UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

Optimization

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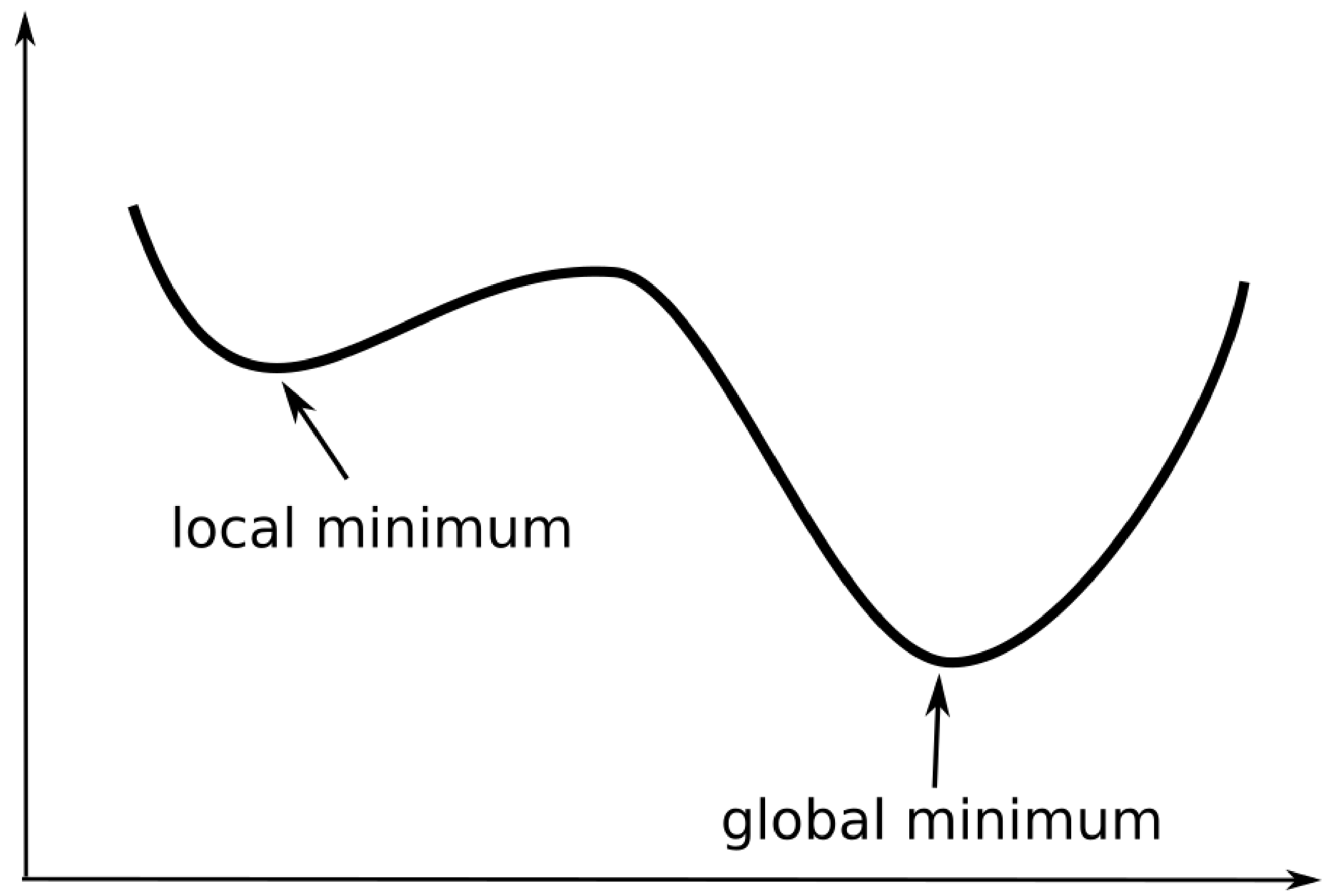
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

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:

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

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

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

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

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

Multivariate optimization : example

- Let's consider this function:

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

- Its gradient is:

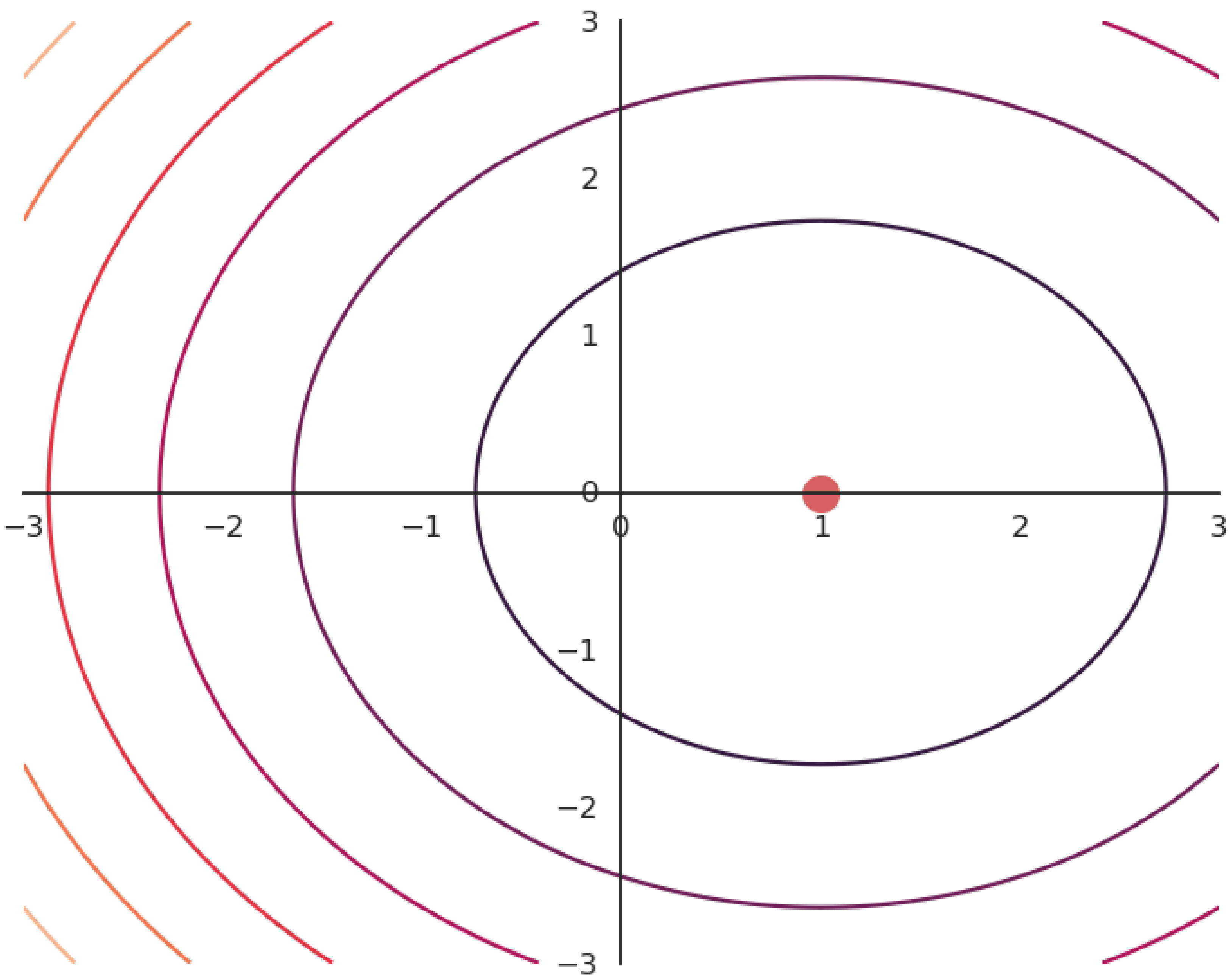
$$\nabla_{x,y}\, f(x, y) = \begin{bmatrix} 2(x-1) \\ 2y \end{bmatrix}$$

