COMP 545: Advanced topics in optimization
From simple to complex ML systems

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 the important class of **convex optimization**
    - Discuss about **convergence rates** and some **lower bounds** on such rates

Convex vs. non-convex optimization

(Naive interpretation of) Space of optimization problems

Convex vs. non-convex optimization

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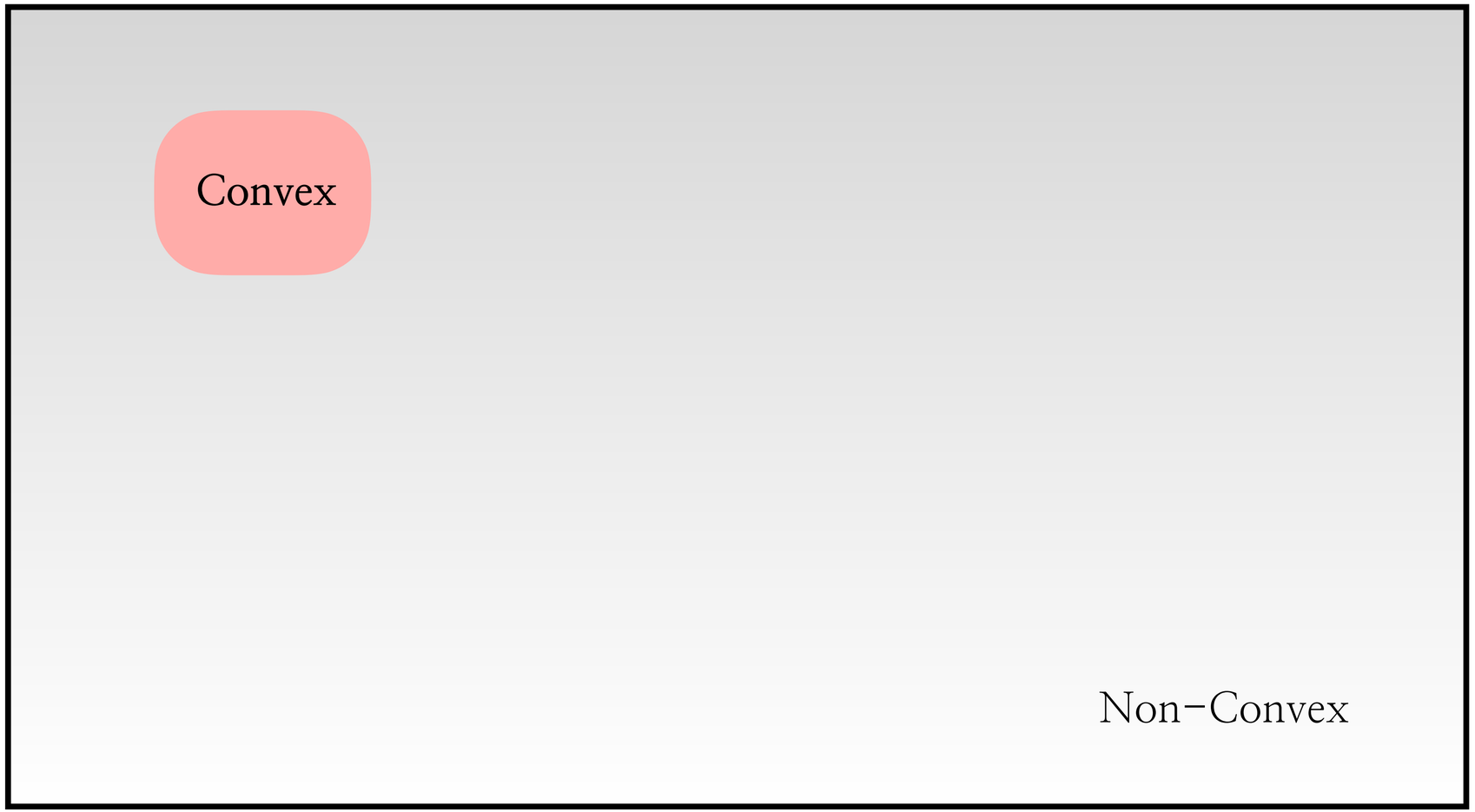
Convex vs. non-convex optimization



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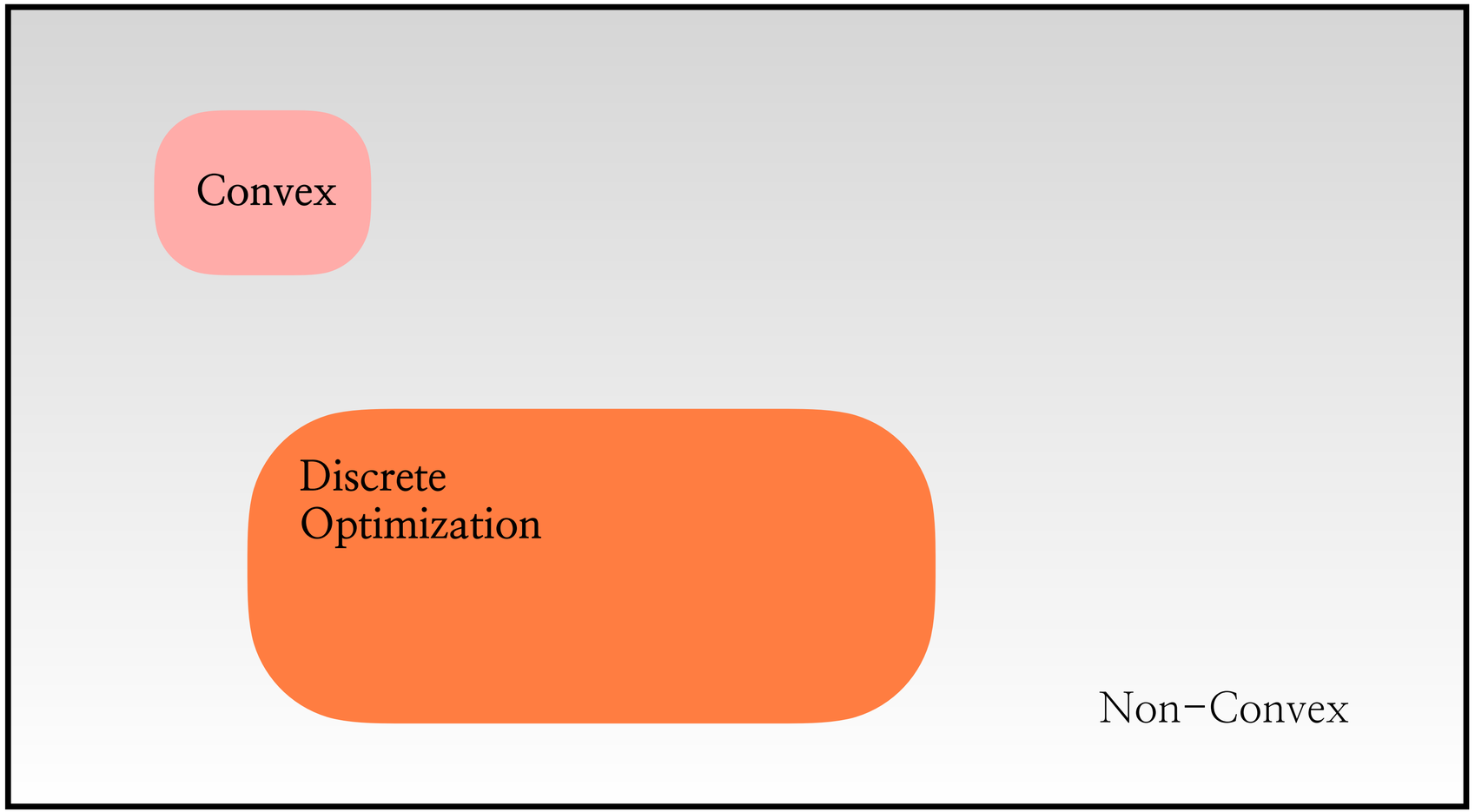

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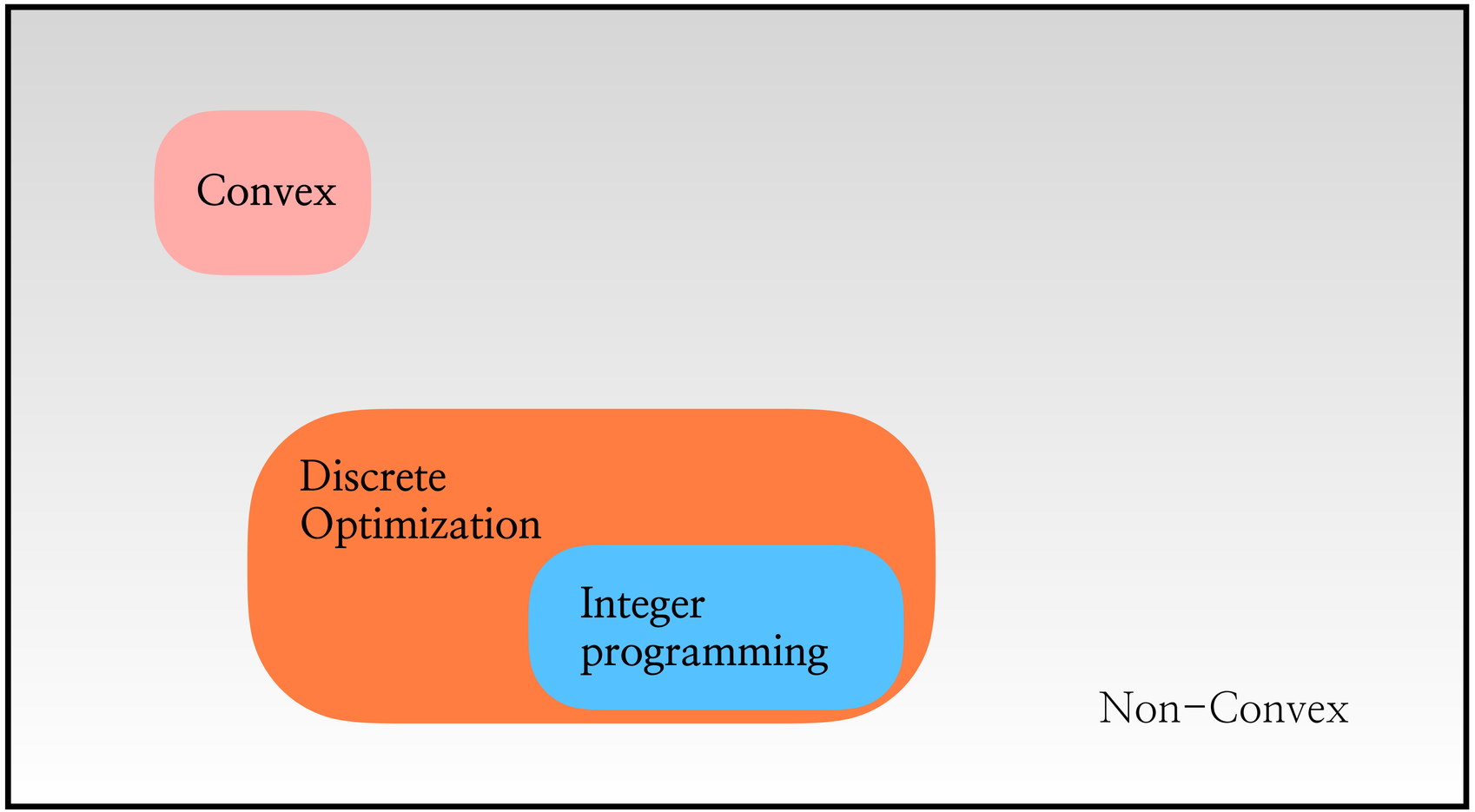

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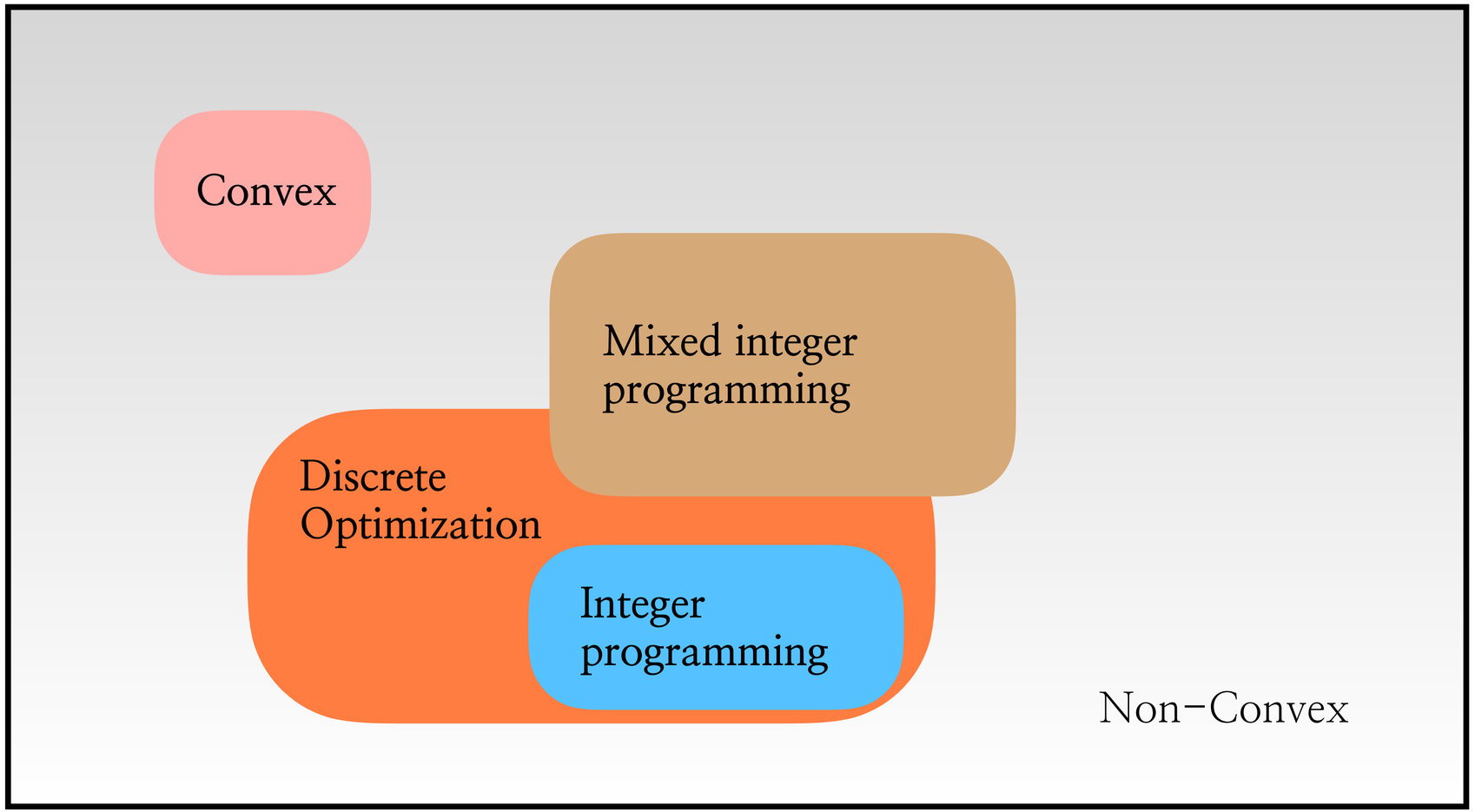

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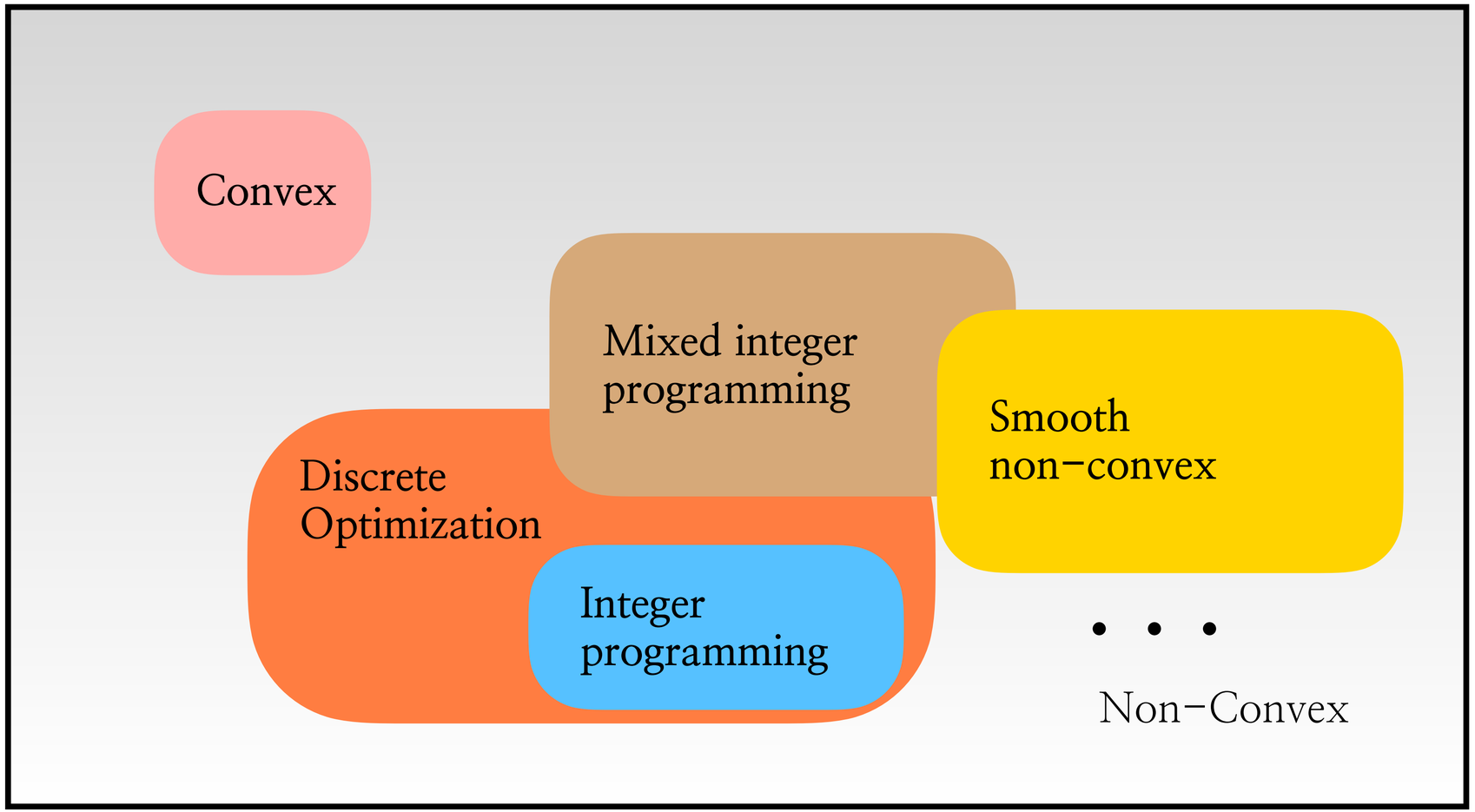

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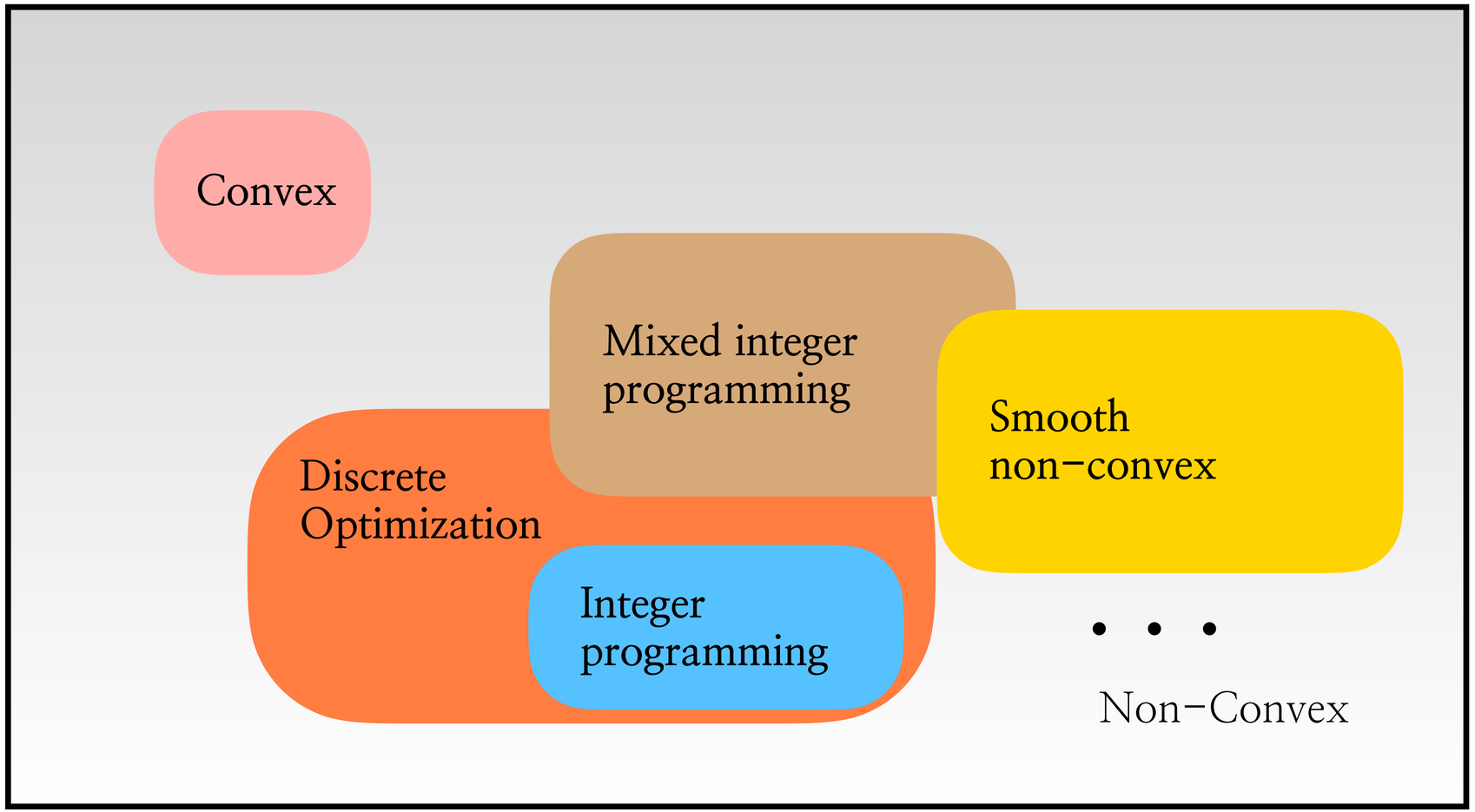

(Naive interpretation of) Space of optimization problems

Derivatives and gradients

- Definition of a **derivative**

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

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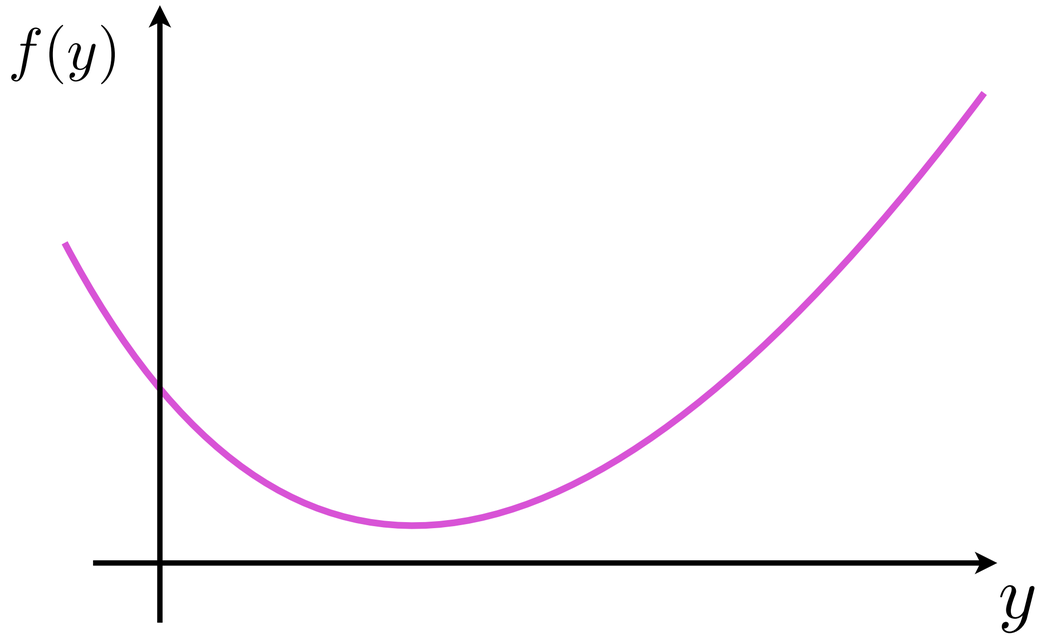

