COMP 414/514: Optimization – Algorithms, Complexity and Approximations

Lecture 2

Overview

$$\min_{x} \quad f(x)$$

$$\text{s.t.} \quad x \in \mathcal{C}$$

- Different objective classes
- Different strategies within each problem
- Different approaches based on computational capabilities
- Different approaches based on constraints

And, always having in mind applications in machine learning, AI and signal processing

Overview

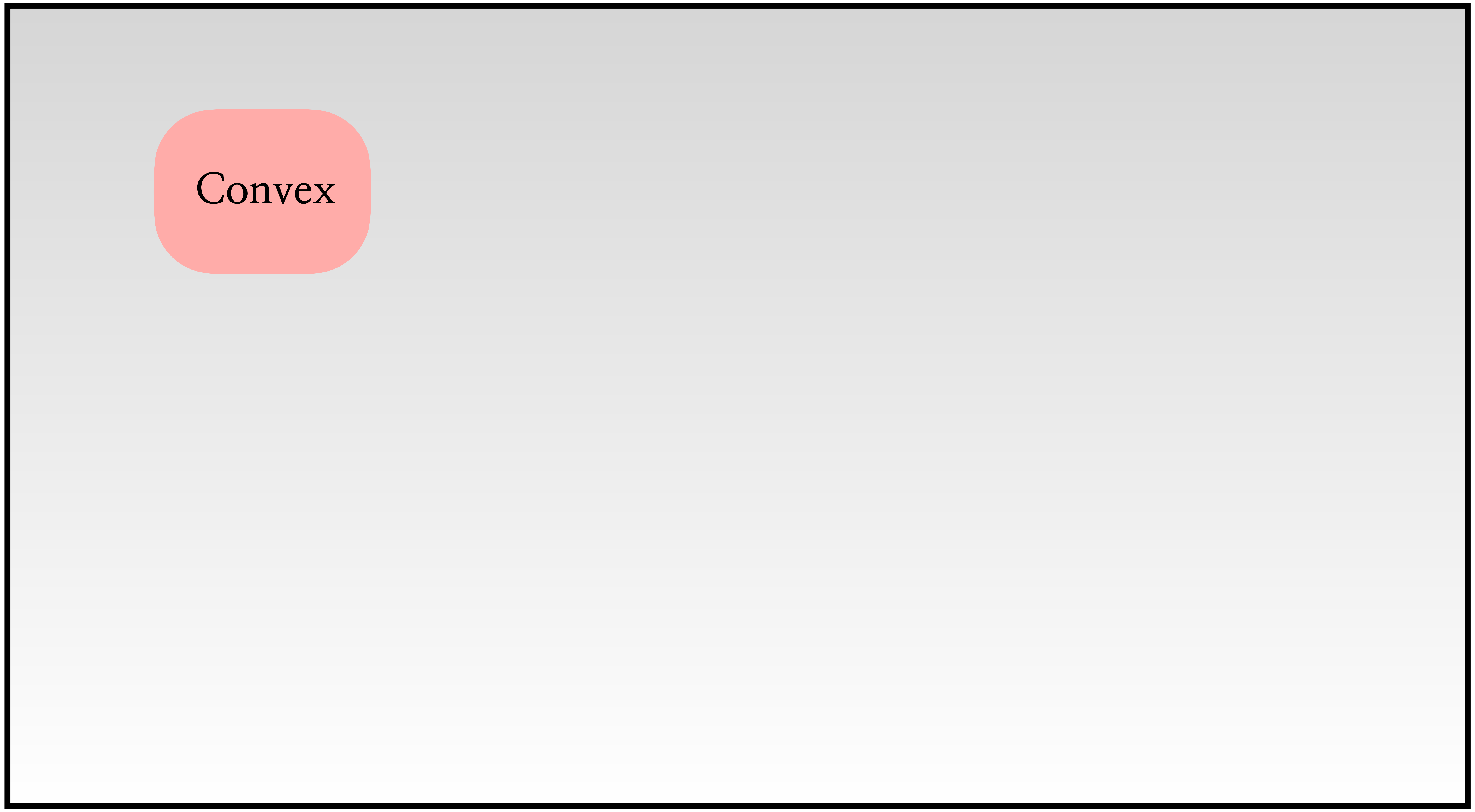
- In the last lecture, we:
    - Introduced some very basic ideas from linear algebra

- In this lecture, we will:
    - Discuss briefly **smooth continuous optimization**
    - Introduce derivatives, Taylor approximation, Lipschitz conditions
    - Discuss about gradient descent, and provide the first **convergence rate**

Convex vs. non−convex optimization

(Naive interpretation of) Space of optimization problems

Convex vs. non−convex optimization



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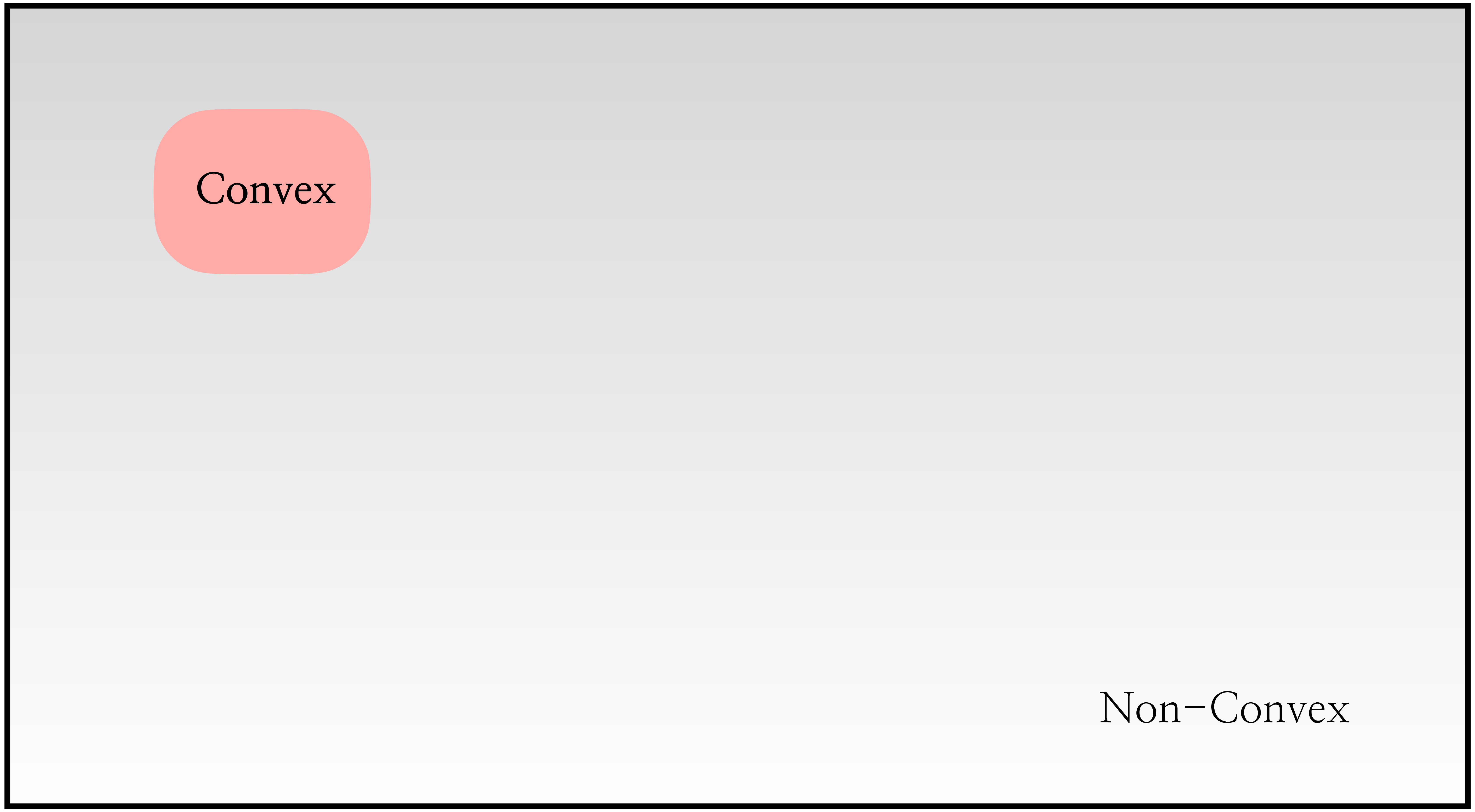

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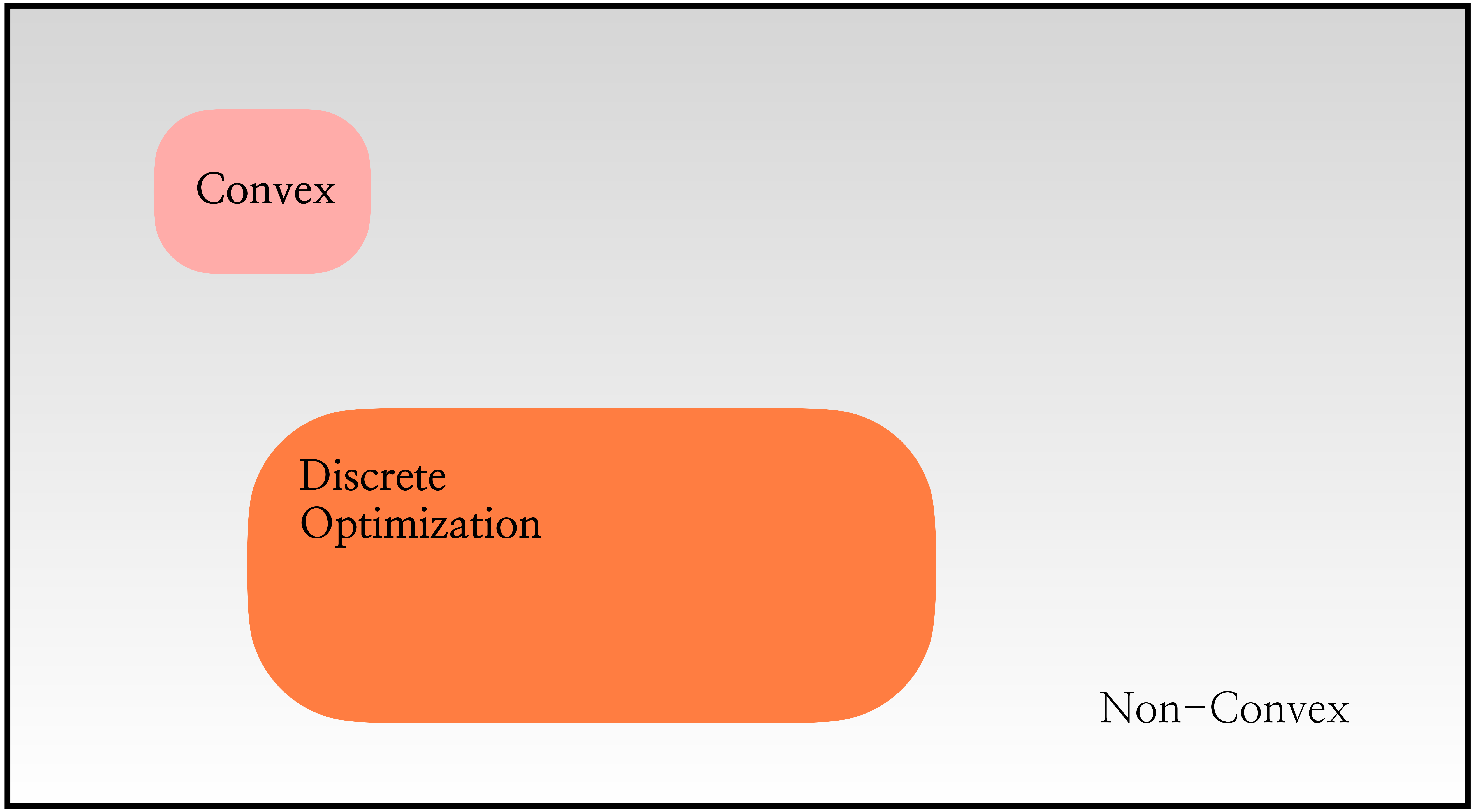

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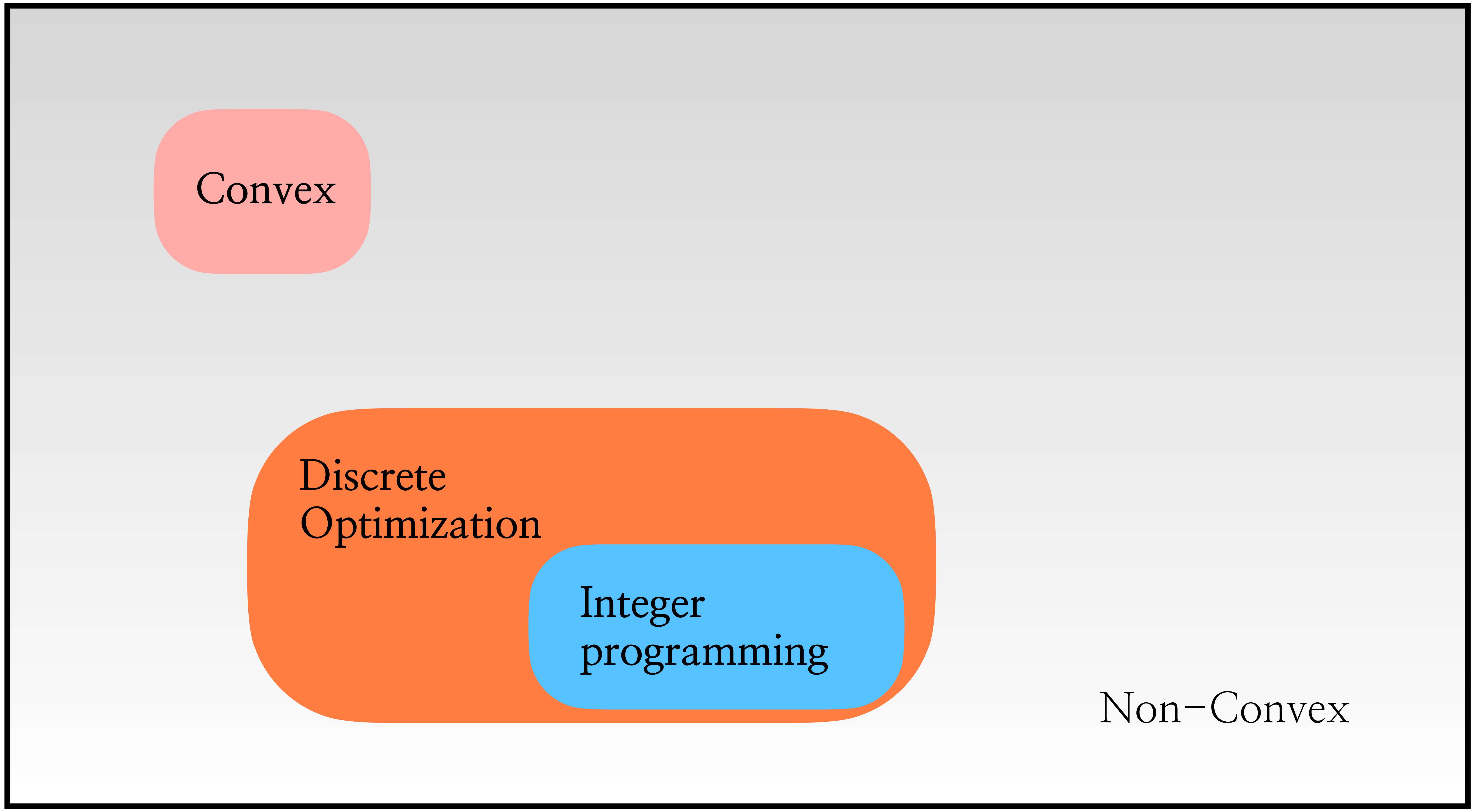

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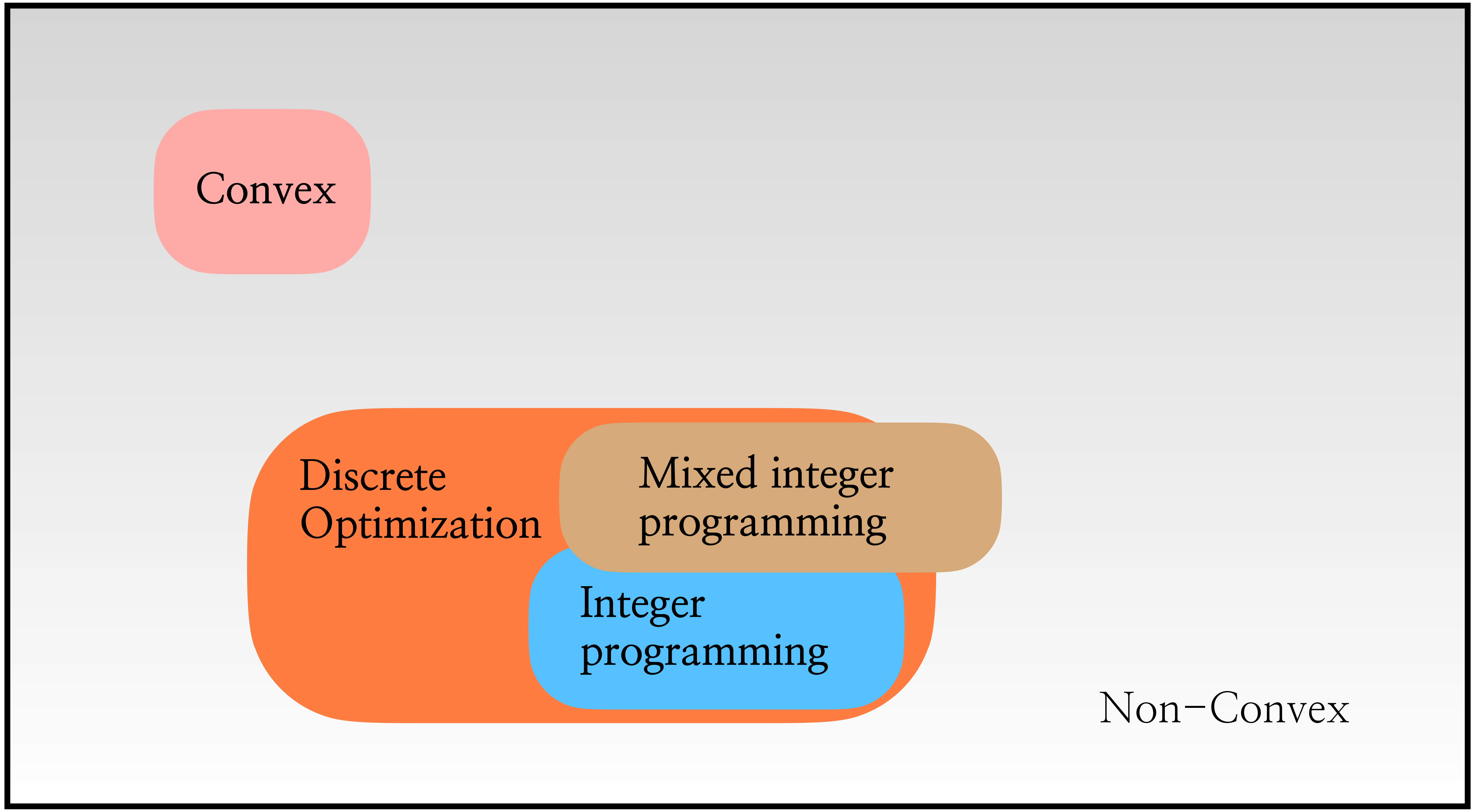

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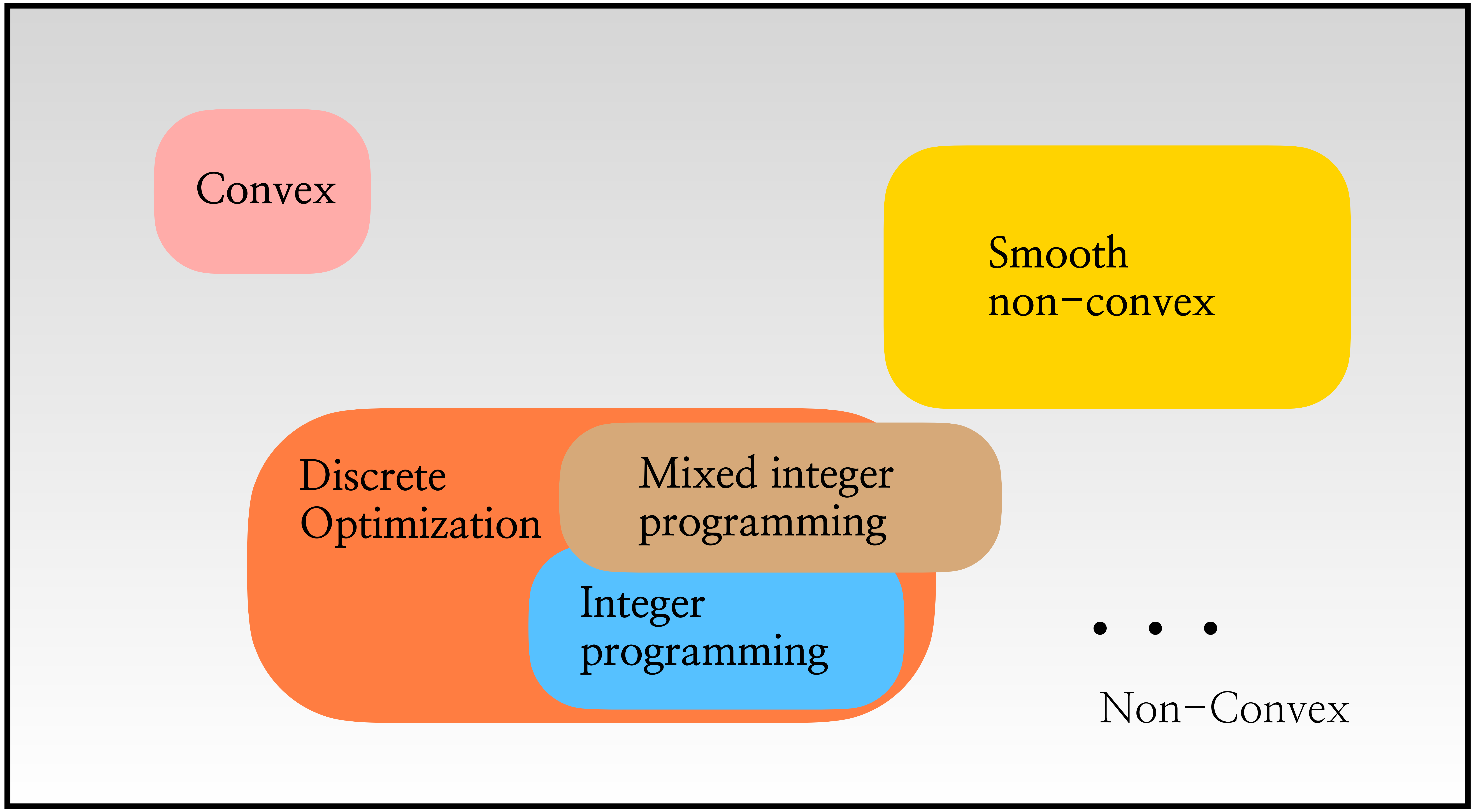

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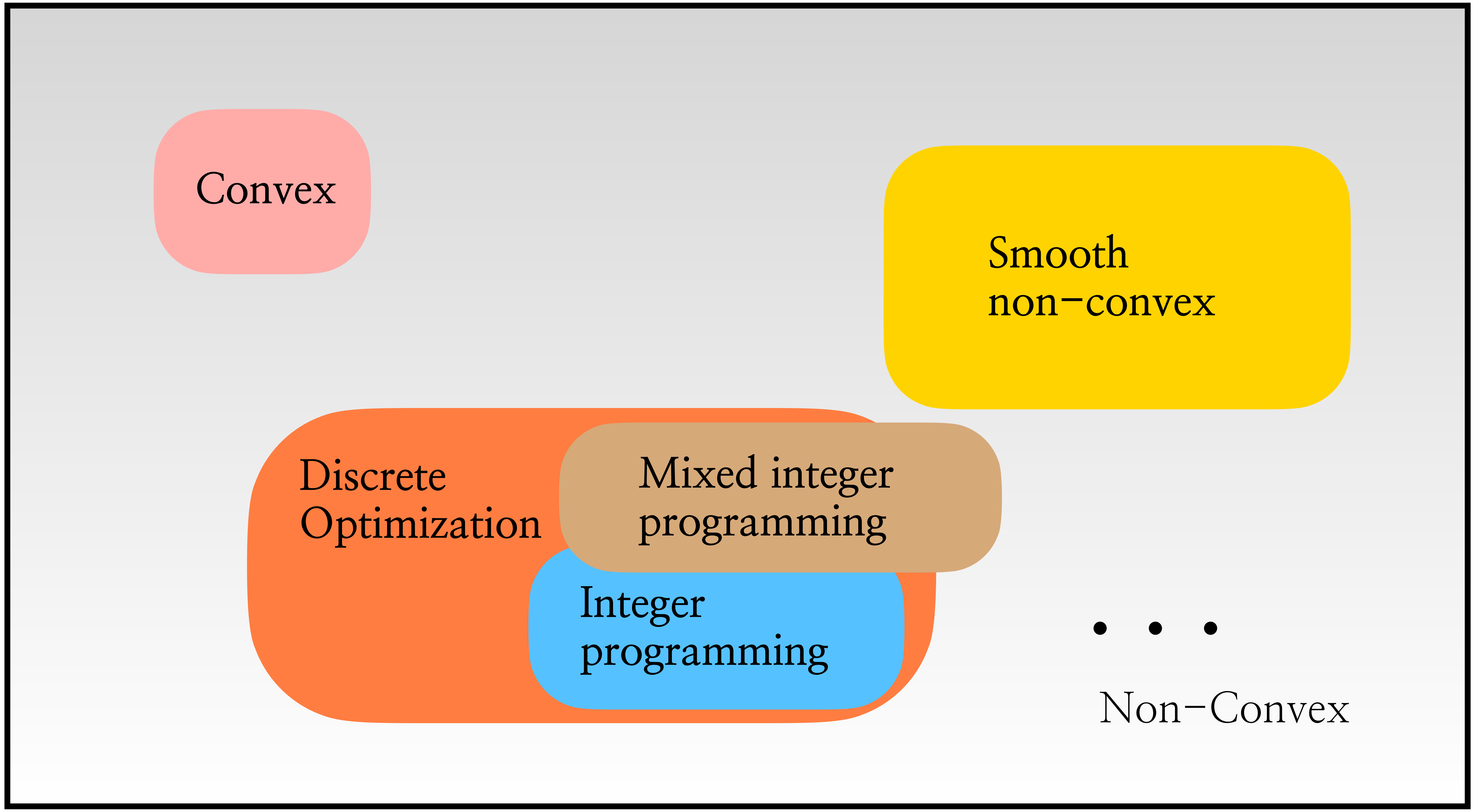

(Naive interpretation of) Space of optimization problems

Derivatives and gradients

– Definition of a **derivative**

$$f : \mathbb{R} \to \mathbb{R} \quad \Bigg| \quad \frac{\partial f}{\partial x} = f'(x) = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

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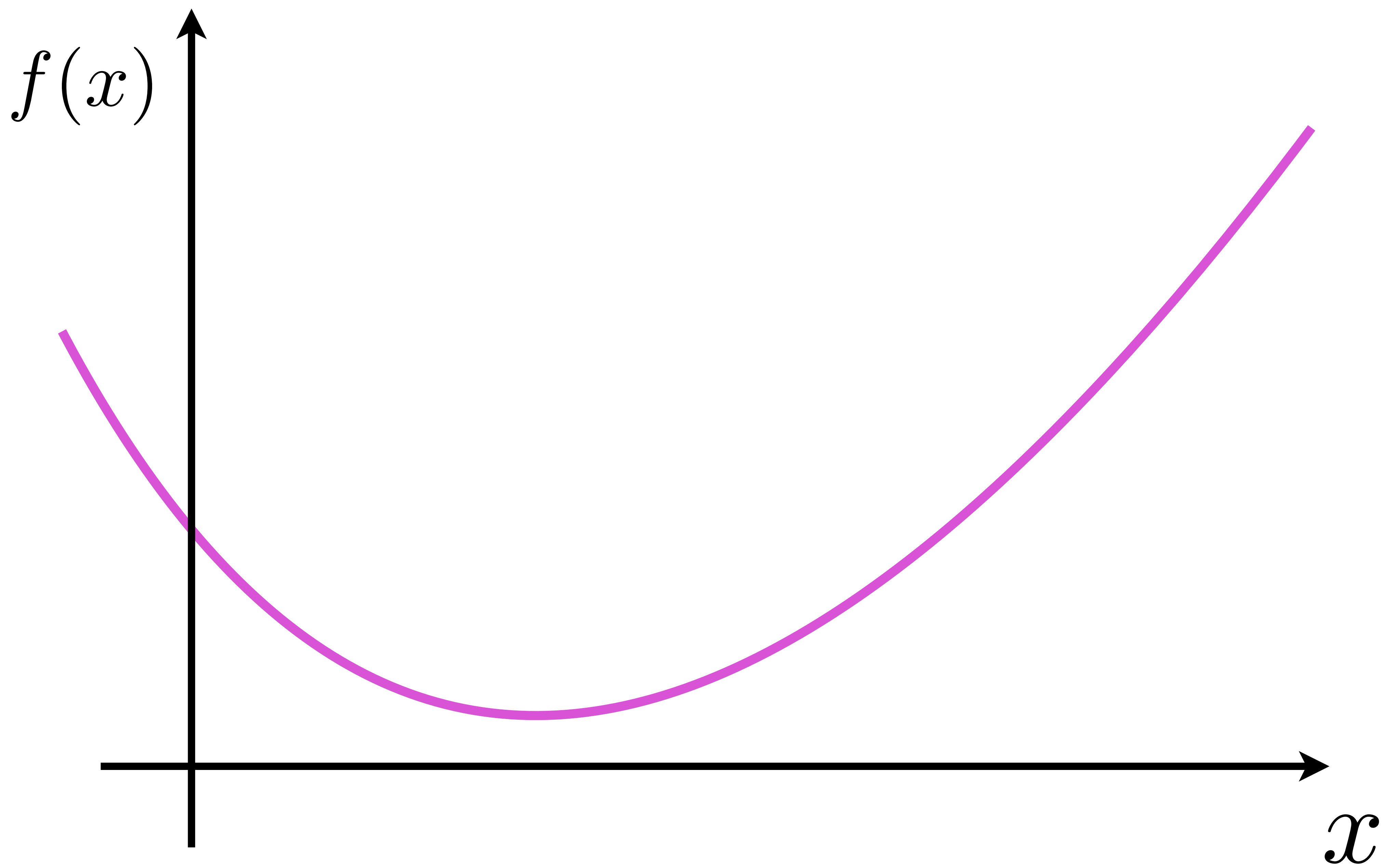

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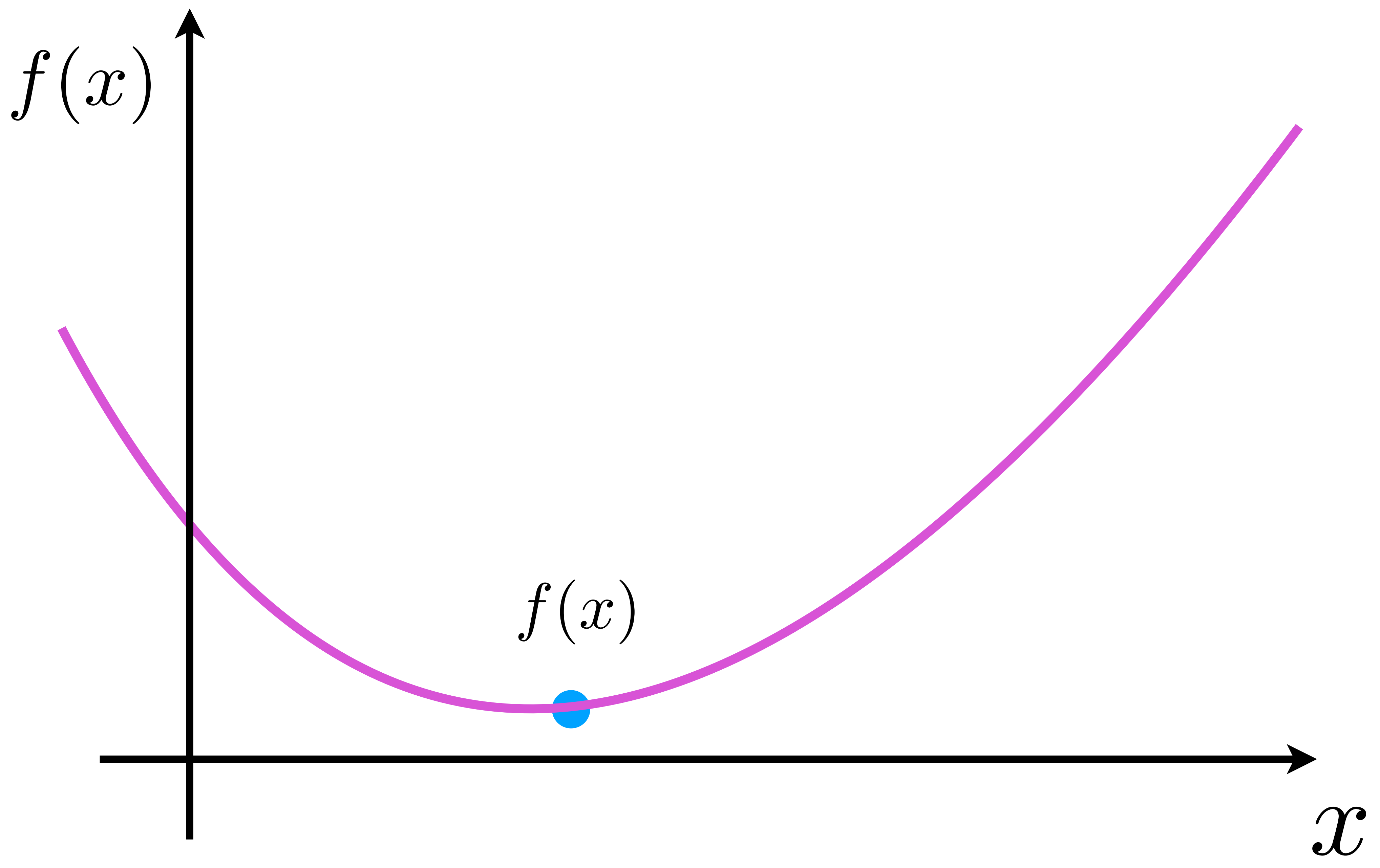