- 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

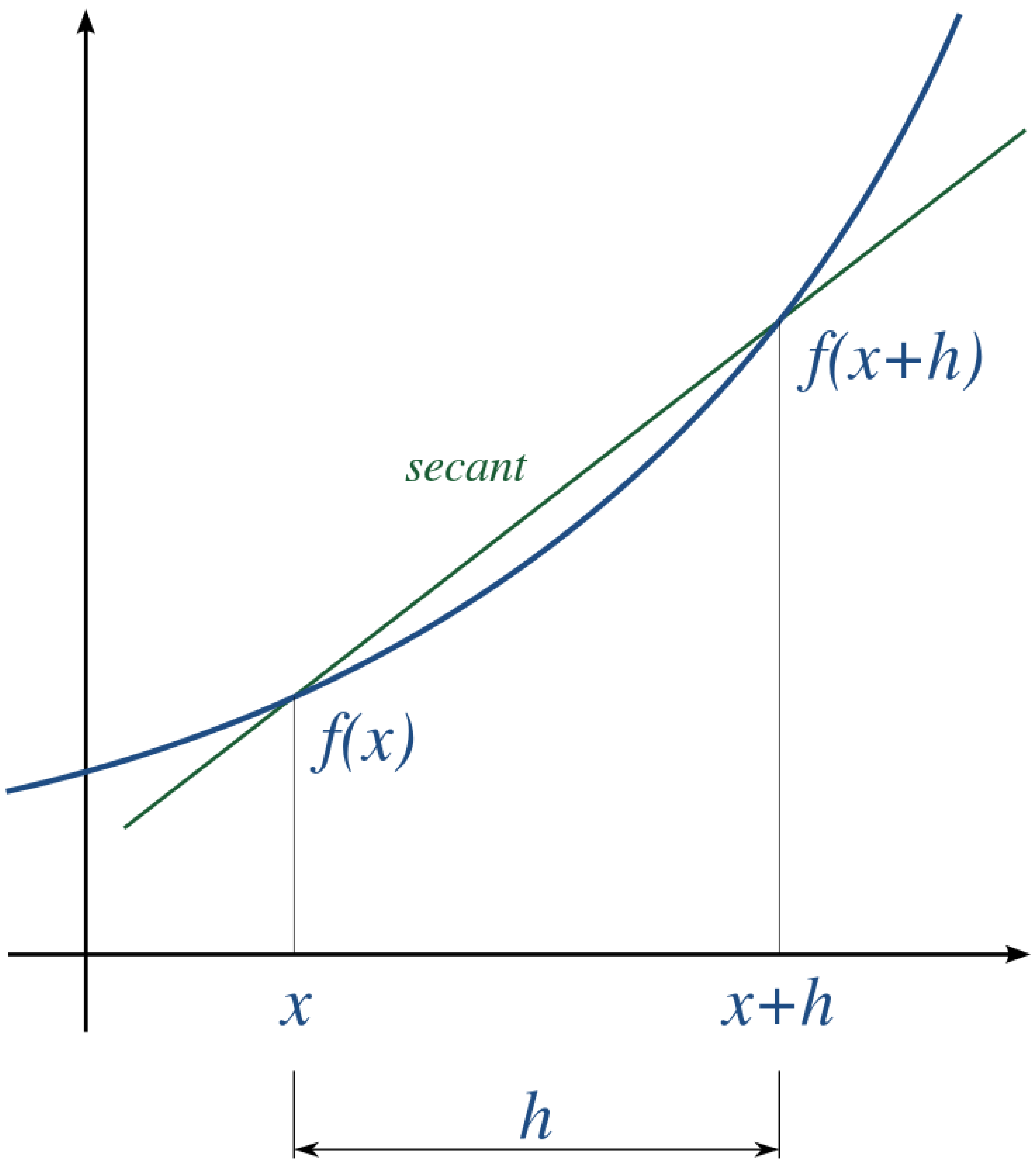
Problem with analytical optimization

- 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:

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

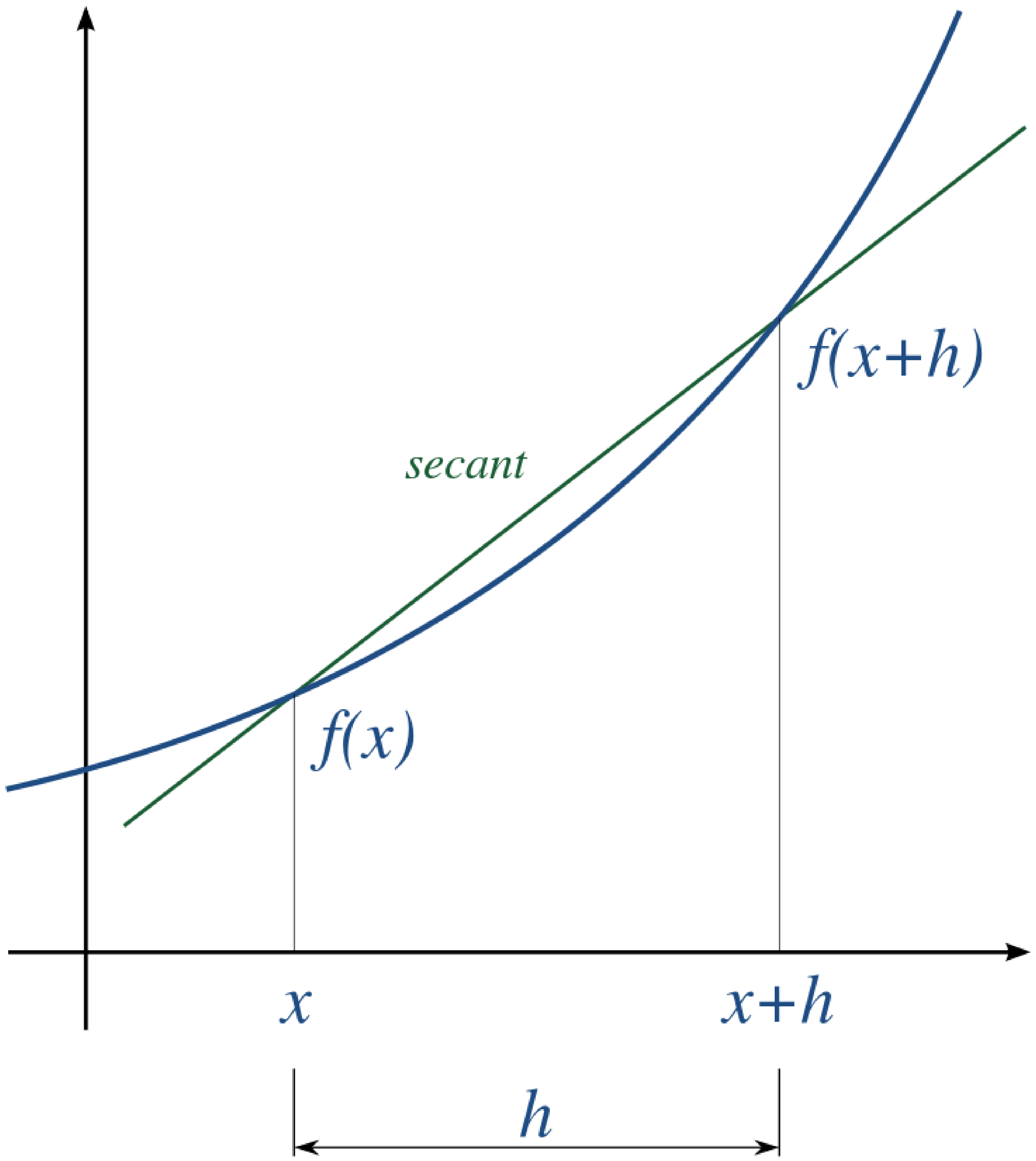
$$= \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- 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:

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

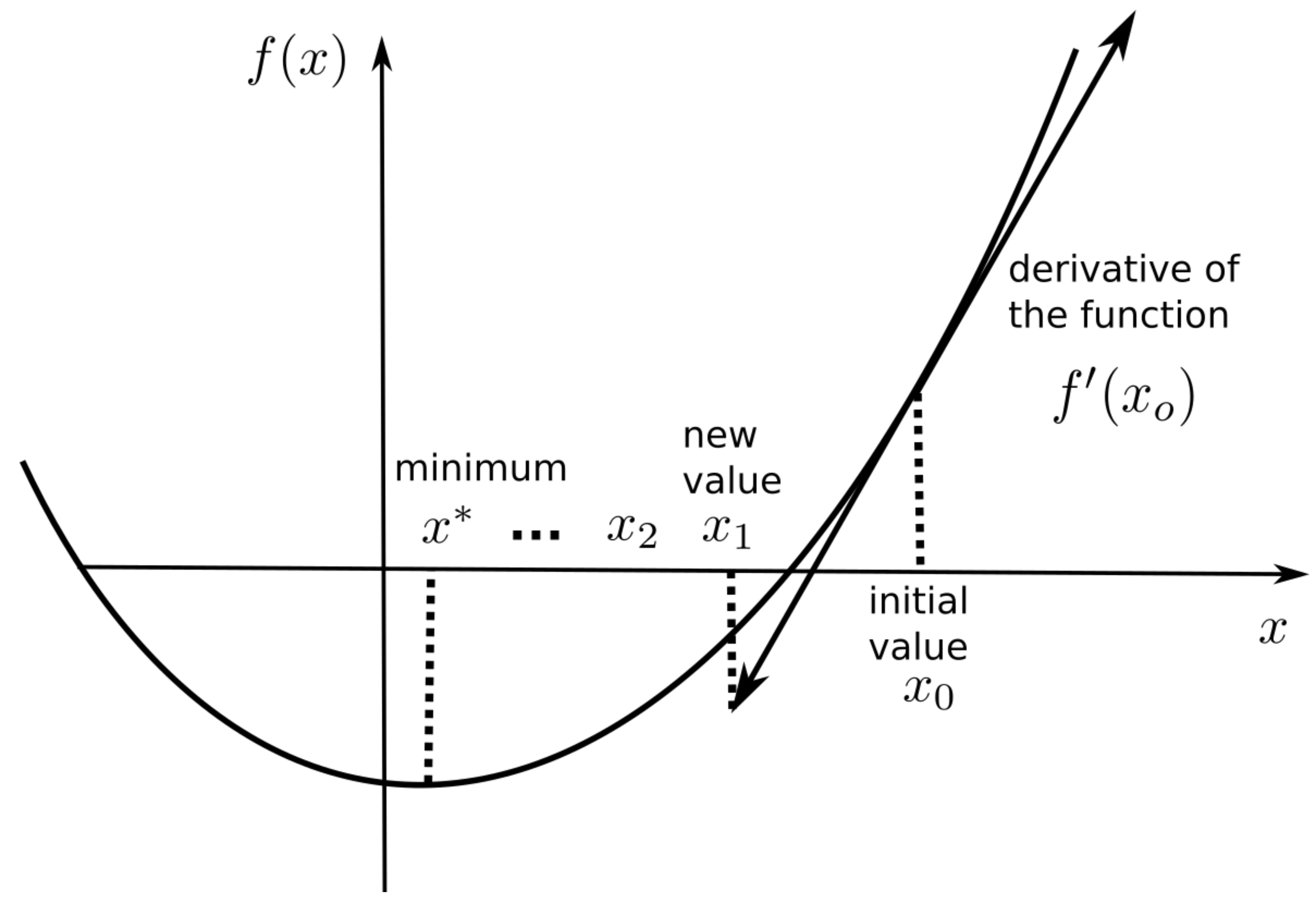
- We therefore want that:

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

- The **change** 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 $[x_0, x_1, x_2, \dots]$ that converge 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:

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

- η is a small parameter between 0 and 1 called the **learning rate**.

