Math for Machine Learning

Week 4.1: Optimization and the Lagrangian Method

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Logistics & Announcements

Lesson Overview

Optimization. Minimize an objective function $f : \mathbb{R}^d \to \mathbb{R}$ with the possible requirement that the minimizer $\mathbf{x}^*$ belongs to a constraint set $\mathscr{C} \subseteq \mathbb{R}^d$.

Lagrangian. For optimization problems with $\mathscr{C}$ defined by equalities/inequalities, the Lagrangian is a function $L : \mathbb{R}^d \times \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ that "unconstrains" the problem.

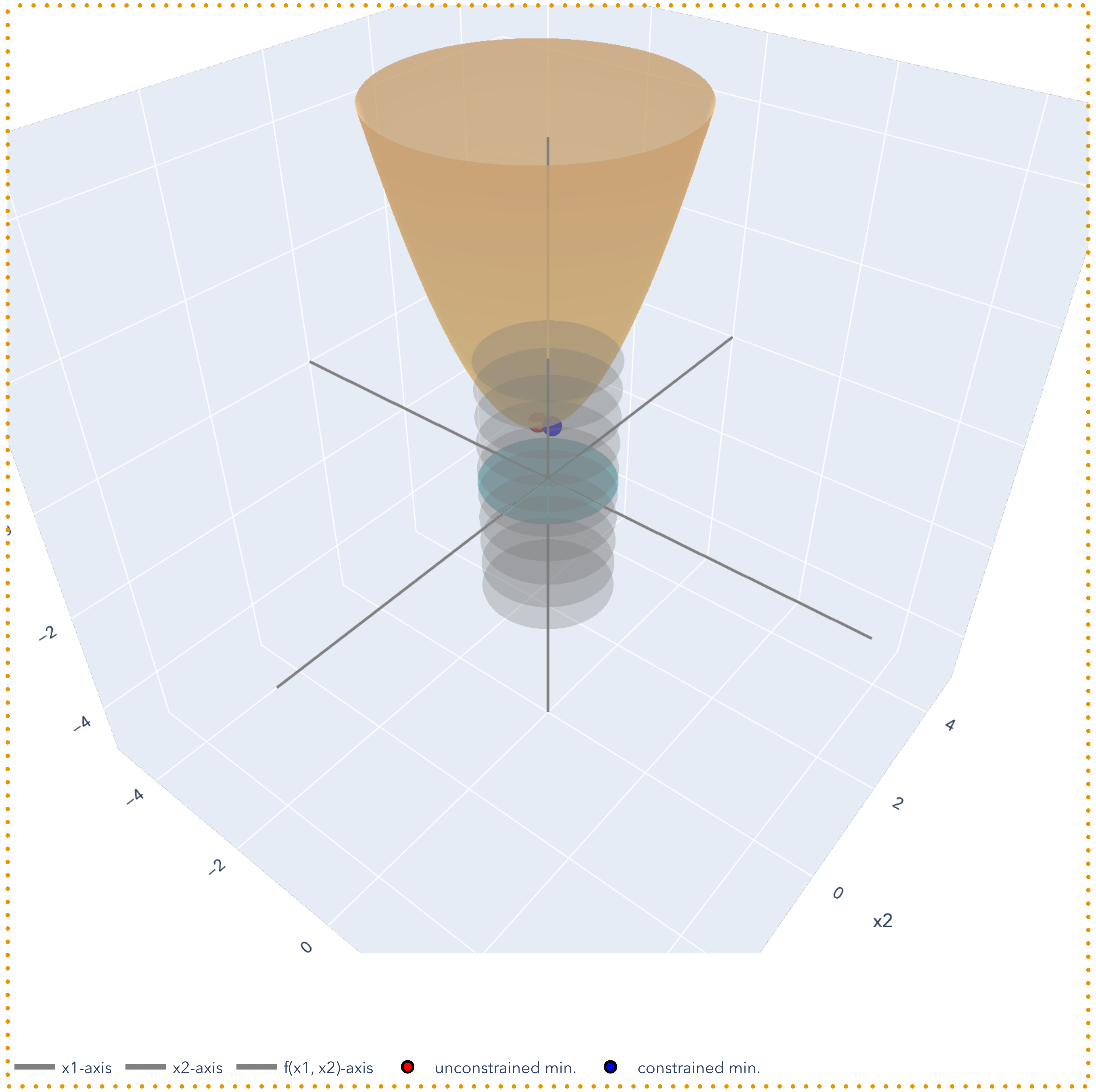
Unconstrained local optima. With no constraints, the standard tools of calculus give conditions for a point $\mathbf{x}^*$ to be optimal, at least to all points close to it.

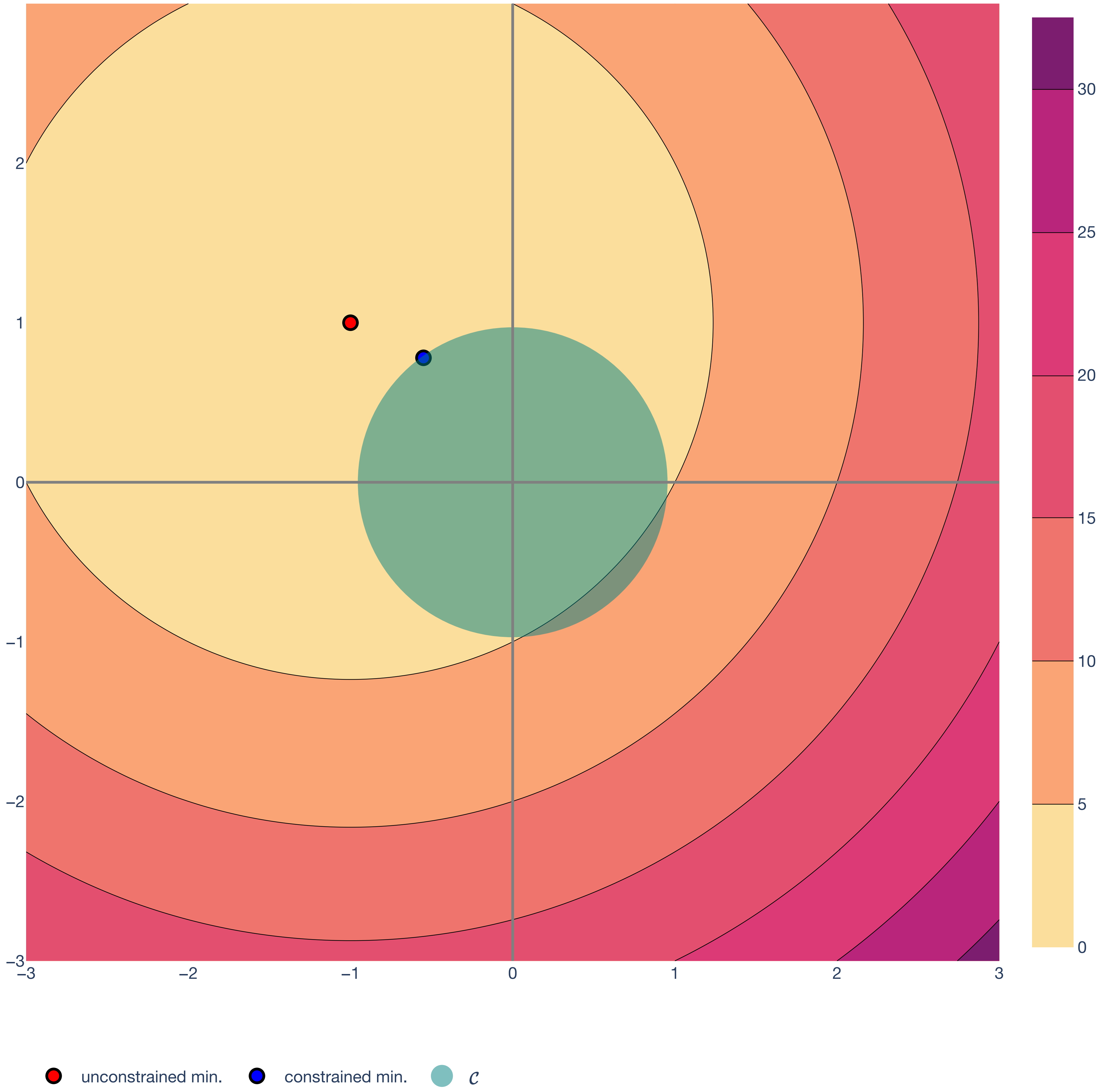
Constrained local optima (Lagrangian and KKT). When $\mathscr{C}$ is represented by inequalities and equalities, we can use the method of Lagrange multipliers and the KKT Theorem to "unconstrain" the problem.

Ridge regression and minimum norm solutions. By constraining the norm of $\mathbf{w}^* \in \mathbb{R}^d$ of least squares (i.e. $\|\mathbf{w}^*\|$), we obtain more "stable" solutions.

Lesson Overview

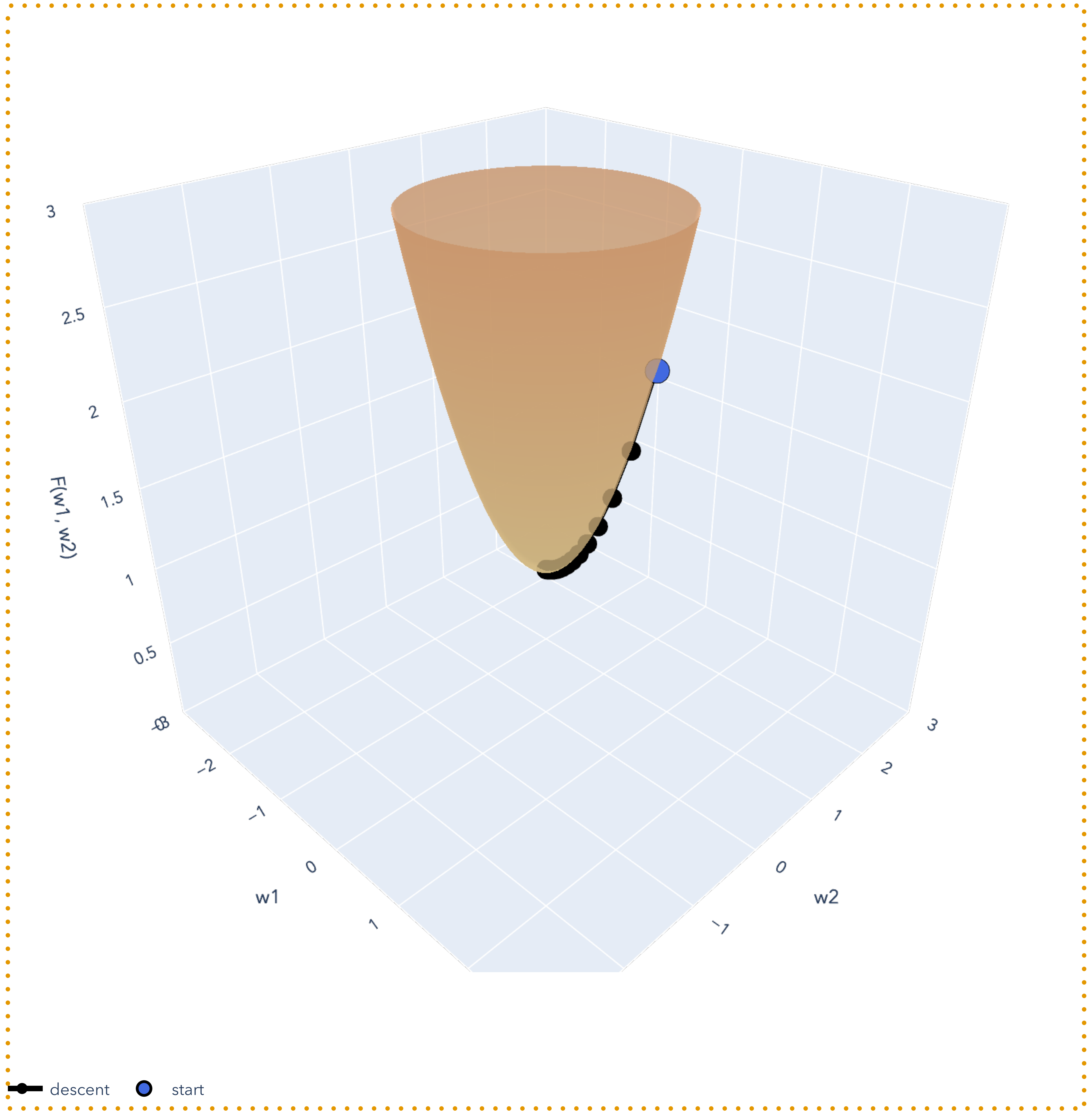
Big Picture: Least Squares

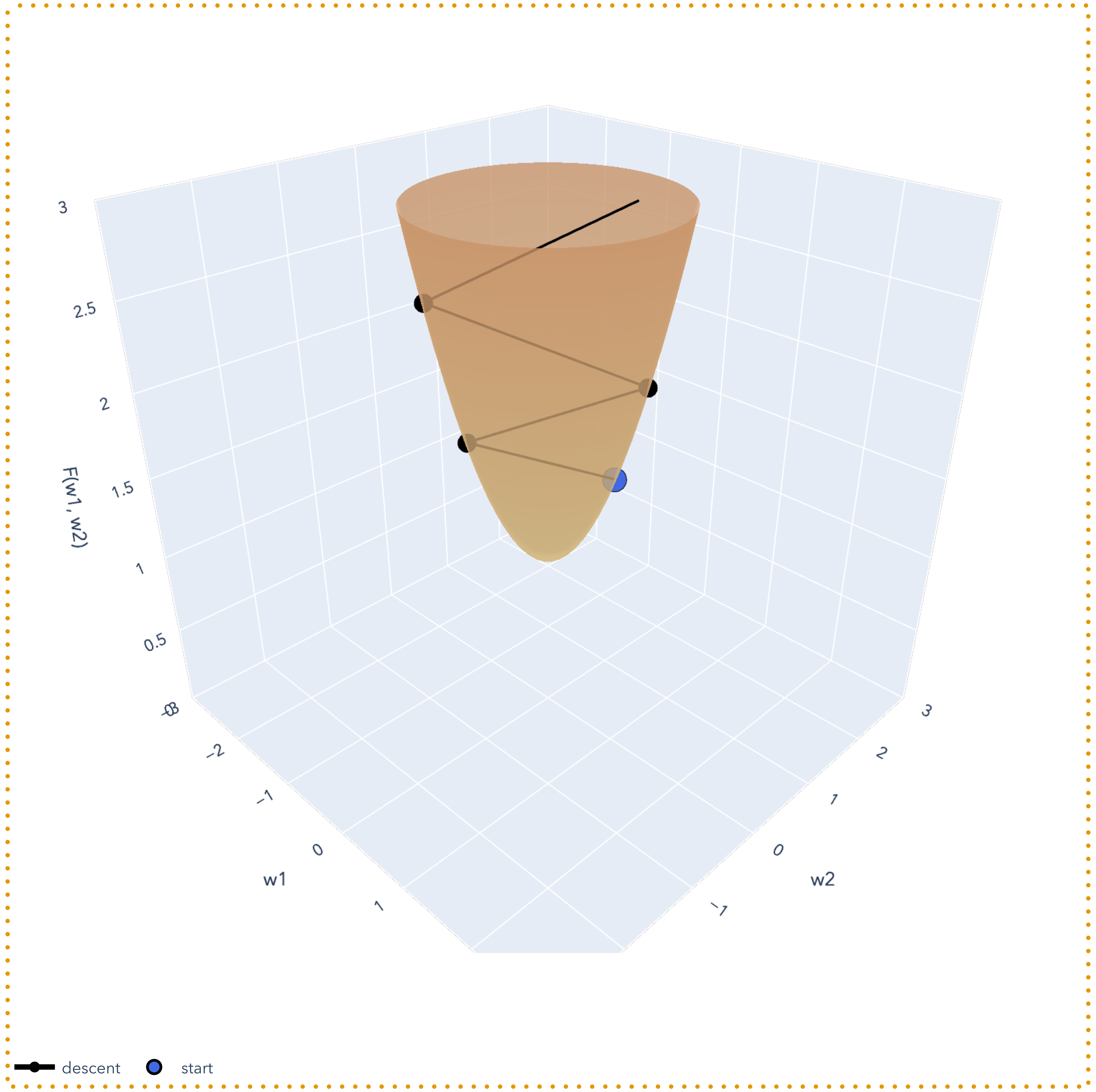




Lesson Overview

Big Picture: Gradient Descent





Optimization Problems

Definition and examples

Motivation

Optimization in calculus

In much of machine learning, we design algorithms for well-defined *optimization problems*.

In an optimization problem, we want to minimize an objective function $f : \mathbb{R}^d \to \mathbb{R}$ with respect to a set of constraints $\mathscr{C} \subseteq \mathbb{R}^d$:

$$\begin{array}{ll} \underset{\mathbf{x} \in \mathbb{R}^d}{\text{minimize}} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Motivation

Components of an optimization problem

$$\begin{aligned} \underset{\mathbf{x}\in\mathbb{R}^d}{\text{minimize}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in \mathscr{C} \end{aligned}$$

$f : \mathbb{R}^d \to \mathbb{R}$ is the objective function. $\mathscr{C} \subseteq \mathbb{R}^d$ is the constraint/feasible set.

$\mathbf{x}^*$ is an optimal solution (global minimum) if

$$\mathbf{x}^* \in \mathscr{C} \quad \text{and} \quad f(\mathbf{x}^*) \leq f(\mathbf{x}), \quad \text{for all } \mathbf{x} \in \mathscr{C}.$$

The optimal value is $f(\mathbf{x}^*)$. Our goal is to find $\mathbf{x}^*$ and $f(\mathbf{x}^*)$.

Note: to maximize $f(\mathbf{x})$, just minimize $-f(\mathbf{x})$. So we'll only focus on *minimization* problems.

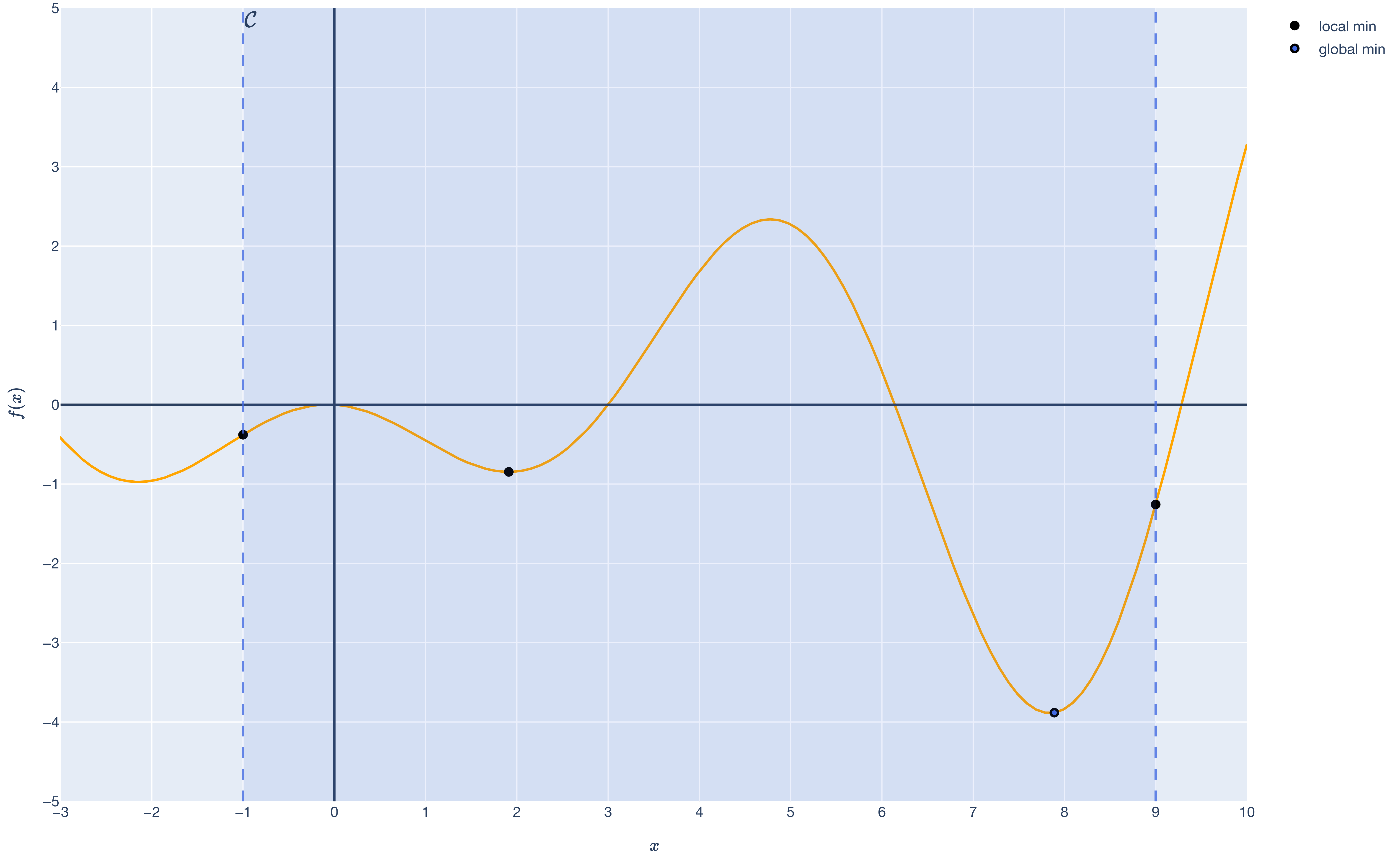
Motivation

Optimization in single-variable calculus

Ultimate goal: Find the *global minimum* of functions.

Intermediary goal: Find the *local minima*.

Now we will focus on constraints!



Motivation

Example: Linear Programming

Let $\mathbf{c} \in \mathbb{R}^d$, $\mathbf{A} \in \mathbb{R}^{n \times d}$, $\mathbf{b} \in \mathbb{R}^n$ be fixed.

Let $\mathbf{x} \in \mathbb{R}^d$ be the decision/free variables.

$$\begin{aligned} \underset{\mathbf{x} \in \mathbb{R}^d}{\text{minimize}} \quad & \mathbf{c}^\top \mathbf{x} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} \preceq \mathbf{b} \end{aligned}$$

$\preceq$ is *element-wise* inequality: $\mathbf{a}_i^\top \mathbf{x} \leq b_i$ for all $i \in [n]$.

Motivation

Example: Linear Programming ($d = 3, n = 7$)

We're cooking some NYC classics again. Suppose we have:

100 bacon,120 egg, 150 cheese, and 300 (sandwich) rolls.

Bacon egg and cheese (BEC) requires 1 bacon, 1 egg, 1 cheese, and 1 roll.

Cost (including labor): \$3

Egg and cheese (EC) requires 0 bacon, 2 egg, 1 cheese, and 1 roll.

Cost (including labor): \$2

Bacon egg omelette (BEO) requires 1 bacon, 3 egg, $1/2$ cheese, and 0 roll.

Cost (including labor): \$1

Motivation

Example: Linear Programming ($d = 3, n = 7$)

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100 bacon, 120 egg, 150 cheese, and 300 (sandwich) rolls.

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Bacon egg omelette (BEO) requires 1 bacon, 3 egg, $1/2$ cheese, and 0 roll.

Cost (including labor): \$1

Decision variables?

$$\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$$

x_1 = number of BEC,

x_2 = number of EC,

x_3 = number of BEO

Constraints?