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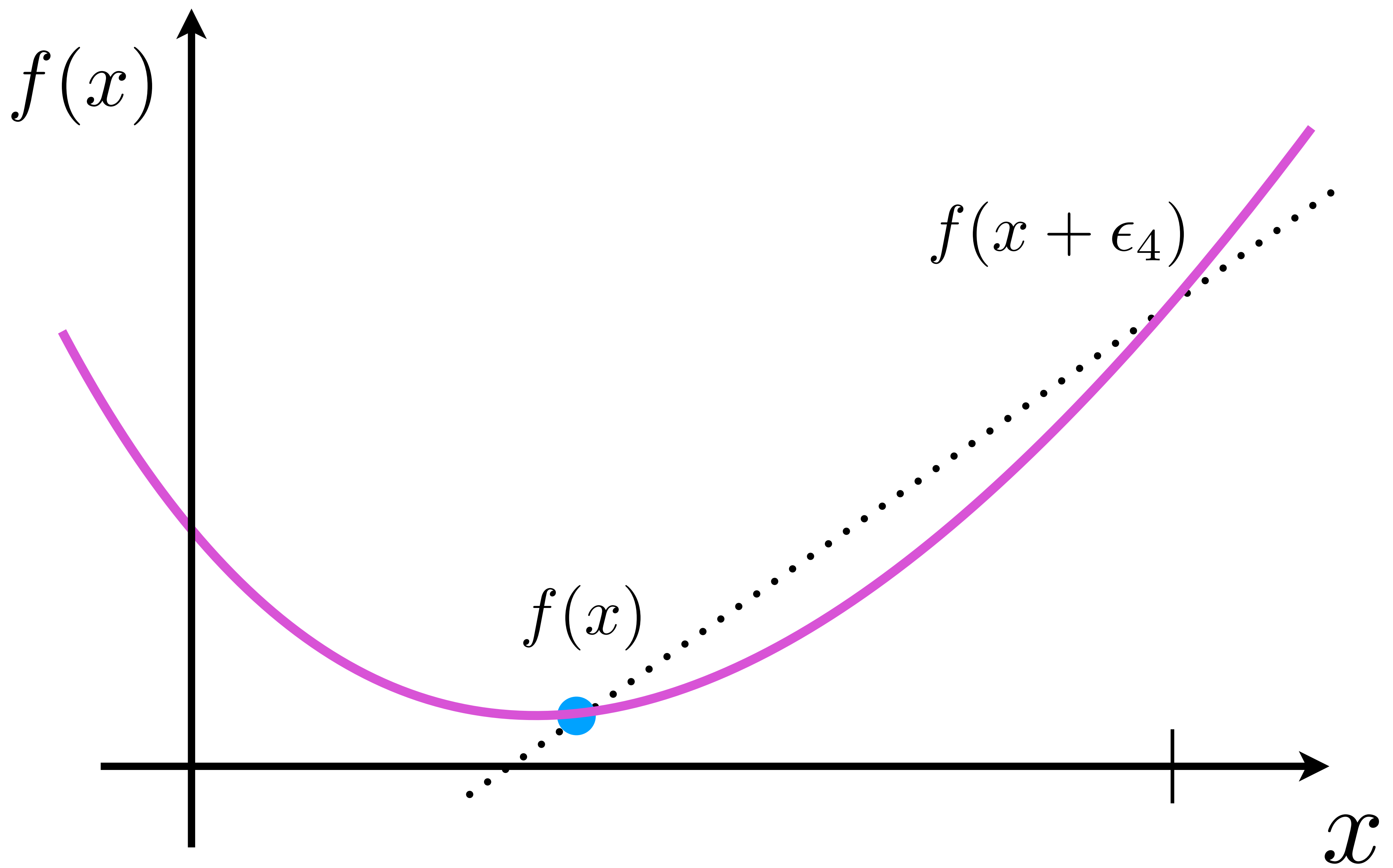

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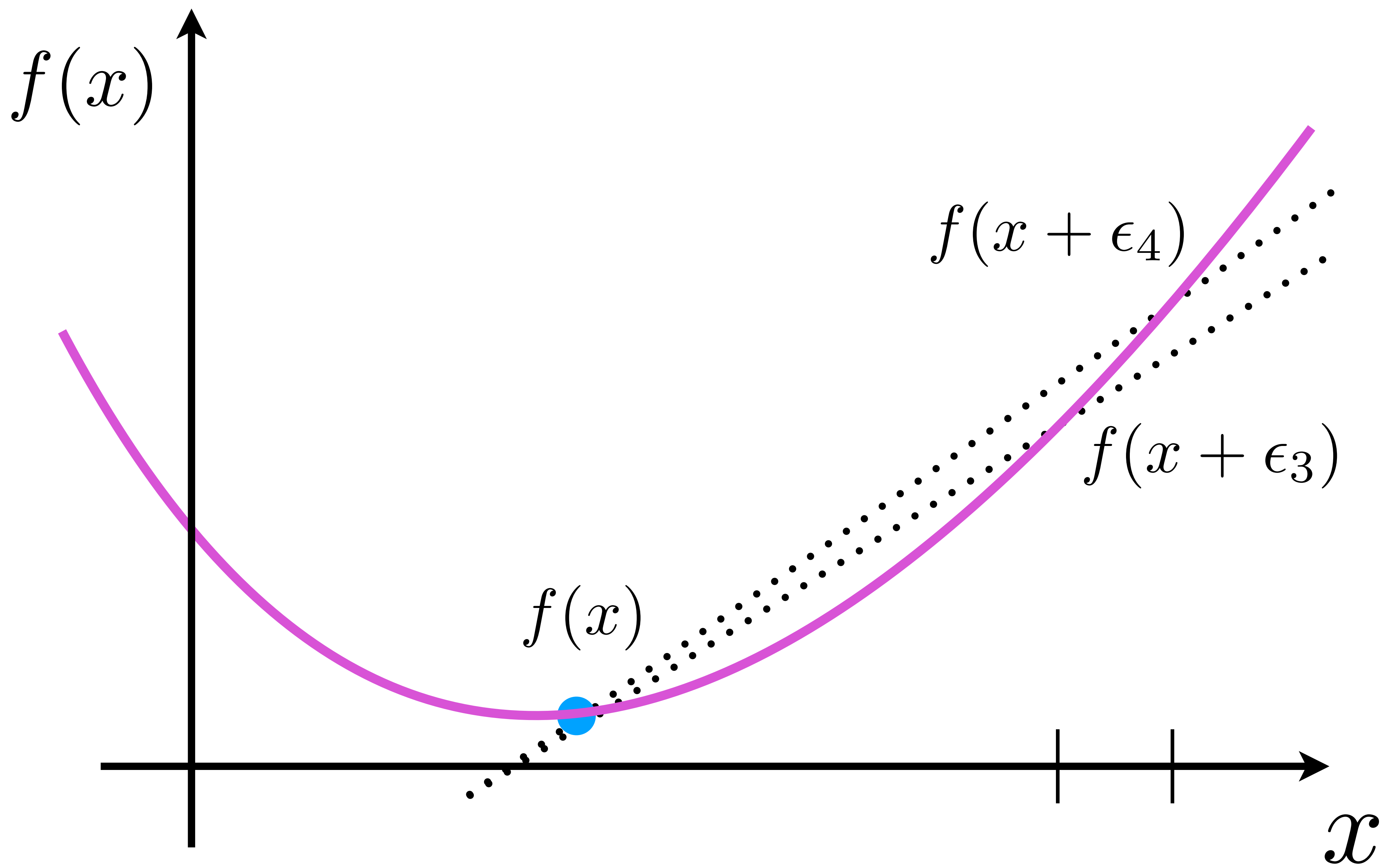

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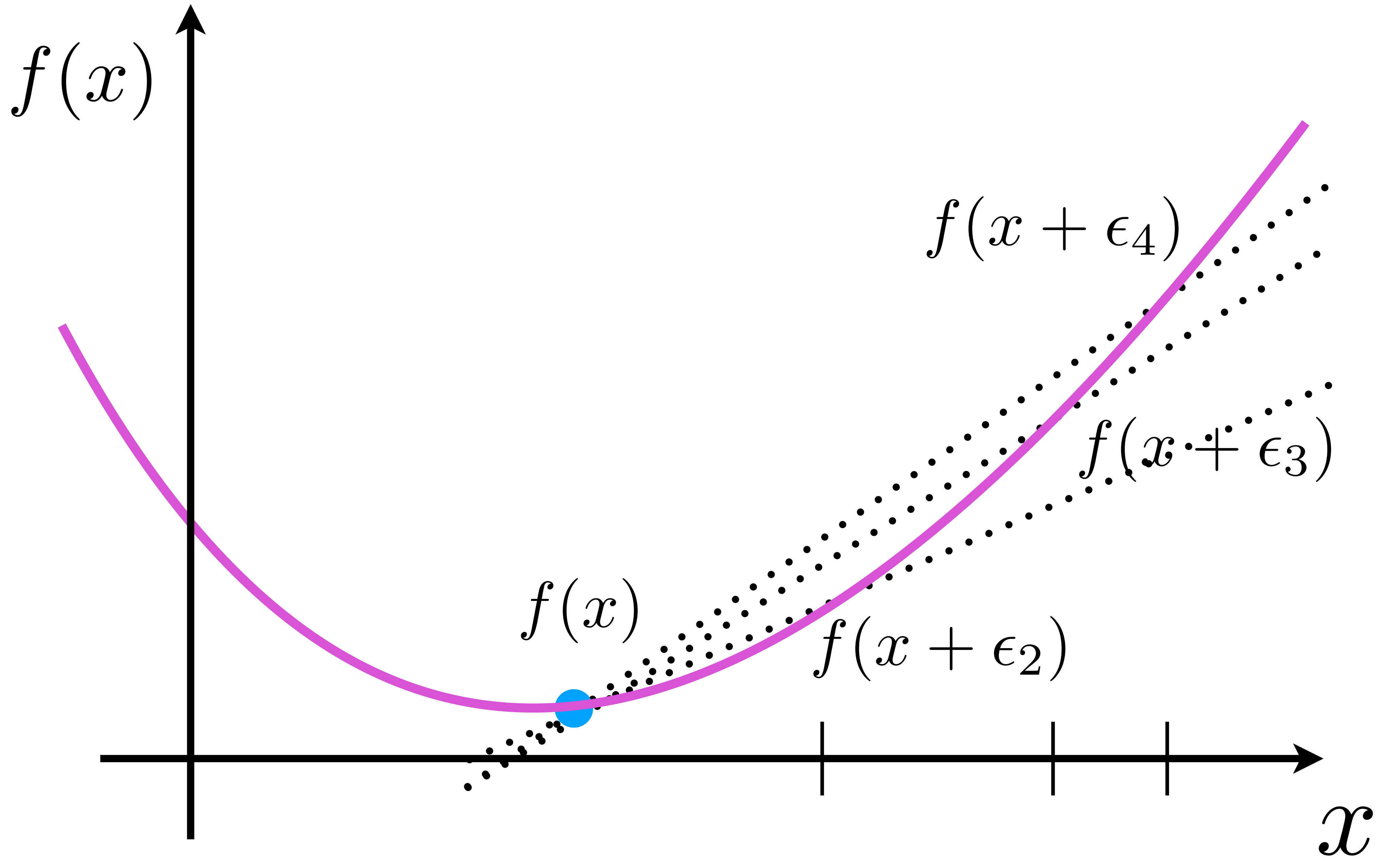

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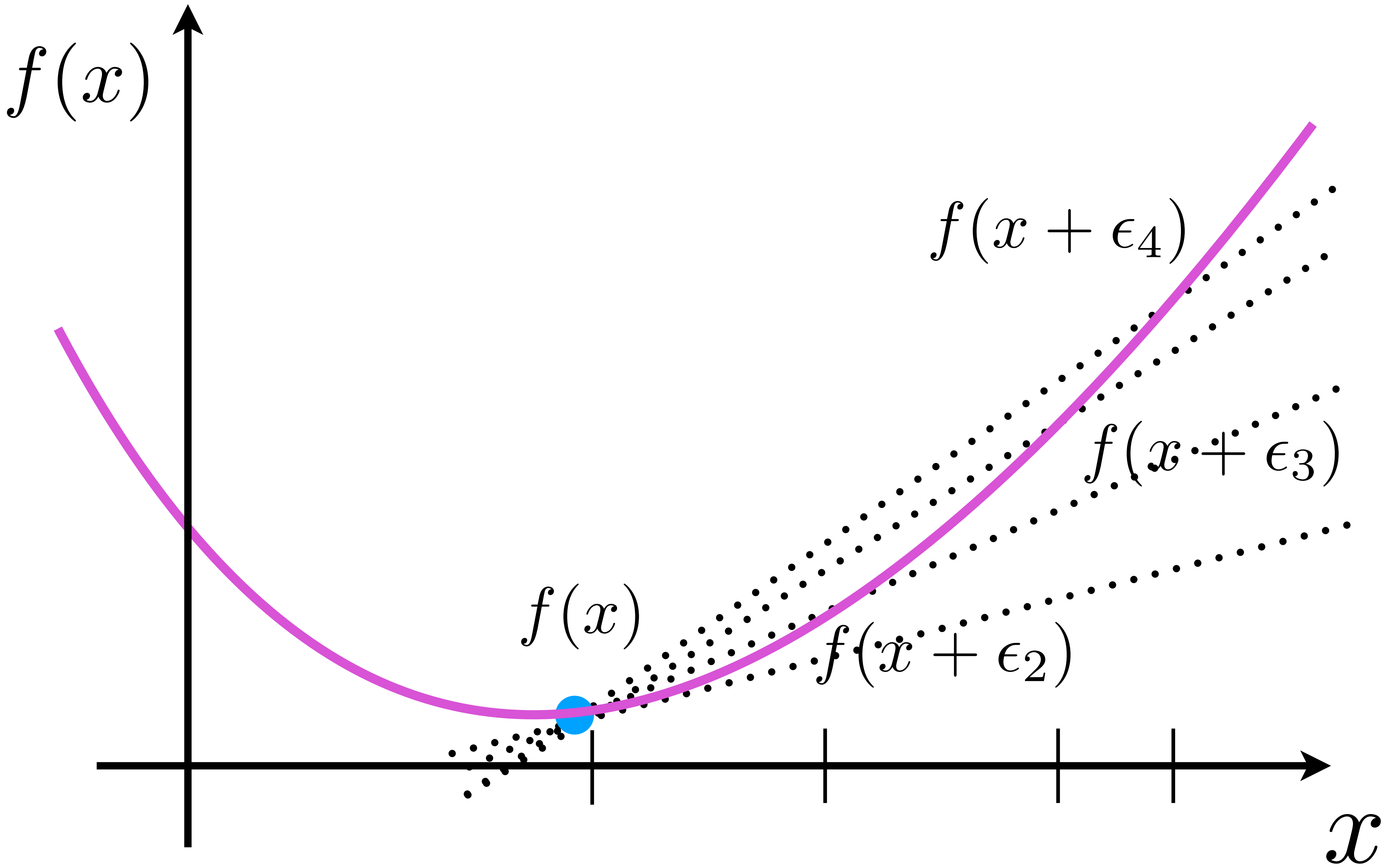

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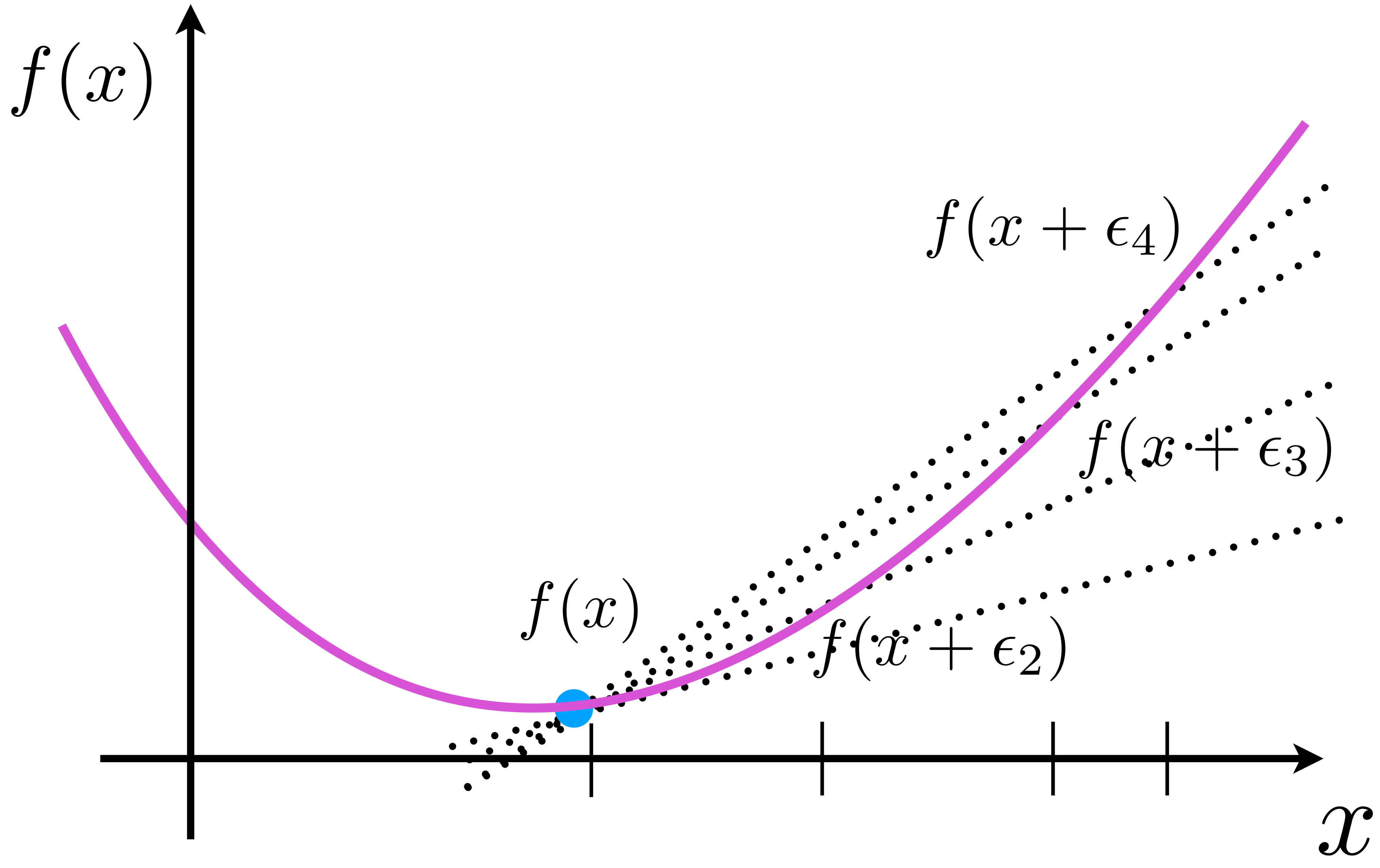

Represents the rate that function changes

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Represents the local curvature:
How the slope of the function changes

Derivatives and gradients

– Generalization to multiple components: **gradient**

$$f : \mathbb{R}^p \to \mathbb{R} \qquad \Big| \qquad \nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_p} \end{bmatrix} \in \mathbb{R}^p$$

where

$$\frac{\partial f}{\partial x_i} = \lim_{\epsilon \to 0} \frac{f(x_1, \ldots, x_{i-1}, x_i + \epsilon, x_{i+1}, \ldots, x_p) - f(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_p)}{\epsilon} = \frac{f(x + \epsilon e_i) - f(x)}{\epsilon}$$

Derivatives and gradients

– **Jacobian** matrix (relates to neural networks)

$$f : \mathbb{R}^p \to \mathbb{R}^m \quad \Big| \quad Df(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_p} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_p} \end{bmatrix} \in \mathbb{R}^{m \times p}$$

– Generalizes the notion of gradient to multiple–output functions

Derivatives and gradients

– **Hessian** matrix

$$f : \mathbb{R}^p \to \mathbb{R} \qquad \Bigg| \qquad \nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_p} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_p} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_p x_1} & \frac{\partial^2 f}{\partial x_p \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_p^2} \end{bmatrix} \in \mathbb{R}^{p \times p}$$

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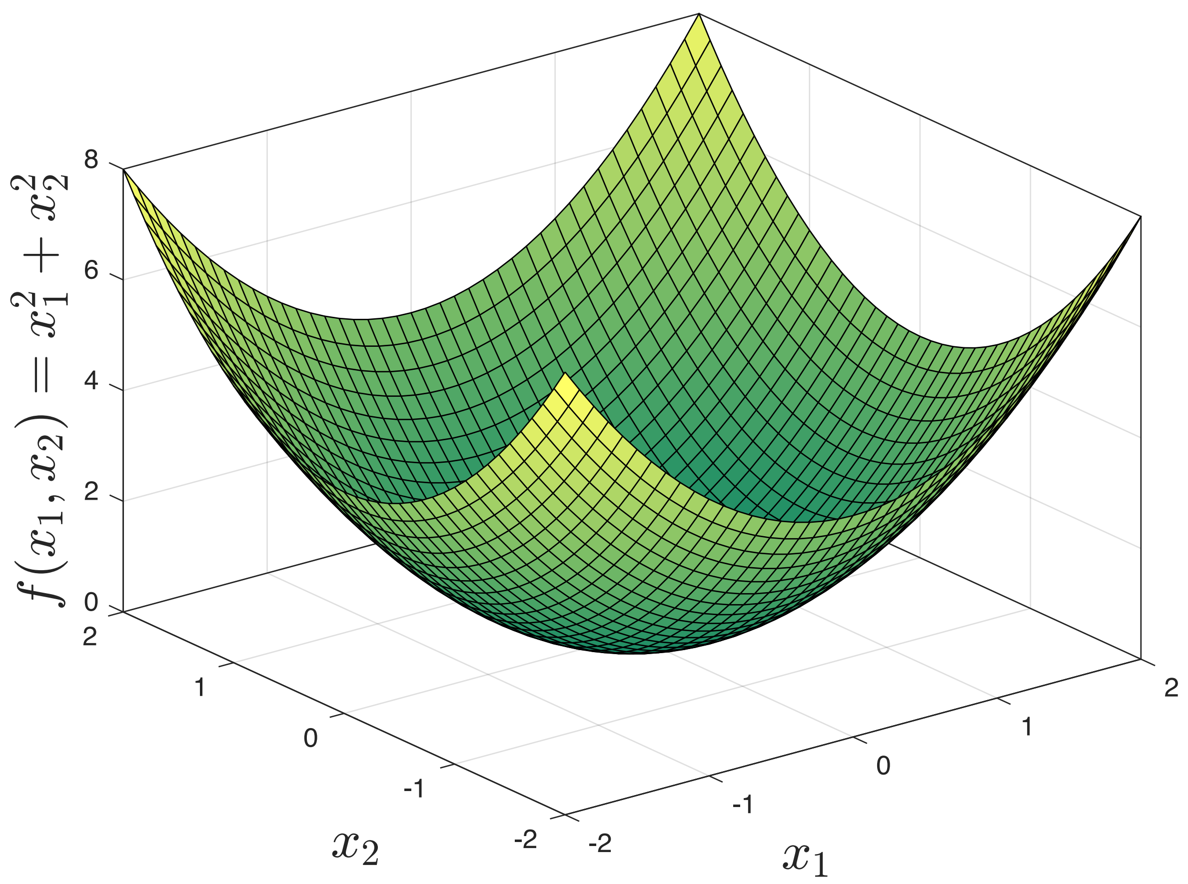
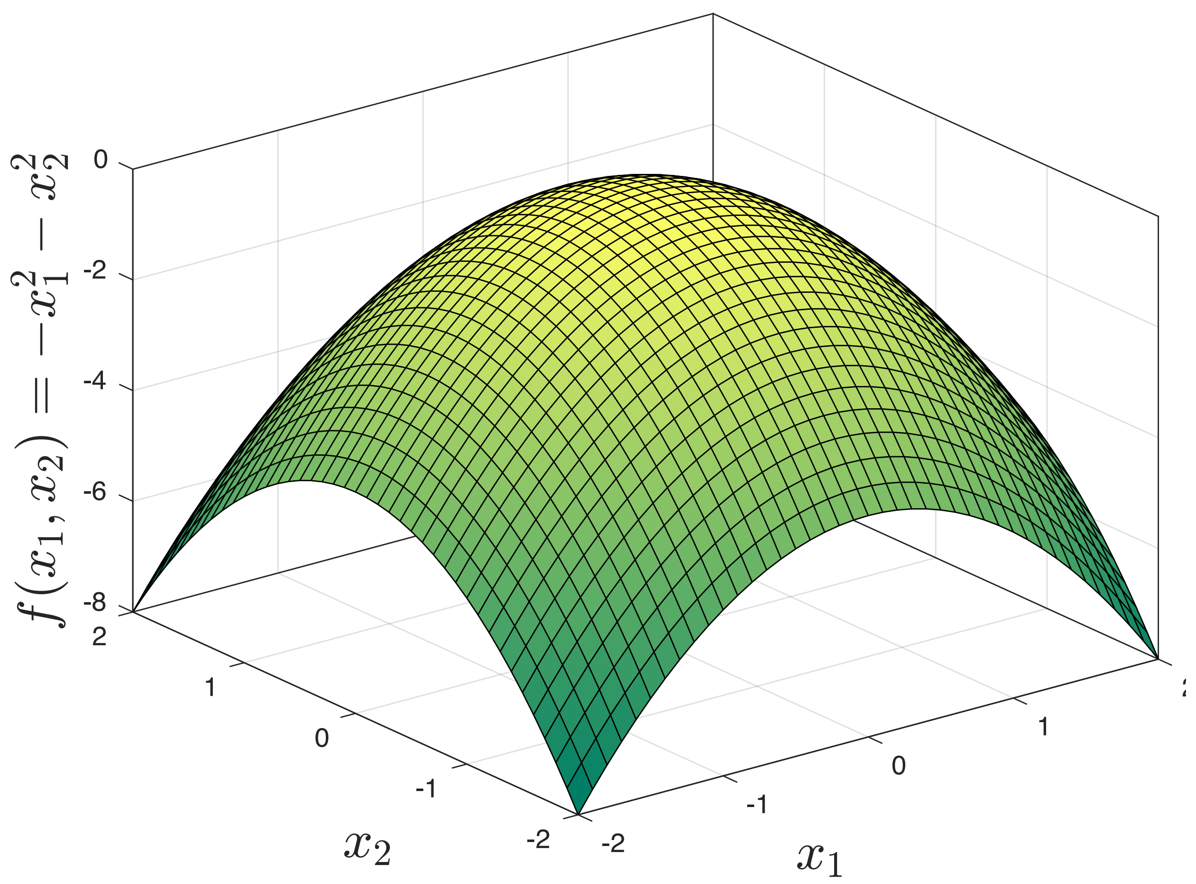


$\nabla^2 f(\cdot) \succ 0$



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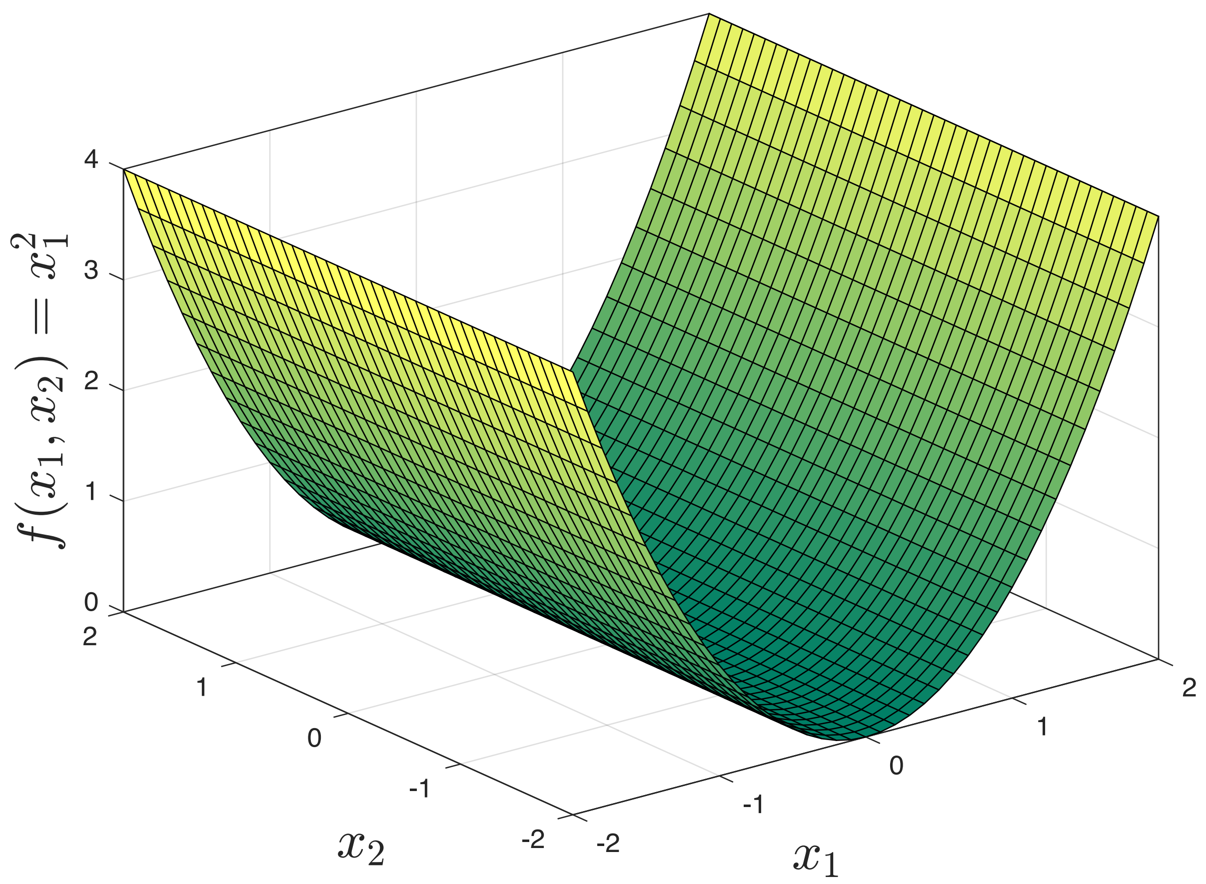

