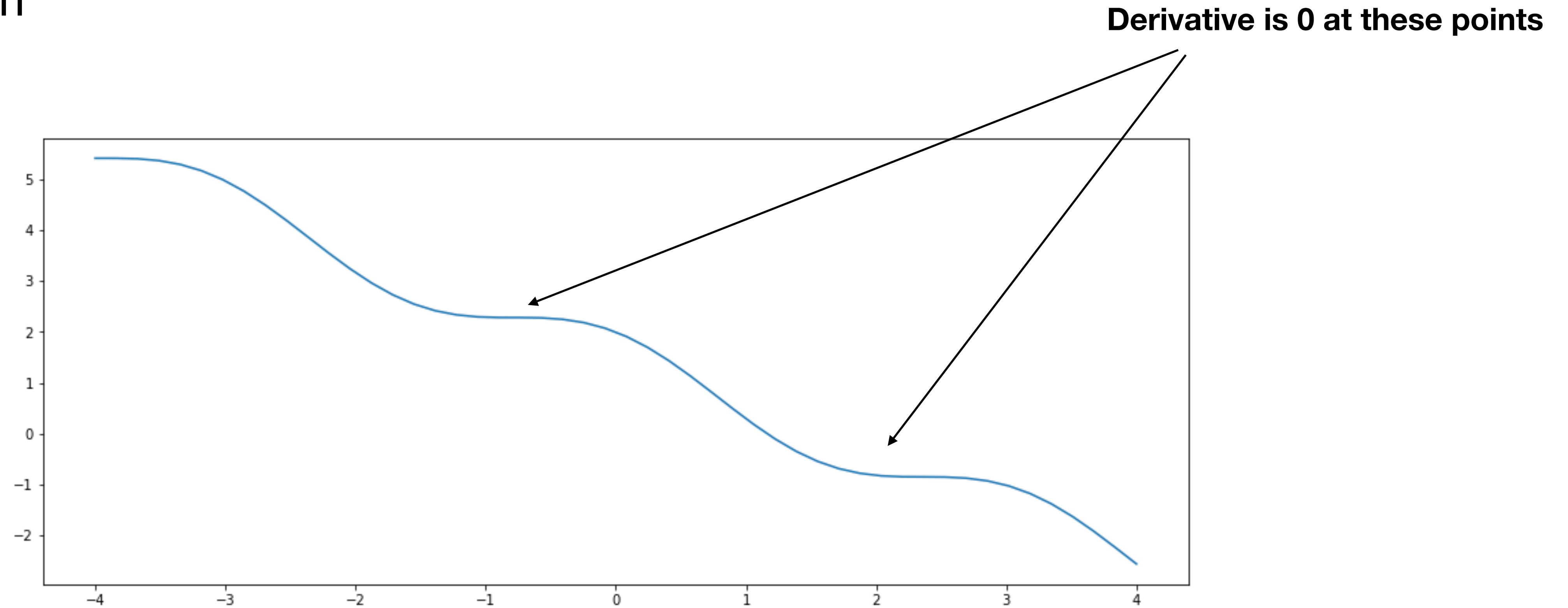
Absence of minimum

- A function may have no minimum

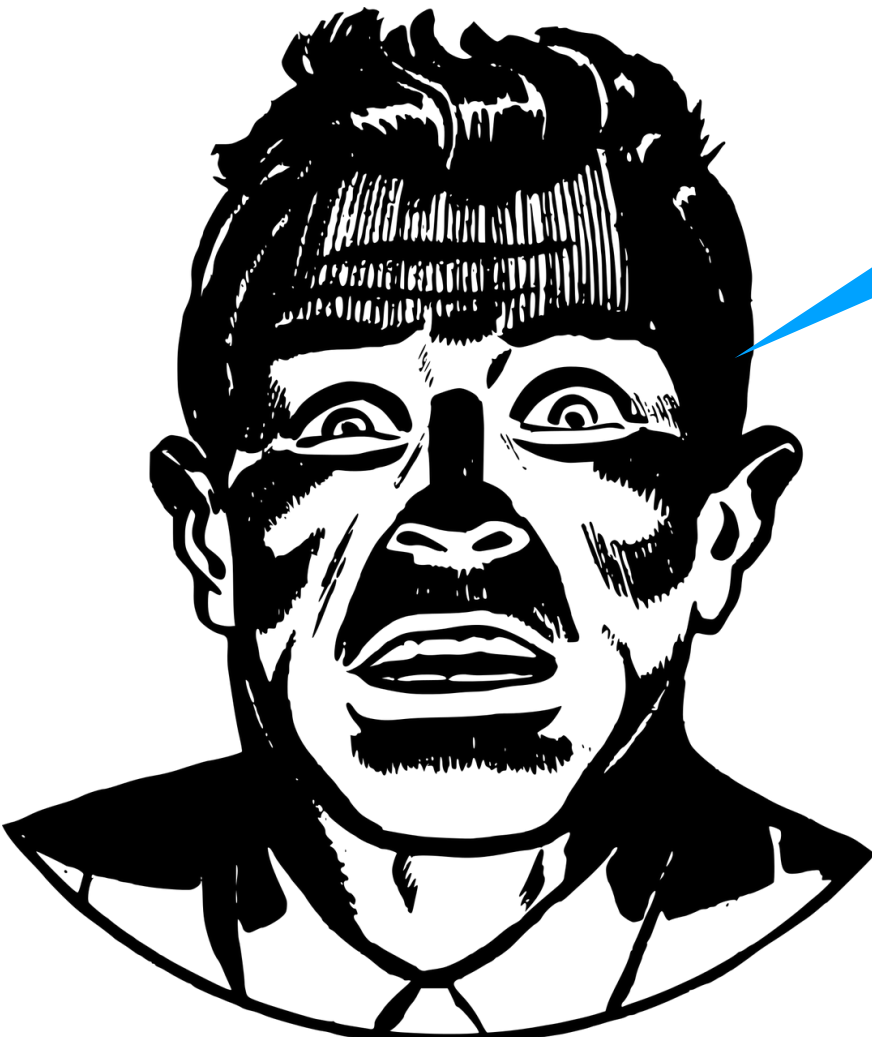


Absence of minimum

- It is even possible for derivative to be 0 even if the function has no minimum



Let us take 15 minutes to review derivatives



Derivatives! Oh no!!



Don't worry. It is a quick review. But in the real world, we rarely have to compute derivatives

Computers do that for us.

Still. It is good to have some basics.

Let us take 15 minutes to review derivatives

- Does everybody remember how to compute derivatives?
- Do not panic if you don't.
 - In practice, we will have functions that can compute the derivatives automatically for us
 - Still, you should understand at least how they work
 - we will review briefly the basics

Different ways of considering derivatives

- We can see derivatives in different ways.
- In high school, derivatives are often introduced as a set of rules that let you compute a derivative from a function.
- Let us review that first.

Computing derivatives

Exercise:

$$\sin(x) + \log(x)$$

$$2 \times \log(x + 1)$$

$$\sin(2x)$$

$$\frac{e^x}{x}$$

$f(x)$	$f'(x)$
$\sin(x)$	$\cos(x)$
$\cos(x)$	$-\sin(x)$
x^n	nx^{n-1}
$\log(x)$	$\frac{1}{x}$
e^x	e^x

$g(h(x))$	$h'(x) \times g'(h(x))$	Composition rule
$g(x) \times h(x)$	$g'(x) \times h(x) + g(x) \times h'(x)$	Leibniz rule
$g(x) + h(x)$	$g'(x) + h'(x)$	Linearity I
$\alpha \cdot h(x)$	$\alpha \cdot h'(x)$	Linearity II

Different ways of considering derivatives

- We can see derivatives in different ways.
- In high school, derivatives are often introduced as a set of rules that let you compute a derivative from a function.
- Let us review that first.
- The other way to see a derivative is as a local linear approximation of a function

What is a derivative?