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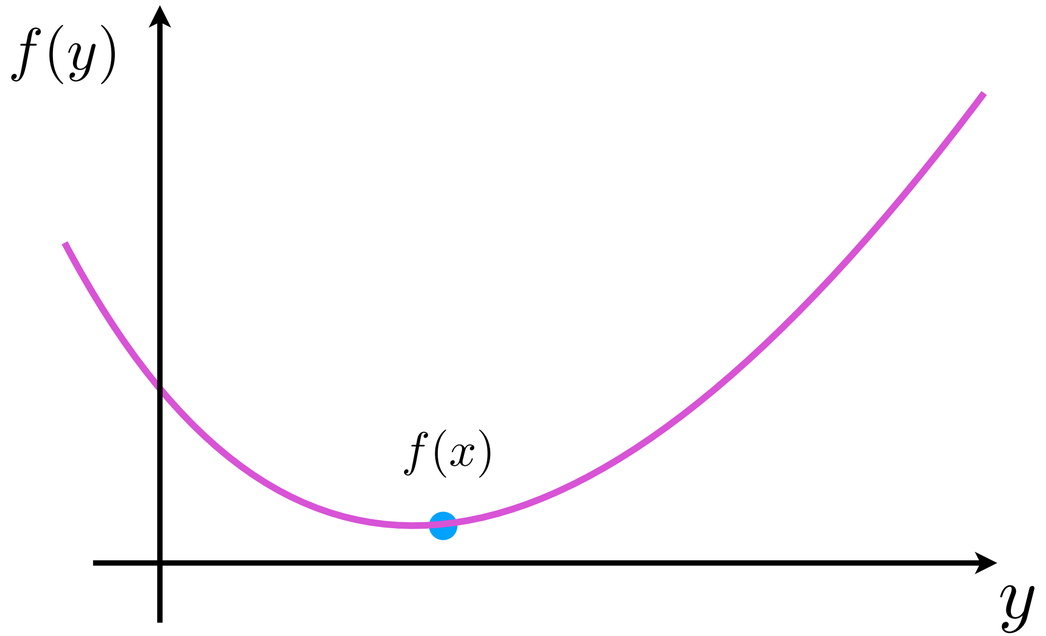

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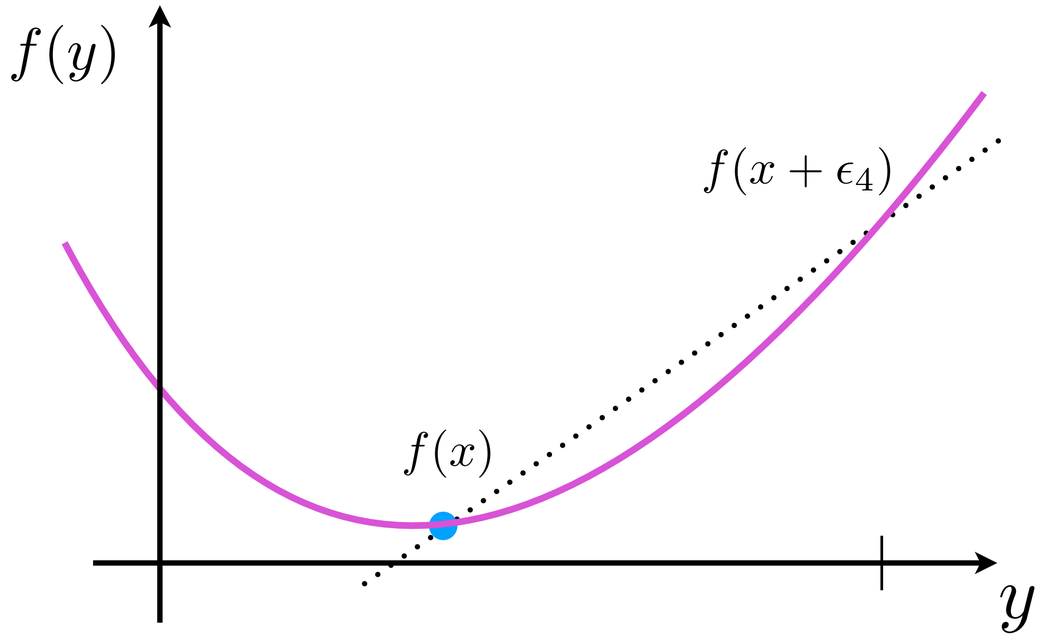

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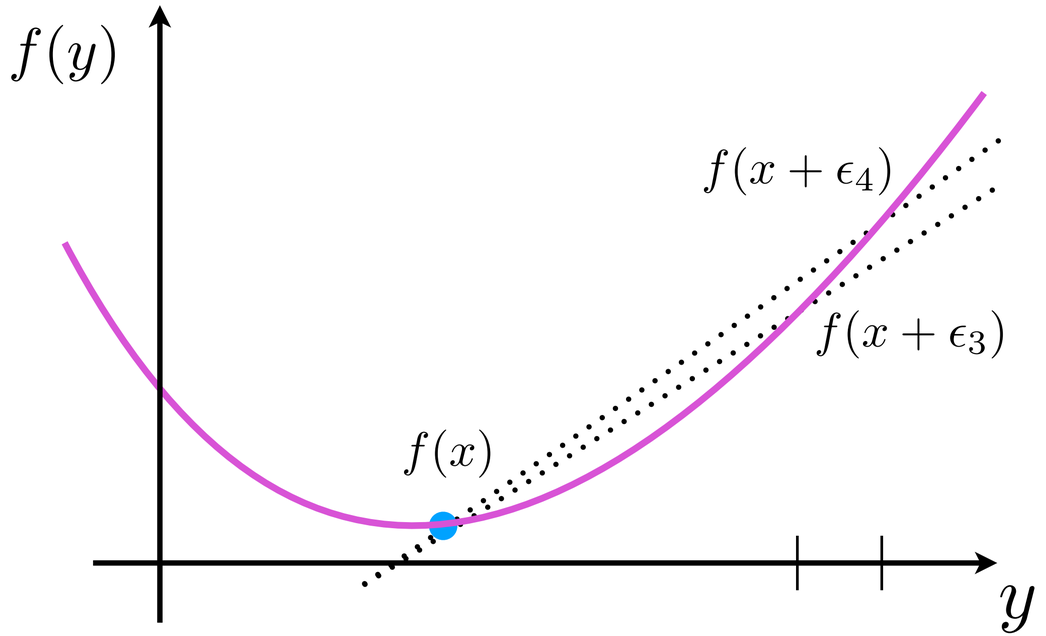

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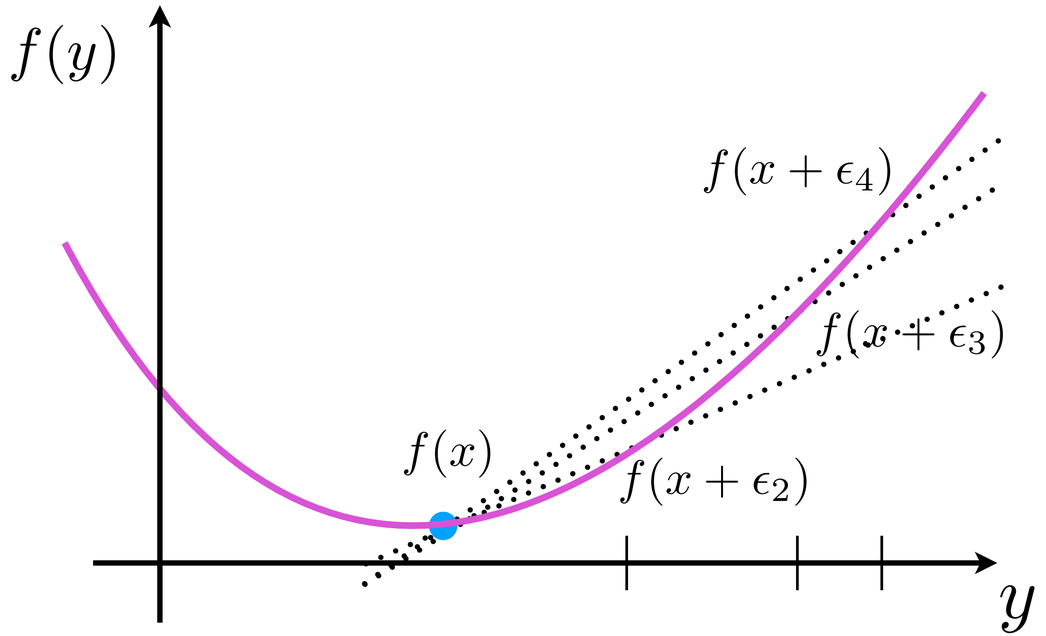

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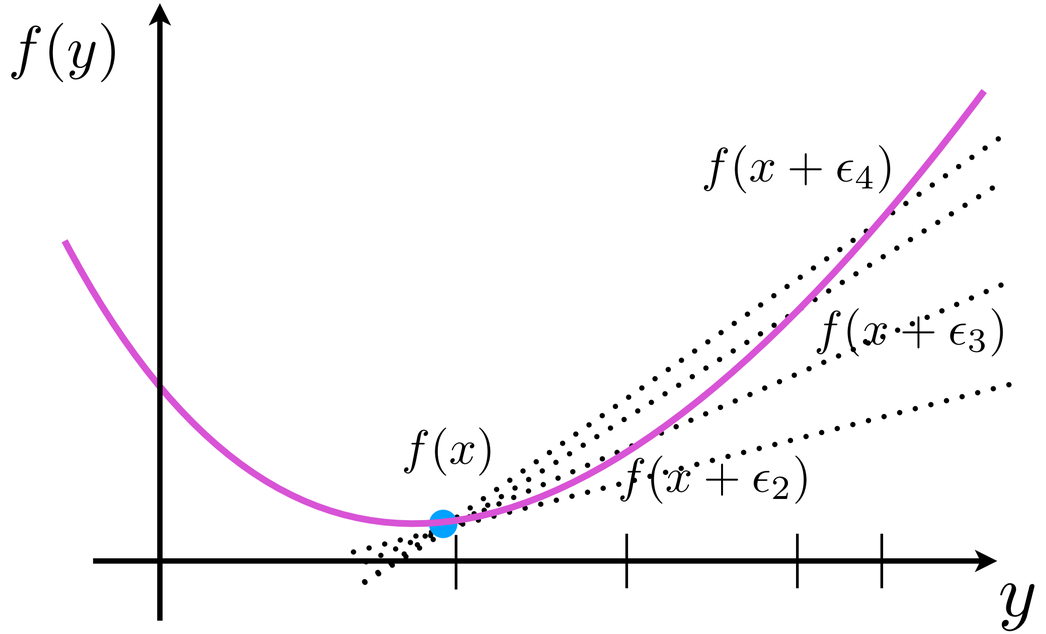

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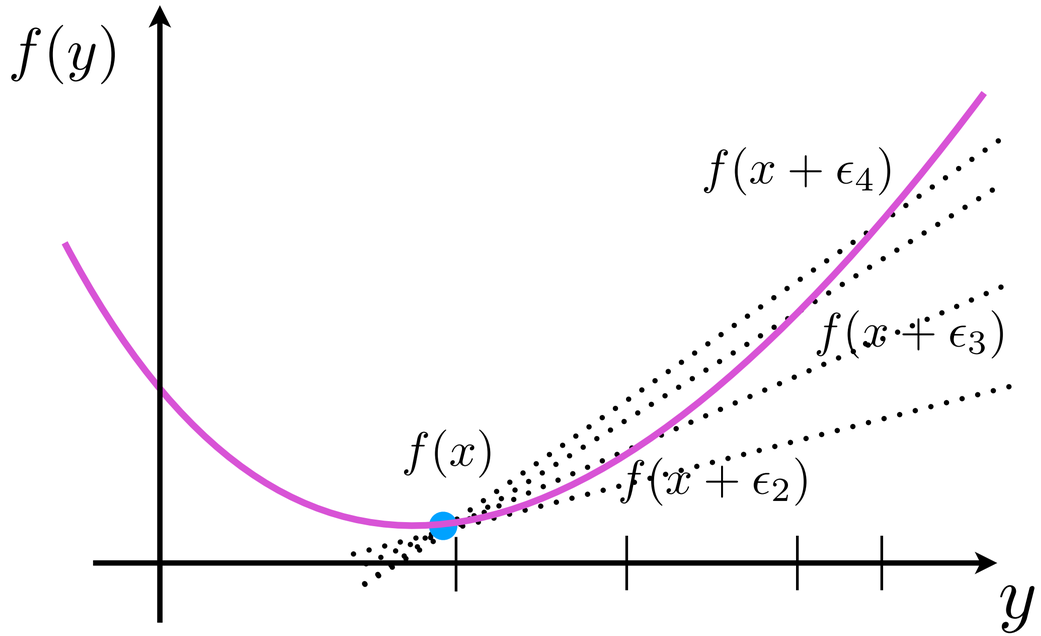

Represents the rate that function changes

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- Definition of **second-order** derivative

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

Derivatives and gradients

- Generalization to multiple components: **gradient**

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

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

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

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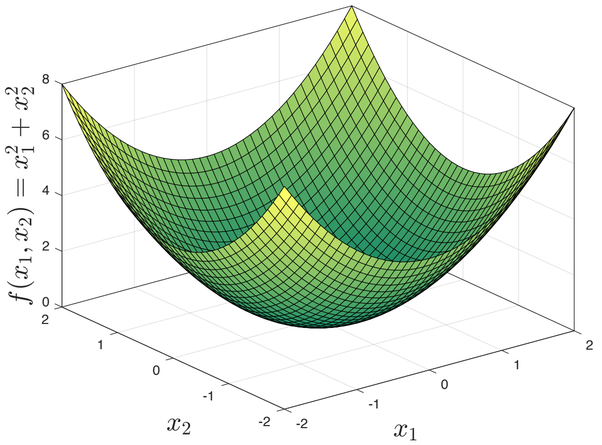
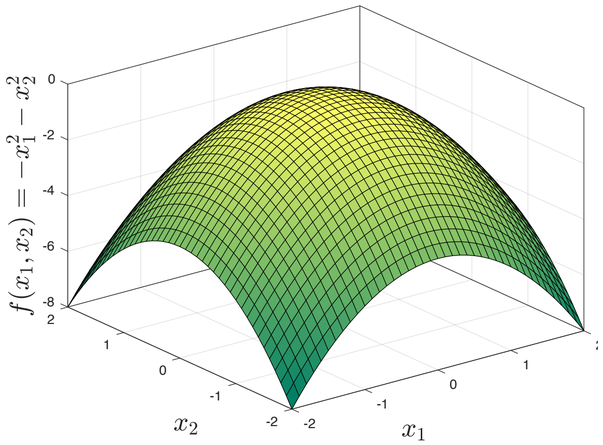


$\nabla^2 f(\cdot) \succ 0$



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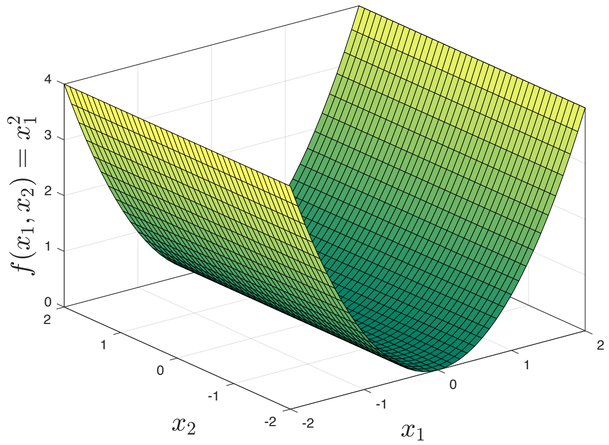

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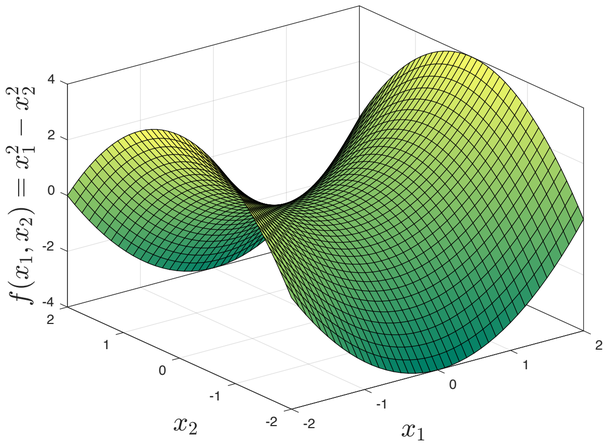
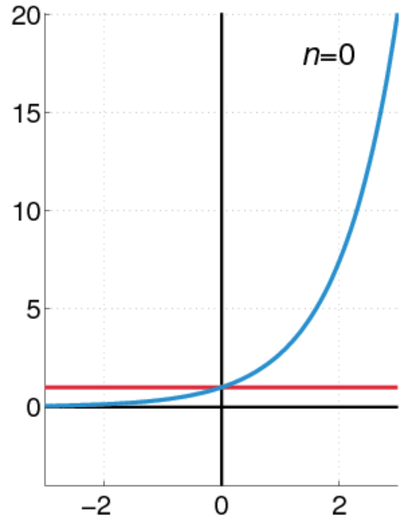


Indefinite

Taylor's expansion

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

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



Example:
exponential function

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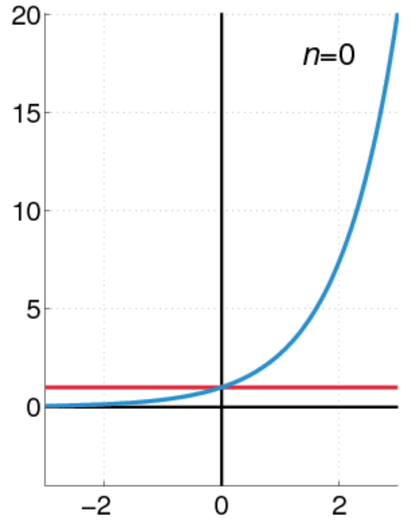

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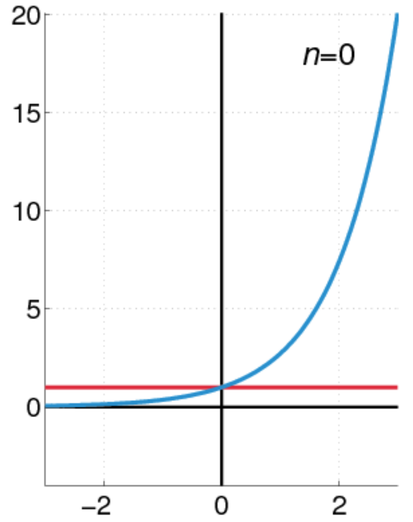

Example: exponential function

- 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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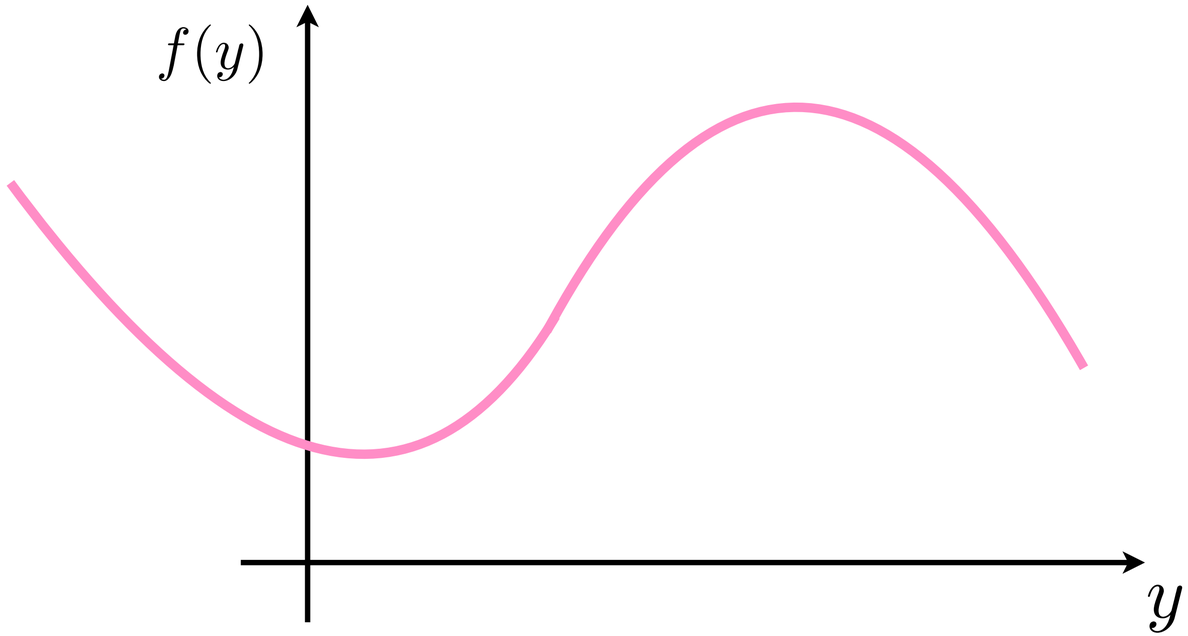

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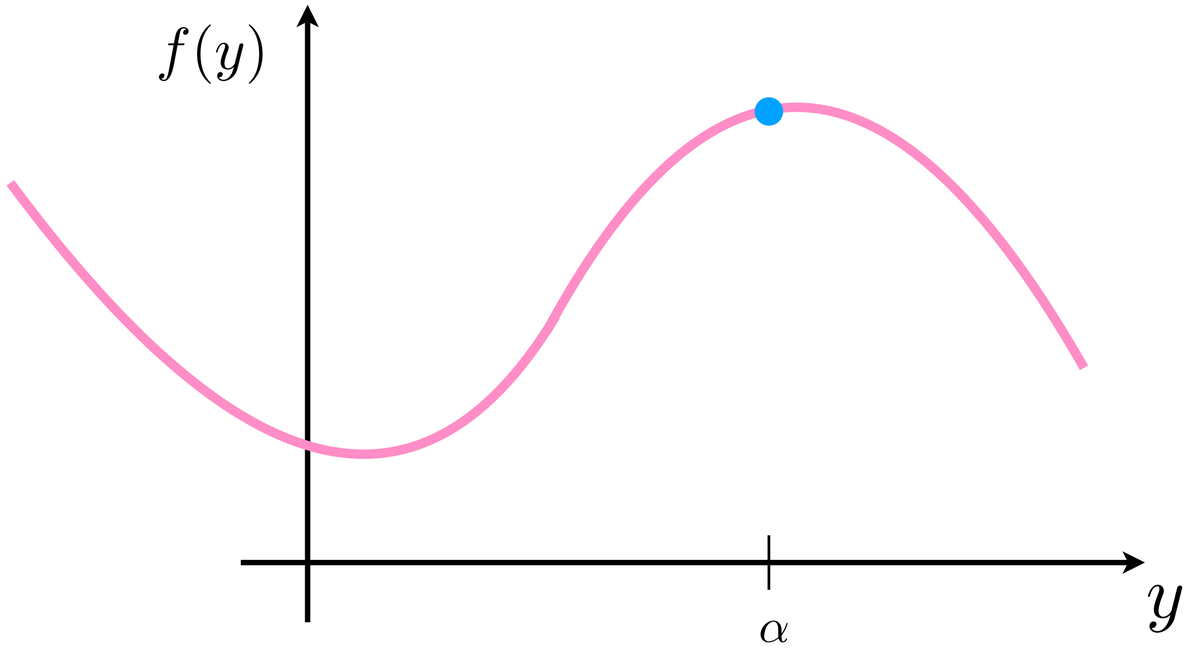

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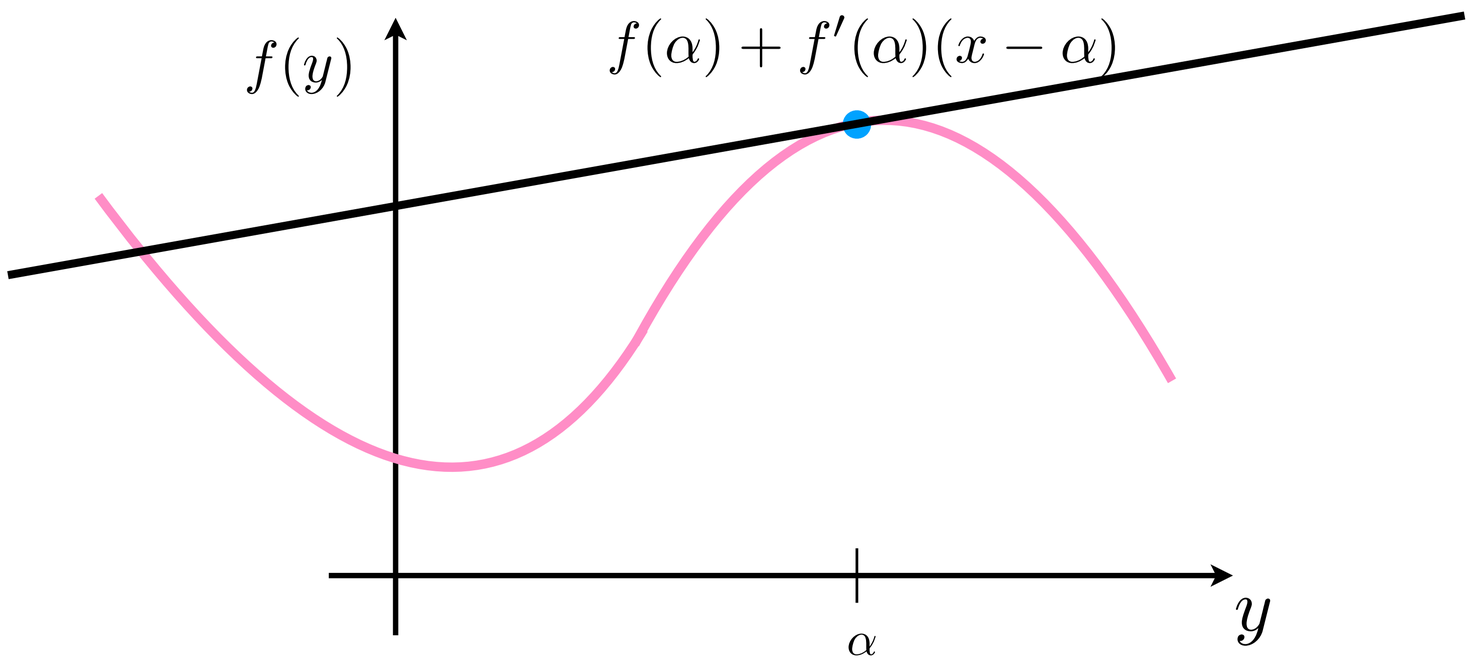