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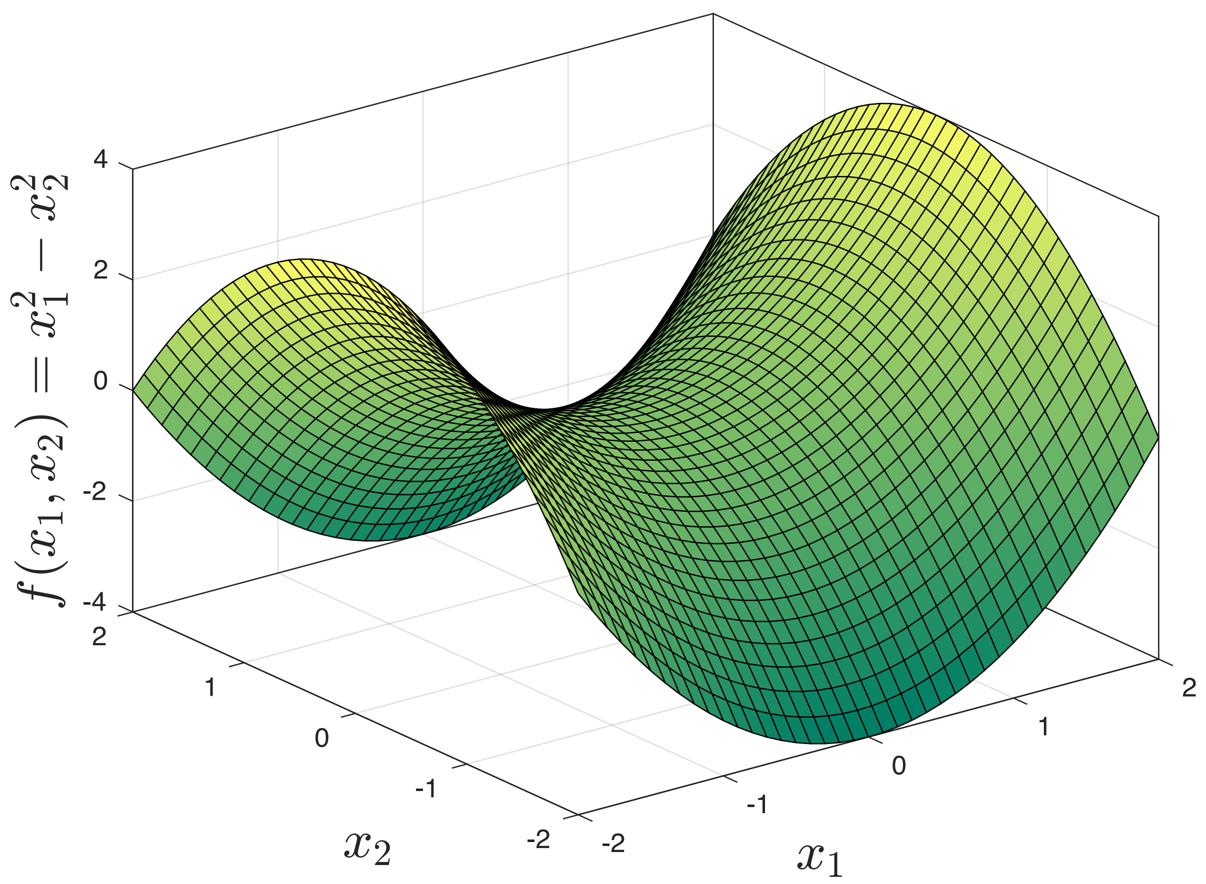
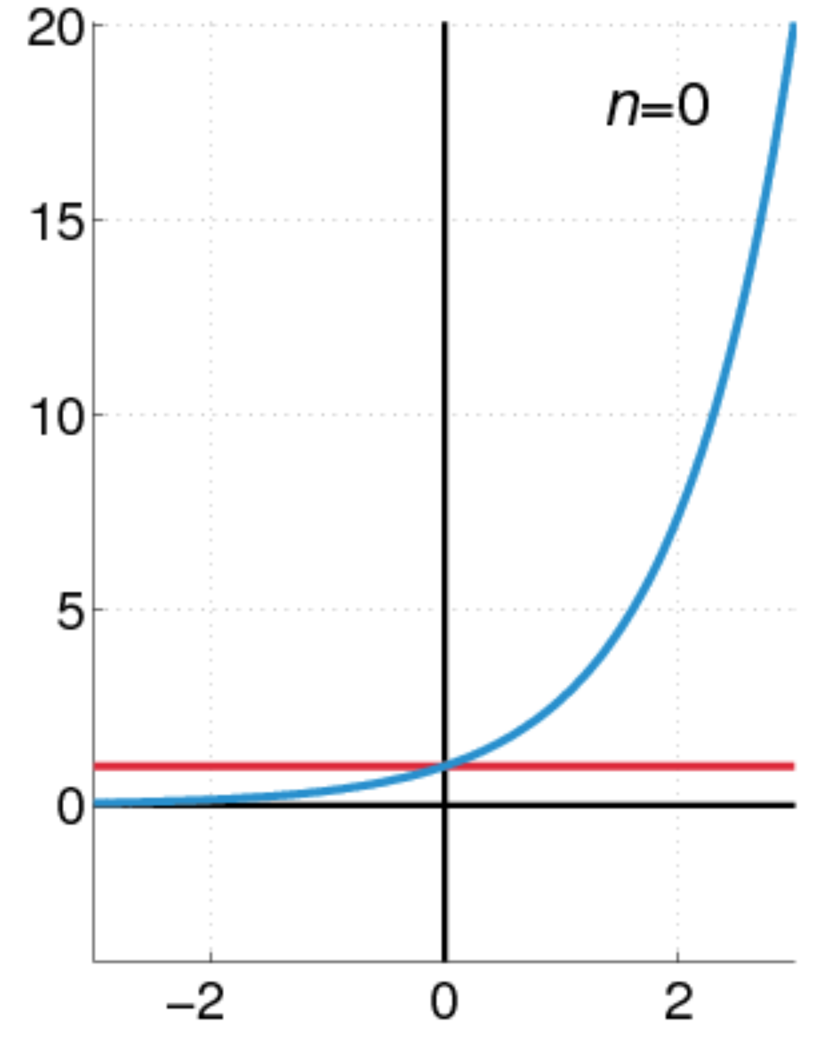


Indefinite

Taylor's expansion

– **Taylor's** expansion: used for (locally) approximating a function

$$f(x)\Big|_{x=\alpha} = f(\alpha) + f'(\alpha)(x-\alpha) + \frac{f''(a)}{2!}(x-\alpha)^2 + \cdots + \frac{f^{(n)}(\alpha)}{n!}(x-\alpha)^n + R_n$$



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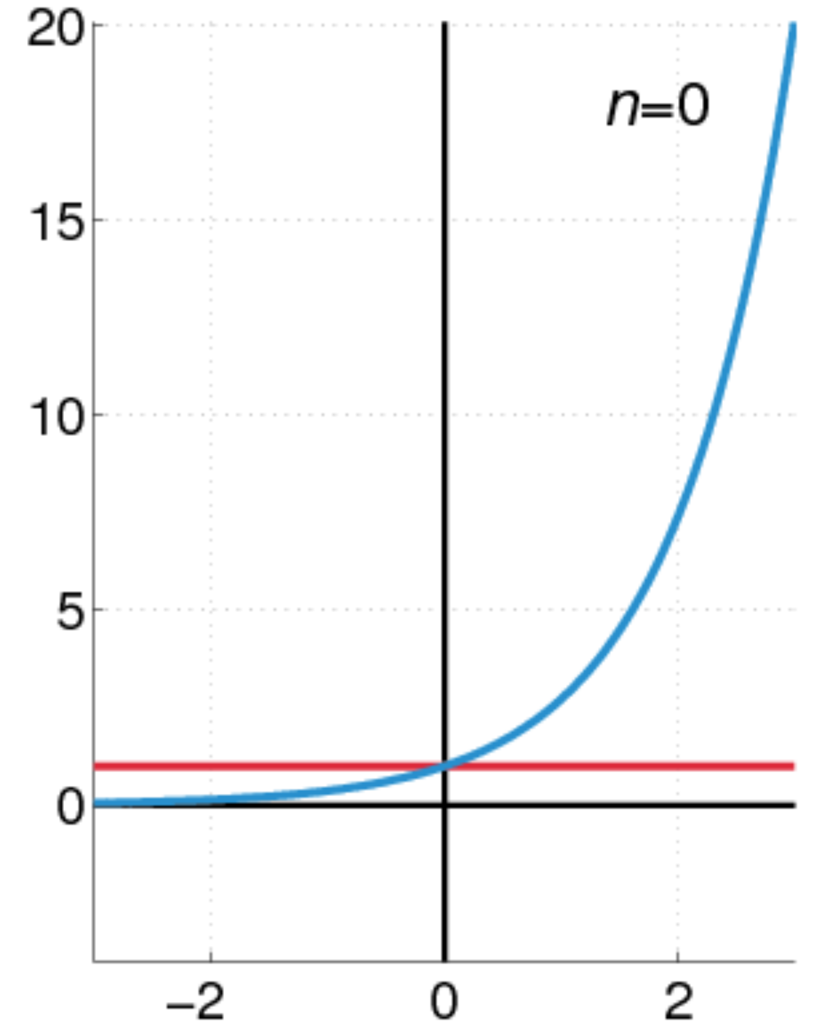

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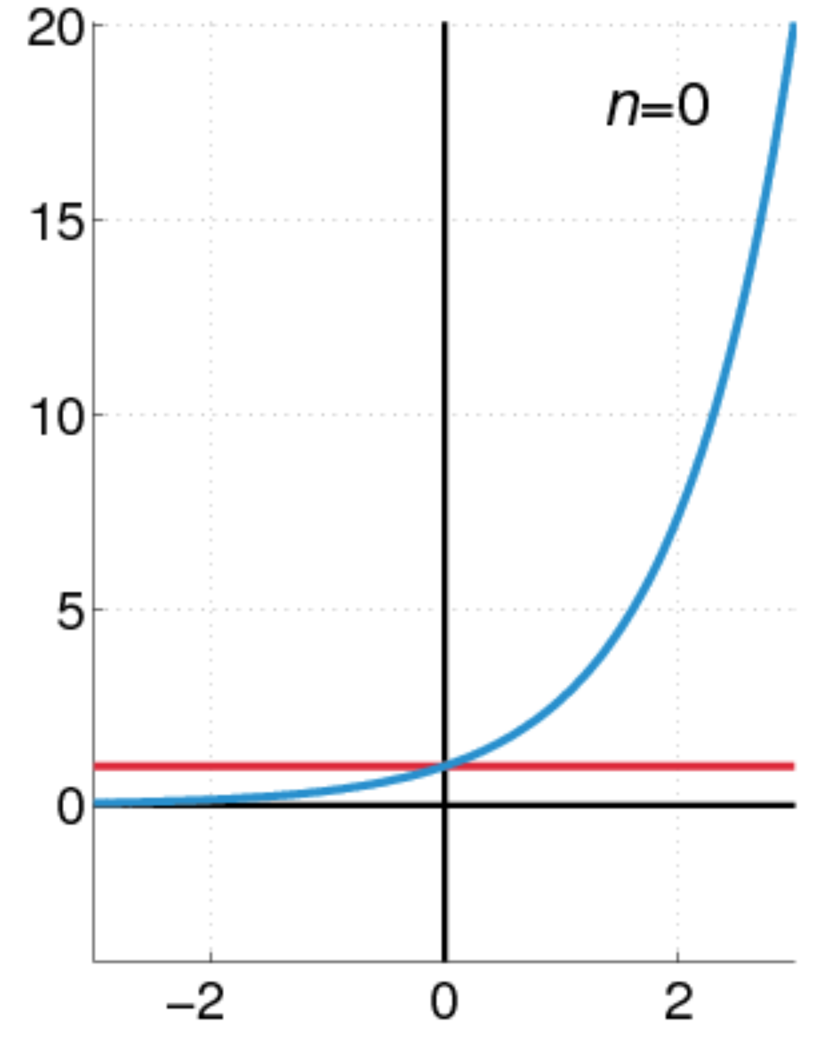

Example: exponential function

- Key properties/assumptions:
  - Function f is differentiable as many times we'd like
  - Provides **(locally)** a good approximation of the function

Taylor's expansion

- First–order Taylor's approximation

$$f : \mathbb{R}^p \to \mathbb{R} \quad \Big| \quad f(x) \approx f(\alpha) + \langle \nabla f(\alpha), x - \alpha \rangle, \alpha \in \mathbb{R}^p$$

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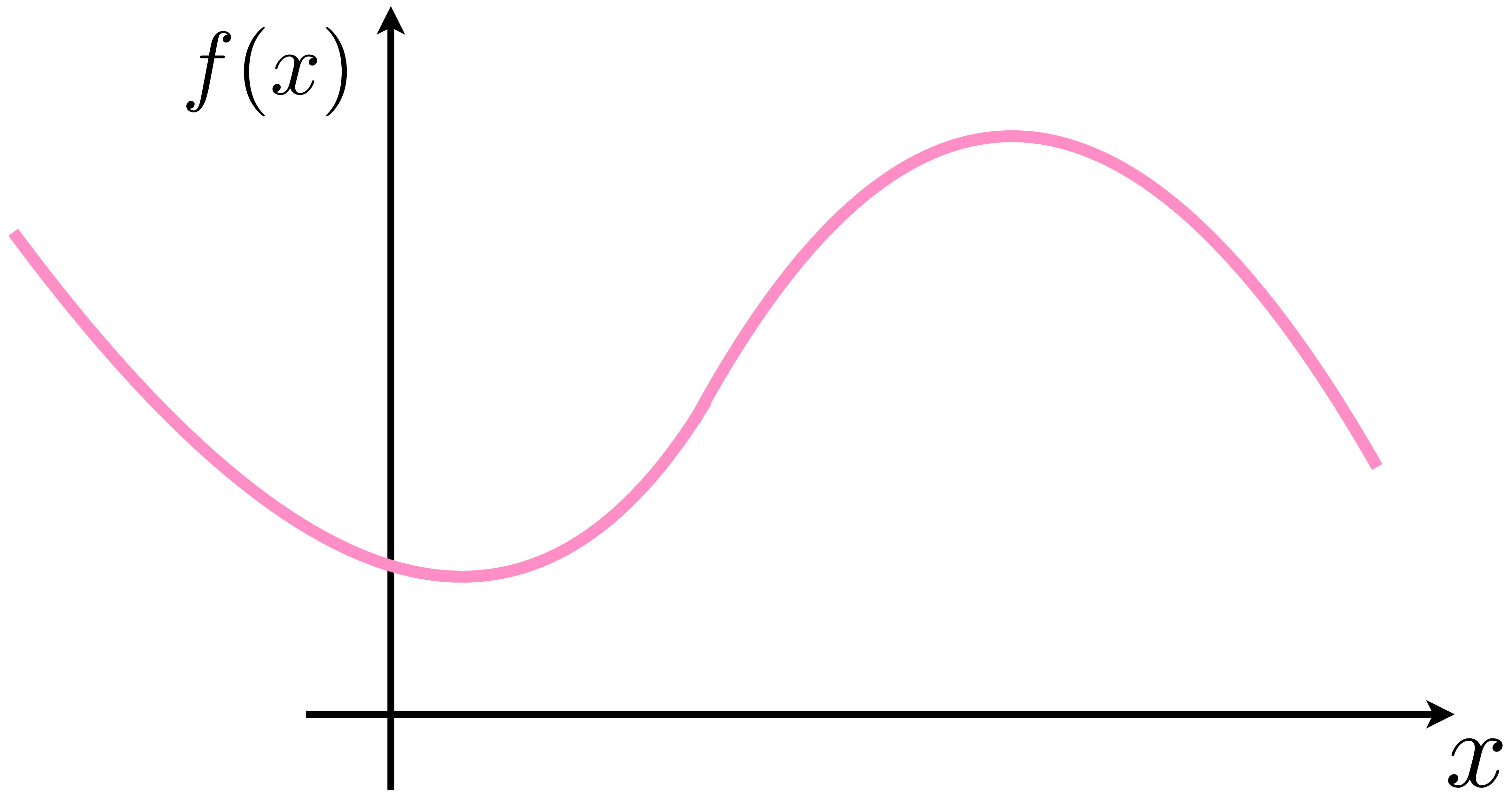

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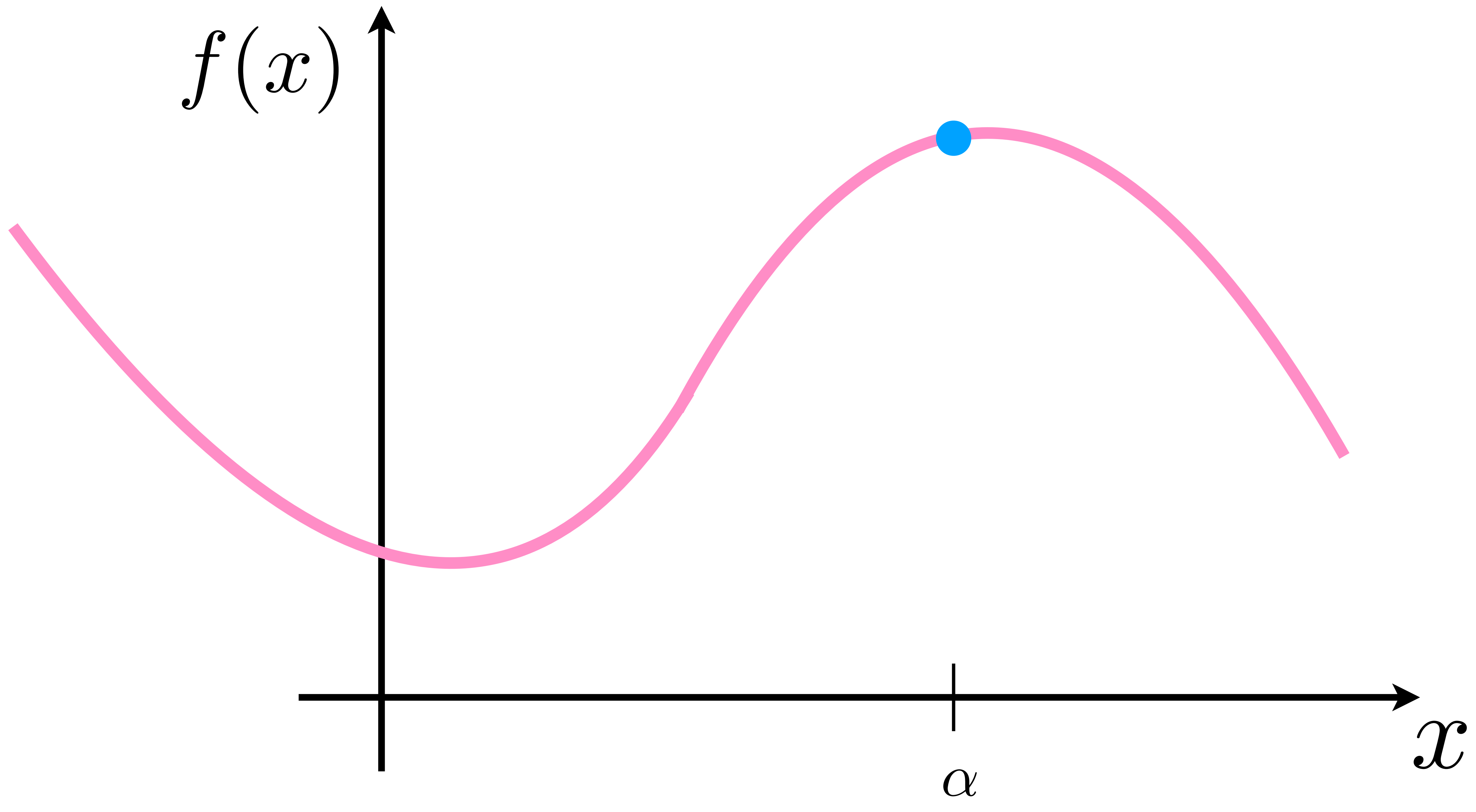

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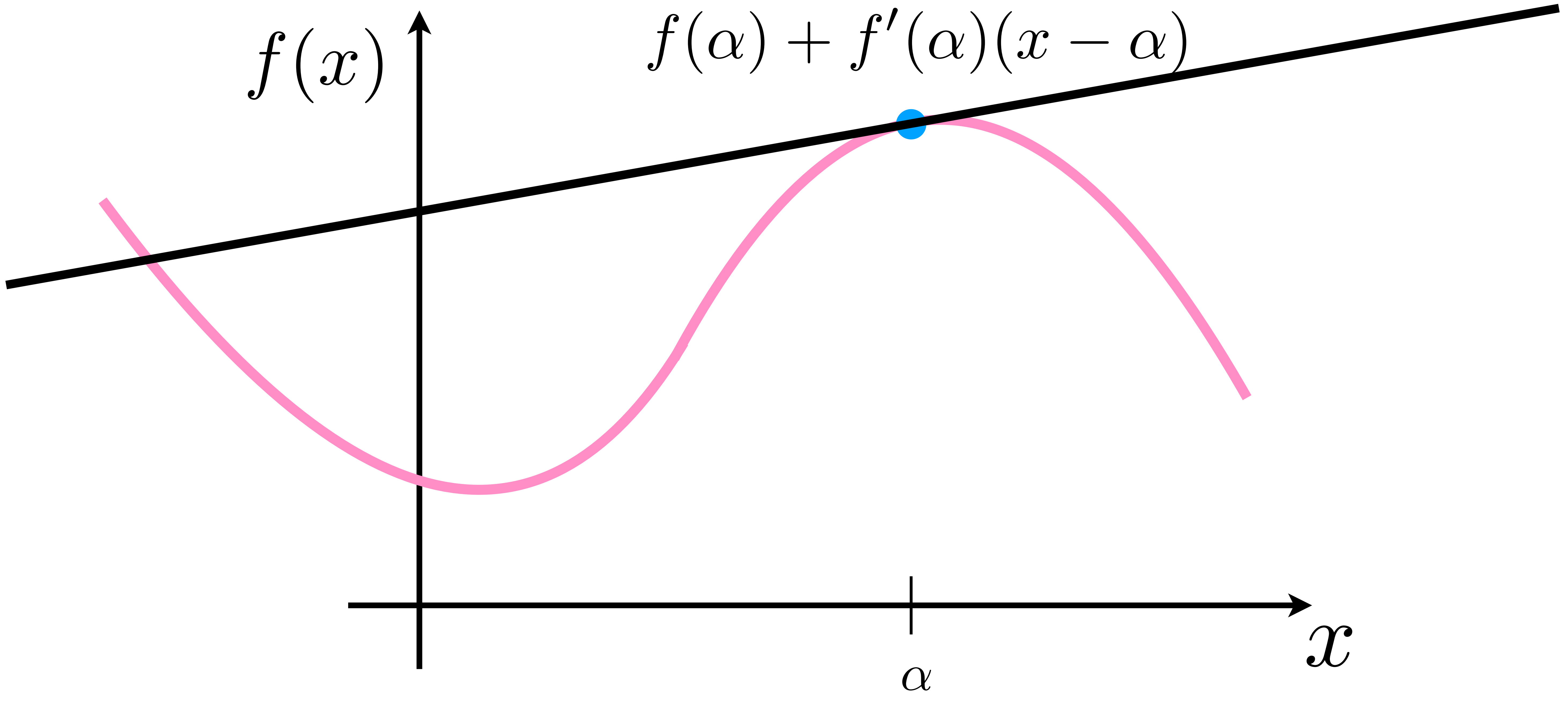

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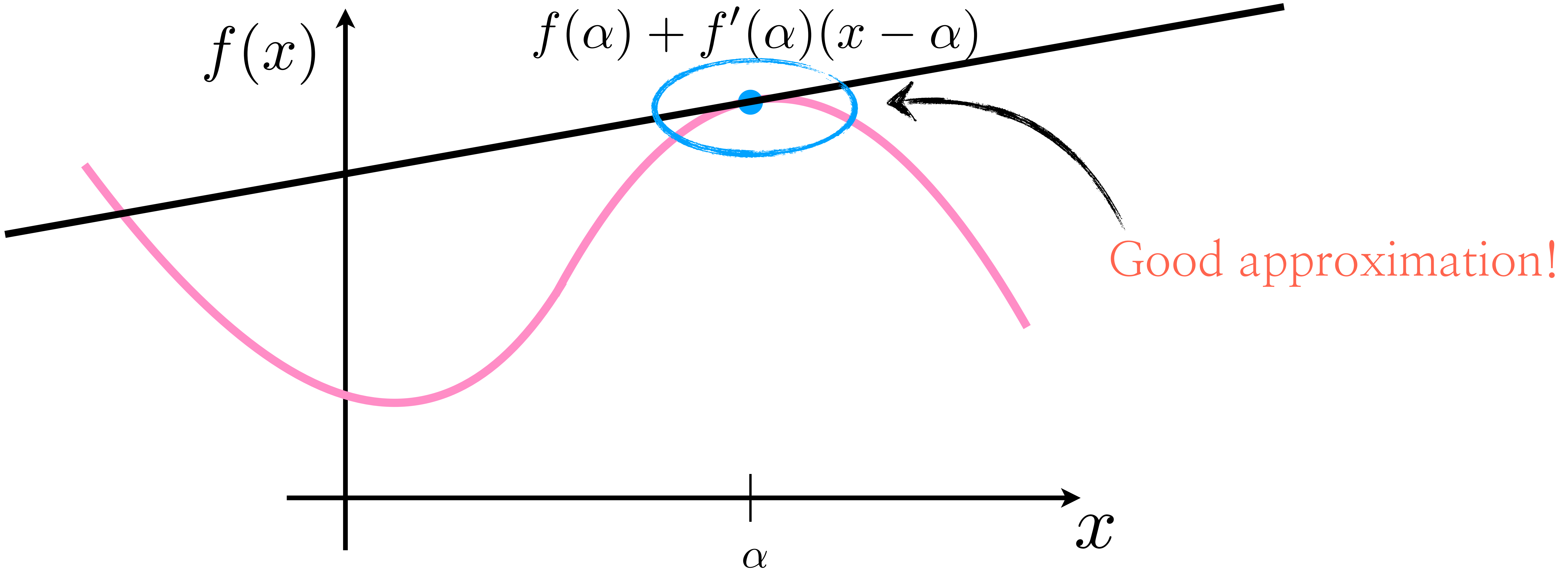

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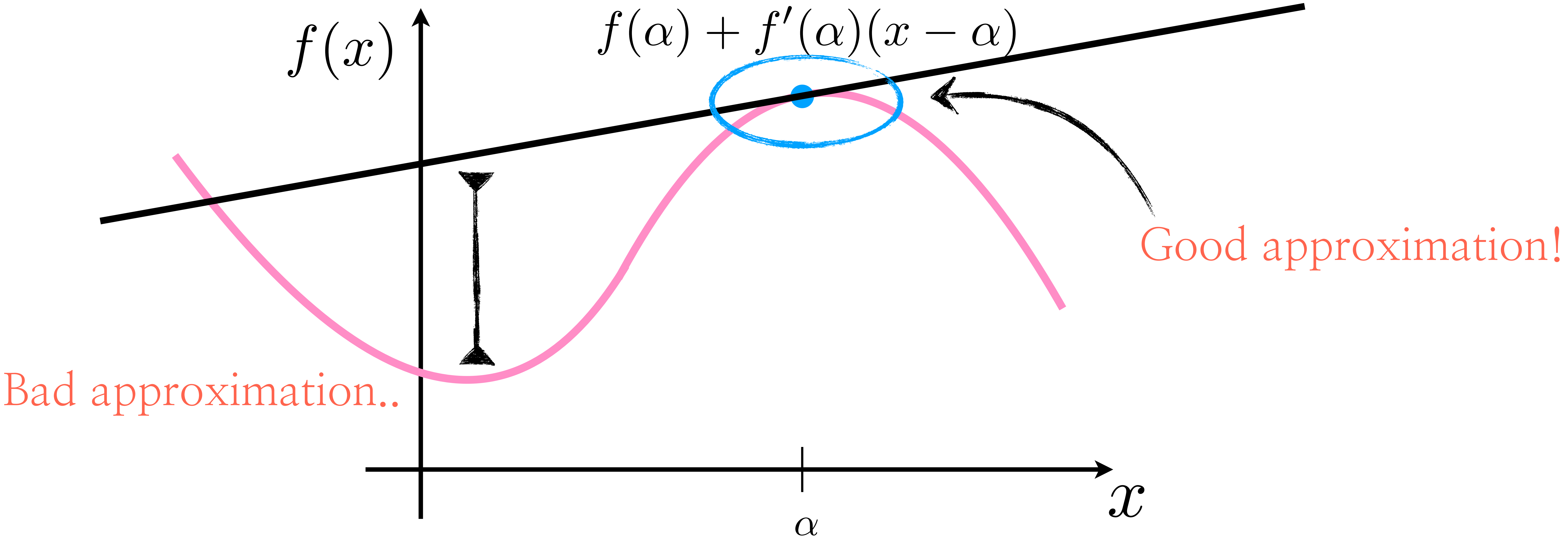

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- Second-order Taylor's approximation

$$f : \mathbb{R}^p \to \mathbb{R} \quad \Big| \quad f(x) \approx f(\alpha) + \langle \nabla f(\alpha), x - \alpha \rangle + \frac{1}{2} \left\langle \nabla^2 f(\alpha)(x - \alpha), x - \alpha \right\rangle, \alpha \in \mathbb{R}^p$$

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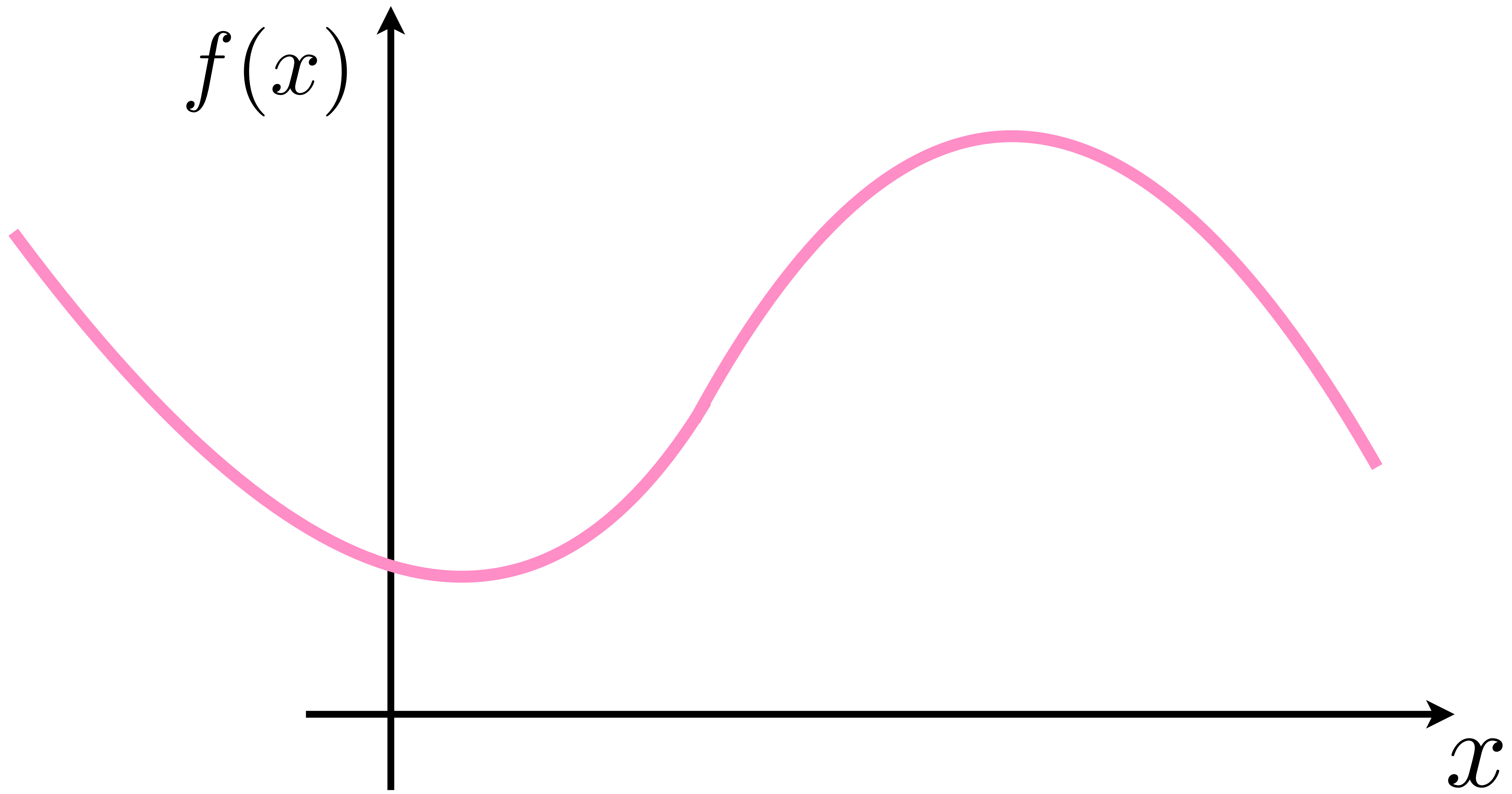

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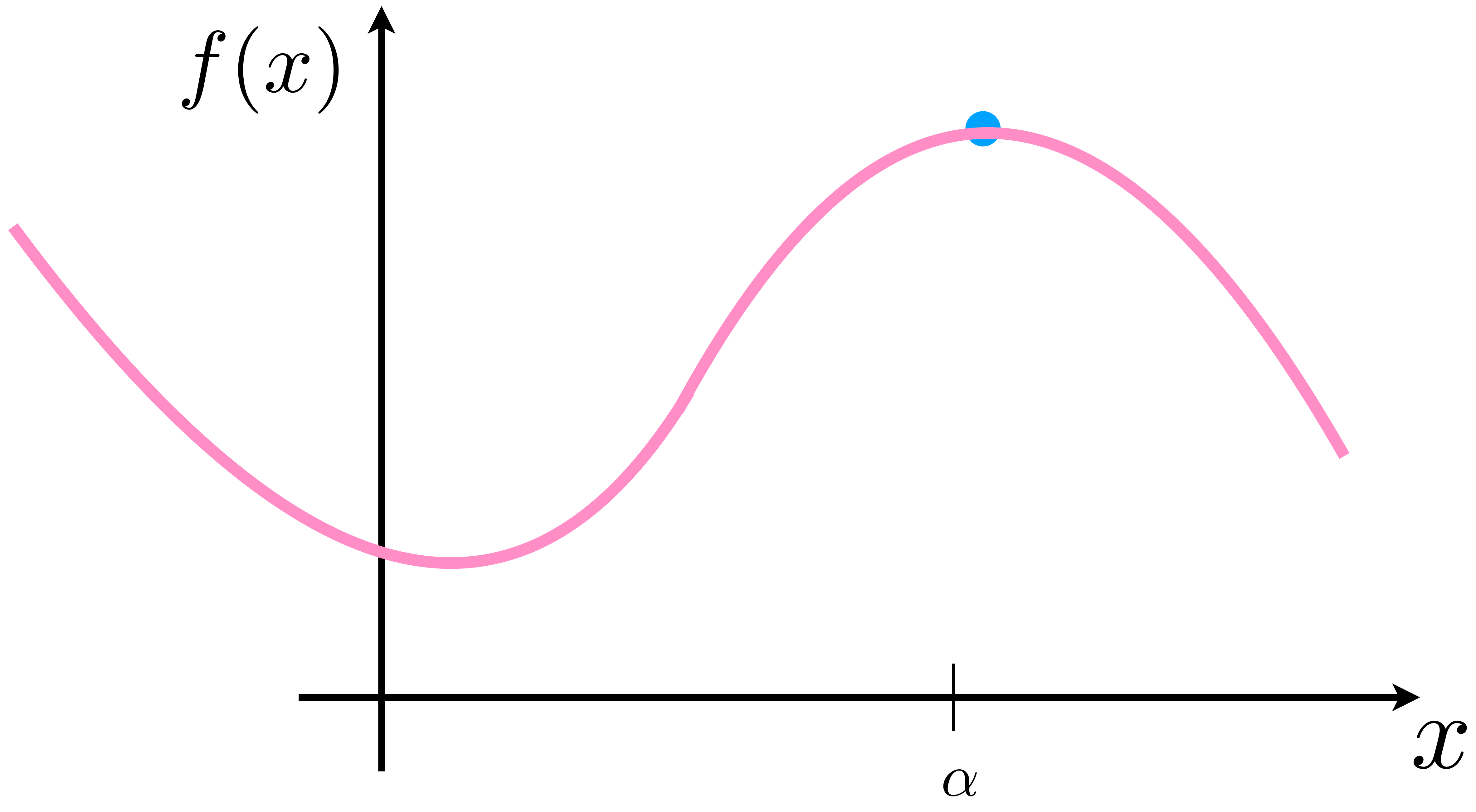

