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.

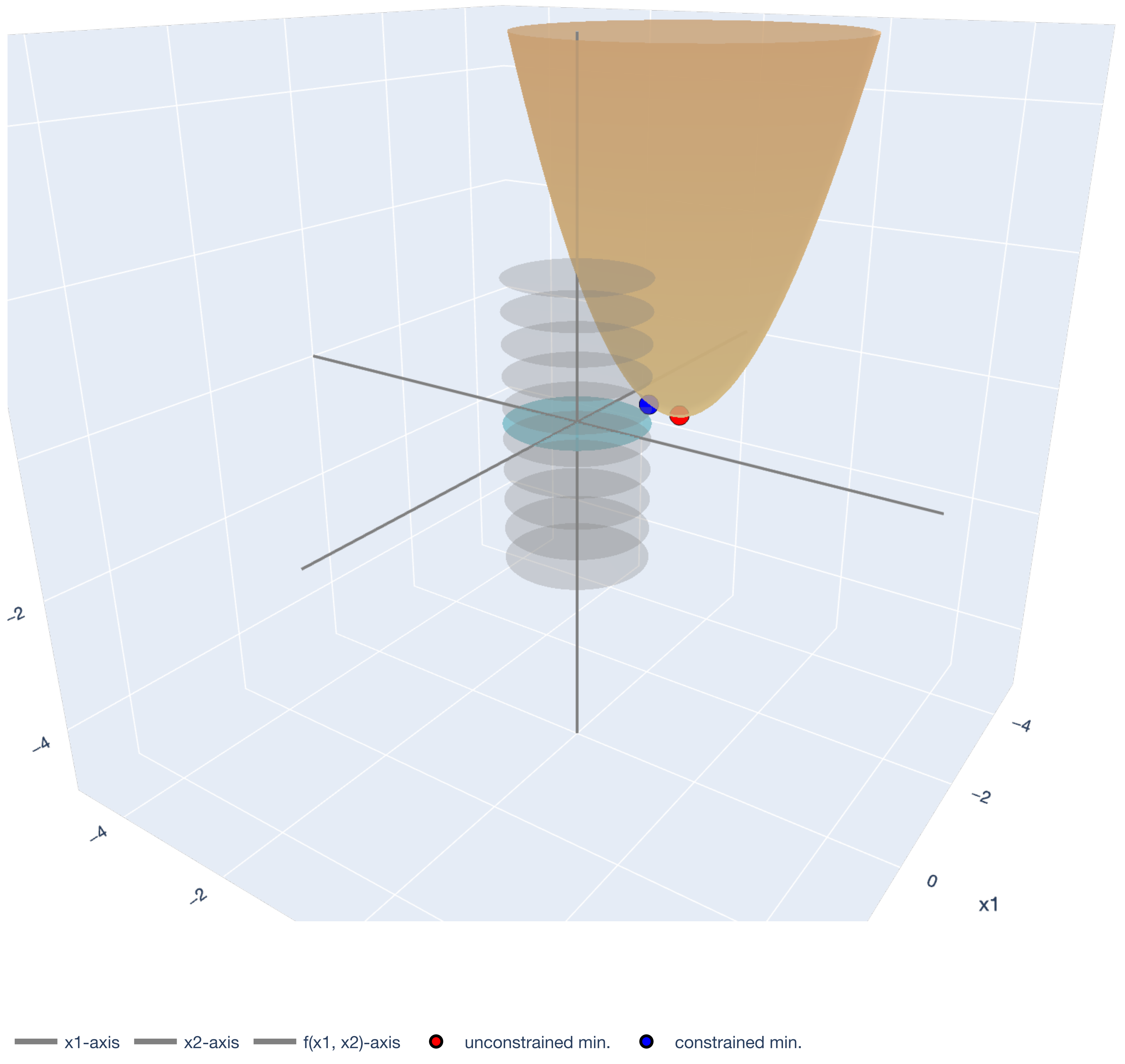
Unconstrained local optima. With no constraints, the standard tools of calculus give conditions for a point $\mathbf{x}^*$ to be optimal, at least to all points close to it.