Bacon: $\mathbf{a}_1 = (1,0,1)$, $b_1 = 100$

Egg: $\mathbf{a}_2 = (1,2,3)$, $b_2 = 120$

Cheese: $\mathbf{a}_3 = (1,1,1/2)$, $b_3 = 150$

Roll: $\mathbf{a}_4 = (1,1,0)$, $b_4 = 300$

Objective?

$$\mathbf{c}^\top \mathbf{x} = 3x_1 + 2x_2 + x_3$$

Motivation

Example: Linear Programming ($d = 3, n = 7$)

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Roll: $\mathbf{a}_4 = (1,1,0)$, $b_4 = 300$

Objective?

$$\mathbf{c}^\top \mathbf{x} = 3x_1 + 2x_2 + x_3$$

Linear program:

$$\begin{aligned} \text{minimize} \quad & 3x_1 + 2x_2 + x_3 \\ \text{subject to} \quad & x_1 + x_3 \leq 100 \\ & x_1 + 2x_2 + 3x_3 \leq 120 \\ & x_1 + x_2 + 0.5x_3 \leq 150 \\ & x_1 + x_2 \leq 300 \\ & x_1 \geq 0 \\ & x_2 \geq 0 \\ & x_3 \geq 0 \end{aligned}$$

Motivation

Example: Linear Programming ($d = 3, n = 7$)

$$
\begin{aligned}
\text{minimize} \quad & 3x_1 + 2x_2 + x_3 \\
\text{subject to} \quad & x_1 + x_3 \leq 100 \\
& x_1 + 2x_2 + 3x_3 \leq 120 \\
& x_1 + x_2 + 0.5x_3 \leq 150 \\
& x_1 + x_2 \leq 300 \\
& x_1 \geq 0 \\
& x_2 \geq 0 \\
& x_3 \geq 0
\end{aligned}
$$

LP in matrix form:

$$
\begin{aligned}
\text{minimize} \quad & 3x_1 + 2x_2 + x_3 \\
\text{subject to} \quad & \mathbf{A}\mathbf{x} \preceq \mathbf{b}
\end{aligned}
$$

$$
\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 2 & 3 \\ 1 & 1 & \frac{1}{2} \\ 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 100 \\ 120 \\ 150 \\ 300 \\ 0 \\ 0 \\ 0 \end{bmatrix}
$$

Regression

Setup (Example View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \ldots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Regression

Setup (Feature View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Least Squares

OLS Theorem

<u>Theorem (Ordinary Least Squares).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$. Let $\hat{\mathbf{w}} \in \mathbb{R}^d$ be the least squares minimizer:

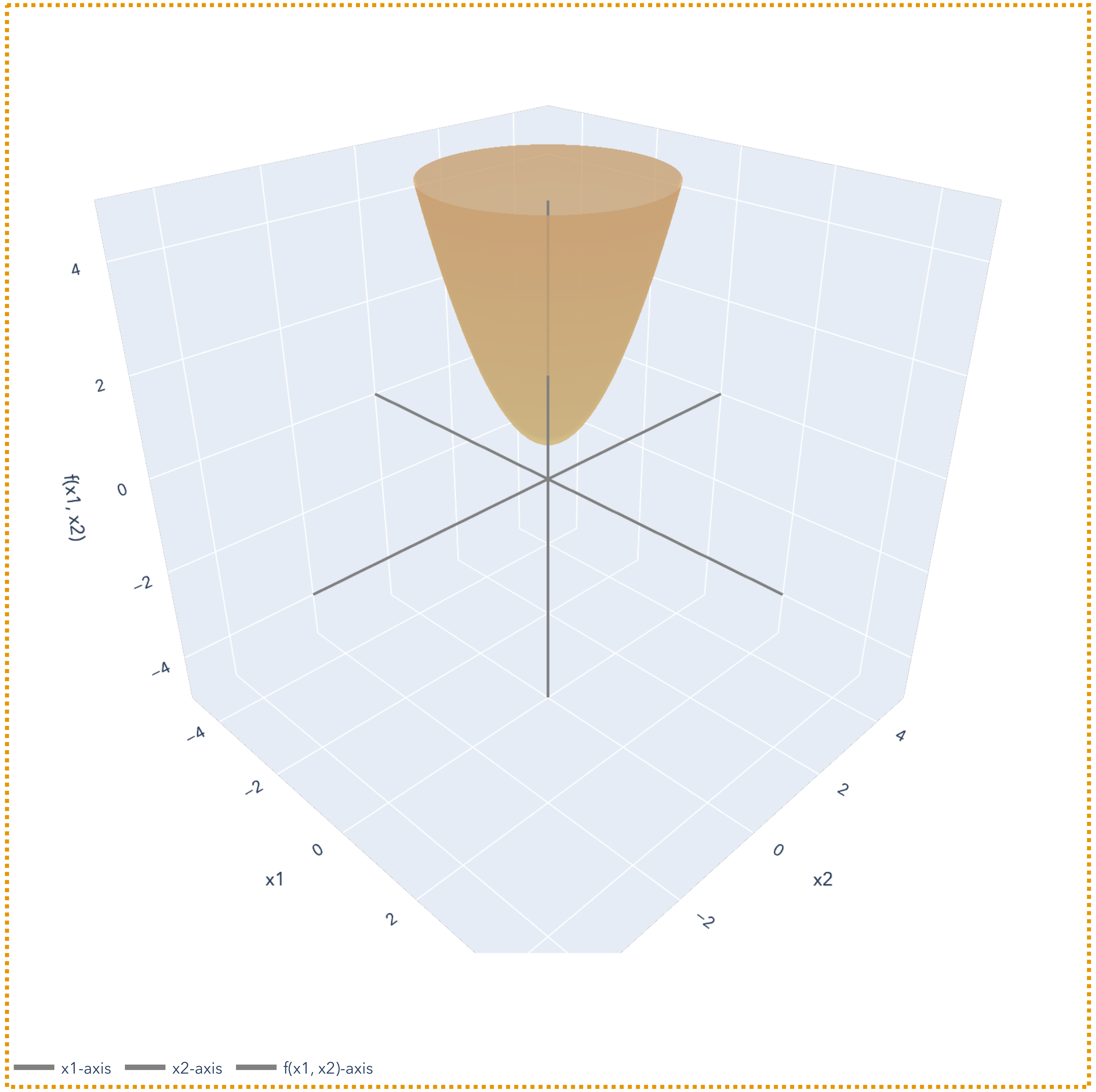
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$



Least Squares

OLS Theorem

Proof (Calculus proof of OLS).

$$f(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \iff f(\mathbf{w}) = \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}$$

"First derivative test." $\nabla_{\mathbf{w}} f(\mathbf{w}) = 2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y}$.

$$2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = \mathbf{0} \implies \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathbf{X}^\top \mathbf{y}$$

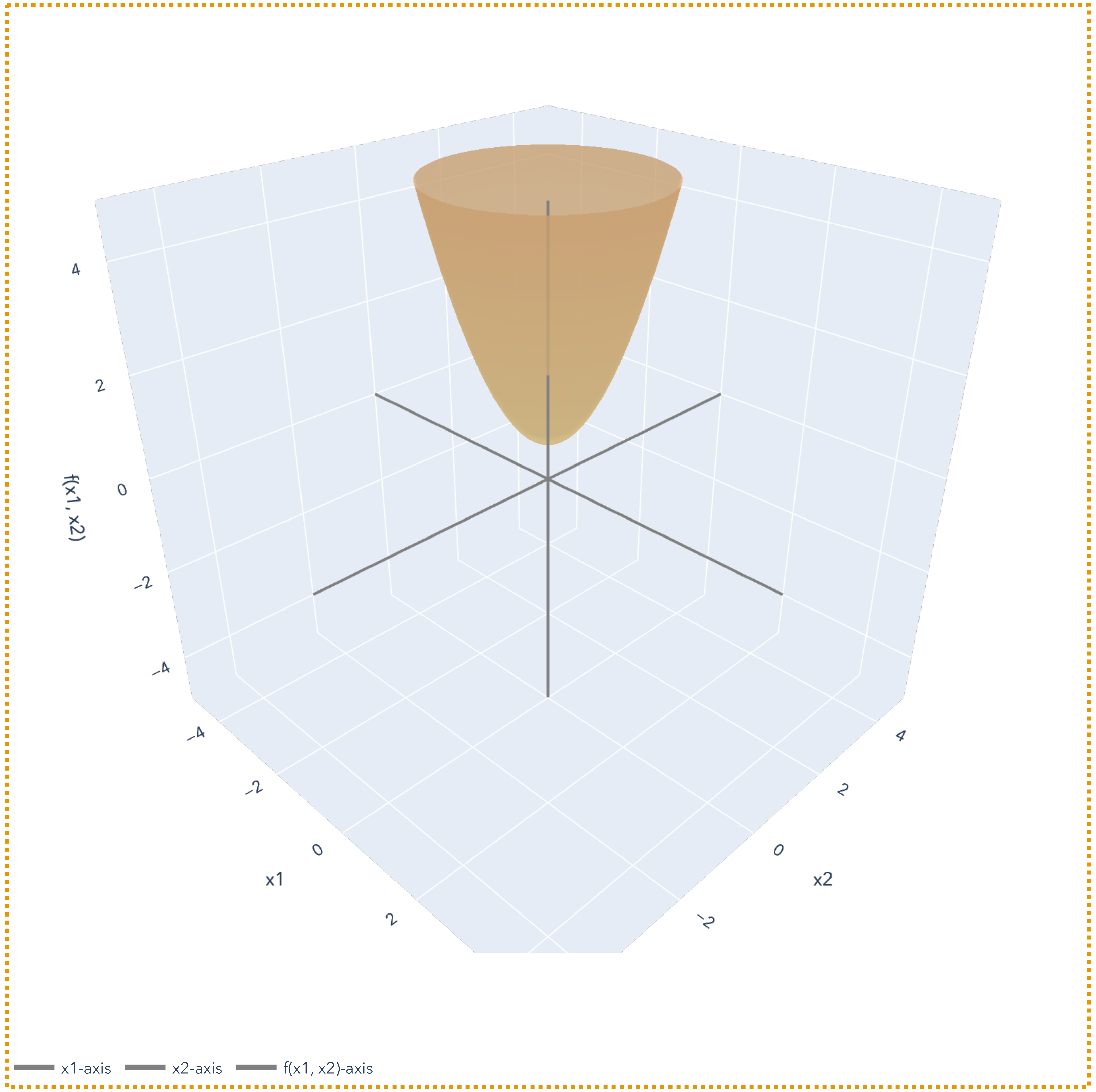
$\operatorname{rank}(\mathbf{X}) = d \implies \operatorname{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \mathbf{X}^\top \mathbf{X}$ is invertible:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." $\nabla^2_{\mathbf{w}} f(\mathbf{w}) = 2\mathbf{X}^\top \mathbf{X}$.

$$\operatorname{rank}(\mathbf{X}) = d \implies \operatorname{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \lambda_1, \ldots, \lambda_d > 0$$

$\implies \mathbf{X}^\top \mathbf{X}$ is positive definite!



Local and global minima

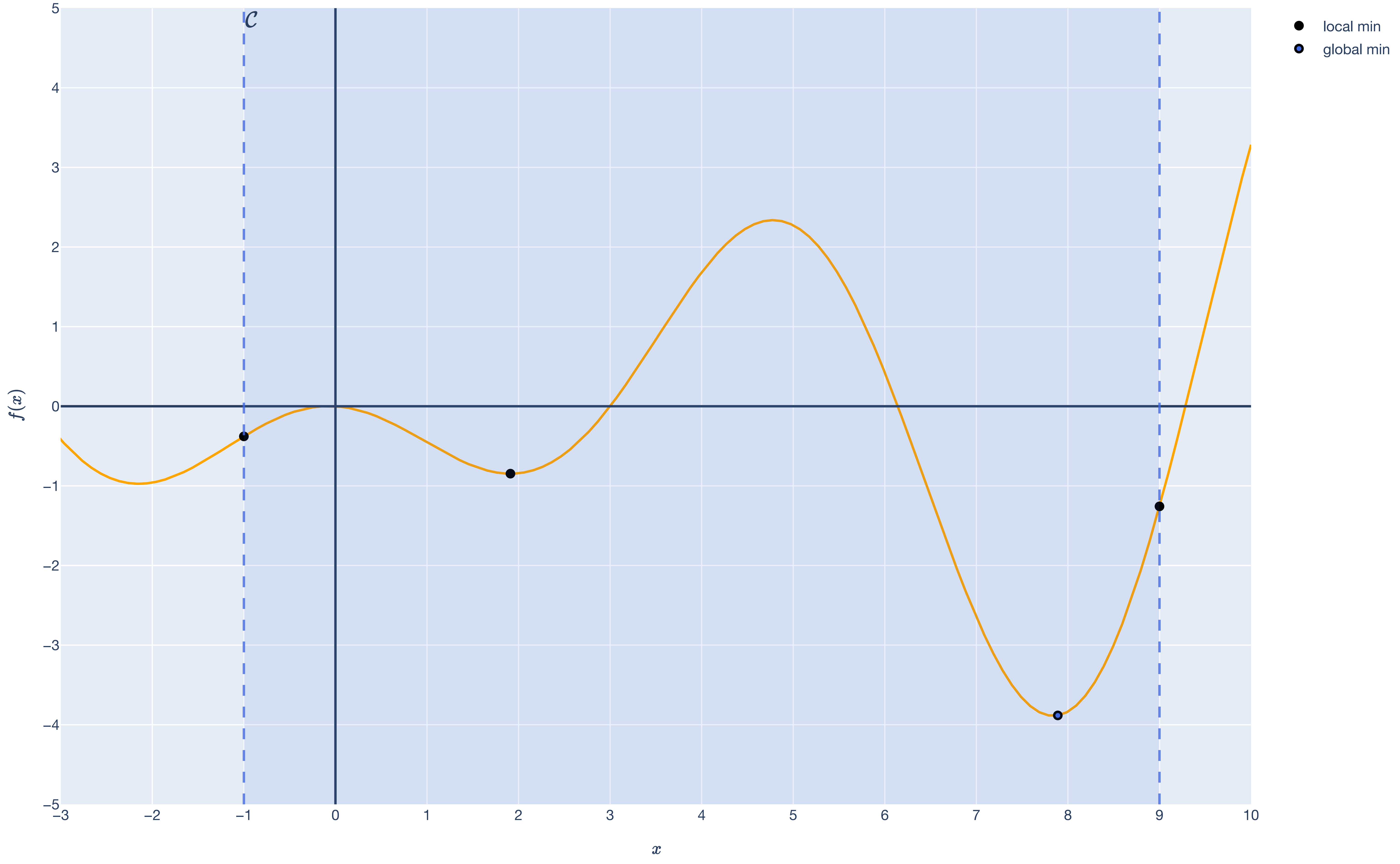
Definition of "locality" and different minima

Motivation

Optimization in single-variable calculus

Ultimate goal: Find the *global minimum* of functions.

Intermediary goal: Find the *local minima*.



“Local” to a Point

Definition of an open ball/neighborhood

Let $\mathbf{x} \in \mathbb{R}^d$ be a point. For some real value $\delta > 0$, the open ball or neighborhood of radius δ around $\mathbf{x}$ is the set of all points:

$$B_\delta(\mathbf{x}) := \{\mathbf{a} \in \mathbb{R}^d : \|\mathbf{x} - \mathbf{a}\| < \delta\} .$$

“Local” to a Point

Definition of an open ball/neighborhood

Example. Consider $\mathbf{x} = (1,1) \in \mathbb{R}^2$. What is the open ball of radius $\delta = 1$ around $\mathbf{x}$?

“Local” to a Point

Definition of the interior of a set

$$B_\delta(\mathbf{x}) := \{\mathbf{a} \in \mathbb{R}^d : \|\mathbf{x} - \mathbf{a}\| < \delta\}$$

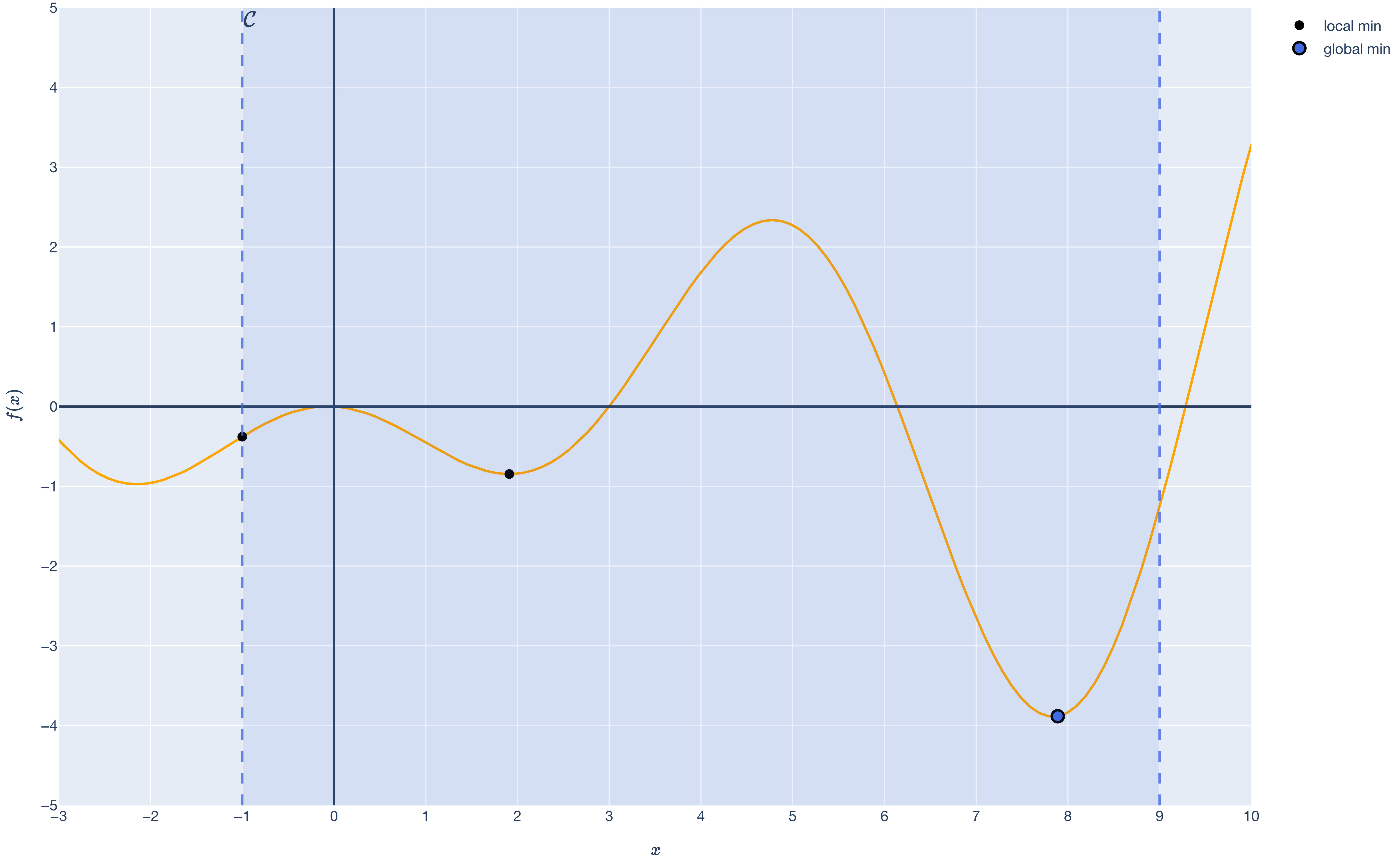
Let $S \subseteq \mathbb{R}^d$ be a set. A point $\mathbf{x} \in S$ is an interior point if there exists a neighborhood $B_\delta(\mathbf{x})$ around $\mathbf{x}$ such that $B_\delta(\mathbf{x}) \subset S$ (where $\subset$ is *proper subset*).

The interior of the set $\mathrm{int}(S)$ is the set of all interior points of S, i.e.

$$\mathrm{int}(S) := \{\mathbf{x} \in S : N_\delta(\mathbf{x}) \subset S\}\,.$$

Types of Minima

Local and global minima



Types of Minima

Local and global minima

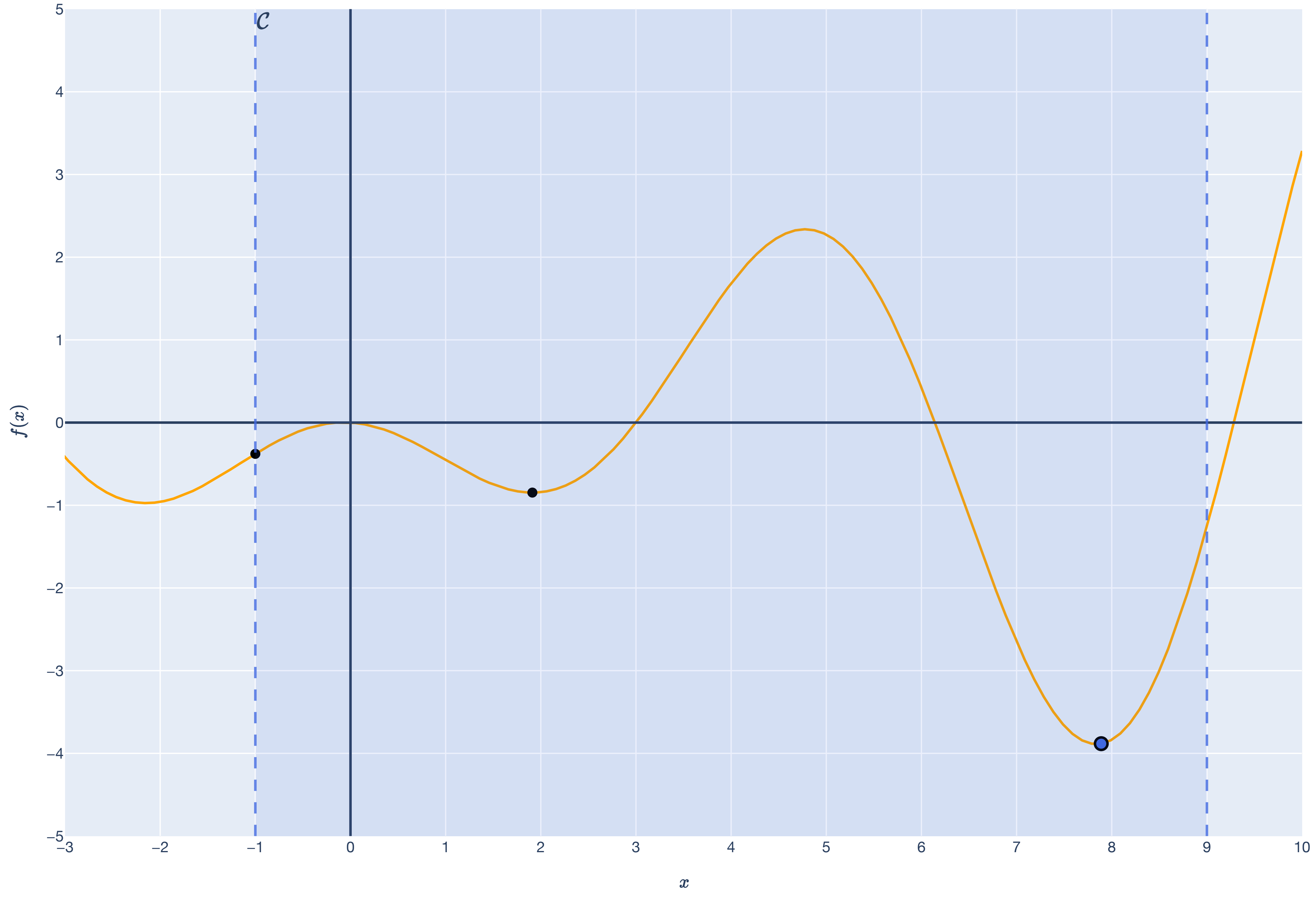
$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

$\hat{\mathbf{x}} \in \mathscr{C}$ is a (constrained) local minimum if there is a neighborhood $B_\delta(\hat{\mathbf{x}})$ around $\hat{\mathbf{x}}$ such that

$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathscr{C} \cap B_\delta(\hat{\mathbf{x}}).$$

$\mathbf{x}^* \in \mathscr{C}$ is a global minimum if

$$f(\mathbf{x}^*) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathscr{C}.$$



Types of Minima

Local and global minima

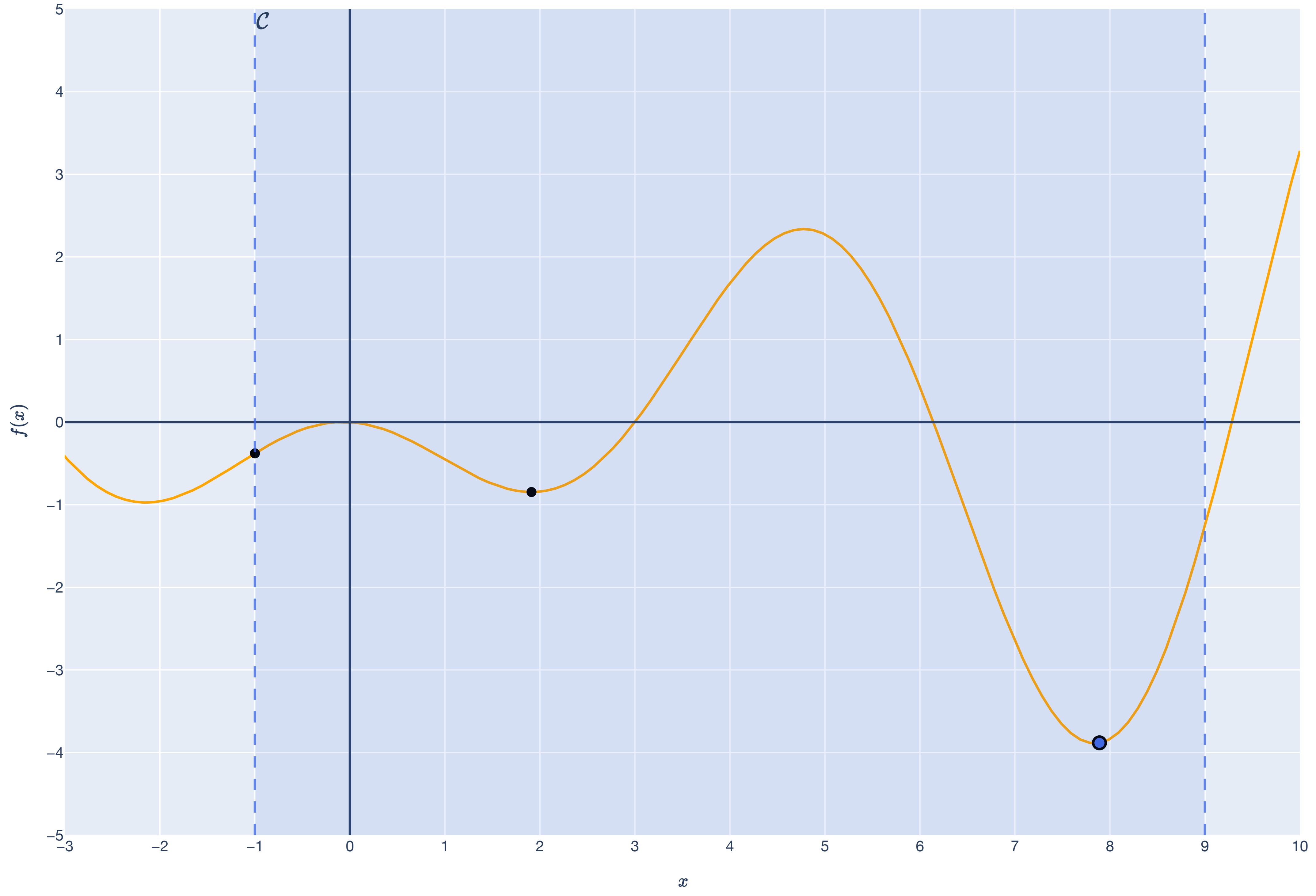
$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

$\hat{\mathbf{x}} \in \mathscr{C}$ is an unconstrained local minimum if there is a neighborhood $B_\delta(\hat{\mathbf{x}}) \subset \mathscr{C}$ around $\hat{\mathbf{x}}$ such that

$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in B_\delta(\hat{\mathbf{x}}).$$

Unconstrained local minima are in $\mathbf{int}(\mathscr{C})$.

