UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

# Neurocomputing

## Optimization

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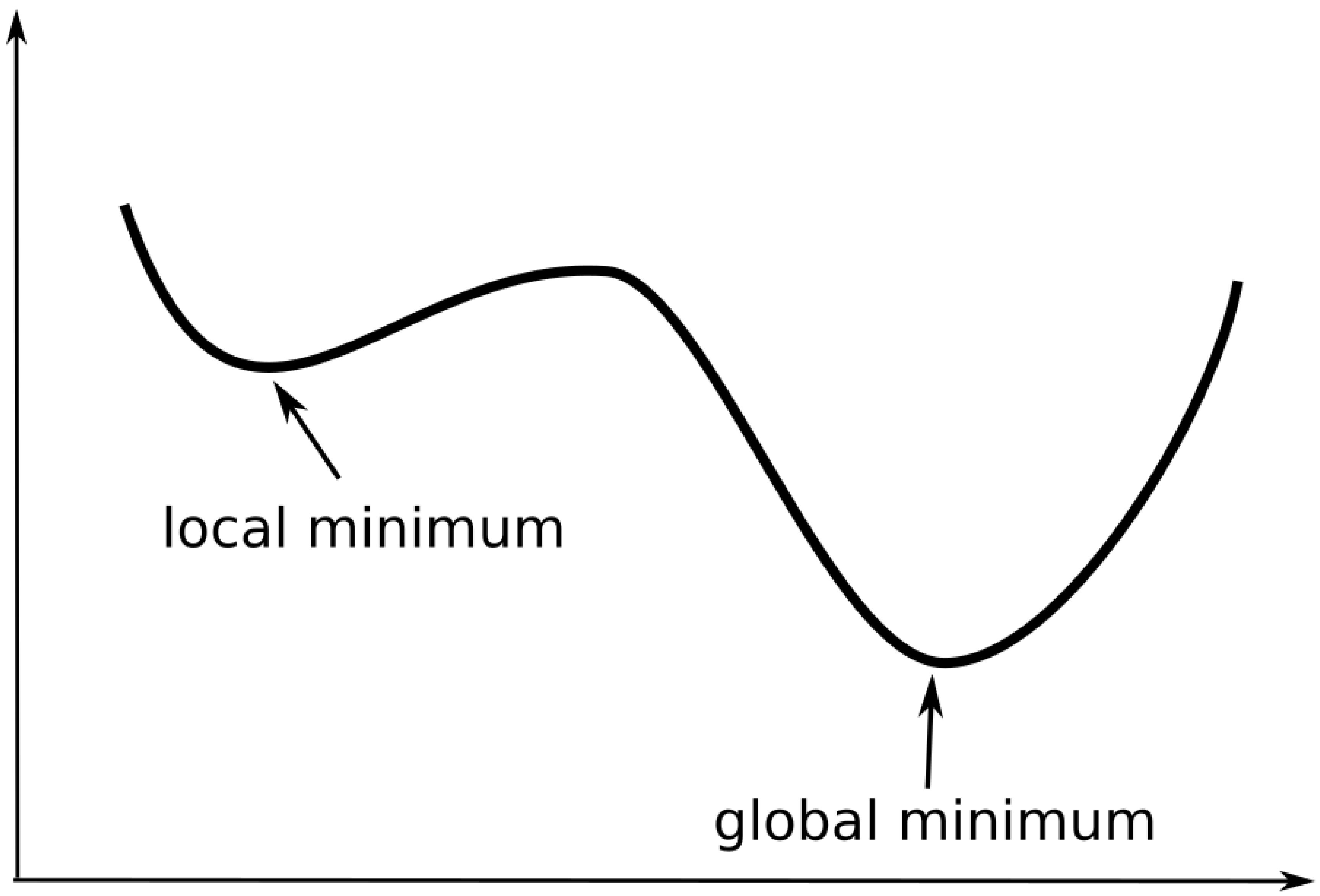
# 1 - Optimization

# Machine learning = Optimization

- Machine learning is all about optimization:
  - Supervised learning minimizes the error between the prediction and the data.
  - Unsupervised learning maximizes the fit between the model and the data
  - Reinforcement learning maximizes the collection of rewards.

- The function to be optimized is called the **objective function**, **cost function** or **loss function**.
- ML searches for the value of **free parameters** which optimize the objective function on the data set.
- The simplest optimization method is the **gradient descent** (or ascent) method.



# Analytical optimization

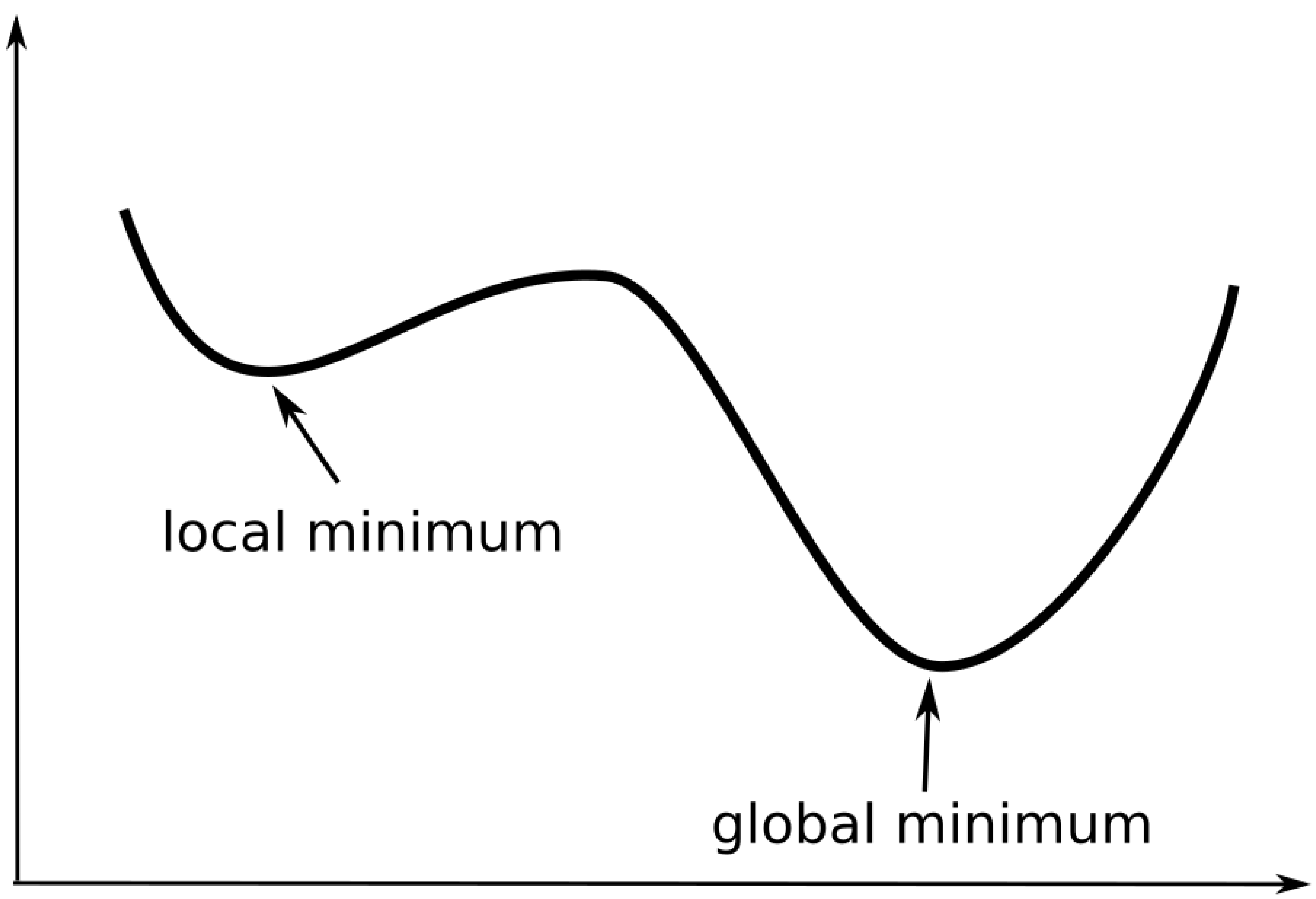
- The easiest method to find the extremum of a function $f(x)$ is to look where its first derivative is equal to 0:

$$x^* = \min_x f(x) \Leftrightarrow f'(x^*) = 0 \text{ and } f''(x^*) > 0$$

$$x^* = \max_x f(x) \Leftrightarrow f'(x^*) = 0 \text{ and } f''(x^*) < 0$$

- The sign of the second order derivative tells us whether it is a maximum or minimum.