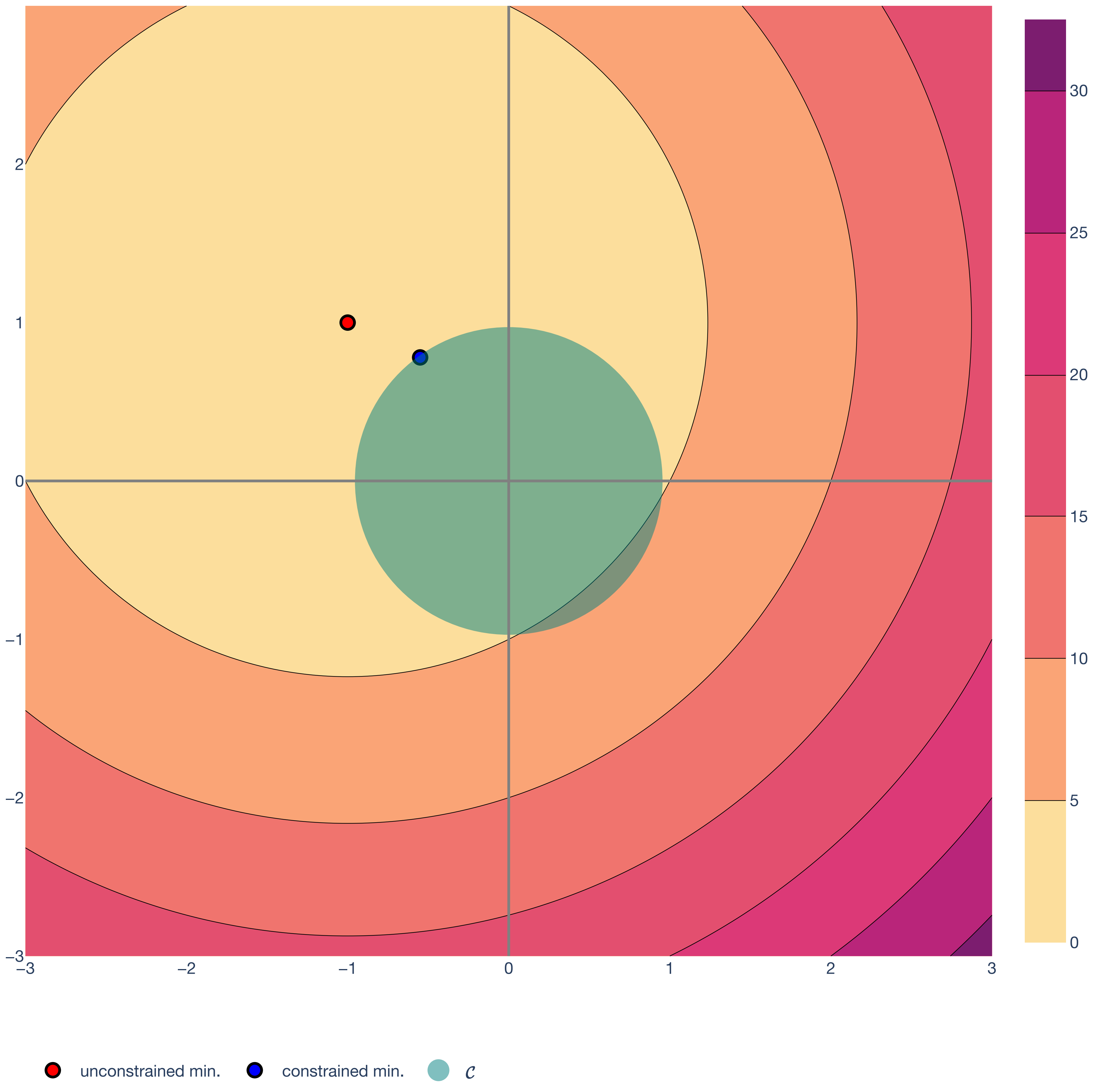
Constrained local optima (Lagrangian and KKT). When $\mathscr{C}$ is represented by inequalities and equalities, we can use the method of *Lagrange multipliers* and the *KKT Theorem* to "unconstrain" the problem.