Constrained local minima can be on the "edge" of the constraint set.



Types of Minima

Which type of minima are each of these points?

$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

constrained local:

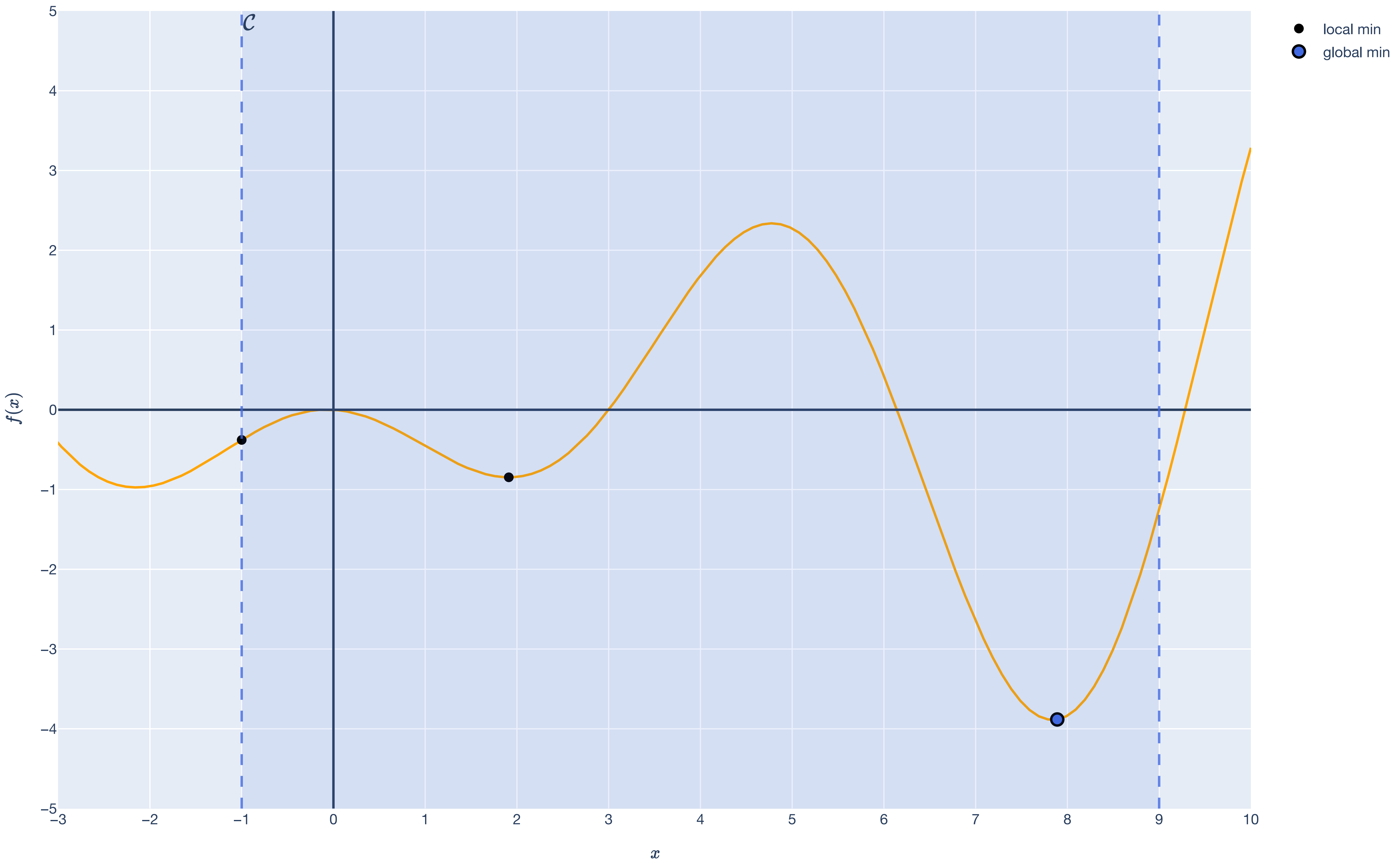
$f(\hat{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathscr{C} \cap B_\delta(\hat{\mathbf{x}})$

unconstrained local:

$f(\hat{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in B_\delta(\hat{\mathbf{x}})$ *and* $B_\delta(\hat{\mathbf{x}}) \subset \mathscr{C}$.

global:

$f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathscr{C}$.



Types of Minima

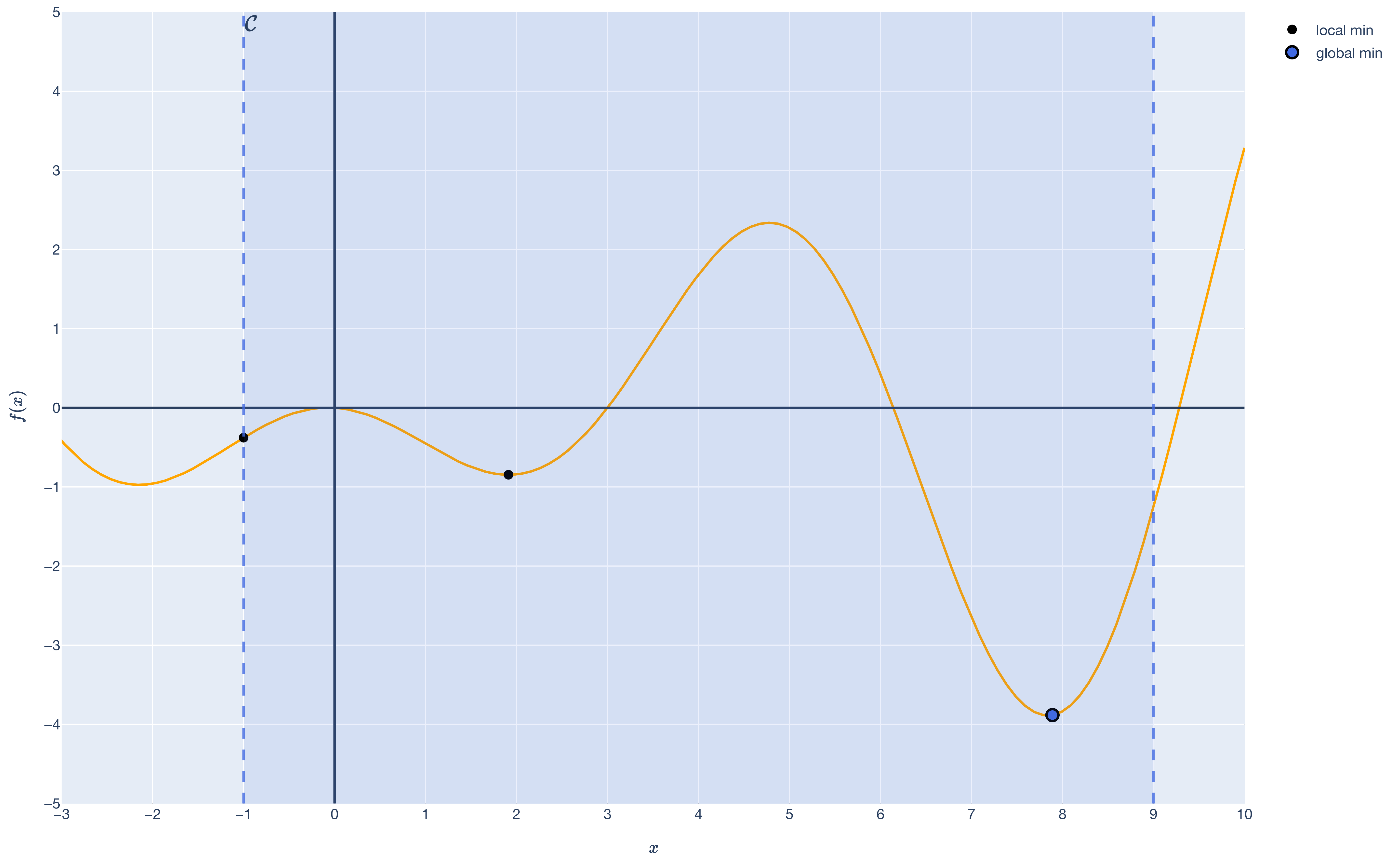
Big picture

We want to find global minima.

Global minima could be either unconstrained local minima or constrained local minima.

> Without $\mathscr{C}$, global minima are just an *unconstrained local minima*.
>
> With $\mathscr{C}$, global minima may lie on the boundary of the constraint set.

Find local minima, then test!



Finding local minima
Big Picture

Necessary and sufficient conditions

Review

$$P \implies Q$$

Q is necessary for P. P is sufficient for Q.

sufficiency: If you assume this, you get your property.

A *sufficient* (not necessary) condition to get an A in this class is to get 100 on every assignment.

necessity: Your property cannot hold unless you assume this.

A *necessary* (not sufficient) condition to get an A in this class is to turn in every assignment.

Unconstrained Minima

How do we find unconstrained minima?

$\hat{\mathbf{x}} \in \mathscr{C}$ is an unconstrained local minimum if there is a neighborhood $B_\delta(\hat{\mathbf{x}}) \subset \mathscr{C}$ around $\hat{\mathbf{x}}$ s.t.

$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in B_\delta(\hat{\mathbf{x}}).$$

From single-variable calculus, this is true if:

$$f'(x) = 0 \text{ and } f''(x) \geq 0.$$

Unconstrained Minima

Intuition from Taylor series

Let $\delta \in \mathbb{R}$ be a scalar increment.

At $x_0 \in \mathbb{R}$, *the second-order Taylor approximation tells us all we need to know:*

$$f(x_0 + \delta) \approx f(x_0) + \underbrace{f'(x_0)\delta}_{f'(x) = 0} + \frac{1}{2}\underbrace{f''(x_0)}_{\substack{f''(x) \geq 0 \\ f''(x) > 0}}\delta^2.$$

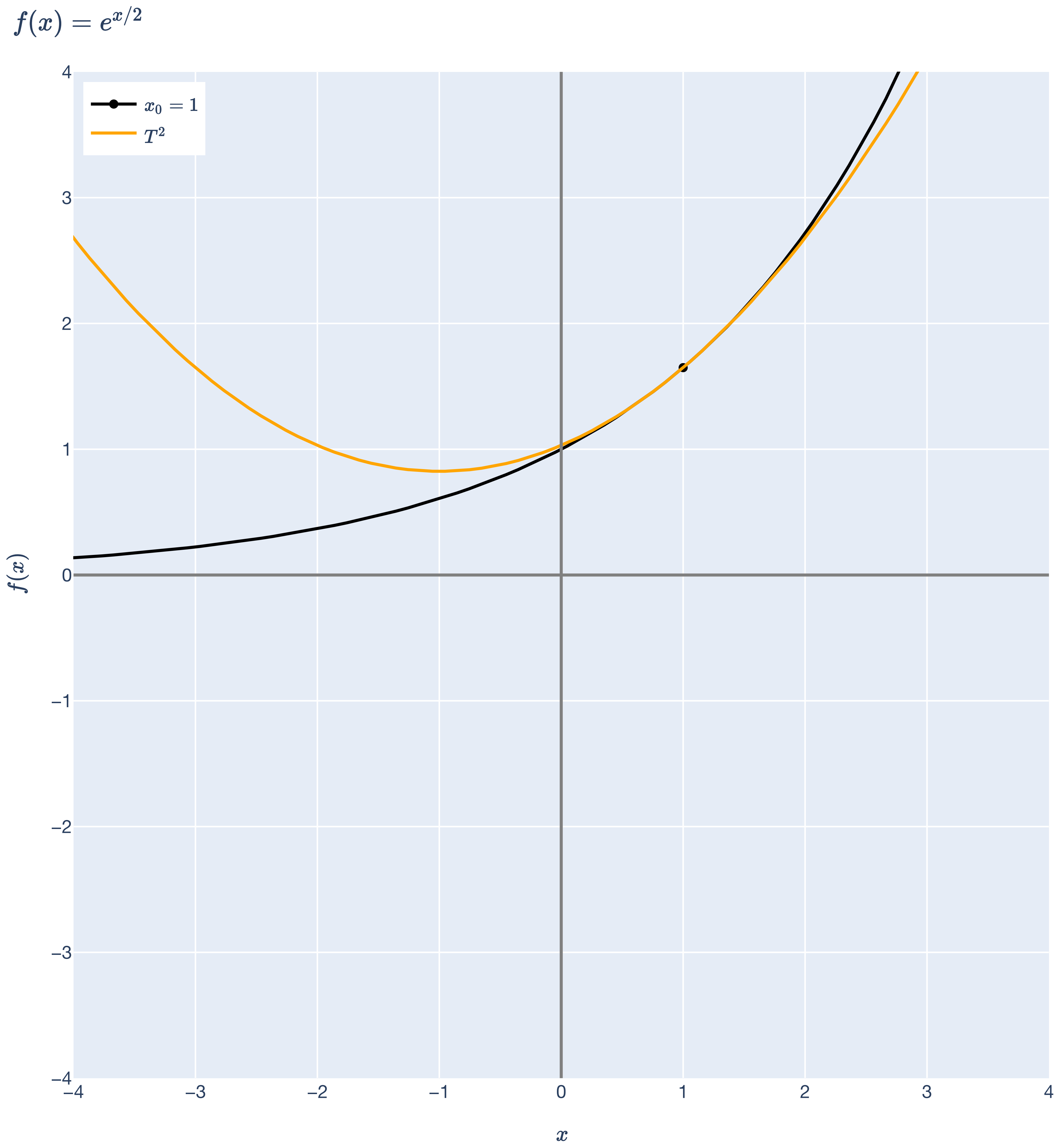
Second-order Taylor Approximation

Single-variable example

$$f(x) = e^{x/2}$$

Second-order Taylor expansion at $x_0 = 1$:

$$T^2(x) = e^{1/2} + \frac{e^{1/2}(x-1)}{2} + \frac{e^{1/2}(x-1)^2}{8}$$



Unconstrained Minima

Intuition from Taylor series

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At $x_0 \in \mathbb{R}$, *the second-order Taylor approximation tells us all we need to know:*

$$f(x_0 + \delta) \approx f(x_0) + \underset{f'(x) = 0}{\overset{f'(x) = 0}{f'(x_0)\delta}} + \frac{1}{2}\underset{f''(x) \geq 0}{\overset{f''(x) \geq 0}{f''(x_0)}}\delta^2.$$

What are the *necessary* conditions for x to be a minimum?

What are the *sufficient* conditions for x to be a minimum?

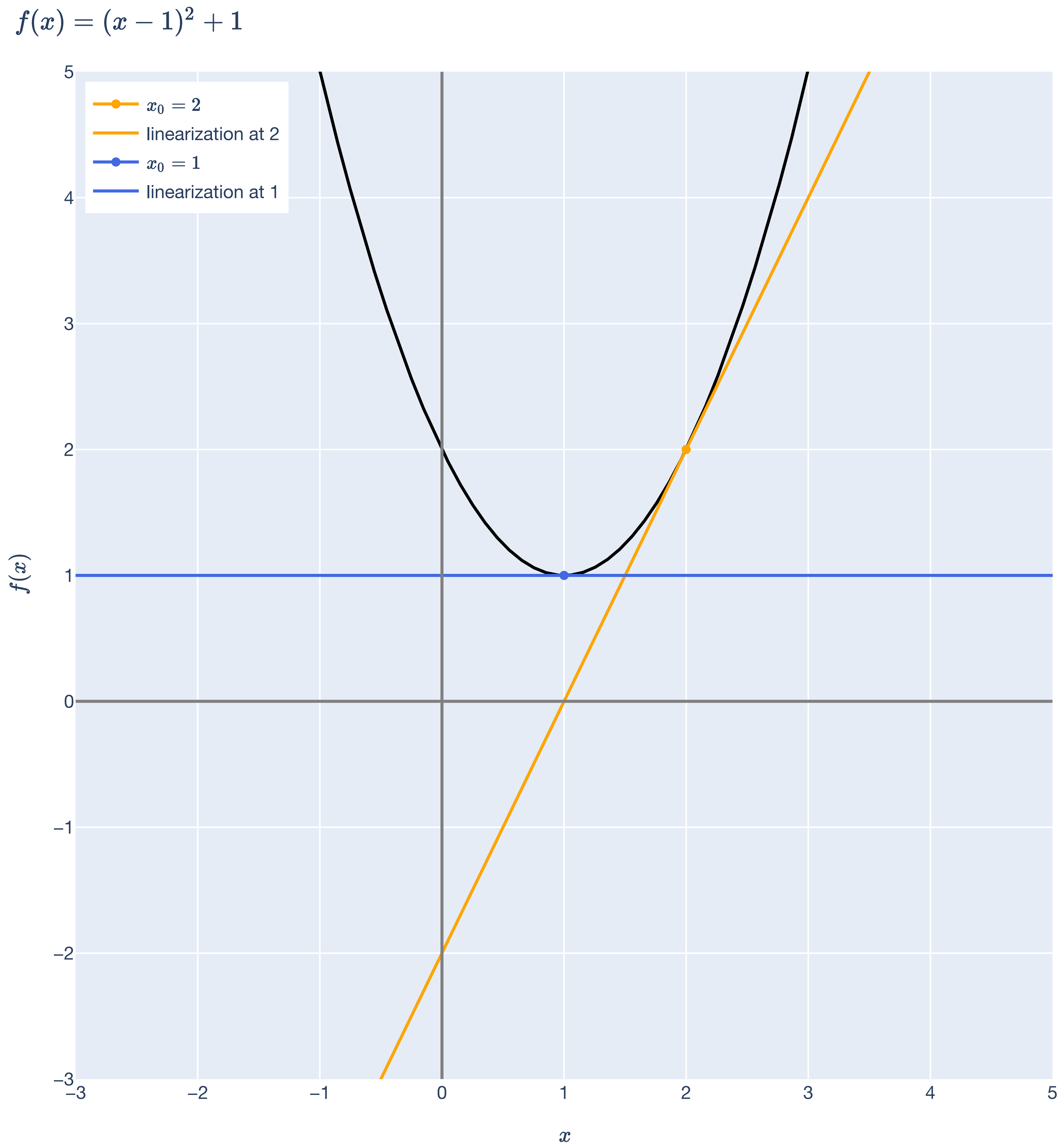
Unconstrained Minima

Sufficient conditions met

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \frac{1}{2} f''(x_0)\delta^2$$

Necessary conditions: $f'(x_0) = 0, f''(x_0) \geq 0.$

Sufficient conditions: $f'(x_0) = 0, f''(x_0) > 0.$



Unconstrained Minima

Necessary, not sufficient

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \frac{1}{2}f''(x_0)\delta^2$$

Necessary conditions: $f'(x_0) = 0, f''(x_0) \geq 0.$

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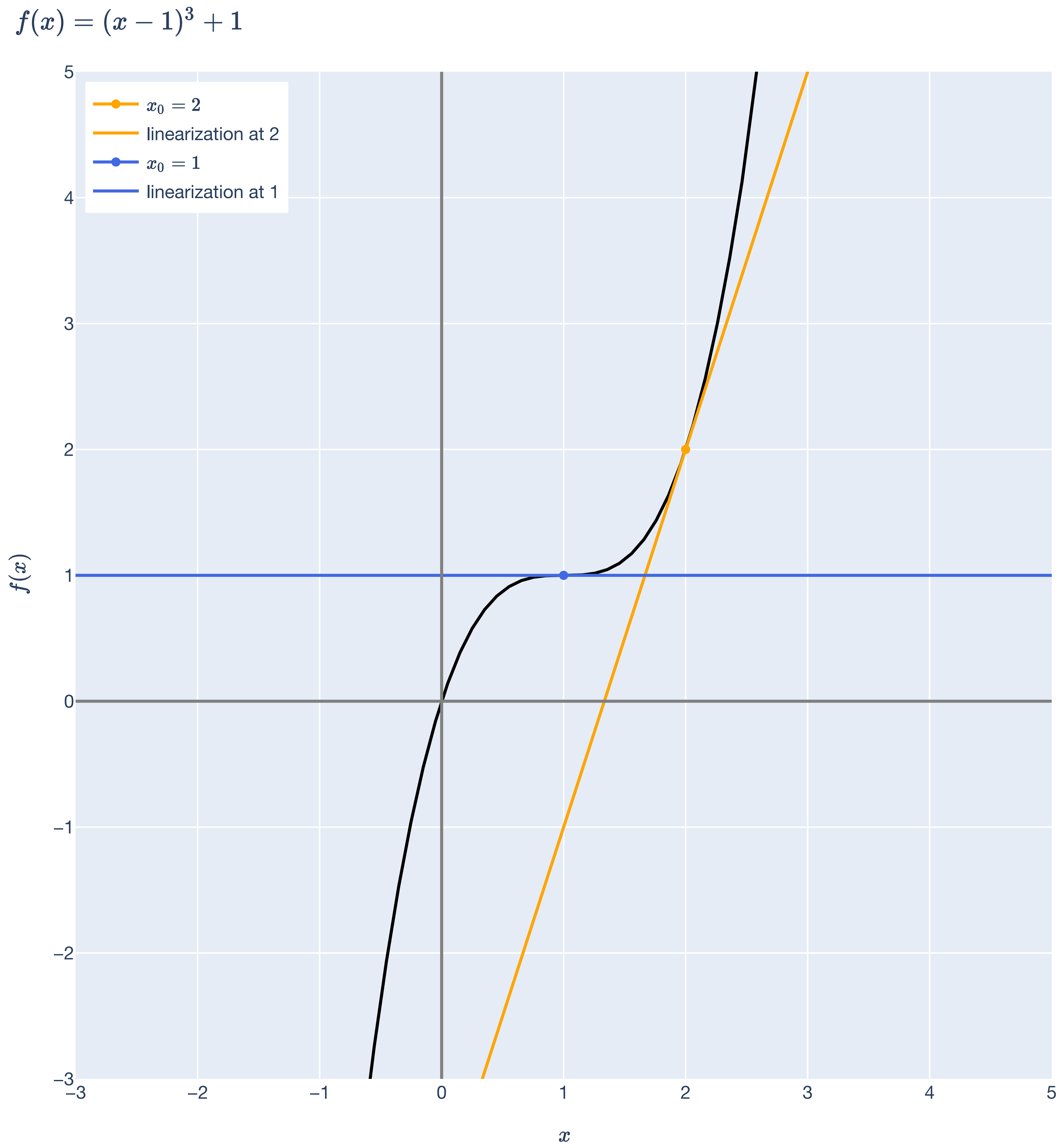

Taylor's Theorem

Intuition

How much do we lose by approximating f with a Taylor approximation?

Remainder: how much more Taylor series is left after "chopping it off" at order n.

First-order approximation:

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top (\mathbf{x} - \mathbf{x}_0)$$

The remainder is:

$$f(\mathbf{x}) - (f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top (\mathbf{x} - \mathbf{x}_0))$$

Taylor's Theorem

Intuition

How much do we lose by approximating f with a Taylor approximation?

Remainder: how much more Taylor series is left after "chopping it off" at order n.

Second-order approximation:

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0)\,.$$

The remainder is:

$$f(\mathbf{x}) - \left(f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) \right).$$

Remainder of Taylor Polynomial

Definition

The remainder of a function and its Taylor polynomial at $\mathbf{x}_0$ is the function:

$$R^n(\mathbf{x}) := f(\mathbf{x}) - T^n_{\mathbf{x}_0}(\mathbf{x})$$

What behavior would we like?

Ideally, $R^n(\mathbf{x}) \to 0$ as $\mathbf{x} \to \mathbf{x}_0$ (the approximation gets better as we approach $\mathbf{x}_0$).