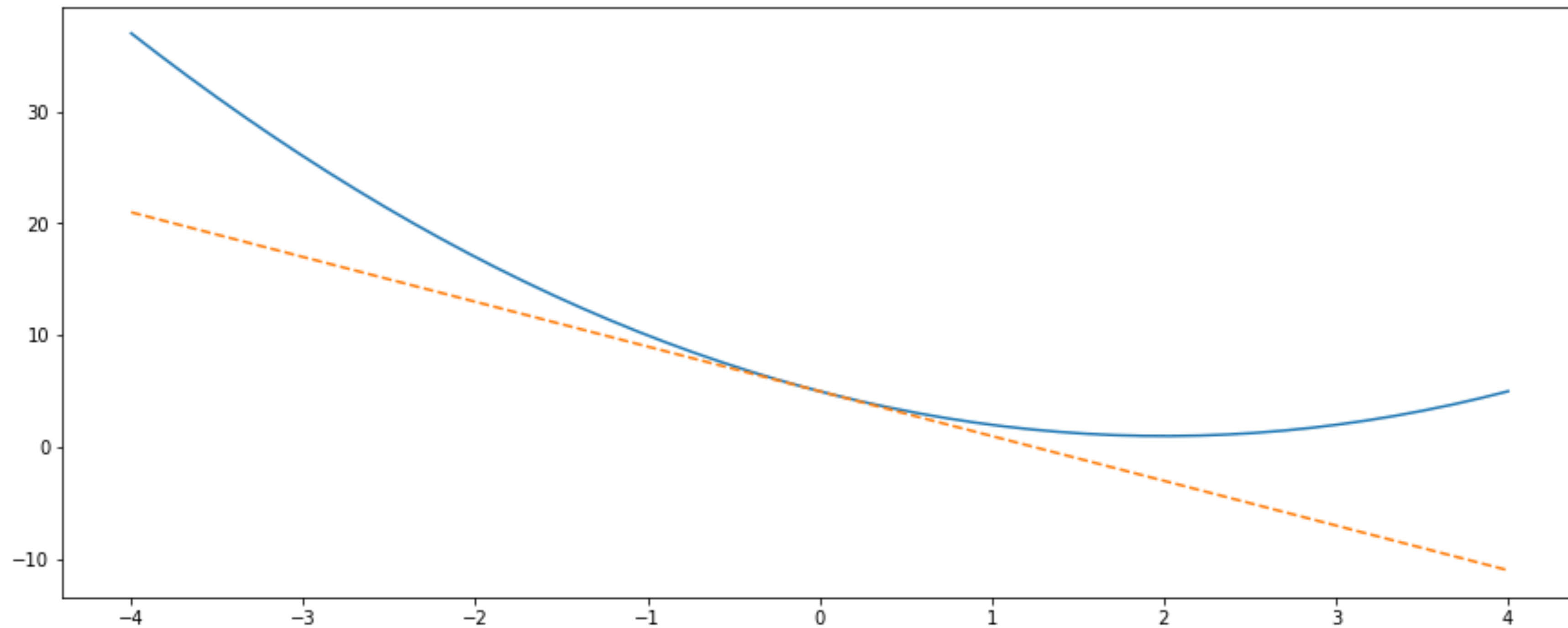
- One definition: the coefficient of the best linear approximation of a function at x
- If h is small: $f(x + h) \approx f(x) + h \cdot f'(x)$
- Example:
 - if we know that $\log(2.3) = 0.832909\dots$
 - How much is $\log(2.4)$?
 - Supposing we cannot compute a log again
 - $2.4 = 2.3 + 0.1$
 - We can approximate: $\log(2.4) \approx \log(2.3) + 0.1 \times \frac{1}{2.3}$
 - Which gives: $\log(2.3) + 0.1 \times \frac{1}{2.3} = 0.876387\dots$
 - The true value is: $\log(2.4) = 0.875468\dots$

Different ways of considering derivatives

- We can see derivatives in different ways.
- In high school, derivatives are often introduced as a set of rules that let you compute a derivative from a function.
- Let us review that first.
- The other way to see a derivative is as a local linear approximation of a function
- Equivalently, the derivative is the slope of the tangent of the function at a point

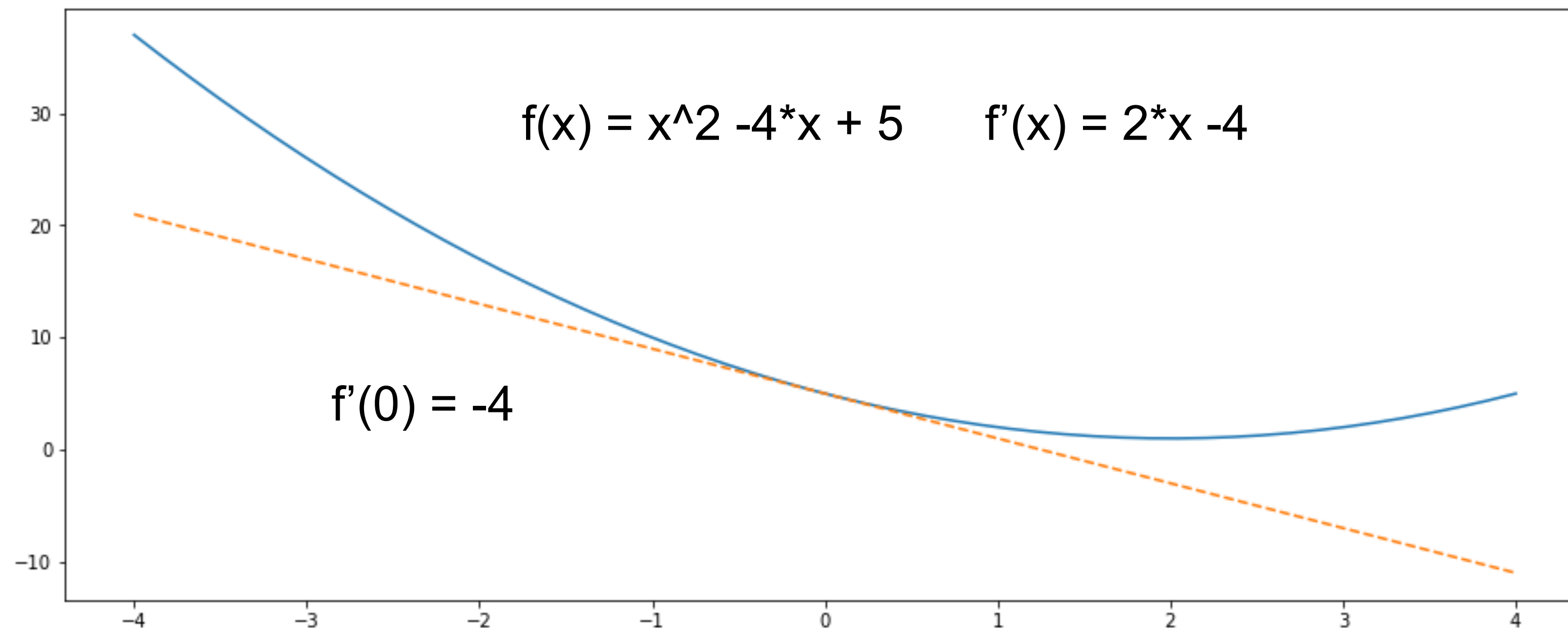
What is a tangent?

- The line that best approximate a line at a point



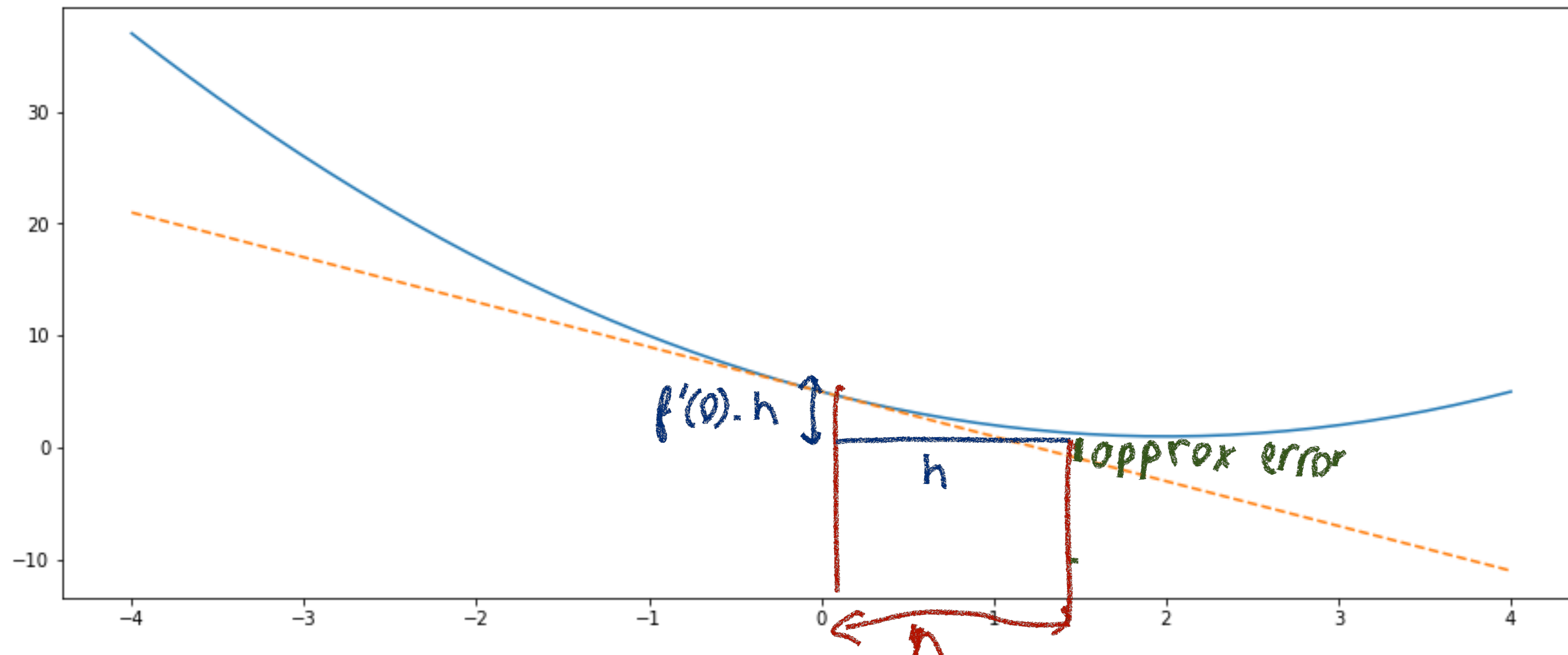
What is a derivative?

- The derivative is also the coefficient of the tangent to the graph of the function.