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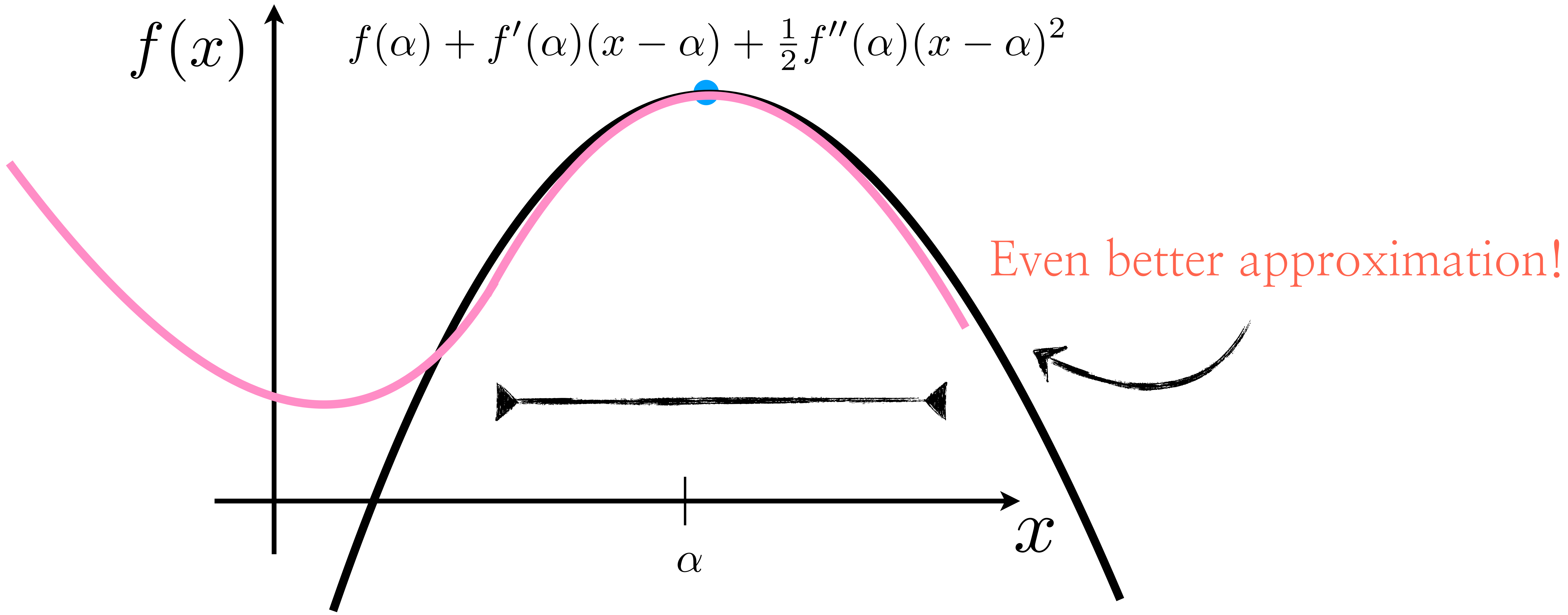

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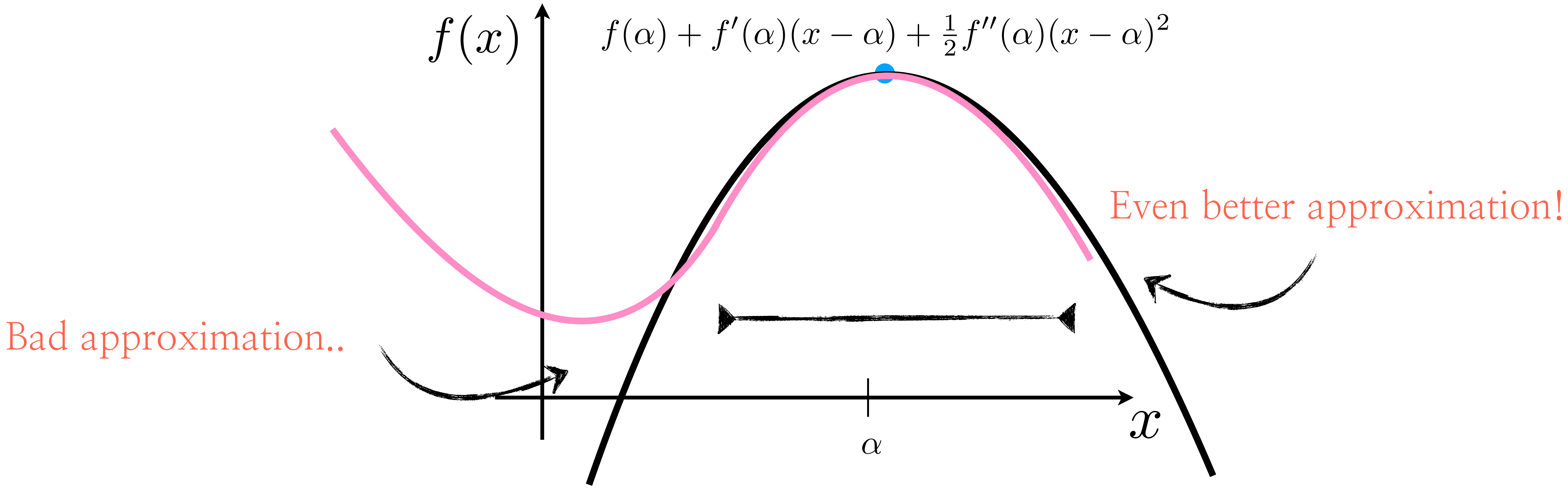

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$$\min_x f(x) \longrightarrow \min_x \left\{ f(x_0) + \nabla f(x_0)^\top (x - x_0) + \frac{1}{2}(x - x_0)^\top \nabla^2 f(x_0)(x - x_0) \right\}$$

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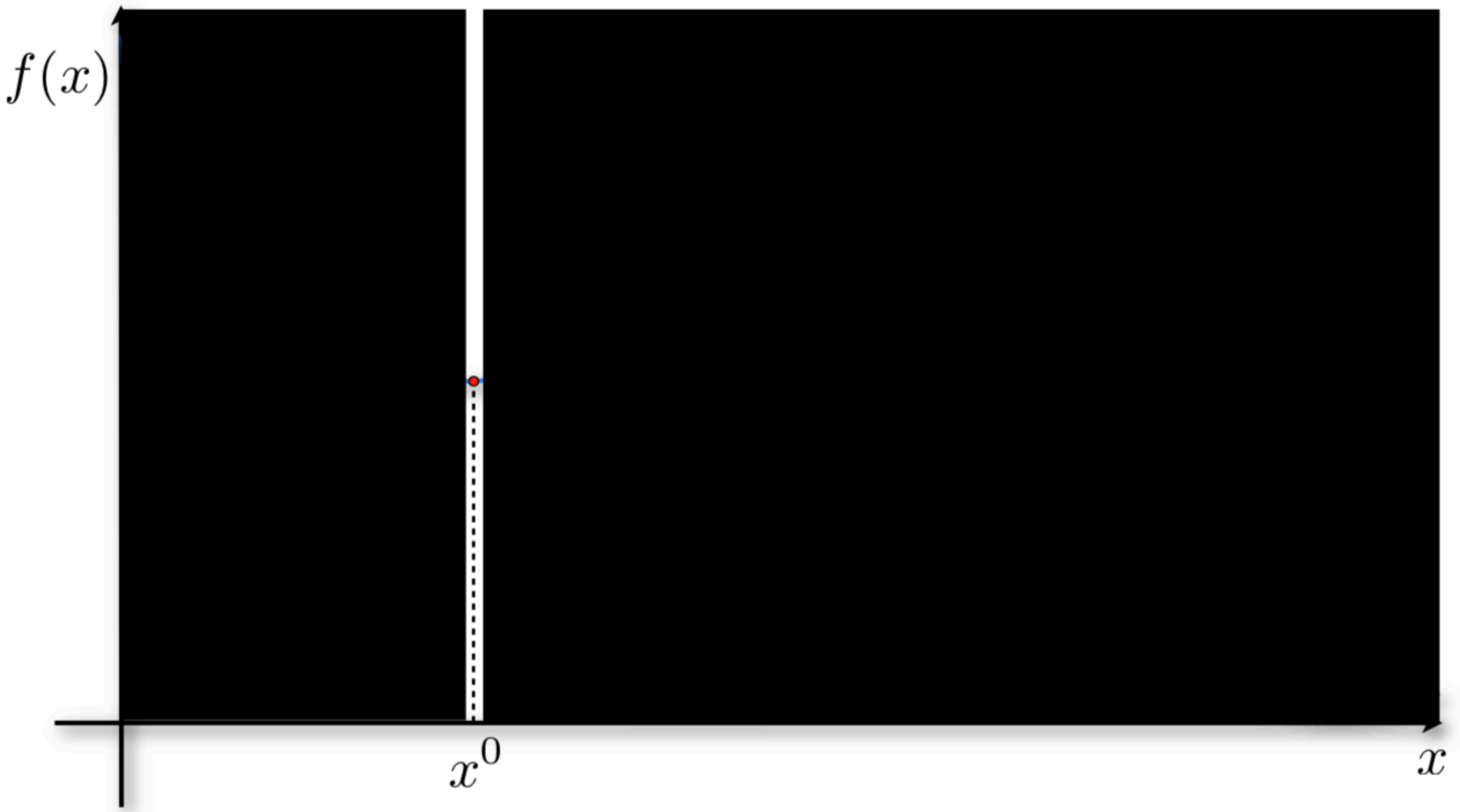
Agnostic optimization

Demo

Agnostic optimization



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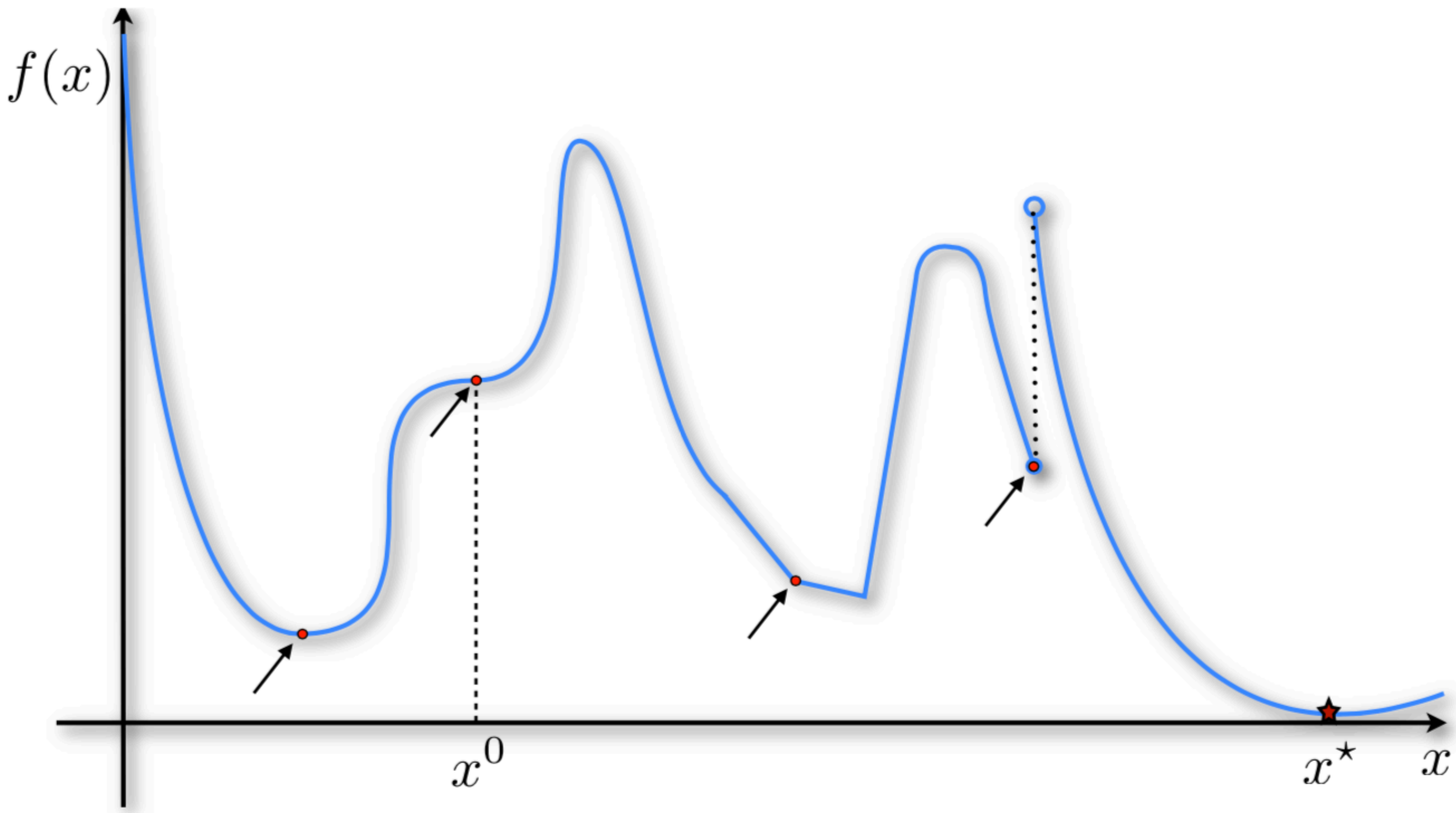

Lipschitz conditions

- **Lipschitz continuity**: $|f(x) - f(y)| \leq M\|x - y\|_2, \quad \forall x, y$

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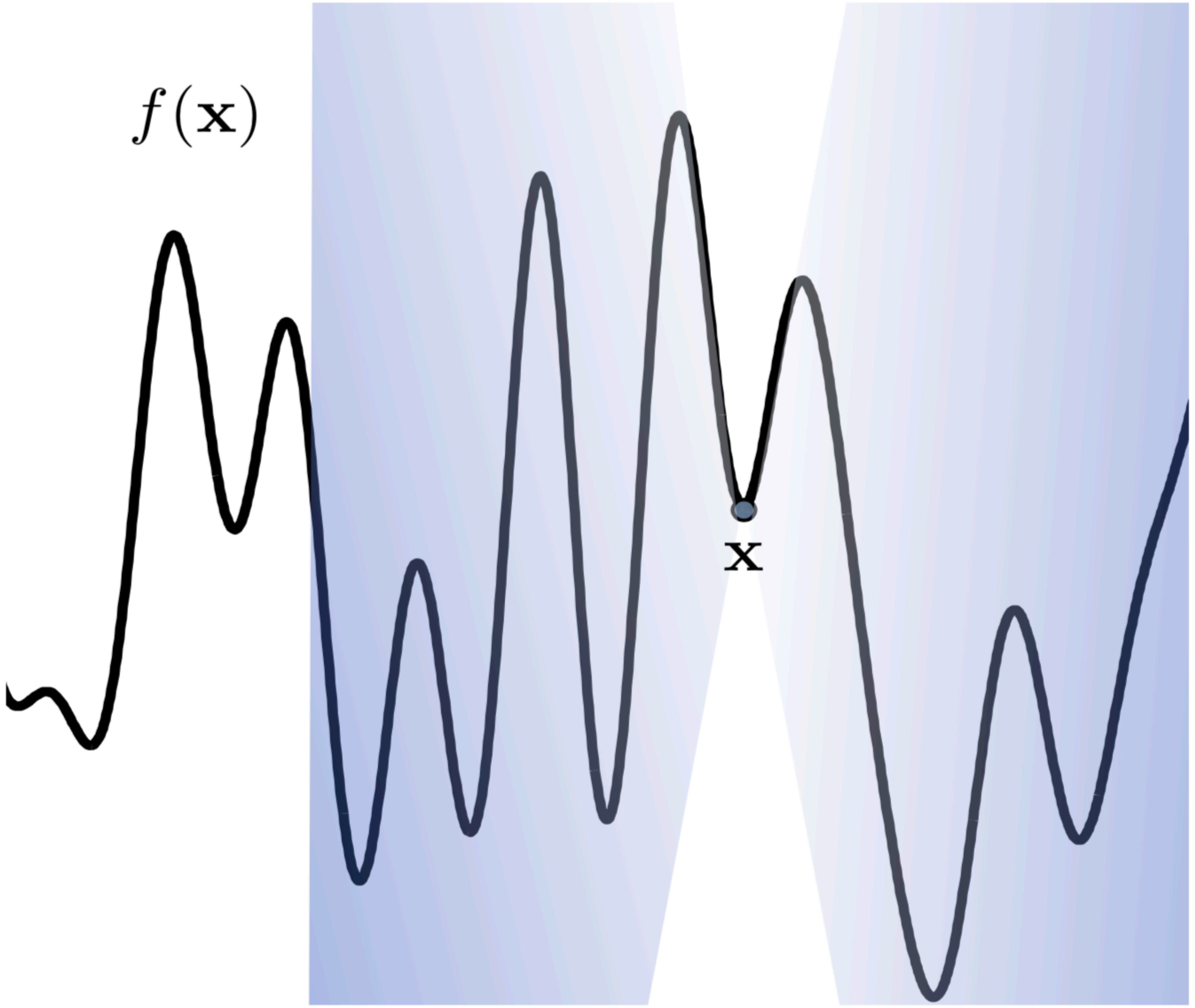
Interpretation via double cone



Function examples:
1. Absolute value
2. Trigonometric functions
3. Quadratics (..)

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    Largest singular value

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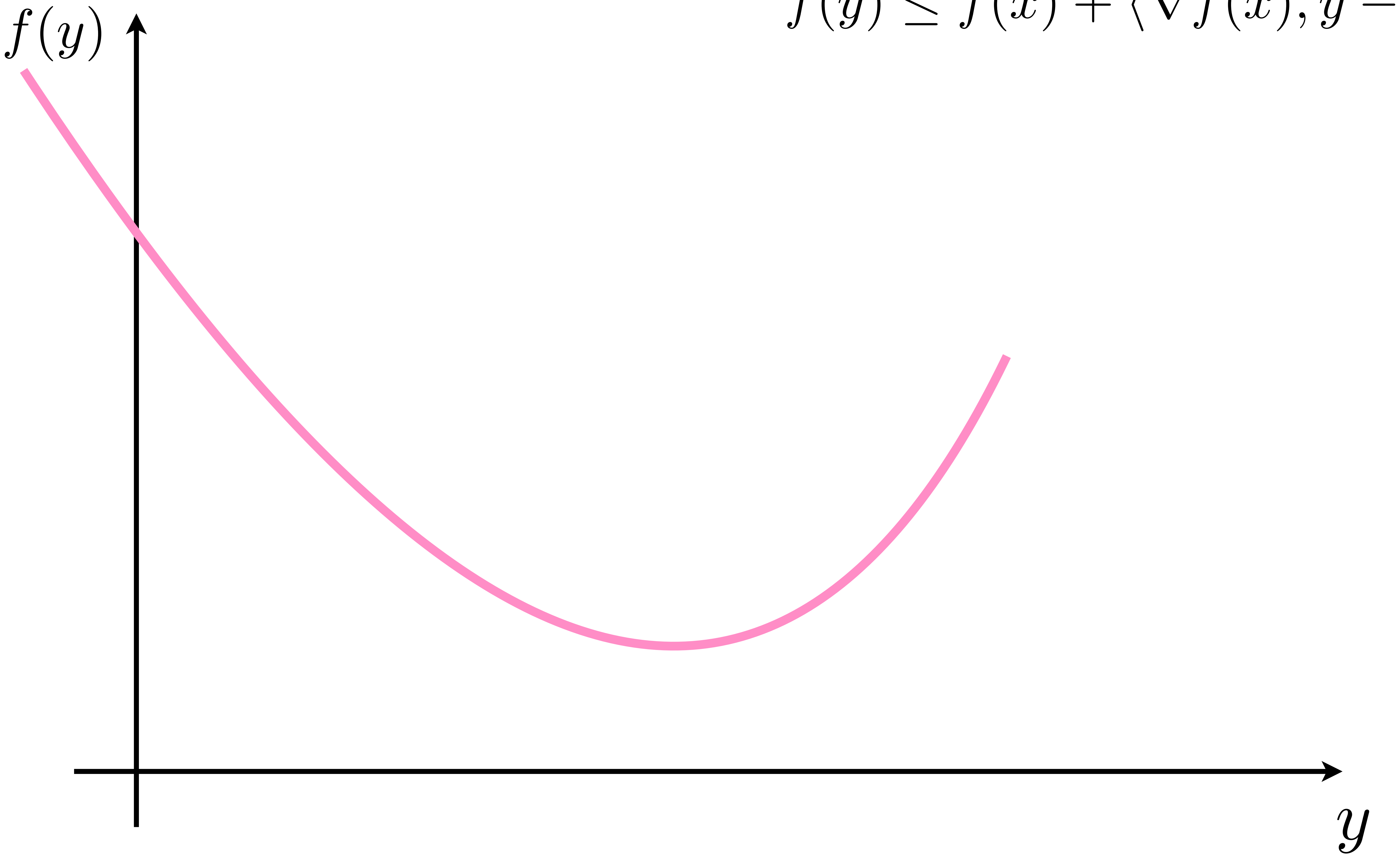

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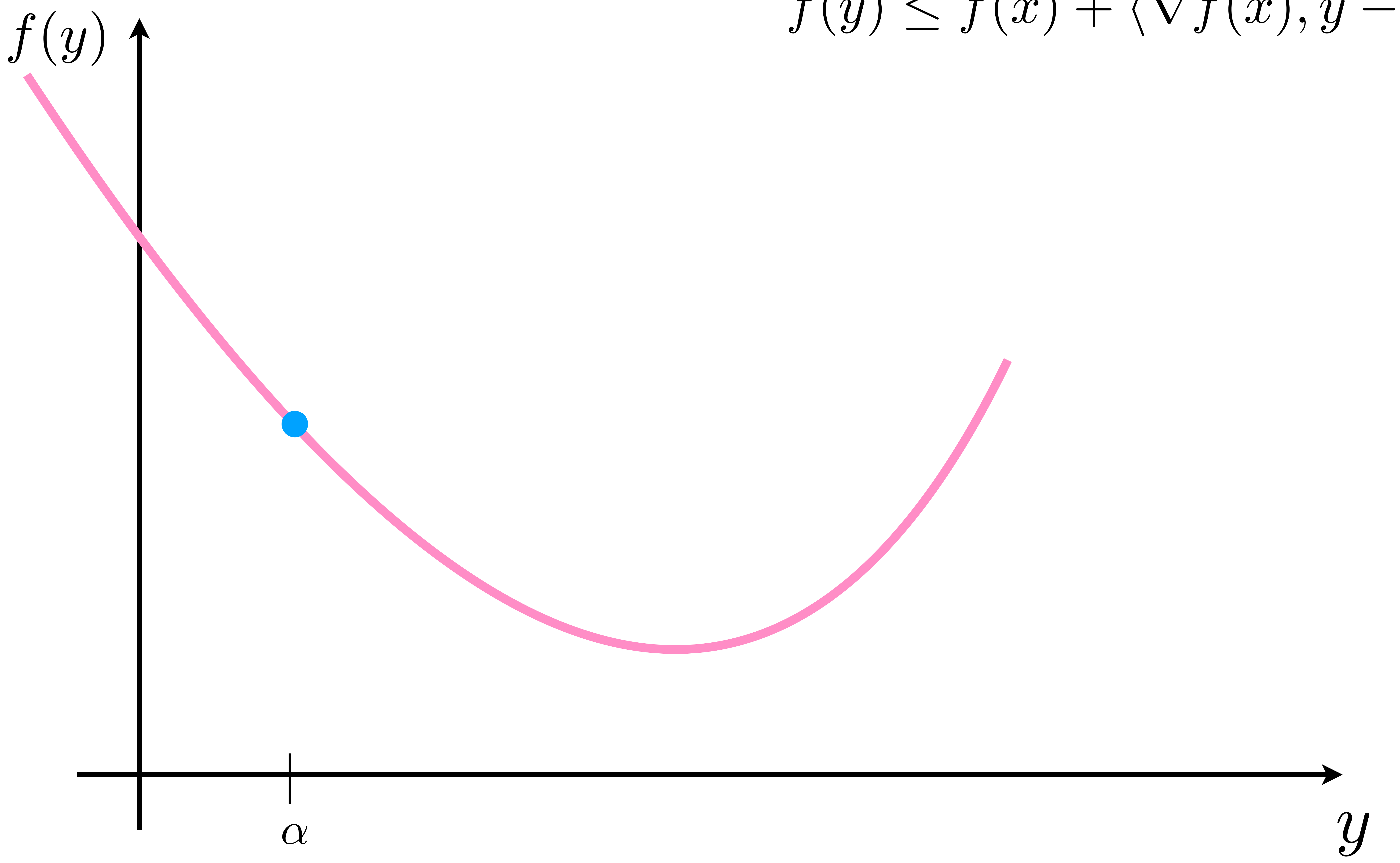

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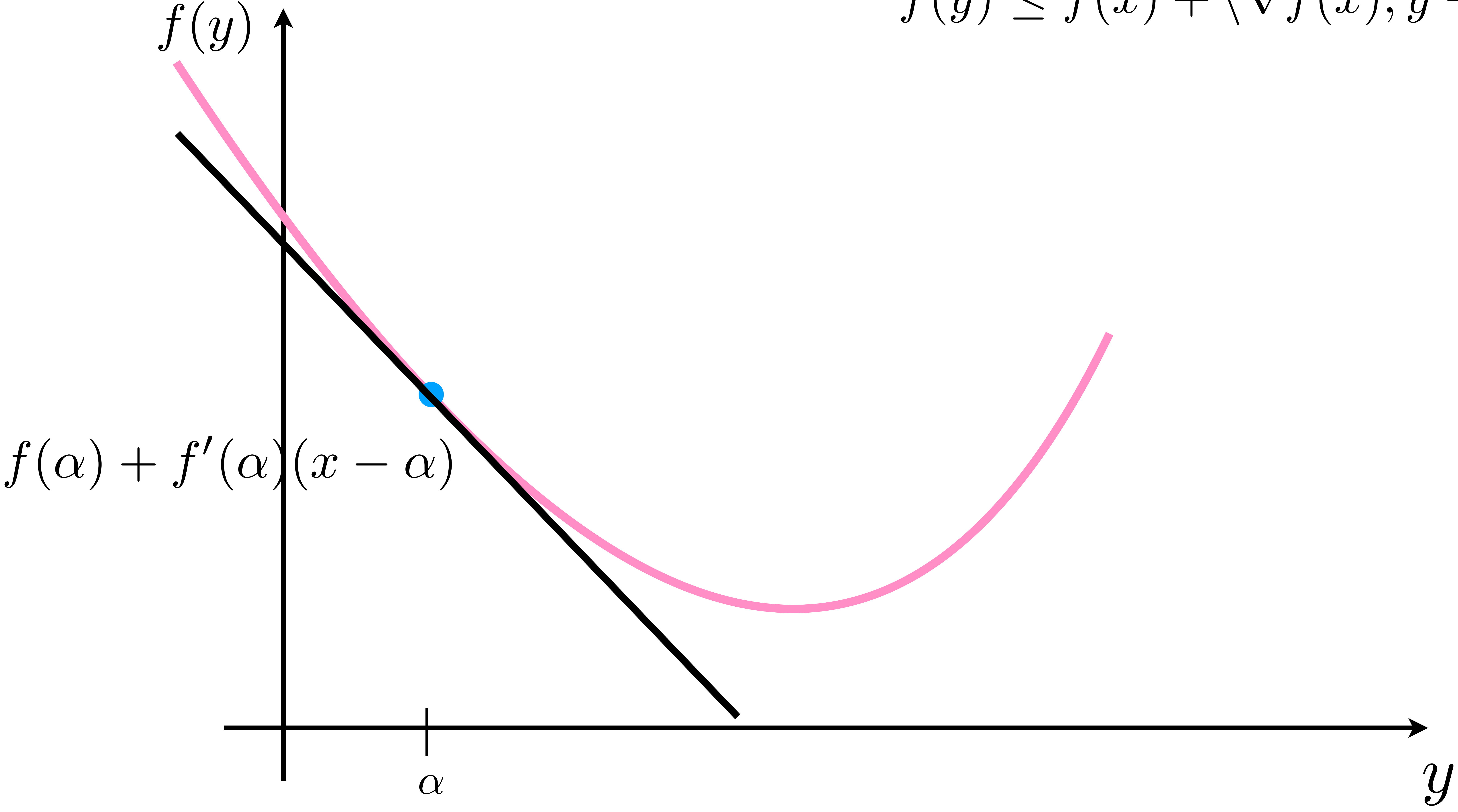

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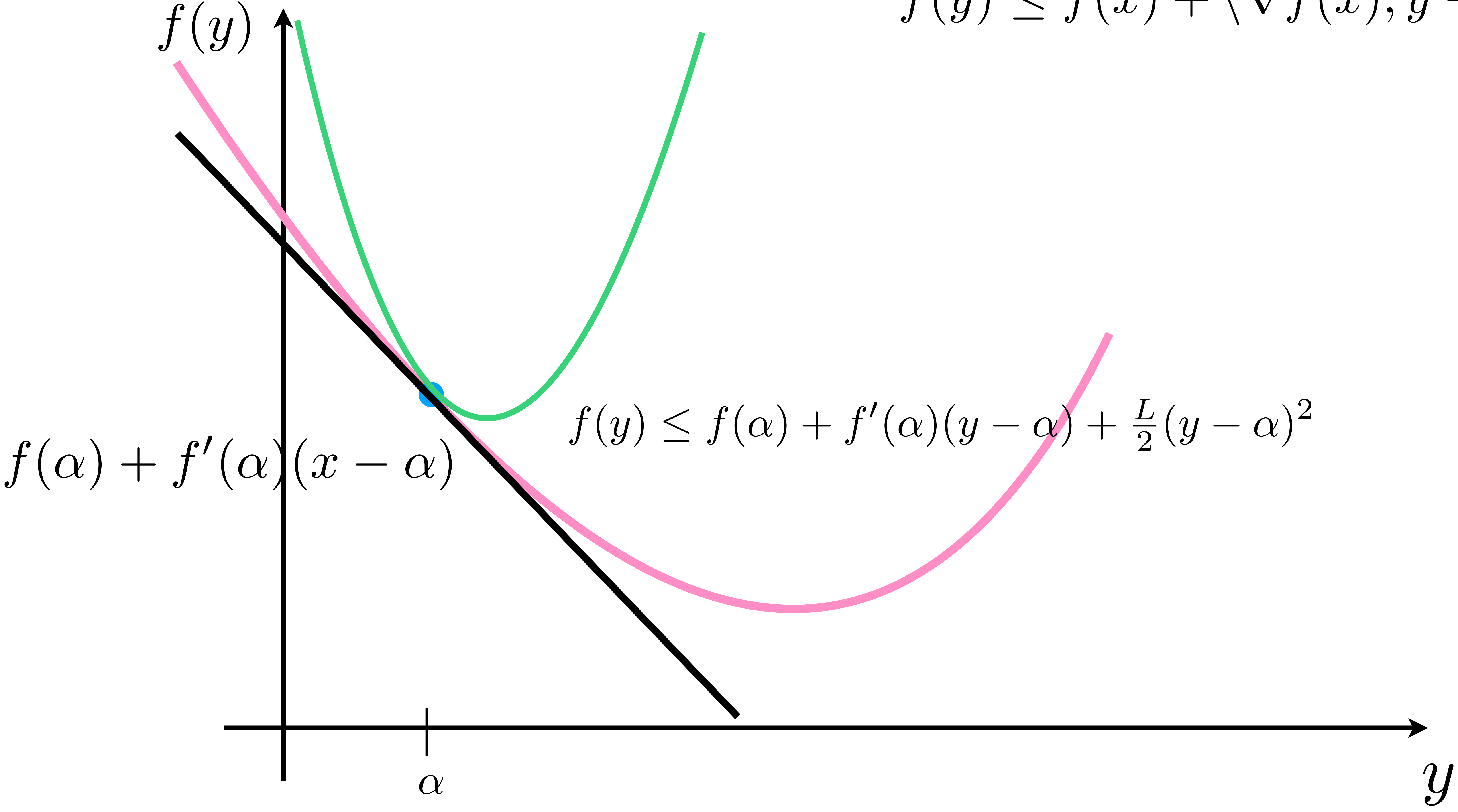