- There can be multiple minima or maxima (or none) depending on the function.
  - The “best” minimum (with the lowest value among all minima) is called the **global minimum**.
  - The others are called **local minima**.



# Multivariate optimization

- A multivariate function is a function of more than one variable, e.g. $f(x, y)$.

- A point $(x^*, y^*)$ is an extremum of $f$ if all partial derivatives are zero at the same time:

$$\begin{cases} \dfrac{\partial f(x^*, y^*)}{\partial x} = 0 \\ \\ \dfrac{\partial f(x^*, y^*)}{\partial y} = 0 \end{cases}$$

- The vector of partial derivatives is called the **gradient of the function**:

$$\nabla_{x,y}\, f(x, y) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} \\ \\ \dfrac{\partial f(x, y)}{\partial y} \end{bmatrix}$$

- Finding the extremum of $f$ is searching for the values of $(x, y)$ where the gradient of the function is the zero vector:

$$\nabla_{x,y}\, f(x^*, y^*) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

# Multivariate optimization : example

- Let's consider this function:

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

- Its gradient is:

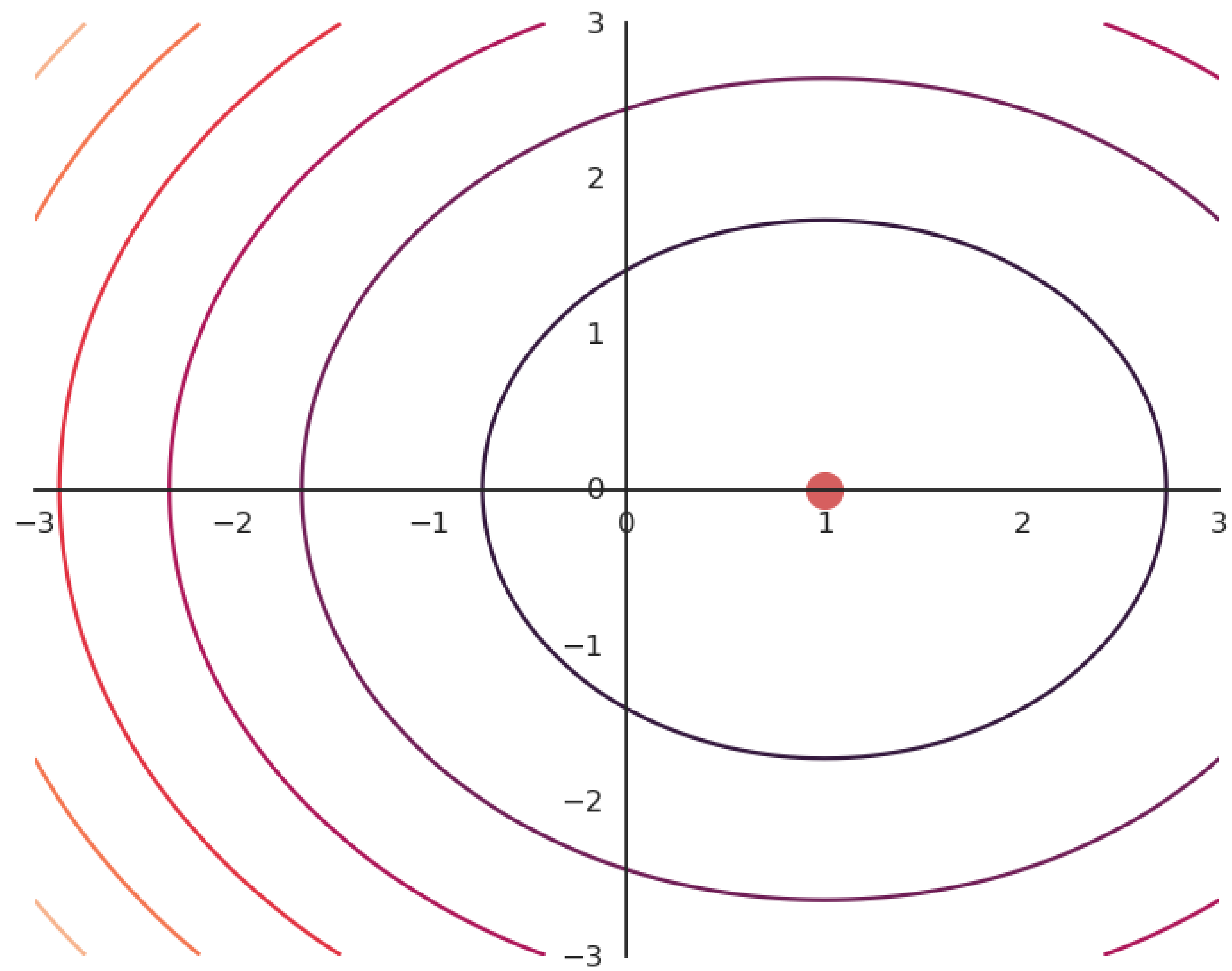
$$\nabla_{x,y} f(x,y) = \begin{bmatrix} 2(x-1) \\ 2y \end{bmatrix}$$

- The gradient is equal to 0 when:

$$\begin{cases} 2\,(x-1) = 0 \\ 2\,y = 0 \end{cases}$$

- $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is the minimum of $f$.

- One should check the second order derivative to know whether it is a minimum or maximum…



# 2 - Gradient descent

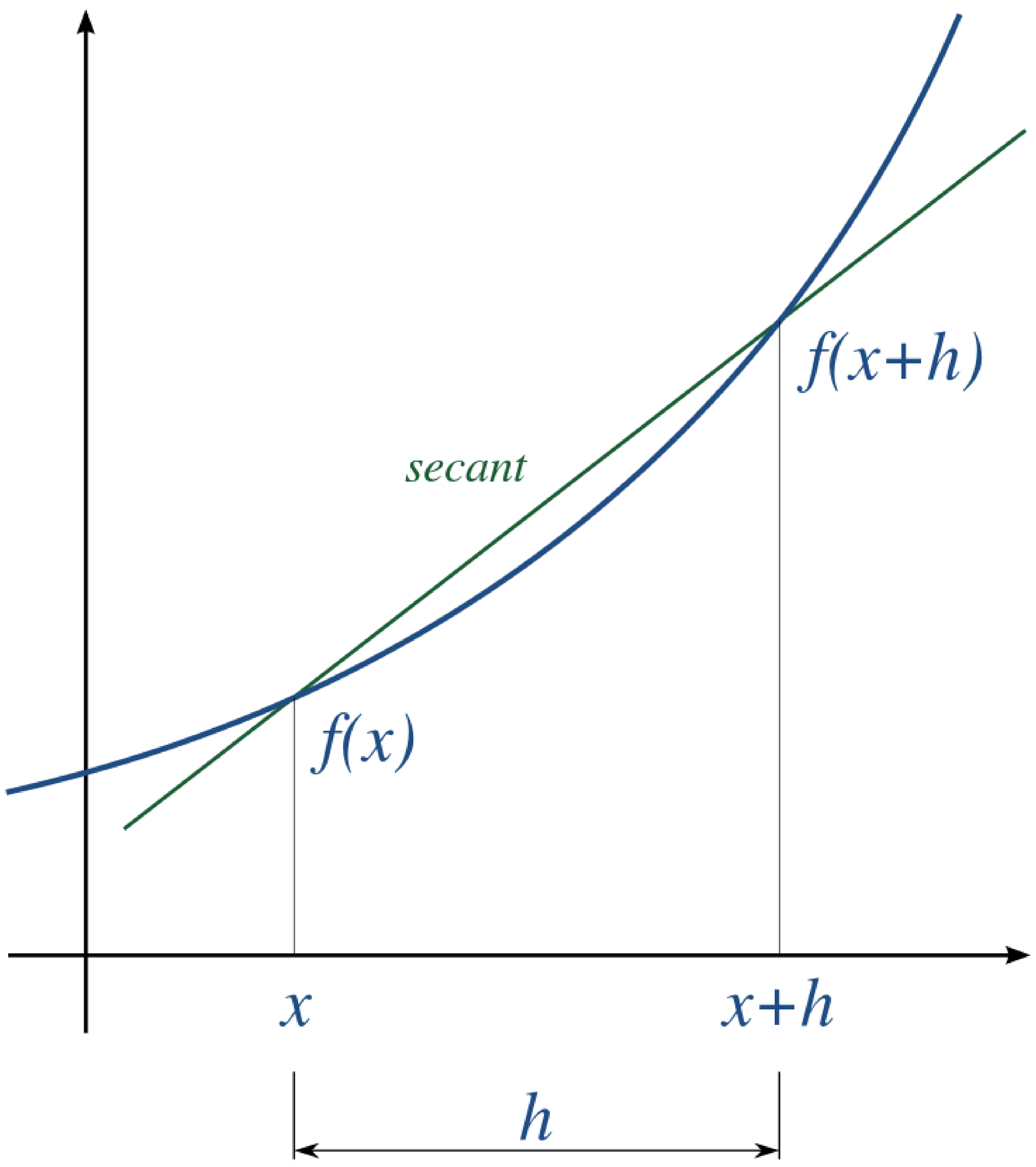
## Problem with analytical optimization

- In machine learning, we generally do not have access to the analytical form of the objective function.
- We can not therefore get its derivative and search where it is 0.
- However, we have access to its value (and derivative) for certain values, for example:

$$f(0, 1) = 2 \qquad f'(0, 1) = -1.5$$

- We can “ask” the model for as many values as we want, but we never get its analytical form.
- For most useful problems, the function would be too complex to differentiate anyway.