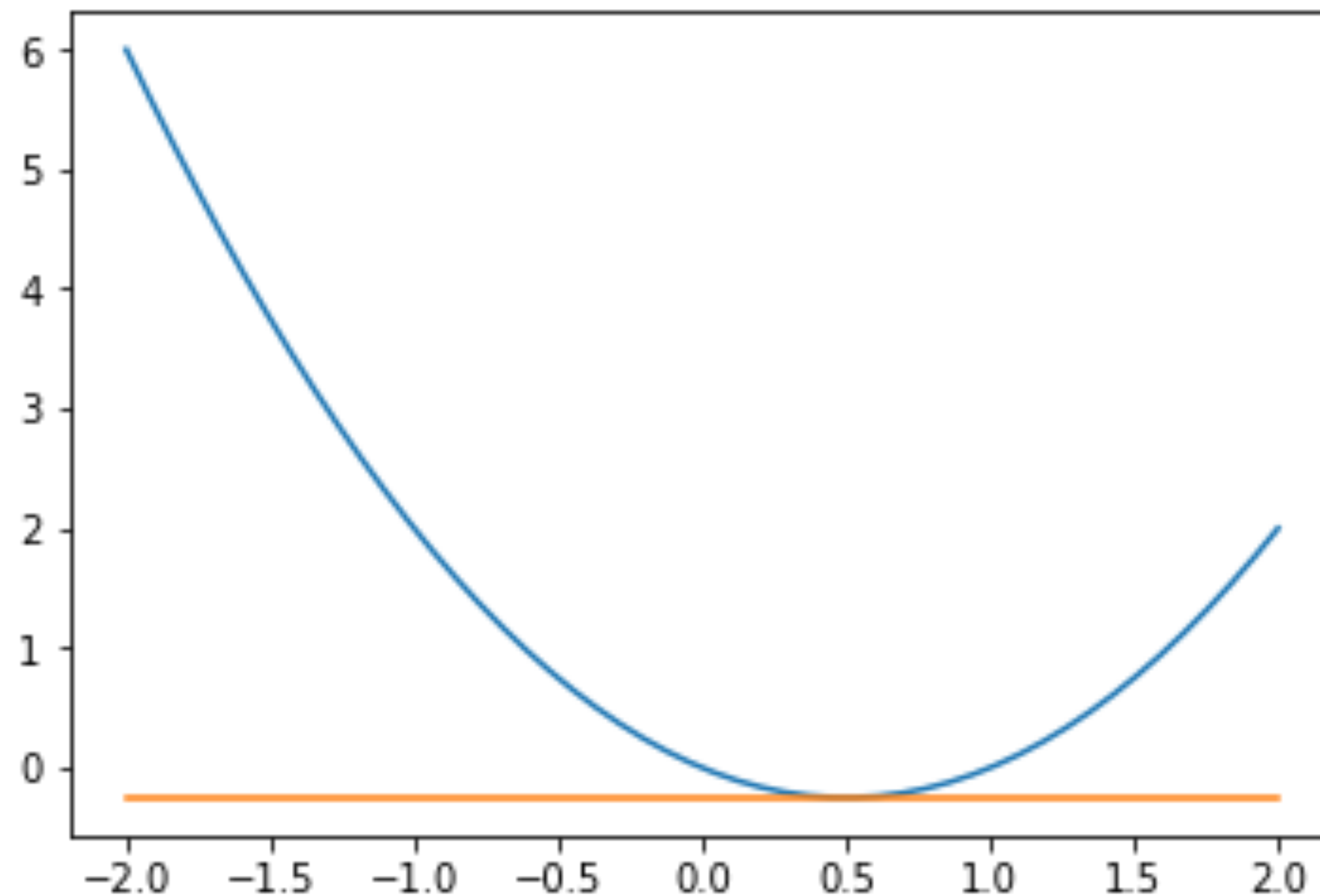
Tangent and derivative

$$f(x + h) \approx f(x) + h \cdot f'(x)$$



Derivative and minimum

- Intuitively, this shows you why the derivative should be zero at a minimum

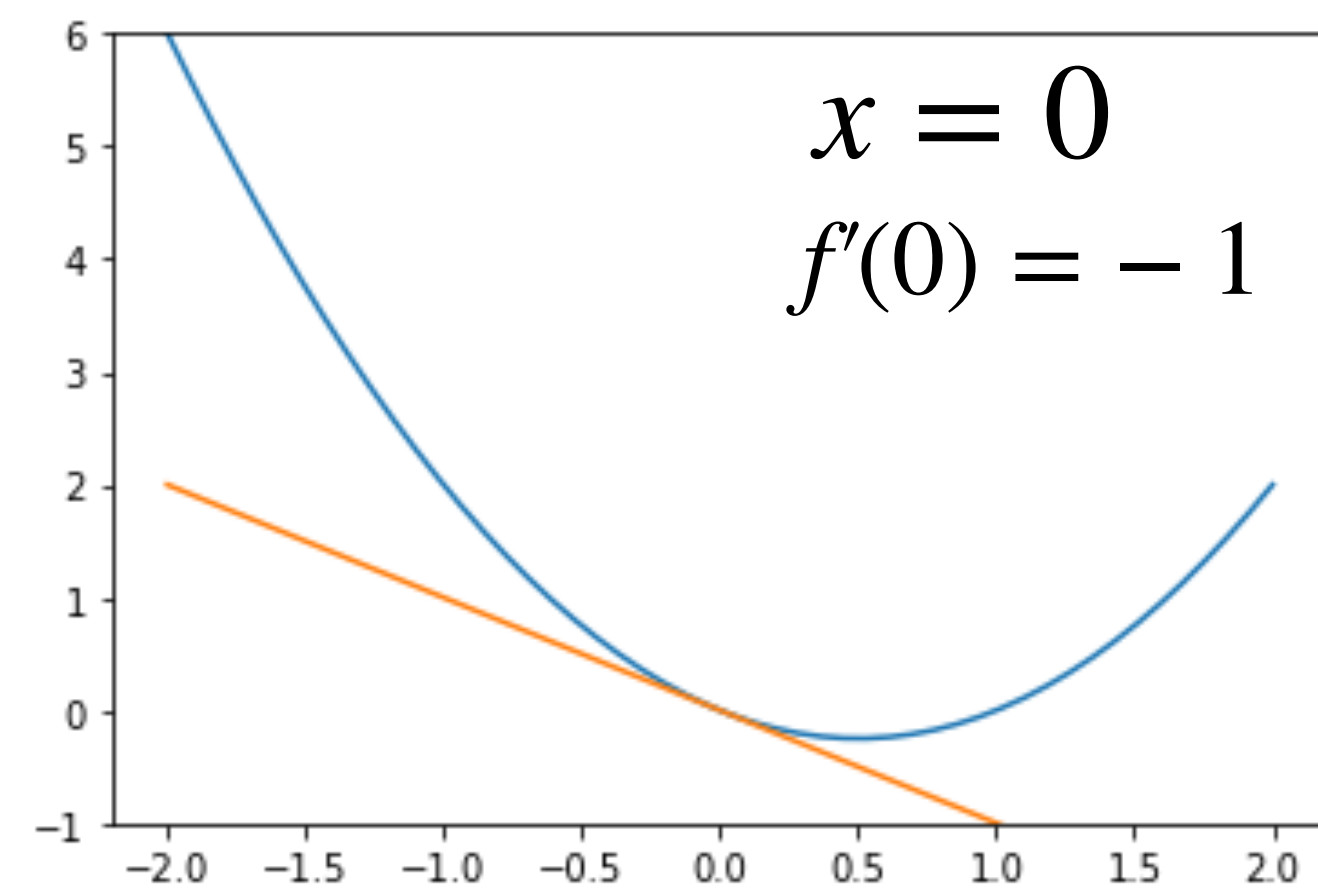


Derivative and minimum

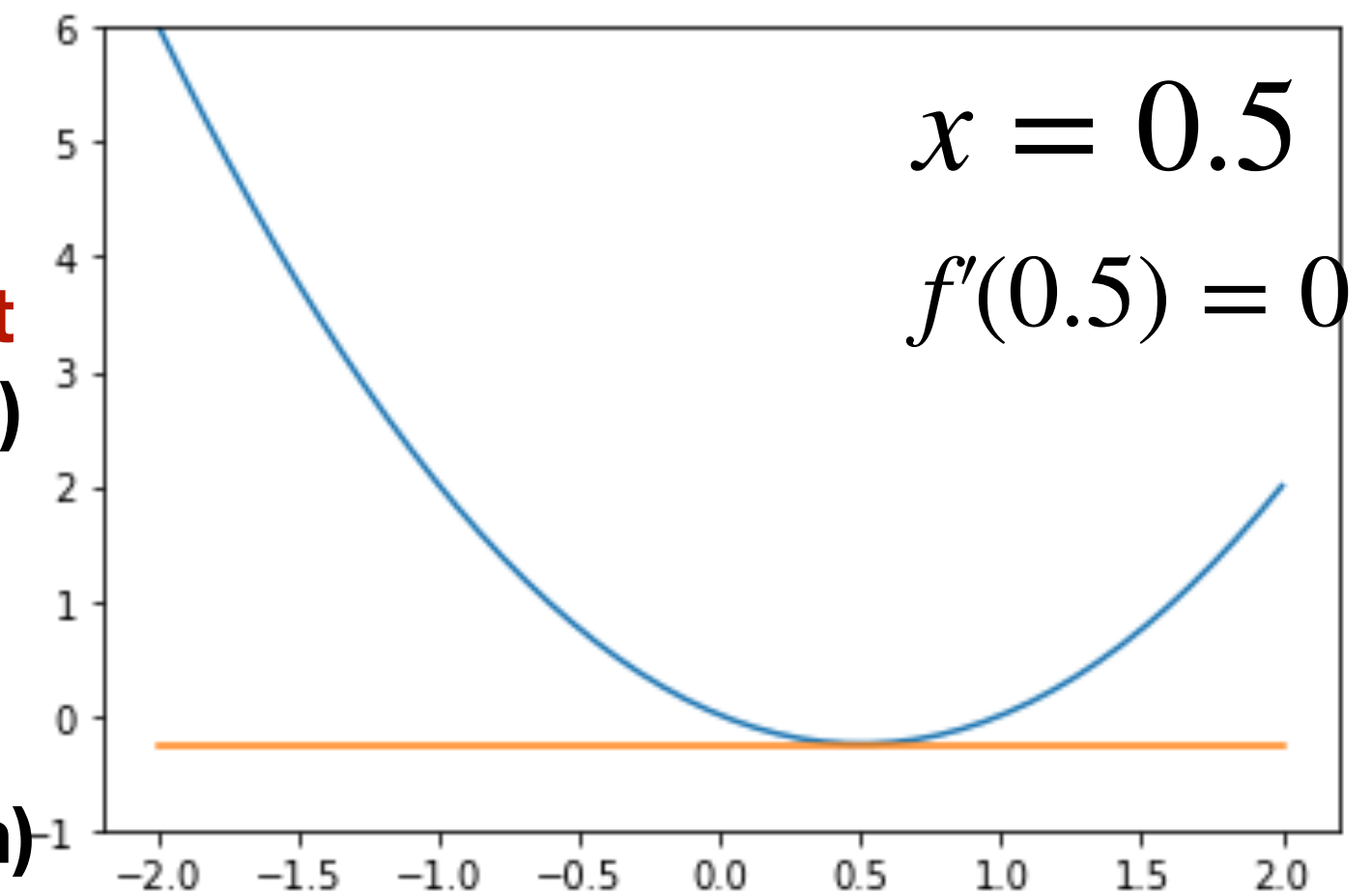