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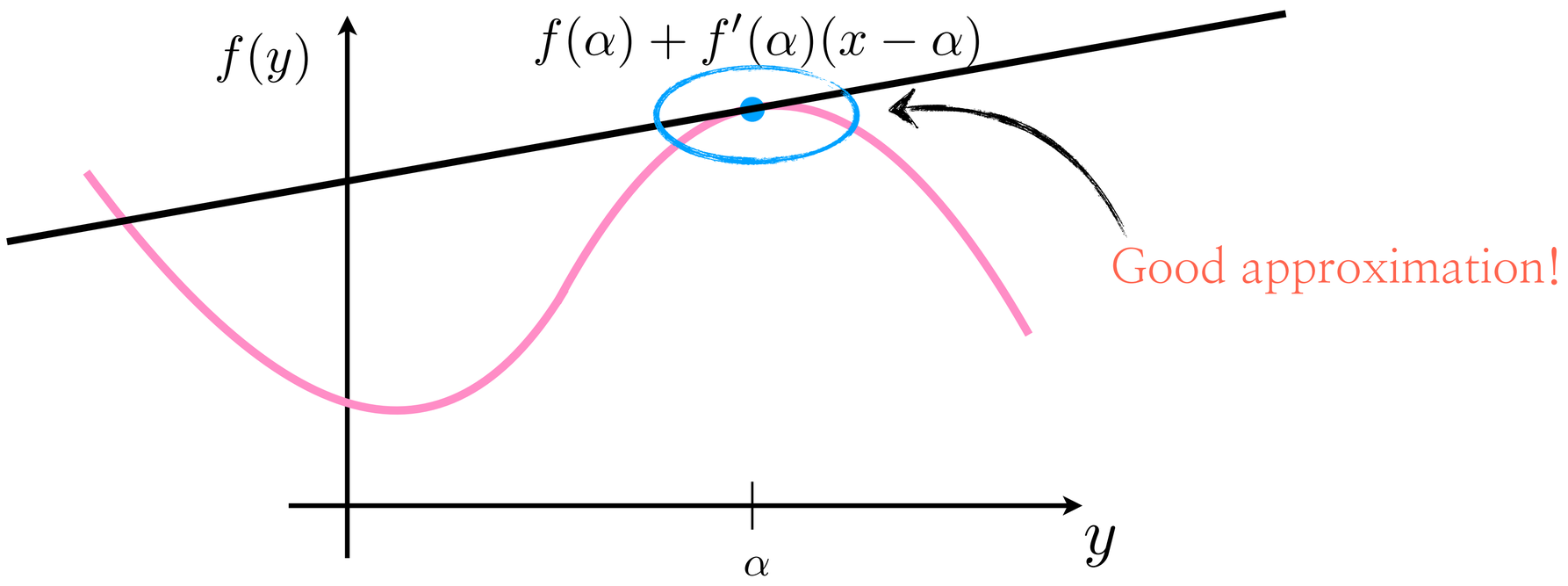

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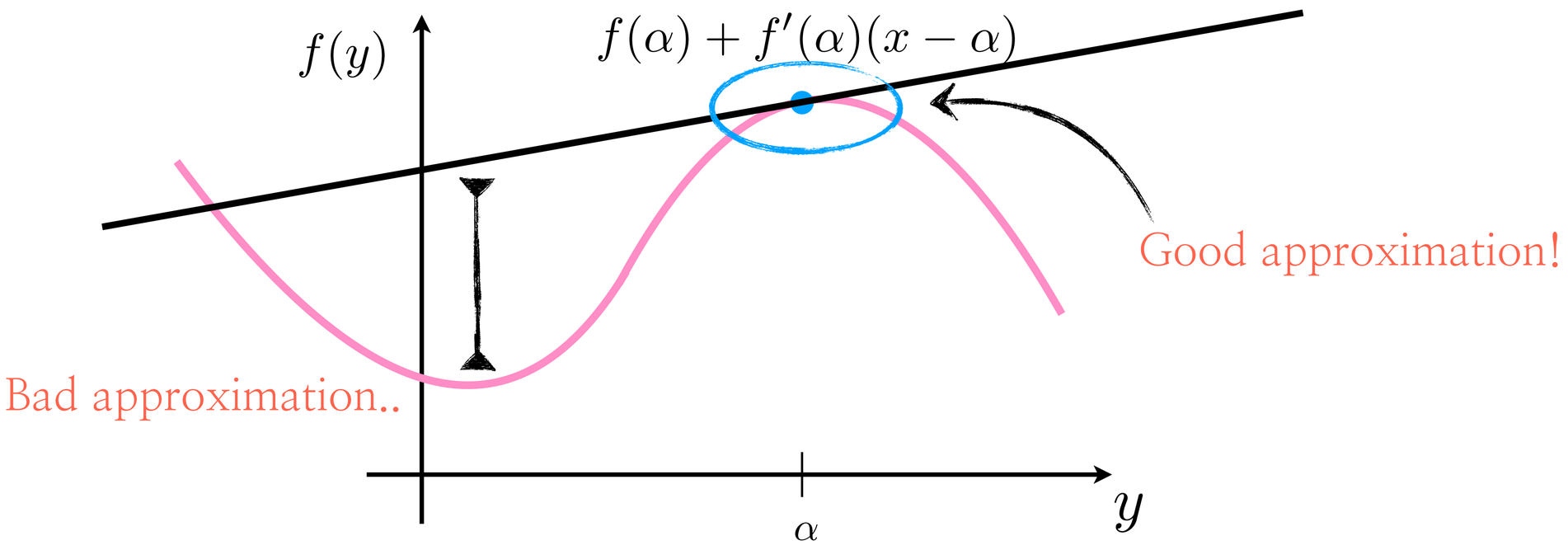

Taylor's expansion

- Second-order Taylor's approximation

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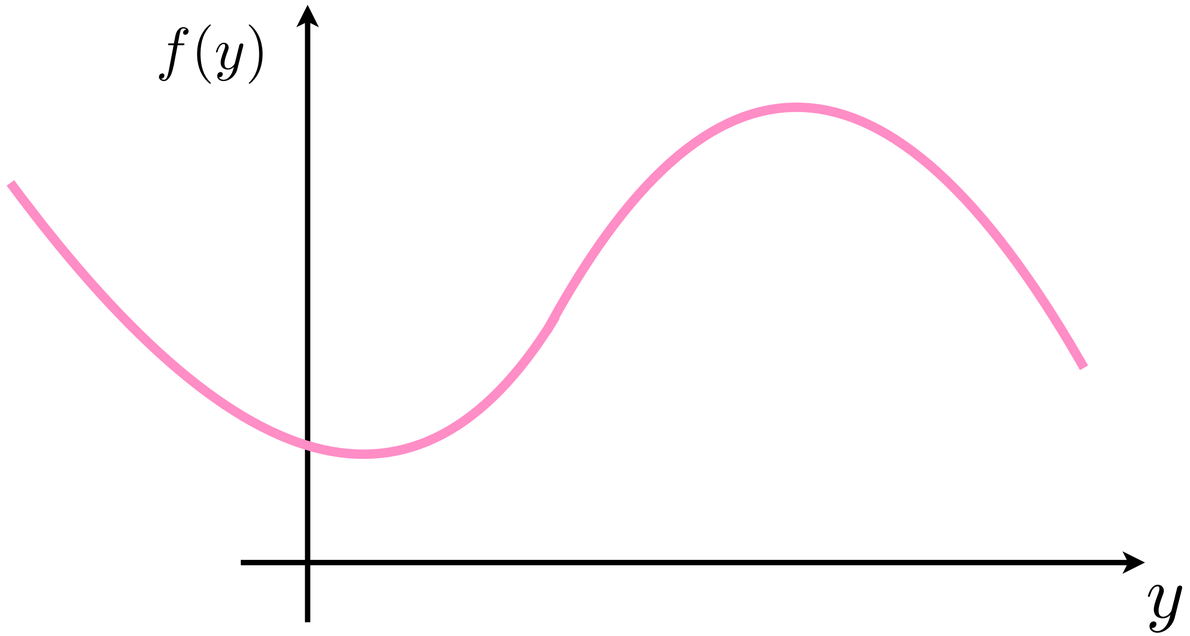

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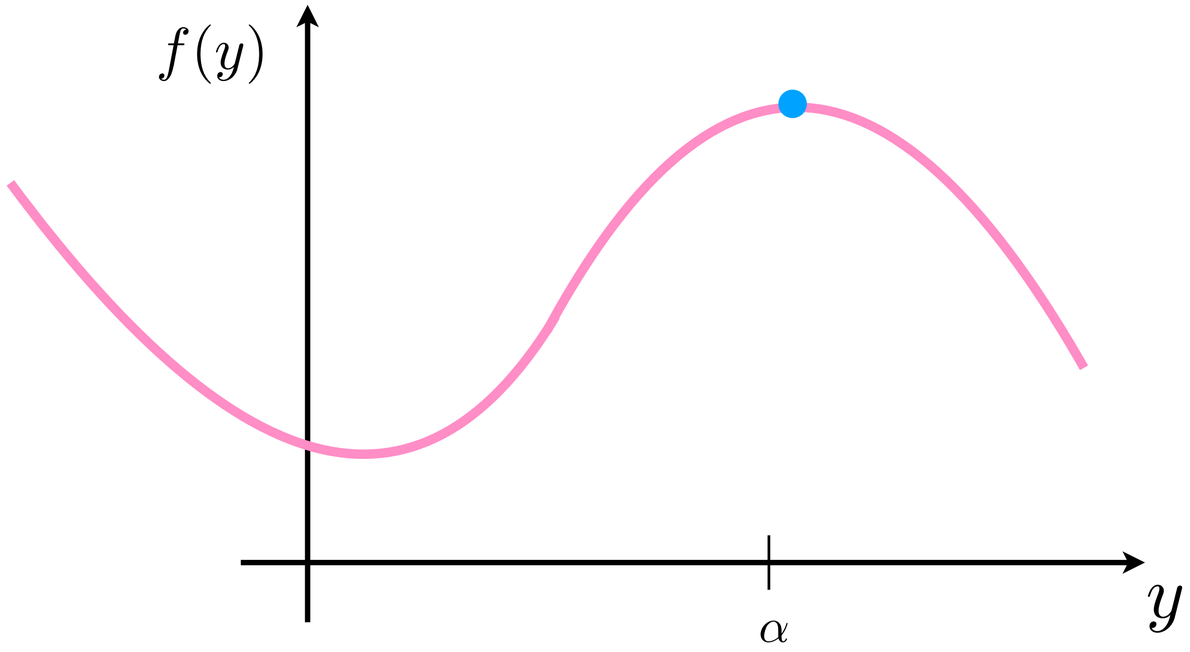

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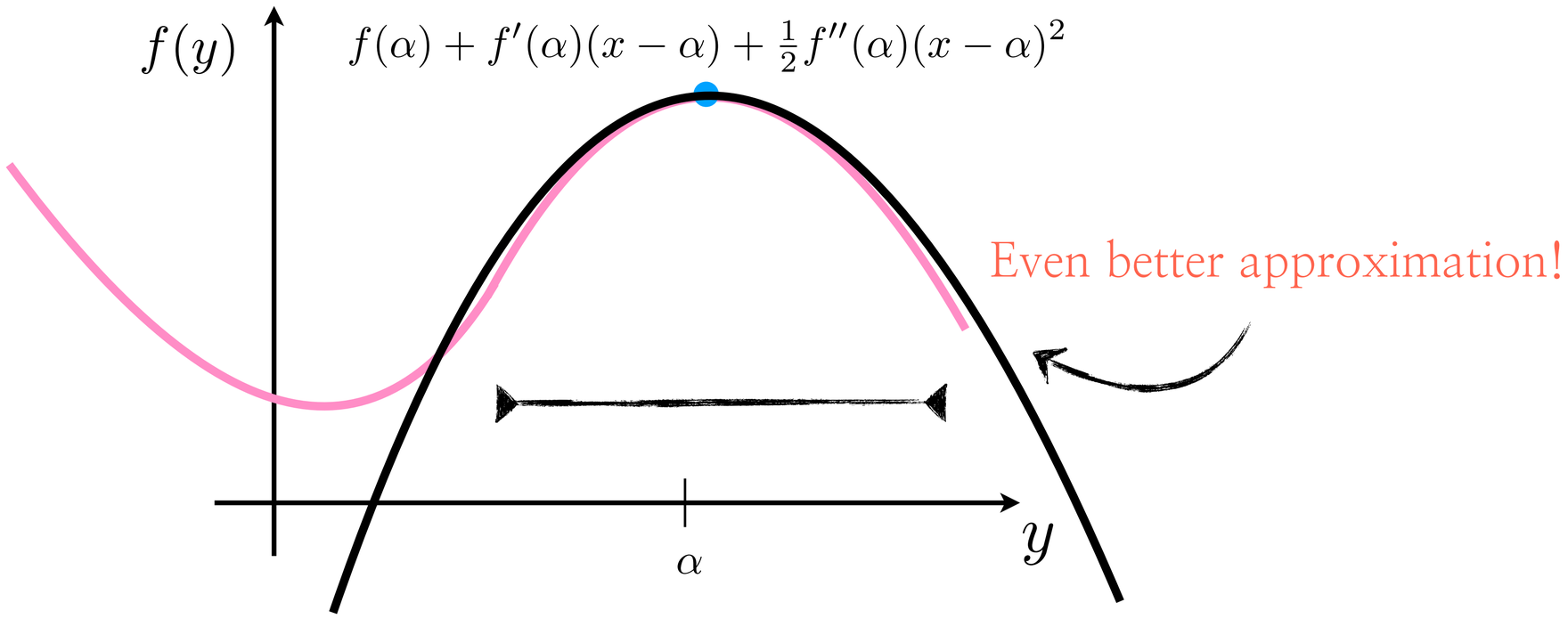

Taylor's expansion

- Second-order Taylor's approximation

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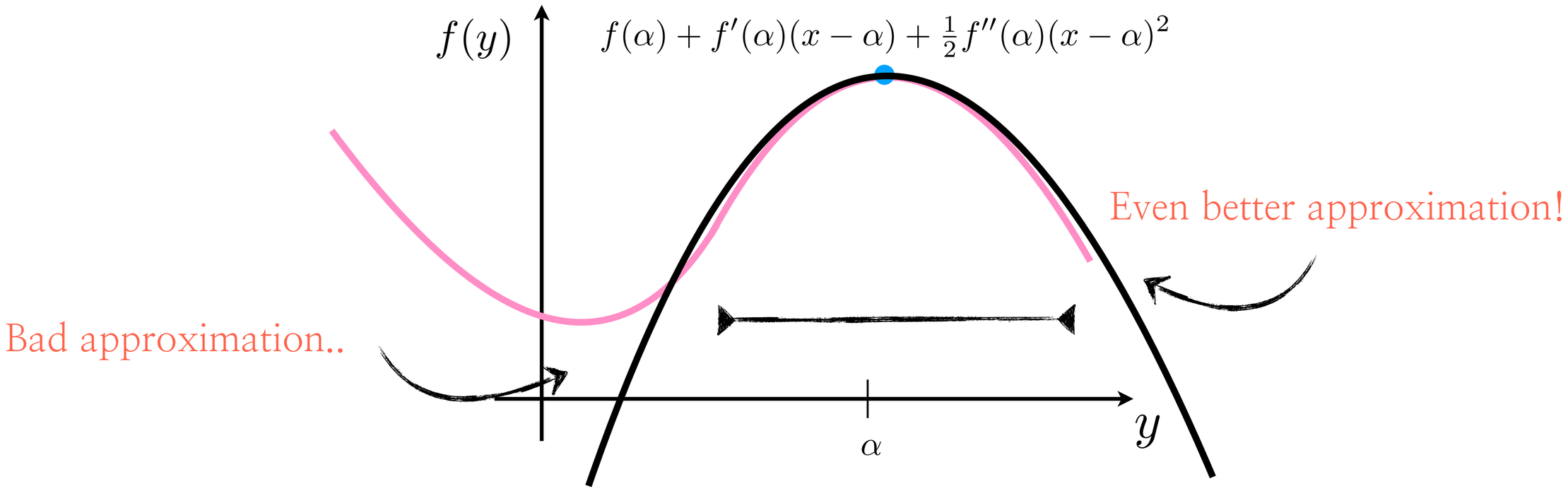

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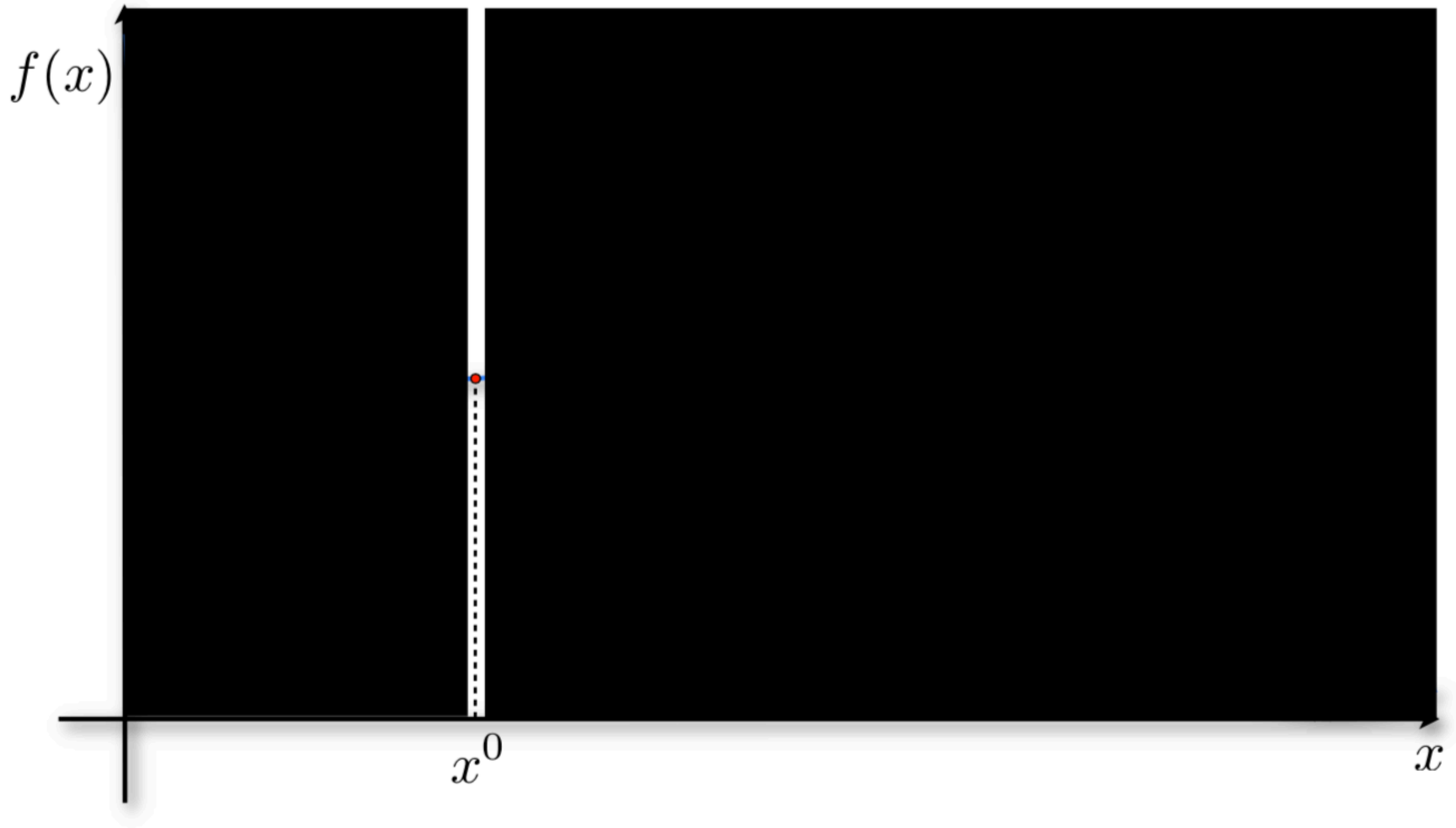
Agnostic optimization

Demo

Agnostic optimization



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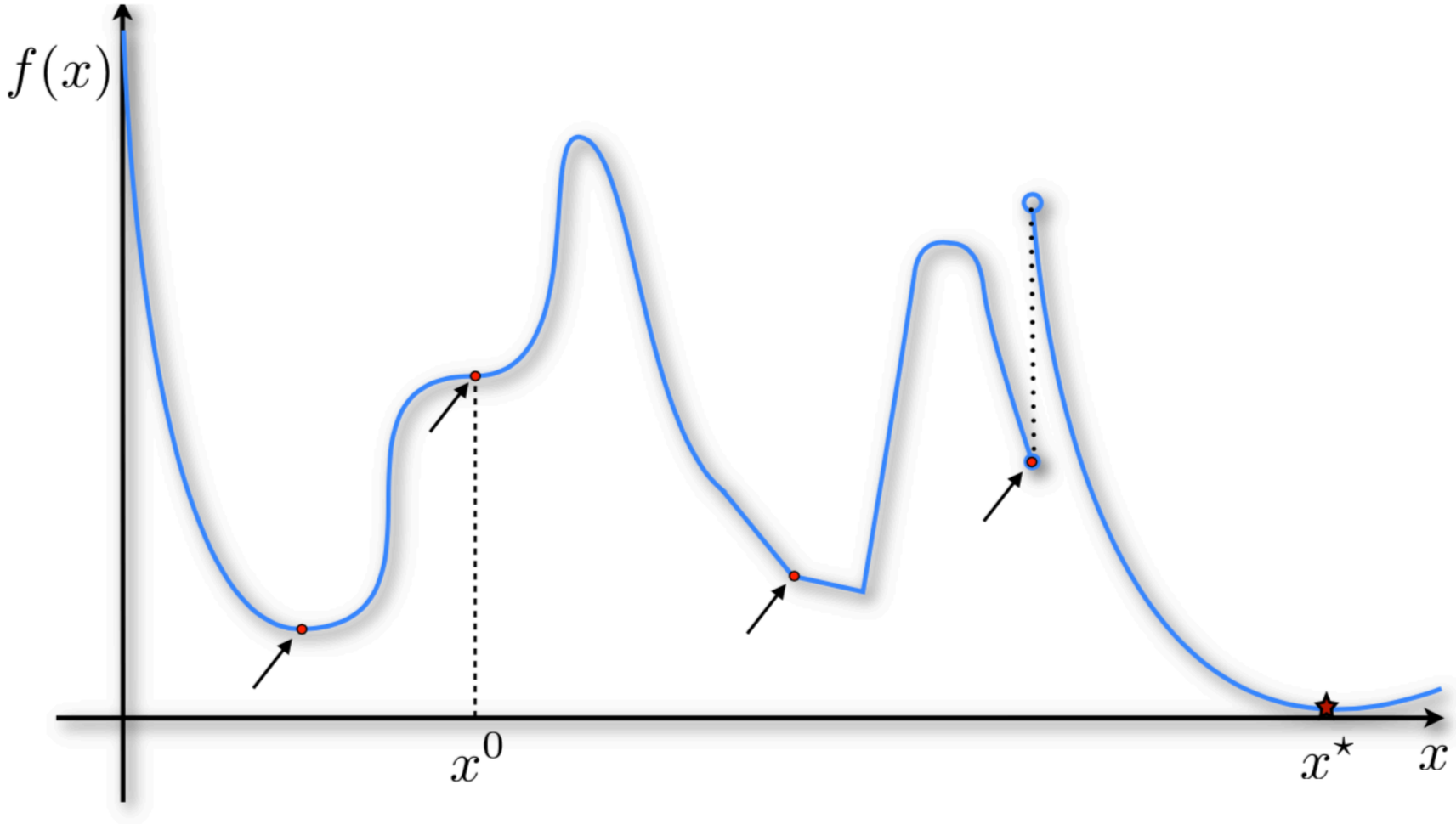