## Euler method




- Let's remember the definition of the derivative of a function. The derivative $f'(x)$ is defined by the slope of the tangent of the function:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{x + h - x}$$

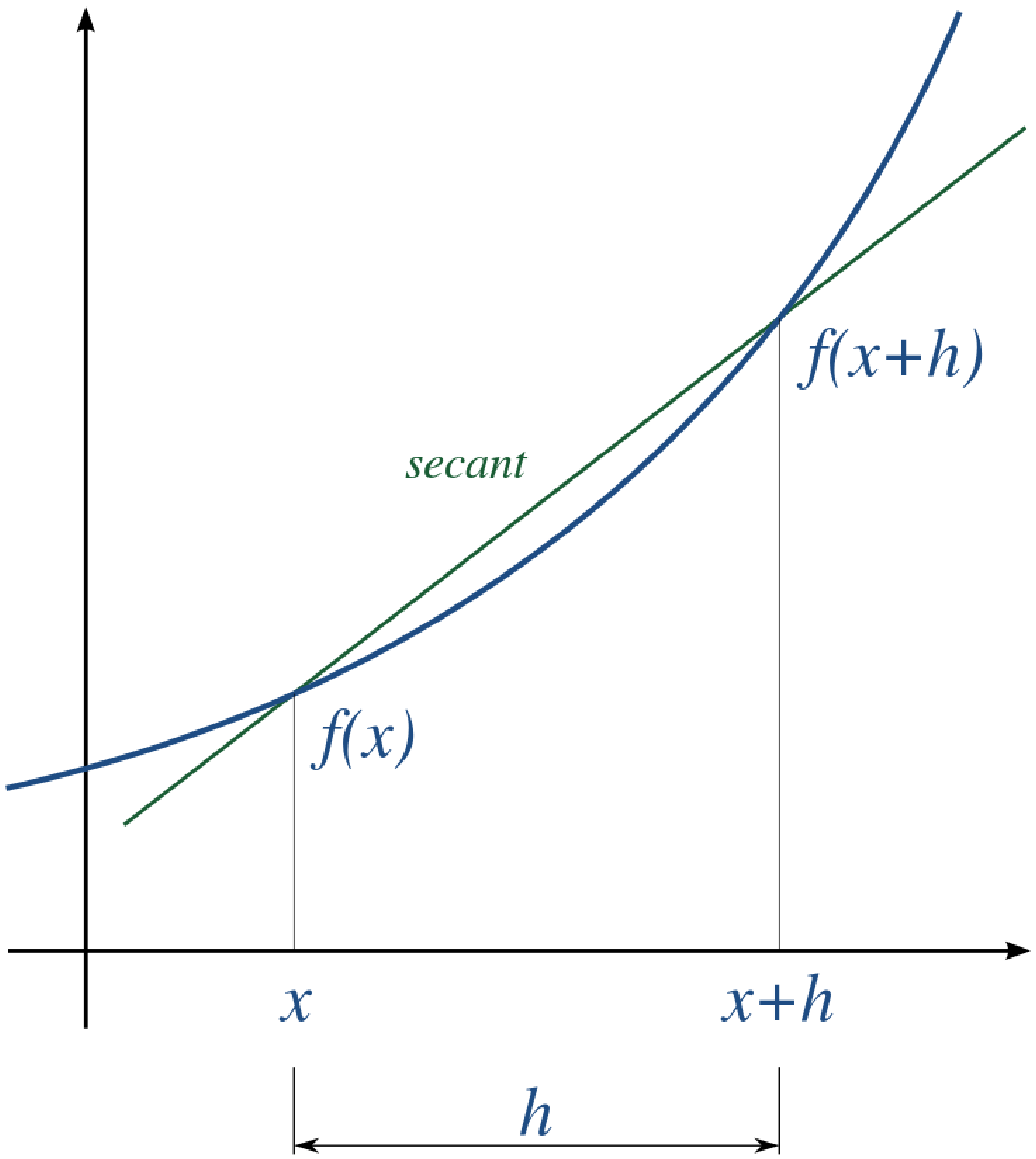
$$= \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- If we take $h$ small enough, we have the following approximation:

$$f(x+h) - f(x) \approx h\, f'(x)$$

- We are making an error, but it is negligible if $h$ is small enough (Taylor series).

# Euler method




- First order approximation:

$$f(x+h) - f(x) \approx h\, f'(x)$$

- If we want $x + h$ to be closer to the minimum than $x$, we want:

$$f(x+h) < f(x)$$

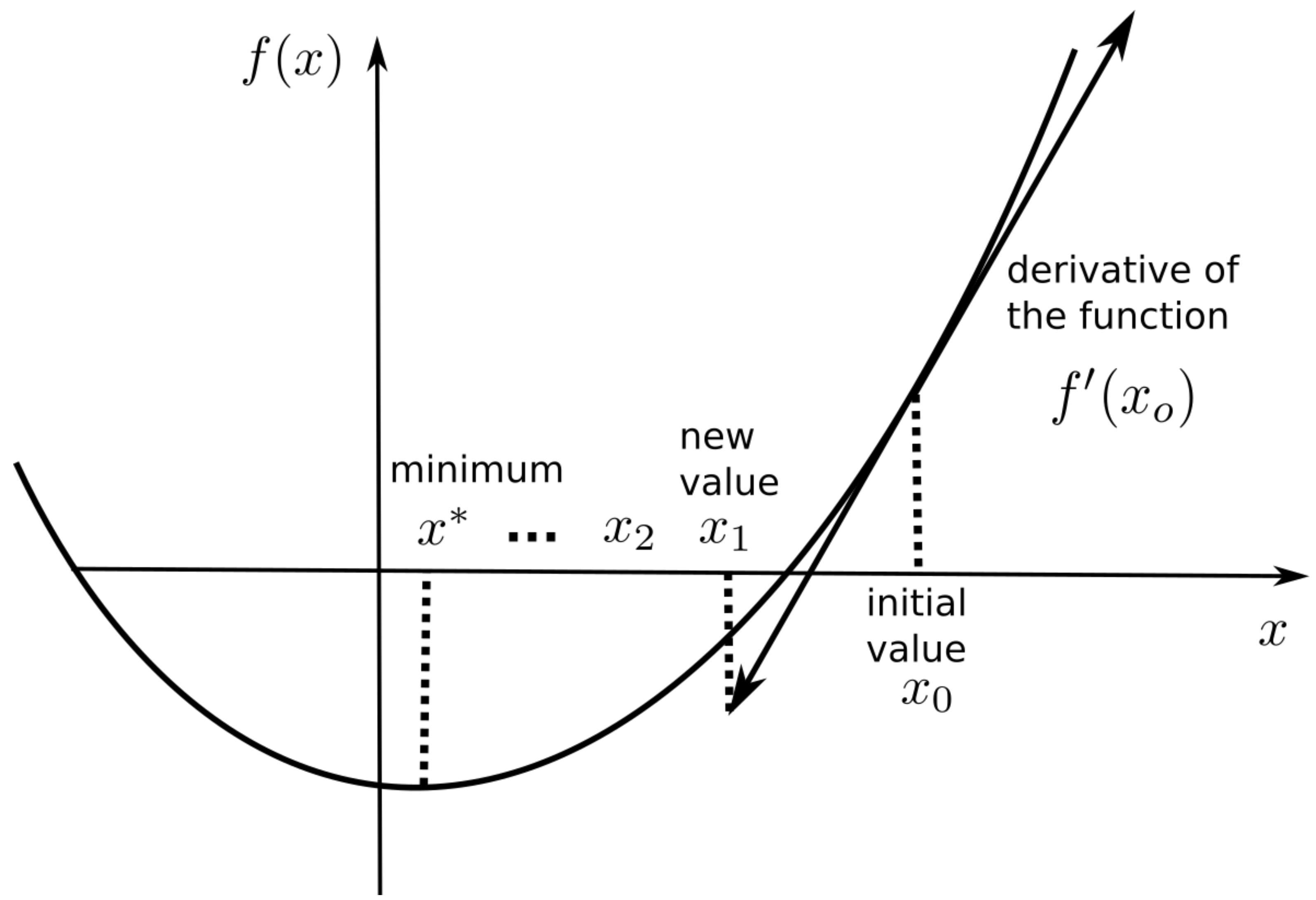
- We therefore want that:

$$h\, f'(x) < 0$$

- The **change** $h$ in the value of $x$ must have the opposite sign of $f'(x)$.
  - If the function is increasing in $x$, the minimum is smaller than $x$.
  - If the function is decreasing in $x$, the minimum is bigger than $x$.