- Let us look again at how a derivative can help us find a minimum

Derivative and minimum

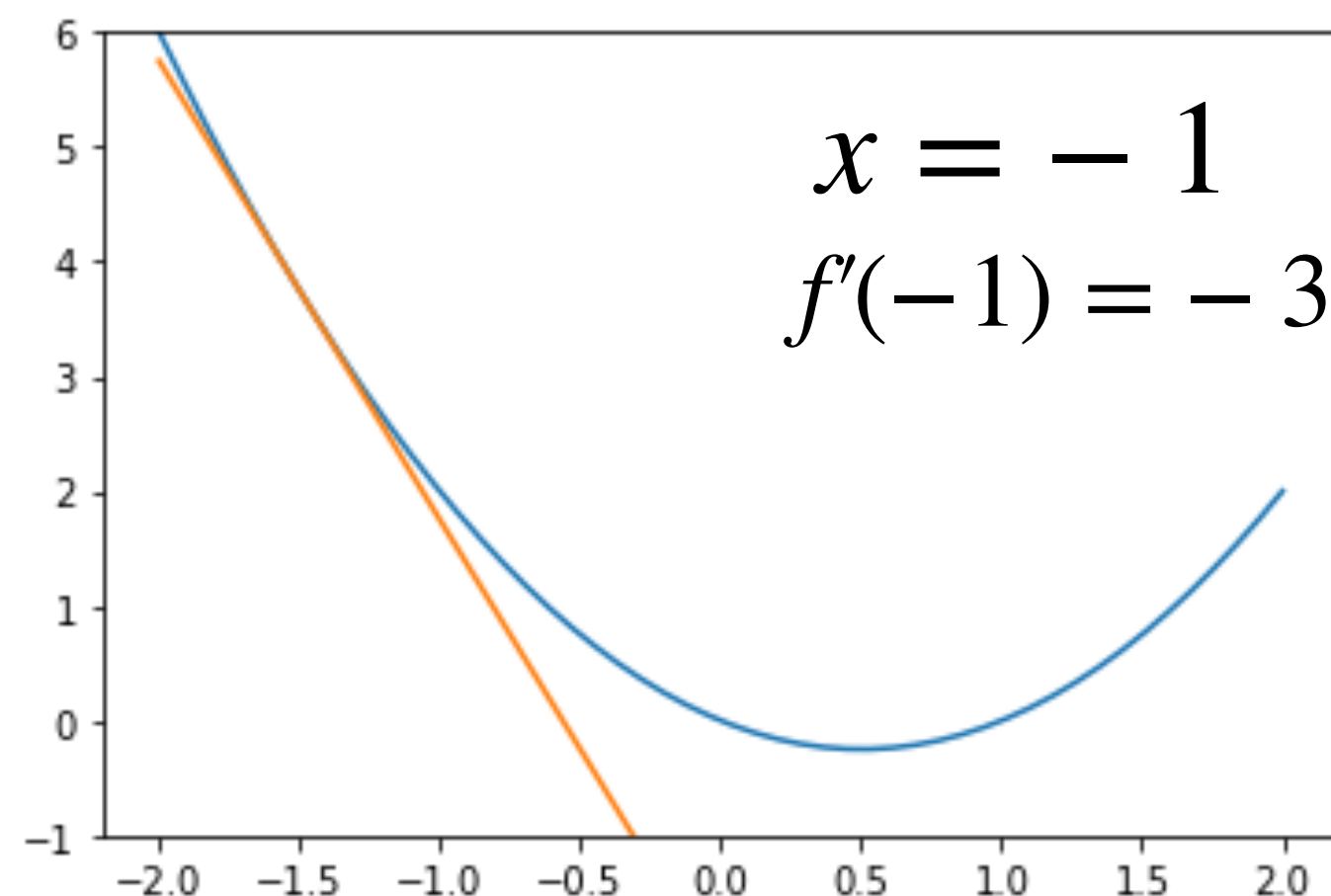
- The derivative tells us in which direction move to find the minimum



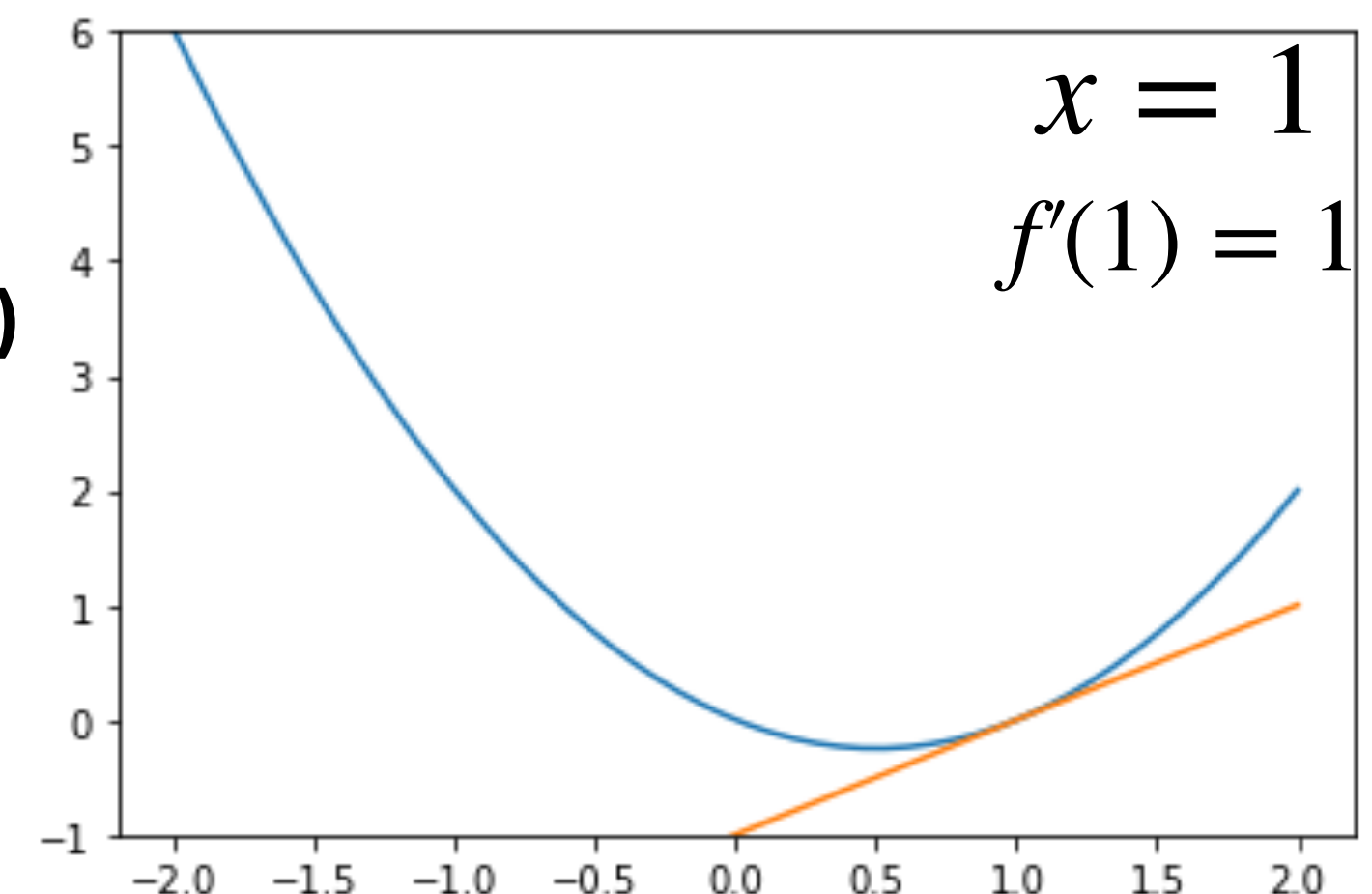
If derivative at x is **negative**, minimum is **on the right**
(we need to increase x to get closer to the minimum)