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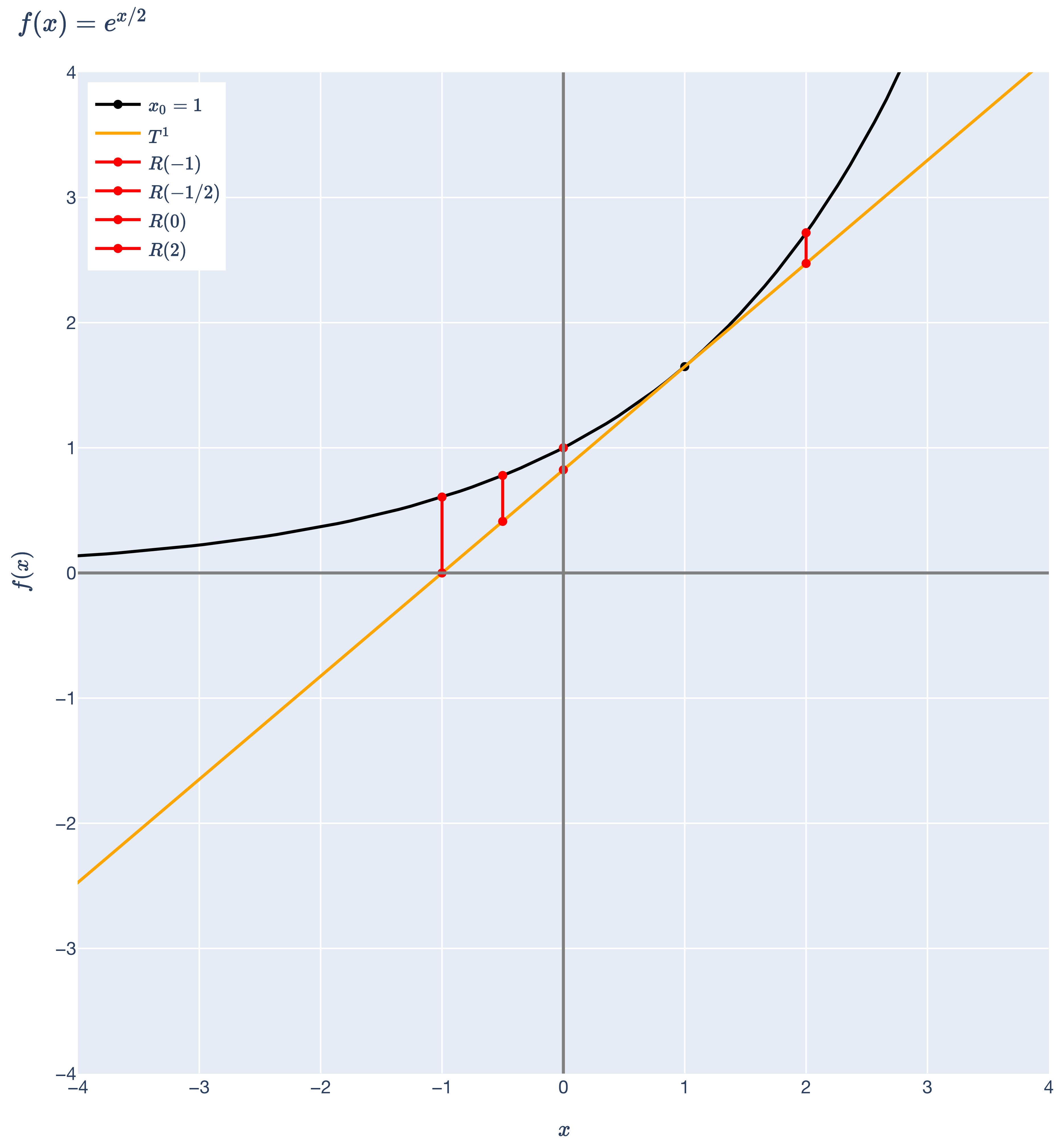
Ideally, $R^n(\mathbf{x}) \to 0$ as $\mathbf{x} \to \mathbf{x}_0$ (the approximation gets better as we approach $\mathbf{x}_0$).



Taylor's Theorem

Peano's Form

Theorem (2nd Order Taylor's Theorem: Peano's Form). Let $f : \mathbb{R}^d \to \mathbb{R}$ be twice differentiable at $\mathbf{x}_0$ and let $\mathbf{d} \in \mathbb{R}^d$. For every $\epsilon > 0$, there exists a neighborhood $B_\delta(\mathbf{0})$ such that

$$\left| f(\mathbf{x}_0 + \mathbf{d}) - \left(f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{d} + \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}_0)\mathbf{d} \right) \right| \leq \epsilon \|\mathbf{d}\|^2$$

for all $\mathbf{d} \in B_\delta(\mathbf{0})$.

However small you want the remainder (ϵ), as long as you are δ-close to $\mathbf{x}_0$, the remainder can get $\epsilon\|\mathbf{d}\|^2$ small.

Unconstrained local minima

Necessary conditions

Least Squares

OLS Theorem

<u>Proof (Calculus proof of OLS).</u>

$$f(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \iff f(\mathbf{w}) = \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}$$

"First derivative test." $\nabla_{\mathbf{w}} f(\mathbf{w}) = 2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y}$.

$$2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = \mathbf{0} \implies \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathbf{X}^\top \mathbf{y}$$

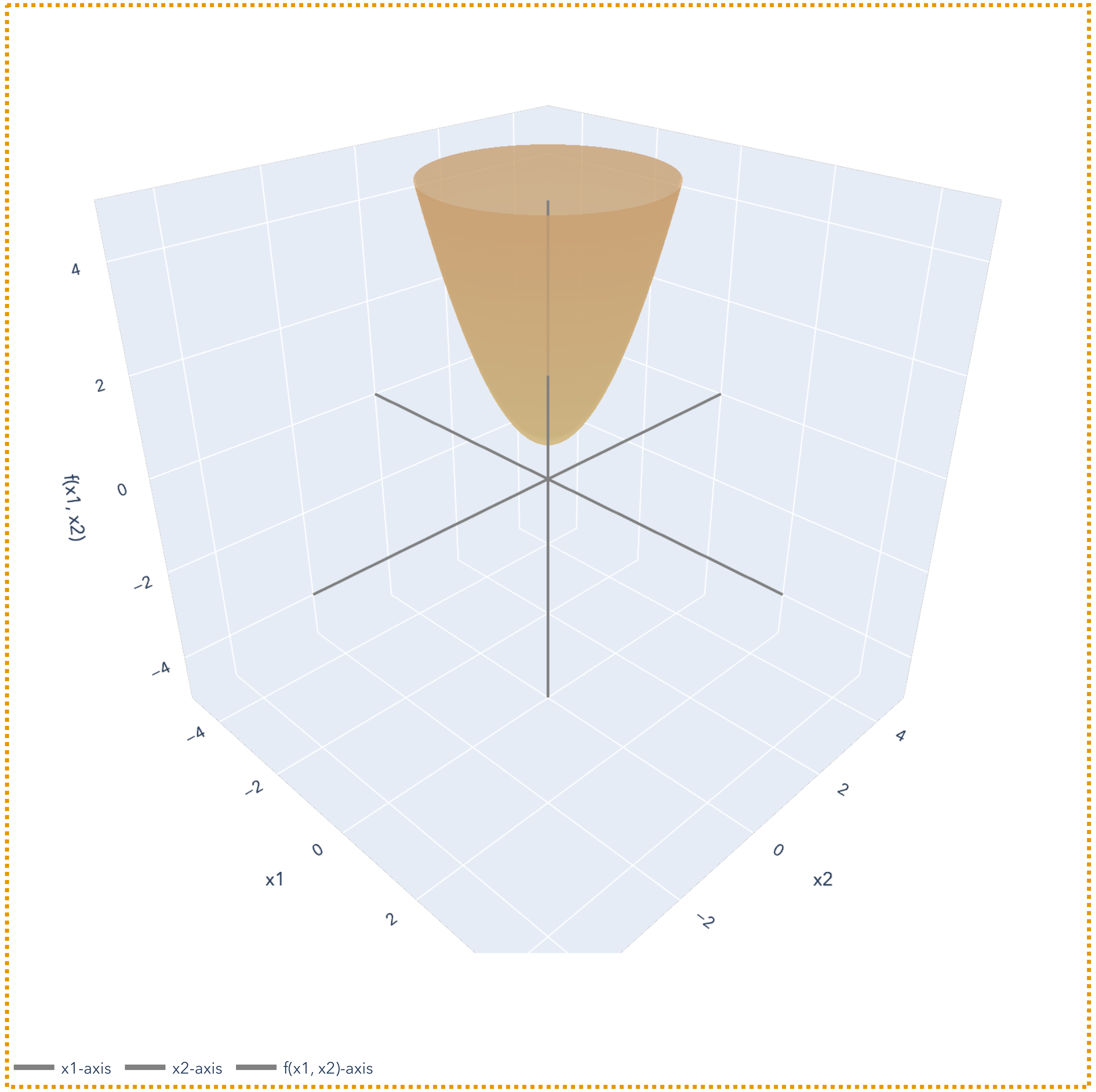
$\mathrm{rank}(\mathbf{X}) = d \implies \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \mathbf{X}^\top \mathbf{X}$ is invertible:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." $\nabla^2_{\mathbf{w}} f(\mathbf{w}) = 2\mathbf{X}^\top \mathbf{X}$.

$$\mathrm{rank}(\mathbf{X}) = d \implies \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \lambda_1, \ldots, \lambda_d > 0$$

$$\implies \mathbf{X}^\top \mathbf{X} \text{ is positive definite!}$$



Necessary Conditions

Comparison to single variable

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \frac{1}{2}f''(x_0)\delta^2$$

when δ is small enough.

Necessary conditions:

$$f'(x_0) = 0, f''(x_0) \geq 0.$$

$$f(\mathbf{x}_0 + \mathbf{d}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{d} + \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}_0)\mathbf{d}$$

when $\|\mathbf{d}\|$ is small enough.

Necessary conditions:

$\nabla f(\mathbf{x}_0) = \mathbf{0}$, $\nabla^2 f(\mathbf{x}_0)$ is PSD.

Differential Calculus

Review: Derivative

at the point where we're taking derivative…

If $f : \mathbb{R}^d \to \mathbb{R}$ is *differentiable* at $\mathbf{x}_0 \in \mathbb{R}^d$…

linear approximation

$$\lim_{\mathbf{x}\to\mathbf{x}_0} \frac{f(\mathbf{x}) - \left(f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top(\mathbf{x} - \mathbf{x}_0)\right)}{\|\mathbf{x} - \mathbf{x}_0\|} = 0$$

as $\mathbf{x}$ gets closer to $\mathbf{x}_0$… …the function is closer and closer to its linear approximation!

Throughout this section, $\mathbf{d} = \mathbf{x} - \mathbf{x}_0$.

Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum).

$$\begin{array}{rl} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Suppose $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$ is an unconstrained local minimum. Then,

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is positive semidefinite, i.e. $\mathbf{v}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{R}^d$.

Proof of first order necessary condition

Step 1: Use definition of gradient for $\alpha\mathbf{d}$

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Choose an arbitrary direction $\alpha\mathbf{d} \in \mathbb{R}^d$, where $\|\mathbf{d}\| = 1$ is a unit vector and $\alpha > 0$ is a scalar.

f is differentiable, so…

$$\lim_{\alpha \to 0} \frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*) - \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d}}{\alpha \|\mathbf{d}\|} = 0$$

which is the same as stating:

$$\boxed{\lim_{\alpha \to 0} \frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)}{\alpha} = \nabla f(\mathbf{x}^*)^\top \mathbf{d}.}$$

Proof of first order necessary condition

Step 2: Use local optimality on difference $f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)$

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

From Step 1,

$$\boxed{\lim_{\alpha \to 0} \frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)}{\alpha} = \nabla f(\mathbf{x}^*)^\top \mathbf{d}.}$$

$\mathbf{x}^*$ is an unconstrained local minimum, so there exists a neighborhood $B_\delta(\mathbf{x}^*)$ such that $f(\mathbf{x}) \geq f(\mathbf{x}^*)$ for all $\mathbf{x} \in B_\delta(\mathbf{x}^*)$. So if $\alpha < \delta$ (sufficiently small),

$$f(\mathbf{x}^* + \alpha\mathbf{d}) \geq f(\mathbf{x}^*) \implies \boxed{\nabla f(\mathbf{x}^*)^\top \mathbf{d} \geq 0.}$$

Proof of first order necessary condition

Step 3: $\mathbf{d} \in \mathbb{R}^n$ was an arbitrary direction.

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

From Step 2, if $\alpha < \delta$ (sufficiently small), $\nabla f(\mathbf{x}^*)^\top \mathbf{d} \geq 0$. But $\mathbf{d} \in \mathbb{R}^d$ was an arbitrary direction with $\|\mathbf{d}\| = 1$.

$\mathbf{d} = \mathbf{e}_1 \implies \nabla f(\mathbf{x}^*)_1 \geq 0$ and $\mathbf{d} = -\mathbf{e}_1 \implies \nabla f(\mathbf{x}^*)_1 < 0$

$\mathbf{d} = \mathbf{e}_2 \implies \nabla f(\mathbf{x}^*)_2 \geq 0$ and $\mathbf{d} = -\mathbf{e}_2 \implies \nabla f(\mathbf{x}^*)_2 < 0$

$\vdots$

$\mathbf{d} = \mathbf{e}_d \implies \nabla f(\mathbf{x}^*)_d \geq 0$ and $\mathbf{d} = -\mathbf{e}_d \implies \nabla f(\mathbf{x}^*)_d < 0$

Therefore, $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum).

$$\begin{array}{rl} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Suppose $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$ is an unconstrained local minimum. Then,

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is positive semidefinite, i.e. $\mathbf{v}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{R}^d$.

Proof of second order necessary condition

Step 1: Use second-order Taylor approximation

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is PSD.

Choose an arbitrary direction $\alpha\mathbf{d} \in \mathbb{R}^d$ where $\alpha > 0$ is a scalar. By Taylor's Theorem (Peano's form) there exists $\delta > 0$ such that for all $\mathbf{d} \in B_\delta(\mathbf{0})$:

$$f(\mathbf{x}^* + \alpha\mathbf{d}) - \left(f(\mathbf{x}^*) + \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} \right) \leq \alpha \|\mathbf{d}\|^2.$$

Proof of second order necessary condition

Step 2: Use first-order condition so $\alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} = 0$

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is PSD.

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - \left(f(\mathbf{x}^*) + \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2} \mathbf{d}^\top \nabla^2 f(\mathbf{x}^*) \mathbf{d} \right) \leq \alpha \|\mathbf{d}\|^2$$

$\mathbf{x}^*$ is an *unconstrained local minimum*, so by first-order condition (just proved):

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - f(\mathbf{x}^*) \leq \frac{\alpha^2}{2} \mathbf{d}^\top \nabla^2 f(\mathbf{x}^*) \mathbf{d} + \alpha \|\mathbf{d}\|^2$$

Proof of second order necessary condition

Step 3: Take $\alpha \to 0$ and use local optimality: $f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*) \geq 0$

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is PSD.

$$f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*) \leq \frac{\alpha^2}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} + \alpha\|\mathbf{d}\|^2.$$

Divide by α^2 everywhere and take the limit as $\alpha \to 0$:

$$\lim_{\alpha \to 0} \frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)}{\alpha^2} - \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} = 0$$

By local optimality of $\mathbf{x}^*$,

$$0 \leq \frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)}{\alpha^2}, \text{ so } 0 \leq \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} \Longrightarrow \nabla^2 f(\mathbf{x}^*) \text{ is PSD (definition of PSD).}$$

Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum).

$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Suppose $\mathbf{x}^* \in \mathrm{int}(\mathscr{C})$ is an unconstrained local minimum. Then,

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is positive semidefinite, i.e. $\mathbf{v}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{R}^d$.

Unconstrained local minima

Sufficient conditions

Least Squares

OLS Theorem

Proof (Calculus proof of OLS).

$$f(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \iff f(\mathbf{w}) = \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}$$

"First derivative test." $\nabla_{\mathbf{w}} f(\mathbf{w}) = 2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y}$.

$$2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = \mathbf{0} \implies \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathbf{X}^\top \mathbf{y}$$

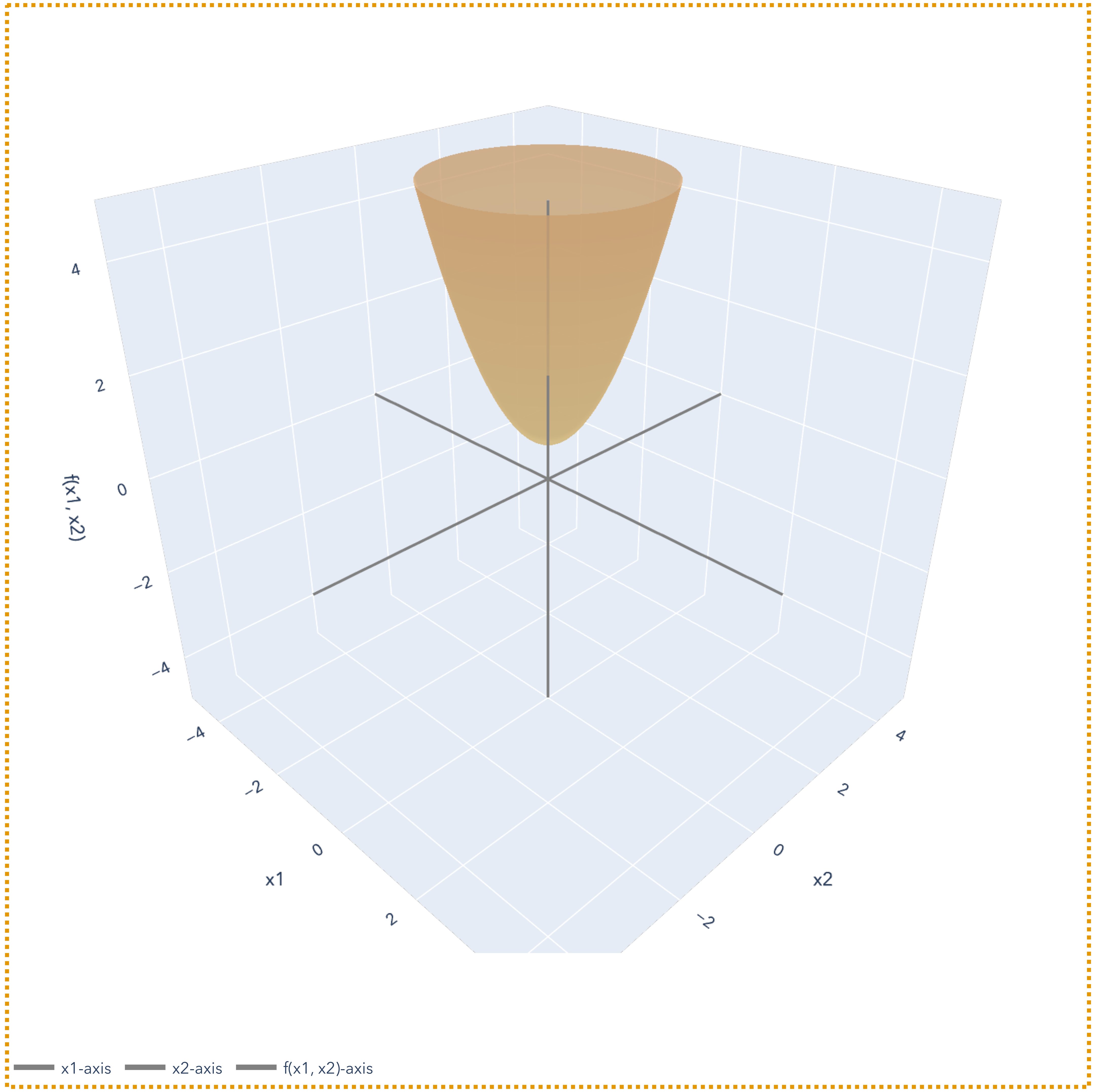
$\mathrm{rank}(\mathbf{X}) = d \Longrightarrow \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \Longrightarrow \mathbf{X}^\top \mathbf{X}$ is invertible:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." $\nabla^2_{\mathbf{w}} f(\mathbf{w}) = 2\mathbf{X}^\top \mathbf{X}$.

$$\mathrm{rank}(\mathbf{X}) = d \implies \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \lambda_1, \ldots, \lambda_d > 0$$

$\implies \mathbf{X}^\top \mathbf{X}$ is positive definite!



Sufficient Conditions

Comparison to single variable

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \frac{1}{2}f''(x_0)\delta^2$$

when δ is small enough.

Necessary conditions:

$$f'(x_0) = 0, f''(x_0) > 0.$$

$$f(\mathbf{x}_0 + \mathbf{d}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{d} + \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}_0)\mathbf{d}$$

when $\|\mathbf{d}\|$ is small enough.

Necessary conditions:

$\nabla f(\mathbf{x}_0) = \mathbf{0}$, $\nabla^2 f(\mathbf{x}_0)$ is PD.

Unconstrained Minima

Sufficient conditions

Theorem (Sufficient Conditions for Unconstrained Local Minimum).

$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Let $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$. If $f \in \mathscr{C}^2$ and

$$\nabla f(\mathbf{x}^*) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}^*) \text{ is positive definite,}$$

then $\mathbf{x}^*$ is a *strict* unconstrained local minimum.

Proof of second order sufficient condition

Step 1: Use second-order Taylor approximation

Second-order condition. If $\nabla^2 f(\mathbf{x}^*)$ is PD, then $\mathbf{x}^*$ is an unconstrained local minimum.

Choose an arbitrary direction $\alpha\mathbf{d} \in \mathbb{R}^d$ where $\alpha > 0$ is a scalar. By Taylor's Theorem (Peano's form) there exists $\delta > 0$ such that for all $\mathbf{d} \in B_\delta(\mathbf{0})$:

$$f(\mathbf{x}^* + \alpha\mathbf{d}) - \left(f(\mathbf{x}^*) + \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} \right) \geq -\alpha\|\mathbf{d}\|^2.$$

Note: Used the negative direction of the statement (which is absolute value).

Proof of second order sufficient condition

Step 2: Eigenvalues of PD matrix are positive

Second-order condition. If $\nabla^2 f(\mathbf{x}^*)$ is PD, then $\mathbf{x}^*$ is an unconstrained local minimum.

From Step 1, for any $\mathbf{d} \in \mathbb{R}^d$ with $\|\mathbf{d}\| = 1$ and $\alpha > 0$,

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - \left(f(\mathbf{x}^*) + \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2} \mathbf{d}^\top \nabla^2 f(\mathbf{x}^*) \mathbf{d} \right) \geq -\alpha \|\mathbf{d}\|^2.$$

Let the eigenvalues of $\nabla^2 f(\mathbf{x}^*)$ be $\lambda_1 \geq \ldots \geq \lambda_d > 0$, and consider the smallest eigenvalue, $\lambda_d > 0$ with unit eigenvector $\mathbf{v}_d$ with $\|\mathbf{v}_d\| = 1$.

$$\implies \frac{\alpha^2}{2} \mathbf{d}^\top \nabla^2 f(\mathbf{x}^*) \mathbf{d} \geq \frac{\alpha^2}{2} \mathbf{v}_d^\top \nabla f(\mathbf{x}^*) \mathbf{v}_d = \frac{\lambda_d \alpha^2}{2}.$$

Proof of second order sufficient condition

Step 3: $\alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} = 0$ from first-order condition

Second-order condition. If $\nabla^2 f(\mathbf{x}^*)$ is PD, then $\mathbf{x}^*$ is an unconstrained local minimum.

Cancel out the first-order term $\alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} = 0$ and plugin the eigenvalue lower bound

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - f(\mathbf{x}^*) \geq \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \underbrace{\frac{\alpha^2}{2} \mathbf{d}^\top \nabla^2 f(\mathbf{x}^*) \mathbf{d}}_{\geq \frac{\lambda_d \alpha^2}{2}} - \alpha \|\mathbf{d}\|^2$$

so this simplifies to…

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - f(\mathbf{x}^*) \geq \frac{\lambda_d \alpha^2}{2} - \alpha \|\mathbf{d}\|^2 = \left(\frac{\lambda_d}{2} - \frac{\|\mathbf{d}\|^2}{\alpha} \right) \alpha^2.$$

Proof of second order sufficient condition

Step 4: Divide by $\|\mathbf{d}\|^2$ and consider small enough $\mathbf{d} \to \mathbf{0}$

Second-order condition. If $\nabla^2 f(\mathbf{x}^*)$ is PD, then $\mathbf{x}^*$ is an unconstrained local minimum.

Take our inequality

$$f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*) \geq \frac{\lambda_d \alpha^2}{2} - \alpha\|\mathbf{d}\|^2 = \left(\frac{\lambda_d}{2} - \frac{\|\mathbf{d}\|^2}{\alpha}\right)\alpha^2.$$

and divide by $\|\mathbf{d}\|^2$ to get:

$$\frac{f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)}{\|\mathbf{d}\|^2} \geq \left(\frac{\lambda_d}{2\|\mathbf{d}\|^2} - \frac{1}{\alpha}\right)\alpha^2,$$ and sufficiently small $\mathbf{d} \to \mathbf{0}$ makes the RHS positive.