Gradient descent

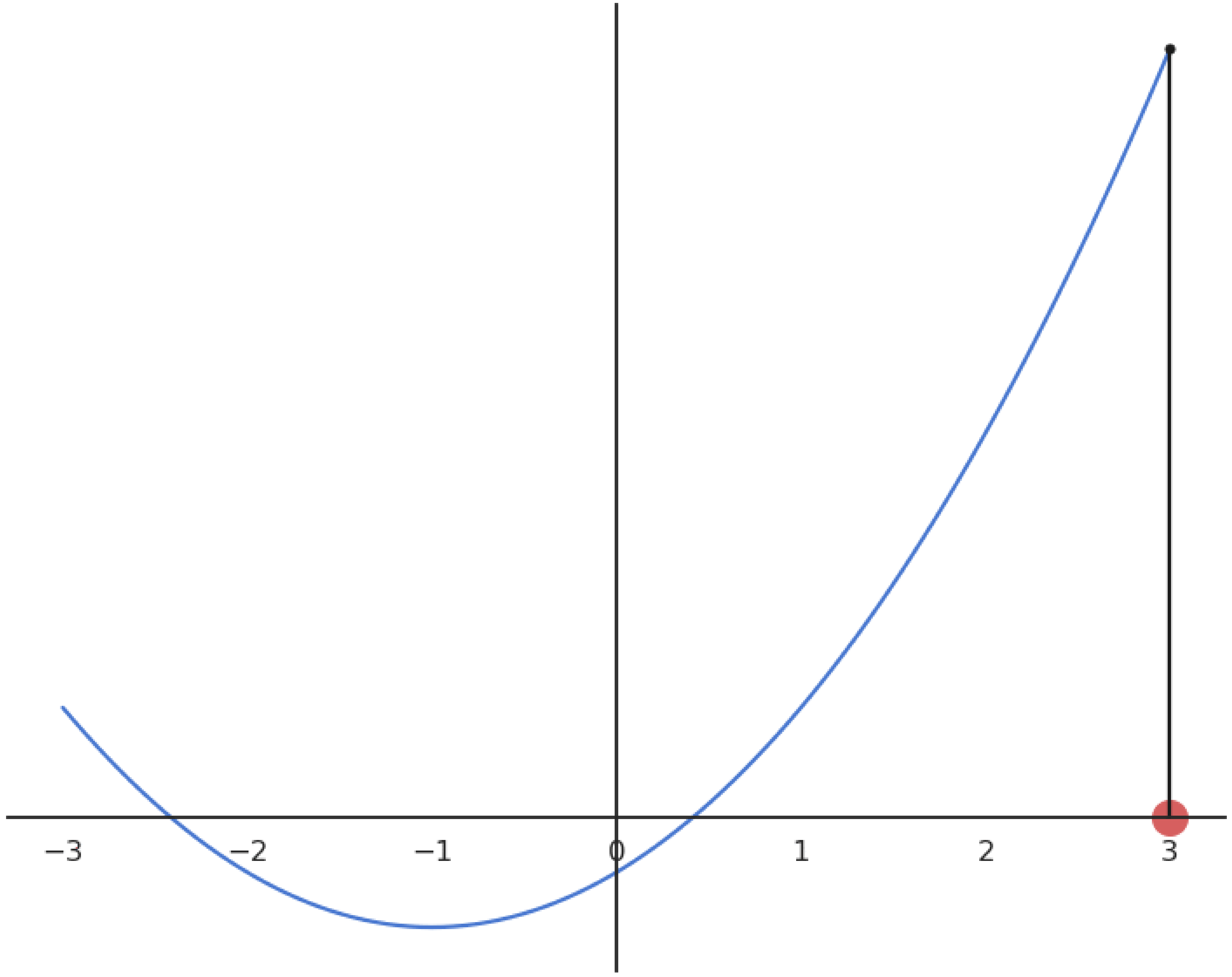
Gradient descent algorithm

- 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 Δx 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:

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

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

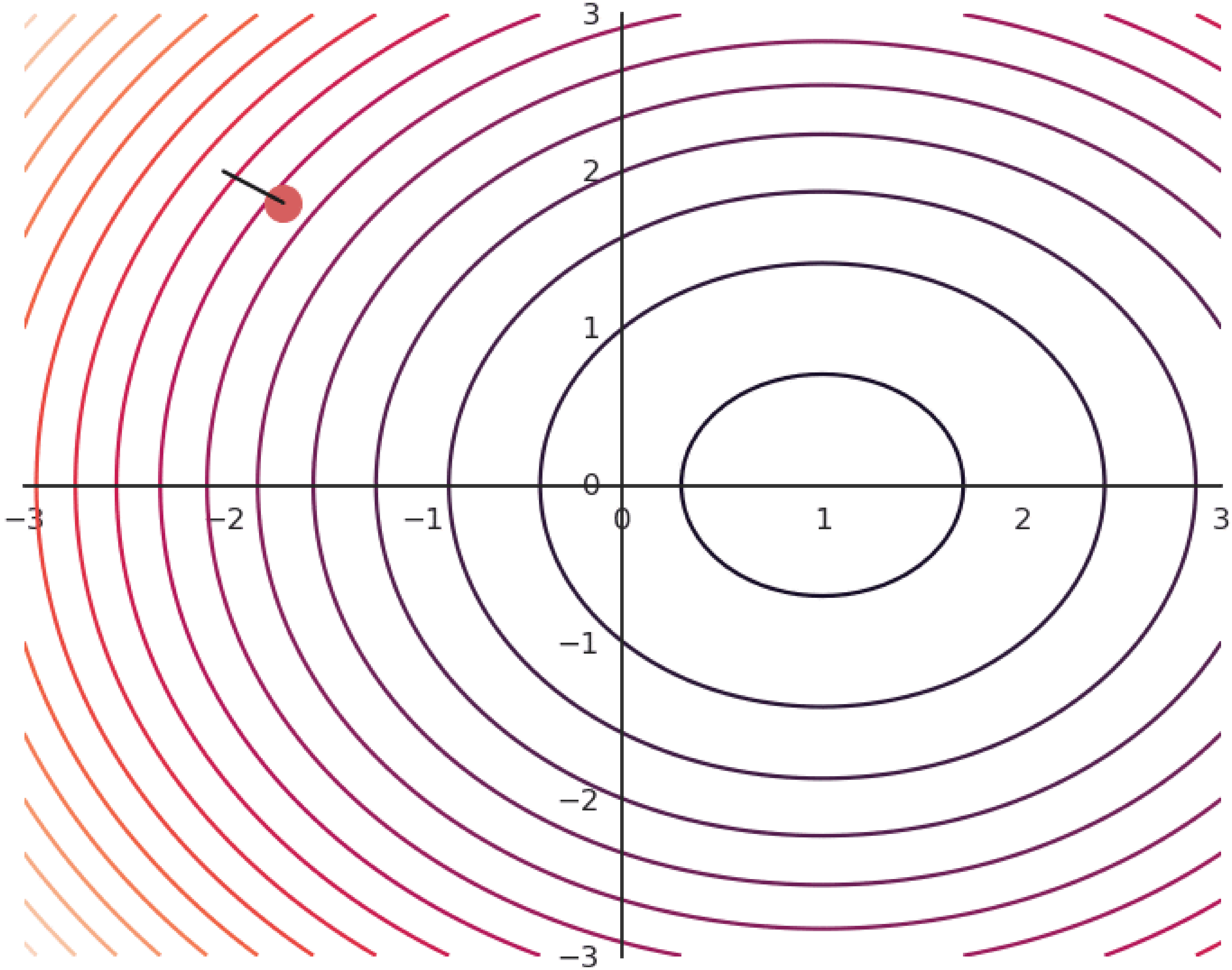
$$\Delta z = z_{n+1} - z_n = -\eta \, \frac{\partial f(x_n, y_n, z_n)}{\partial z}$$