Lipschitz conditions

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

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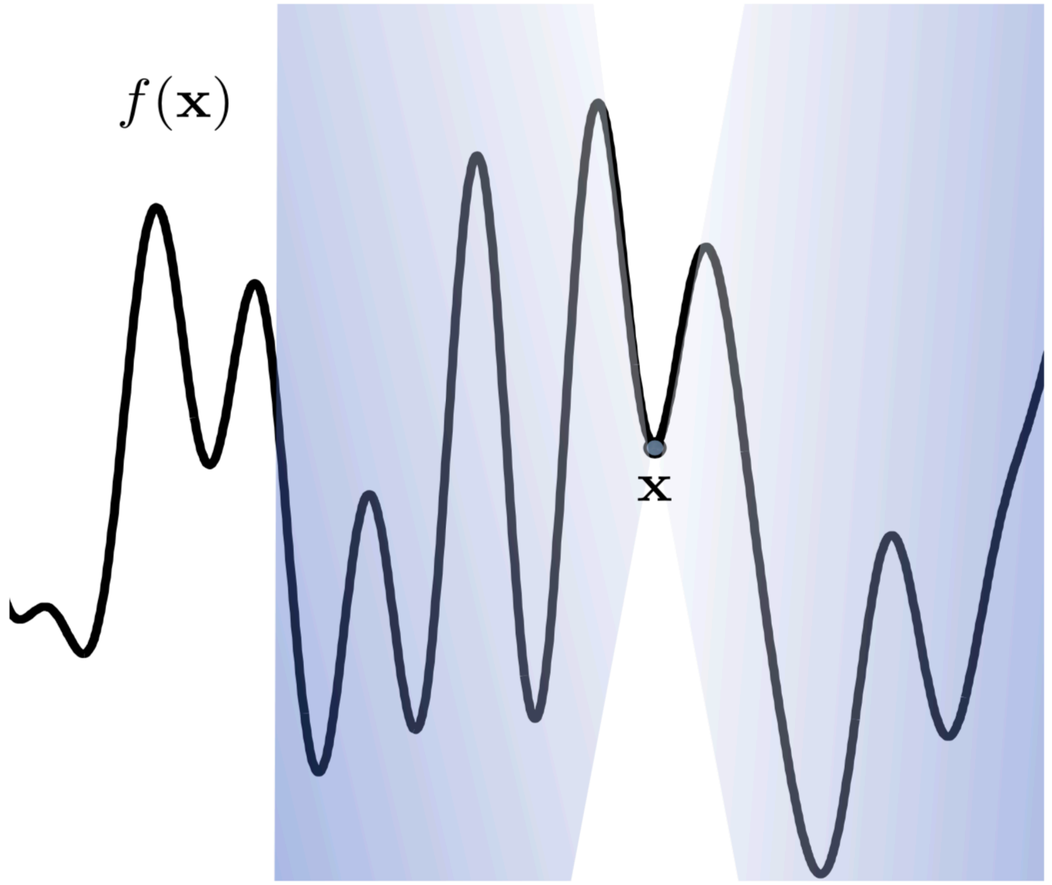
Interpretation via double cone



Function examples:

1. Absolute value
2. Trigonometric functions
3. Quadratics (..)

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    Largest singular value

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f(y) &\leq f(x) + \langle \nabla f(x), y - x \rangle + \tfrac{L}{2}\|x - y\|_2^2 \\
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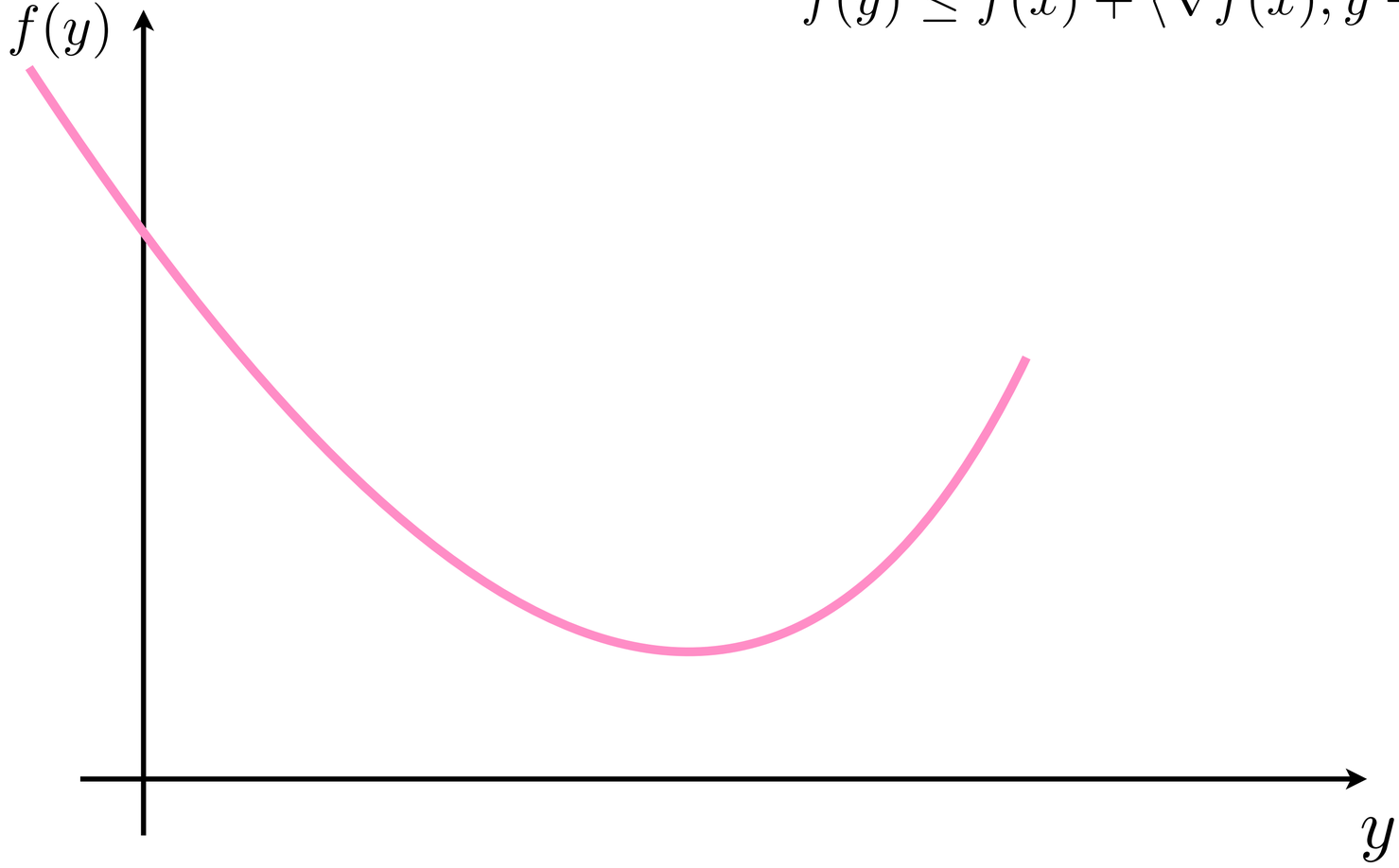

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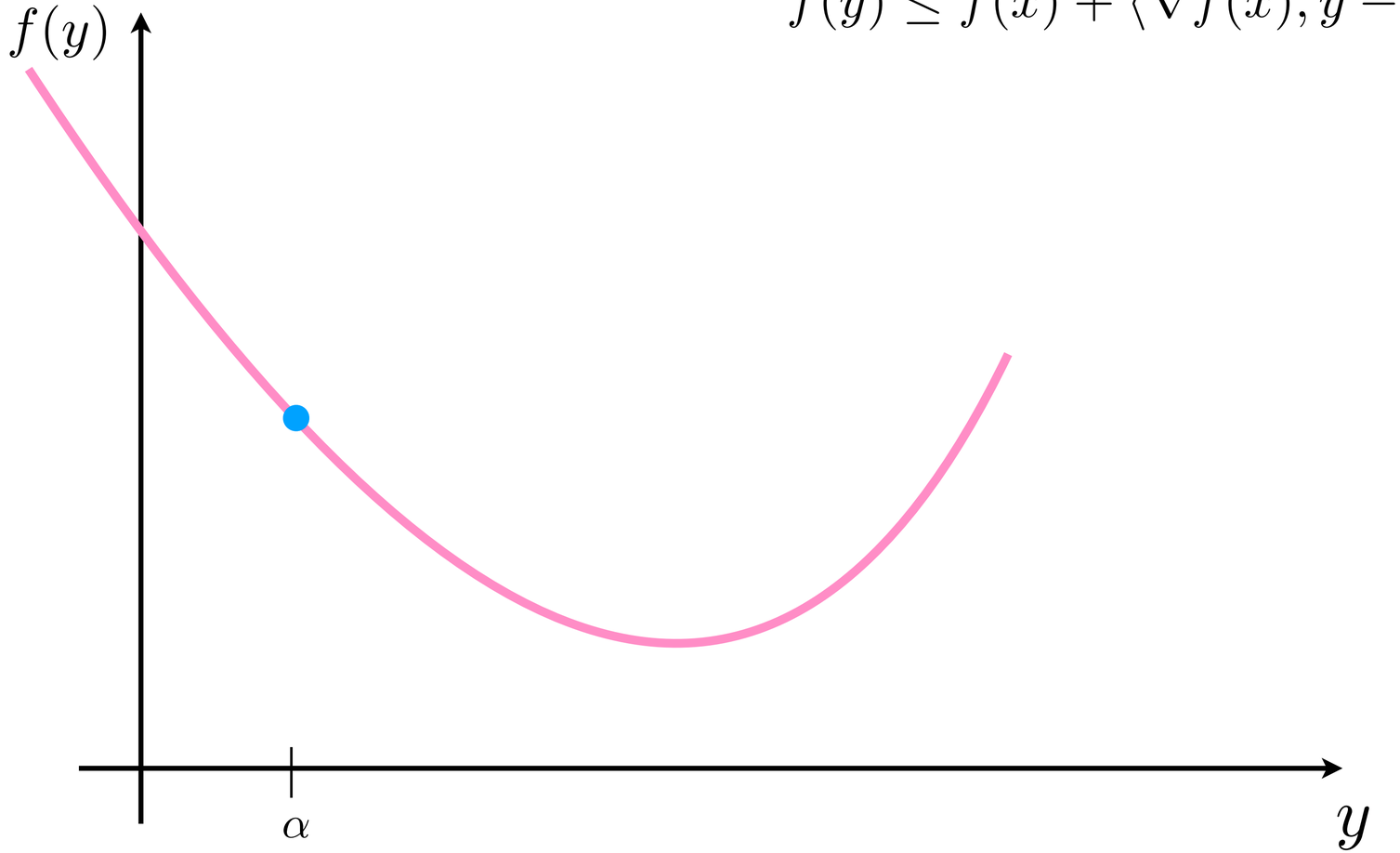

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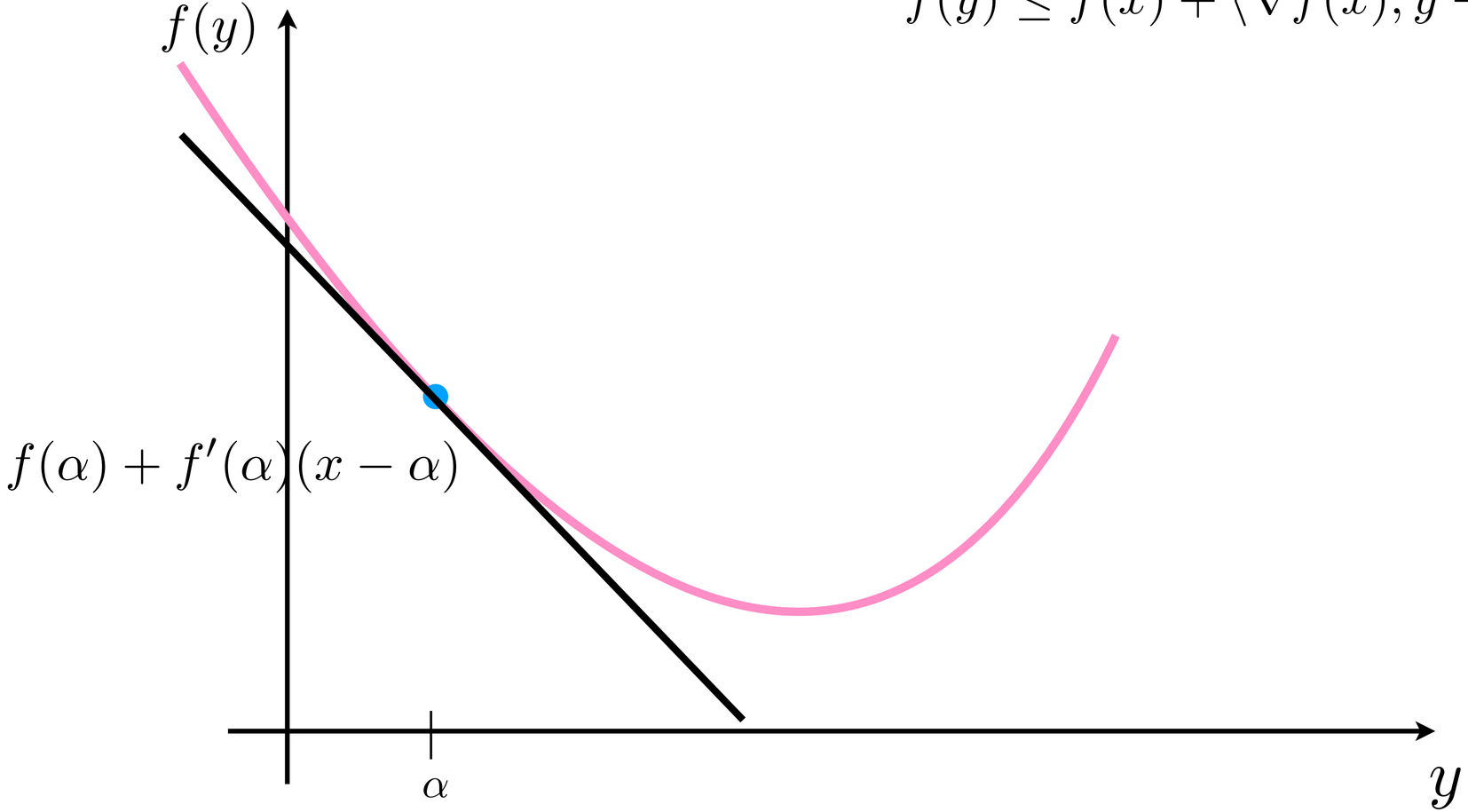

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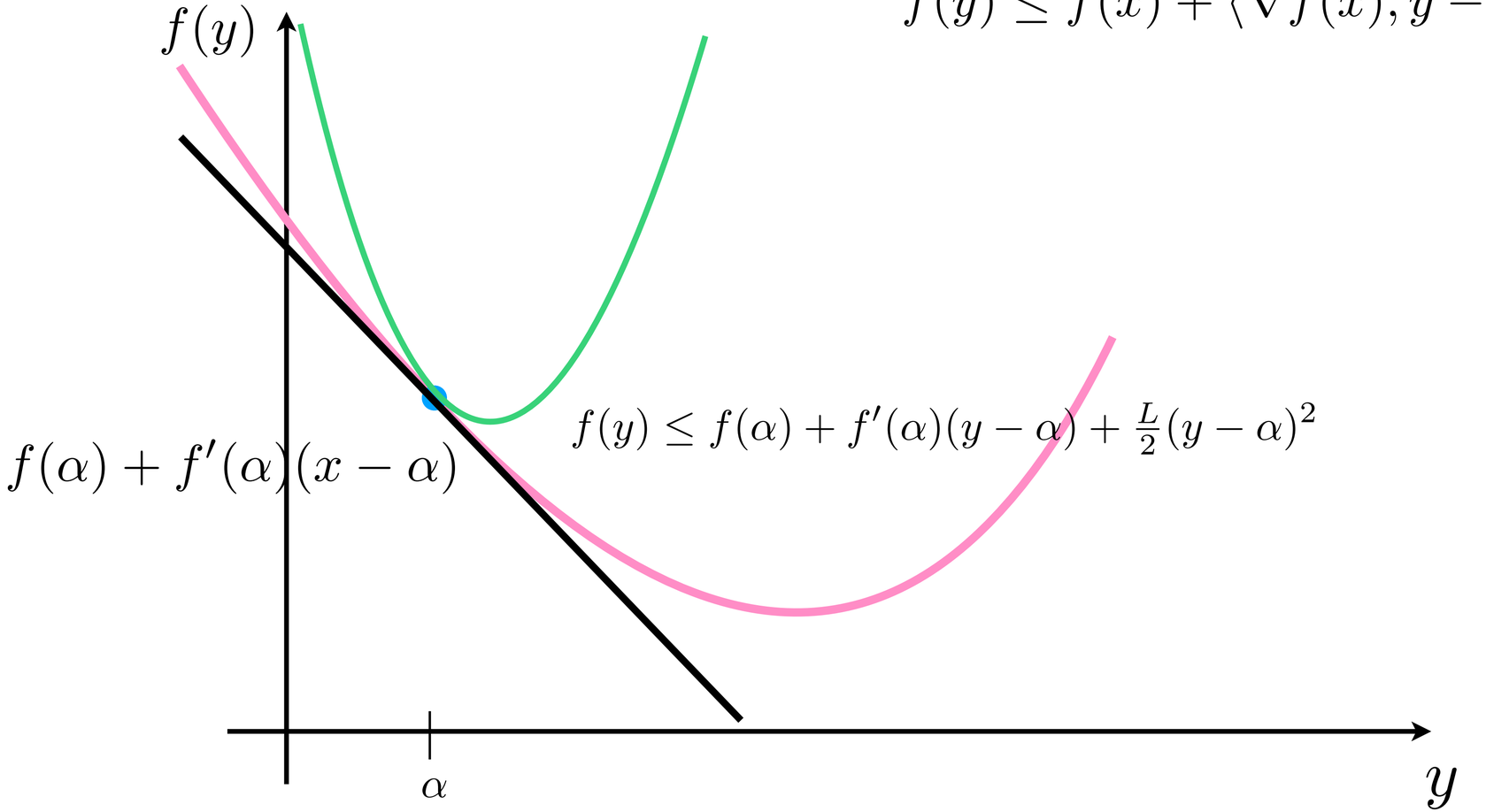

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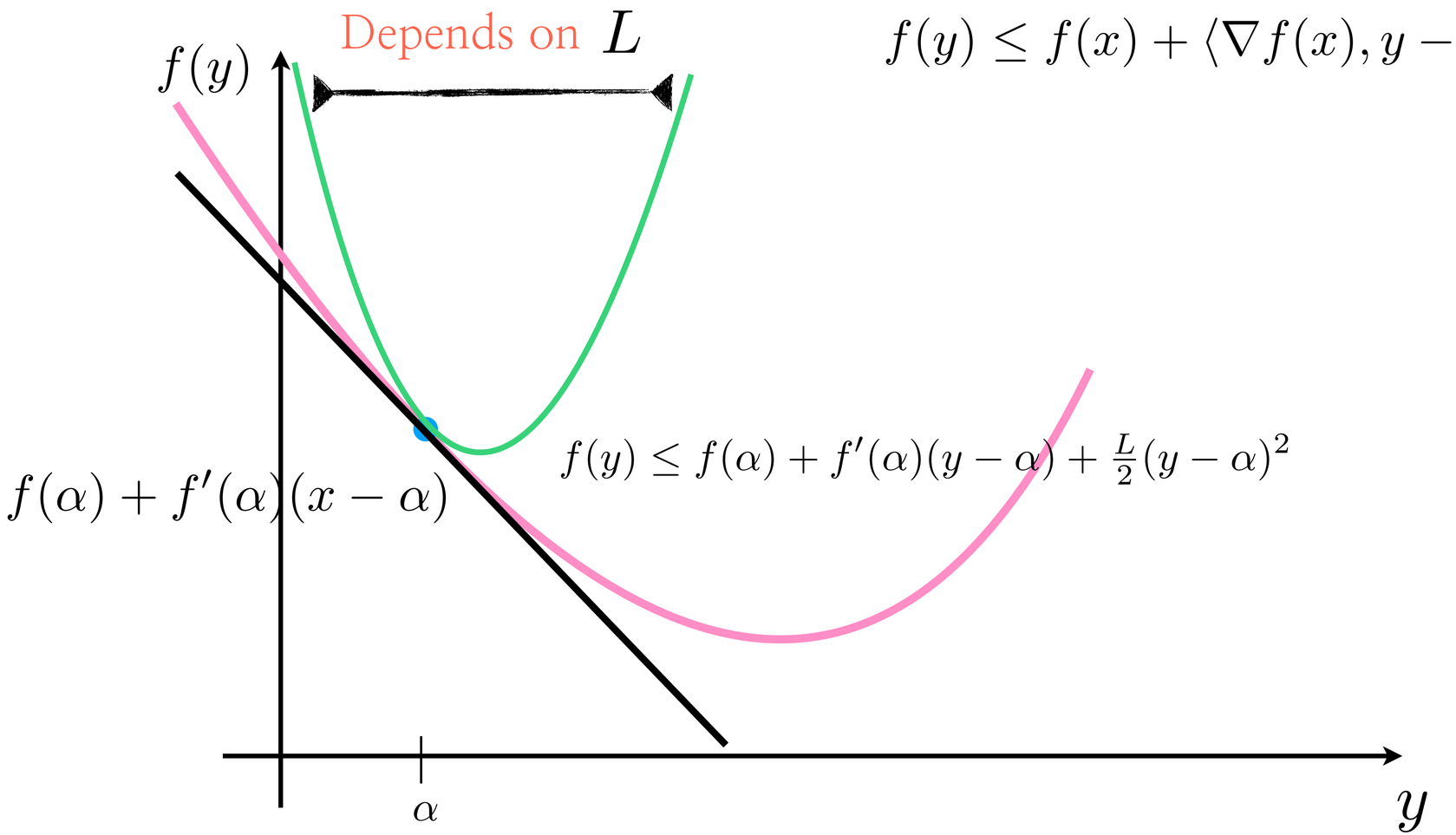

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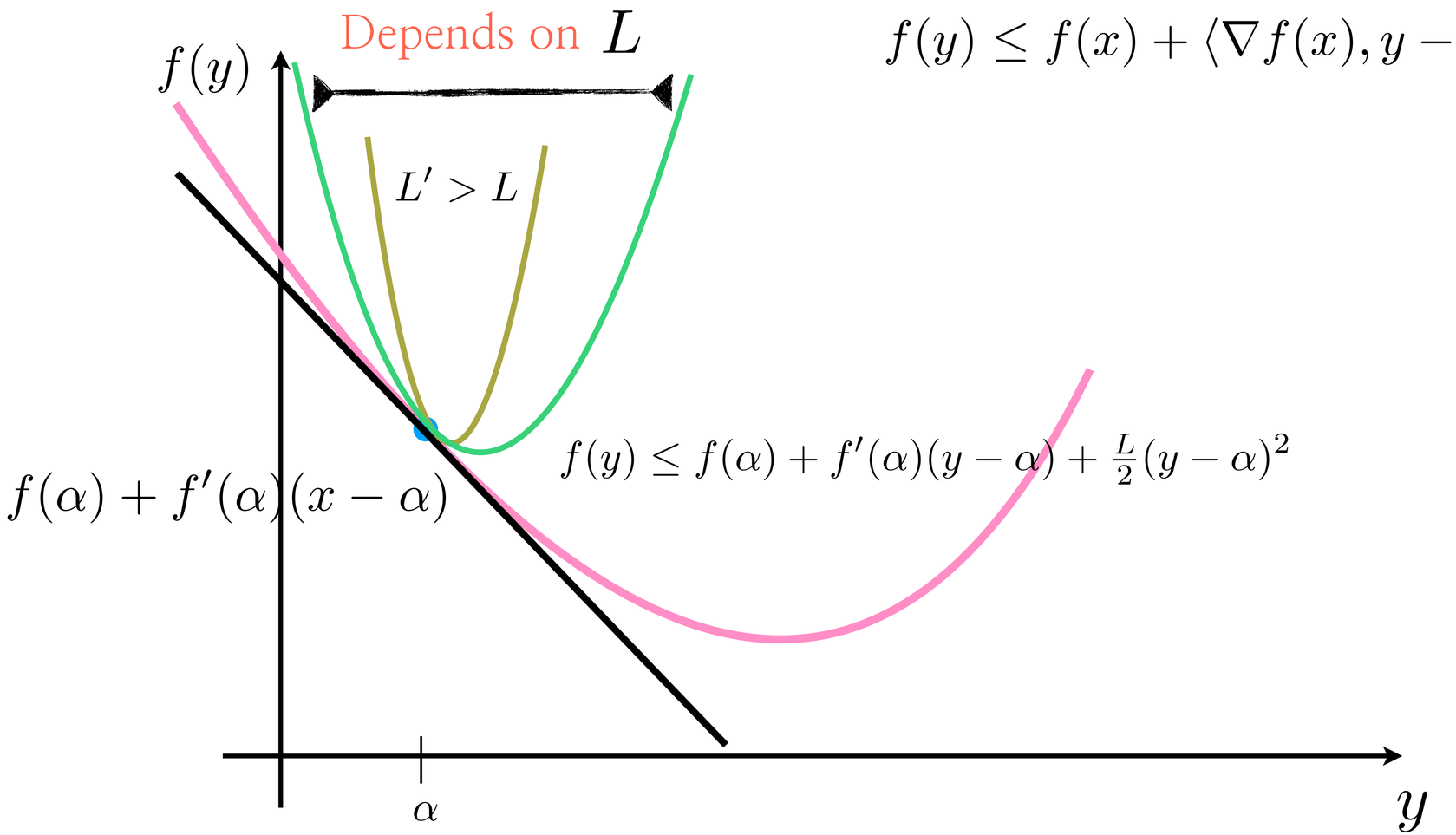