Least Squares

OLS Theorem

Proof (Calculus proof of OLS).

$$f(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \iff f(\mathbf{w}) = \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}$$

"First derivative test." $\nabla_{\mathbf{w}} f(\mathbf{w}) = 2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y}$.

$$2(\mathbf{X}^\top \mathbf{X})\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = \mathbf{0} \implies \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathbf{X}^\top \mathbf{y}$$

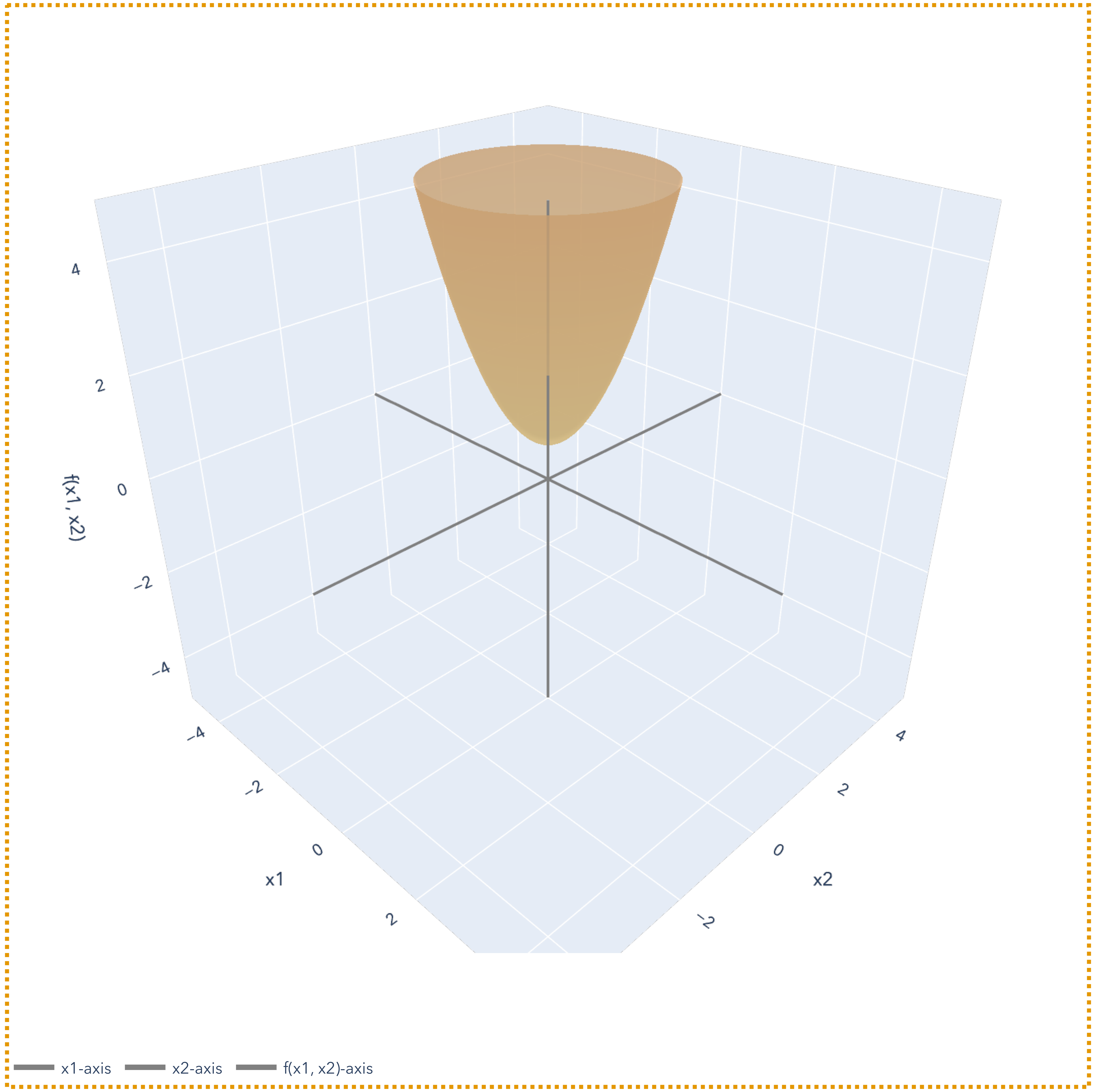
$\mathrm{rank}(\mathbf{X}) = d \Longrightarrow \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \Longrightarrow \mathbf{X}^\top \mathbf{X}$ is invertible:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." $\nabla^2_{\mathbf{w}} f(\mathbf{w}) = 2\mathbf{X}^\top \mathbf{X}$.

$$\mathrm{rank}(\mathbf{X}) = d \implies \mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d \implies \lambda_1, \ldots, \lambda_d > 0$$

$$\implies \mathbf{X}^\top \mathbf{X} \text{ is positive definite!}$$



Finding global minima

Introducing constraint sets

Types of Minima

Big picture

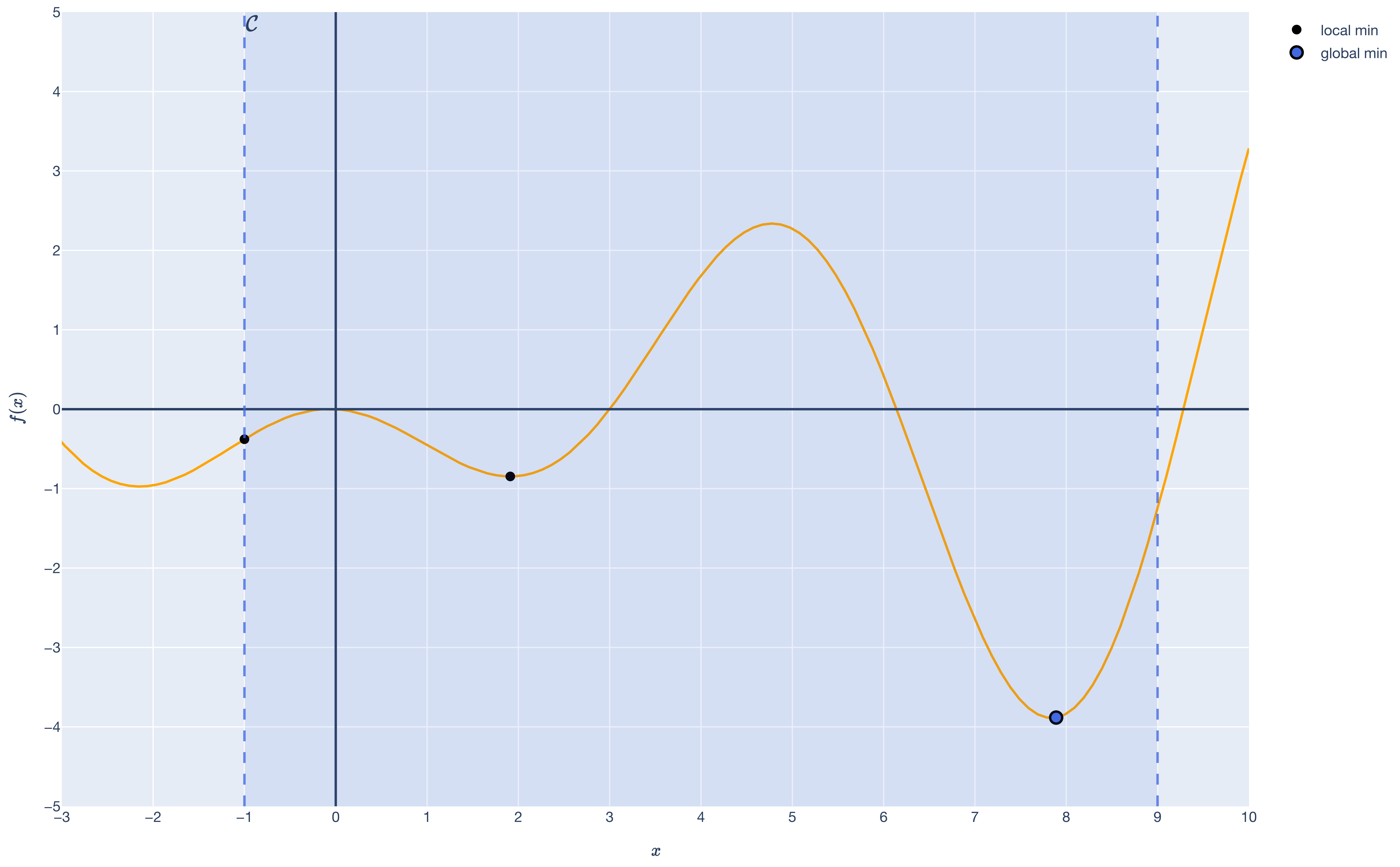
We want to find global minima.

Global minima could be either unconstrained local minima or constrained local minima.

> Without $\mathscr{C}$, global minima are just an *unconstrained local minima*.

> With $\mathscr{C}$, global minima may lie on the boundary of the constraint set.

Find local minima, then test!



Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum).

$$\begin{array}{rl} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

Suppose $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$ is an unconstrained local minimum. Then,

First-order condition. If f is differentiable at $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Second-order condition. If f is twice-differentiable at $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is positive semidefinite, i.e. $\mathbf{v}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{R}^d$.

Finding global minima

Using necessary conditions with constraints

Necessary conditions for unconstrained local minima:

$$\nabla f(\mathbf{x}^*) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}^*) \geq 0.$$

How do we find the *global* minimum from this?

1. Find *unconstrained local minima* from first-order condition
   $M := \{\mathbf{x}^* \in \operatorname{int}(\mathscr{C}) : \nabla f(\mathbf{x}^*) = \mathbf{0}\}$.

2. Find the set of "boundary" points $B := \mathscr{C} \backslash \operatorname{int}(\mathscr{C}) = \{\mathbf{x} \in \mathscr{C} : \mathbf{x} \notin \operatorname{int}(\mathscr{C})\}$.

3. The global minimum must be in the set $M \cup B$, so evaluate f on all $\mathbf{x} \in M \cup B$.

Finding global minima

Using necessary conditions with constraints

Necessary conditions for unconstrained local minima:

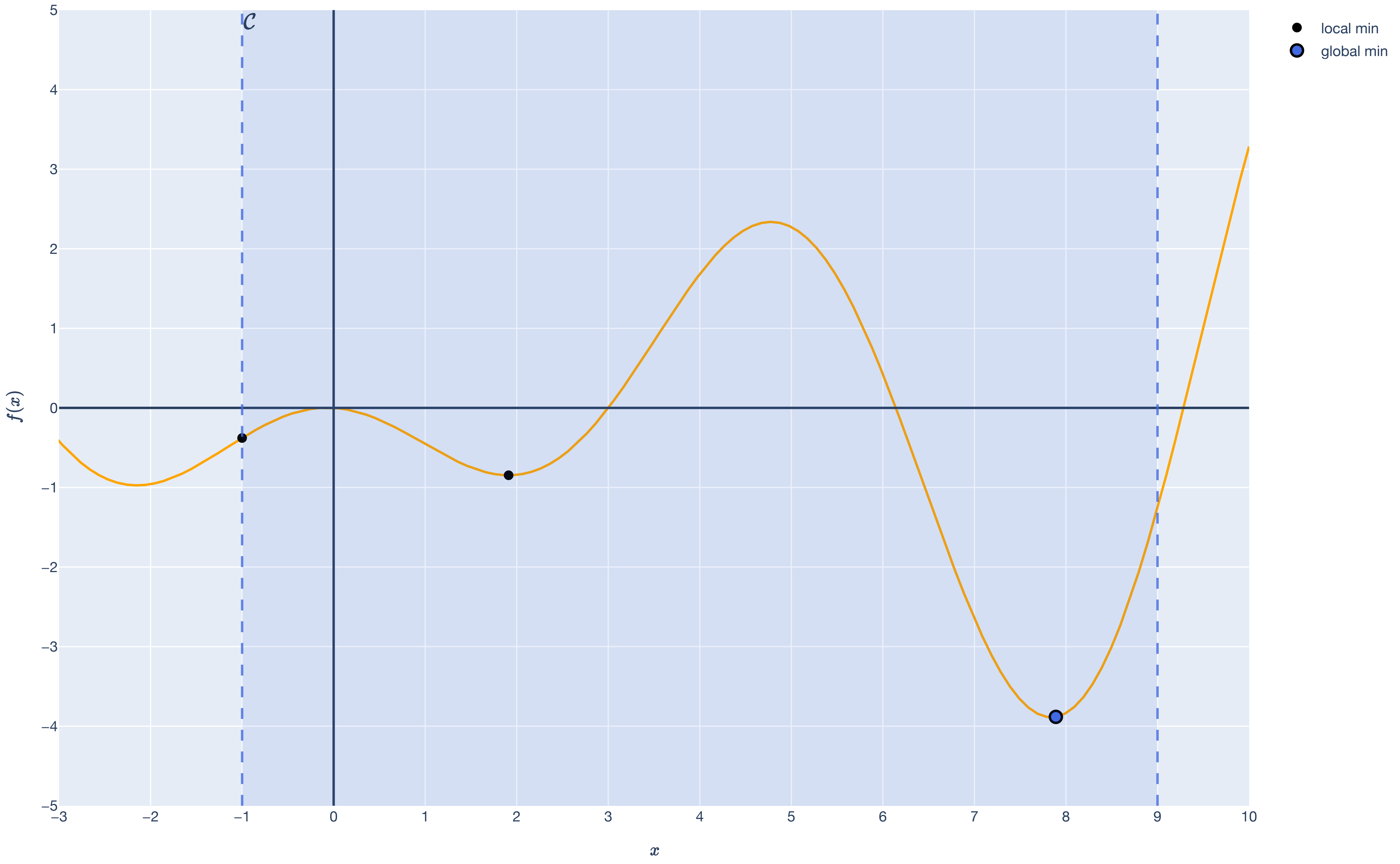
$$\nabla f(\mathbf{x}^*) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}^*) \geq 0.$$

How do we find the *global* minimum from this?

1. Find *unconstrained local minima* from first-order condition $M := \{\mathbf{x}^* \in \text{int}(\mathscr{C}) : \nabla f(\mathbf{x}^*) = \mathbf{0}\}$.

2. Find the set of “boundary” points $B := \mathscr{C} \backslash \text{int}(\mathscr{C}) = \{\mathbf{x} \in \mathscr{C} : \mathbf{x} \notin \text{int}(\mathscr{C})\}$.

3. The global minimum must be in the set $M \cup B$, so evaluate f on all $\mathbf{x} \in M \cup B$.



Finding global minima

Using necessary conditions without constraints

Necessary conditions for unconstrained local minima:

$$\nabla f(\mathbf{x}^*) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}^*) \succeq 0.$$

How do we find the *global* minimum from this when $\mathscr{C} = \mathbb{R}^d$?

1. Find *unconstrained local minima* from first-order condition $M := \{\mathbf{x}^* \in \mathbb{R}^d : \nabla f(\mathbf{x}^*) = \mathbf{0}\}$.
2. There are no boundary points! ($B := \mathscr{C} \setminus \mathrm{int}(\mathscr{C}) = \{\mathbf{x} \in \mathscr{C} : \mathbf{x} \notin \mathrm{int}(\mathscr{C})\} = \varnothing$)
3. The global minimum must be in the set M, so evaluate f on all $\mathbf{x} \in M$.

Finding global minima

Using necessary conditions without constraints

Necessary conditions for unconstrained local minima:

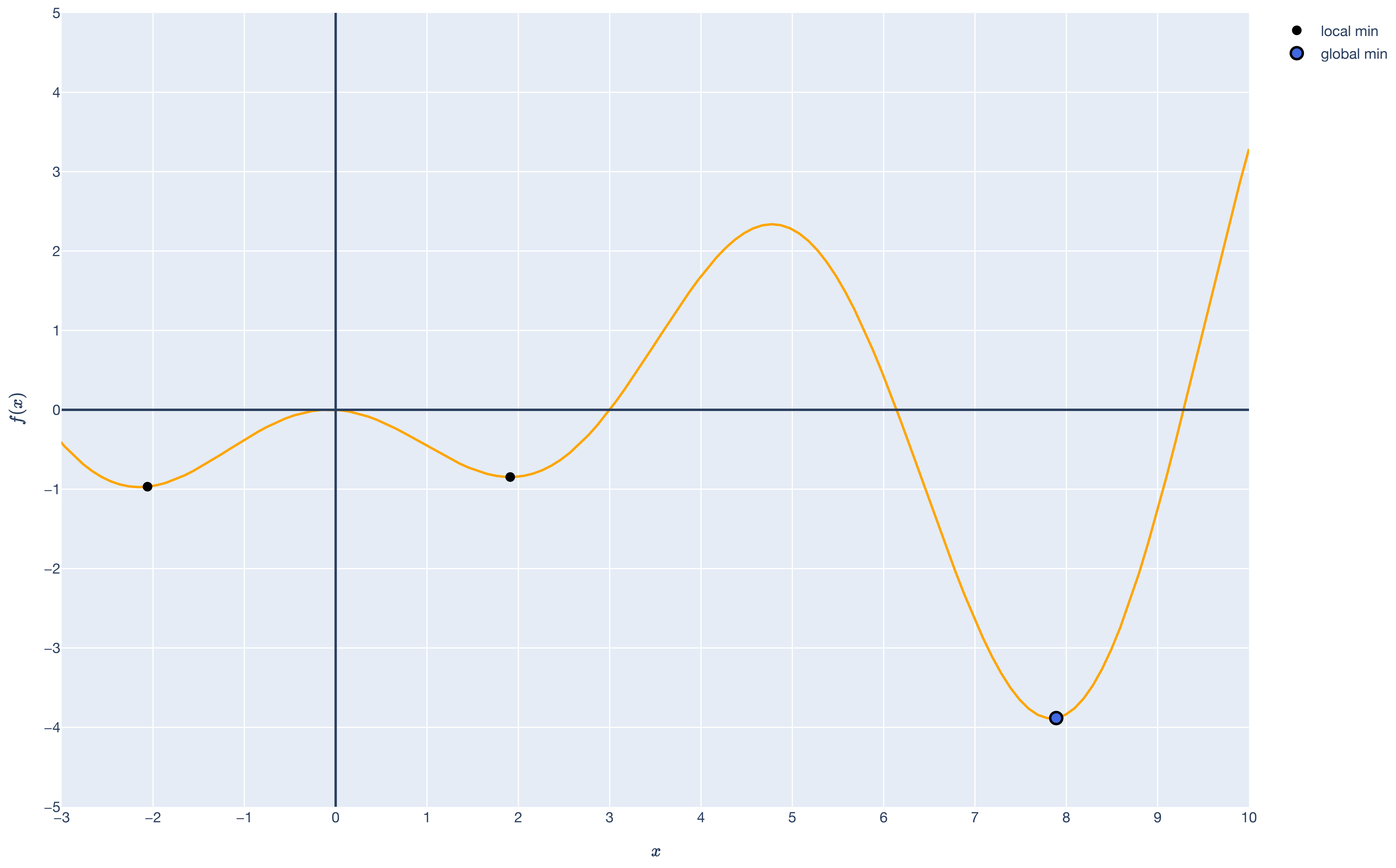
$$\nabla f(\mathbf{x}^*) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}^*) \succeq 0.$$

How do we find the *global* minimum from this when $\mathscr{C} = \mathbb{R}^d$?

1. Find *unconstrained local minima* from first-order condition $M := \{\mathbf{x}^* \in \mathbb{R}^d : \nabla f(\mathbf{x}^*) = \mathbf{0}\}$.

2. There are no boundary points!
   $(B := \mathscr{C} \backslash \mathrm{int}(\mathscr{C}) = \{\mathbf{x} \in \mathscr{C} : \mathbf{x} \notin \mathrm{int}(\mathscr{C})\} = \varnothing)$

3. The global minimum must be in the set M, so evaluate f on all $\mathbf{x} \in M$.



Unconstrained Minima

Example

$$\begin{array}{ll} \text{minimize} & x^2 \\ \text{subject to} & x \in [1,3] \end{array}$$

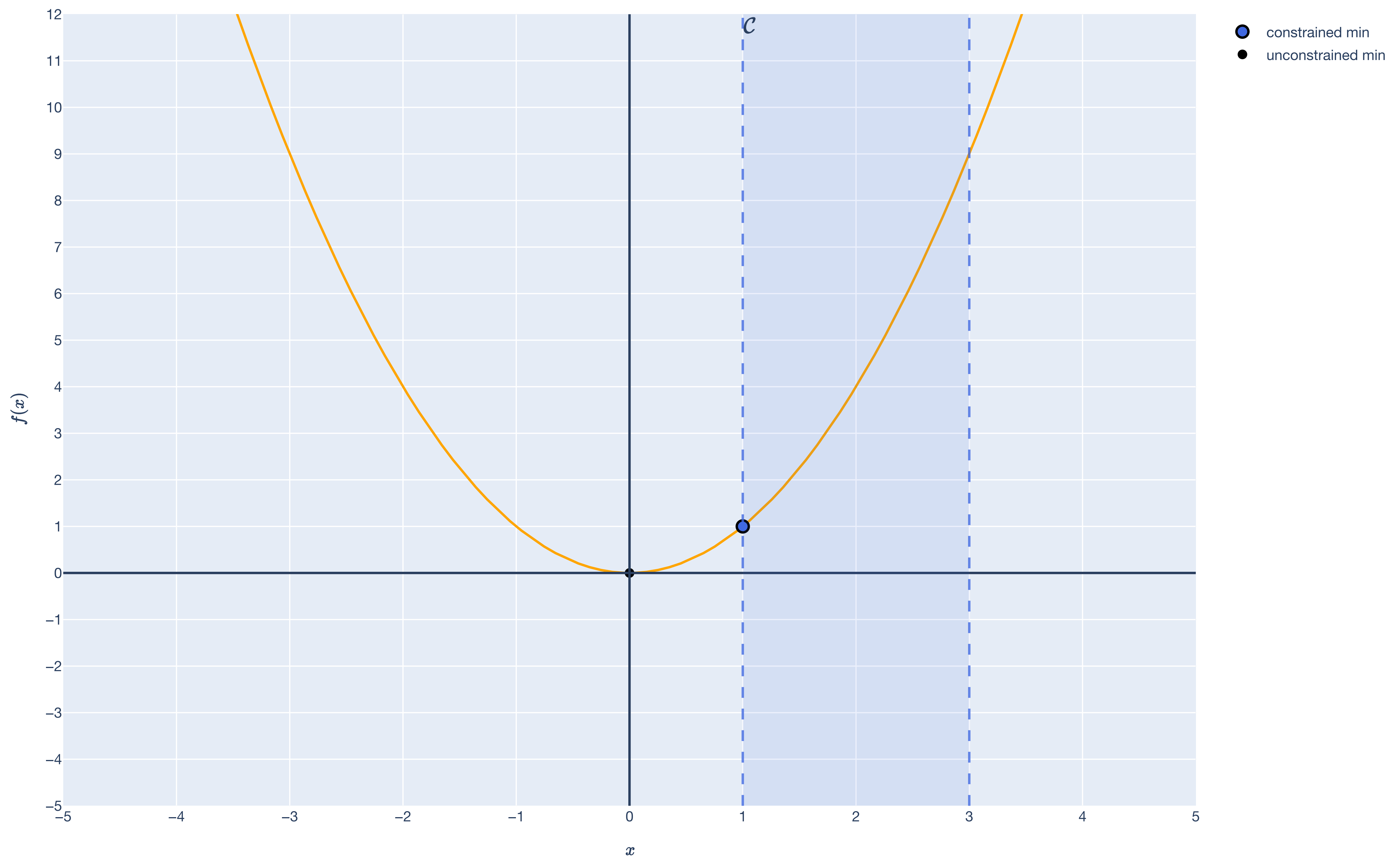
When $f : \mathbb{R} \to \mathbb{R}$ is one-dimensional on $\mathscr{C} = [a, b]$ and differentiable on $\mathrm{int}(\mathscr{C}) := (a, b)$.

Unconstrained Minima

Example

$$\begin{array}{ll} \text{minimize} & x^2 \\ \text{subject to} & x \in [1,3] \end{array}$$

When $f : \mathbb{R} \to \mathbb{R}$ is one-dimensional on $\mathscr{C} = [a, b]$ and differentiable on $\operatorname{int}(\mathscr{C}) := (a, b)$.



Unconstrained Minima

Example: Why haven't we solved optimization?

$$\begin{aligned} \text{minimize} \quad & f(x_1, x_2) \\ \text{subject to} \quad & x_1^2 + x_2^2 \le 1 \end{aligned}$$

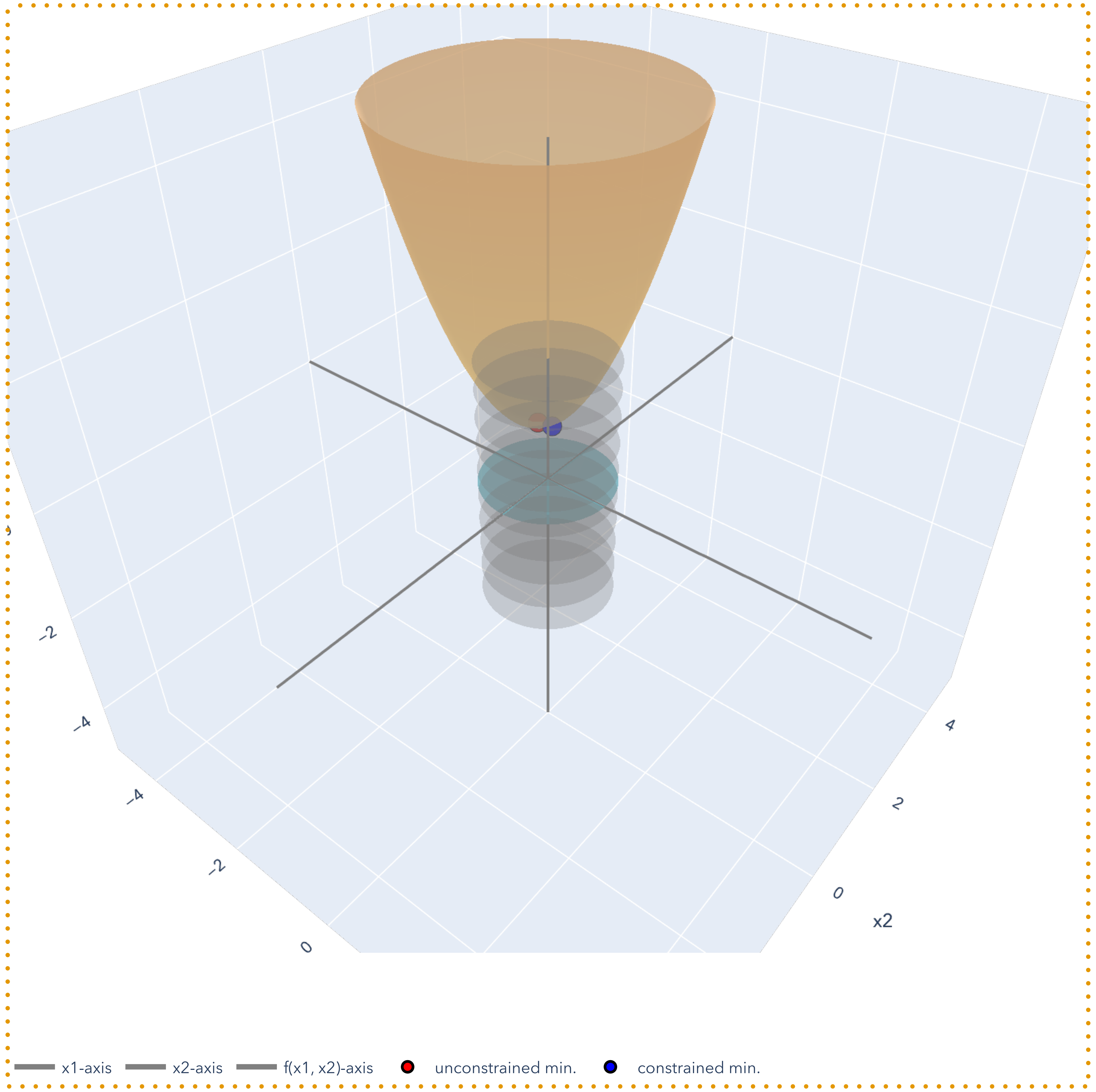
Need to evaluate f on the infinite number of points on the boundary of the circle,
$\mathscr{C} \setminus \mathrm{int}(\mathscr{C}) := \{\mathbf{x} \in \mathbb{R}^2 : x_1^2 + x_2^2 = 1\}$!