Multivariate Gradient descent

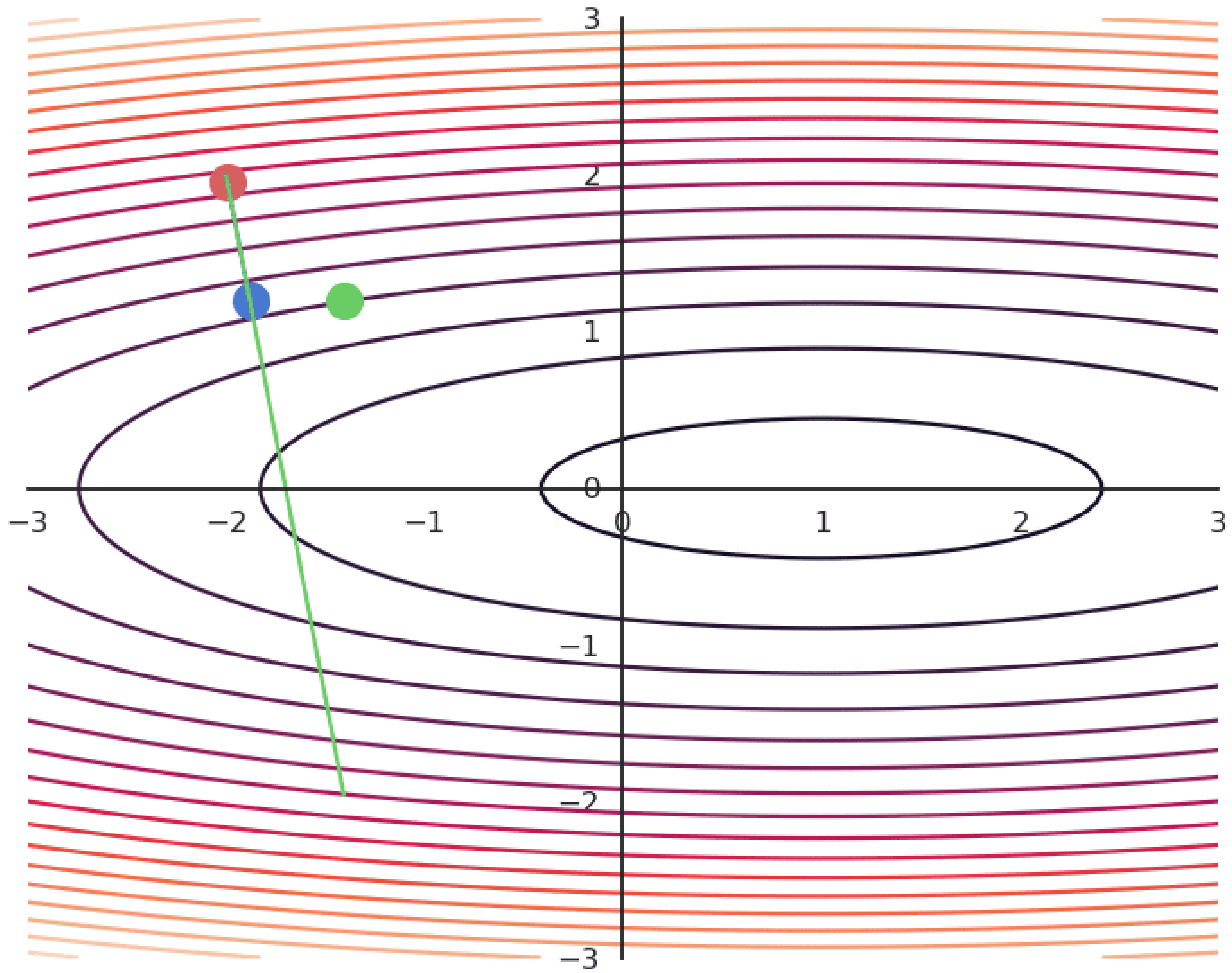
- We can also use the vector notation to use the **gradient operator**:

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

Multivariate gradient descent

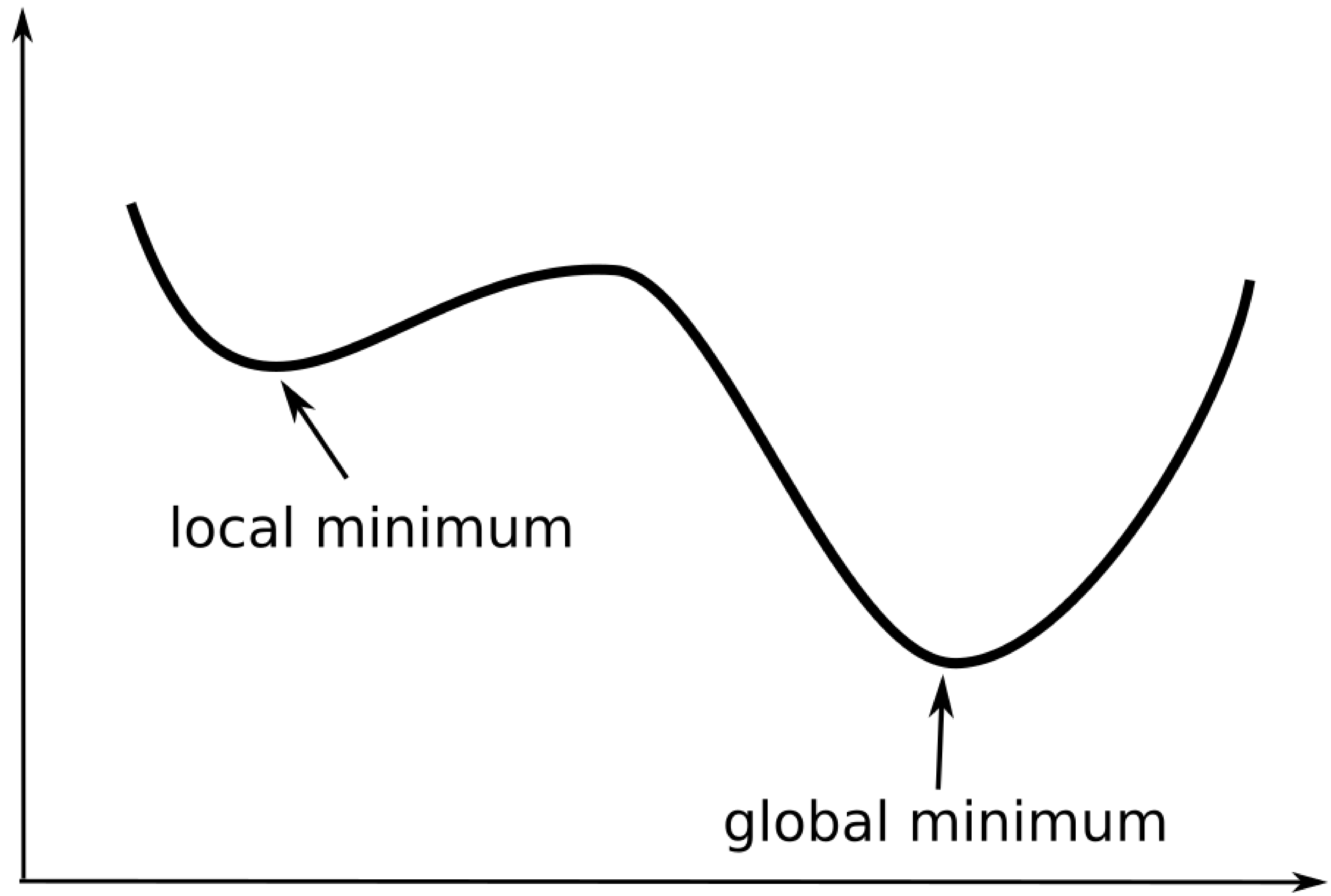


Influence of the learning rate



- The parameter η is called the learning rate (or step size) and regulates the speed of convergence.
- The choice of the learning rate η 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