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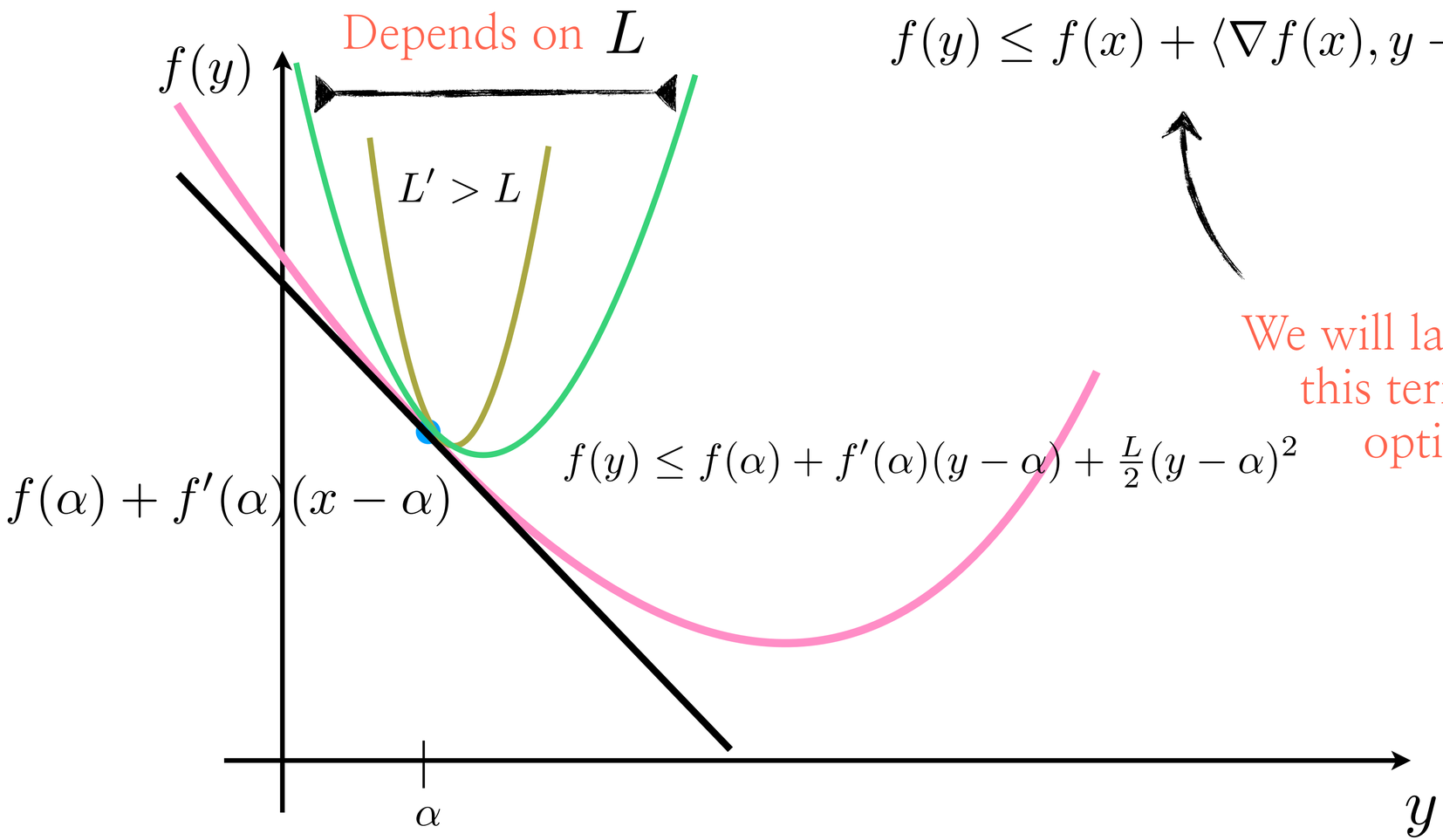

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We will later on see how this term appear in optimization

Lipschitz conditions

- How does this relate to Taylor's expansion?

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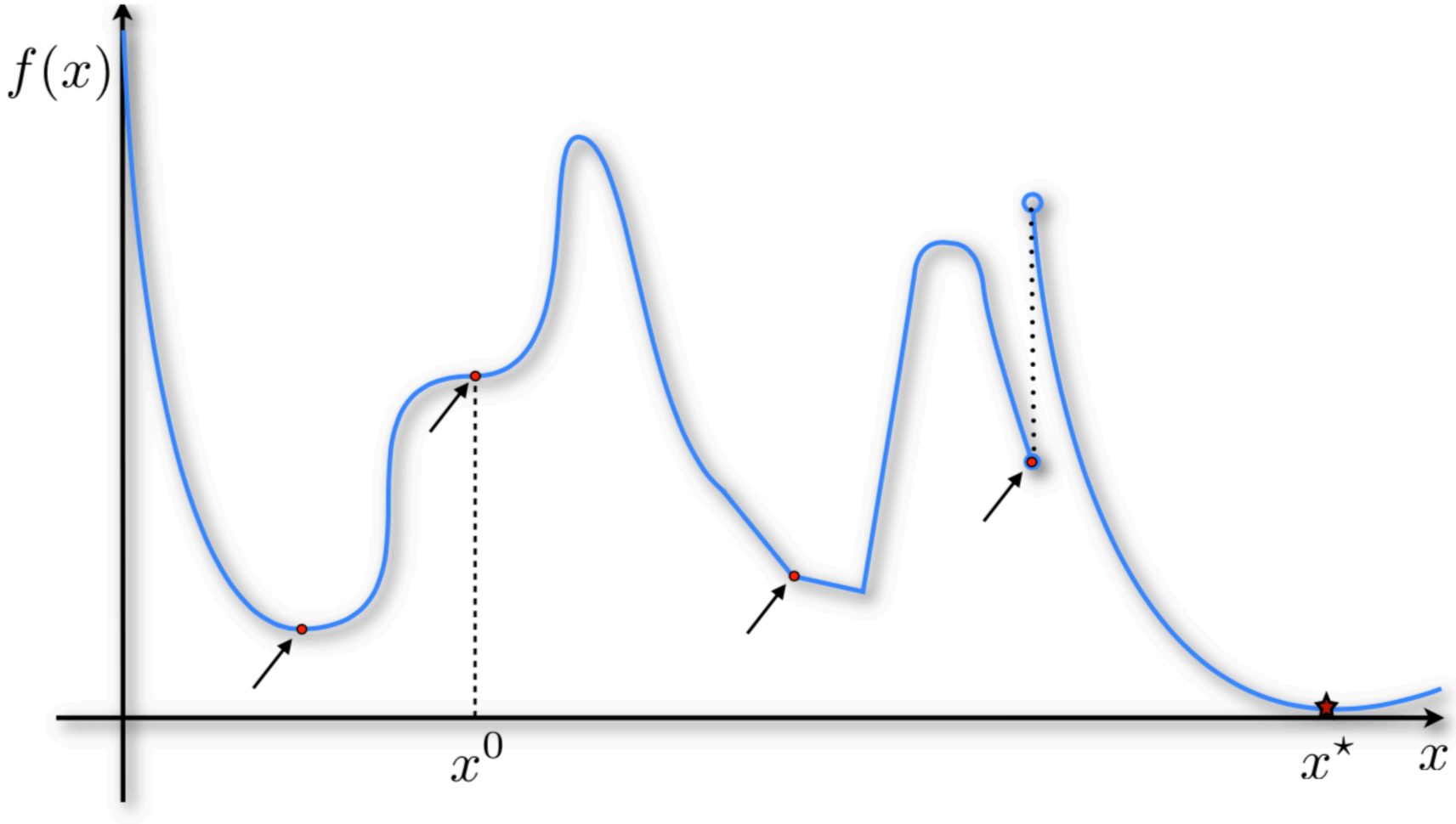
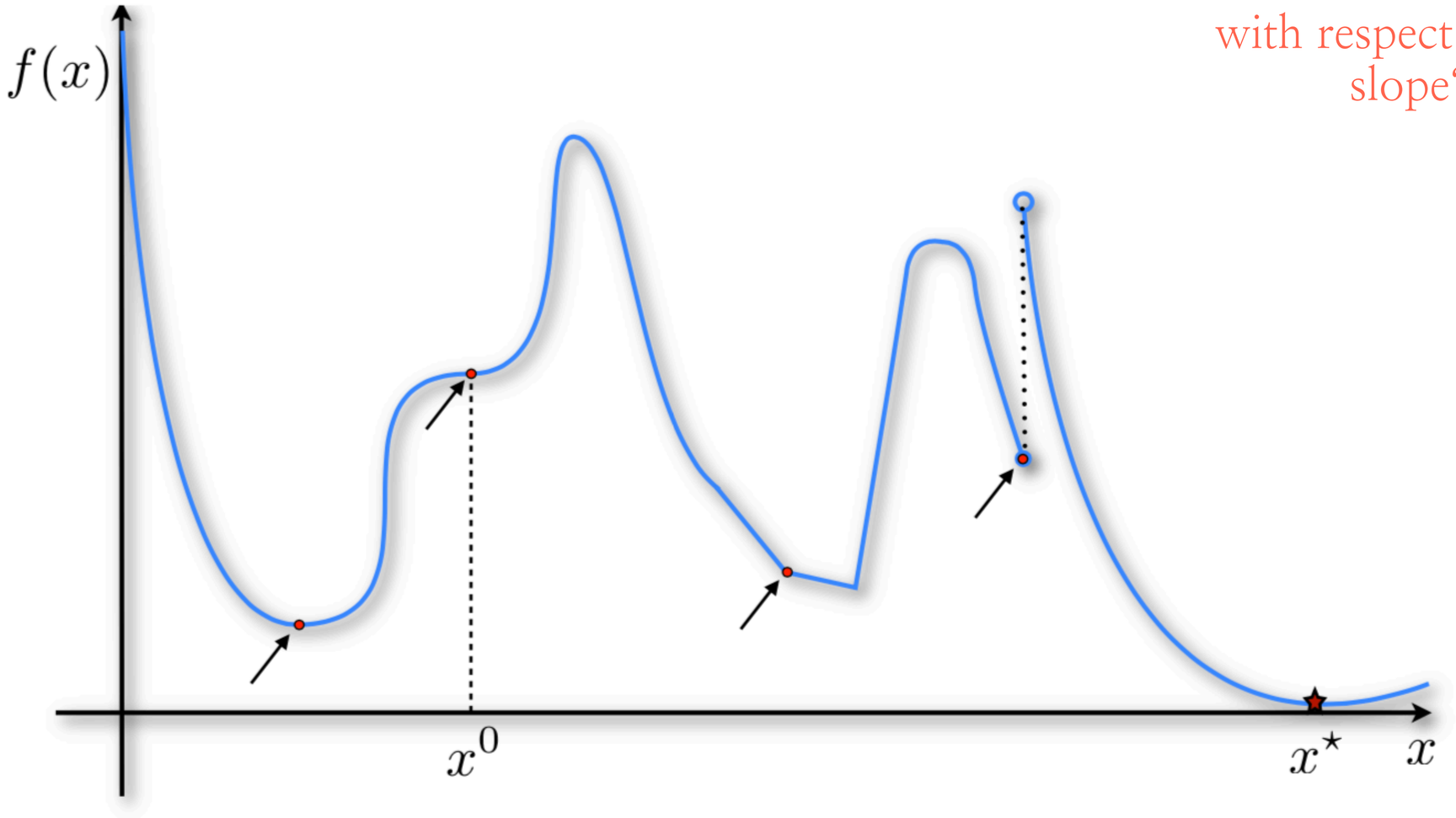
Agnostic optimization



Agnostic optimization

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



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Necessary

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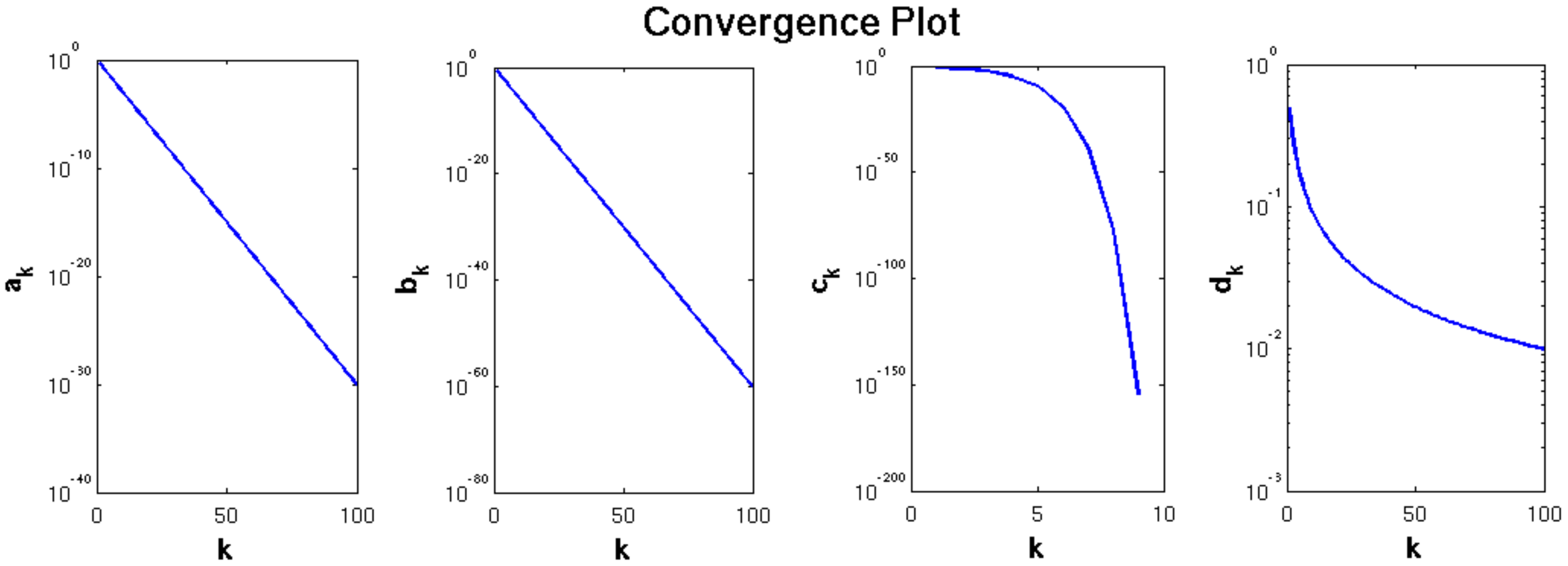
First convergence result

Whiteboard

Convergence rates 101

(Source: Wikipedia)



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$q^k,\ q \in (0,1)$

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$O(1/\varepsilon^2),\ O(1/\varepsilon),\ O(1/\sqrt{\varepsilon})$

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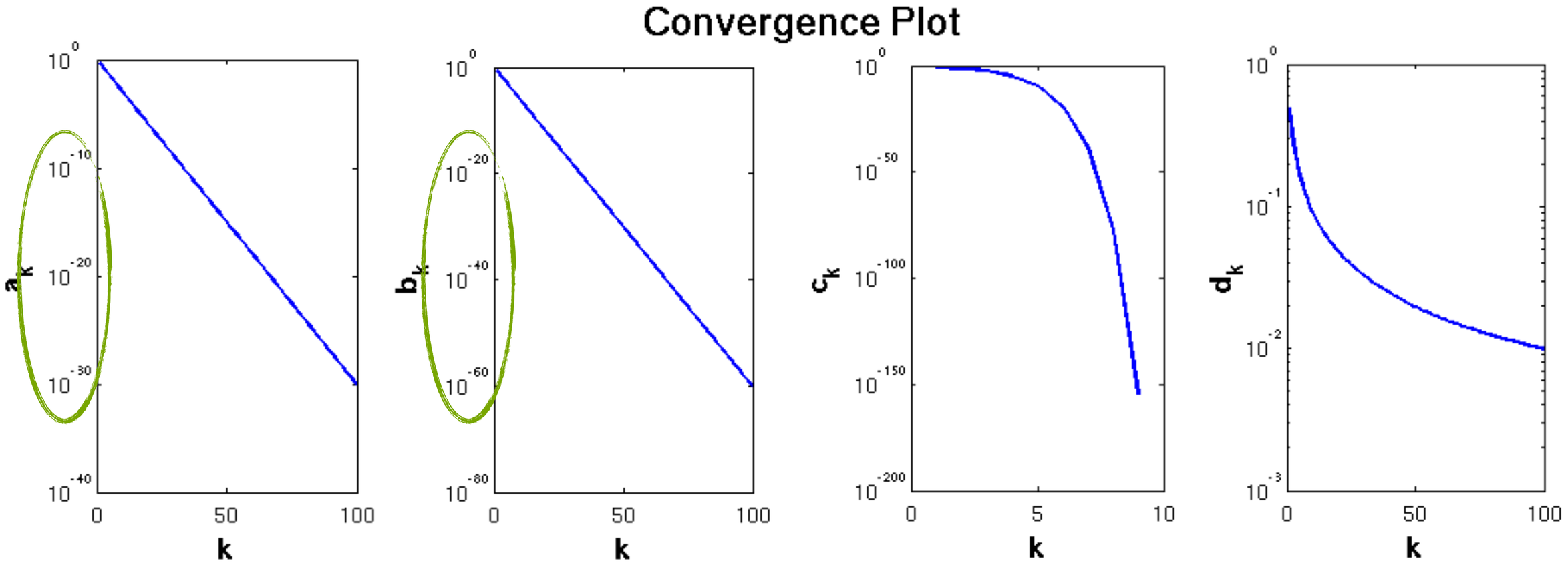

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$O(1/k^2), O(1/k), O(\sqrt{(k)})$

First convergence result

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

"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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Whiteboard

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Whiteboard

"But these are actually convex!"

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

Demo

“What does convexity bring onto the table?”

Convex functions

- General definition:

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y),\ \forall a \in [0,1]$$

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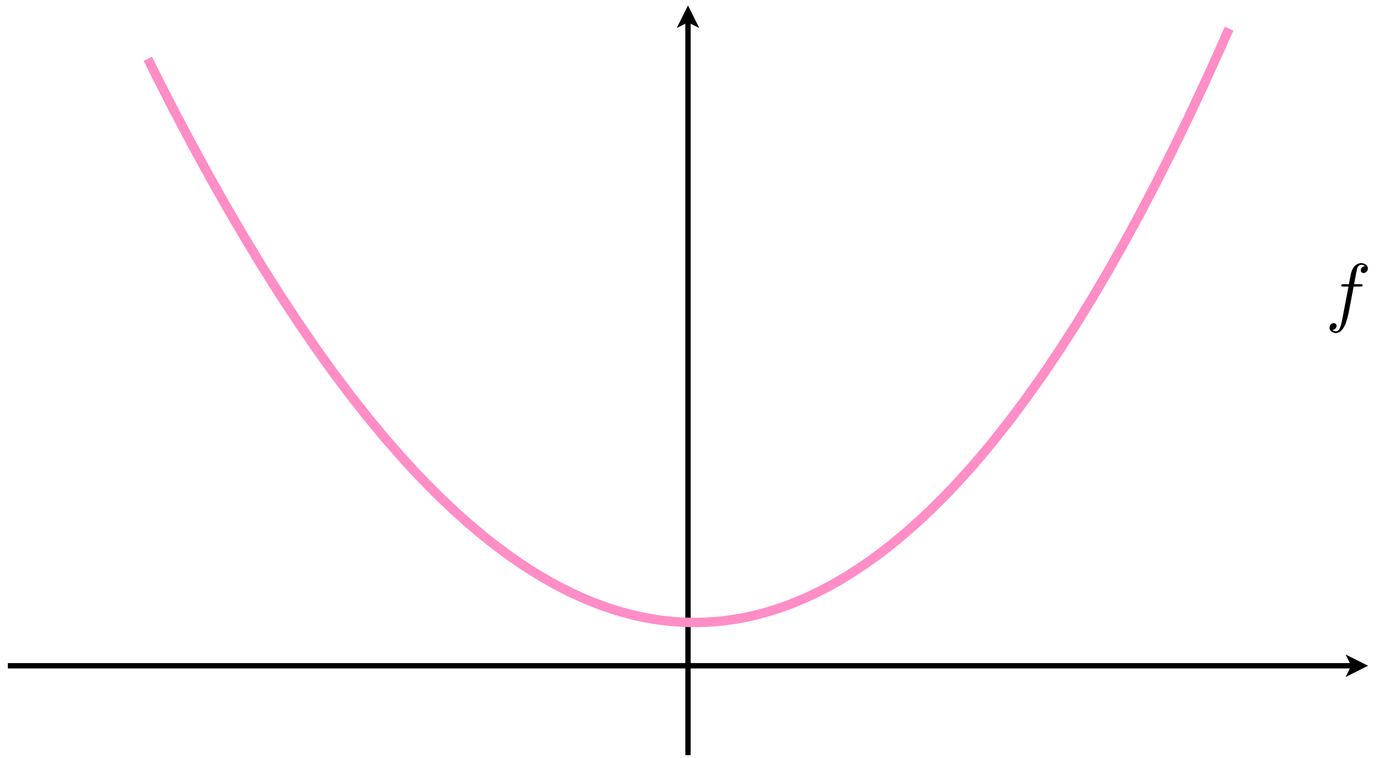

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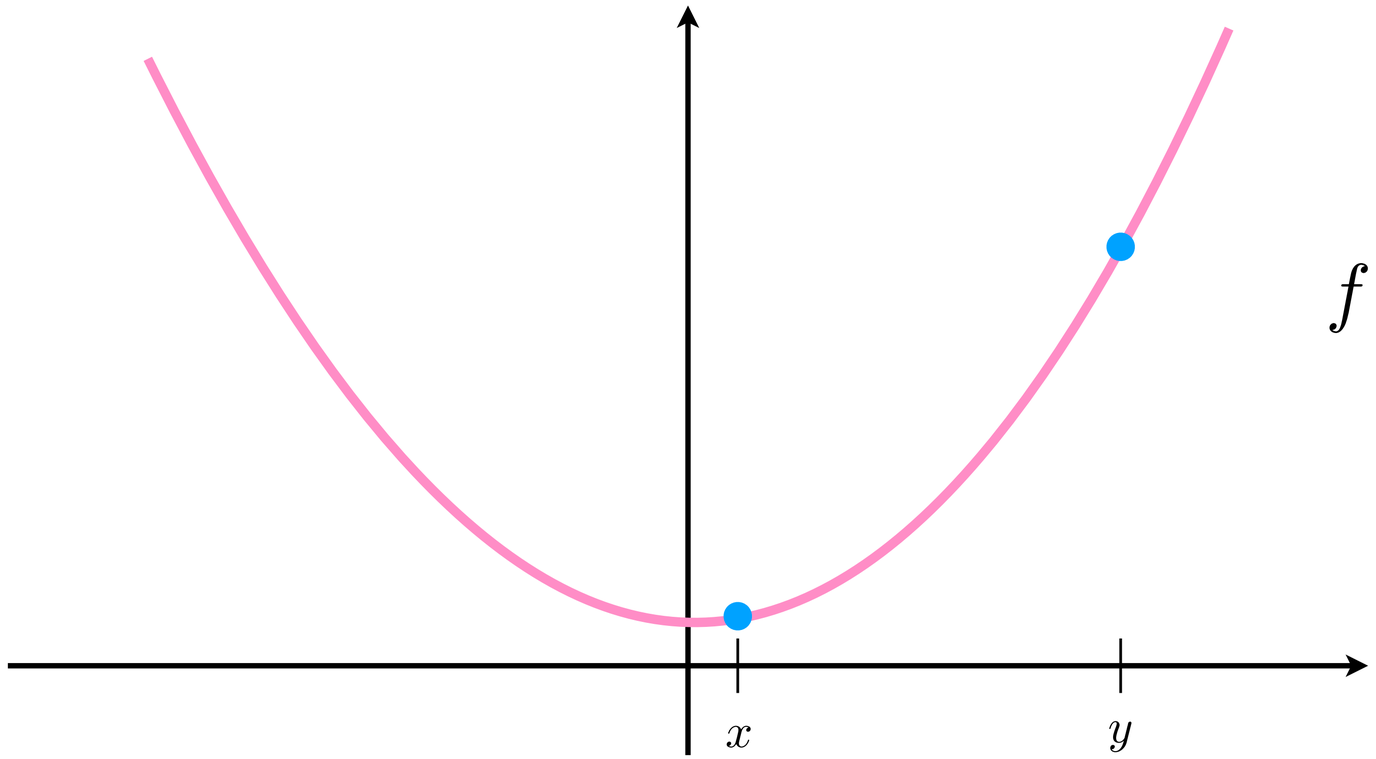