If derivative at x is **positive**, minimum is **on the left**
(we need to decrease x to get closer to the minimum)



If derivative at x is **zero**, x should be a **minimum**
(not necessarily in theory, but in our cases, it will be)



Gradient Descent Algorithm

- This suggests some procedure for finding a minimum:
 - Start at any x (eg. $x = 0$)
 - Compute $f'(x)$
 - If $f'(x) > 0$: Decrease x a bit
 - If $f'(x) < 0$: Increase x a bit
 - Repeat

Gradient Descent Algorithm

- This suggests some procedure for finding a minimum:
 - Start at any x (eg. $x = 0$)
 - Compute $f'(x)$
 - If $f'(x) > 0$: Decrease x a bit
 - If $f'(x) < 0$: Increase x a bit
 - Repeat



In practice, we do this:

$$x := x - lr \cdot f'(x)$$

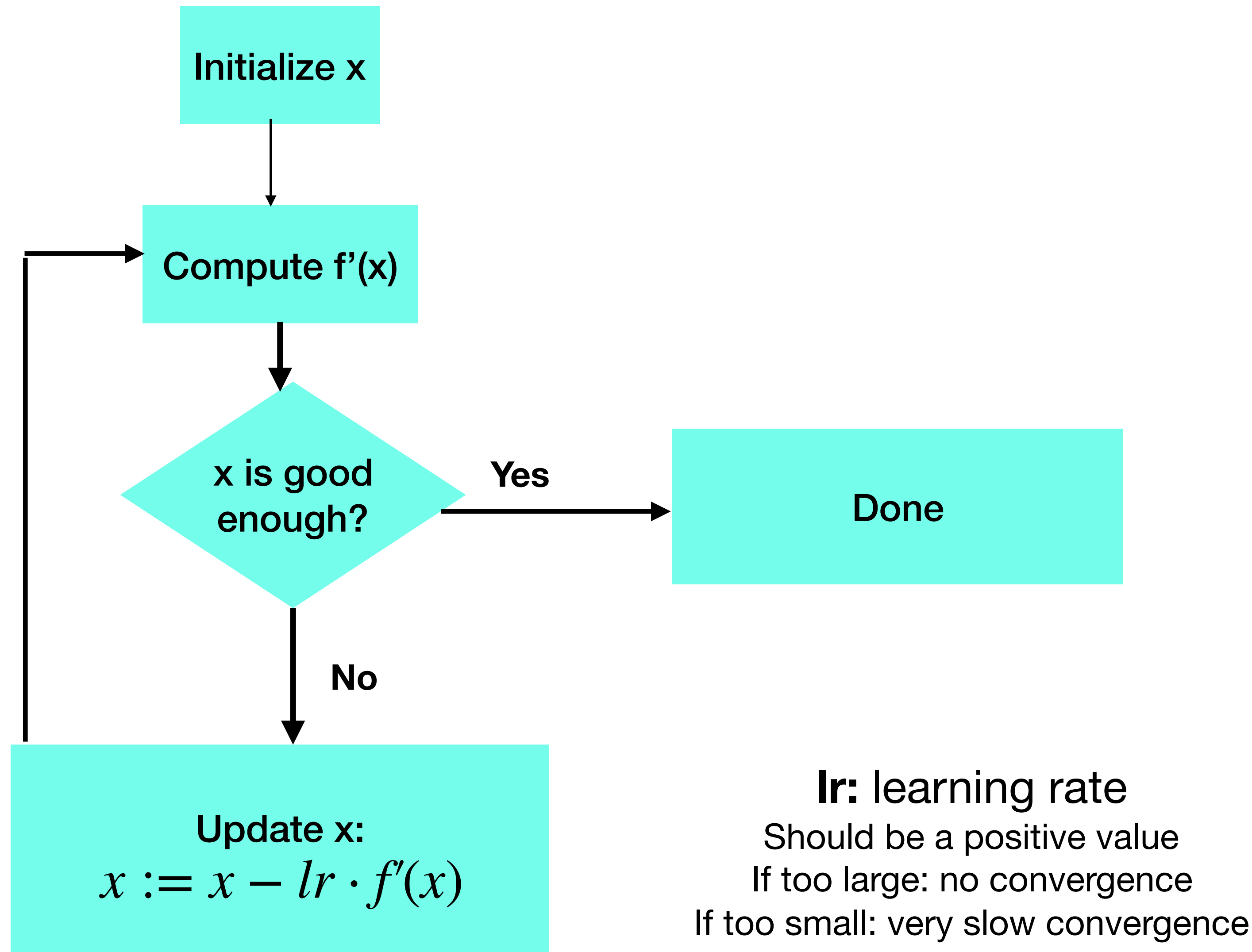
lr: learning rate

Should be a positive value

If too large: no convergence

If too small: very slow convergence

Gradient Descent algorithm



$$f(x) = x^2 - x$$

$$f'(x) = 2x - 1$$

$$\arg \min_x f(x) = 0.5$$

$$lr = 0.2$$

$$x = 0$$
$$f'(x) = -1$$

$$x = 0.2$$
$$f'(x) = -0.6$$

$$x = 0.32$$
$$f'(x) = -0.36$$

$$x = 0.392$$

...

...

...

...

$$x = 0.493$$
$$f'(x) = -0.014$$

STOP?

Gradient Descent algorithm

- Let us try to see a bit more how it works in practice using Jupiter Notebooks
- <https://colab.research.google.com/drive/1Pdn4laPkbt-DU3w2EdidFiqdXAq63QJu>
- bit.ly/2KDOoTP

Gradient Descent Algorithm

- Gradient descent works well **even** when we have functions of millions of variable
 - This is why it is so useful for Machine Learning and Neural Networks
 - Other methods will not be practical in such settings
- Convergence will depend on the choice of a good **learning rate**
 - In experiments, a good deal of time is often spent finding an optimal learning rate
 - **Too large** learning rate: **no** convergence (ie. the system learn nothing)
 - **Too small** learning rate: **slow** convergence (ie. the system takes a long time to learn)

Minimizing a function of
several variables

Functions of several variables

- A function of several variables is just that: a function which has several variables

$$f : \mathbb{R}^3 \rightarrow \mathbb{R}$$

$$f(x, y, z) = (x - y)^2 + z^2 - z$$

$$f(0,0,0) = 0$$

$$f(1,2,3) = 7$$

$$f(-1,2,2) = 11$$

$$f(0,1,1) = ?$$

$$f(2,2,0) = ?$$

- Like before, we want to find its minimum:

$$\arg \min_{x,y,z} f(x, y, z) = (0,0,0.5)$$

Parameterized functions

- By fixing one of the variable, we can obtain a function with one less variable

Function of 3 variables: $f(x, y, z) = (x - y)^2 + z^2 - z$

Fixing z:

$$\downarrow$$
$$z = 2$$

$$\downarrow$$
$$f(x, y, 2) = (x - y)^2 + 4 - 2$$

Function of 2 variables: $f(x, y) = (x - y)^2 + 2$

Parameterized functions

- By fixing one of the variable, we can obtain a function with one less variable

Function of 3 variables: $f(x, y, z) = (x - y)^2 + z^2 - z$

Fixing y:

$$\downarrow$$
$$y = 2$$

$$\downarrow$$
$$f(x, 2, z) = (x - 2)^2 + z^2 - z$$

Function of 2 variables: $f(x, z) = (x - 2)^2 + z^2 - z$

Parameterized functions

- By fixing one of the variable, we can obtain a function with one less variable

Function of 3 variables: $f(x, y, z) = (x - y)^2 + z^2 - z$



Fixing y and z:

$$y = 2$$

$$z = 3$$



$$f(x, 2, 3) = (x - 2)^2 + 9 - 3$$

Function of 1 variable: $f(x) = (x - 2)^2 + 6$

Parameterized functions

- Therefore, in this case, variables **y** and **z** can be used to describe a “family” of functions.
- We say they parameterize the

Function of 3 variables: $f(x, y, z) = (x - y)^2 + z^2 - z$



Fixing y and z:

$$y = 2$$

$$z = 3$$

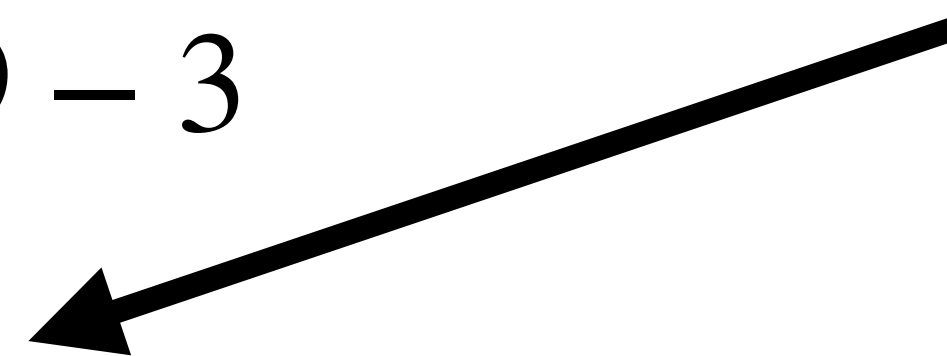


$$f(x, 2, 3) = (x - 2)^2 + 9 - 3$$

**For each value of y and z,
we have one function of
one variable**

Function of 1 variable:

$$f(x) = (x - 2)^2 + 6$$



Parameterized functions

- Therefore, in this case, variables **y** and **z** can be used to describe a “family” of functions
- In such a case, we will say that **f** is a function *parameterized* by **y** and **z**
- And we note the parameters separately, as subscripts