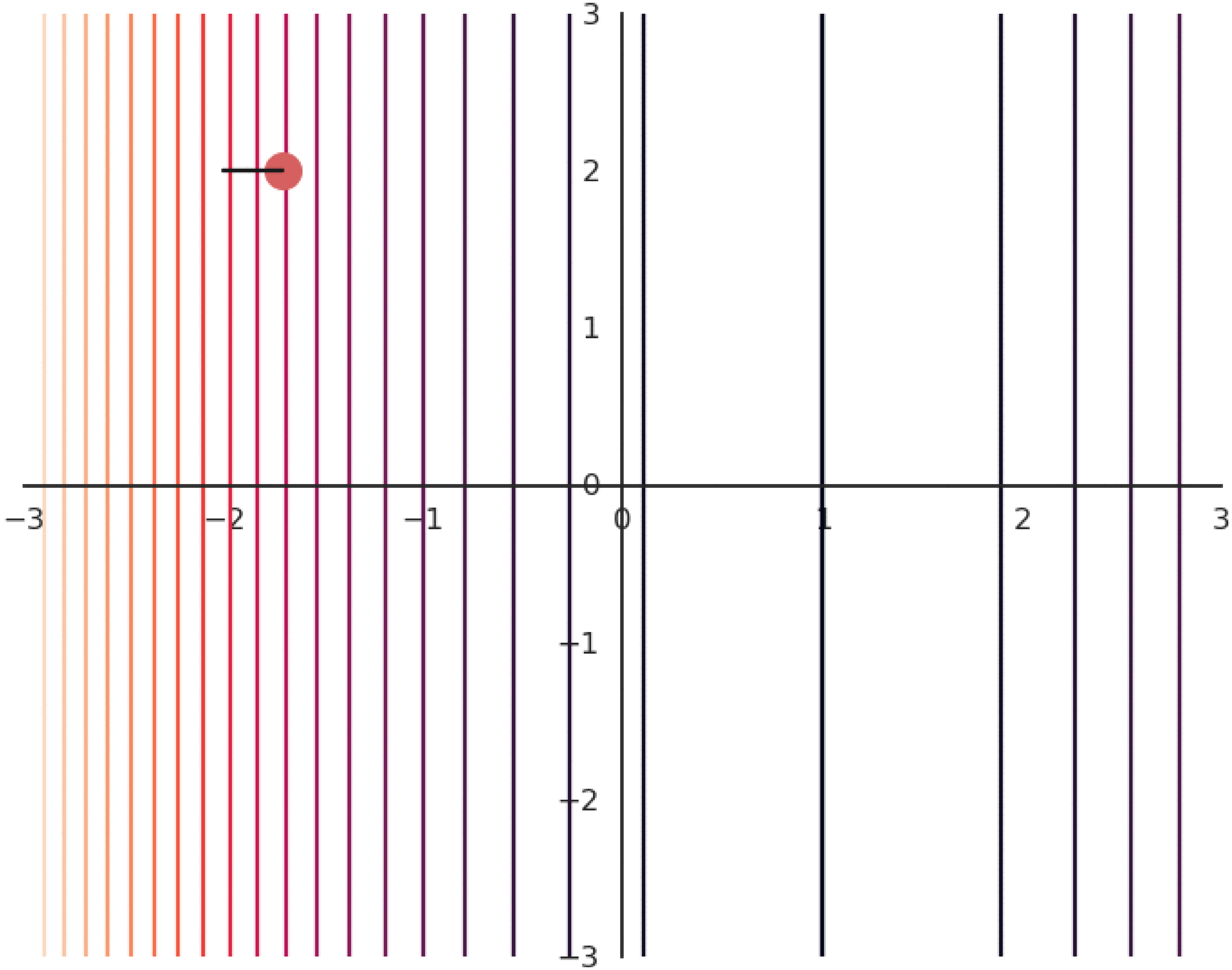
Regularization

- 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** λ:

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

L2 - Regularization

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

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

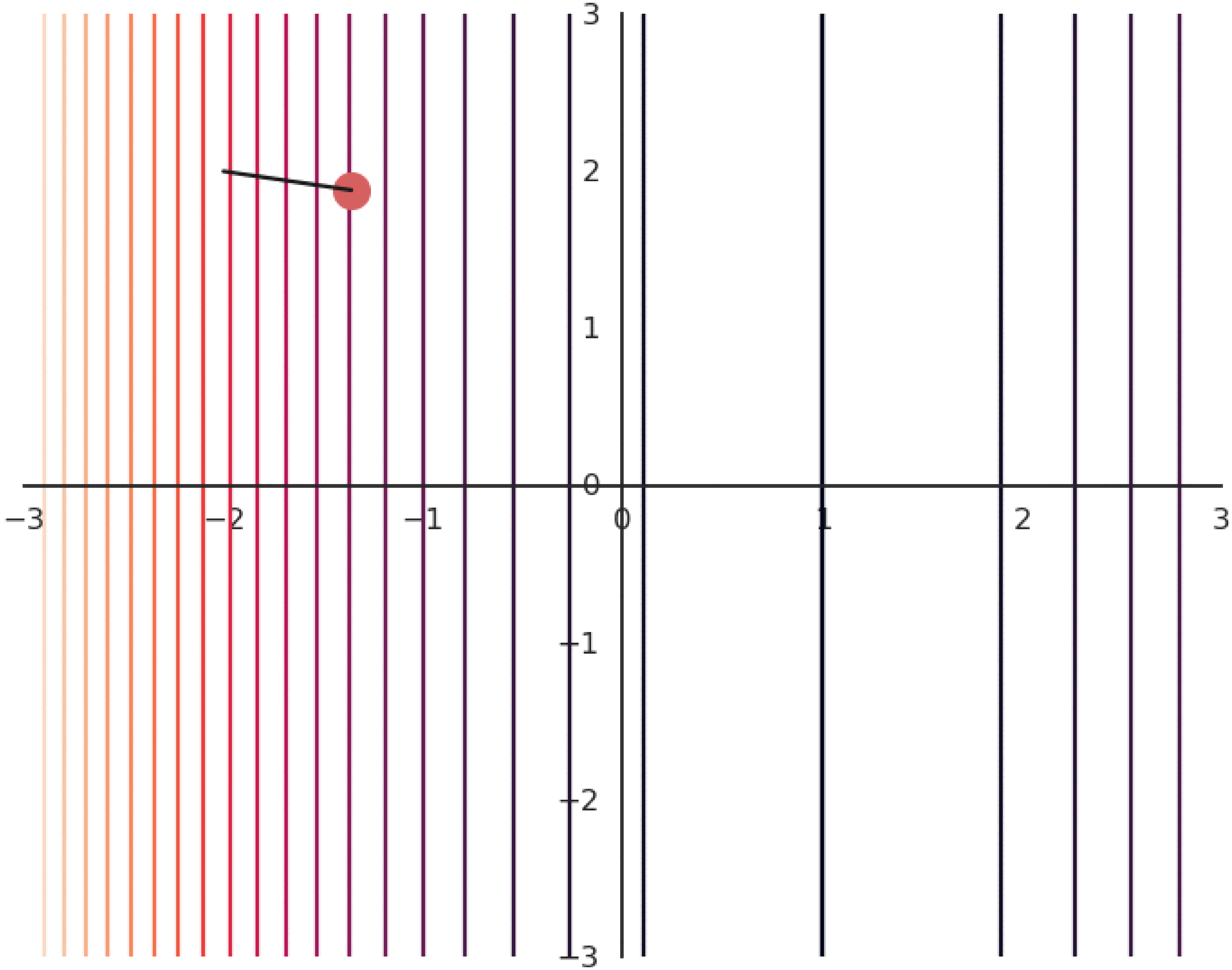
- We just need to compute its gradient:

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

and apply gradient descent iteratively:

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

L2 - Regularization

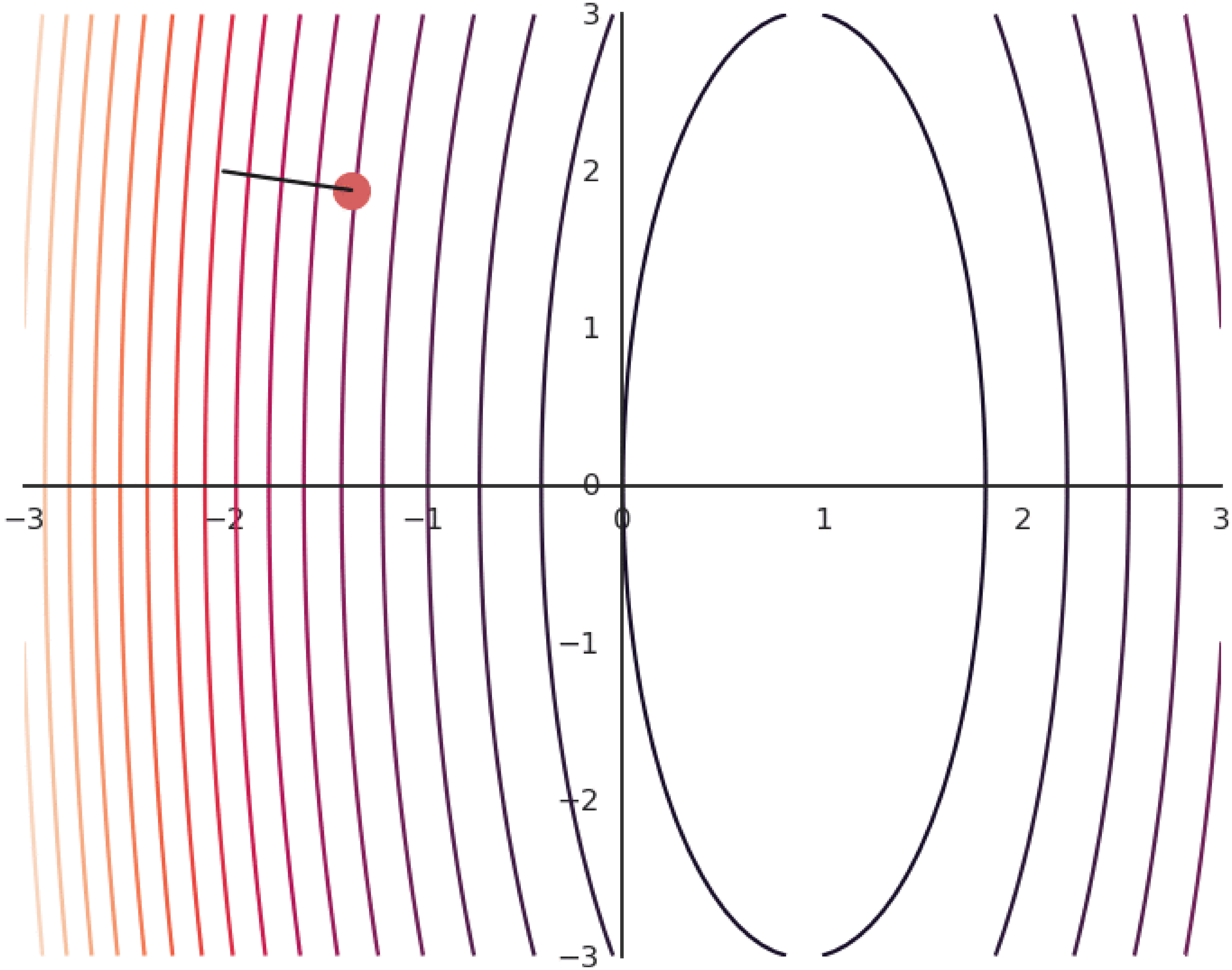


L2 - Regularization

- 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.