# Gradient descent

- **Gradient descent** (GD) is a first-order method to iteratively find the minimum of a function $f(x)$.




- It creates a series of estimates $[x_0, x_1, x_2, \ldots]$ that converges to a local minimum of $f$.
- Each element of the series is calculated based on the previous element and the derivative of the function in that element:

$$x_{n+1} = x_n + \Delta x = x_n - \eta\, f'(x_n)$$

- $\eta$ is a small parameter between 0 and 1 called the **learning rate**.

# Gradient descent

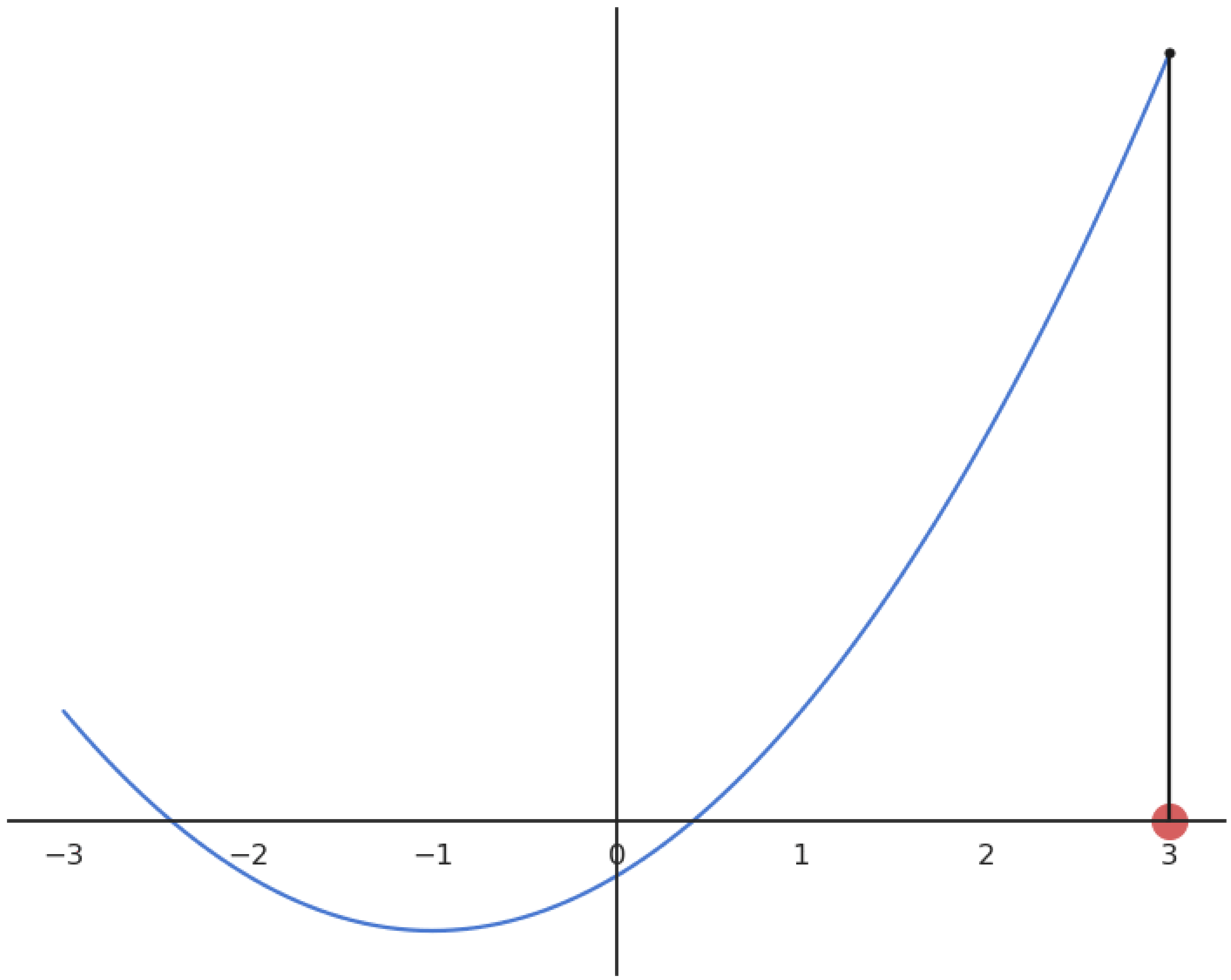
**Gradient descent algorithm**

- We start with an initially wrong estimate of $x$: $x_0$
- for $n \in [0, \infty]$:
    - We compute or estimate the derivative of the loss function in $x_n$: $f'(x_n)$
    - We compute a new value $x_{n+1}$ for the estimate using the **gradient descent update rule**:

$$\Delta x = x_{n+1} - x_n = -\eta \, f'(x_n)$$

- There is theoretically no end to the GD algorithm: we iterate forever and always get closer to the minimum.
- The algorithm can be stopped when the change $\Delta x$ is below a threshold.

# Gradient descent



## Multivariate gradient descent

- Gradient descent can be applied to multivariate functions:

$$\min_{x, y, z} \qquad f(x, y, z)$$

- Each variable is updated independently using partial derivatives:

$$\Delta x = x_{n+1} - x_n = - \eta \, \frac{\partial f(x_n, y_n, z_n)}{\partial x}$$

$$\Delta y = y_{n+1} - y_n = - \eta \, \frac{\partial f(x_n, y_n, z_n)}{\partial y}$$

$$\Delta z = z_{n+1} - z_n = - \eta \, \frac{\partial f(x_n, y_n, z_n)}{\partial z}$$