How do we deal with the possible constrained local minima induced by $\mathscr{C}$?

Unconstrained Minima

Example: Why haven't we solved optimization?

$$\begin{array}{ll} \text{minimize} & f(x_1, x_2) \\ \text{subject to} & x_1^2 + x_2^2 \leq 1 \end{array}$$



Need to evaluate f on the infinite number of points on the boundary of the circle, $\mathscr{C} \backslash \mathrm{int}(\mathscr{C}) := \{\mathbf{x} \in \mathbb{R}^2 : x_1^2 + x_2^2 = 1\}$!

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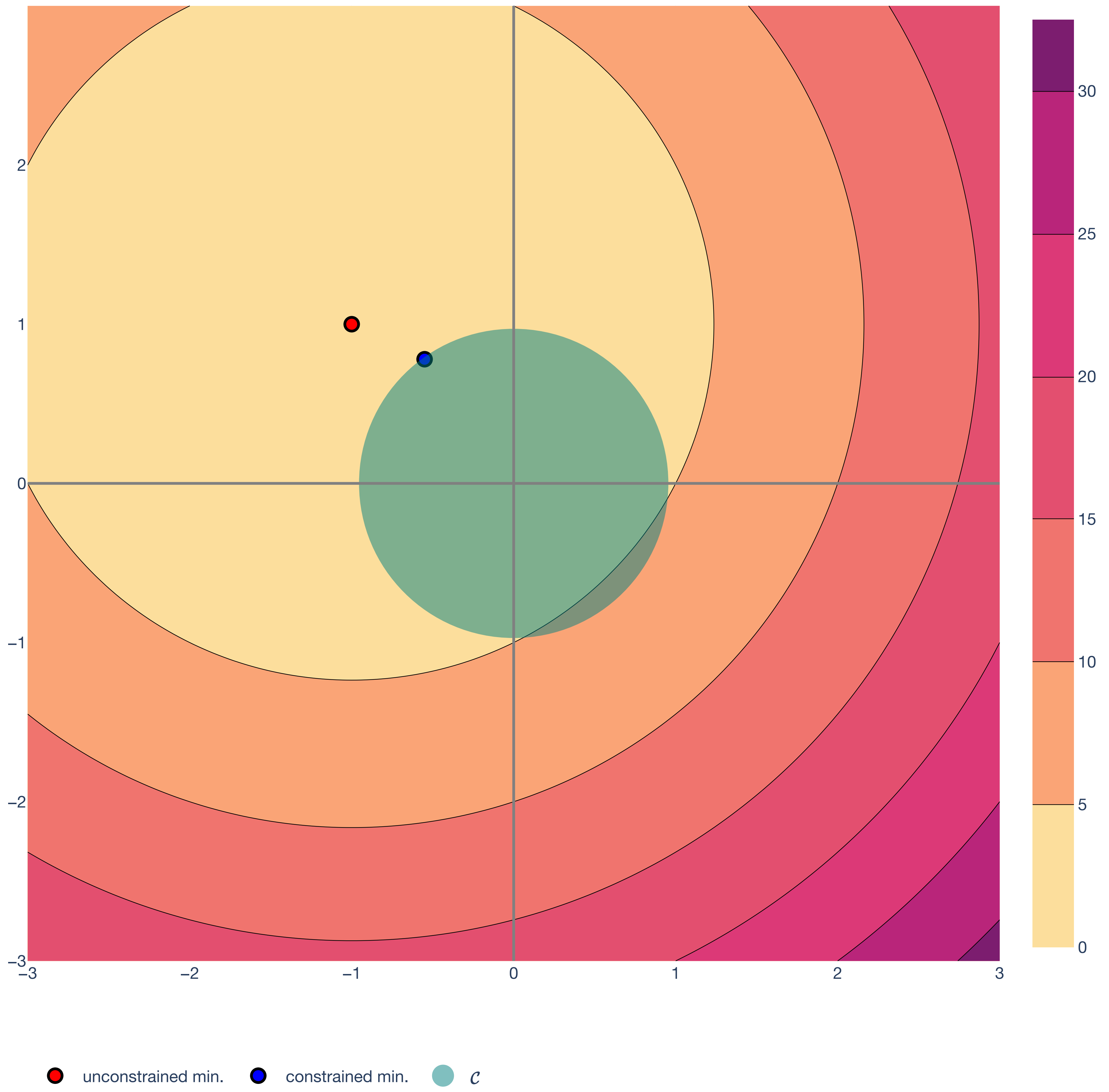


Constrained Minima

Equality Constraints and the Lagrangian

Types of Minima

Which type of minima are each of these points?

$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathscr{C} \end{array}$$

<u>constrained local:</u>

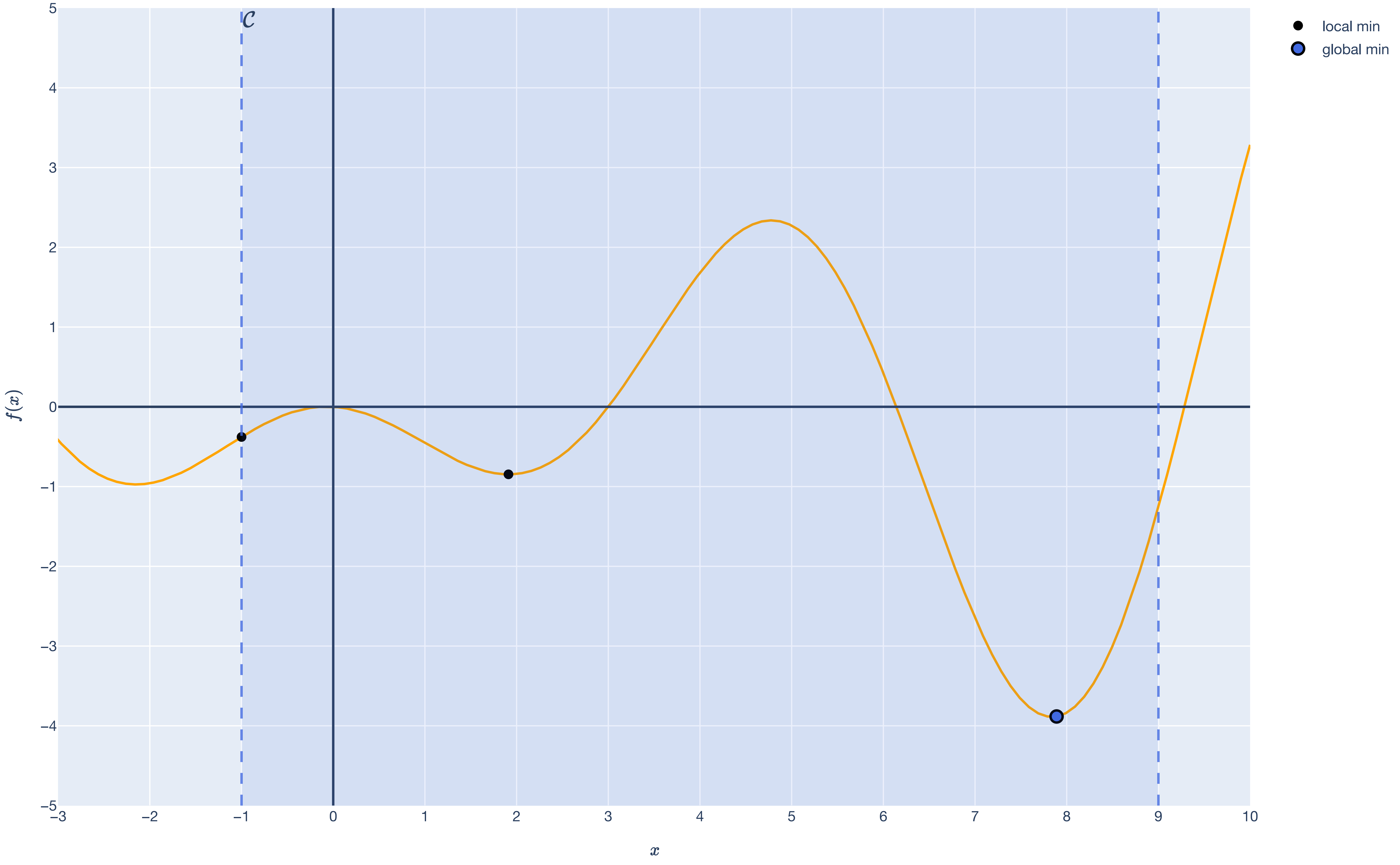
$f(\hat{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathscr{C} \cap B_\delta(\hat{\mathbf{x}})$

<u>unconstrained local:</u>

$f(\hat{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in B_\delta(\hat{\mathbf{x}})$ *and* $B_\delta(\hat{\mathbf{x}}) \subset \mathscr{C}$.

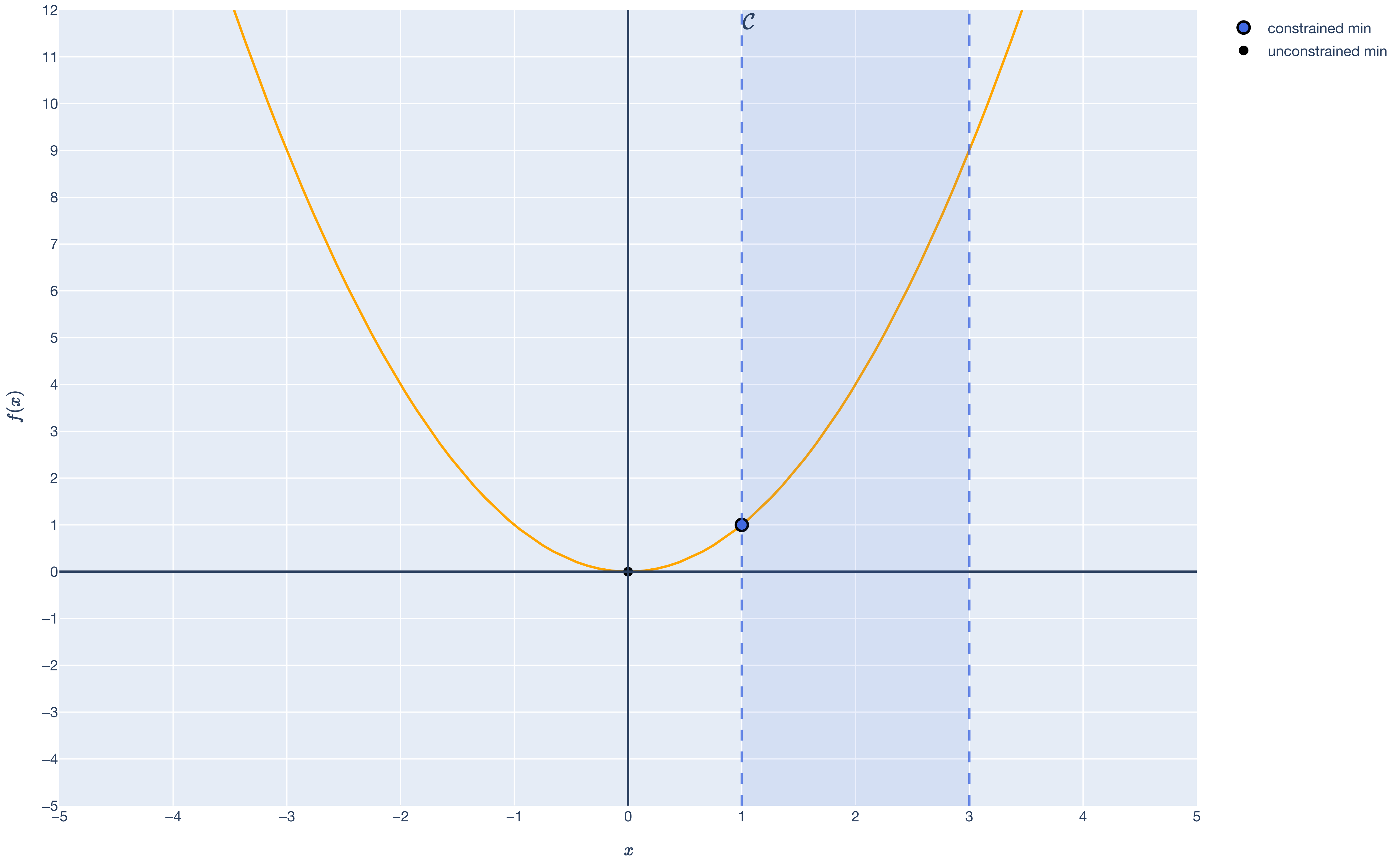
<u>global:</u>

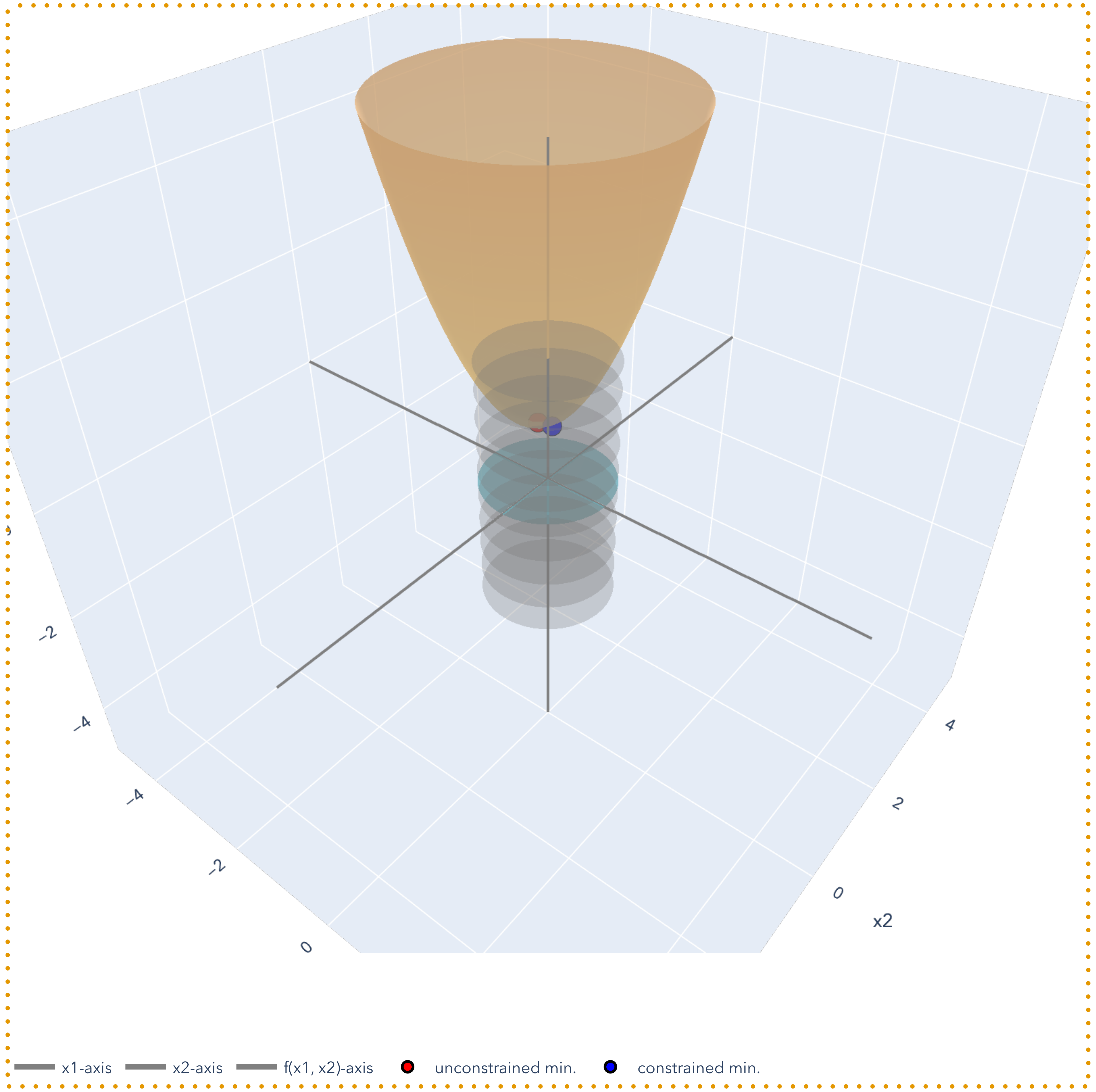
$f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathscr{C}$.



Constrained Local Minima

Minimum values on the “edge of the constraint set”





Constrained Minima

Equality constrained optimization

$$\begin{aligned} \text{minimize} \quad & \boxed{f(\mathbf{x})} \quad \text{objective function} \\ \text{subject to} \quad & \boxed{h_1(\mathbf{x}) = 0} \\ & \quad \vdots \\ & \boxed{h_m(\mathbf{x}) = 0} \quad \text{equality constraints} \end{aligned}$$

Objective function $f : \mathbb{R}^d \to \mathbb{R}$ like before.

$h_1, \ldots, h_m$ are $\mathscr{C}^1$ functions $h_i : \mathbb{R}^d \to \mathbb{R}$ that form $\mathscr{C}$, the constraint set.

Constrained Minima

Equality constrained optimization

$$
\begin{aligned}
\text{minimize} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & h_1(\mathbf{x}) = 0 \\
& \vdots \\
& h_m(\mathbf{x}) = 0
\end{aligned}
$$

The $= 0$ constraint is without loss of generality:

If we want $h_j(\mathbf{x}) = c$ then we can always consider $h_j'(\mathbf{x}) = h_j(\mathbf{x}) - c = 0$ instead.

Constrained Minima: Equality Constraints

Example: Maximum Volume Box

$$\begin{aligned} \text{minimize} \quad & x_1x_2x_3 \\ \text{subject to} \quad & x_1x_2 + x_2x_3 + x_1x_3 - c/2 = 0 \end{aligned}$$

Objective function: $f(\mathbf{x}) = x_1x_2x_3$

Single equality constraint: $h : \mathbb{R}^3 \to \mathbb{R}$, defined as $h(\mathbf{x}) = x_1x_2 + x_2x_3 + x_1x_3 - c/2$.

Constrained Minima: Equality Constraints

Idea

Convert *constrained* optimization problem into an *unconstrained* optimization problem.

Then deal with unconstrained problem as we did before:

$$\nabla f(\mathbf{x}) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\mathbf{x}) \geq 0.$$

The unconstrained optimization problem will have m more variables (for each constraint h_j for $j \in [m]$), represented by a vector $\lambda \in \mathbb{R}^m$ (the Lagrange multipliers).

Constrained Minima: Equality Constraints

Definition of the Lagrangian

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & h_1(\mathbf{x}) = 0 \\ & \quad \vdots \\ & h_m(\mathbf{x}) = 0 \end{aligned}$$

The associated Lagrangian function $L : \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R}$ is

$$L(\mathbf{x}, \lambda) := f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i h_i(\mathbf{x}).$$

Constrained Minima: Equality Constraints

Regularity Conditions

$$\begin{array}{rl} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & h_1(\mathbf{x}) = 0, \ldots, h_m(\mathbf{x}) = 0 \end{array}$$

A point $\mathbf{x} \in \mathbb{R}^d$ is a regular point if:

1. $\mathbf{x}$ is feasible, i.e. $h_1(\mathbf{x}) = 0, \ldots, h_m(\mathbf{x}) = 0$.

2. The gradients $\nabla h_1(\mathbf{x}), \ldots, \nabla h_m(\mathbf{x})$ are linearly independent.

Constraints are "non-redundant." This is a property of how we write down our problem.

Constrained Minima: Equality Constraints

Lagrange Multiplier Theorem: Necessary Conditions

Theorem (Lagrange Multiplier Theorem - Necessary). Let $\mathbf{x}^* \in \mathbb{R}^d$ be a local minimum that is a regular point. Then, there exists a unique vector $\lambda \in \mathbb{R}^m$ called a Lagrange multiplier such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) = 0$$

Constrained Minima: Equality Constraints

Lagrange Multiplier Theorem: Necessary Conditions

Theorem (Lagrange Multiplier Theorem - Necessary). Let $\mathbf{x}^* \in \mathbb{R}^d$ be a local minimum that is a regular point. Then, there exists a unique vector $\lambda \in \mathbb{R}^m$ called a Lagrange multiplier such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) = 0$$

If, in addition, f and $h_1, \ldots, h_m$ are twice continuously differentiable,

$$\mathbf{d}^\top \left(\nabla^2 f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla^2 h_i(\mathbf{x}^*) \right) \mathbf{d} \geq 0$$

for all $\mathbf{d} \in \mathbb{R}^d$ such that $\nabla h_j(\mathbf{x}^*)^\top \mathbf{d} = 0$ for all $j \in [m]$.

Constrained Minima: Equality Constraints

How to remember the Lagrange multiplier theorem

$$\nabla f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}) = 0$$

Remember the necessary conditions for unconstrained local minima:

$$\nabla f(\mathbf{x}) = \mathbf{0} \text{ and } \nabla^2 f(\mathbf{x}) \geq 0.$$

Applying first-order necessary conditions for Lagrangian, so local minimum $(\mathbf{x}^*, \lambda^*)$ must satisfy

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*) = \mathbf{0} \text{ and } \nabla_{\lambda} L(\mathbf{x}^*, \lambda^*) = \mathbf{0}.$$

Notice that $\nabla_{\lambda} L(\mathbf{x}^*, \lambda^*) = \mathbf{0}$ is the same as requiring feasibility: $h_j(\mathbf{x}^*) = 0$ for all $j \in [m]$.

Constrained Minima: Equality Constraints

Lagrange Multiplier Theorem: Sufficient Conditions

Theorem (Lagrange Multiplier Theorem - Sufficient Conditions). Let f and $\mathbf{h}$ be $\mathscr{C}^2$ functions, such that $\mathbf{x}* \in \mathbb{R}^d$ and $\lambda* \in \mathbb{R}^m$ satisfy

$$\nabla_{\mathbf{x}} L(\mathbf{x}*, \lambda*) = 0 \text{ and } \nabla_{\lambda} L(\mathbf{x}*, \lambda*) = 0$$

$$\mathbf{d}^\top \nabla^2_{\mathbf{x},\mathbf{x}} L(\mathbf{x}*, \lambda*)\mathbf{d} > 0, \text{ for all } \mathbf{d} \in \mathbb{R}^d \text{ such that } \nabla h_j(\mathbf{x}*)^\top \mathbf{d} = 0 \text{ for all } j \in [m].$$

Then, $\mathbf{x}*$ is a local minimum.

Constrained Minima: Equality Constraints

How do we use the Lagrangian?

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i h_i(\mathbf{x}) \,.$$

Assuming a global minimum exists, to find it…

1. Find the set $(\mathbf{x}^*, \lambda^*)$ of regular points satisfying the first-order necessary conditions:

   $$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*) = 0 \text{ and } \nabla_{\lambda} L(\mathbf{x}^*, \lambda^*) = 0.$$

2. Find the set of all non-regular points.

3. The global minima must be among the points in (1) or (2).

Constrained Minima: Equality Constraints

Example: Maximum Volume Box

$$\begin{aligned} \text{minimize} \quad & x_1 x_2 x_3 \\ \text{subject to} \quad & x_1 x_2 + x_2 x_3 + x_1 x_3 - c/2 = 0 \end{aligned}$$

Constrained Minima

Inequality Constraints and the KKT Theorem

Constrained Minima

Inequality constrained optimization

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & h_1(\mathbf{x}) = 0, \ldots, h_m(\mathbf{x}) = 0 \\ & g_1(\mathbf{x}) \leq 0, \ldots, g_r(\mathbf{x}) \leq 0 \end{aligned}$$

objective function

equality constraints

inequality constraints

Objective function $f : \mathbb{R}^d \to \mathbb{R}$ like before.

$h_1, \ldots, h_m$ are $\mathscr{C}^1$ functions $h_i : \mathbb{R}^d \to \mathbb{R}$ that form $\mathscr{C}$, the constraint set.

$g_1, \ldots, g_r$ are $\mathscr{C}^1$ functions $g_i : \mathbb{R}^d \to \mathbb{R}$ that form $\mathscr{C}$, the constraint set.