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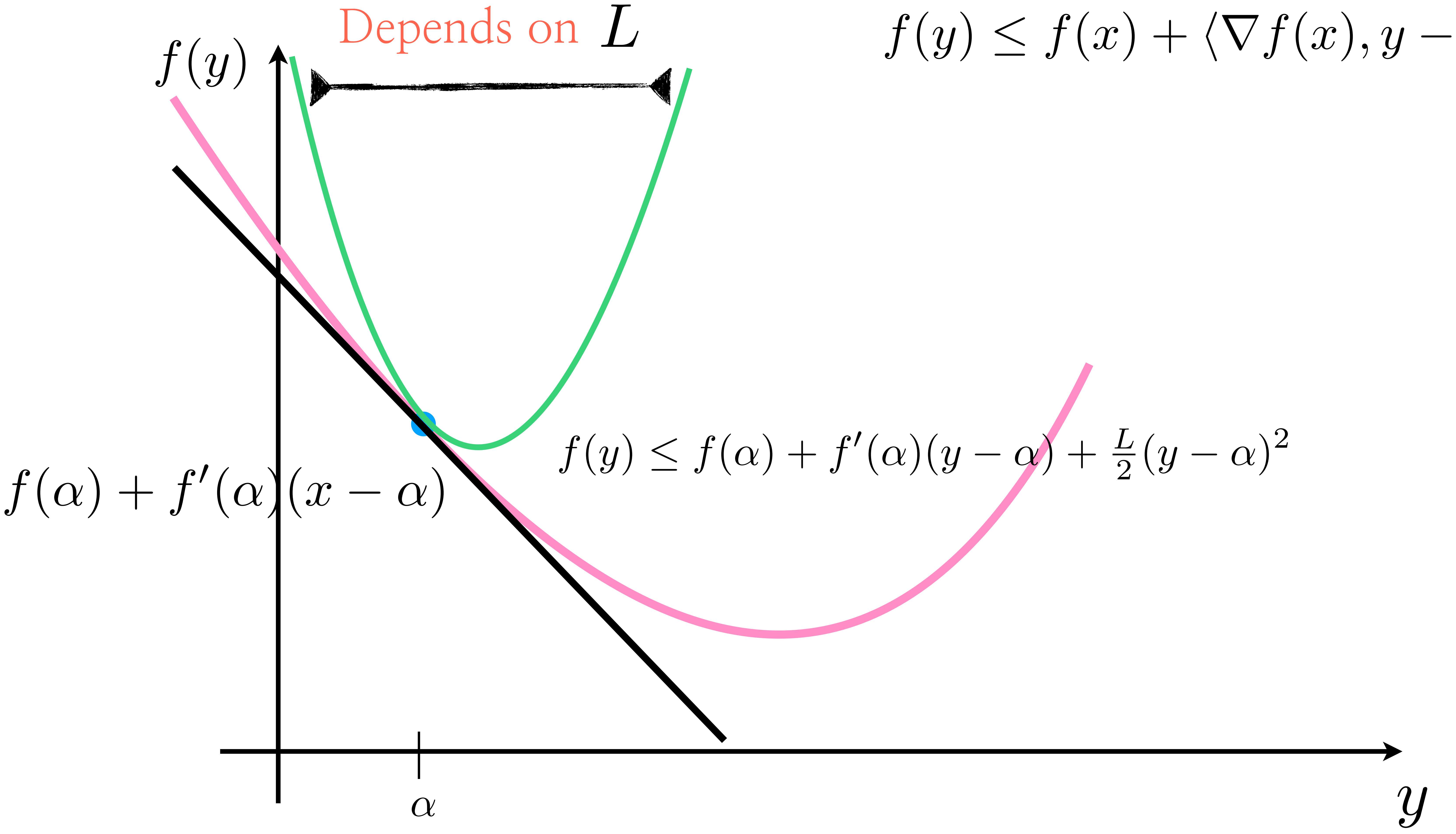

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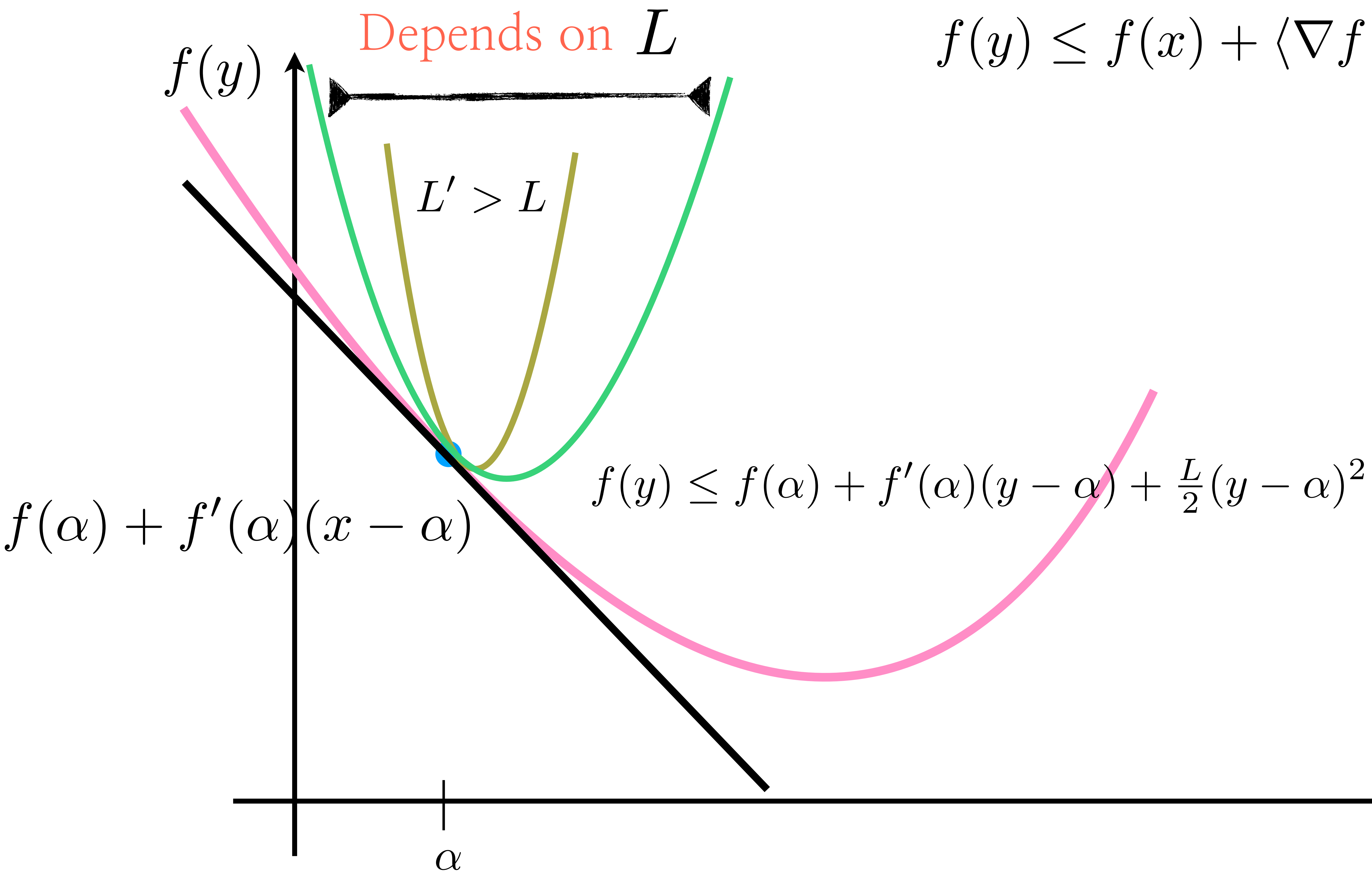

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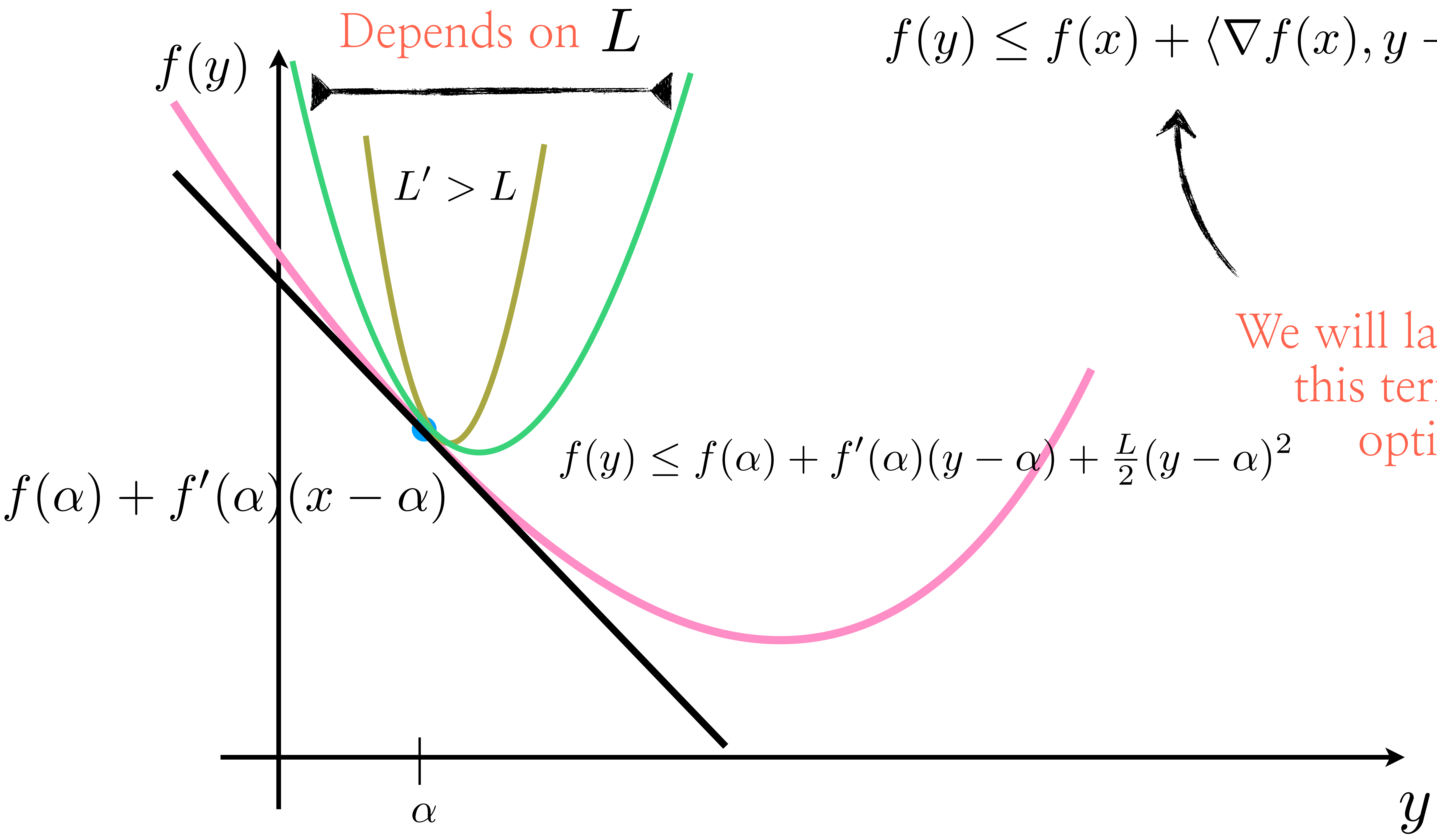

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We will later on see how this term appear in optimization

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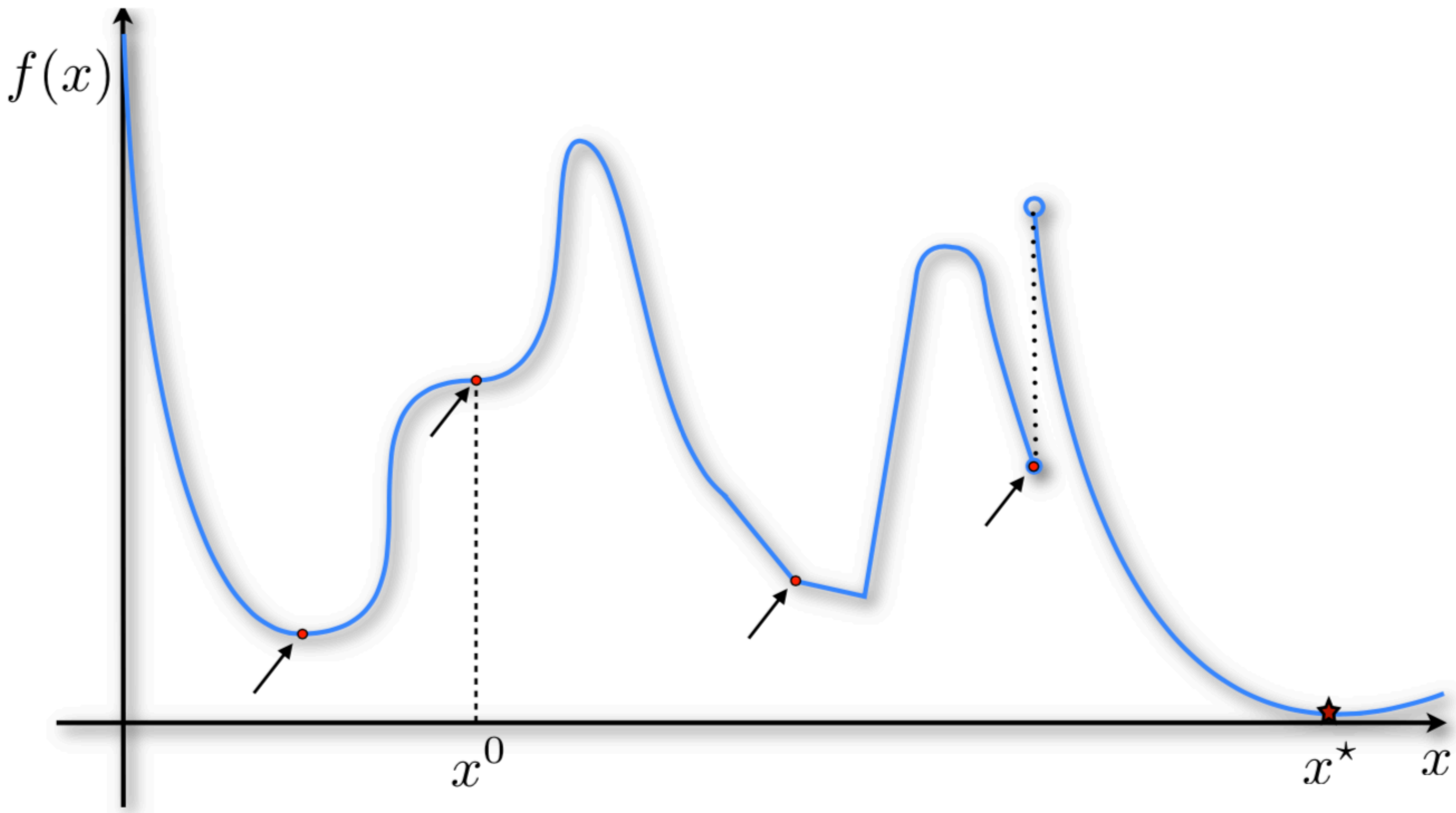
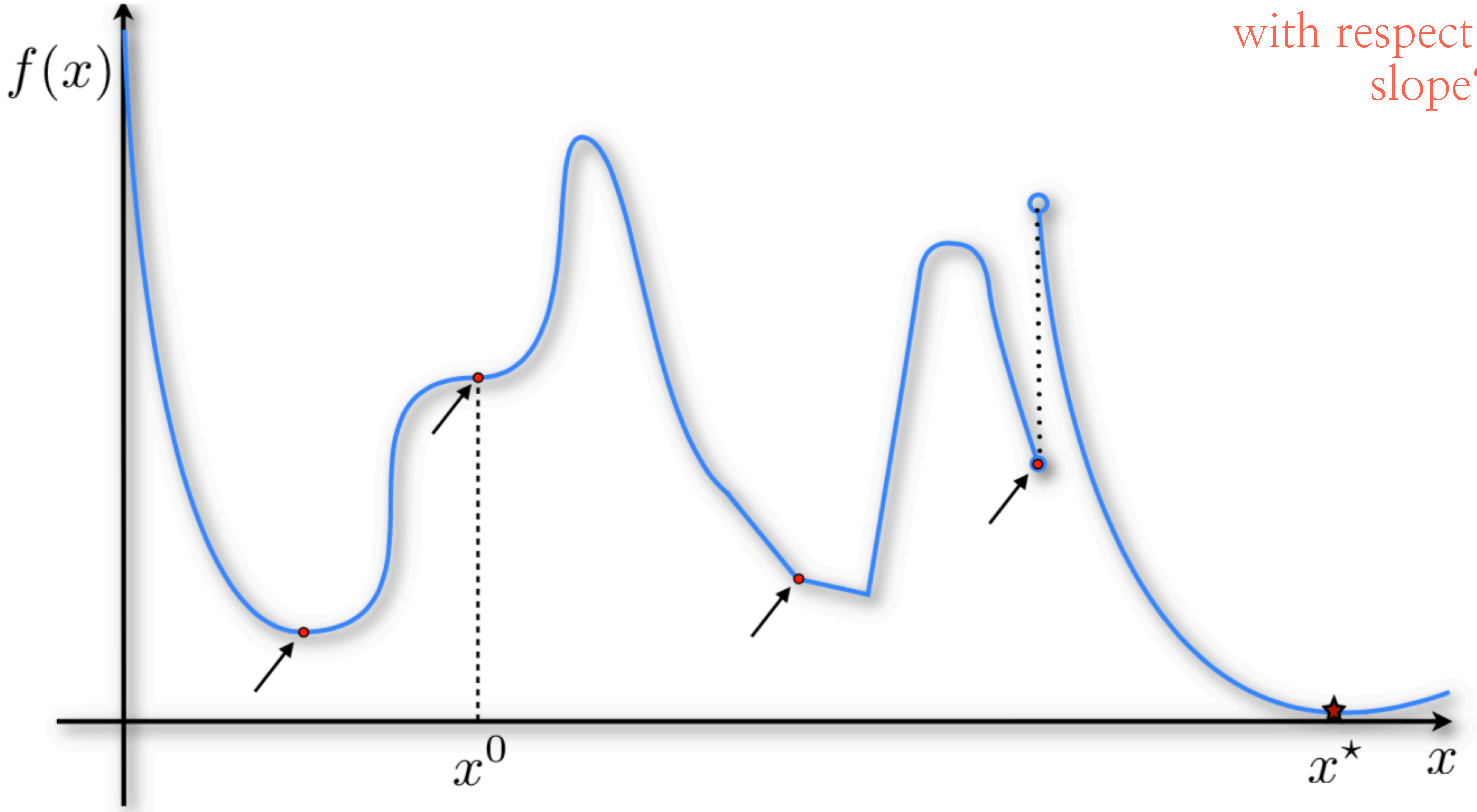
Agnostic optimization



Agnostic optimization

What do you observe at local minima/maxima with respect to their slope?



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Necessary

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Gradient descent

Gradient as local information (short story)

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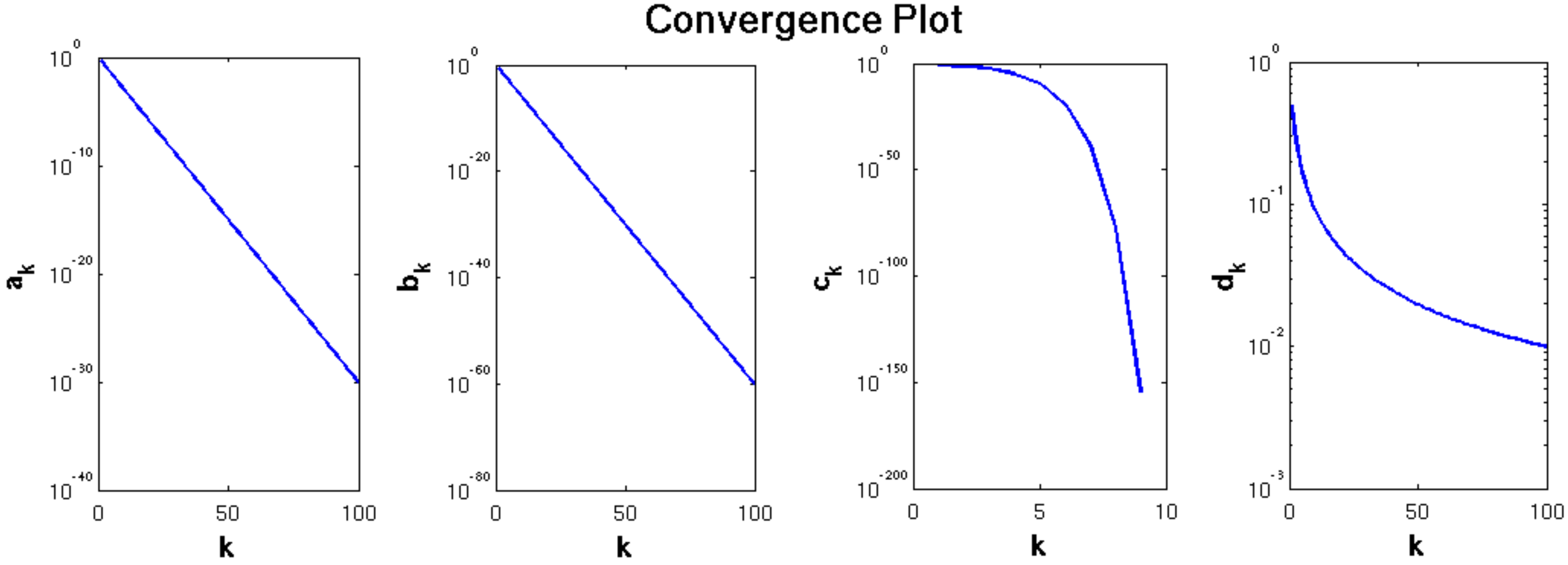
First convergence result

Whiteboard

Convergence rates 101

(Source: Wikipedia)



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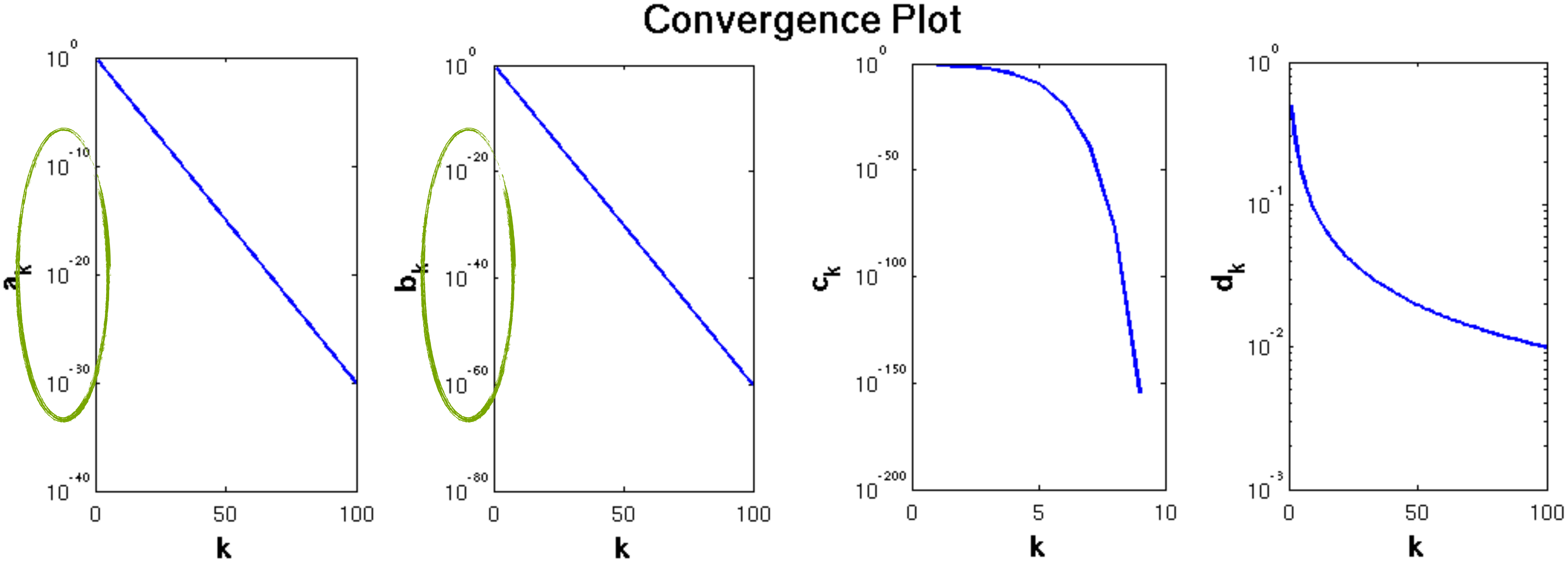

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$$\min_{x \in \mathbb{R}^p} f(x)$$

“Assume the objective is has Lipschitz continuous gradients. Then, gradient descent:

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

with step size

$$\eta = \frac{1}{L}$$

converges sublinearly to a stationary point; i.e.,

$$\min_t \|\nabla f(x_t)\|_2 \leq \sqrt{\frac{2L}{T+1}} \cdot \left(f(x_0) - f(x^\star)\right)^{1/2} = O\left(\frac{1}{\sqrt{T}}\right)$$ “

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Whiteboard

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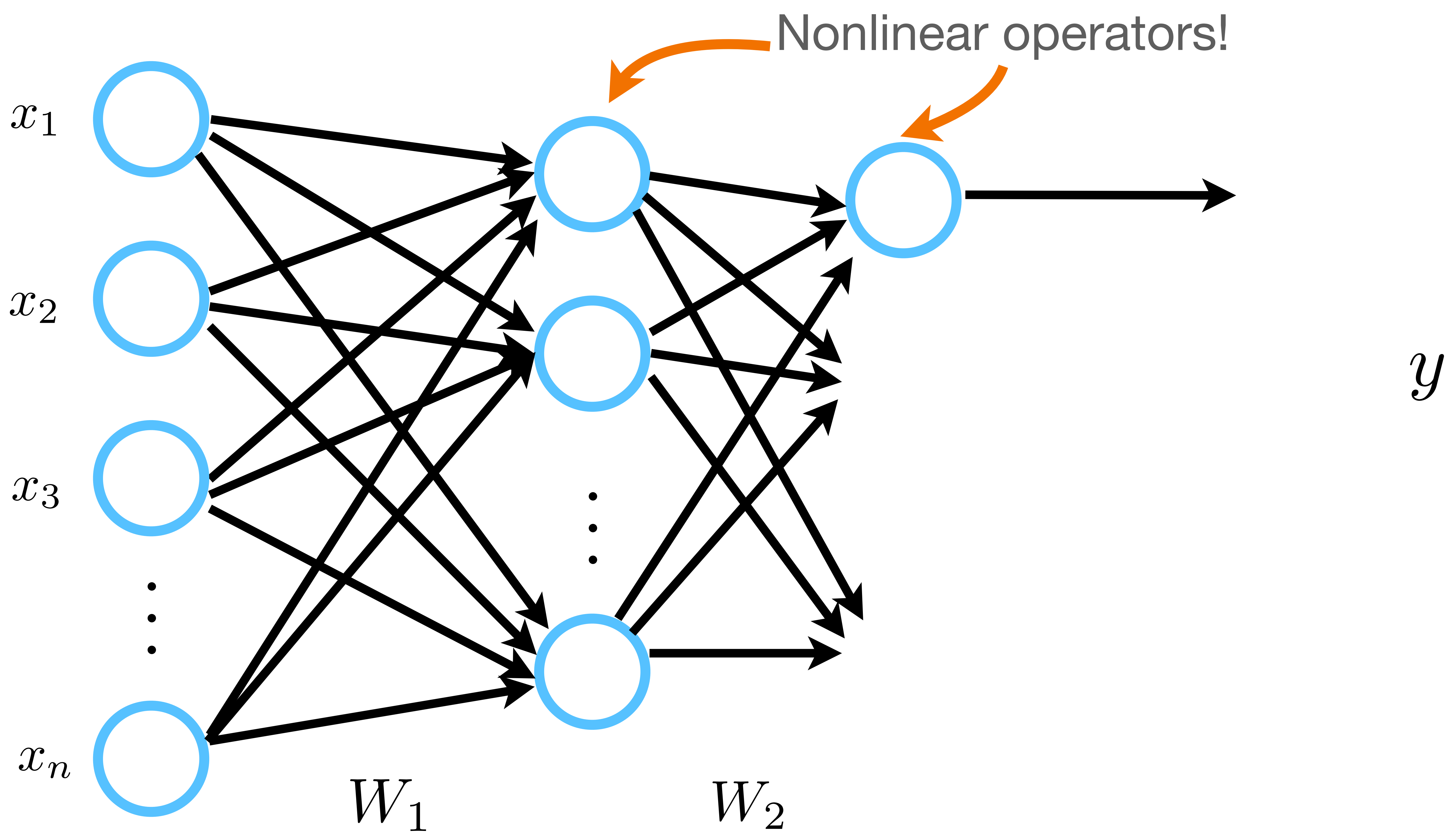
– Non−convex objective: $f(x) = x^2 + 3\sin^2(x)$

Demo

Combining all these things together: MLP



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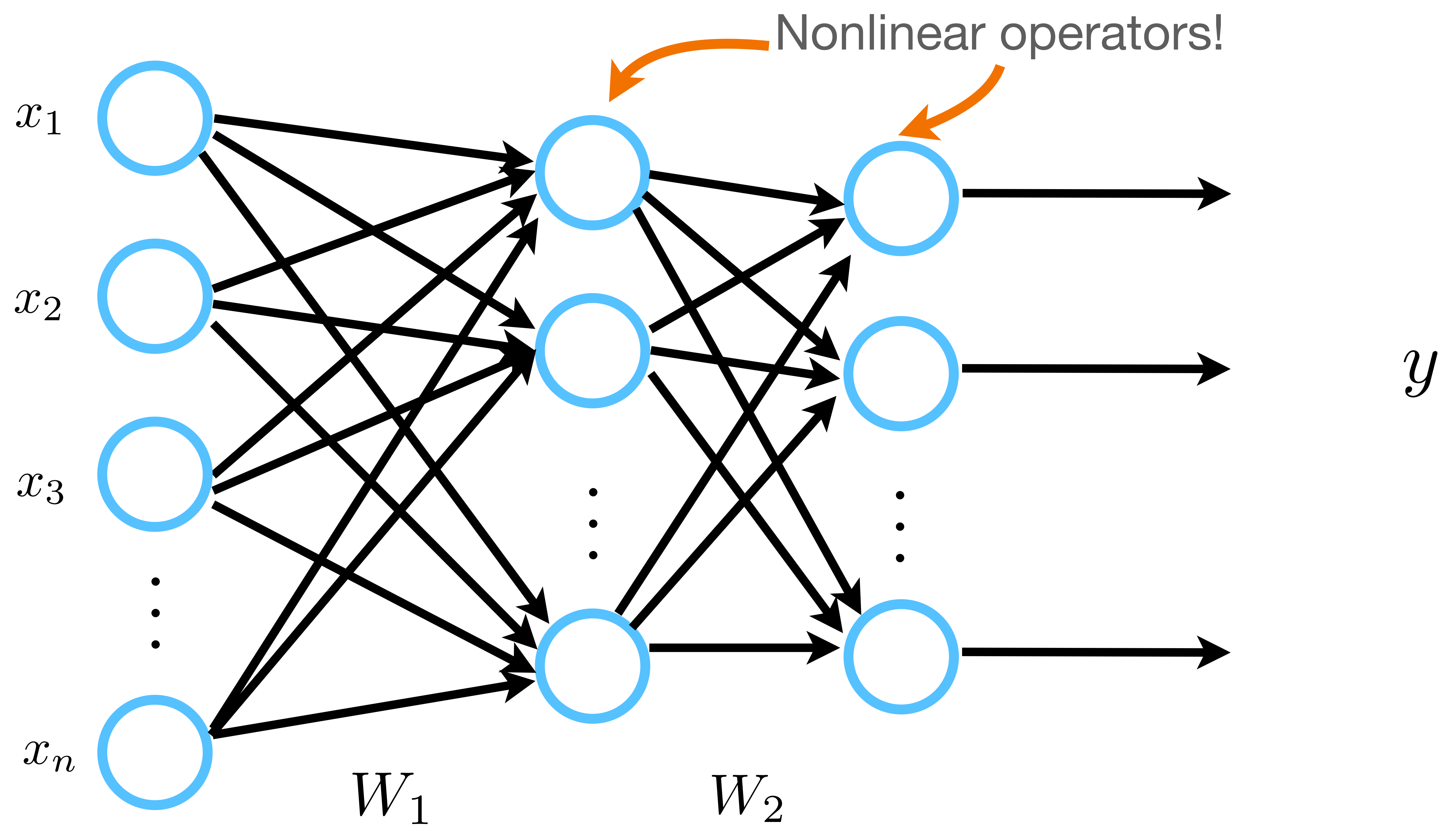
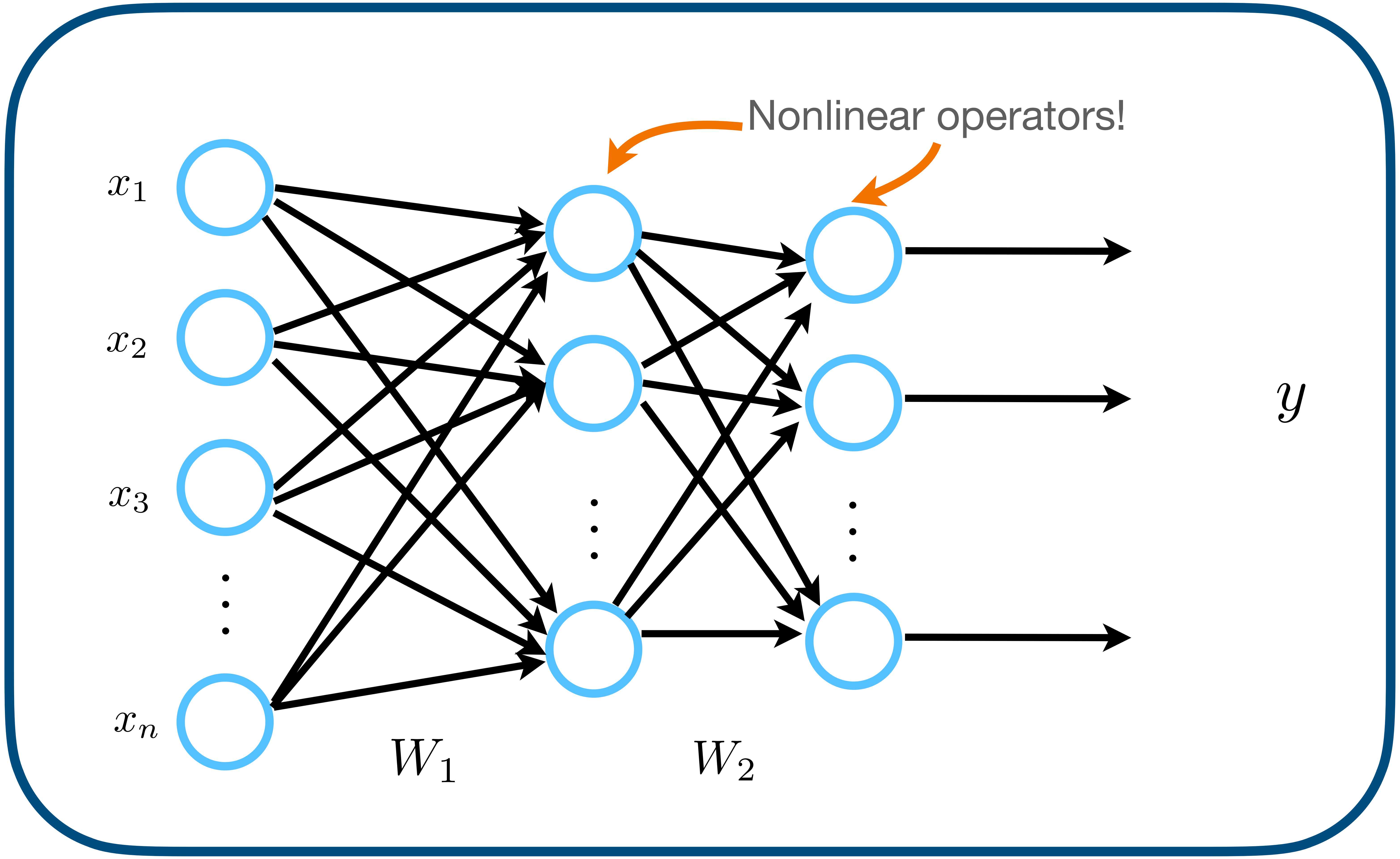