Function of 3 variables: $f_{y,z}(x) = (x - y)^2 + z^2 - z$

Fixing y and z:

$$y = 2 \quad z = 3$$

**For each value of y and z,
we have one function of
one variable**

$$f_{2,3}(x) = (x - 2)^2 + 9 - 3$$

$$f_{2,3}(x) = (x - 2)^2 + 6$$

Function of 1 variable:

$$f_{0,0}(x) = x^2$$

$$f_{0,2}(x) = x^2 + 2$$

Partial derivatives

- What is the equivalent of our “high school” derivatives when we have several variables?
- One part of the answer is ***partial derivatives***
- Partial derivatives are computed by choosing one variable and fixing the others
- In other words, we see the function of several variables as a parameterized function of one variable

Partial derivatives

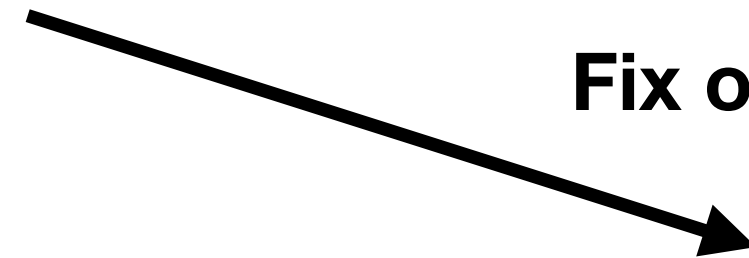
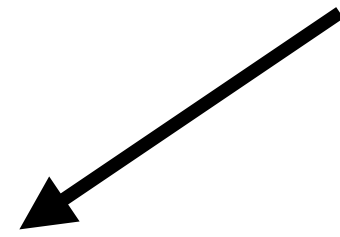
- What is the equivalent of our “high school” derivatives when we have several variables?
- One part of the answer is ***partial derivatives***
- Partial derivatives are computed by choosing one variable and fixing the others
- In other words, we see the function of several variables as a parameterized function of one variable
- Indeed, if we choose y , and fix x and z , we can see $f(x, y, z)$ as a function of one variable and compute its derivative

$$f(x, y, z) = (x - y)^2 + z^2 - z$$

$$\bullet \quad \frac{\partial f}{\partial x} = 2(x - y) \qquad \frac{\partial f}{\partial y} = 2(y - x) \qquad \frac{\partial f}{\partial z} = 2z - 1$$

Partial derivatives

$$f(x, y, z) = (x - y)^2 + z^2 - z$$



Fix other variables

$$f_{y,z}(x) = (x - y)^2 + z^2 - z$$

$$f_{x,z}(y) = (x - y)^2 + z^2 - z$$

$$f_{x,y}(z) = (x - y)^2 + z^2 - z$$



Compute derivative

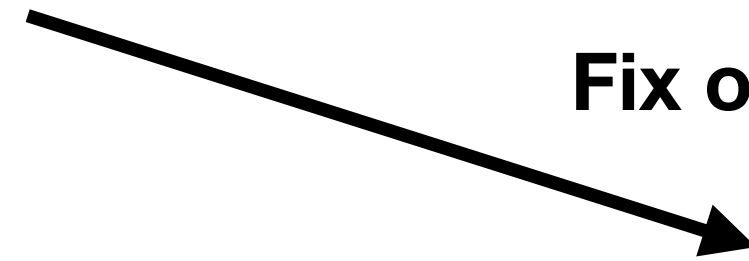
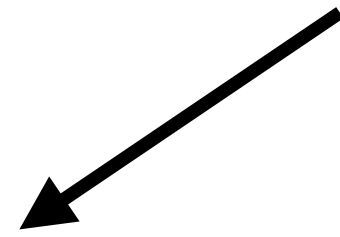
$$f'_{y,z}(x) = 2(x - y)$$

$$f'_{x,z}(y) = 2(y - x)$$

$$f'_{x,y}(z) = 2z - 1$$

Partial derivatives

$$f(x, y, z) = (x - y)^2 + z^2 - z$$



Fix other variables

$$f_{y,z}(x) = (x - y)^2 + z^2 - z$$

$$f_{x,z}(y) = (x - y)^2 + z^2 - z$$

$$f_{x,y}(z) = (x - y)^2 + z^2 - z$$



Compute derivative



$$f'_{y,z}(x) = 2(x - y)$$

$$f'_{x,z}(y) = 2(y - x)$$

$$f'_{x,y}(z) = 2z - 1$$

In practice, we use this notation for partial derivatives:

$$\frac{\partial f}{\partial x} = 2(x - y)$$

$$\frac{\partial f}{\partial y} = 2(y - x)$$

$$\frac{\partial f}{\partial z} = 2z - 1$$

Computing the partial derivatives

$$f(x, y, z) = (x - y)^2 + z^2 - z$$

$$\frac{\partial f}{\partial x} =$$

$$\frac{\partial f}{\partial y} =$$

$$\frac{\partial f}{\partial z} =$$

Partial derivatives

- Exercise: Compute the partial derivatives

$$f(x, y, z) = xyz - z^2 - y^2$$

$$f(x, y, z) = e^{x+y} - \log(z)$$

Partial derivatives

- Exercise: Compute the partial derivatives

$$f(x, y, z) = xyz - z^2 - y^2$$

Choice A:

$$\frac{\partial f}{\partial x} = yz$$

$$\frac{\partial f}{\partial y} = xz - 2y$$

$$\frac{\partial f}{\partial z} = xy - 2z$$

Choice B:

$$\frac{\partial f}{\partial x} = x - z^2 - y^2$$

$$\frac{\partial f}{\partial y} = y - 2y - z^2$$

$$\frac{\partial f}{\partial z} = z - 2z - y^2$$

Partial derivatives

- Exercise: Compute the partial derivatives

$$f(x, y, z) = e^{x+y} - \log(z)$$

Choice A:

$$\frac{\partial f}{\partial x} = e^{x+y}$$

$$\frac{\partial f}{\partial y} = e^{x+y}$$

$$\frac{\partial f}{\partial z} = -\frac{1}{z}$$

Choice B:

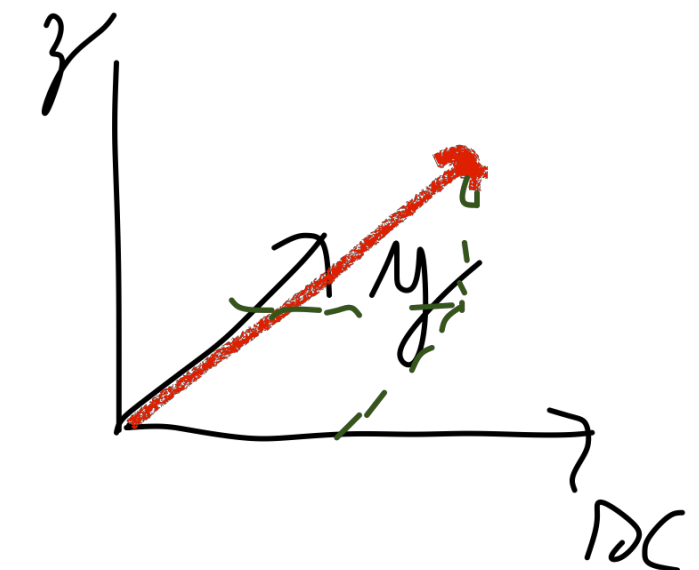
$$\frac{\partial f}{\partial x} = e^{x+y} - \log(z)$$

$$\frac{\partial f}{\partial y} = e^{x+y} - \log(z)$$

$$\frac{\partial f}{\partial z} = e^{x+y} - \frac{1}{z}$$

Vectors

- What are vectors?
- You probably have used vectors in Physics classes to represent force and speed
 - 3-dimensional vectors: [2.3, 4.5, -1]
- In Machine Learning, we also use them a lot
- Except that they can have more than 3 dimensions
 - 5-dimensional vector: [-1, 3, 4.1, 5.2, 4]
 - We often note the set of all n-dimensional vectors $\mathbb{R}^n$



$$[1, 2.1, 4.1, -1, -1] \in \mathbb{R}^5$$

Vectors (Continued)

- For now, we only need to know the following about vectors:
 - A n-dimensional Vector is a list of n numbers
 - We can add 2 vectors (if they have the same dimension)
$$[2.1, 3.4, 1.1, 3.2] + [-1, 2.1, 3.1, -2] = [1.1, 5.5, 4.2, 1.2]$$
$$[2.1, 3.4] + [-1, 2.1, 3.1, -2] = \text{X}$$
 - We can multiply a vector by a number
$$0.5 \times [2, 3, -1, -2] = [1, 1.5, -1.5, -1]$$

Vectors(Continued)

- We will usually denote a vector by a letter with an arrow on it: $\vec{x}$
- We denote the i^{th} component of $\vec{x}$ by x_i
- If $\vec{x} = [1, 2.2, -1, 4]$
 - Then we have $x_0=1$, $x_1=2.2$, $x_2=-1$, $x_3=4$

Vectors: Exercise

$$\overrightarrow{x} = [1, 5, -2, 0.5]$$

$$\overrightarrow{y} = [2, 2, 10, 10]$$

$$\overrightarrow{z} = [3, -3, 0]$$

- Dimensions of $\overrightarrow{x}, \overrightarrow{y}, \overrightarrow{z}$?