Constrained Minima

Inequality constrained optimization

$$
\begin{array}{rl}
\text{minimize} & f(\mathbf{x}) \\
\text{subject to} & h_1(\mathbf{x}) = 0, \ldots, h_m(\mathbf{x}) = 0 \\
& g_1(\mathbf{x}) \le 0, \ldots, g_r(\mathbf{x}) \le 0
\end{array}
$$

To solve: Reduce to *equality constrained optimization.*

The only difference is that each *inequality constraint* can either be active or not.

A constraint $j \in [r]$ is active if $g_j(\mathbf{x}) = 0$.

Constrained Minima: Inequality Constraints

Definition of active constraints

For feasible $\mathbf{x} \in \mathbb{R}^d$ the set of active inequality constraints is

$$\mathscr{A}(\mathbf{x}) := \{j : g_j(\mathbf{x}) = 0\} \subseteq [r] \,.$$

A point $\mathbf{x} \in \mathbb{R}^d$ is a regular point if it is feasible and the gradients

$$\{\, \nabla h_1(\mathbf{x}), \ldots, \nabla h_m(\mathbf{x})\} \cup \{\, \nabla g_j(\mathbf{x}) : j \in \mathscr{A}(\mathbf{x})\}$$

are linearly independent.

Constrained Minima: Inequality Constraints

Lagrangian in Inequality Constrained Optimization

$$\begin{array}{rl} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & h_1(\mathbf{x}) = 0, \ldots, h_m(\mathbf{x}) = 0 \\ & g_1(\mathbf{x}) \le 0, \ldots, g_r(\mathbf{x}) \le 0 \end{array}$$

The Lagrangian function $L : \mathbb{R}^d \times \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ is the function

$$L(\mathbf{x}, \lambda, \mu) := f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i h_i(\mathbf{x}) + \sum_{j=1}^{r} \mu_j g_j(\mathbf{x}).$$

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem

Theorem (KKT Theorem - Necessary Conditions). Let $\mathbf{x}^* \in \mathbb{R}^d$ be a local minimum that is a regular point. Then, there exists unique vectors $\lambda \in \mathbb{R}^m$ and $\mu \in \mathbb{R}^r$ called Lagrange multipliers such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) + \sum_{j=1}^{r} \mu_j^* \nabla g_j(\mathbf{x}^*) = 0,$$

where $\mu_j^* \geq 0$ for all $j \in [r]$ and $\mu_j^* = 0$ for all non-active constraints $j \notin \mathscr{A}(\mathbf{x}^*)$ (complementary slackness).

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem

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$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) + \sum_{j=1}^{r} \mu_j^* \nabla g_j(\mathbf{x}^*) = 0,$$

where $\mu_j^* \geq 0$ for all $j \in [r]$ and $\mu_j^* = 0$ for all non-active constraints $j \notin \mathscr{A}(\mathbf{x}^*)$ (complementary slackness).

If, in addition, f and the h_i are all twice continuously differentiable,

$$\mathbf{d}^\top \left(\nabla^2 f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla^2 h_i(\mathbf{x}^*) \right) \mathbf{d} \geq 0$$

for all $\mathbf{d} \in \mathbb{R}^d$ such that $\nabla h_j(\mathbf{x}^*)^\top \mathbf{d} = 0$ for all $j \in [m]$.

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem

$$L(\mathbf{x}, \lambda, \mu) := f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i h_i(\mathbf{x}) + \sum_{j=1}^{r} \mu_j g_j(\mathbf{x}),$$

Write the previous necessary conditions at the local optimum $(\mathbf{x}^*, \lambda^*, \mu^*)$ as:

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*, \mu^*) = 0, \ \mathbf{h}(\mathbf{x}^*) = 0, \ \mathbf{g}(\mathbf{x}^*) \leq 0$$

where we *also* require the complementary slackness *conditions*:

$\mu^* \geq 0$ and $\mu_j^* g_j(\mathbf{x}^*) = 0, \ \forall j \in [r].$

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem: Sufficient Conditions

Theorem (KKT Theorem - Sufficient Conditions). Let f, $\mathbf{h}$, and $\mathbf{g}$ be $\mathscr{C}^2$ functions, such that $\mathbf{x}^* \in \mathbb{R}^d$, $\lambda \in \mathbb{R}^m$, $\mu^* \in \mathbb{R}^r$ satisfy

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*, \mu^*) = 0,\ \mathbf{h}(\mathbf{x}^*) = 0,\ \mathbf{g}(\mathbf{x}^*) \leq 0$$

$$\mu^* \geq 0 \text{ and } \mu_j^* g_j(\mathbf{x}^*) = 0,\ \forall j \in [r]$$

$$\mathbf{d}^\top \nabla^2_{\mathbf{x},\mathbf{x}} L(\mathbf{x}^*, \lambda^*, \mu^*)\mathbf{d} > 0,$$

for all $\mathbf{d}$ such that $\nabla h_i(\mathbf{x}^*)^\top \mathbf{d} = 0$ for all $i \in [m]$ and $\nabla g_j(\mathbf{x}^*)^\top \mathbf{d} = 0,\ \forall j \in \mathscr{A}(\mathbf{x}^*)$.

Then, $\mathbf{x}^*$ is a local minimum.

Constrained Minima: Inequality Constraints

How do we use the Lagrangian?

$$L(\mathbf{x}, \lambda, \mu) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i h_i(\mathbf{x}) + \sum_{j=1}^{r} \mu_j g_j(\mathbf{x})$$

Assuming a global minimum exists, to find a global minimum…

1. Find the set $(\mathbf{x}^*, \lambda^*, \mu^*)$ satisfying the necessary conditions:

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*, \mu^*) = 0,\ \mathbf{h}(\mathbf{x}^*) = 0,\ \mathbf{g}(\mathbf{x}^*) \leq 0$$ (first-order conditions)

$\mu^* \geq 0$ and $\mu_j^* g_j(\mathbf{x}^*) = 0,\ \forall j \in [r]$ (complementary slackness)

2. Find the set of all non-regular points.

3. The global minima must be among the points in (1) or (2).

Constrained Minima: Inequality Constraints

Example: Smallest point in a halfspace

$$
\begin{array}{ll}
\text{minimize} & \dfrac{1}{2}\|\mathbf{x}\|_2^2 \\
\text{subject to} & x_1 + x_2 + x_3 \leq -3
\end{array}
$$

Least Squares Regression

Regularization and Ridge Regression

Regression

Setup (Example View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^{n}$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

<u>Goal:</u> For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \ldots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Regression

Setup (Feature View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Least Squares

OLS Theorem

<u>Theorem (Ordinary Least Squares).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$. Let $\hat{\mathbf{w}} \in \mathbb{R}^d$ be the least squares minimizer:

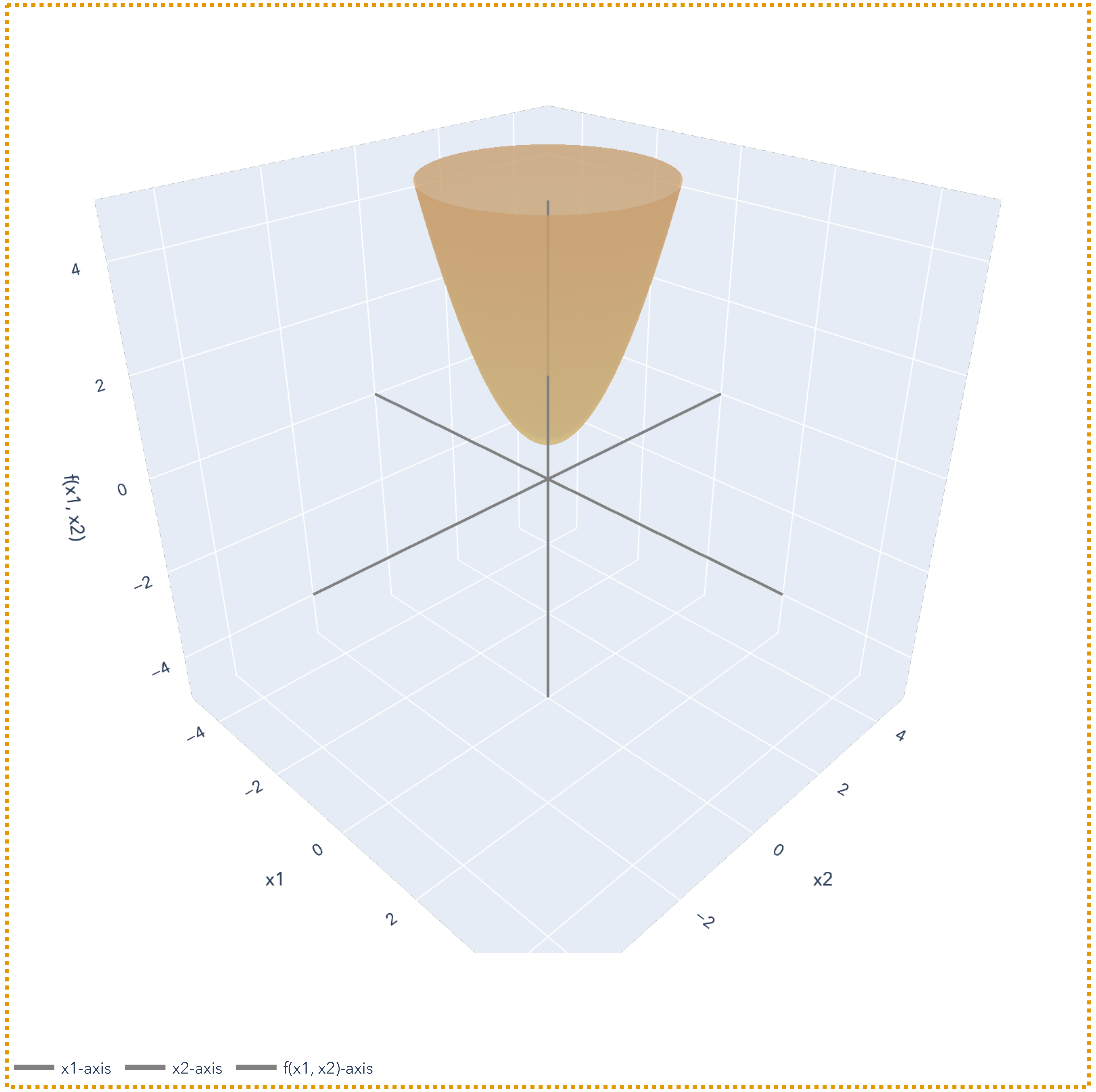
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$



Least Squares

Least norm exact solution

For $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\operatorname{rank}(\mathbf{X}) = n$,

$$\begin{aligned} \underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} \quad & \|\mathbf{w}\| \\ \text{subject to} \quad & \mathbf{X}\mathbf{w} = \mathbf{y} \end{aligned}$$

We already know how to solve this – use the pseudoinverse!

Least Squares

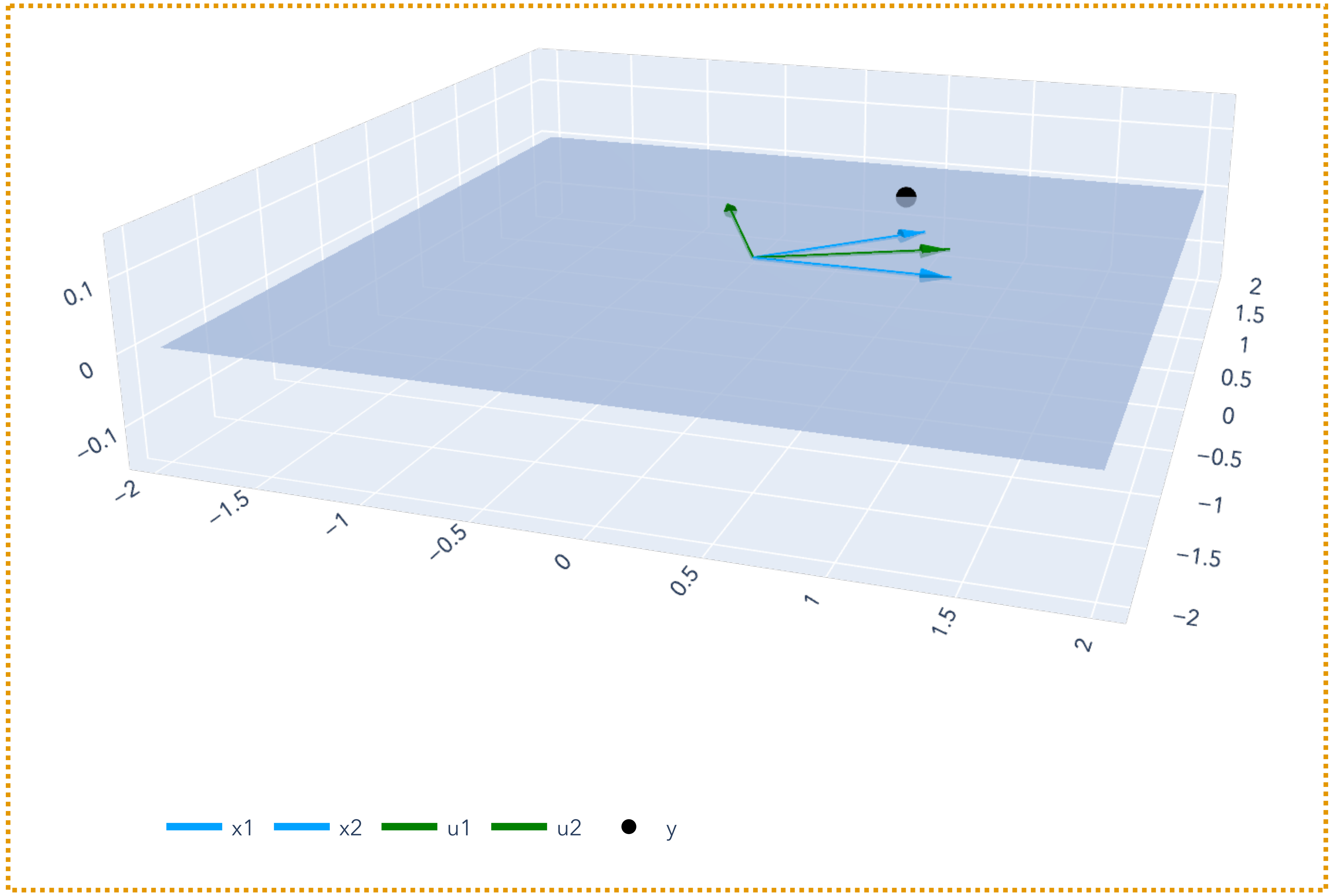
Least norm exact solution

For $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\operatorname{rank}(\mathbf{X}) = n$,

$$\begin{array}{ll} \underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} & \|\mathbf{w}\| \\ \text{subject to} & \mathbf{X}\mathbf{w} = \mathbf{y} \end{array}$$

<u>Theorem (Minimum norm least squares solution).</u>
Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, let $d \geq n$, and let $\operatorname{rank}(\mathbf{X}) = n$. Then, $\hat{\mathbf{w}} = \mathbf{X}^+\mathbf{y} = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^\top\mathbf{y}$ is the exact solution $\mathbf{X}\hat{\mathbf{w}} = \mathbf{y}$ with smallest Euclidean norm:

$$\|\mathbf{w}\|_2^2 \geq \|\hat{\mathbf{w}}\|_2^2 \text{ for all } \mathbf{w} \in \mathbb{R}^d.$$



Least Squares

Least norm exact solution

$$\begin{array}{ll} \underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} & \|\mathbf{w}\| \\ \text{subject to} & \mathbf{X}\mathbf{w} = \mathbf{y} \end{array}$$

Alternate proof (through Lagrangian). For Lagrange multipliers $\lambda \in \mathbb{R}^n$,

$$L(\mathbf{w}, \lambda) = \|\mathbf{w}\| + \lambda^\top(\mathbf{X}\mathbf{w} - \mathbf{y})$$

First-order conditions: $\nabla_{\mathbf{w}} L(\mathbf{w}, \lambda) = 2\mathbf{w} + \mathbf{X}^\top\lambda$ and $\nabla_\lambda L(\mathbf{w}, \lambda) = \mathbf{X}\mathbf{w} - \mathbf{y}$.

Setting equal to zero: $2\mathbf{w} + \mathbf{X}^\top\lambda = \mathbf{0}$ and $\mathbf{X}\mathbf{w} - \mathbf{y} = \mathbf{0} \Longrightarrow \mathbf{w} = -\frac{1}{2}\mathbf{X}^\top\lambda$ and $\mathbf{X}\mathbf{w} = \mathbf{y}$

Solve for λ: $\mathbf{X}\mathbf{w} = -\frac{1}{2}\mathbf{X}\mathbf{X}^\top\lambda \implies -\frac{1}{2}(\mathbf{X}\mathbf{X}^\top)\lambda = \mathbf{y} \implies \lambda = -2(\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{y}$.

Plug λ back in to solve for $\mathbf{w}$: $\mathbf{w} = -\frac{1}{2}\mathbf{X}^\top\lambda = -\frac{1}{2}\mathbf{X}^\top\left(-2(\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{y}\right) \implies \mathbf{w} = \mathbf{X}^\top(\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{y} = \mathbf{X}^+\mathbf{y}$. *The pseudoinverse!*

Least Squares

Least norm exact solution

For $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\mathrm{rank}(\mathbf{X}) = n$,

$$\begin{aligned} \underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} \quad & \|\mathbf{w}\| \\ \text{subject to} \quad & \mathbf{X}\mathbf{w} = \mathbf{y} \end{aligned}$$

<u>Theorem (Minimum norm least squares solution).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, let $d \geq n$, and let $\mathrm{rank}(\mathbf{X}) = n$. Then, $\hat{\mathbf{w}} = \mathbf{X}^{+}\mathbf{y} = \mathbf{V}\boldsymbol{\Sigma}^{+}\mathbf{U}^{\top}\mathbf{y}$ is the exact solution $\mathbf{X}\hat{\mathbf{w}} = \mathbf{y}$ with smallest Euclidean norm:

$$\|\mathbf{w}\|_2^2 \geq \|\hat{\mathbf{w}}\|_2^2 \text{ for all } \mathbf{w} \in \mathbb{R}^d.$$

Least Squares

Ridge Regression

Our goal will now be to minimize two objectives:

$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \text{ and } \|\mathbf{w}\|^2.$$

Writing this as an optimization problem:

$$\underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma \|\mathbf{w}\|^2$$

where $\gamma > 0$ is a fixed tuning parameter.

This optimization problem is known as ridge/Tikhonov/ℓ_2-regularized regression.

Least Squares

Ridge Regression

Our goal will now be to minimize two objectives:

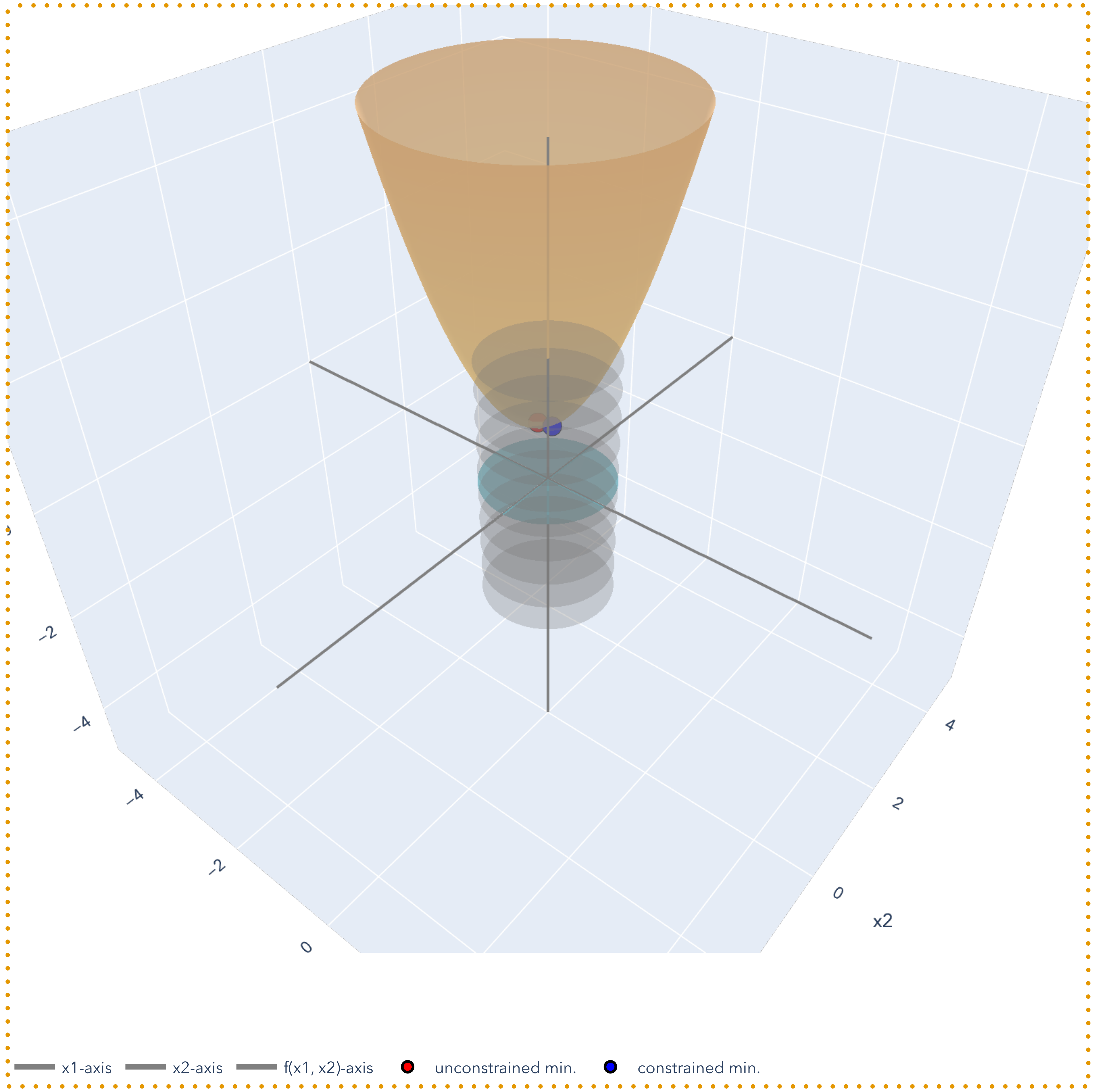
$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \text{ and } \|\mathbf{w}\|^2.$$

Writing this as an optimization problem:

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma\|\mathbf{w}\|^2$$

where $\gamma > 0$ is a fixed tuning parameter.

This optimization problem is known as ridge/Tikhonov/ℓ_2-regularized regression.



Least Squares

Ridge Regression

Our goal will now be to minimize two objectives:

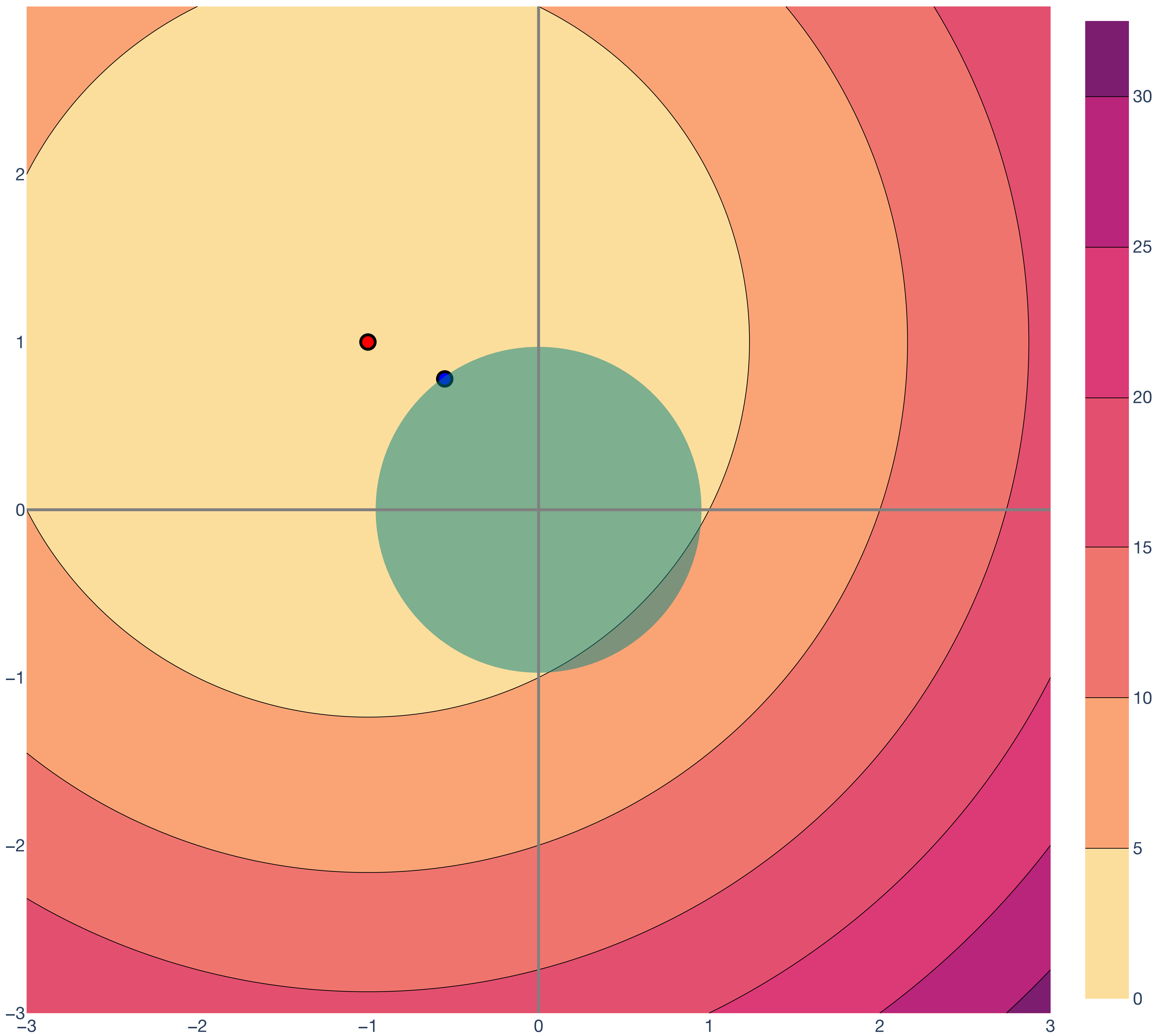
$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \text{ and } \|\mathbf{w}\|^2.$$

Writing this as an optimization problem:

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma\|\mathbf{w}\|^2$$

where $\gamma > 0$ is a fixed tuning parameter.