Combining all these things together: MLP

Feedforward/fully connected neural network



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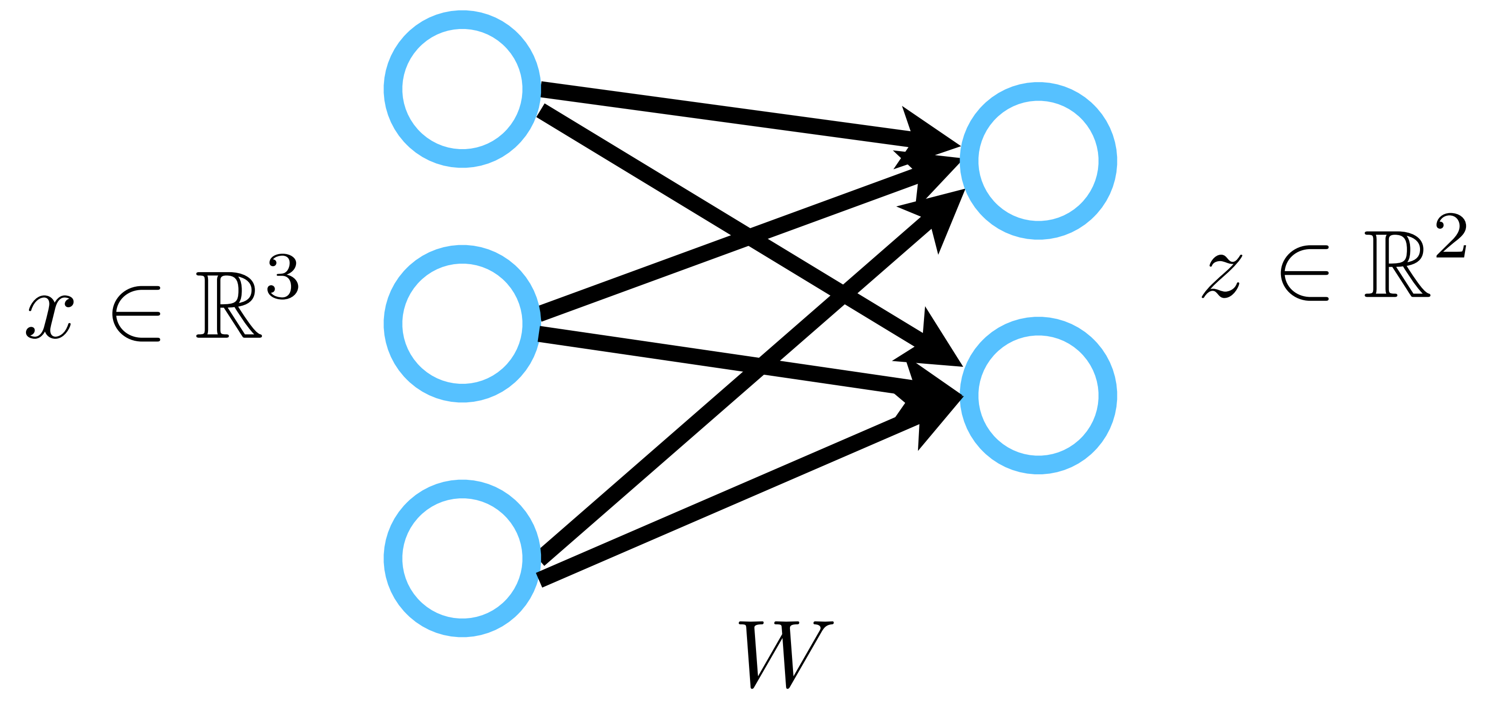

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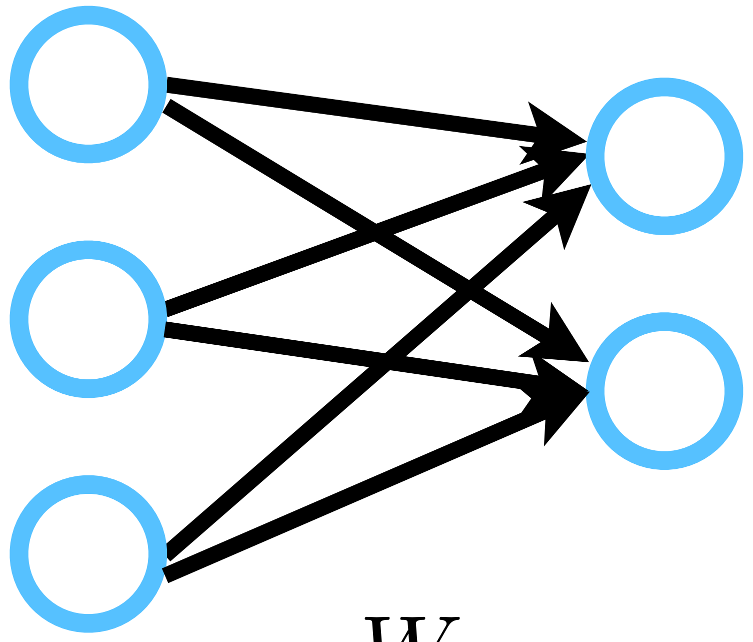

$z \in \mathbb{R}^2$

W

$$z = Wx = \begin{bmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

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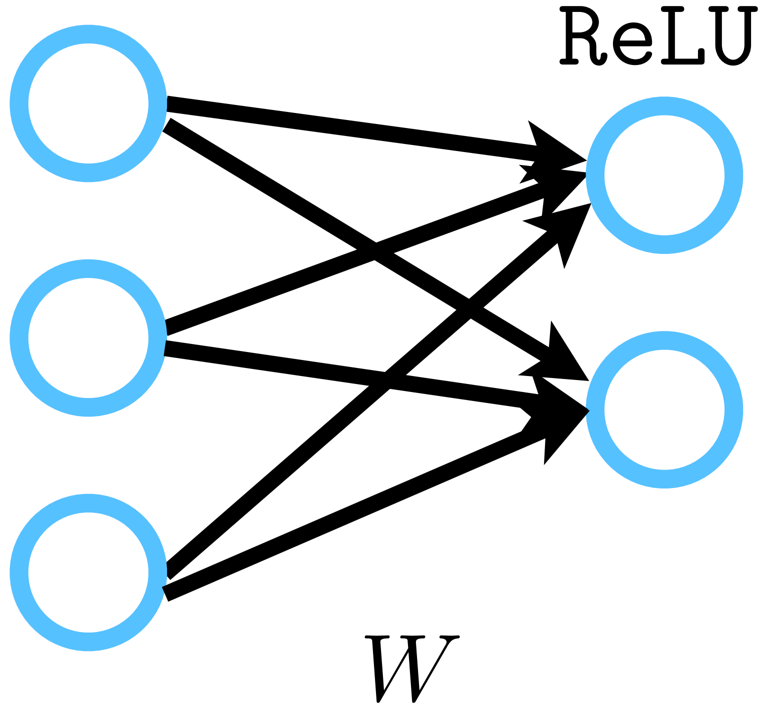

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$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} \texttt{ReLU}(W_{1,:}x) \\ \texttt{ReLU}(W_{2,:}x) \end{bmatrix}$$

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Goal: make loss as small as possible over the whole dataset ($\{x_i, y_i\}_{i=1}^n$)

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Learns from data: input could be pixels or words - usually no other information provided.
(This highlights the difference with the so far procedure: hand-crafted representation learning)

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(Quite abstract for now)

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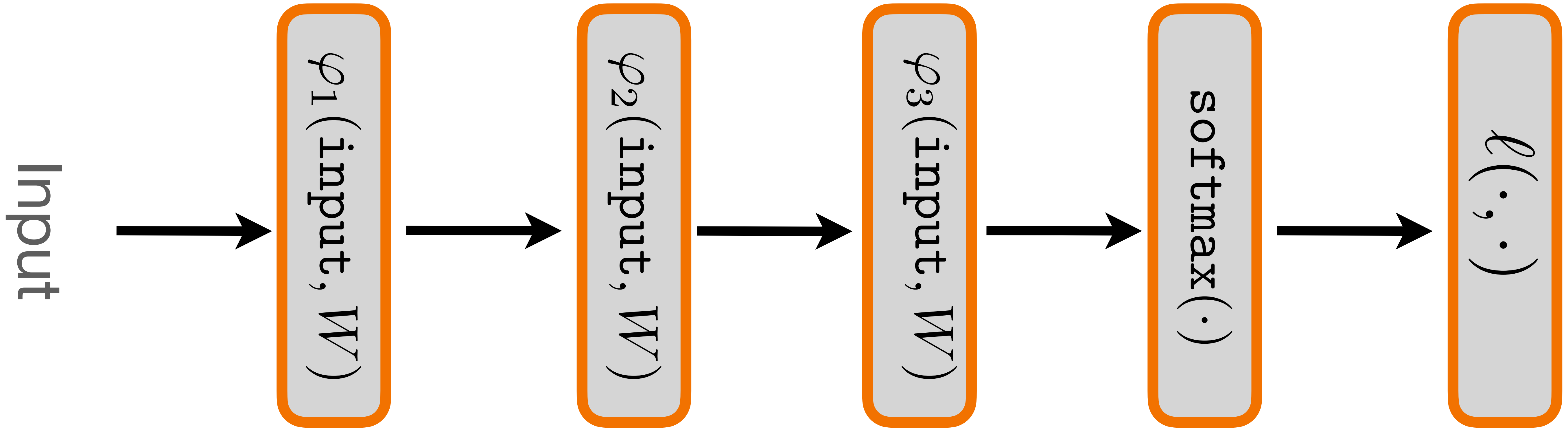

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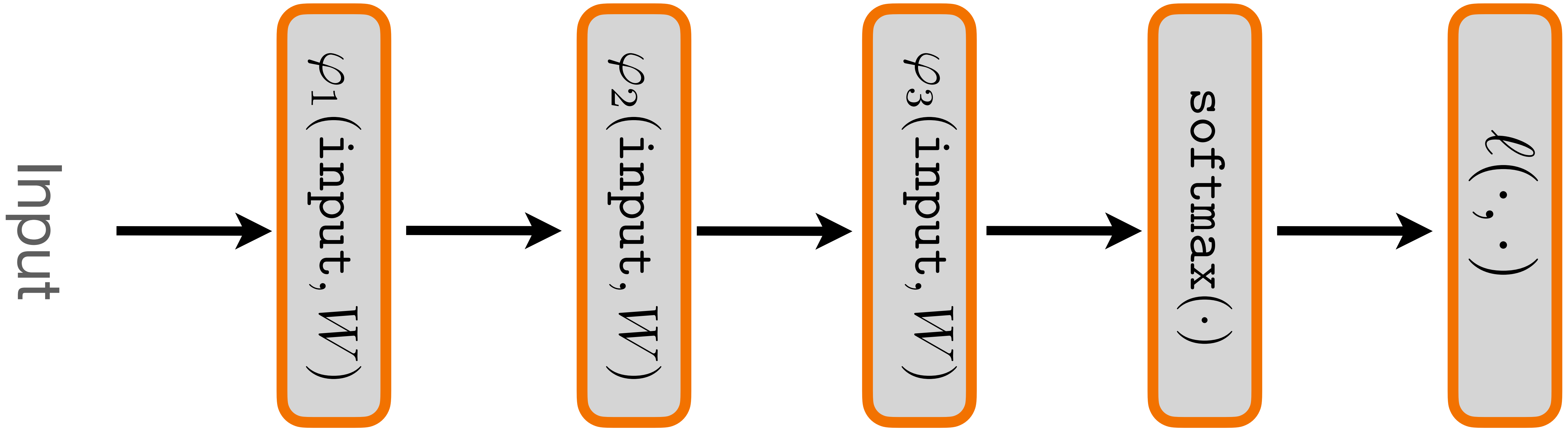

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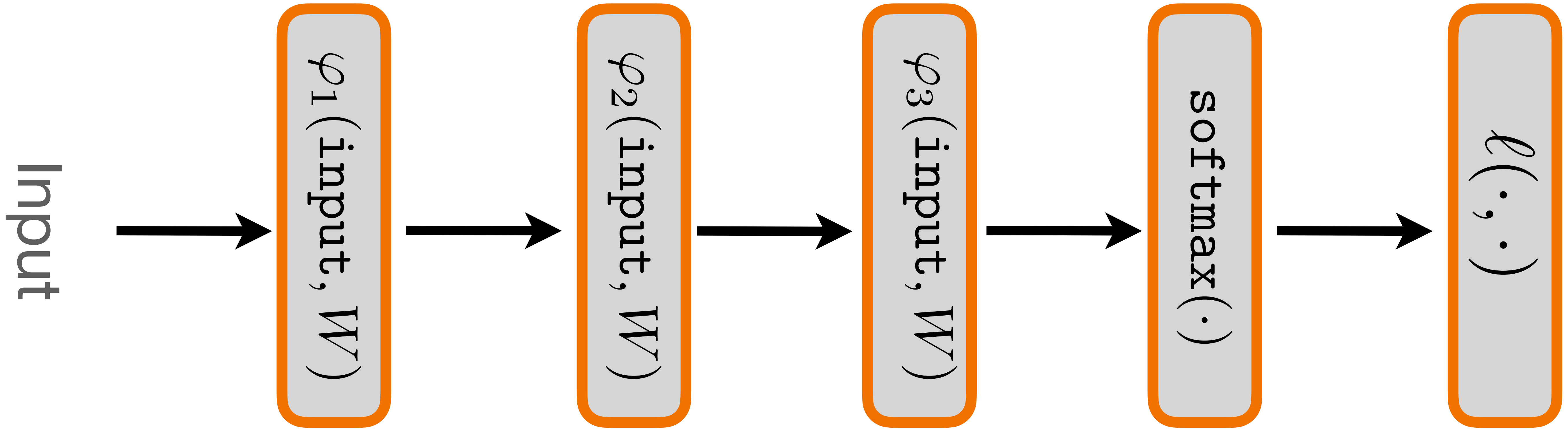

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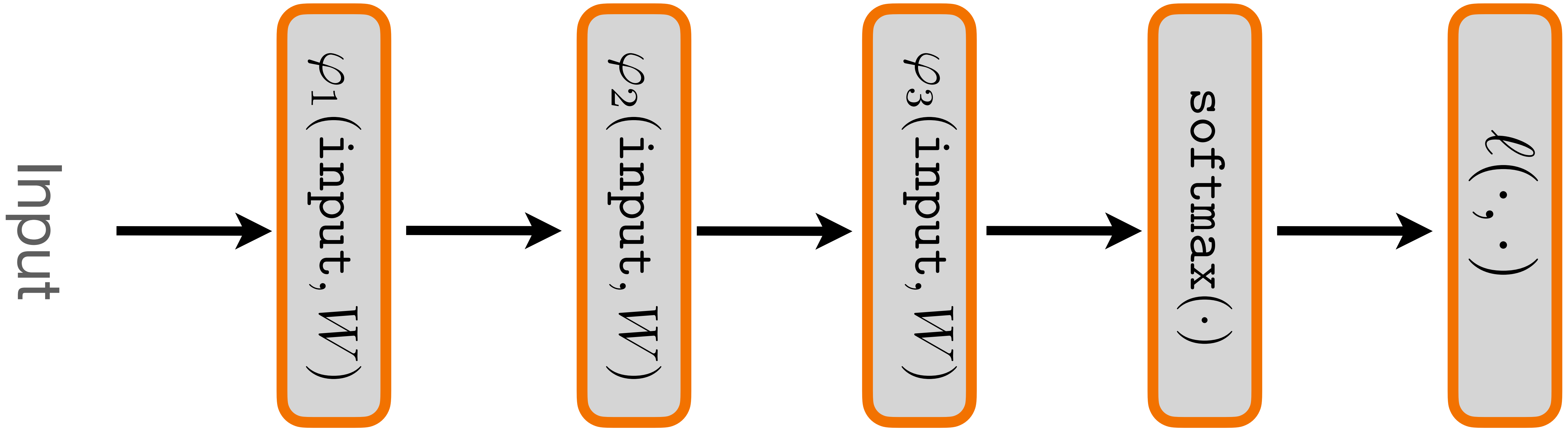

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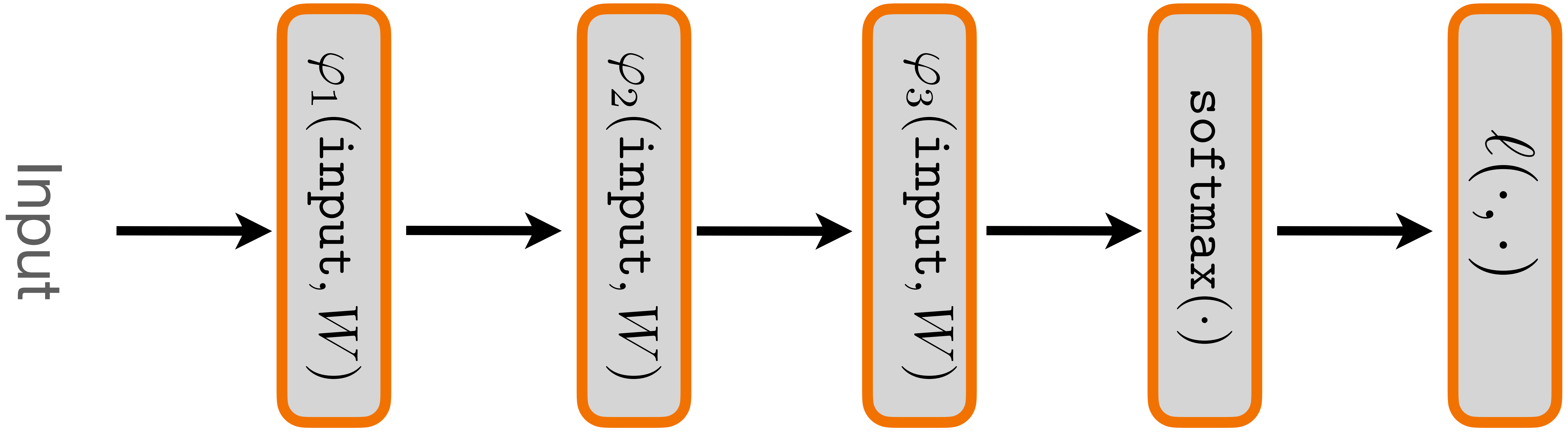

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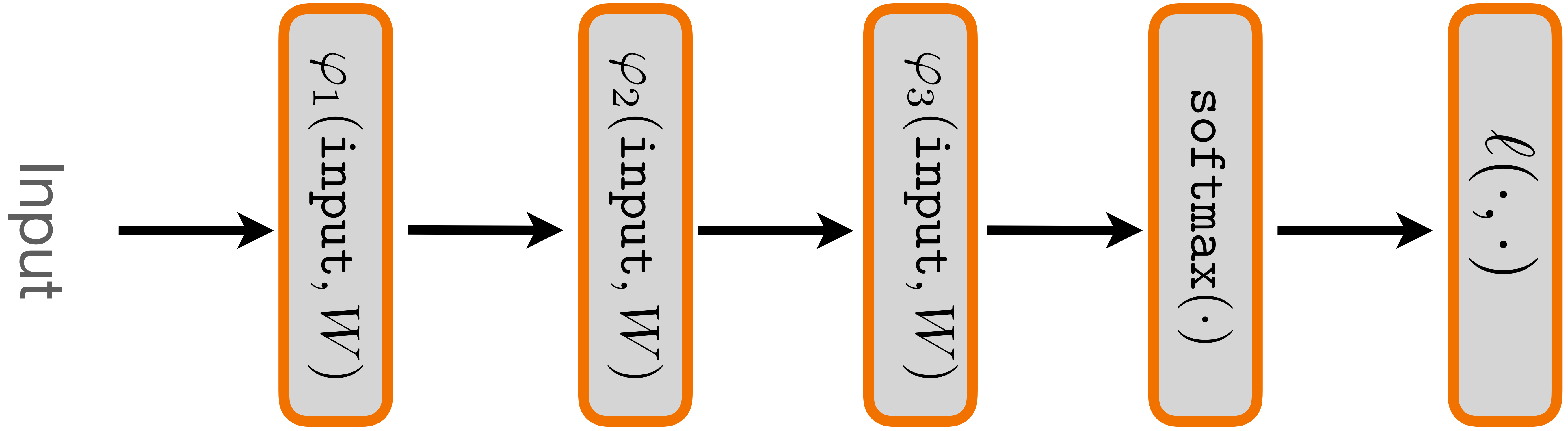

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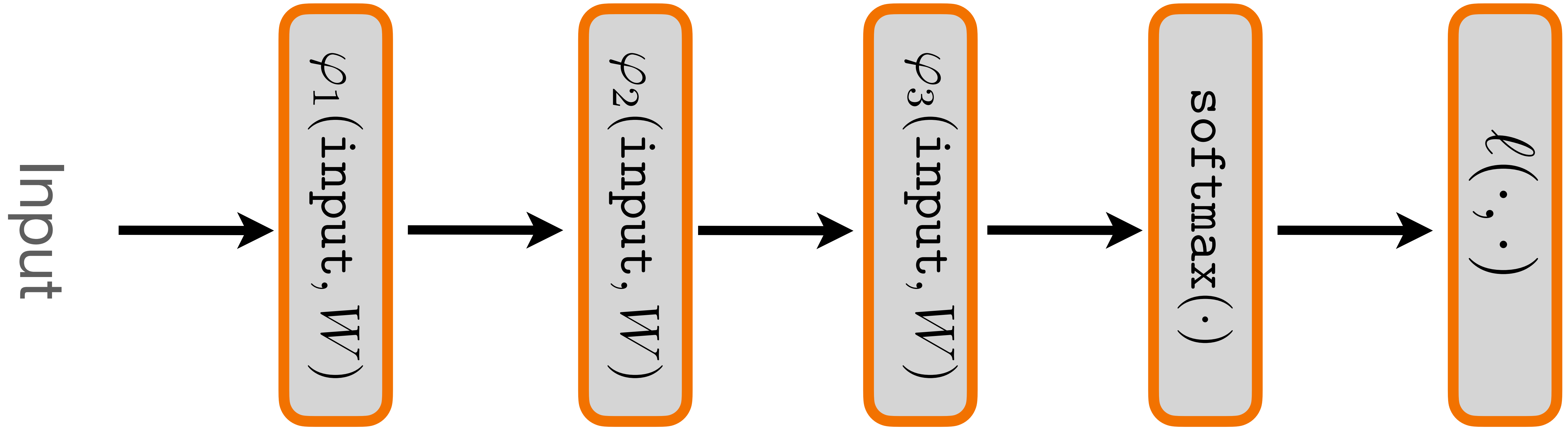

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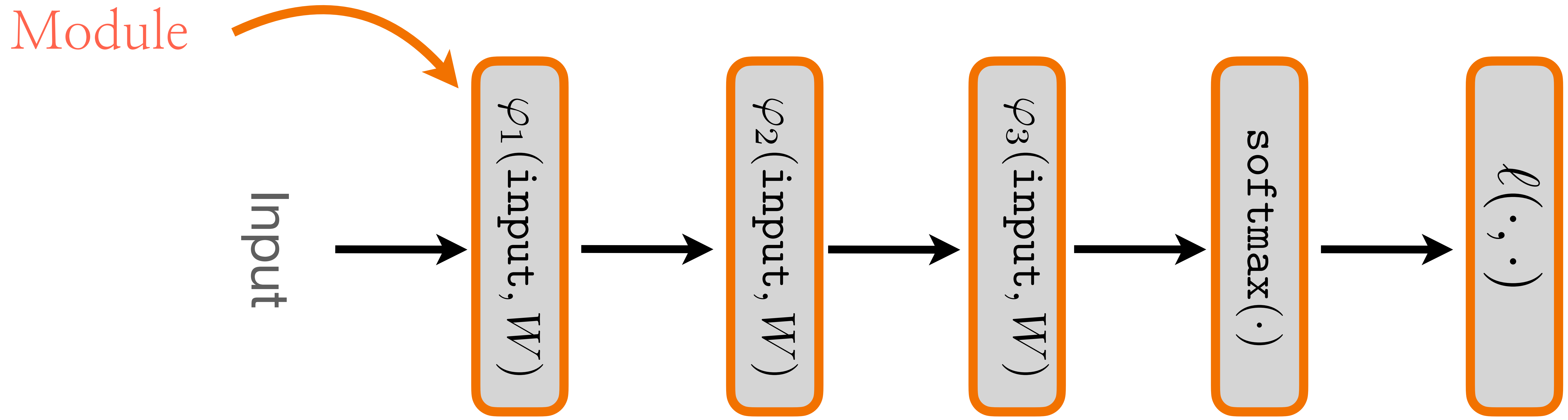

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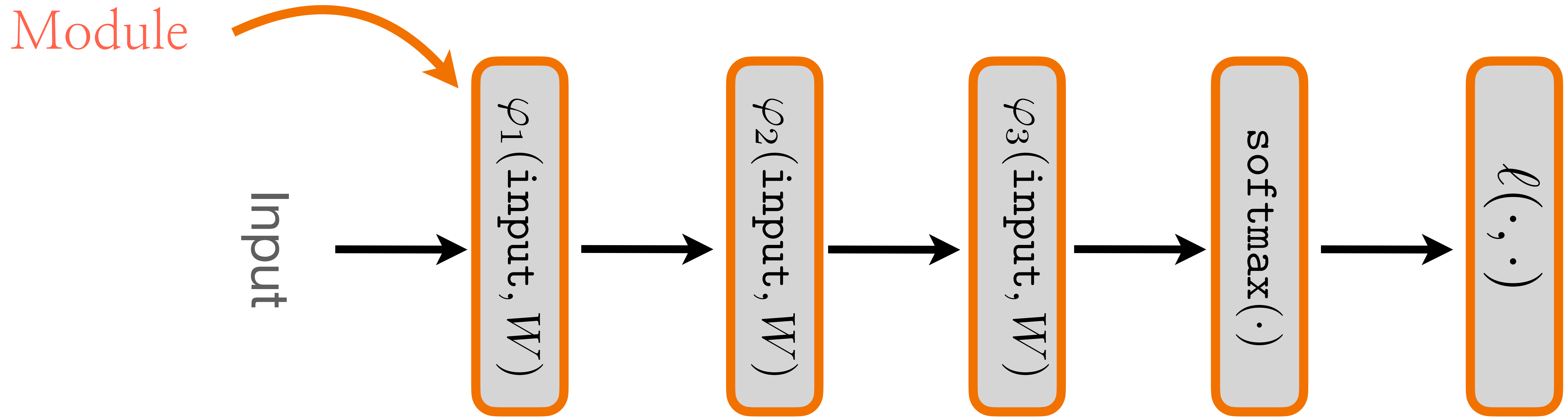

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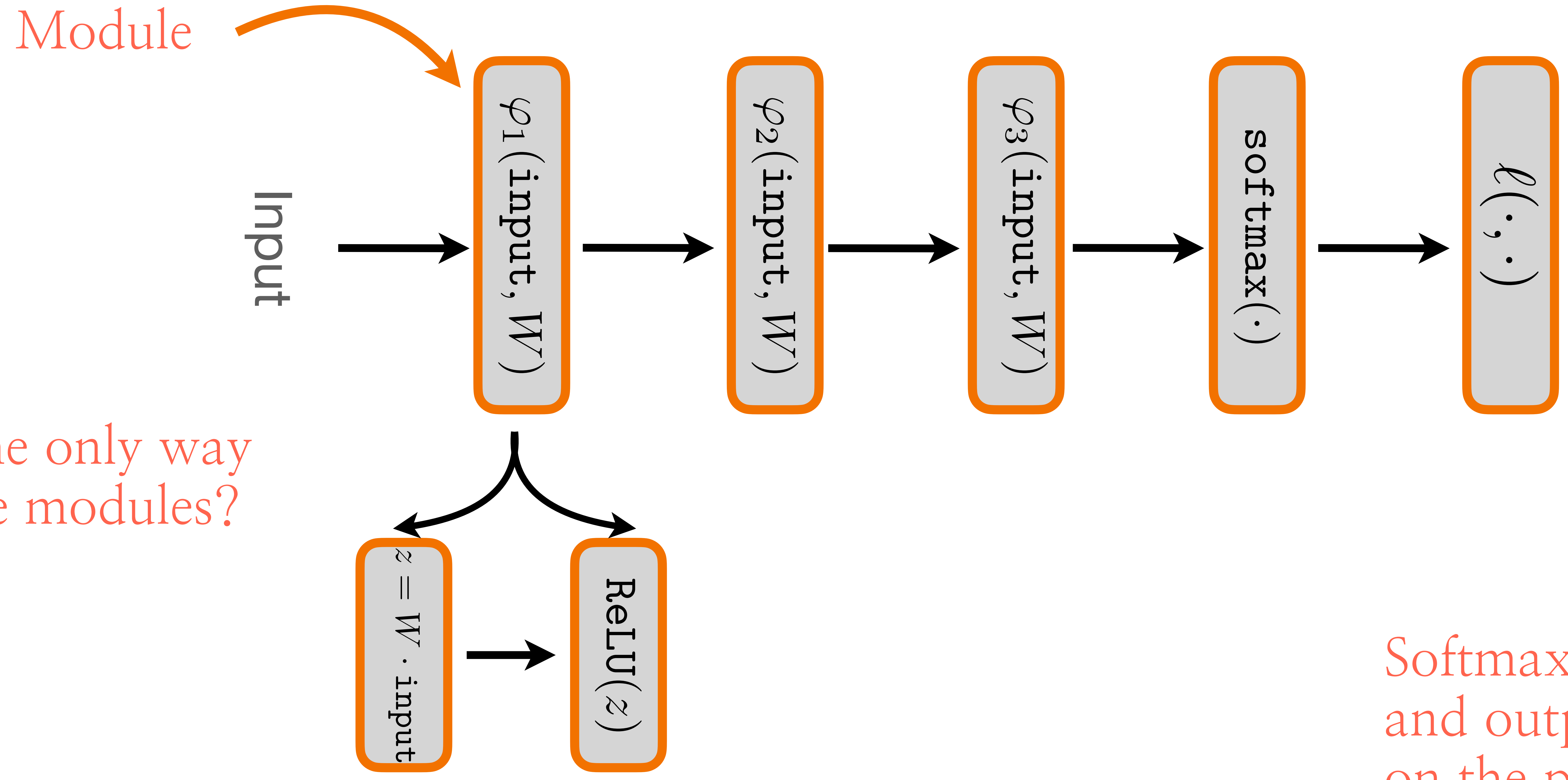