- Values of x_1, y_2, z_0, y_0 ?

- Compute:
$$\overrightarrow{x} + \overrightarrow{y}$$
$$\overrightarrow{x} + 0.5 \times \overrightarrow{y}$$
$$\overrightarrow{y} + \overrightarrow{z}$$

Vectors and Multivariate functions

- For now, we have represented the variables of a multivariate function with the letters x, y, z as in:
$$f(x, y, z) = (x - y)^2 + z^2 - z$$

- In practice, we can have any number of variables. So it is more convenient to use:

- x_0 (instead of x) , x_1 (instead of y), x_2 (instead of z), $x_3 \dots x_n$ (if we need more than 3 variables)

$$f(x_0, x_1, x_2) = (x_0 - x_1)^2 + x_2^2 - x_2$$

- We can also use a vectorial notation to represent all of the variables as one vector variable:

$$\overrightarrow{x} = [x_0, x_1, x_2] \qquad f(\overrightarrow{x}) = (x_0 - x_1)^2 + x_2^2 - x_2$$

- So, keep in mind that the 3 following expressions actually refer to the same function:

$$f(x, y, z) = (x - y)^2 + z^2 - z$$

$$f(x_0, x_1, x_2) = (x_0 - x_1)^2 + x_2^2 - x_2$$

- $$f(\overrightarrow{x}) = (x_0 - x_1)^2 + x_2^2 - x_2$$

Gradient

- The partial derivatives become the component of a vector we call the ***gradient***

$$\text{grad} \cdot f(x, y, z) = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right]$$

- For example: $f(x, y, z) = (x - y)^2 + z^2 - z$
- $\text{grad} \cdot f(x, y, z) = [2(x - y), 2(y - x), 2z - 1]$

Gradient

$$\text{grad} \cdot f(x, y, z) = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right]$$

- In this case, the function has 3 variables. Therefore the gradient is a vector of size 3
- If the gradient has n variables, it is a vector of size n
- More precisely, the gradient of f is itself a function that return a vector

$$f : \mathbb{R}^n \rightarrow \mathbb{R}$$

$$f(x_1, x_2, \dots, x_n)$$

$$\text{grad} \cdot f : \mathbb{R}^n \rightarrow \mathbb{R}^n$$

$$\text{grad} \cdot f(x_1, x_2, \dots, x_n) = [g_1, \dots, g_n]$$

Interpreting the gradient

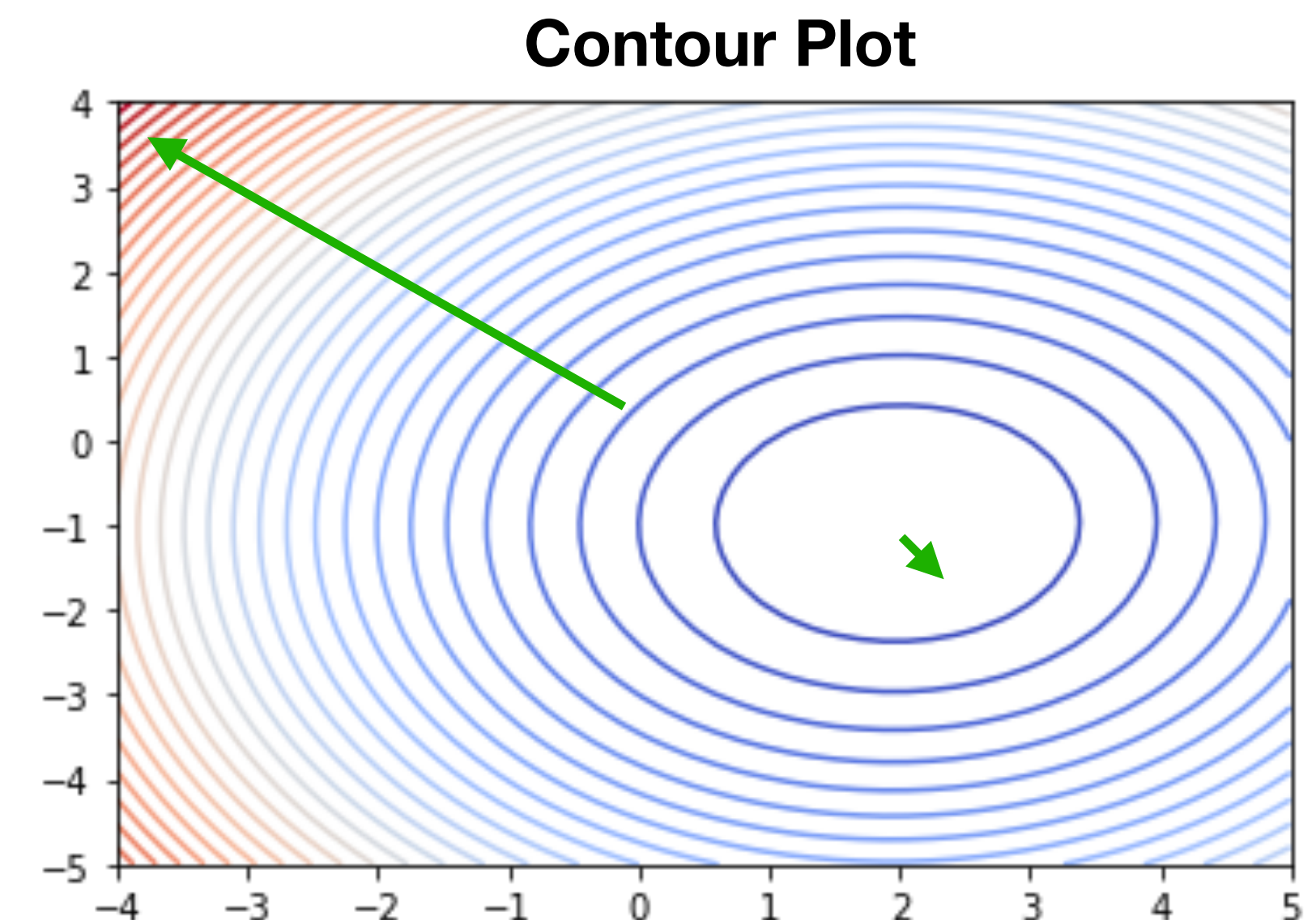
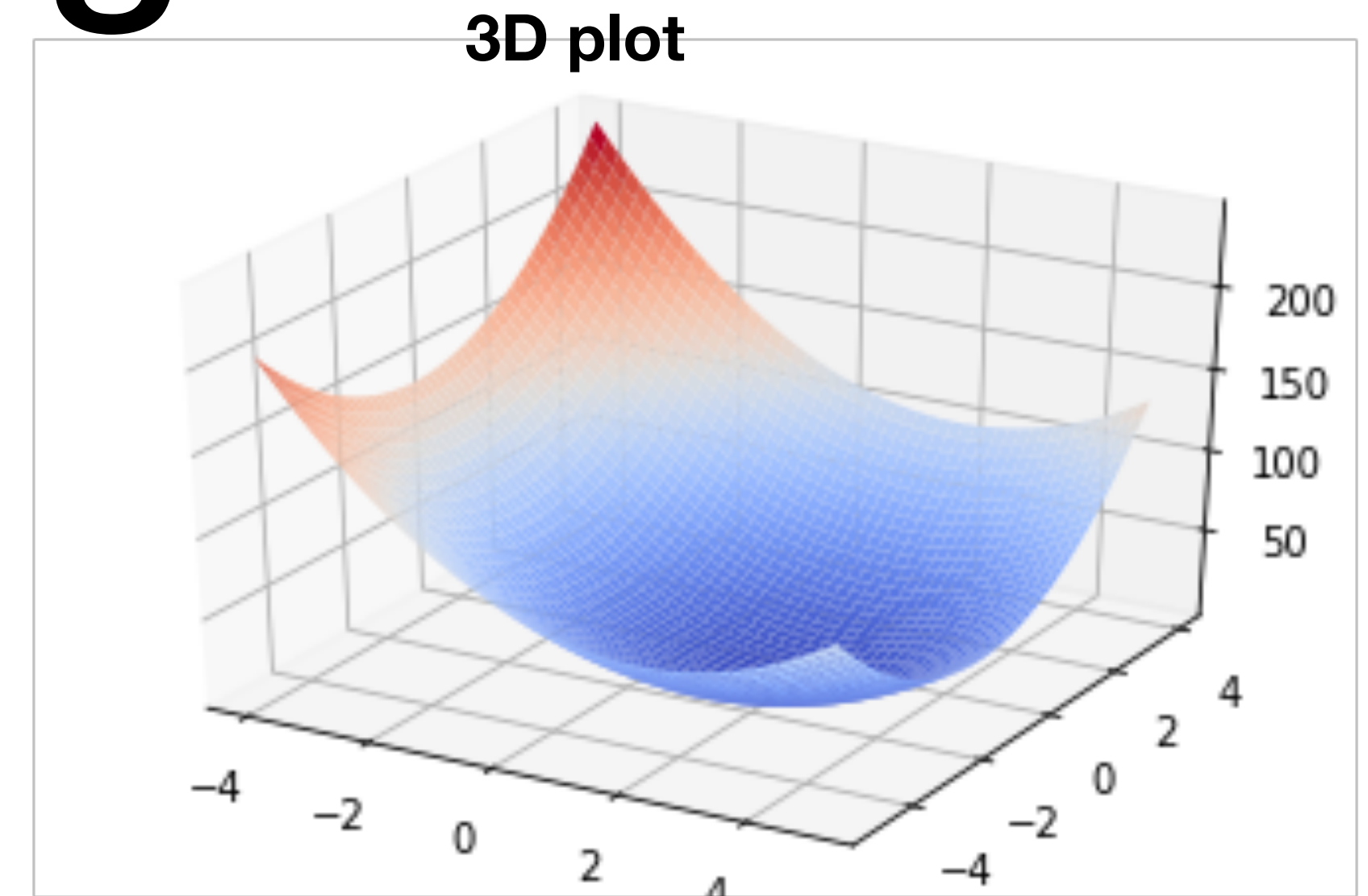
- At a given point, the gradient is the direction for which the value of the function increase fastest
- Therefore, in general, it points in the direction **opposite to the minimum**