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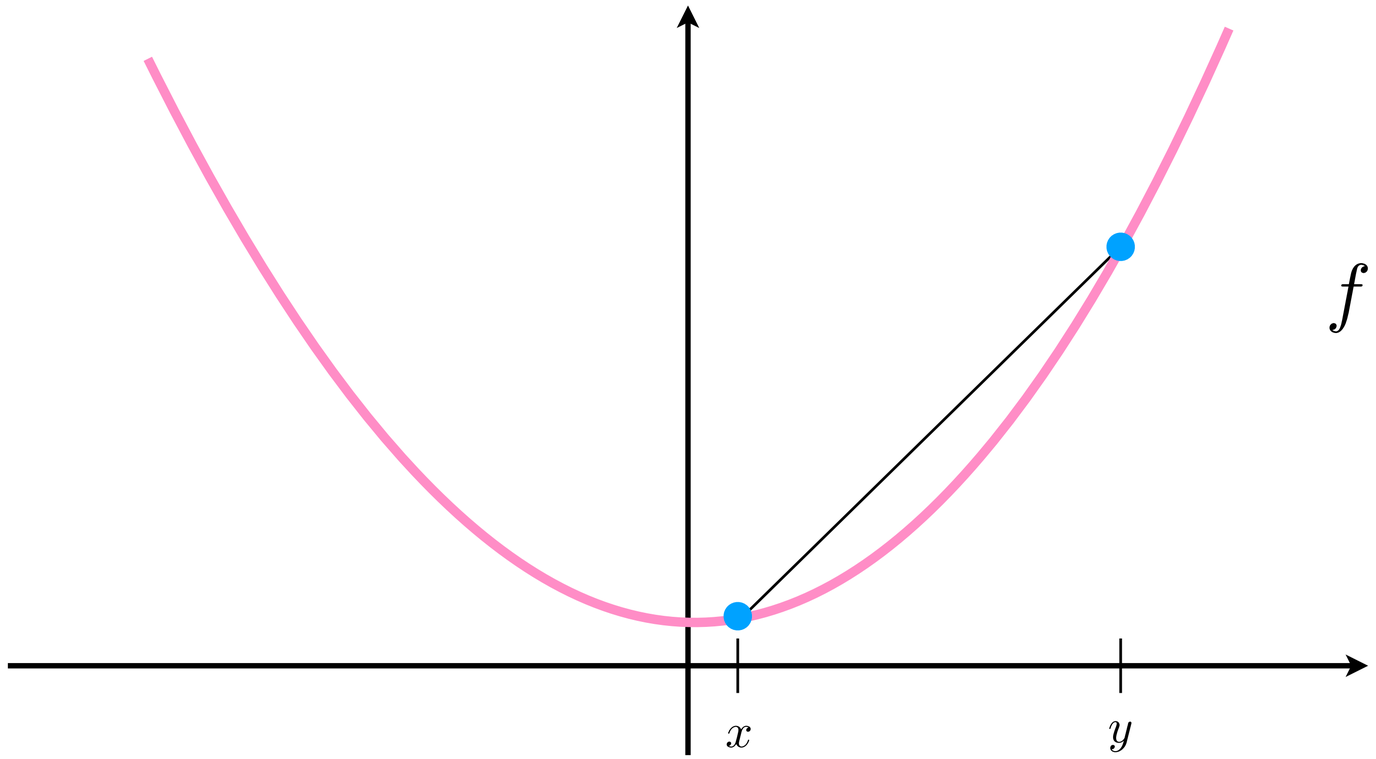

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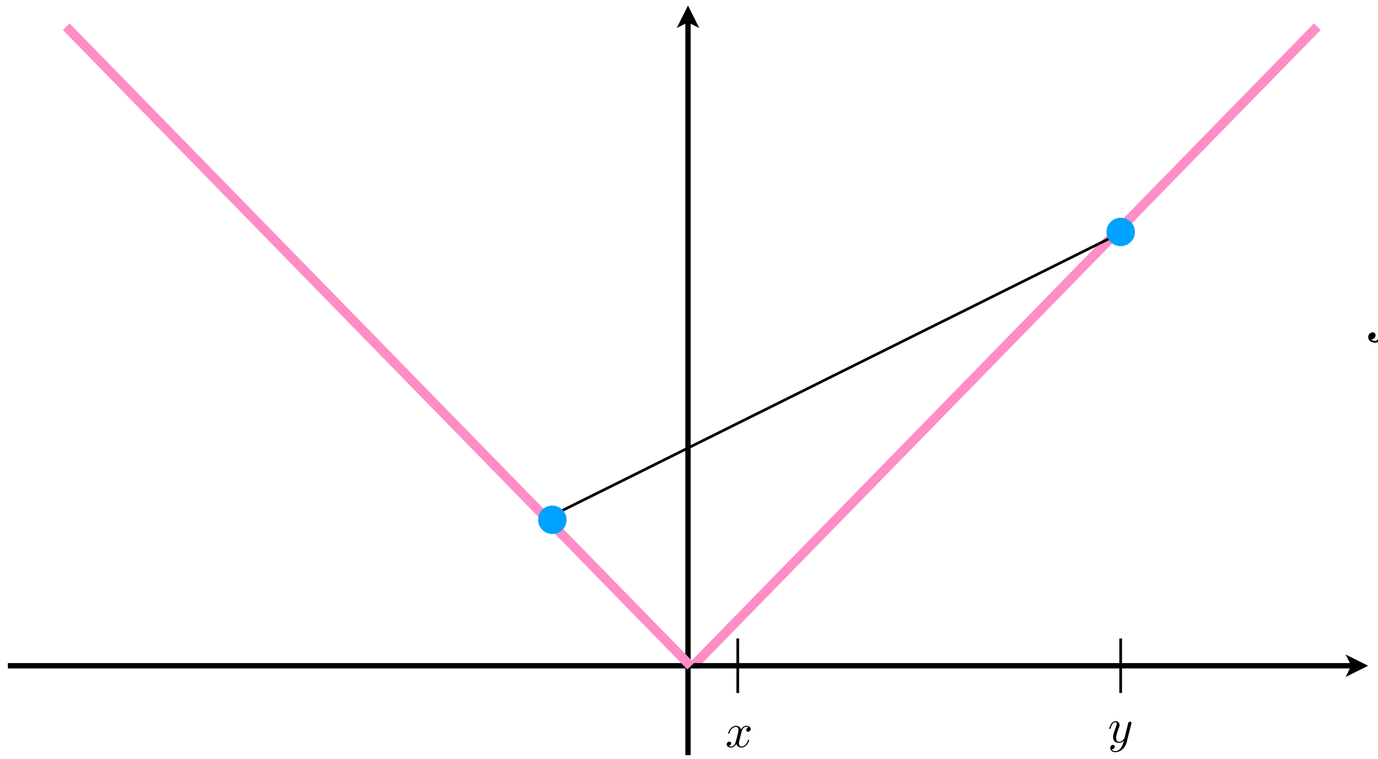

$$f(x) = |x|$$

Convex functions

- Examples:

Function	Example	Attributes
ℓ_p vector norms, $p \geq 1$	$\|\mathbf{x}\|_2, \|\mathbf{x}\|_1, \|\mathbf{x}\|_\infty$	convex
ℓ_p matrix norms, $p \geq 1$	$\|\mathbf{X}\|_* = \sum_{i=1}^{\text{rank}(\mathbf{X})} \sigma_i$	convex
Square root function	$\sqrt{x}$	concave, nondecreasing
Maximum of functions	$\max\{x_1, \ldots, x_n\}$	convex, nondecreasing
Minimum of functions	$\min\{x_1, \ldots, x_n\}$	concave, nondecreasing
Sum of convex functions	$\sum_{i=1}^n f_i$, f_i convex	convex
Logarithmic functions	$\log(\det(\mathbf{X}))$	concave, assumes $\mathbf{X} \succ 0$
Affine/linear functions	$\sum_{i=1}^n X_{ii}$	both convex and concave
Eigenvalue functions	$\lambda_{max}(\mathbf{X})$	convex, assumes $\mathbf{X} = \mathbf{X}^T$

Convex functions

- Alternative (more practical) definitions of convexity

$$f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle \,, \quad \forall x, y$$

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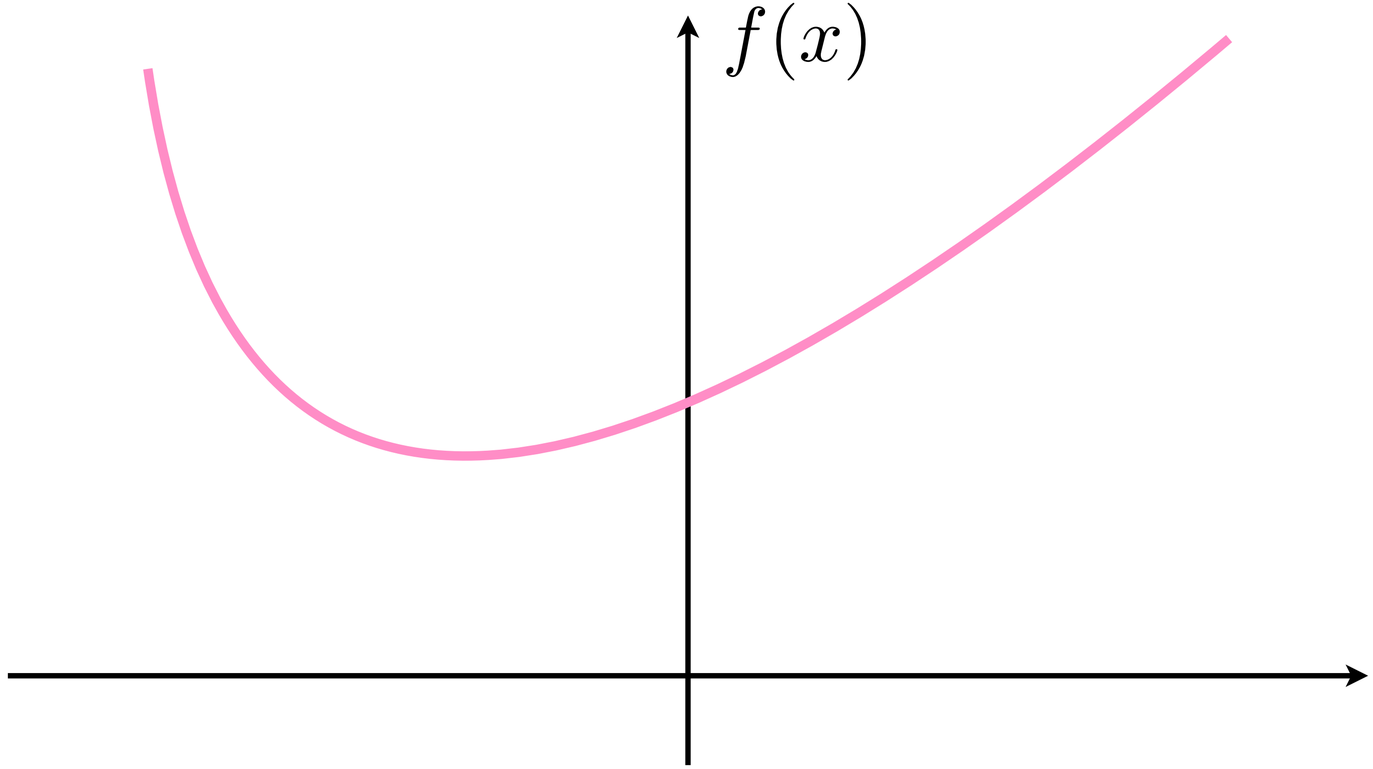

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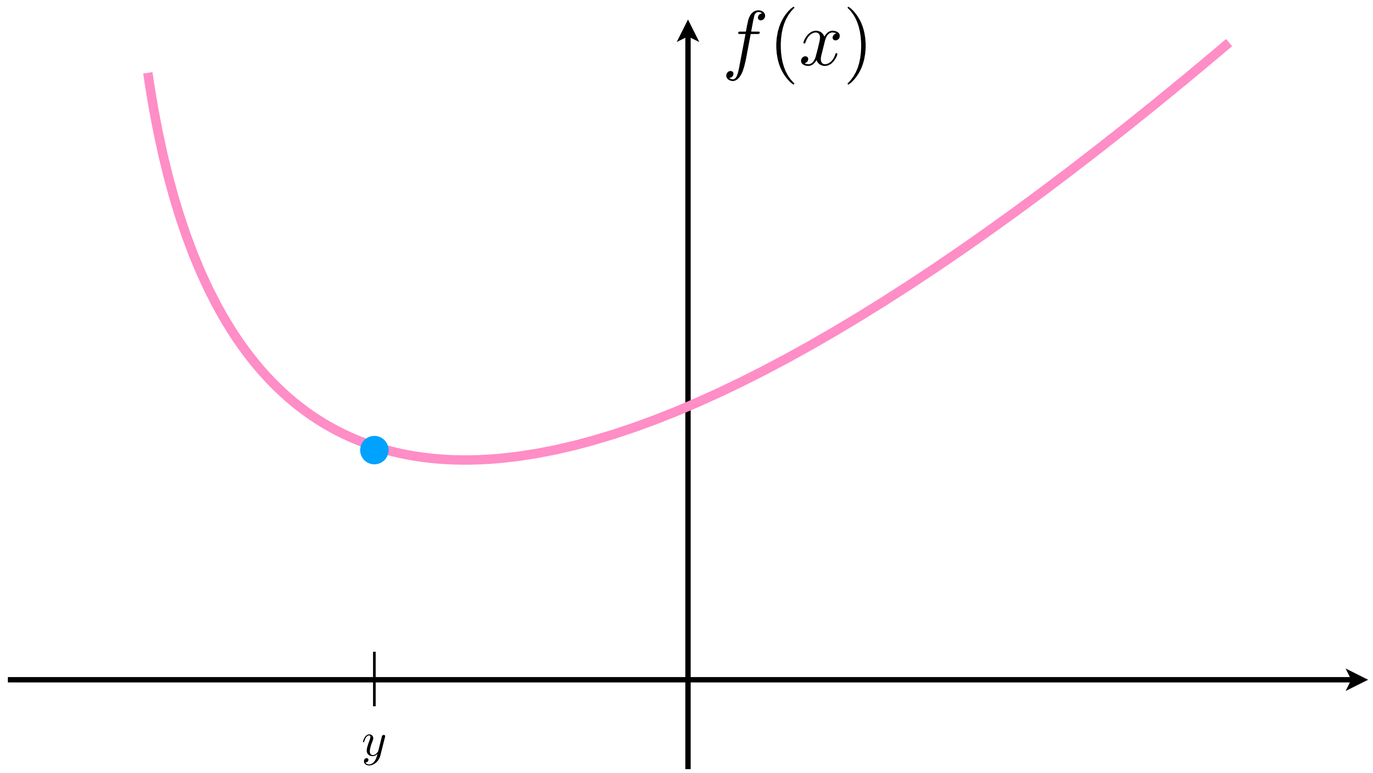

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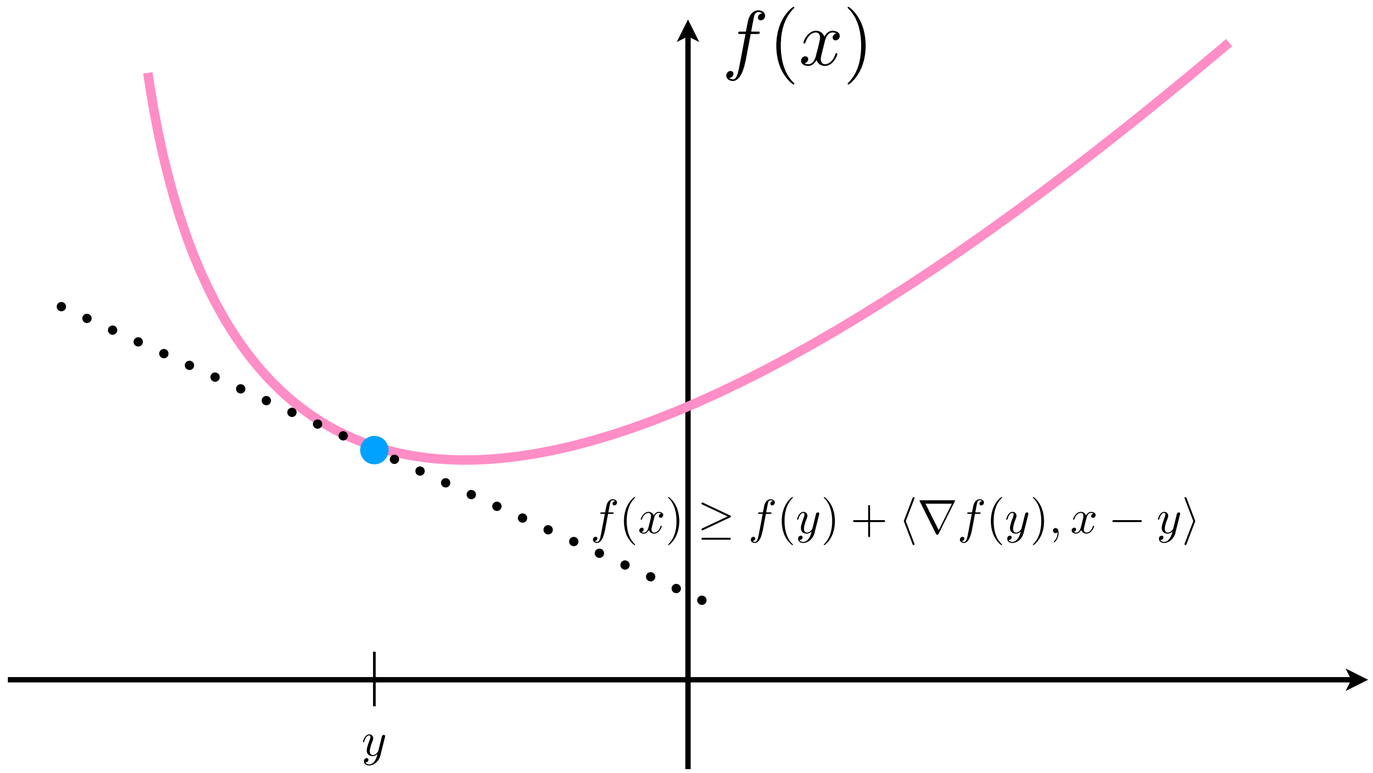

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(Assuming the function is twice differentiable)

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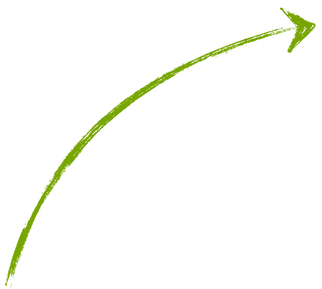

Any interpretations?

Convex functions

- Key consequences of convexity

“Any stationary point is a global minimum”

Proof:

Convex functions

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Proof: Assume a stationary point $x^\star$. This implies $\nabla f(x^\star) = 0$

Convex functions

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"Any stationary point is a global minimum"

Proof: Assume a stationary point $x^\star$. This implies $\nabla f(x^\star) = 0$

By convexity:

$$f(x) \geq f(x^\star) + \langle \nabla f(x^\star), x - x^\star \rangle = f(x^\star), \ \forall x$$

- This is what makes convex optimization preferable.

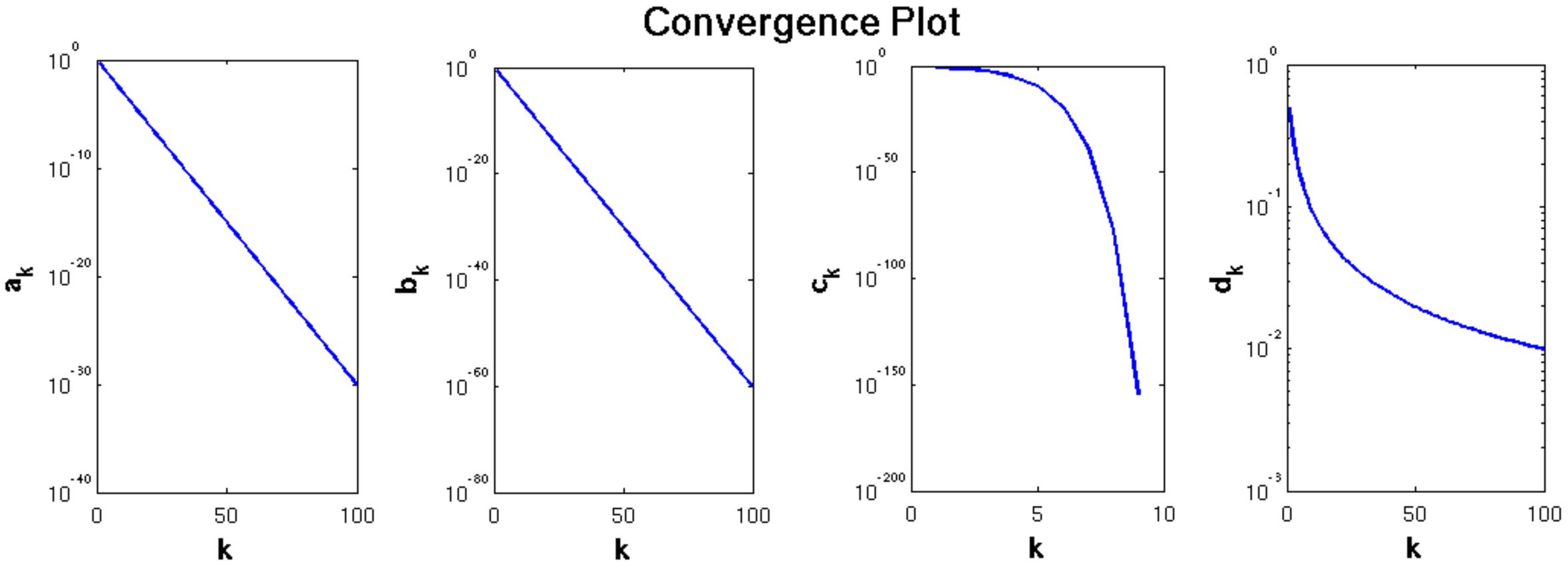
(Any local solution is actually global –
this does not mean that convex optimization is necessarily tractable!)

Does convexity improve guarantees?

Whiteboard

Convergence rates 101

(Source: Wikipedia)



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$q^k,\ q \in (0,1)$

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$O(1/\varepsilon^2),\ O(1/\varepsilon),\ O(1/\sqrt{\varepsilon})$

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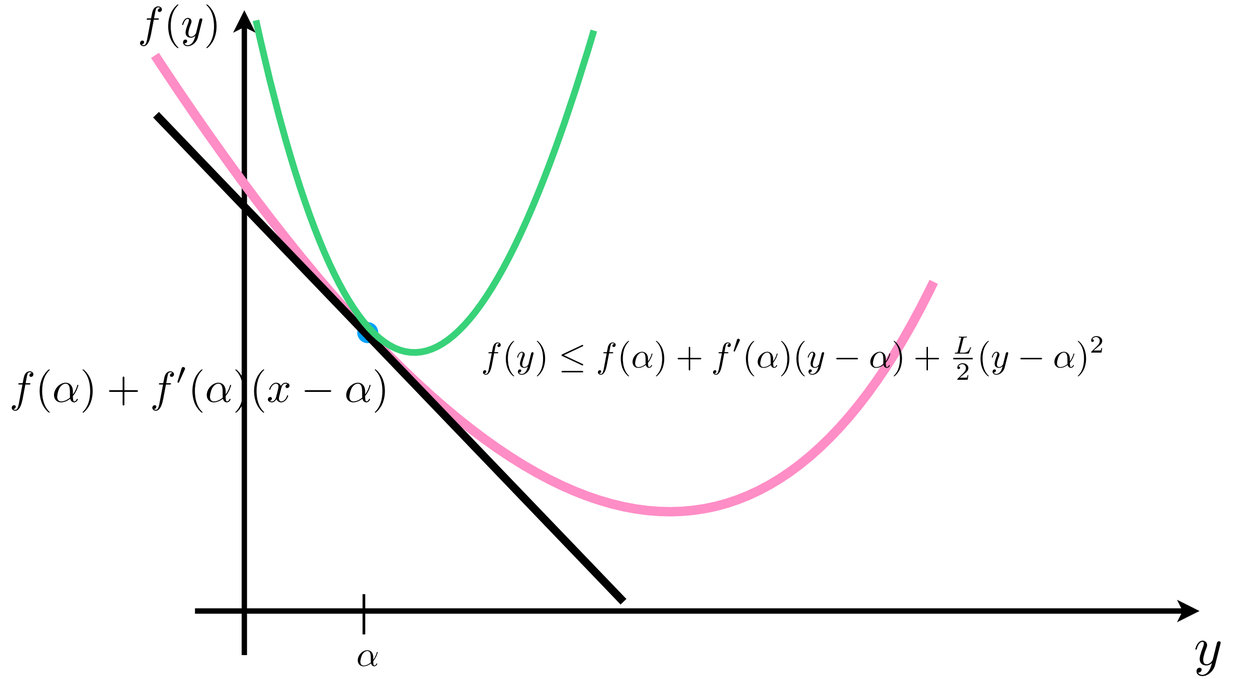
Can we achieve a better performance?