This optimization problem is known as ridge/Tikhonov/ℓ_2-regularized regression.



For bigger γ, bigger "constraint" ball!

Ridge Regression

Property: PSD to PD matrices

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w}-\mathbf{y}\|^2 + \gamma\|\mathbf{w}\|^2$$

How do we solve this using the first and second order conditions?

Property (Perturbing PSD matrices). Let $\mathbf{A} \in \mathbb{R}^{d\times d}$ be a positive semidefinite matrix. Then, for any $\gamma > 0$, the matrix $\mathbf{A} + \gamma\mathbf{I}$ is positive definite.

Proof. Let $\mathbf{v} \in \mathbb{R}^d$ be any vector. $\mathbf{v}^\top(\mathbf{A}+\gamma\mathbf{I})\mathbf{v} = \mathbf{v}^\top(\mathbf{A}\mathbf{v}+\gamma\mathbf{v}) = \mathbf{v}^\top\mathbf{A}\mathbf{v} + \gamma\mathbf{v}^\top\mathbf{v}$

$$= \underbrace{\mathbf{v}^\top\mathbf{A}\mathbf{v}}_{\geq 0} + \underbrace{\gamma\|\mathbf{v}\|^2}_{>0 \text{ unless } \mathbf{v}=\mathbf{0}.}$$

Ridge Regression

First-order conditions

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w}-\mathbf{y}\|^2 + \gamma\|\mathbf{w}\|^2$$

Take the gradient and set to $\mathbf{0}$:

$$\nabla_{\mathbf{w}}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|^2 + \nabla_{\mathbf{w}}\|\mathbf{w}\|^2 = 2\mathbf{X}^\top\mathbf{X}\mathbf{w} - 2\mathbf{X}^\top\mathbf{y} + 2\gamma\mathbf{w}$$

$$2\mathbf{X}^\top\mathbf{X}\mathbf{w} - 2\mathbf{X}^\top\mathbf{y} + 2\gamma\mathbf{w} = \mathbf{0} \implies (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})\mathbf{w} = \mathbf{X}^\top\mathbf{y}$$

By property (perturbing PSD matrices), $\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I}$ is PD, so:

$$\mathbf{w}^* = (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}.$$

Least Squares

Solving ridge regression

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \quad \|\mathbf{X}\mathbf{w}-\mathbf{y}\|^2+\gamma\|\mathbf{w}\|^2$$

Candidate minimizer: $\mathbf{w}^* = (\mathbf{X}^\top\mathbf{X}+\gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}.$

Gradient: $\nabla_{\mathbf{w}}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|^2+\nabla_{\mathbf{w}}\|\mathbf{w}\|^2 = 2\mathbf{X}^\top\mathbf{X}\mathbf{w}-2\mathbf{X}^\top\mathbf{y}+2\gamma\mathbf{w}$

Taking the Hessian,

$\nabla^2 f(\mathbf{w}) = \mathbf{X}^\top\mathbf{X}+\gamma\mathbf{I}$, which is positive definite.

Sufficient condition for optimality applies!

Ridge Regression

Theorem

<u>Theorem (Ridge Regression).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$, and $\gamma > 0$. Then,

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \; \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma \|\mathbf{w}\|^2$$

has the form:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Least Squares

Comparison with ridge solution

<u>Theorem (Ridge Regression).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$, and $\gamma > 0$. Then, the ridge minimizer:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma \|\mathbf{w}\|^2$$

has the form:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

<u>Theorem (Ordinary Least Squares).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$. Let $\hat{\mathbf{w}} \in \mathbb{R}^d$ be the least squares minimizer:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Error in (OLS) Regression

Error using least squares model

Choose a weight vector that "fits the training data": $\hat{\mathbf{w}} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\hat{\mathbf{w}} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

But $\hat{\mathbf{y}}$ might not be a perfect fit to $\mathbf{y}$!

Model this using a *true weight vector* $\mathbf{w}^* \in \mathbb{R}^d$ and an *error term* $\epsilon = (\epsilon_1, \ldots, \epsilon_n) \in \mathbb{R}^n$.

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i \text{ for all } i \in [n]$$

$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$$

Error in (OLS) Regression

Error using least squares model

True labels: $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$.

What happens when we use the OLS weights $\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$?

$$\begin{aligned}
\hat{\mathbf{w}} &= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y} \\
&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top(\mathbf{X}\mathbf{w}^* + \epsilon) \\
&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{X}\mathbf{w}^* + (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon \\
&= \mathbf{w}^* + (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon
\end{aligned}$$

Error in (OLS) Regression

Error using least squares model

True labels: $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$.

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&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top(\mathbf{X}\mathbf{w}^* + \epsilon) \\
&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{X}\mathbf{w}^* + (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon \\
&= \mathbf{w}^* + (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon
\end{aligned}$$

When $\epsilon = 0$ ($\mathbf{y}$ is linearly related to $\mathbf{X}$), this is perfect: $\hat{\mathbf{w}} = \mathbf{w}^*$!

Error in (OLS) Regression

Error using least squares model

True labels: $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$.

What happens when we use the OLS weights $\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$?

$$\begin{aligned}
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&= \mathbf{w}^* + (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon
\end{aligned}$$

When $\epsilon \neq 0$, we are off by $\hat{\mathbf{w}} - \mathbf{w}^* = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon$.

Error in (OLS) Regression

Eigendecomposition perspective

Weight vector's error: $\hat{\mathbf{w}} - \mathbf{w}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \epsilon$.

We know that $\mathbf{X}^\top \mathbf{X}$ (the *covariance matrix*) is PSD, so it is diagonalizable:

$$\mathbf{X}^\top \mathbf{X} = \mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^\top \implies (\mathbf{X}^\top \mathbf{X})^{-1} = \mathbf{V}^\top \boldsymbol{\Lambda}^{-1} \mathbf{V}\,.$$

The inverse of the diagonal matrix $\boldsymbol{\Lambda}^{-1}$:

$$\boldsymbol{\Lambda}^{-1} = \begin{bmatrix} 1/\lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1/\lambda_d \end{bmatrix}$$, so if λ_i is small, the entries of $\hat{\mathbf{w}}$ blow up!

Error in Regression

Error using ridge regression

True labels: $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$.

What happens when we use the ridge regression weights $\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}$?

$$\begin{aligned}
\hat{\mathbf{w}} &= (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y} \\
&= (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top(\mathbf{X}\mathbf{w}^* + \epsilon) \\
&= (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{X}\mathbf{w}^* + (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\epsilon
\end{aligned}$$

When $\epsilon = 0$ ($\mathbf{y}$ is linearly related to $\mathbf{X}$), this is no longer perfect:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{X}\mathbf{w}^*, \text{ but...}$$

Error in Regression

Error using ridge regression

True labels: $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$.

What happens when we use the ridge regression weights $\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}$?

$$
\begin{aligned}
\hat{\mathbf{w}} &= (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y} \\
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\end{aligned}
$$

When $\epsilon \neq 0$, we have more stable errors!

Error in Ridge Regression

Eigendecomposition perspective

Ridge weights: $\hat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}$.

We know that $\mathbf{X}^\top\mathbf{X}$ is positive semidefinite, so it is diagonalizable:

$$\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\top + \mathbf{V}(\gamma\mathbf{I})\mathbf{V}^\top \implies (\mathbf{X}^\top\mathbf{X} + \gamma\mathbf{I})^{-1} = \mathbf{V}^\top(\boldsymbol{\Lambda} + \gamma\mathbf{I})^{-1}\mathbf{V}.$$

The inverse of the diagonal matrix $(\boldsymbol{\Lambda} + \gamma\mathbf{I})^{-1}$:

$$(\boldsymbol{\Lambda} + \gamma\mathbf{I})^{-1} = \begin{bmatrix} \frac{1}{\lambda_1 + \gamma} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\lambda_d + \gamma} \end{bmatrix}$$, so $\dfrac{1}{\lambda_i + \gamma}$ entries are never bigger than $\dfrac{1}{\gamma}$!

Least Squares

Ridge Regression

<u>Theorem (Ridge Regression).</u> Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$, and $\gamma > 0$. Then,

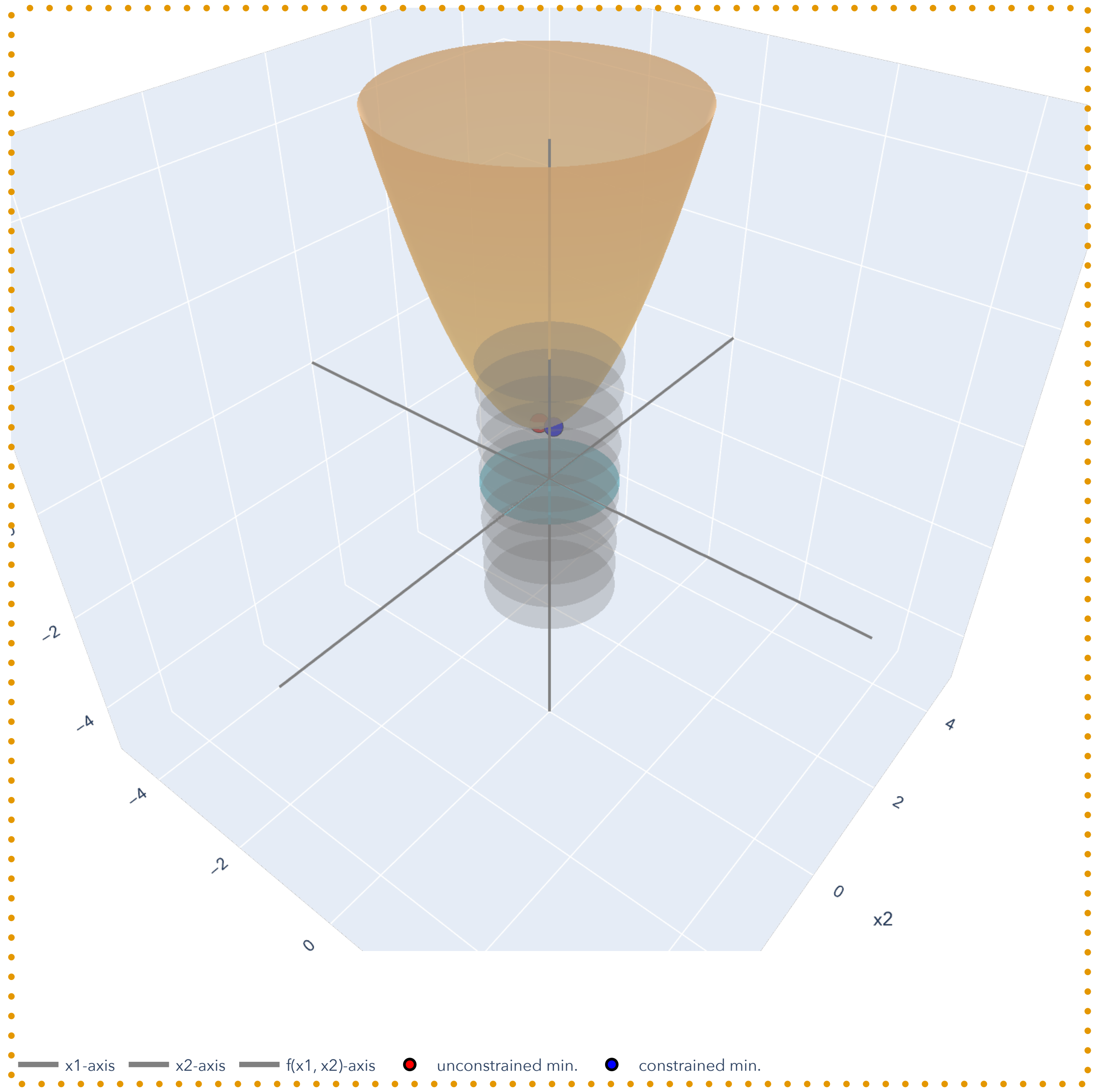
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma\|\mathbf{w}\|^2$$

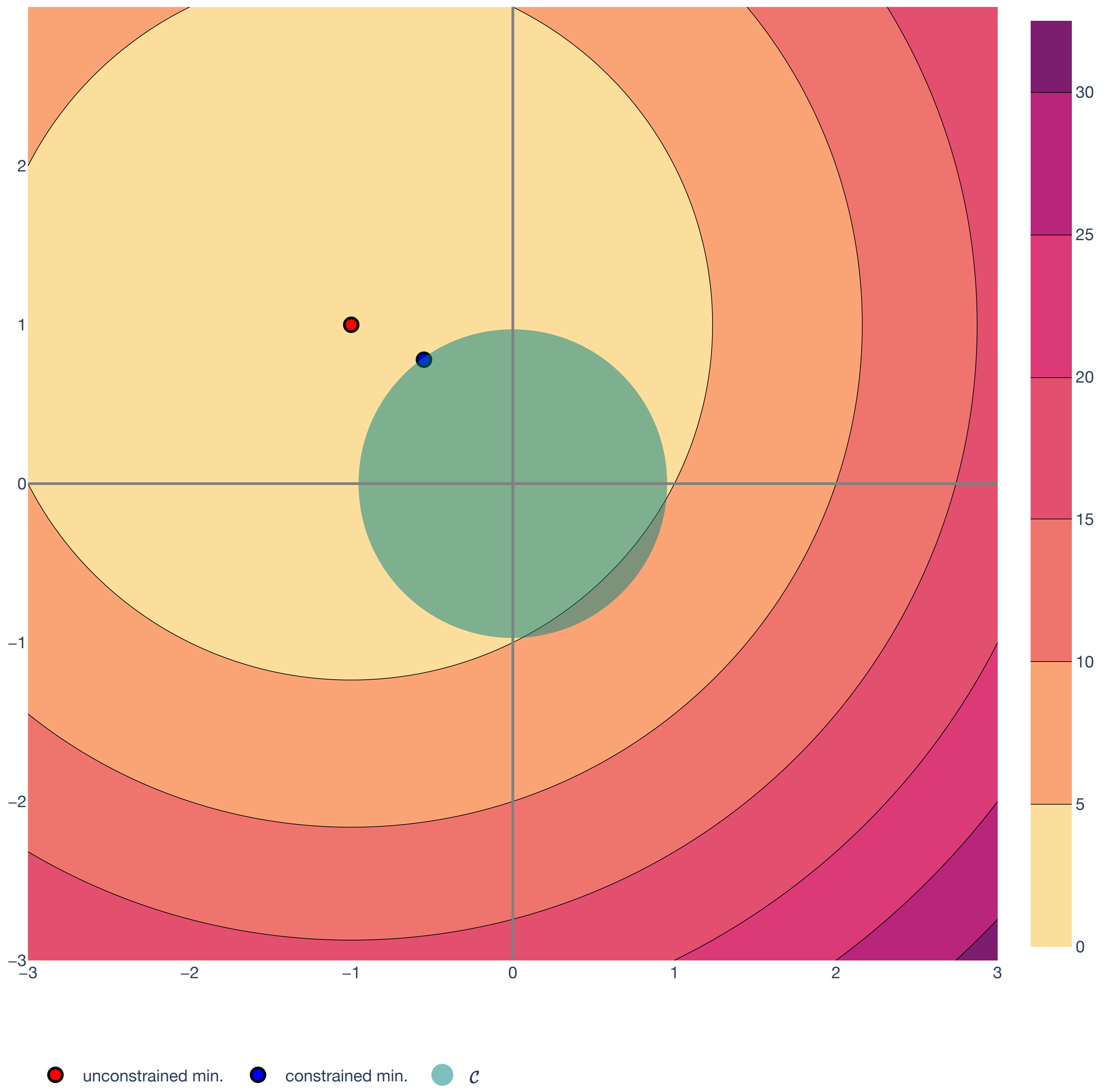
has the form:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1}\mathbf{X}^\top \mathbf{y}.$$

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \gamma \mathbf{I})^{-1}\mathbf{X}^\top \mathbf{y}.$$





For bigger γ, bigger "constraint" ball!

Recap

Lesson Overview

Optimization. Minimize an objective function $f : \mathbb{R}^d \to \mathbb{R}$ with the possible requirement that the minimizer $\mathbf{x}^*$ belongs to a constraint set $\mathscr{C} \subseteq \mathbb{R}^d$.

Lagrangian. For optimization problems with $\mathscr{C}$ defined by equalities/inequalities, the Lagrangian is a function $L : \mathbb{R}^d \times \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ that "unconstrains" the problem.

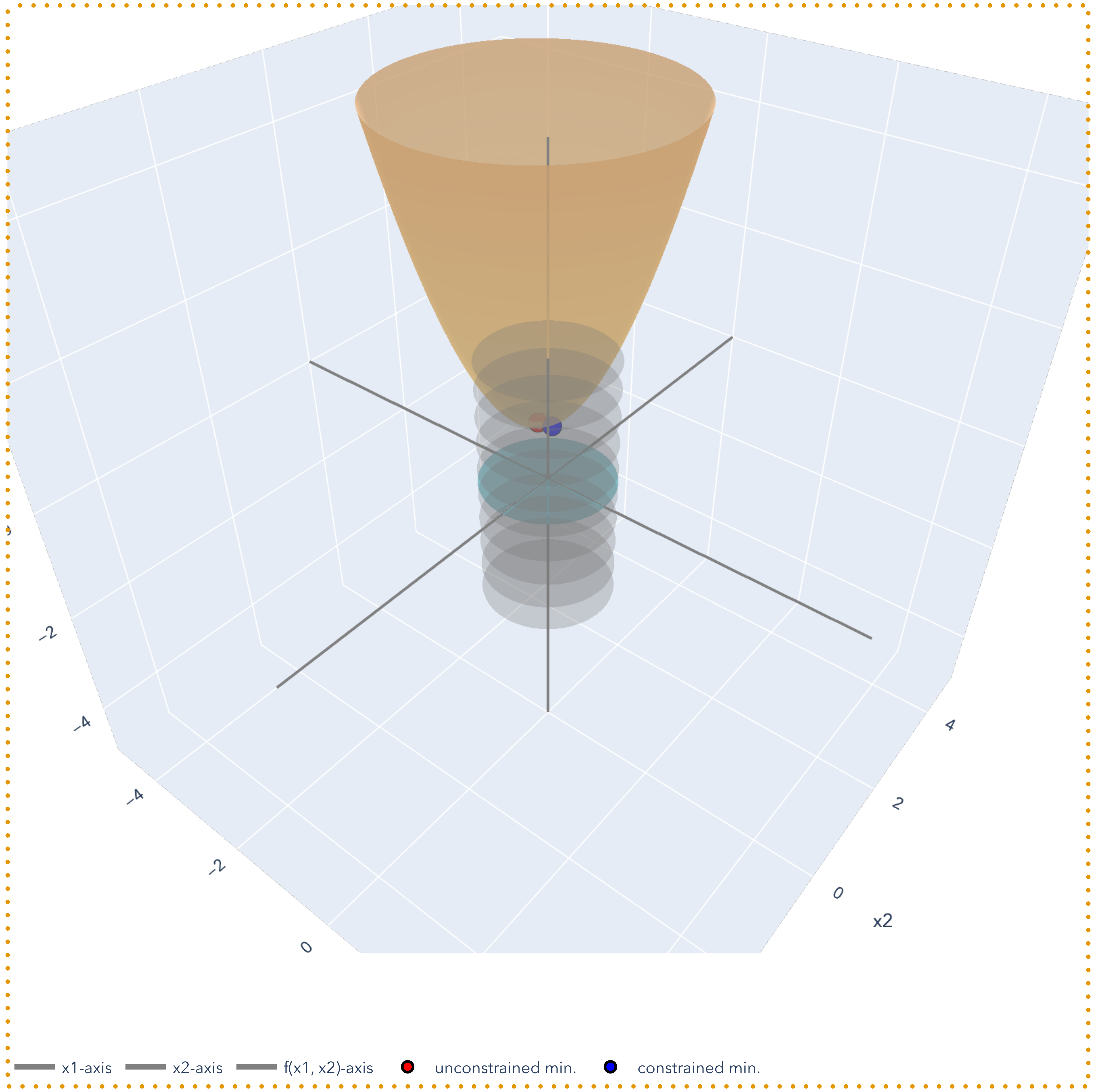
Unconstrained local optima. With no constraints, the standard tools of calculus give conditions for a point $\mathbf{x}^*$ to be optimal, at least to all points close to it.

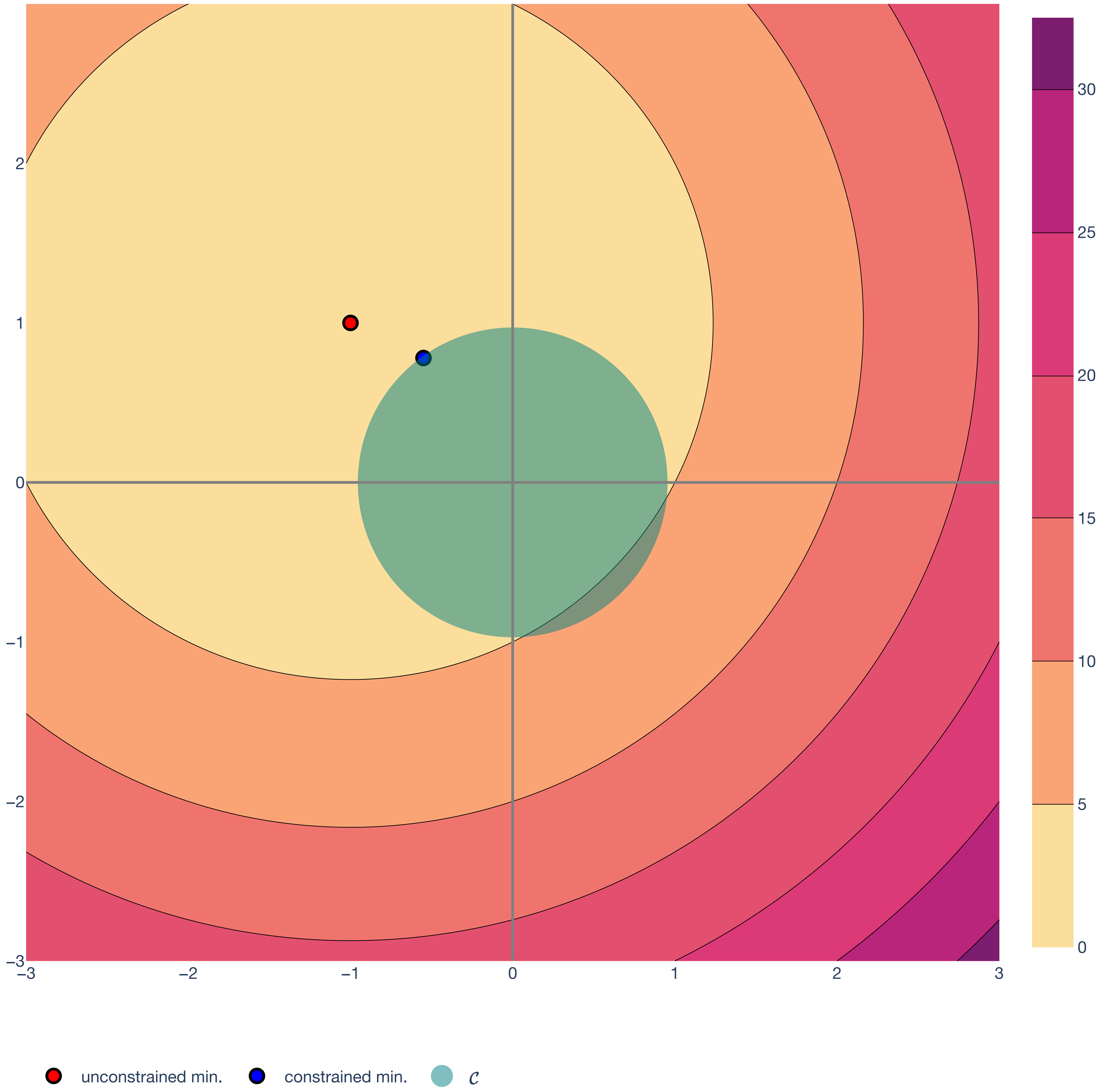
Constrained local optima (Lagrangian and KKT). When $\mathscr{C}$ is represented by inequalities and equalities, we can use the method of Lagrange multipliers and the KKT Theorem to "unconstrain" the problem.

Ridge regression and minimum norm solutions. By constraining the norm of $\mathbf{w}^* \in \mathbb{R}^d$ of least squares (i.e. $\|\mathbf{w}^*\|$), we obtain more "stable" solutions.

Lesson Overview

Big Picture: Least Squares





Lesson Overview

Big Picture: Gradient Descent