$$f(x, y) = 4(x - 2)^2 + 4(y + 1)^2 - 0.1xy$$

$$\text{grad} \cdot f(x, y) = [8(x - 2) - 0.1y, 8(y + 1) - 0.1x]$$

$$\text{grad} \cdot f(0, 0) = [-16, 16]$$

$$\text{grad} \cdot f(2, -1) = [0.1, -0.2]$$



Gradient Descent

- Because we know that the gradient point in a direction opposite to the minimum, we can use the same idea as in the case of one variable

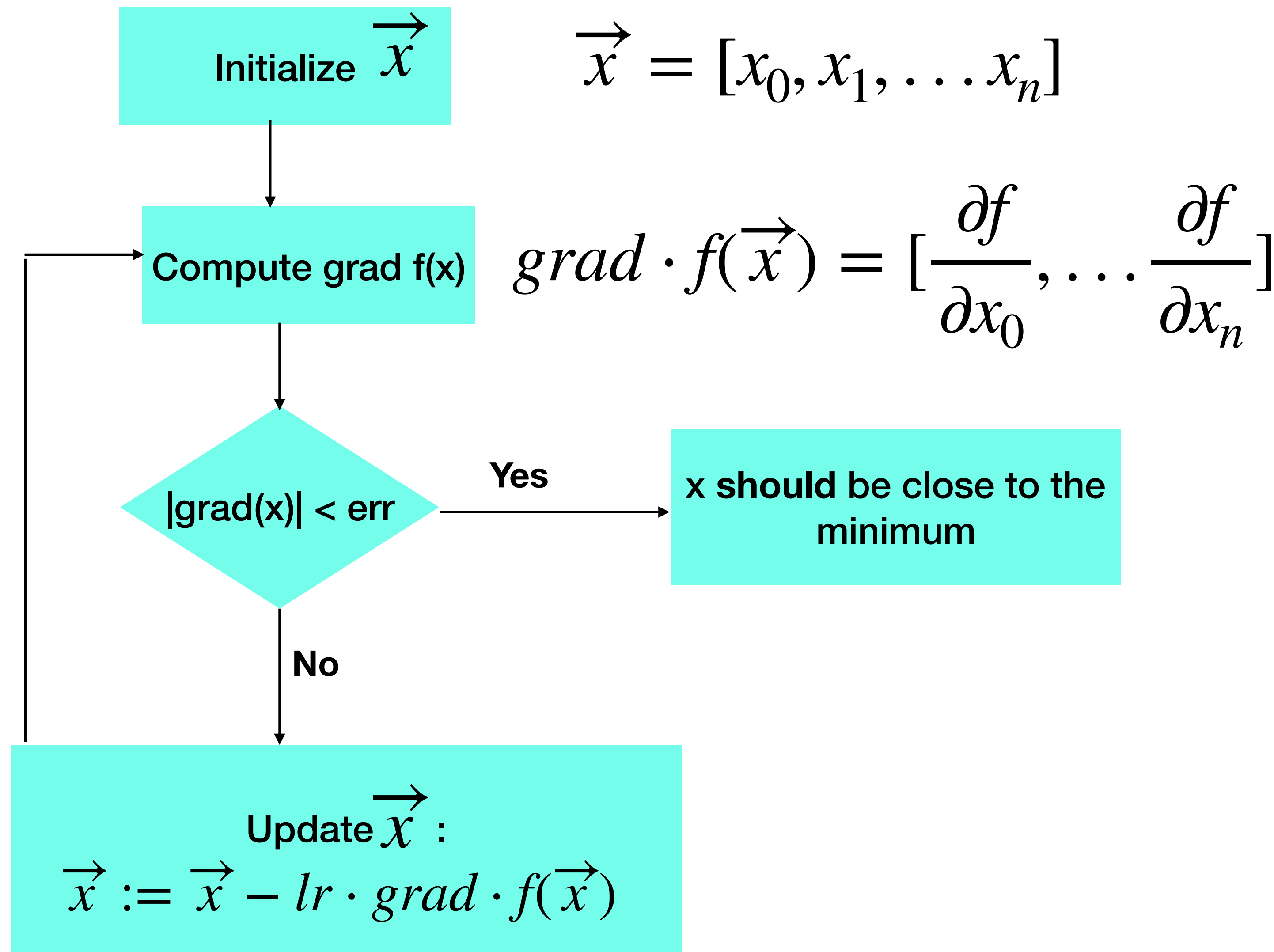
One variable:

$$x := x - lr \cdot f'(x)$$

Multiple variables:

$$\vec{x} := \vec{x} - lr \cdot grad \cdot f(\vec{x})$$

Gradient Descent algorithm



$$f(\vec{x}) = (x_0 - x_1)^2 + x_2^2 - x_2$$
$$\text{grad} \cdot f(\vec{x}) = [2(x_0 - x_1), 2(x_1 - x_0), 2x_2 - 1]$$

$$lr = 0.2$$

$$\vec{x} = (0, 1, 0)$$
$$\text{grad} \cdot f(\vec{x}) = [-2, 2, -1]$$

$$\vec{x} = (0.4, 0.6, 0.2)$$
$$\text{grad} \cdot f(\vec{x}) = [-0.4, 0.4, -0.6]$$

$$\vec{x} = (0.41, 0.43, 0.51)$$
$$\text{grad} \cdot f(\vec{x}) = [-0.04, 0.04, 0.01]$$

- Let us check gradient descent in practice with some notebook
- On google colab: <http://bit.ly/2vertEi>
- (or full url: <https://colab.research.google.com/drive/16MvnIY0TH8HTEiDCgRoWLZOqzGPu4np8>)
-

What is the equivalent of second derivative for multivariate functions?

- It is the Hessian Matrix:

$$\begin{vmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial x \partial z} & \frac{\partial^2 f}{\partial y \partial z} & \frac{\partial^2 f}{\partial z^2} \end{vmatrix}$$

- But thankfully, we will not need to use it
- But for your information, this would be the equivalent of the “High School” minimization when we have several variables:

-

- To minimize $f(x, y, z)$:
1. Compute gradient of $f(x, y, z)$
 2. Compute hessian of $f(x)$
 3. Find x, y, z such that $\text{grad } f(x, y, z) = 0$
 4. If hessian of $f(x, y, z)$ is definite positive then (x, y, z) is a local minimum of f

Gradient Descent Algorithm

- You can see that, in the case of the gradient descent, the algorithm is the same for univariate functions and multivariate functions
- It is a simple algorithm, but it scales very well
- There exists many variations of it:
 - Gradient Descent with momentum
 - Stochastic Gradient Descent
 - Adagrad, Adadelata, Adam, ...

Gradient Descent with Momentum

- Compute a “gradient with momentum” at each iteration:
-

$$gm_t = 0.6grad \cdot f(\vec{x}) + 0.4gm_{t-1}$$

Update $\vec{x}$:

$$\vec{x} := \vec{x} - lr \cdot gm_t$$

Stochastic Gradient Descent

- What happens if the gradient is noisy?
- That is, we can only compute a value that is equal to the true gradient “on average”?
- A bit like if you are drunk and trying to get home

Stochastic Gradient Descent

- What happens if the gradient is noisy?
- That is, we can only compute a value that is equal to the true gradient “on average”?
 - A bit like if you are drunk and trying to get home
- It turns out it works.
 - But you have to decrease your learning rate over time to stabilize $lr = \frac{lr_0}{\sqrt{(t+1)}}$
 - Convergence will be slower
- Very interesting because a noisy gradient can be million times faster to compute than a “true” gradient

Optimization libraries

- You can also minimize a function by using a specialized library
- It gives you access to more sophisticated minimization algorithms
- However these more sophisticated algorithms do not scale as well as Gradient Descent
- Which is one Gradient Descent and its variants are still the main tool for large scale Machine Learning (In particular, Deep Learning)

```
In [103]: scipy.optimize.minimize(f_numpy, np.array([0,0]), jac=grad_f_numpy, method="L-BFGS-B")
```

```
Out[103]:      fun: 0.1969057665260197
      hess_inv: <2x2 LbfgsInvHessProduct with dtype=float64>
      jac: array([-3.88578059e-16,  2.77555756e-17])
      message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
      nfev: 5
      nit: 4
      status: 0
      success: True
      x: array([ 1.9878106 , -0.97515237])
```