- Strong convexity: $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2}\|x - y\|_2^2, \ \forall x, y$
  - Strong convexity parameter: $\mu > 0$

"Strong convexity implies that f should be steep enough to make progress"



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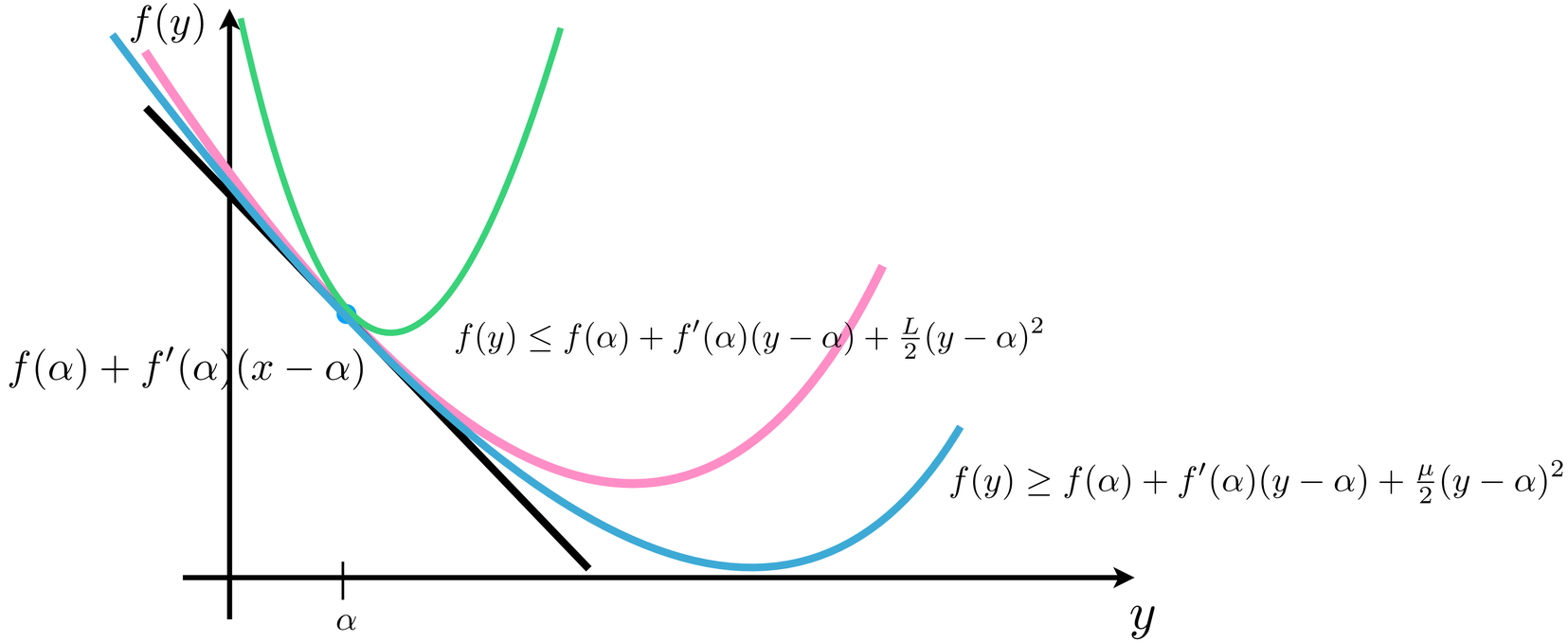

Strong convexity

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$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|_2^2$$

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{1}{2\mu}\|\nabla f(x) - \nabla f(y)\|_2^2$$

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- What if we also have Lipschitz continuous gradients?

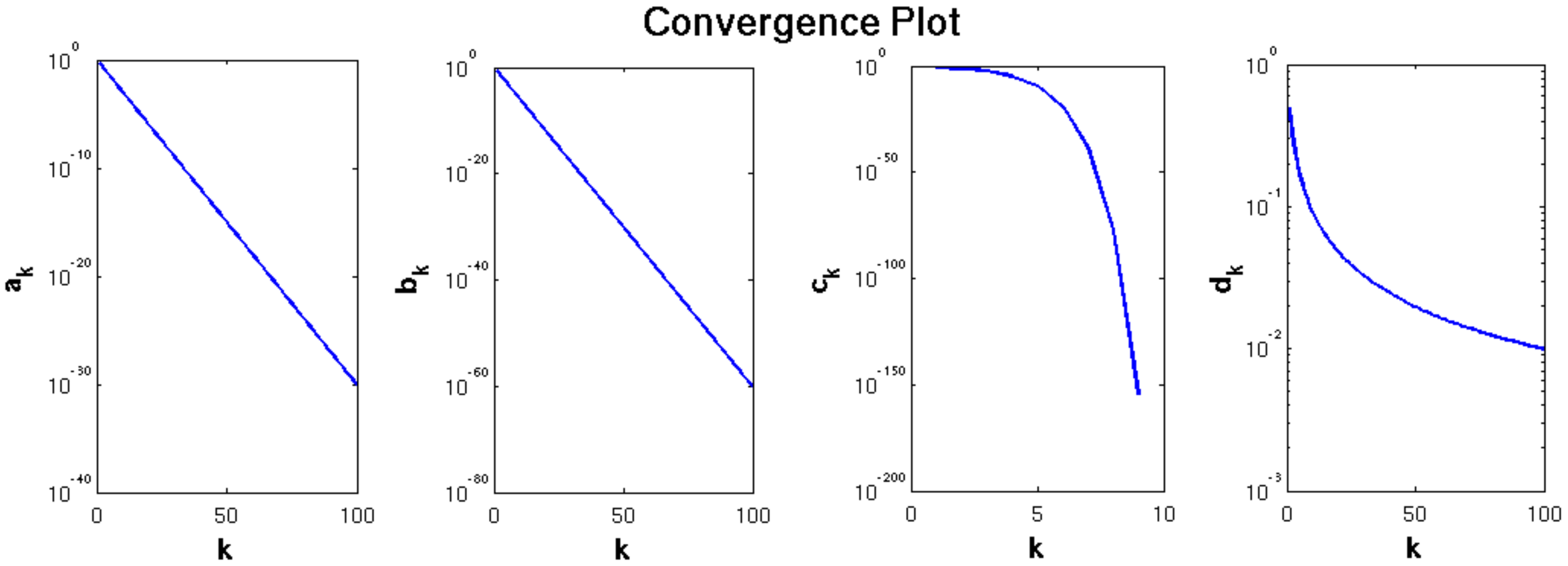
$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \frac{\mu L}{\mu + L}\|x - y\|_2^2 + \frac{1}{\mu + L}\|\nabla f(x) - \nabla f(y)\|_2^2$$

What is the gain?

Whiteboard

Convergence rates 101

(Source: Wikipedia)



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What should be our expectations: Lower bounds

- For objectives with Lipschitz continuous gradients:

$$f(x_t) - f(x^\star) \geq \frac{3L\|x_0 - x^\star\|_2^2}{32(t+1)^2}$$

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- In addition, for objectives that are strongly convex:

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- In future lectures: acceleration techniques that achieves these rates

Convex optimization

Demo

Are there other, more powerful, global assumptions?

- Remember, our analysis is based on: $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2, \quad \forall x, y$

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- Polyak–Lojasiewicz (PL) inequality

$$\frac{1}{2}\|\nabla f(x)\|_2^2 \geq \xi(f(x) - f(x^\star)), \quad \forall x, \quad \text{for some } \xi > 0$$

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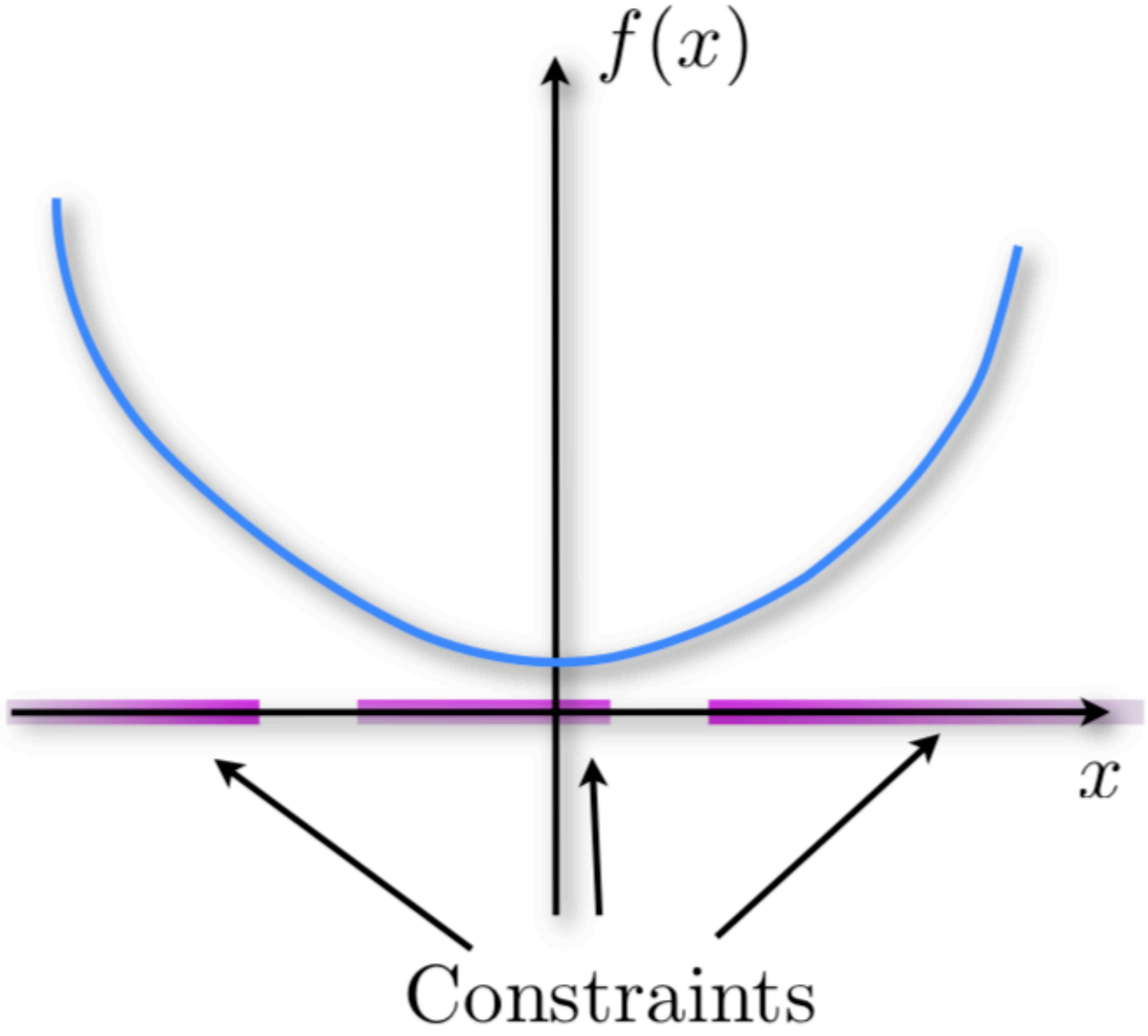
- Does not use **convexity**: holds for invex functions (stationary = global)

Convex optimization is not only about the objective



- Back to the first slide:

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

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

(We will worry about this in the lectures to follow!)

Convex sets

$\mathcal{C} \subseteq \mathbb{R}^p$ is convex if $\forall x_1, x_2 \in \mathcal{C}$, it holds $\forall \alpha \in [0,1] : \alpha x_1 + (1-\alpha) x_2 \in \mathcal{C}$

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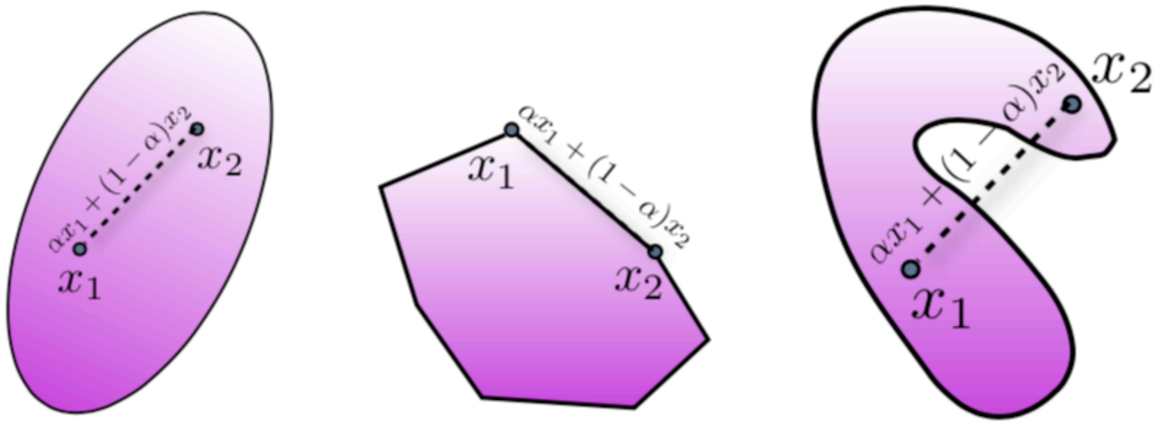

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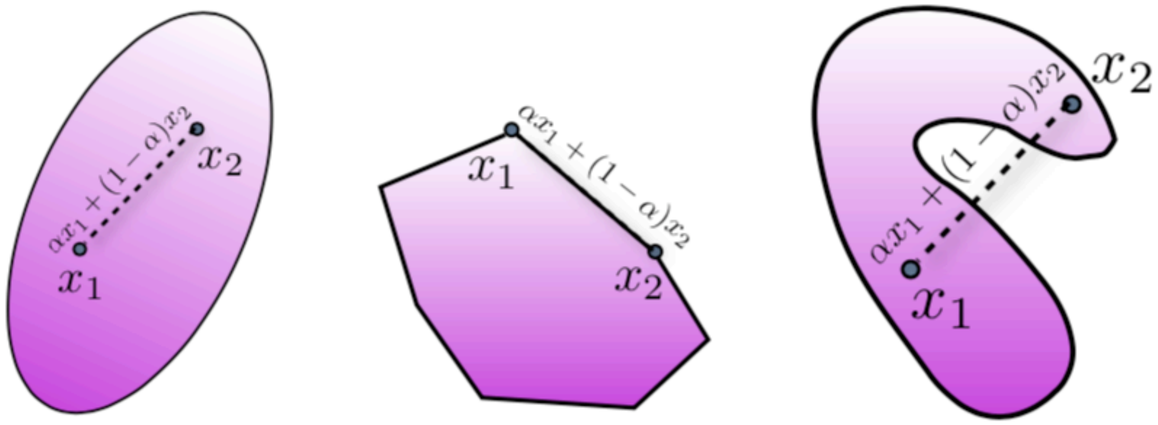

– Convex hull of points: $\text{conv}(\mathcal{V}) = \left\{ \sum_{i=1}^{|\mathcal{V}|} \alpha_i x_i \;:\; \sum_{i=1}^{|\mathcal{V}|} \alpha_i = 1,\ \alpha_i \geq 0, x_i \in \mathcal{V} \right\}$

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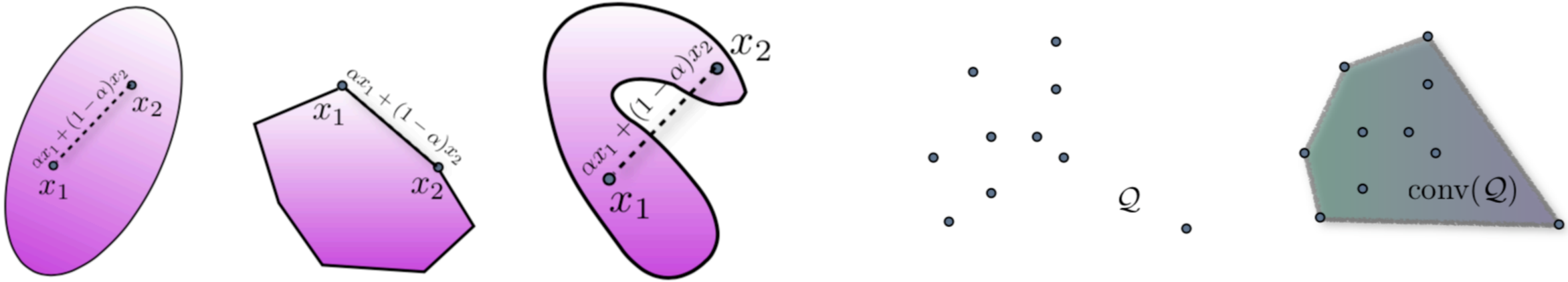

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Projections onto convex sets

$$\Pi_{\mathcal{C}}(x) = \arg\min_{y \in \mathcal{C}} \|x - y\|_2^2$$

(The use of Euclidean norm is arbitrary and often depends on the application)

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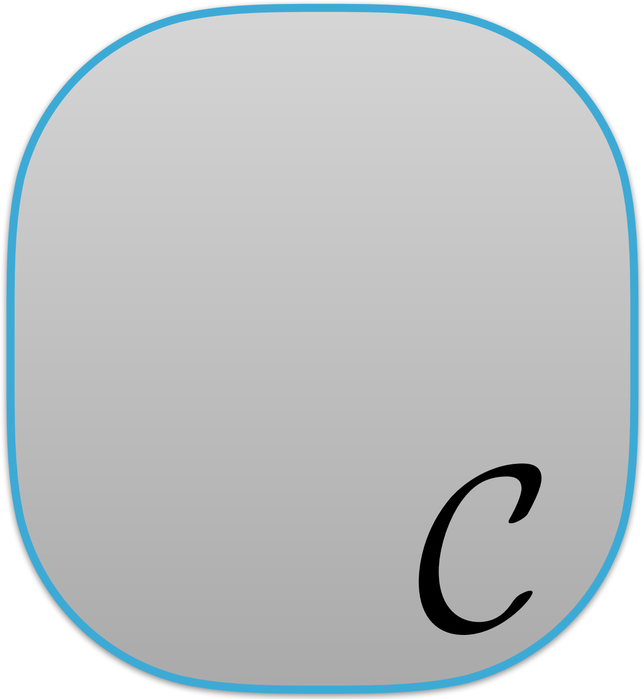

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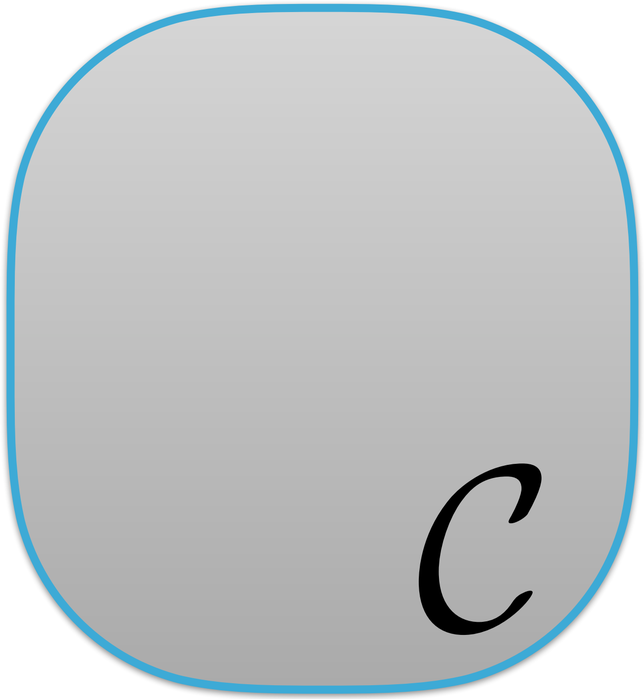

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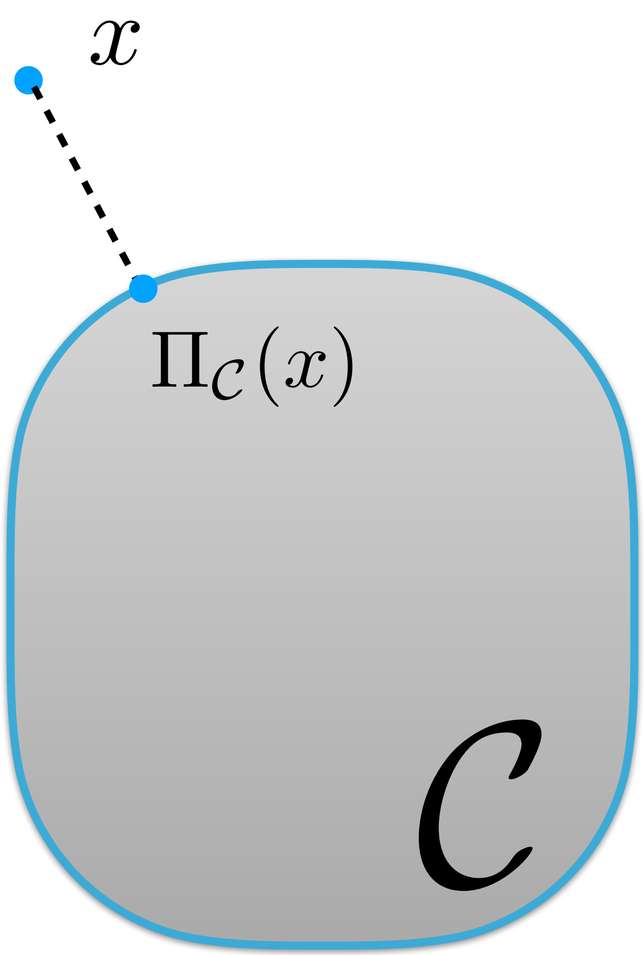

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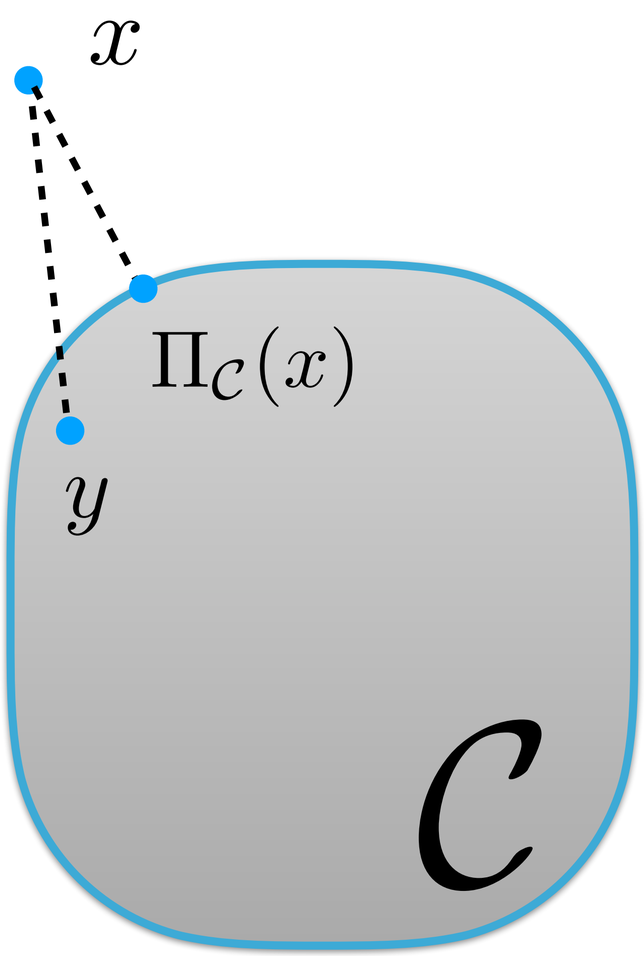

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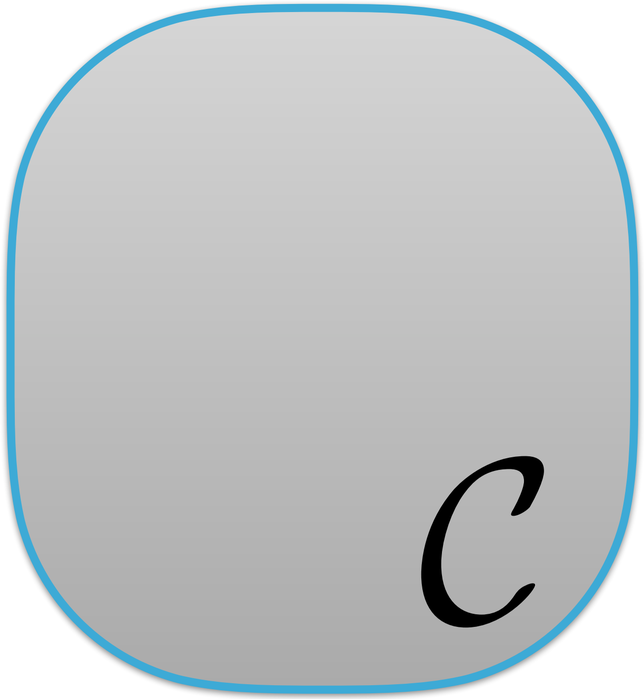