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

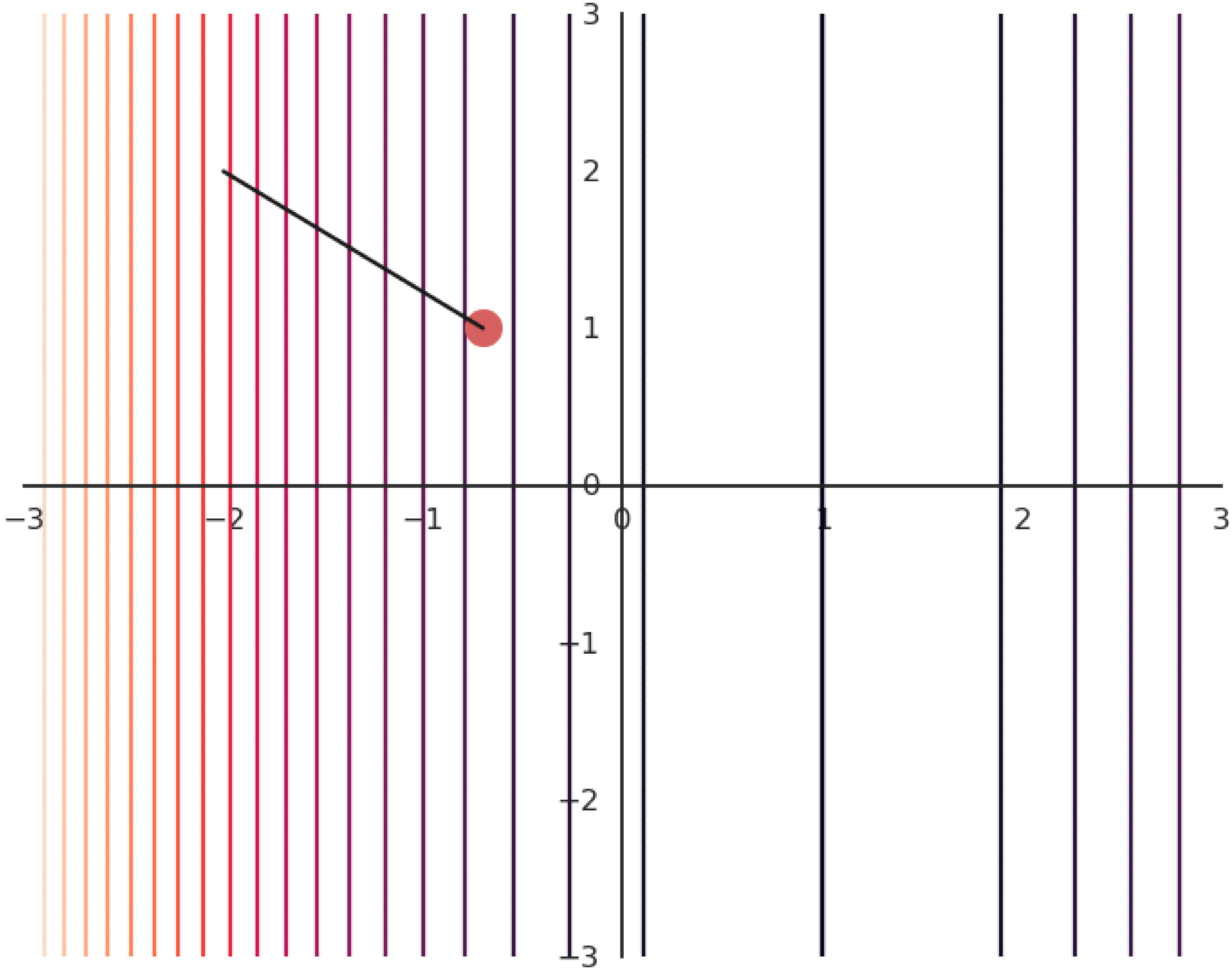
L2 - Regularization



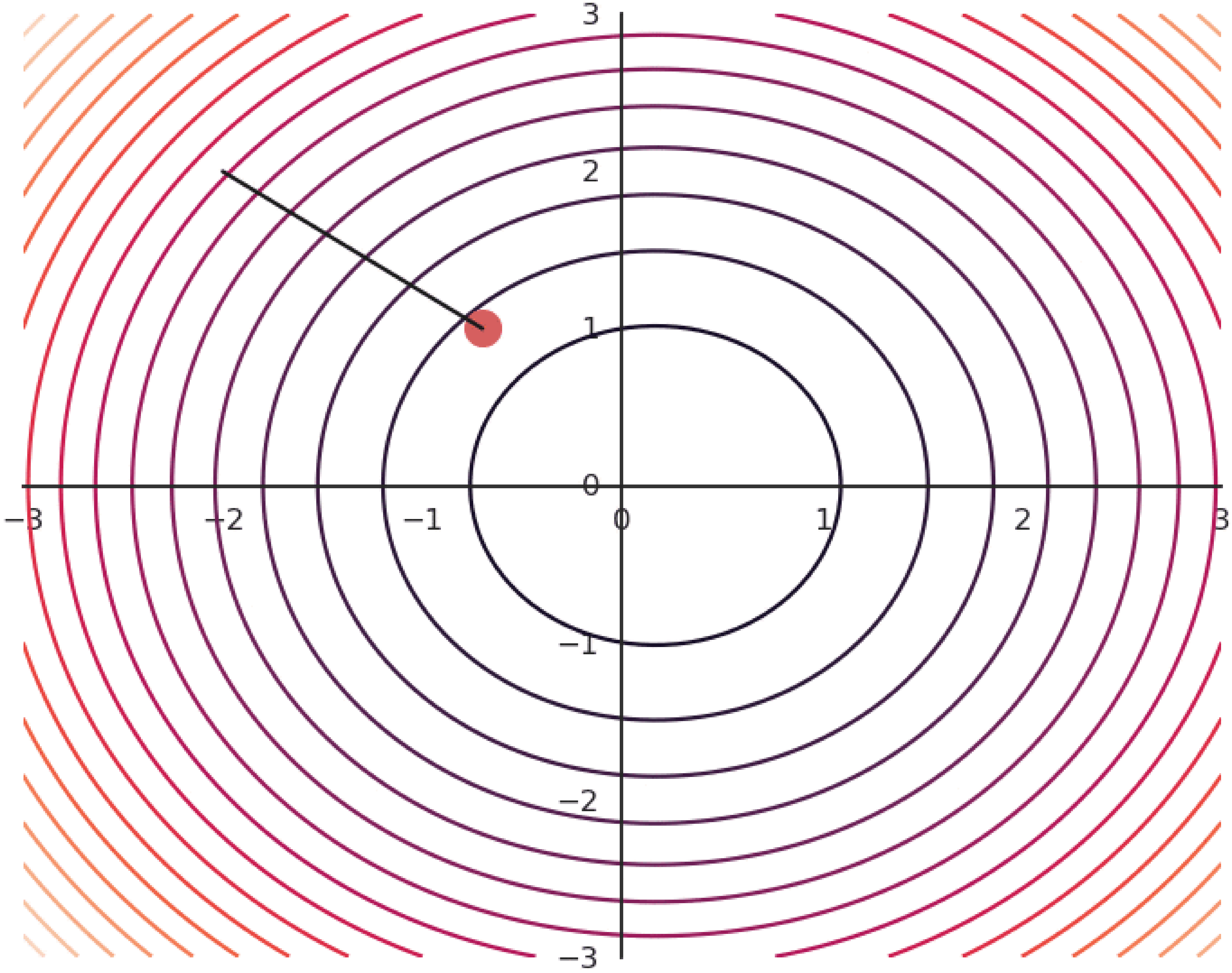
L2 - Regularization

- 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 λ (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.

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

- λ controls which of the two objectives, $f(x, y)$ or $x^2 + y^2$, has the priority:
    - When λ is small, $f(x, y)$ dominates and the norm of $\mathbf{x}$ can be anything.
    - When λ 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 λ 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:

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

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

L1 - Regularization