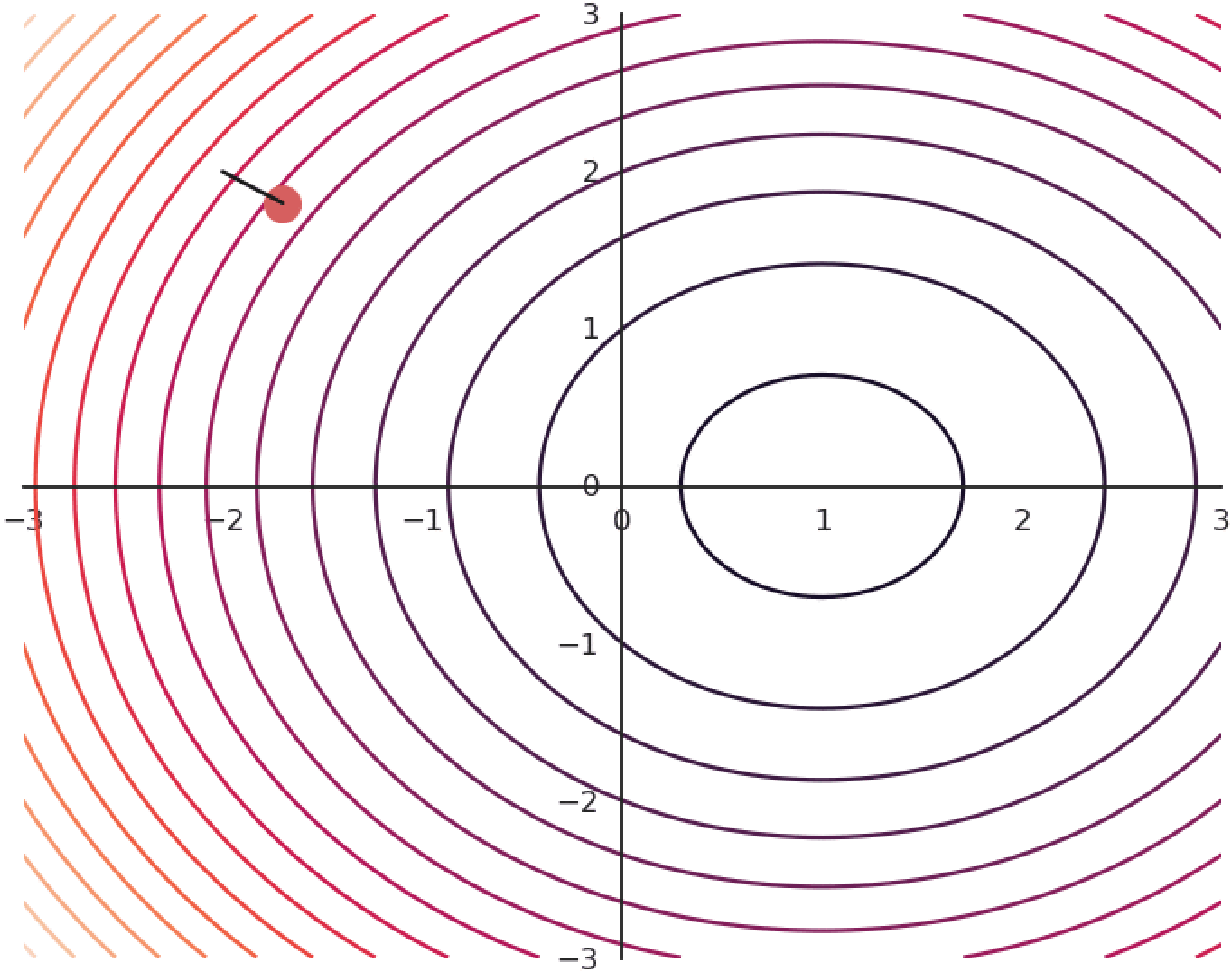
- We can also use the vector notation to use the **gradient operator**:

$$\mathbf{x}_n = \begin{bmatrix} x_n \\ y_n \\ z_n \end{bmatrix} \quad \text{and} \quad \nabla_\mathbf{x} \, f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(x, y, z)}{\partial x} \\ \frac{\partial f(x, y, z)}{\partial y} \\ \frac{\partial f(x, y, z)}{\partial z} \end{bmatrix}$$

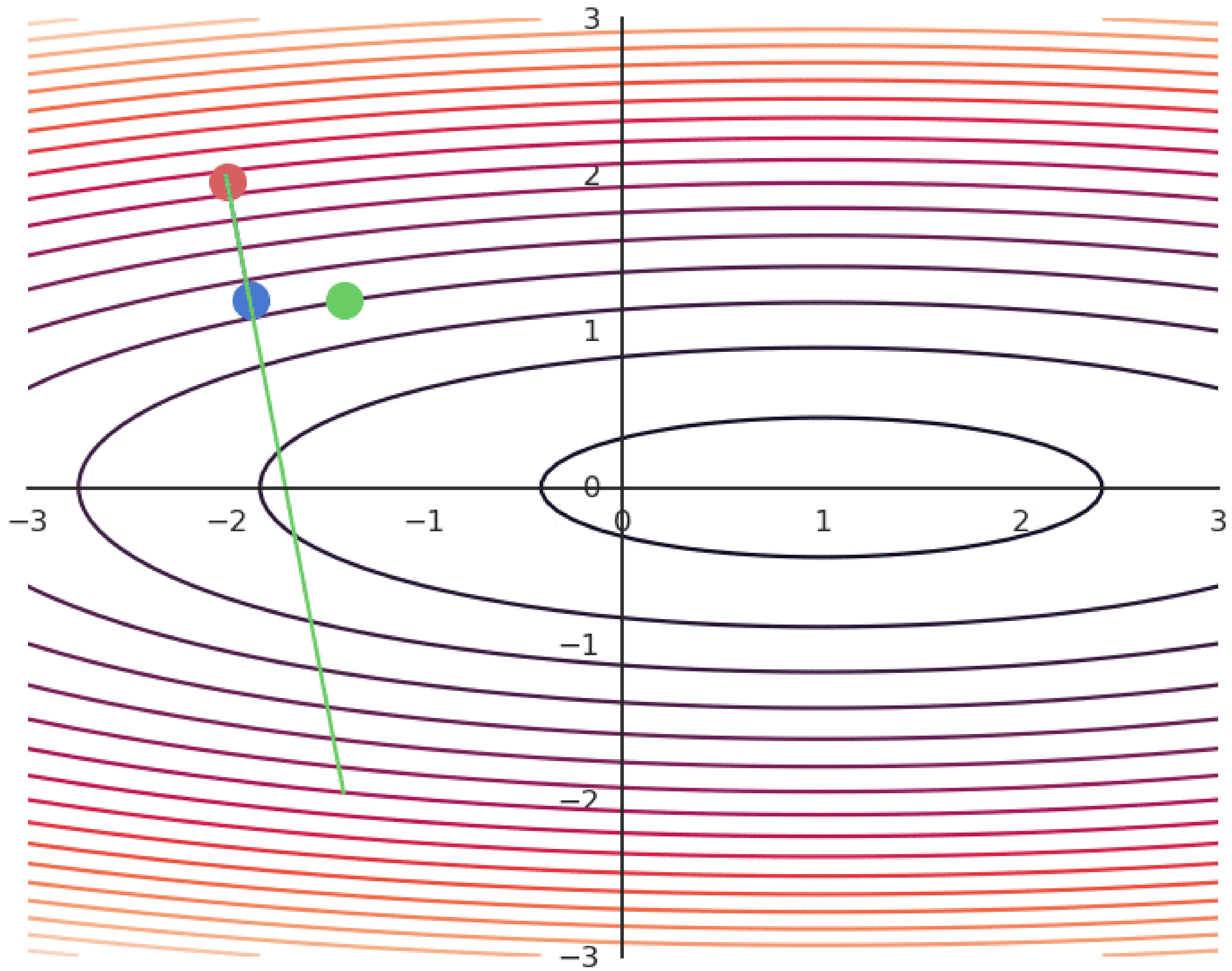
which gives:

$$\Delta \mathbf{x} = - \eta \, \nabla_\mathbf{x} \, f(\mathbf{x}_n)$$

# Multivariate gradient descent

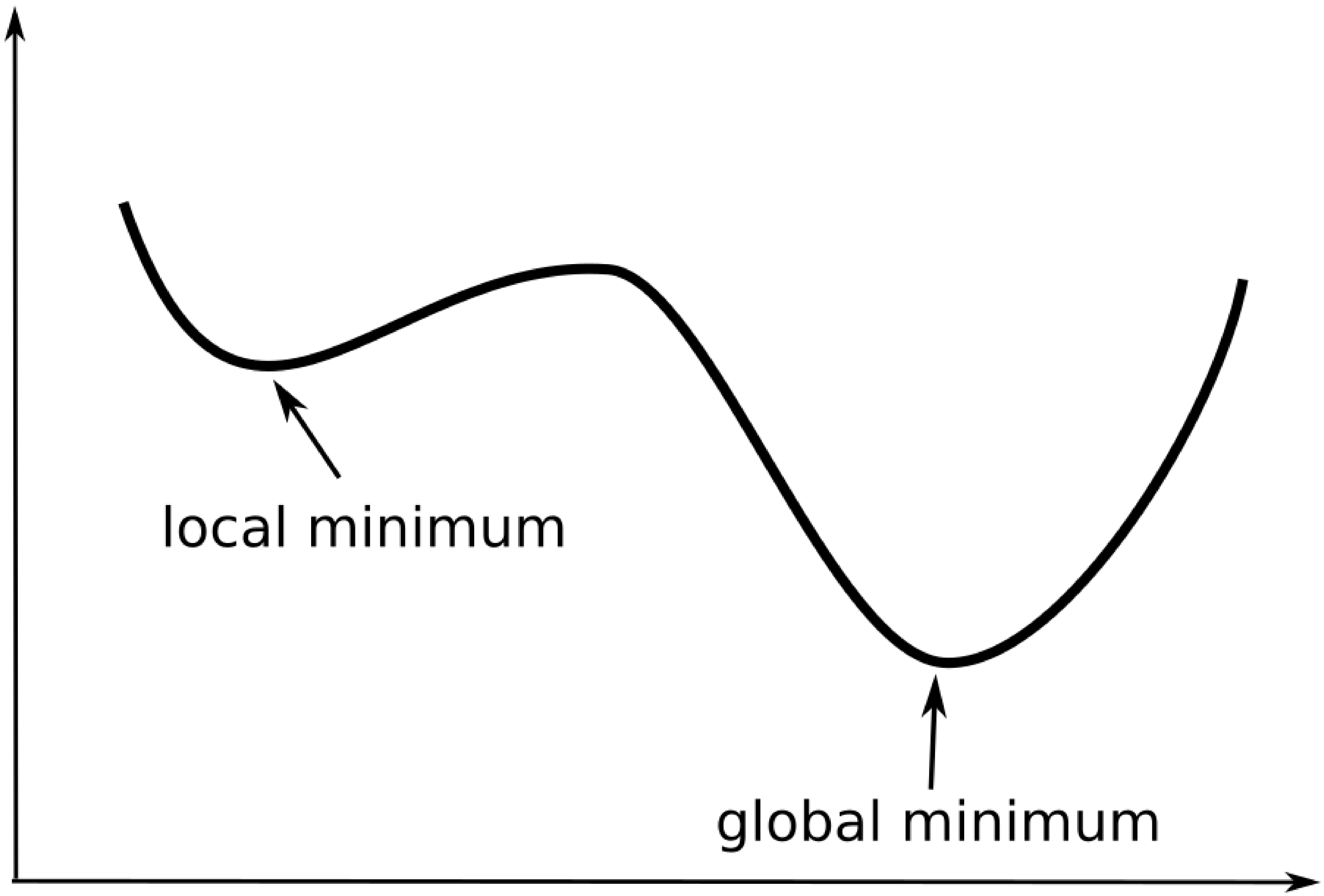


# Influence of the learning rate




- The parameter $\eta$ is called the learning rate (or step size) and regulates the speed of convergence.
- The choice of the learning rate $\eta$ is critical:
  - If it is too small, the algorithm will need a lot of iterations to converge.
  - If it is too big, the algorithm can oscillate around the desired values without ever converging.

# Optimality of gradient descent




- Gradient descent is not optimal: it always finds a local minimum, but there is no guarantee that it is the global minimum.
- The found solution depends on the initial choice of $x_0$. If you initialize the parameters near to the global minimum, you are lucky. But how?
- This will be a big issue in neural networks.

# 3 - Regularization

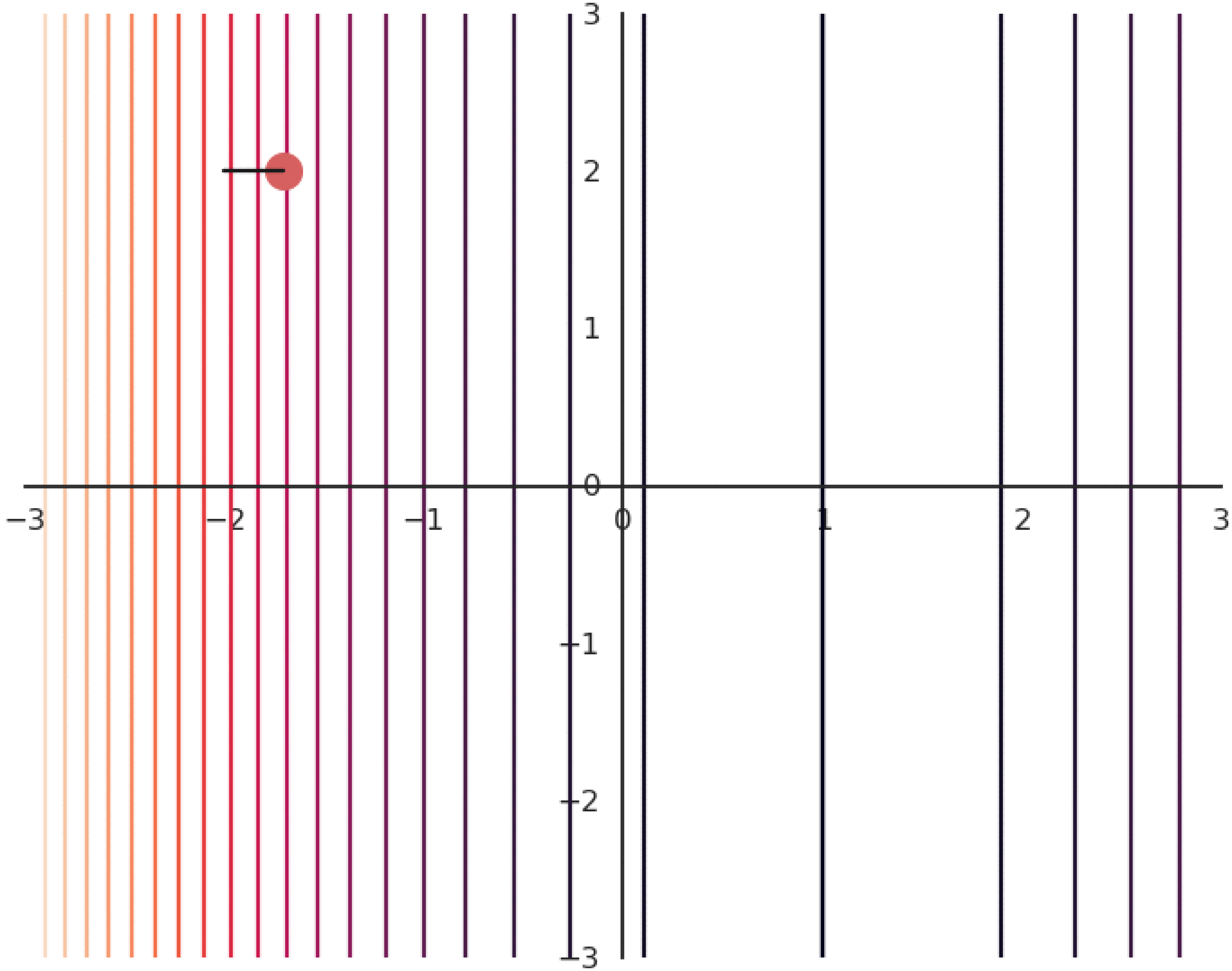
# Regularization

- Most of the time, there are many minima to a function, if not an infinity.
- As GD only converges to the “closest” local minimum, you are never sure that you get a good solution.
- Consider the following function:

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

- As it does not depend on $y$, whatever initial value $y_0$ will be considered as a solution.
- As we will see later, this is something we do not want.

# Regularization



# L2 - Regularization

- We may want to put the additional **constraint** that $x$ and $y$ should be as small as possible.
- One possibility is to also minimize the **Euclidian norm** (or **L2-norm**) of the vector $\mathbf{x} = [x, y]$.

$$\min_{x, y} ||\mathbf{x}||^2 = x^2 + y^2$$

- Note that this objective is in contradiction with the original objective: $(0, 0)$ minimizes the norm, but not the function $f(x, y)$.
- We construct a new function as the sum of $f(x, y)$ and the norm of $\mathbf{x}$, weighted by the **regularization parameter** $\lambda$:

$$\mathcal{L}(x, y) = f(x, y) + \lambda \, (x^2 + y^2)$$

# L2 - Regularization

- For a fixed value of $\lambda$, for example 0.1, we now minimize using gradient descent the following loss function function:

$$\mathcal{L}(x, y) = f(x, y) + \lambda \, (x^2 + y^2)$$

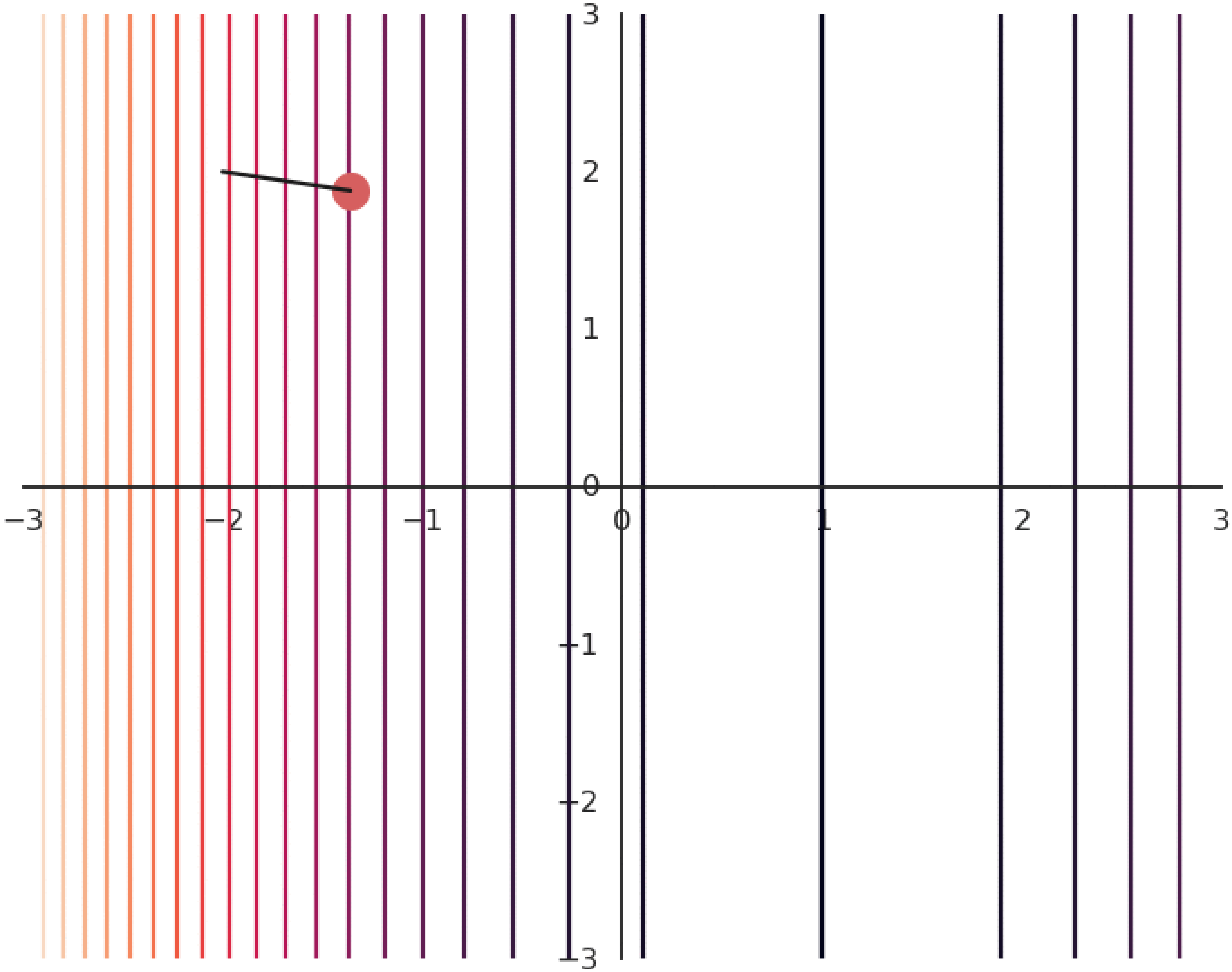
- We just need to compute its gradient:

$$\nabla_{x,y} \, \mathcal{L}(x, y) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} + 2 \, \lambda \, x \\ \\ \dfrac{\partial f(x, y)}{\partial y} + 2 \, \lambda \, y \end{bmatrix}$$

and apply gradient descent iteratively:

$$\Delta \begin{bmatrix} x \\ y \end{bmatrix} = - \eta \, \nabla_{x,y} \, \mathcal{L}(x, y) = - \eta \, \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} + 2 \, \lambda \, x \\ \\ \dfrac{\partial f(x, y)}{\partial y} + 2 \, \lambda \, y \end{bmatrix}$$

# L2 - Regularization

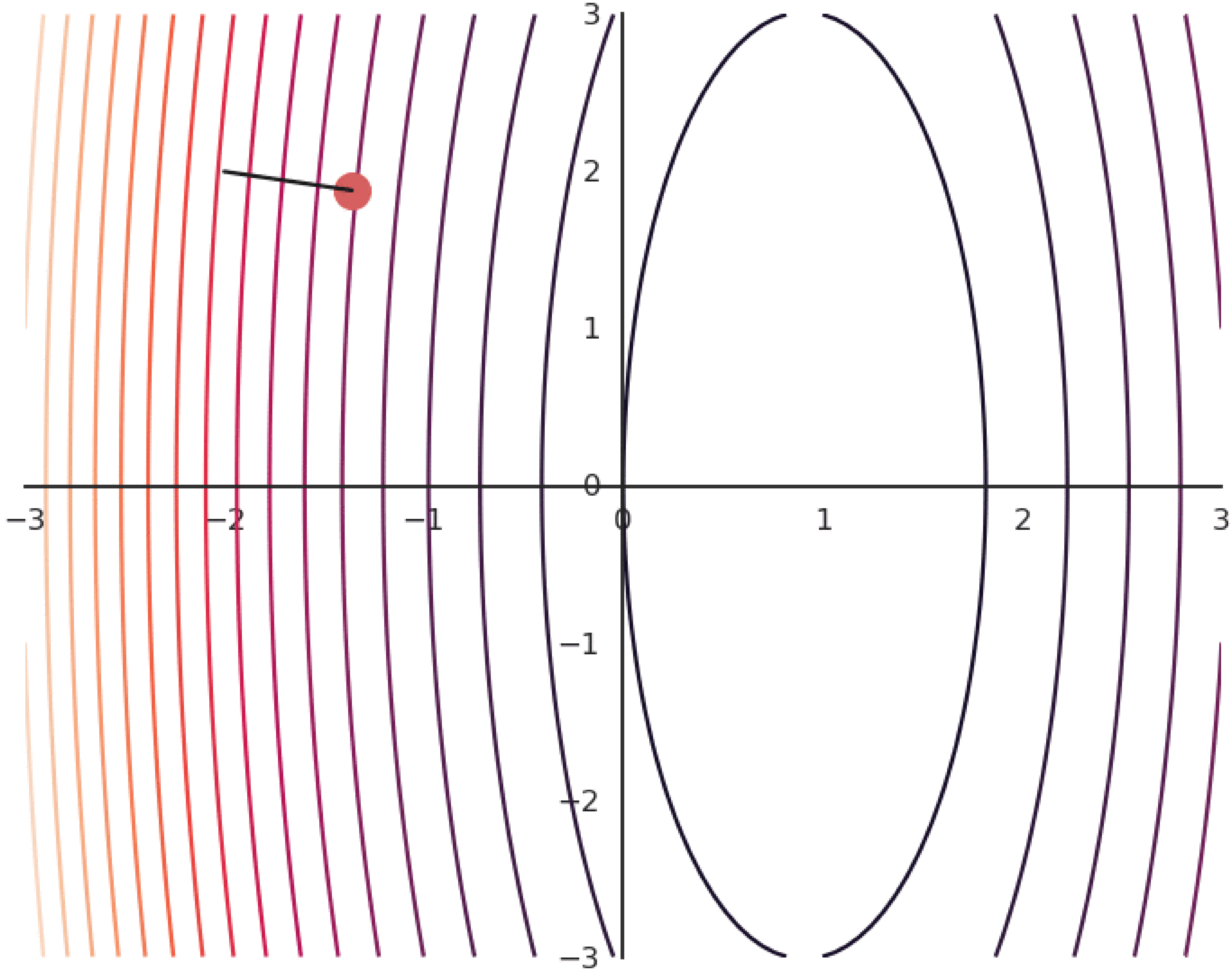


## L2 - Regularization

- You may notice that the result of the optimization is a bit off, it is not exactly $(1, 0)$.
- This is because we do not optimize $f(x, y)$ directly, but $\mathcal{L}(x, y)$.
- Let's look at the real landscape of the function.