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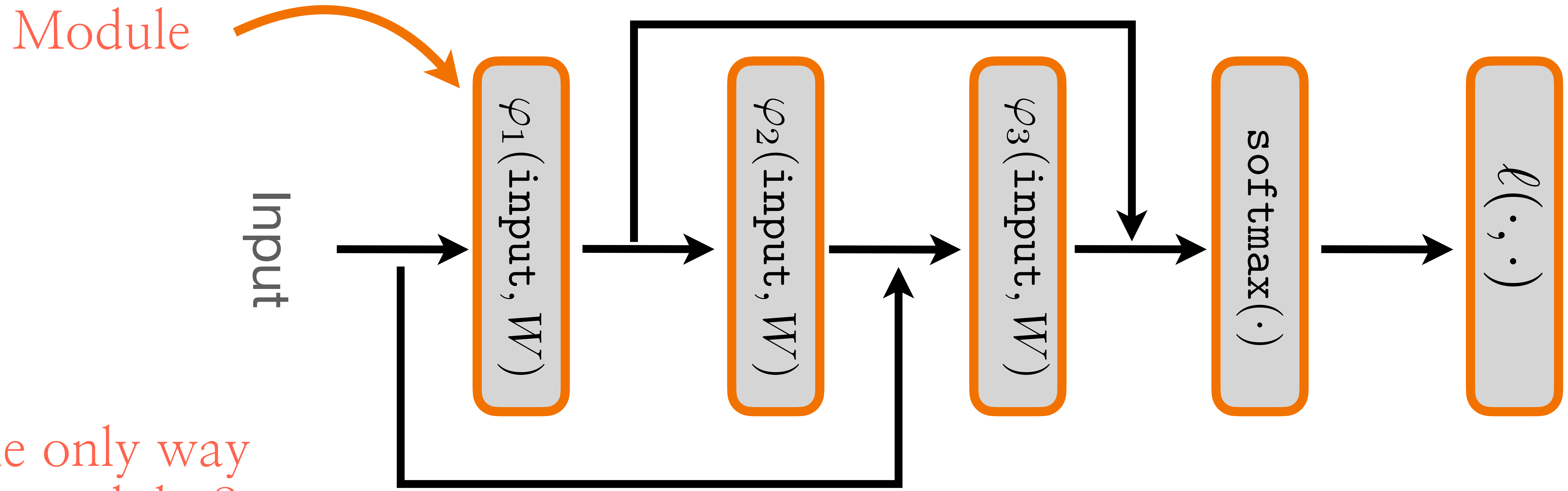

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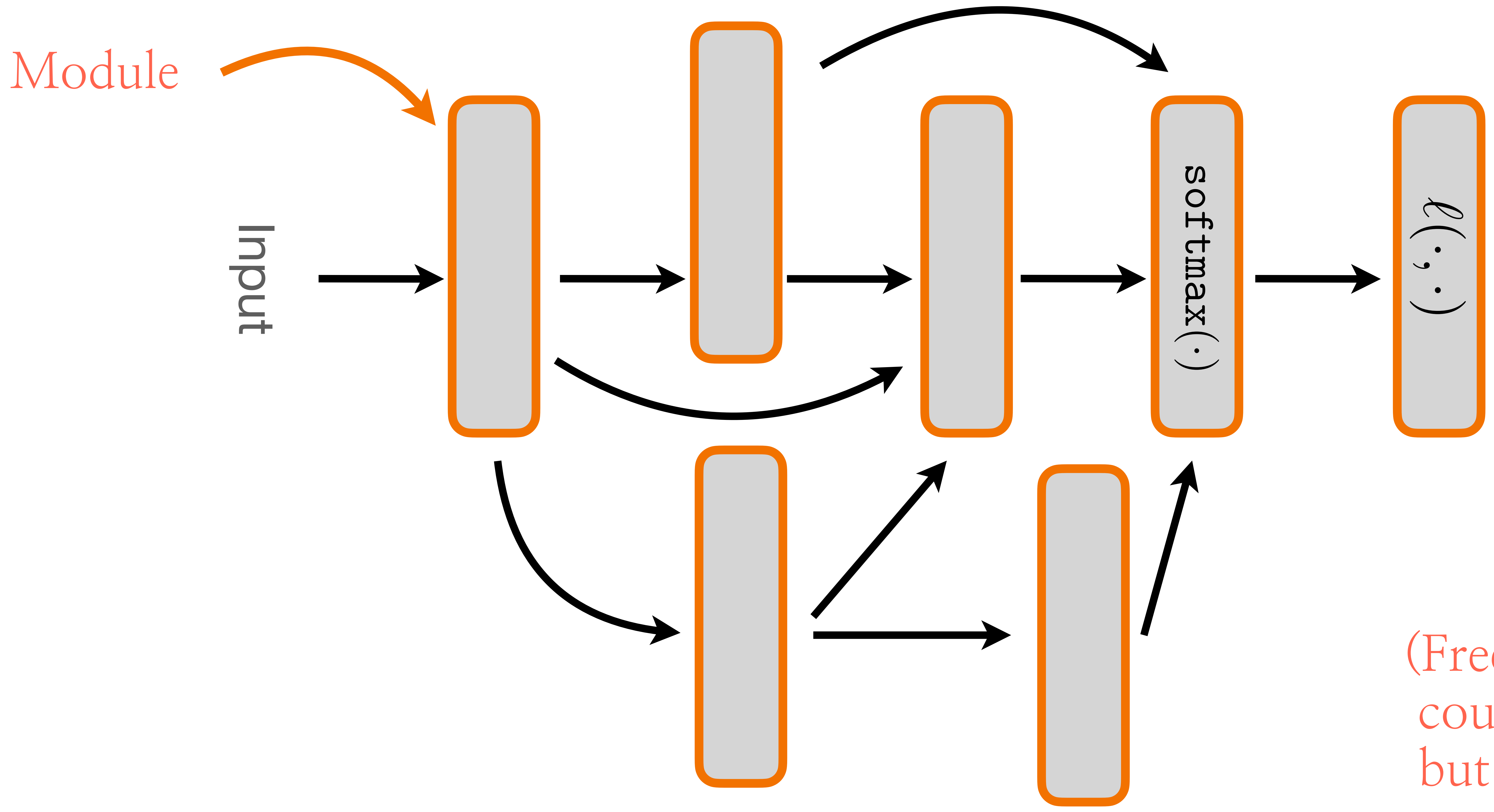

(Free lunch theorem: user bias could help you in one case, but can hurt you in another)

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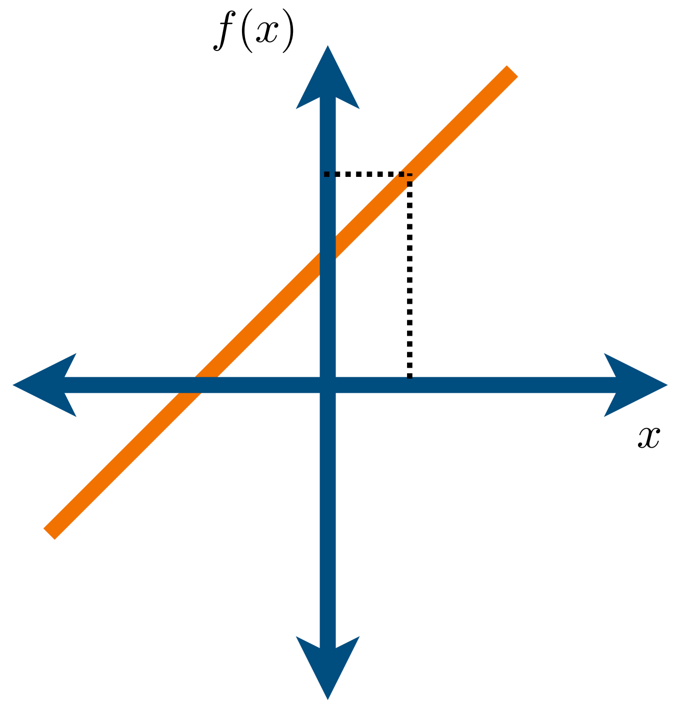

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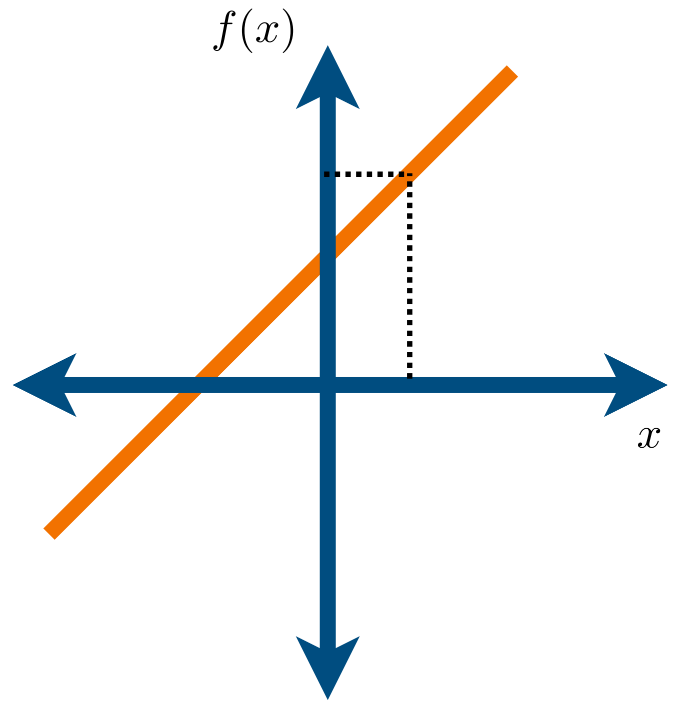
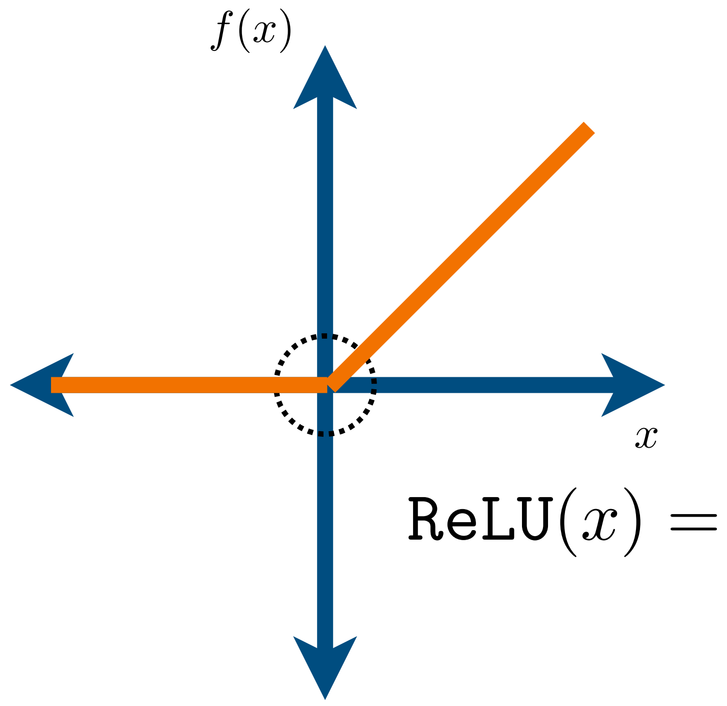
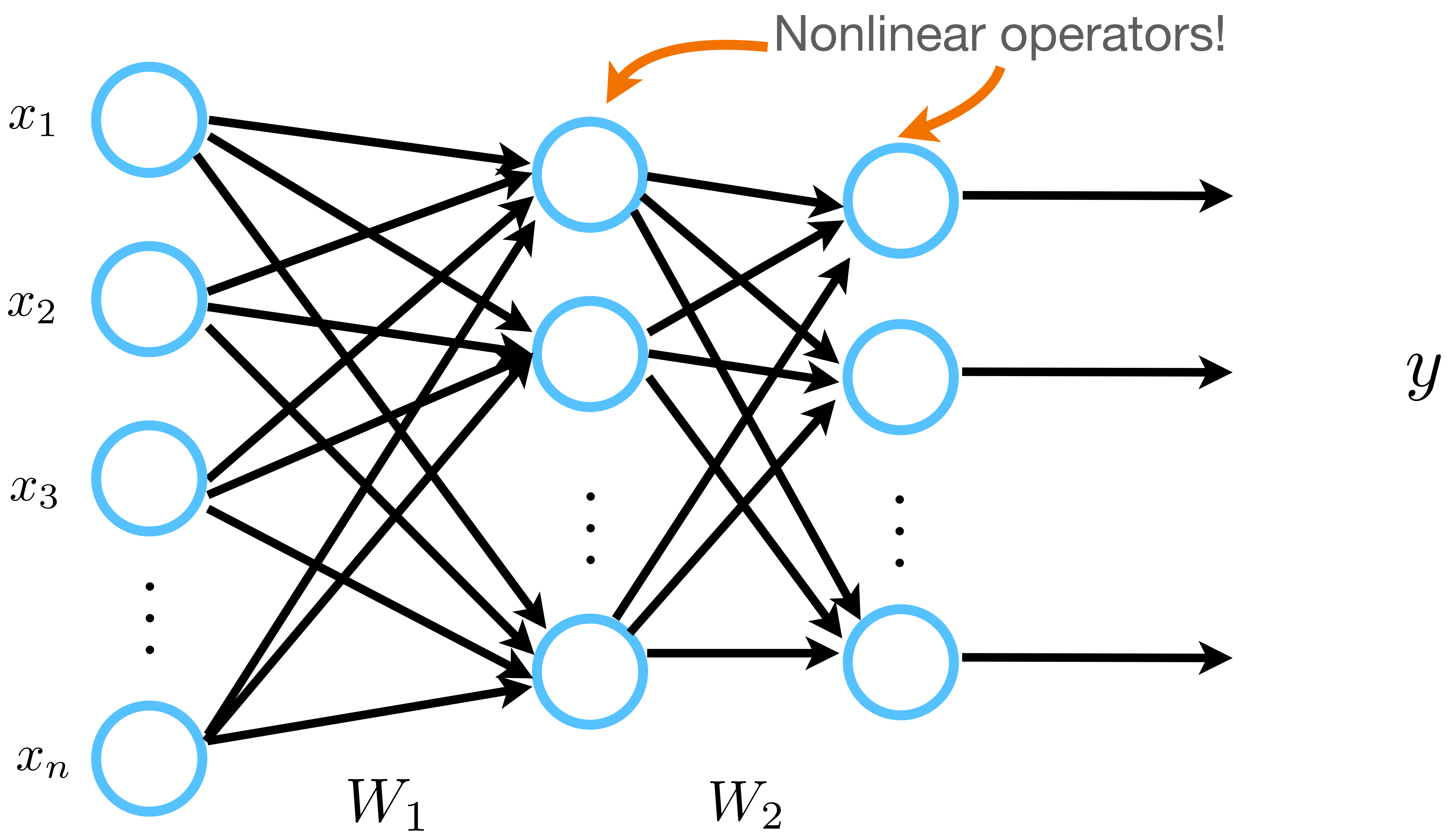




$$\texttt{ReLU}(x) = \begin{cases} x, & x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

Fully connected neural networks or MLPs



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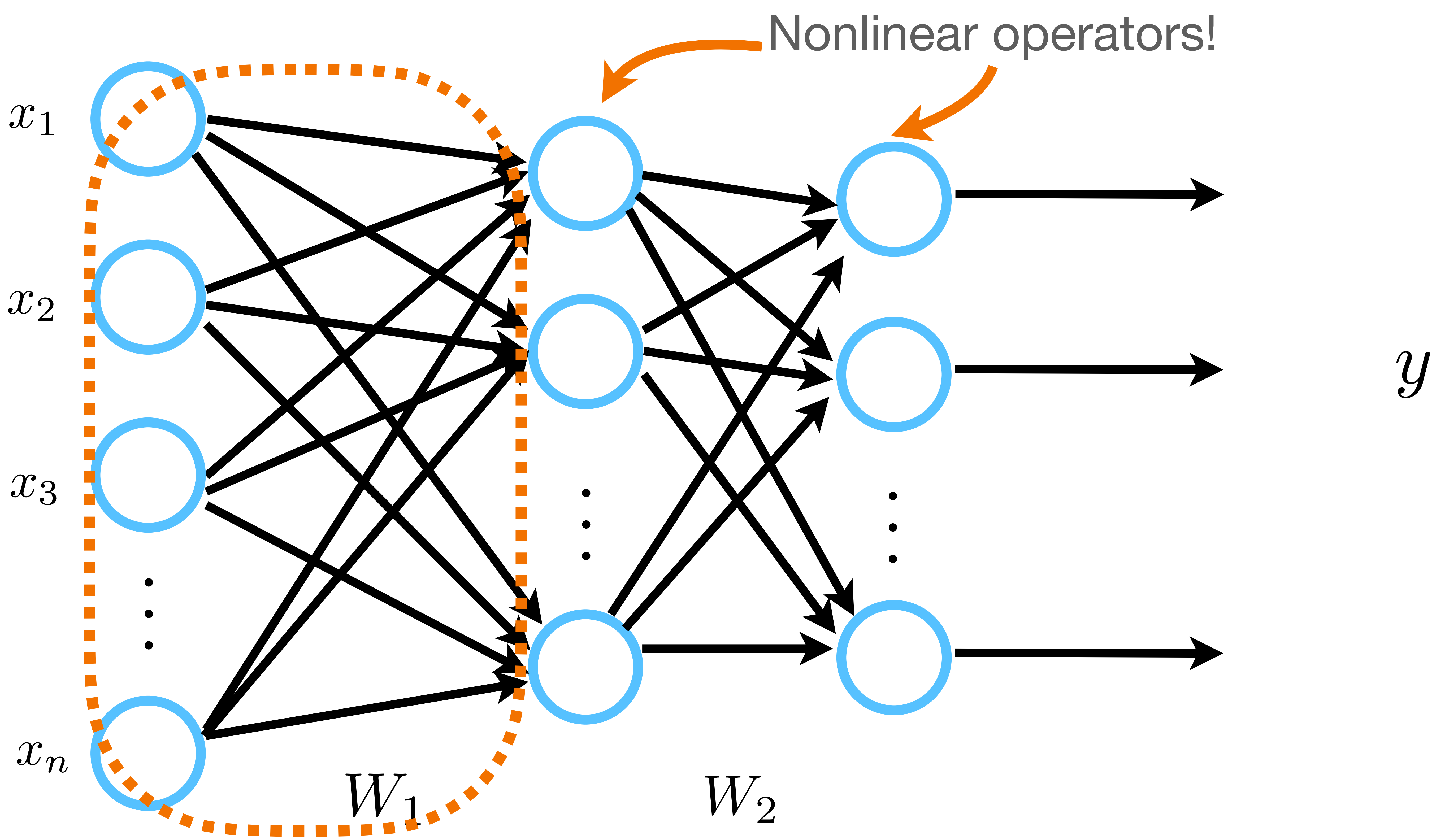

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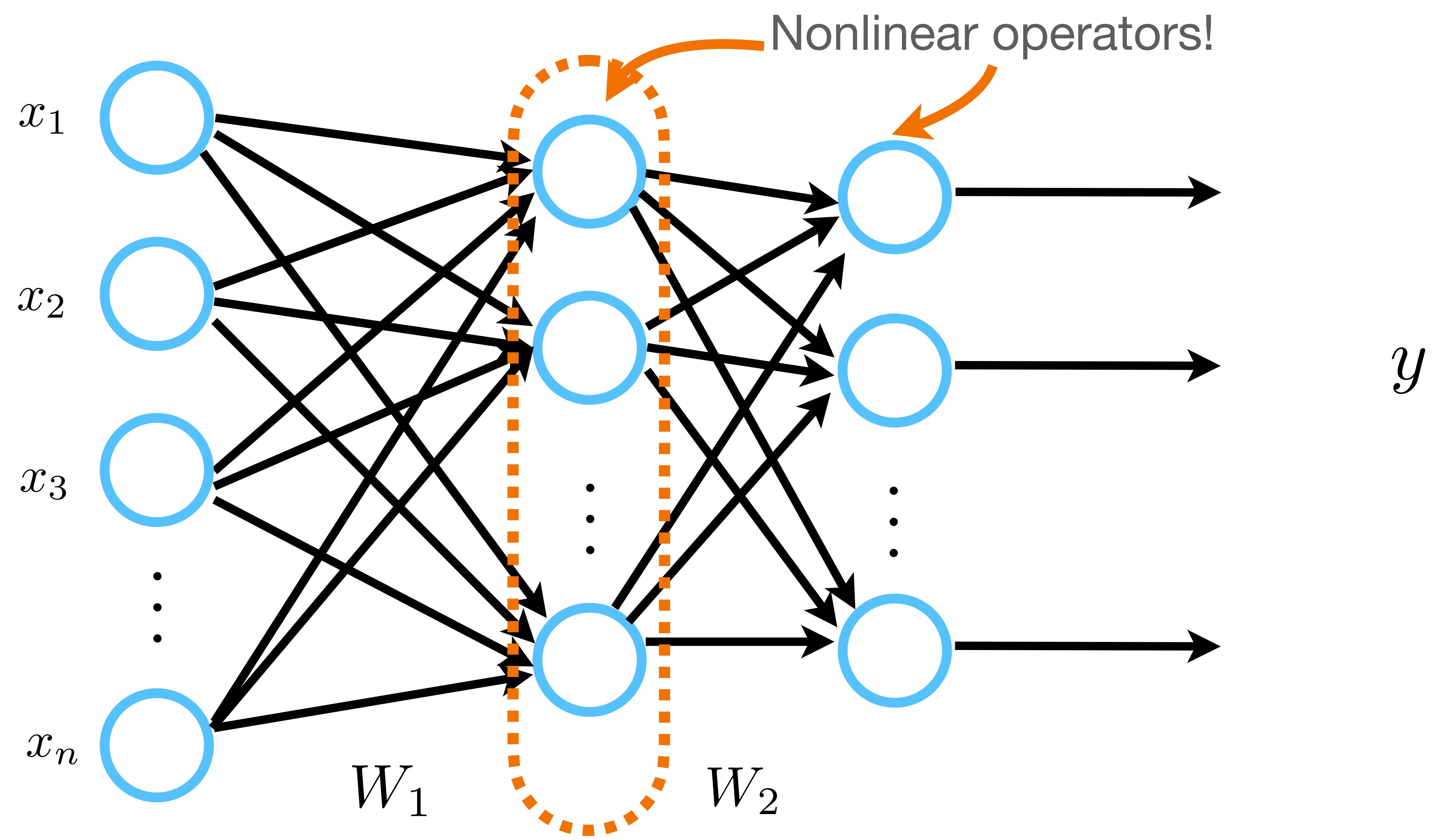

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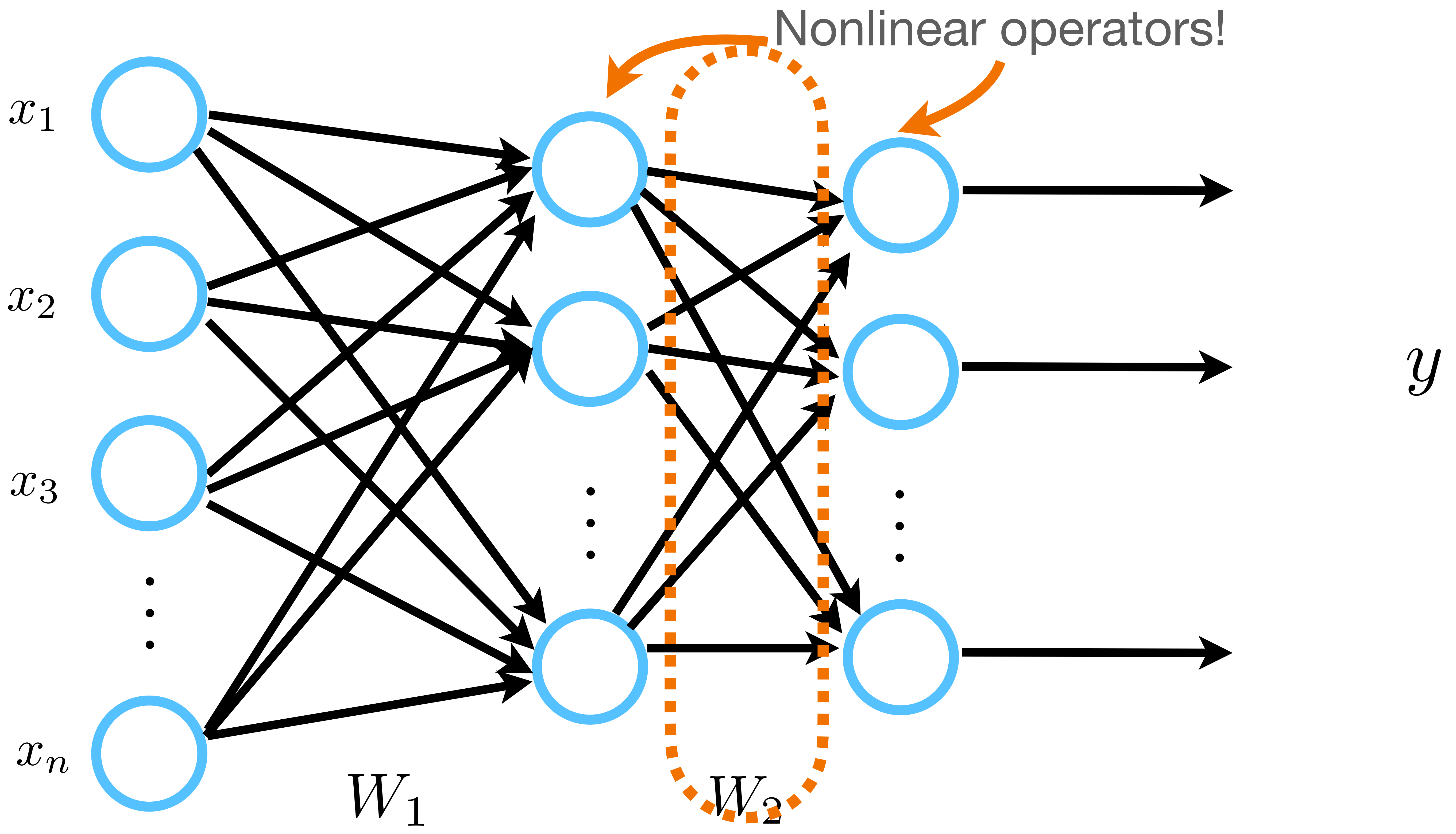

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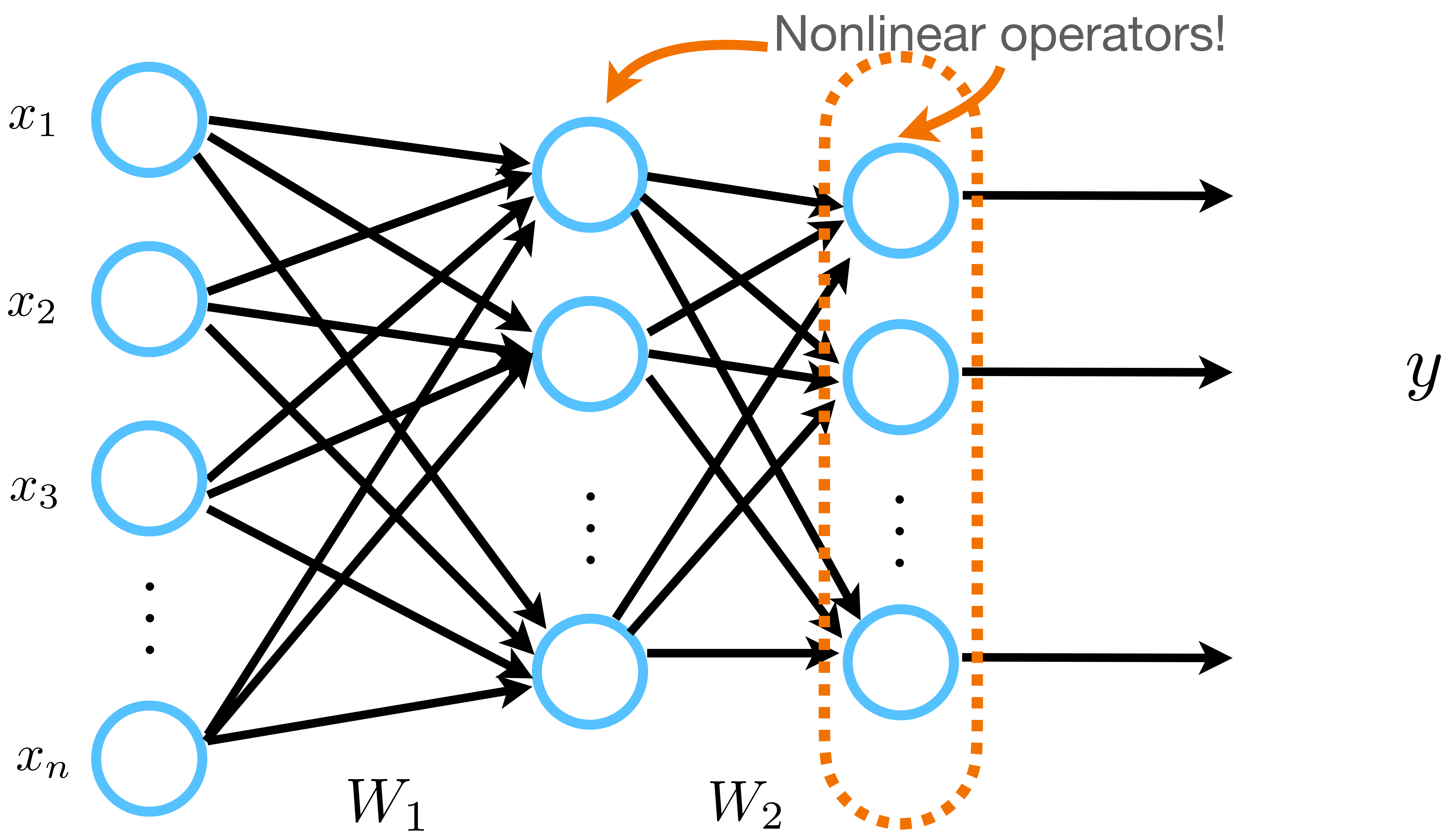
Fully connected neural networks or MLPs



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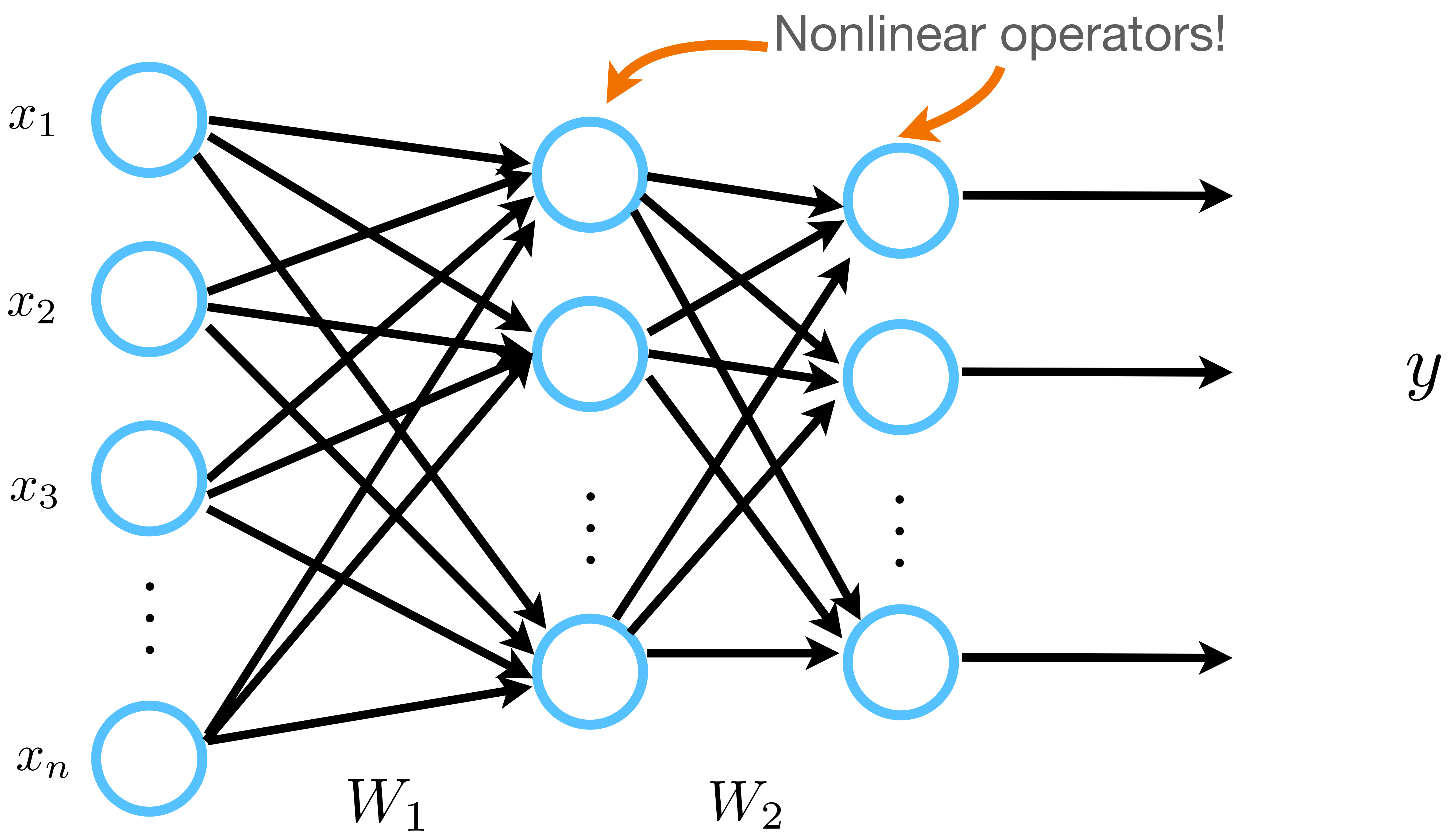

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- Famous architecture due to simplicity and theoretical guarantees