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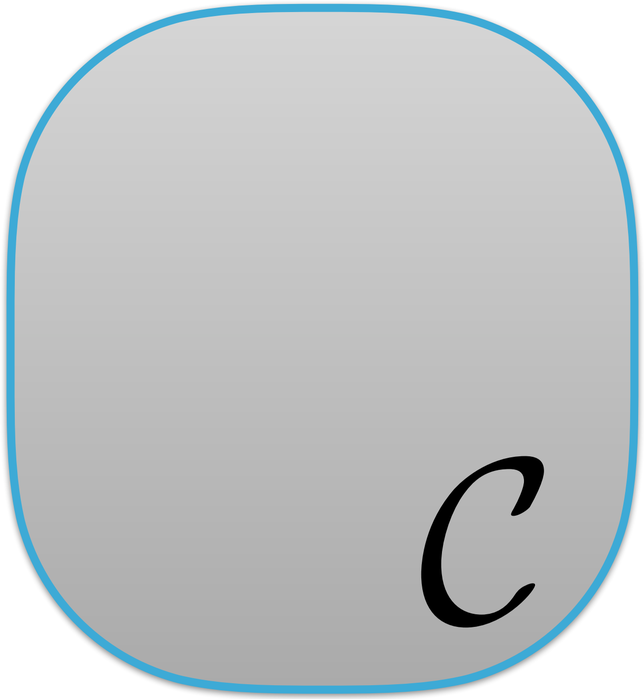

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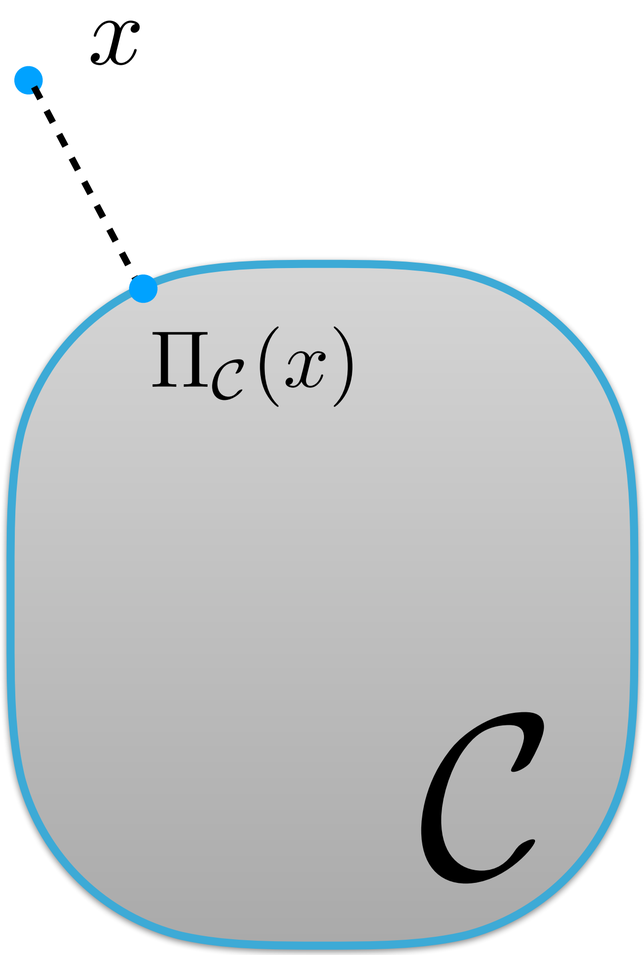

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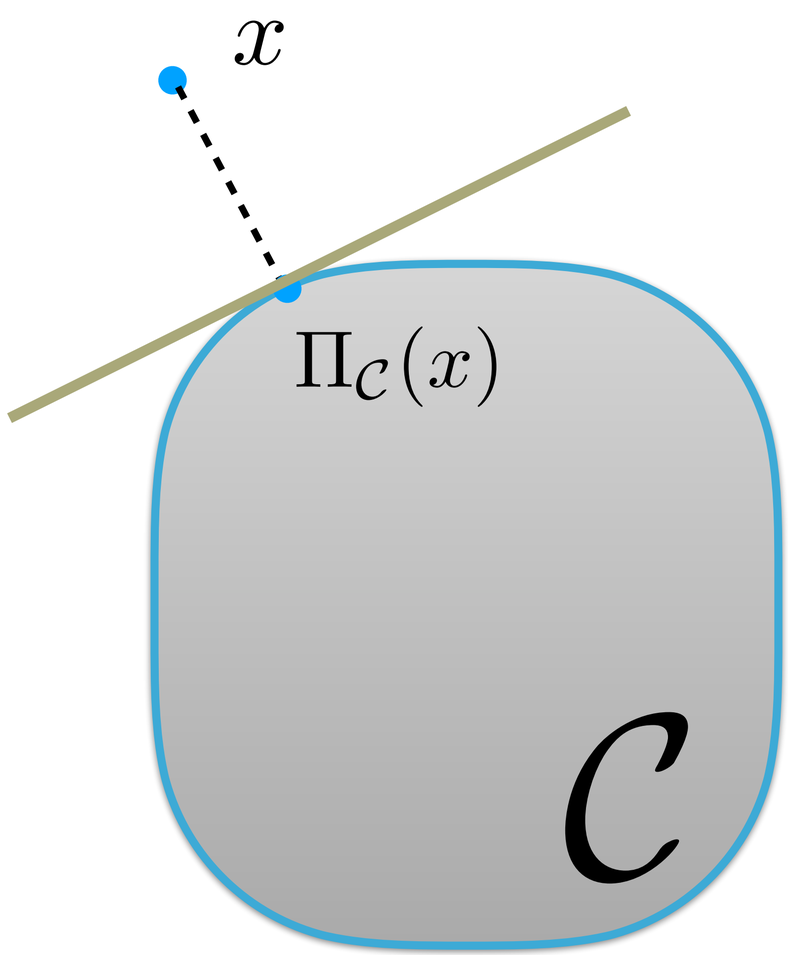

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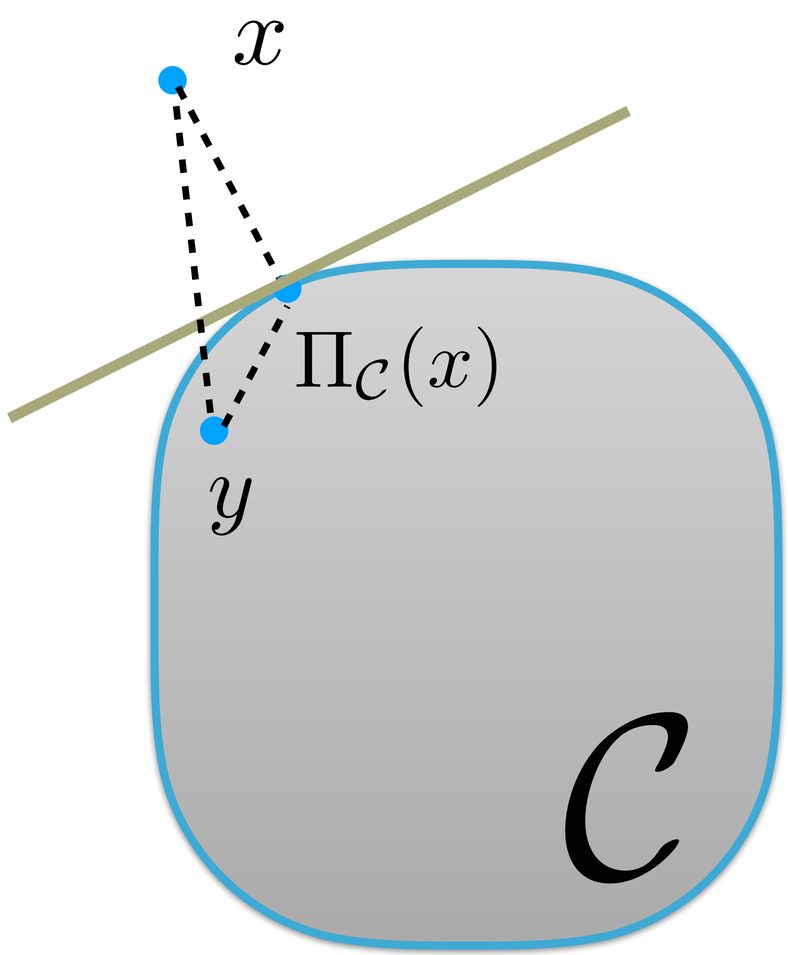

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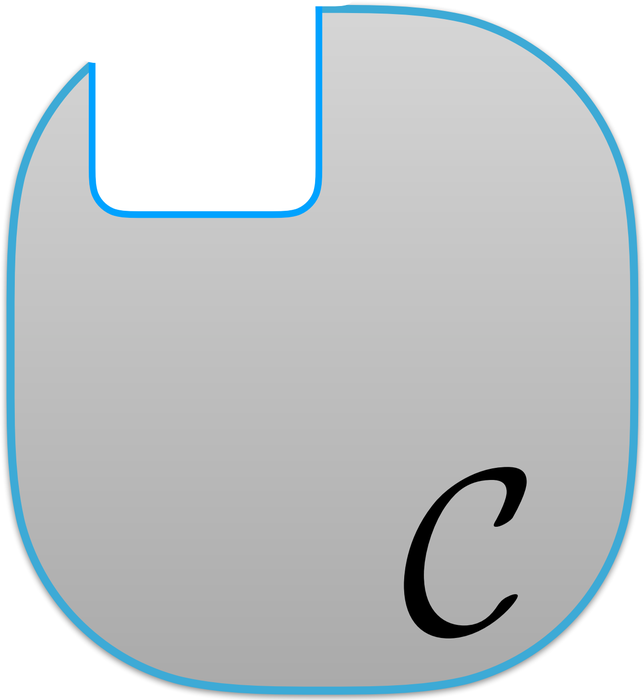

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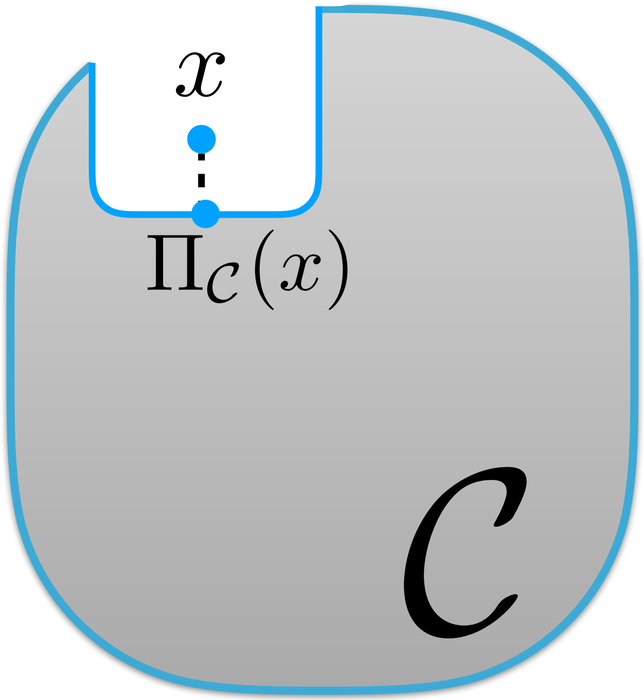

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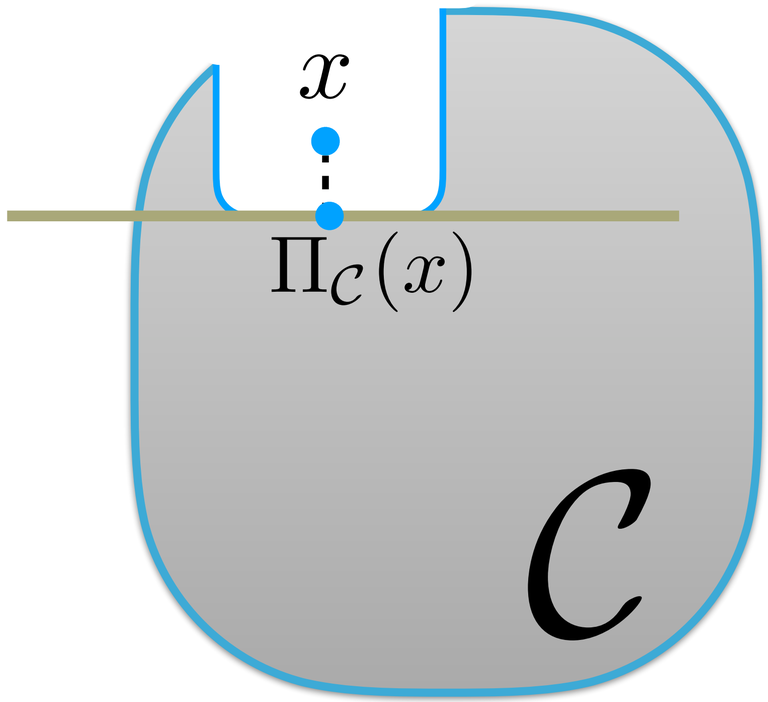

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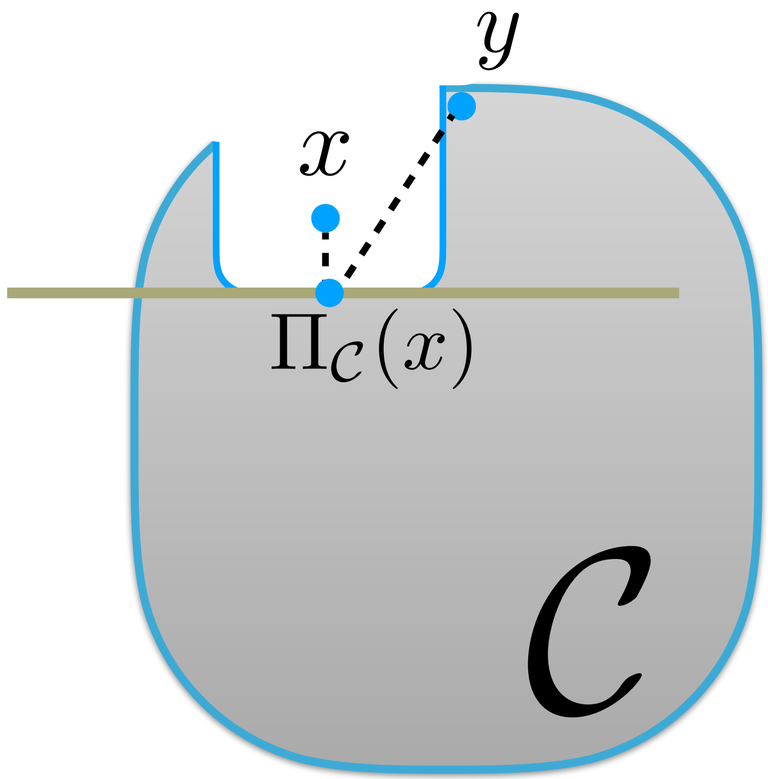

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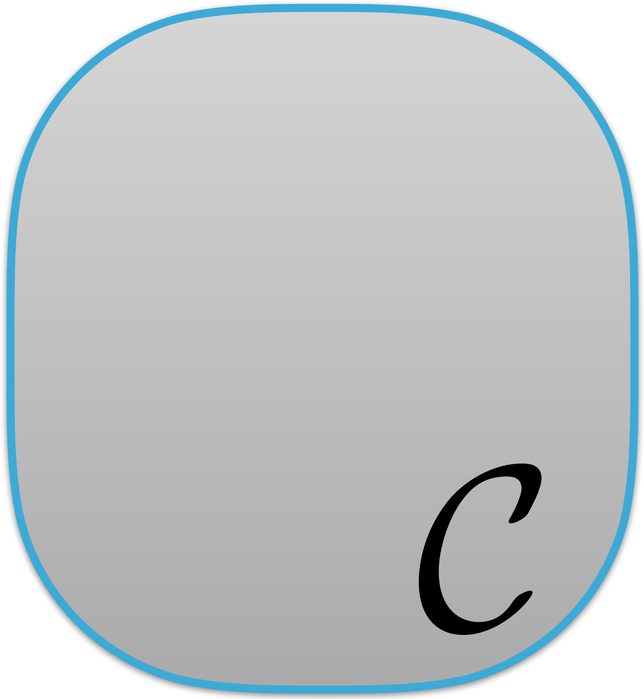

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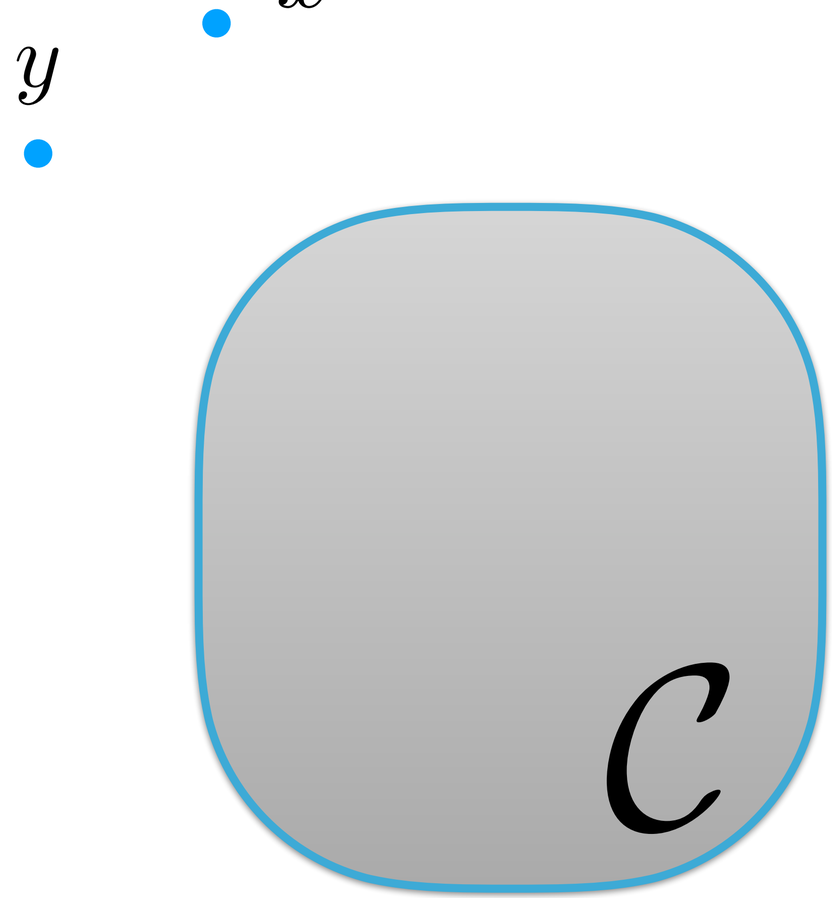

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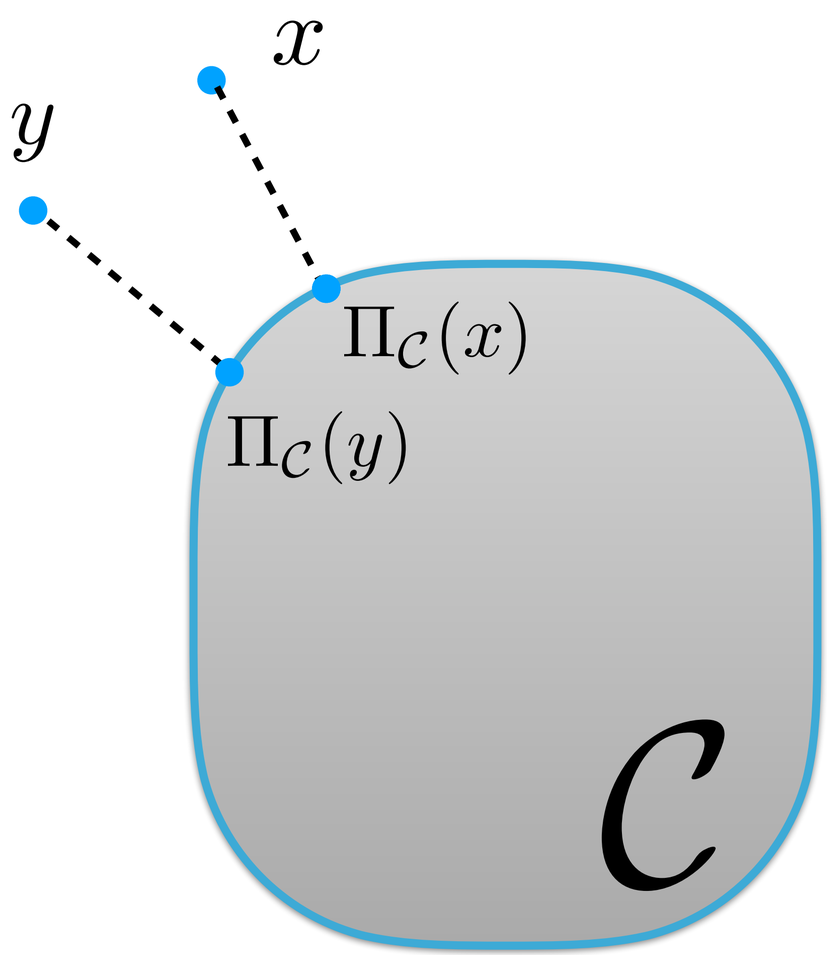

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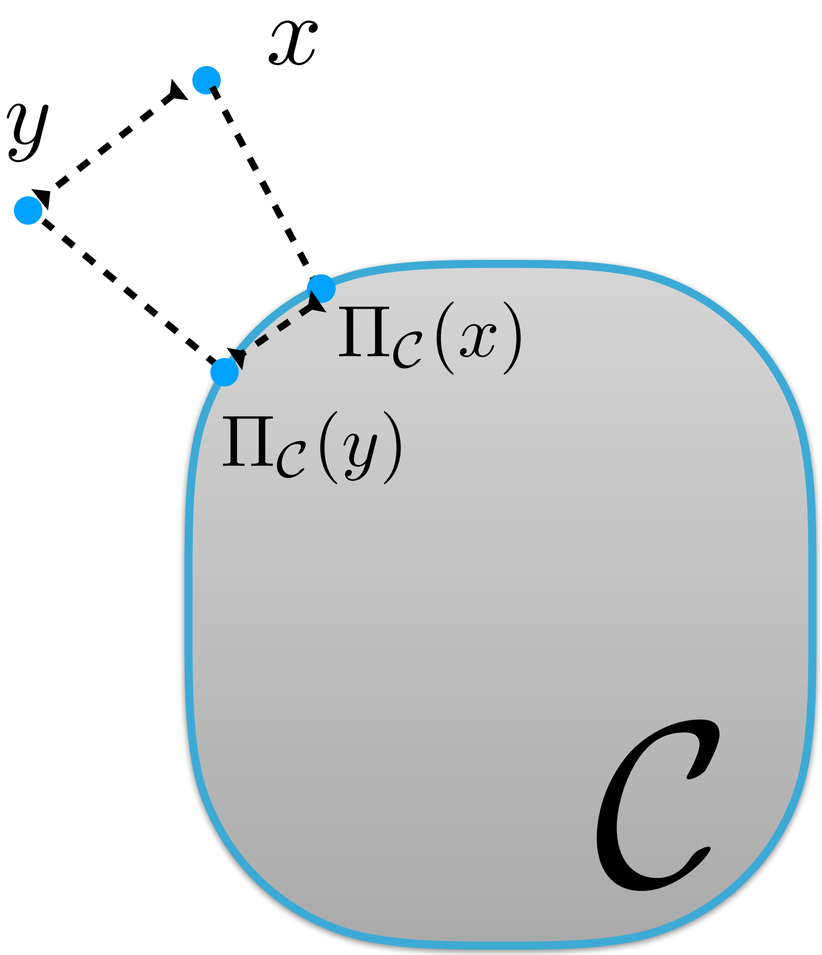

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Demo

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Whiteboard

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Is this set convex? If no or yes, why?

- But we observed that, despite non-convexity, it works just fine..

(Thus, a different analysis is needed, depending on the problem at hand)

But, constrained optimization can be hard..

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- There are constrained problems where we need exponentially many bits even to describe the solution..

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Operations Research is an area where multiple, difficult constraints appear

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- Prof. Richard Tapia is teaching a course on constrained convex opt.

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- Why should we still care about convex optimization?

Several practical problems are actually convex
Many practical problems can be approximated by convex ones
If one doesn't understand convex opt., why even try understanding non-convex opt.?

Papers to review – due next Tuesday

(Select one of the following papers)

- "Linear convergence of gradient and proximal-gradient methods under the Polyak-Łojasiewicz condition", Karimi et al., 2016.

(Focus on Sections 1,2,4,5 – and the corresponding appendix)

(Rule: as you read, think of extensions – feel free to find me for more discussions)

Conclusion

- Gradient descent has nice properties (even for non-convex problems)
- Further global assumptions lead to better convergence guarantees
- Convex optimization has nice properties (local = global)

..but can be intractable!

Next lecture

- Provide a taxonomy of alternative approaches
- Focus on more computational side and how we can accelerate opt. methods