$$\mathcal{L}(x, y) = f(x, y) + \lambda \left(x^2 + y^2\right)$$

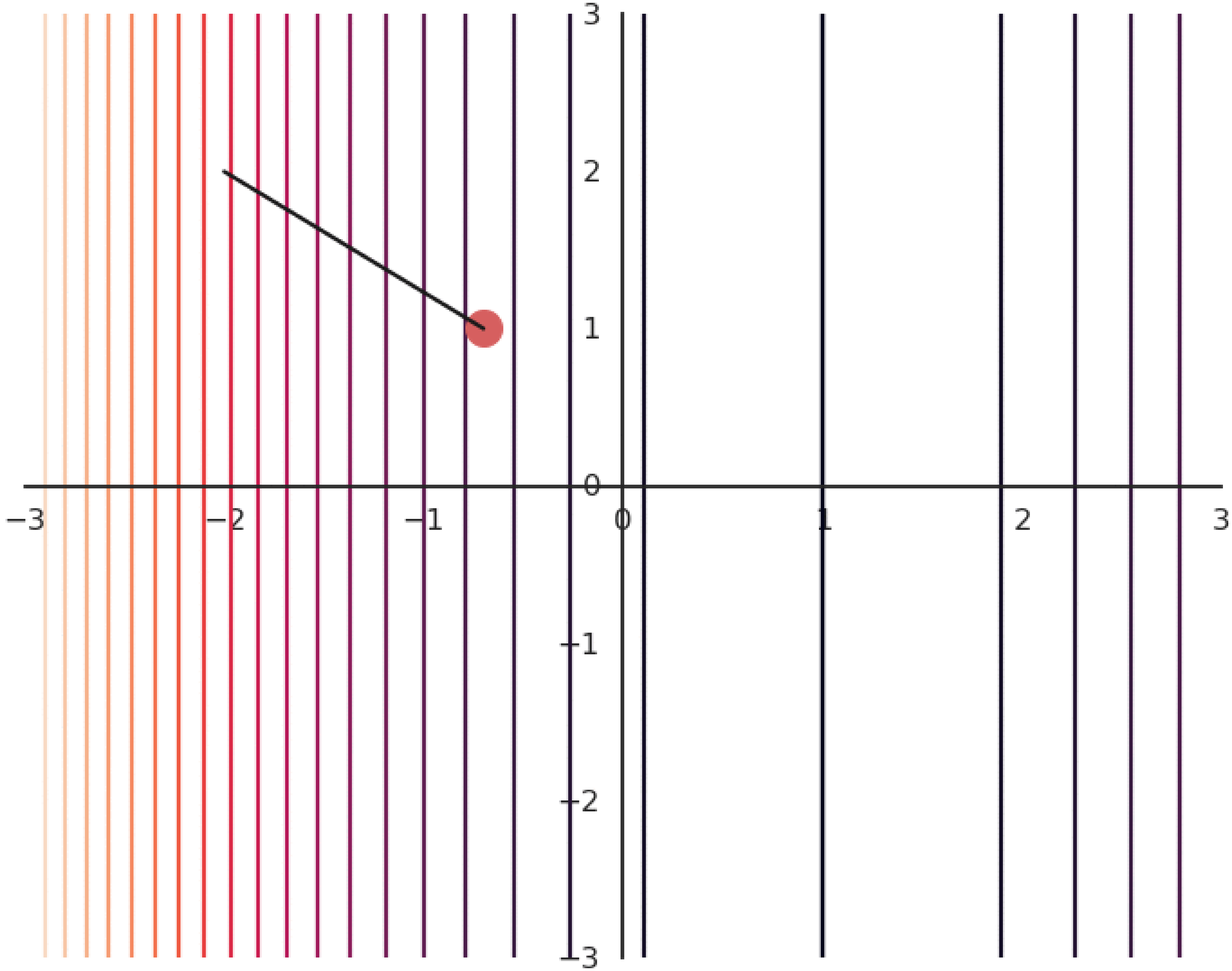
# L2 - Regularization



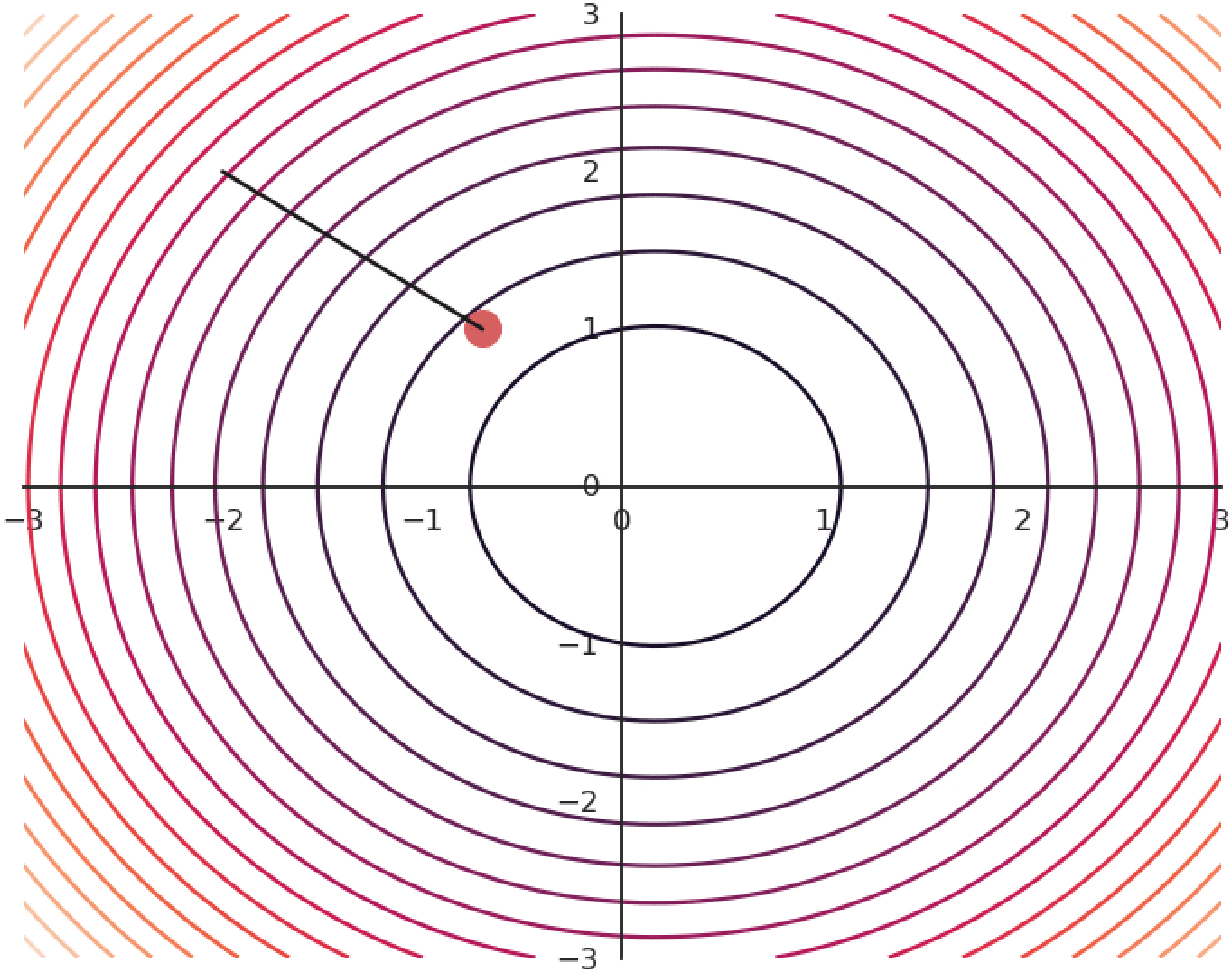
## L2 - Regularization

- The optimization with GD works, it is just that the function is different.
- The constraint on the Euclidian norm “attracts” or “distorts” the function towards $(0, 0)$.
- This may seem counter-intuitive, but we will see with deep networks that we can live with it.
- Let’s now look at what happens when we increase $\lambda$ (to 5.0).

# L2 - Regularization



# L2 - Regularization



# L2 - Regularization

- Now the result of the optimization is totally wrong: the constraint on the norm completely dominates the optimization process.

$$\mathcal{L}(x, y) = f(x, y) + \lambda \, (x^2 + y^2)$$

- $\lambda$ controls which of the two objectives, $f(x, y)$ or $x^2 + y^2$, has the priority:
  - When $\lambda$ is small, $f(x, y)$ dominates and the norm of $\mathbf{x}$ can be anything.
  - When $\lambda$ is big, $x^2 + y^2$ dominates, the result will be very small but $f(x, y)$ will have any value.
- The right value for $\lambda$ is hard to find. We will see later methods to experimentally find its most adequate value.

## L1 - Regularization

- Another form of regularization is **L1 - regularization** using the L1-norm (absolute values):

$$\mathcal{L}(x, y) = f(x, y) + \lambda \, (|x| + |y|)$$

- Its gradient only depend on the sign of $x$ and $y$:

$$\nabla_{x, y} \, \mathcal{L}(x, y) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} + \lambda \, \text{sign}(x) \\ \\ \dfrac{\partial f(x, y)}{\partial y} + \lambda \, \text{sign}(y) \end{bmatrix}$$

- It tends to lead to **sparser** value of $(x, y)$, i.e. either $x$ or $y$ will be 0.

# L1 - Regularization