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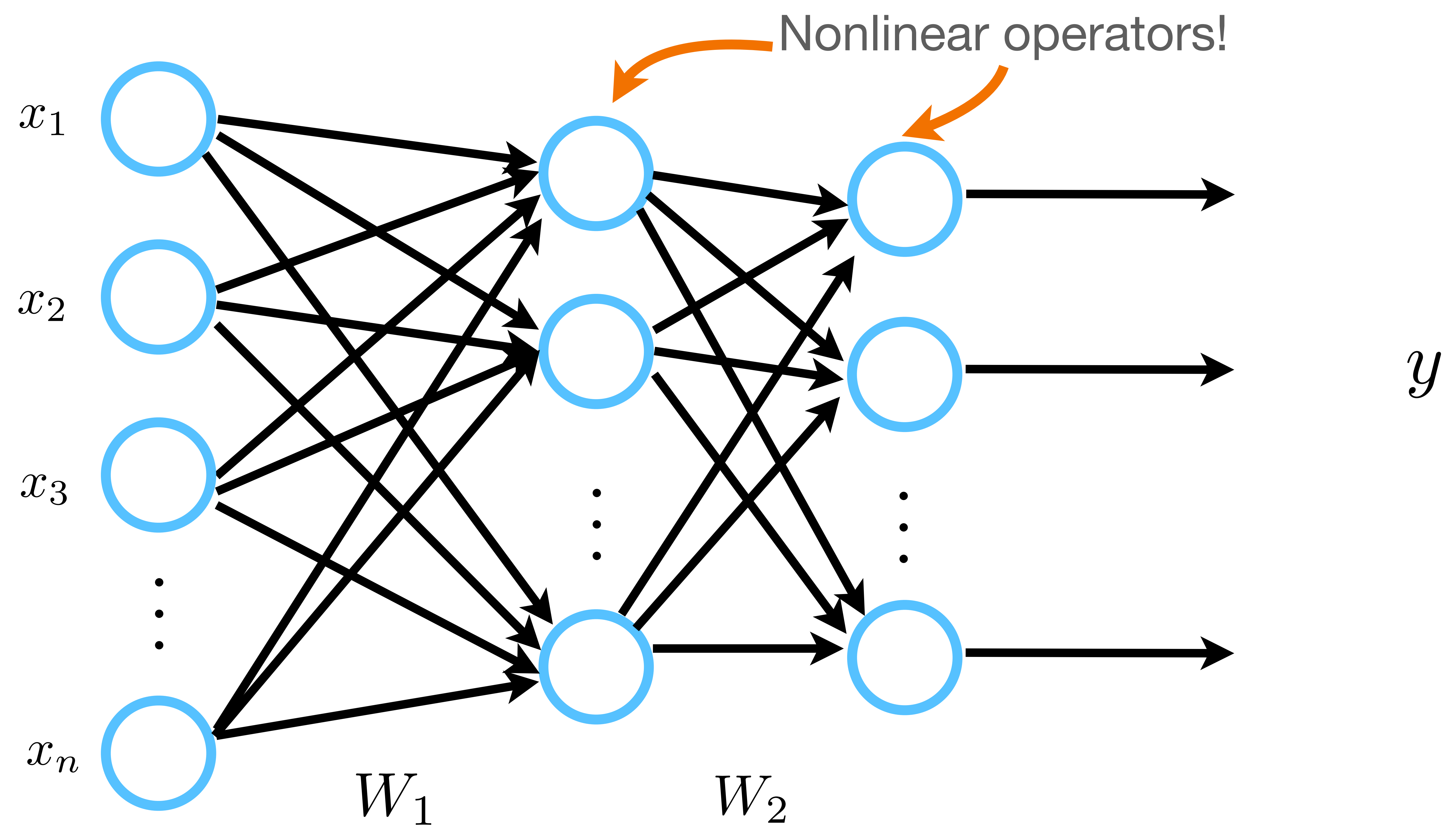

This sequence of operations is also known as the **forward pass on the neural network**

You can think of forward pass as function evaluation

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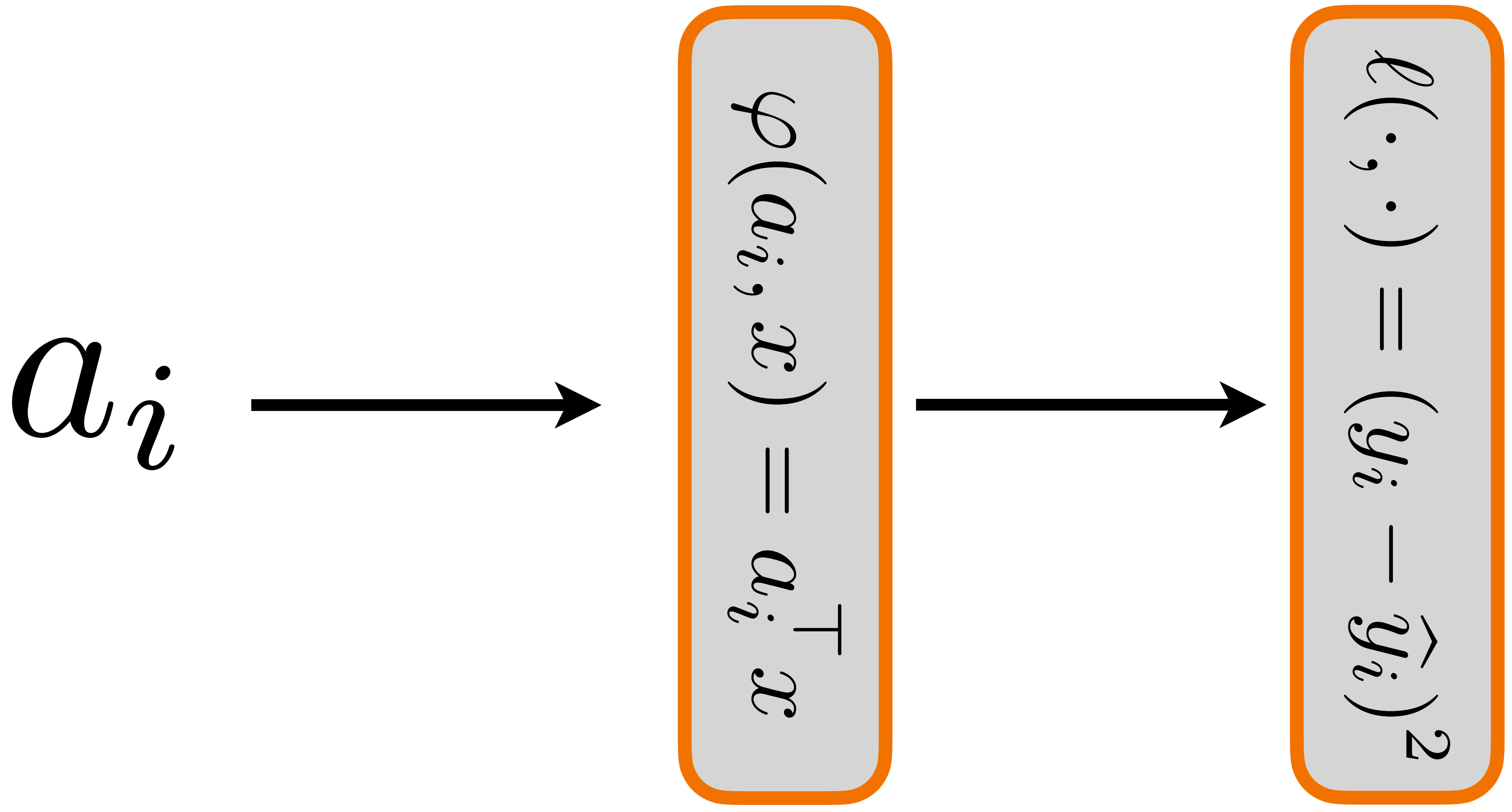

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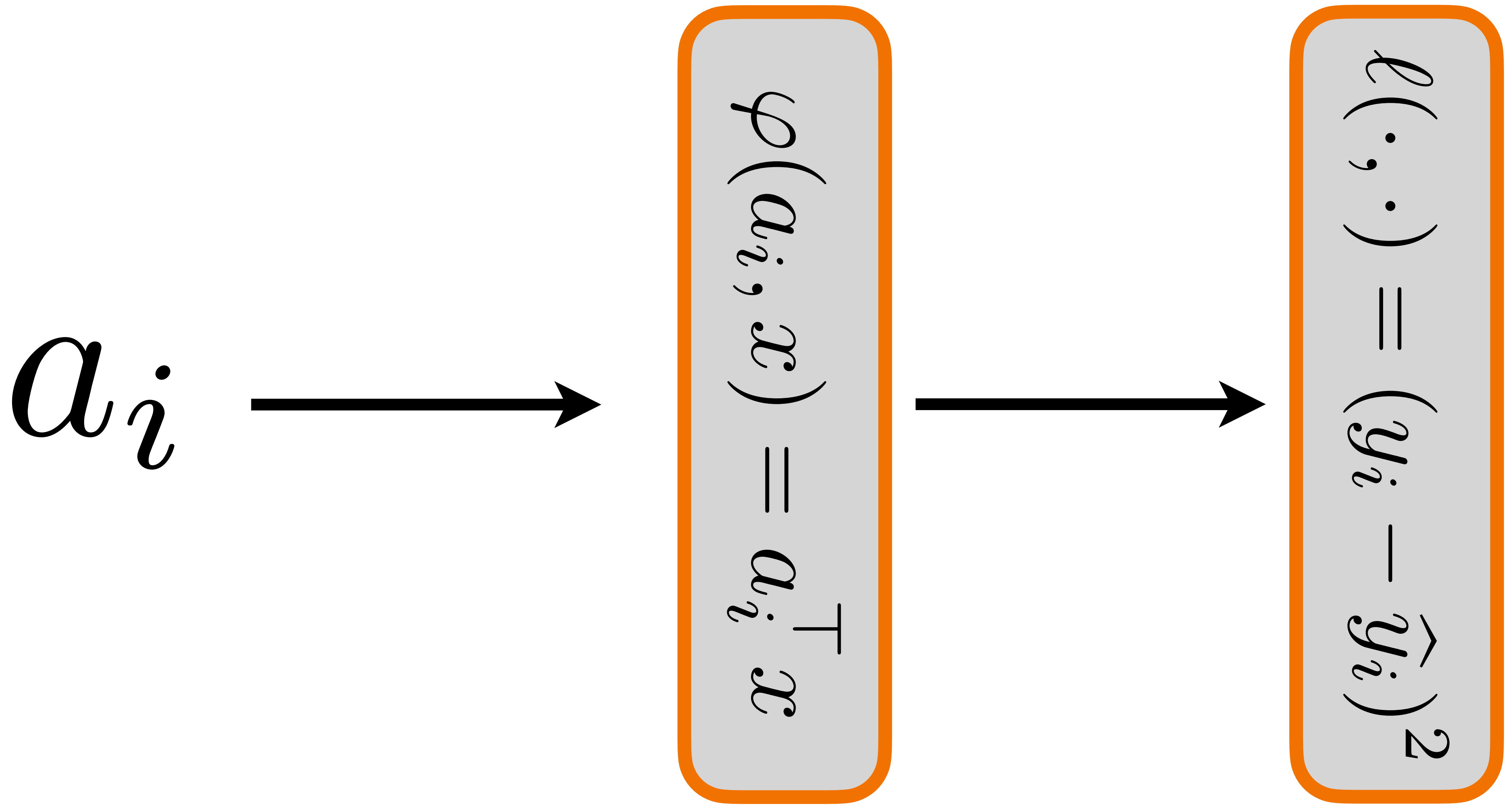

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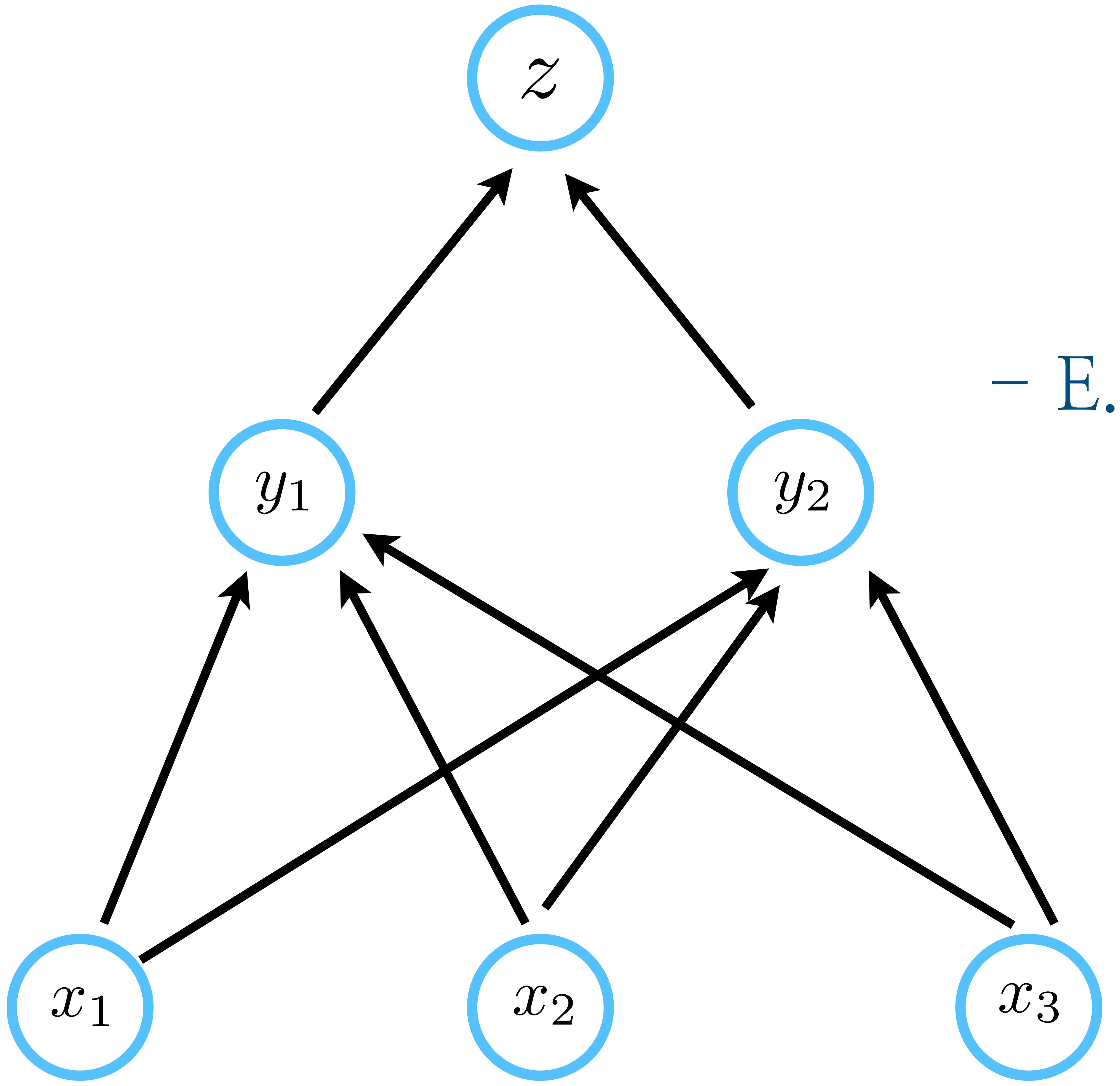
&= -2a_i(y_i - a_i^\top x)
\end{aligned}$$

(chain rule of derivatives)



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$$

– E.g.,

$$\frac{\partial z}{\partial x_3} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_3} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_3}$$

(Follow all relevant paths)

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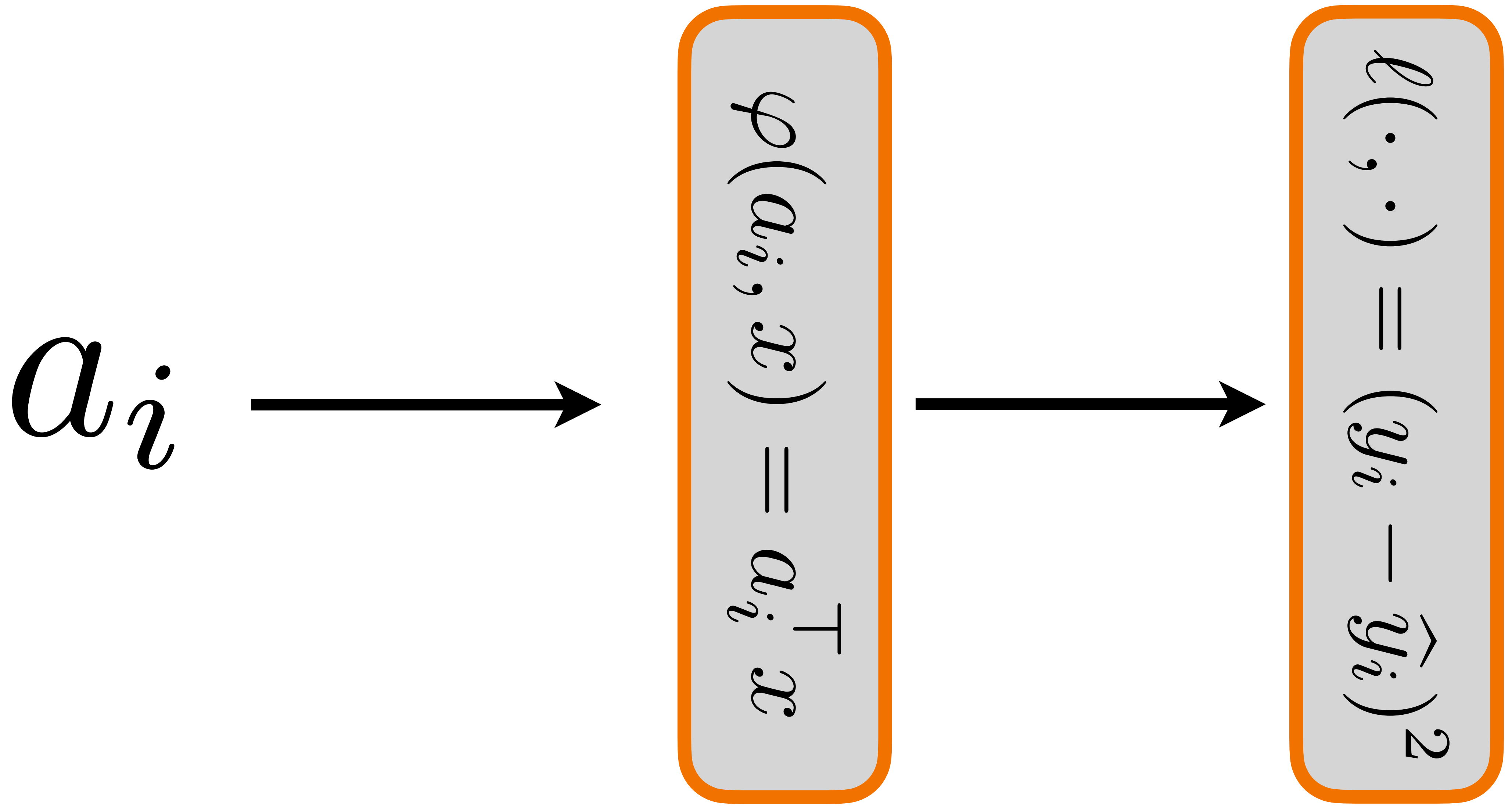

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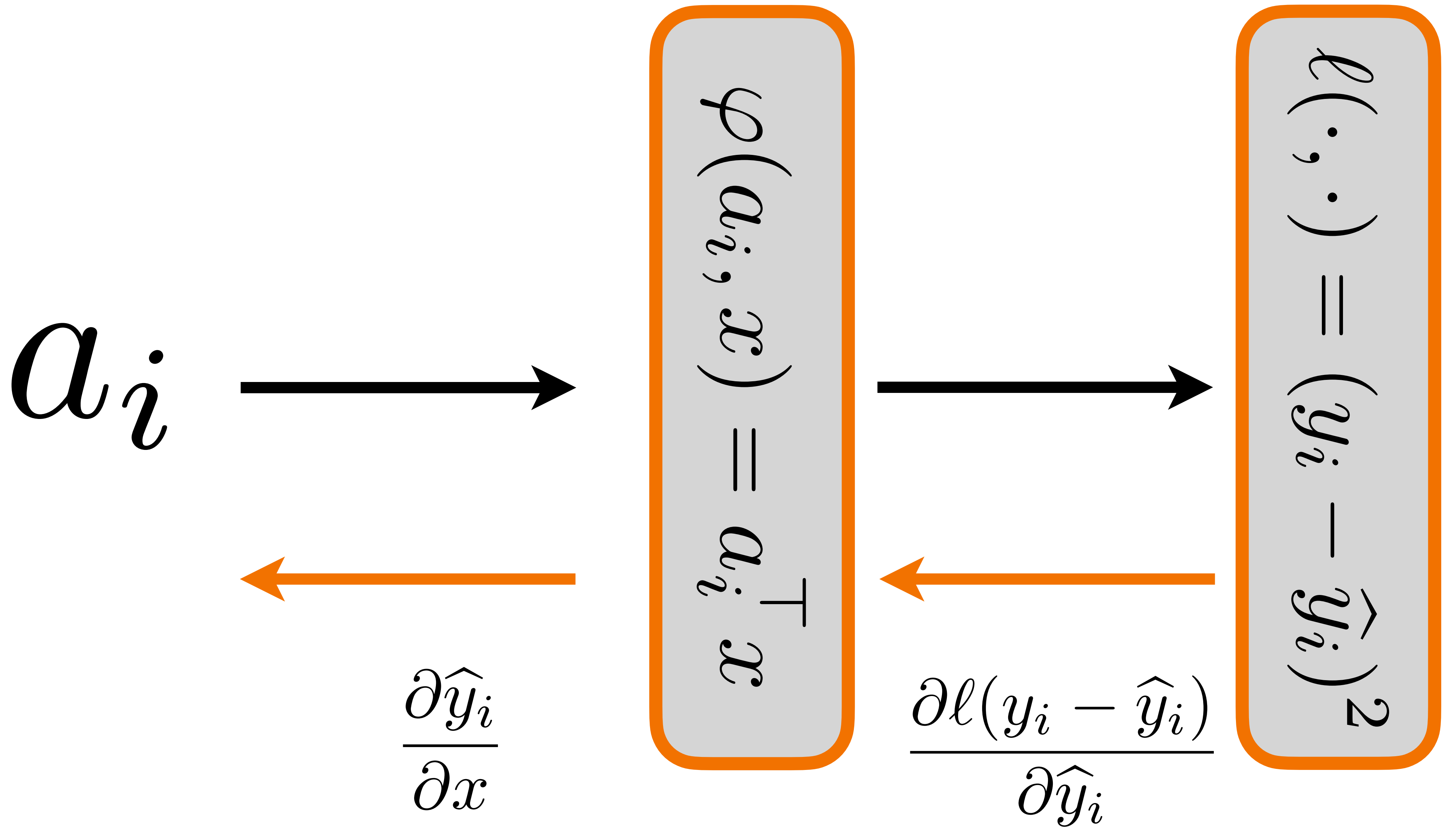

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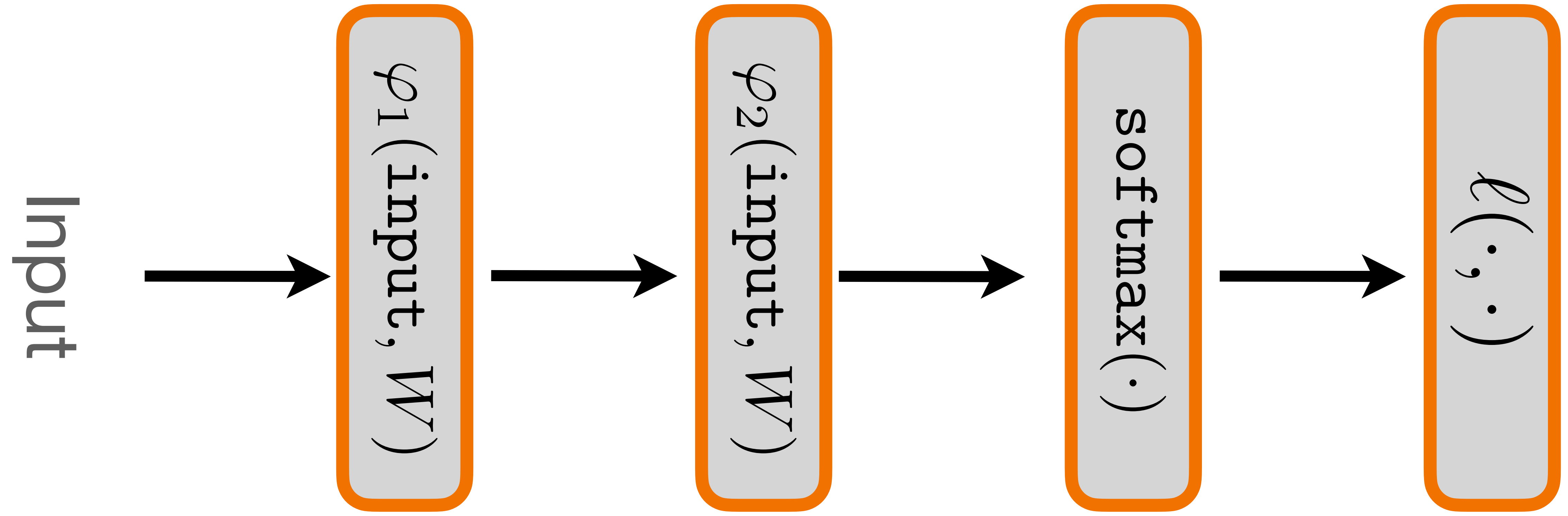

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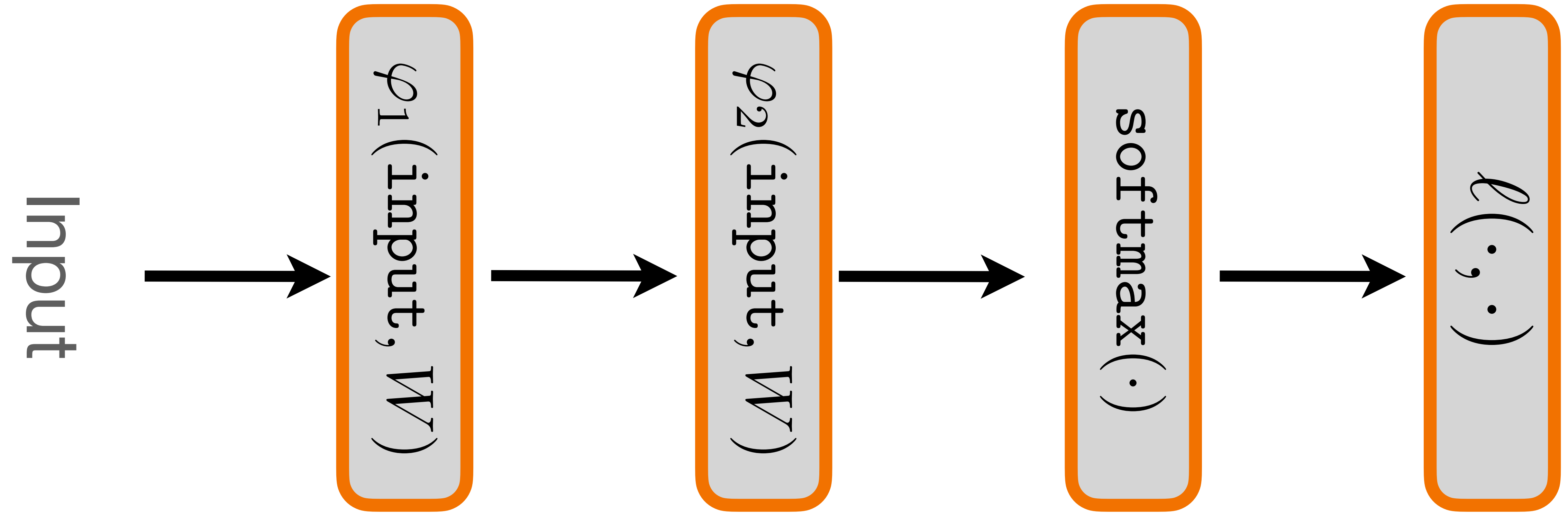

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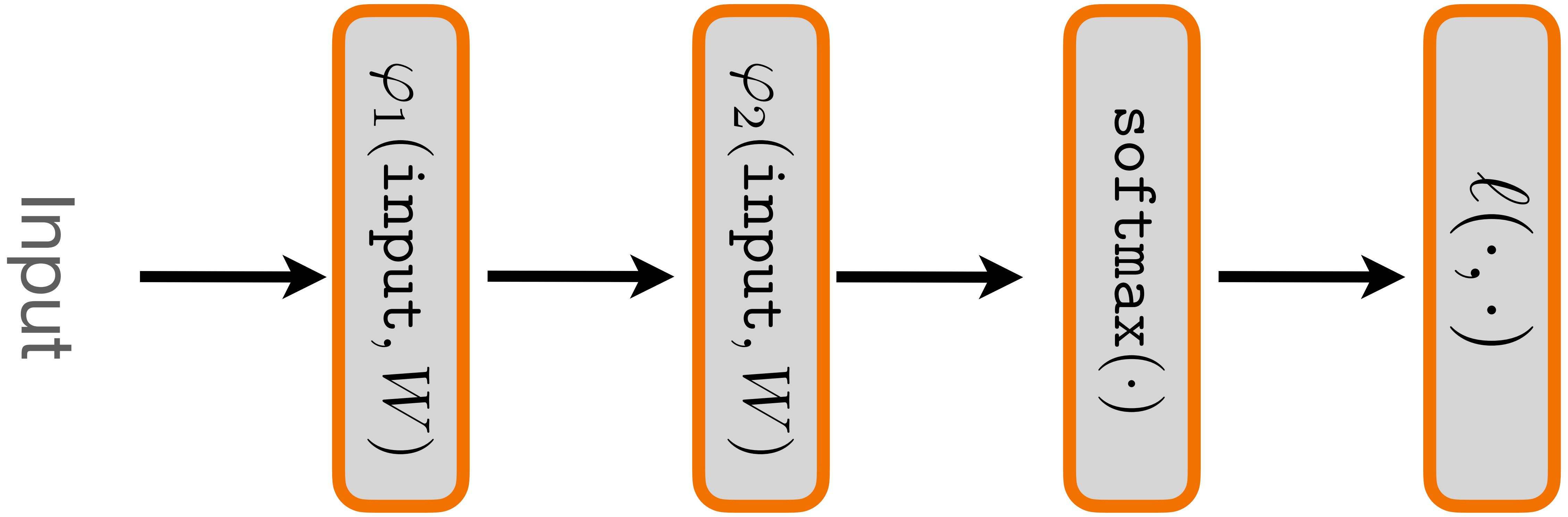

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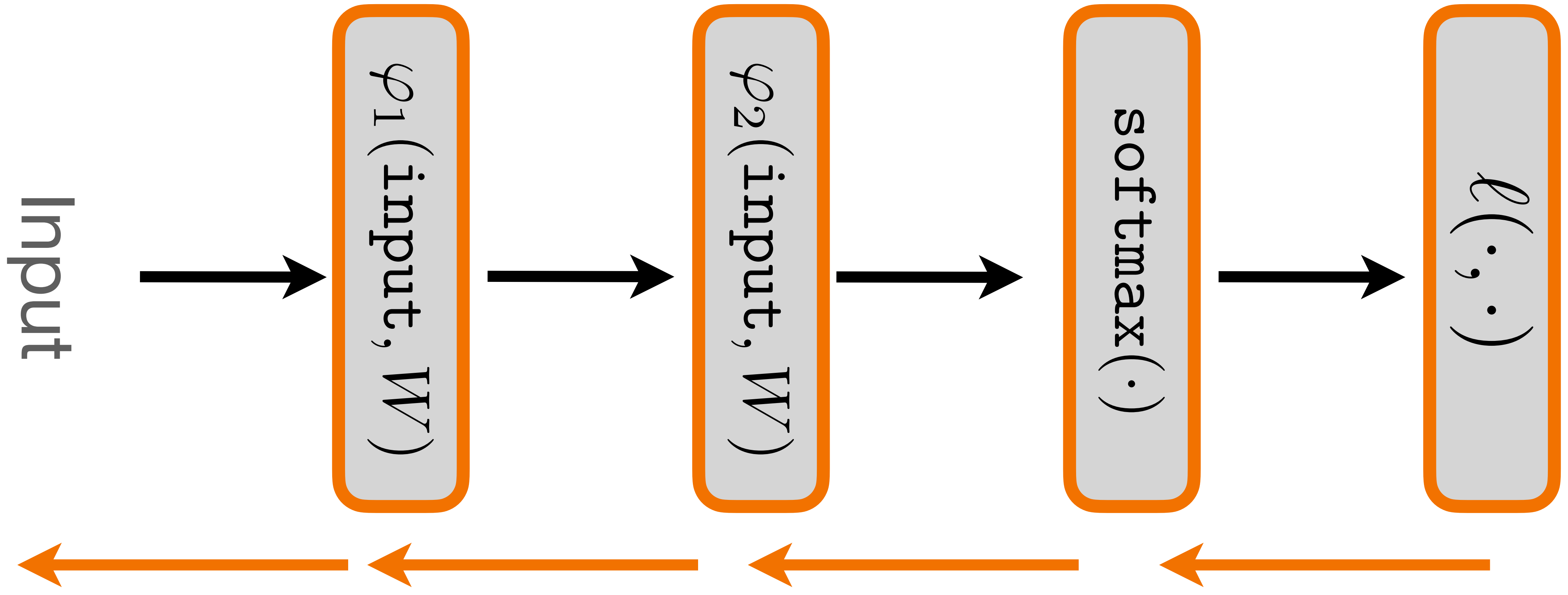

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Backpropagation = Gradient descent

(Just done efficiently on graphs, without redoing calculations)

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- We have set up background of smooth optimization
- We have provided the first convergence rate result, and defined different convergence rates that could be attainable

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Next lecture

– Brief introduction to convex optimization and related topics