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

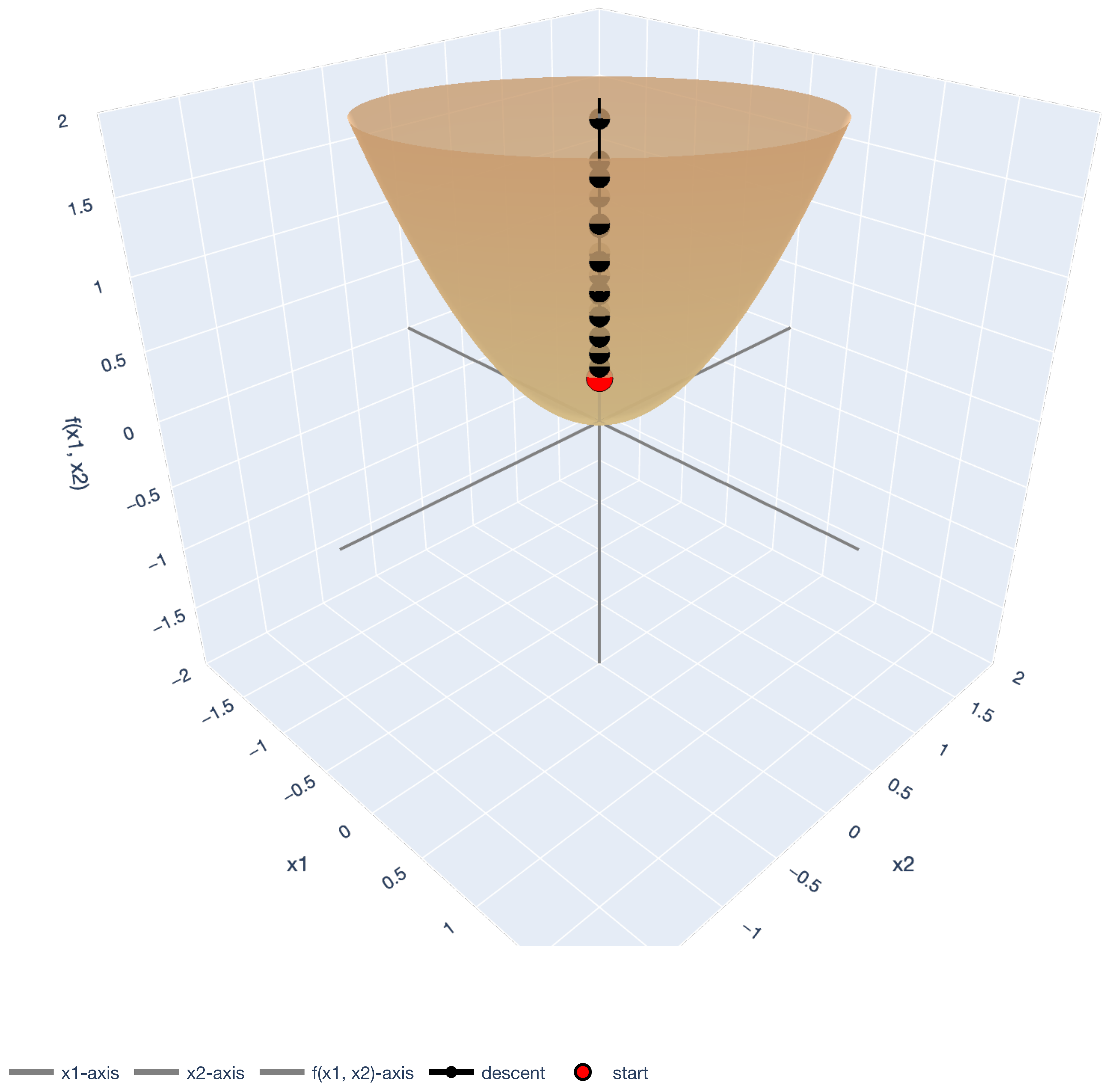
Big Picture: Least Squares

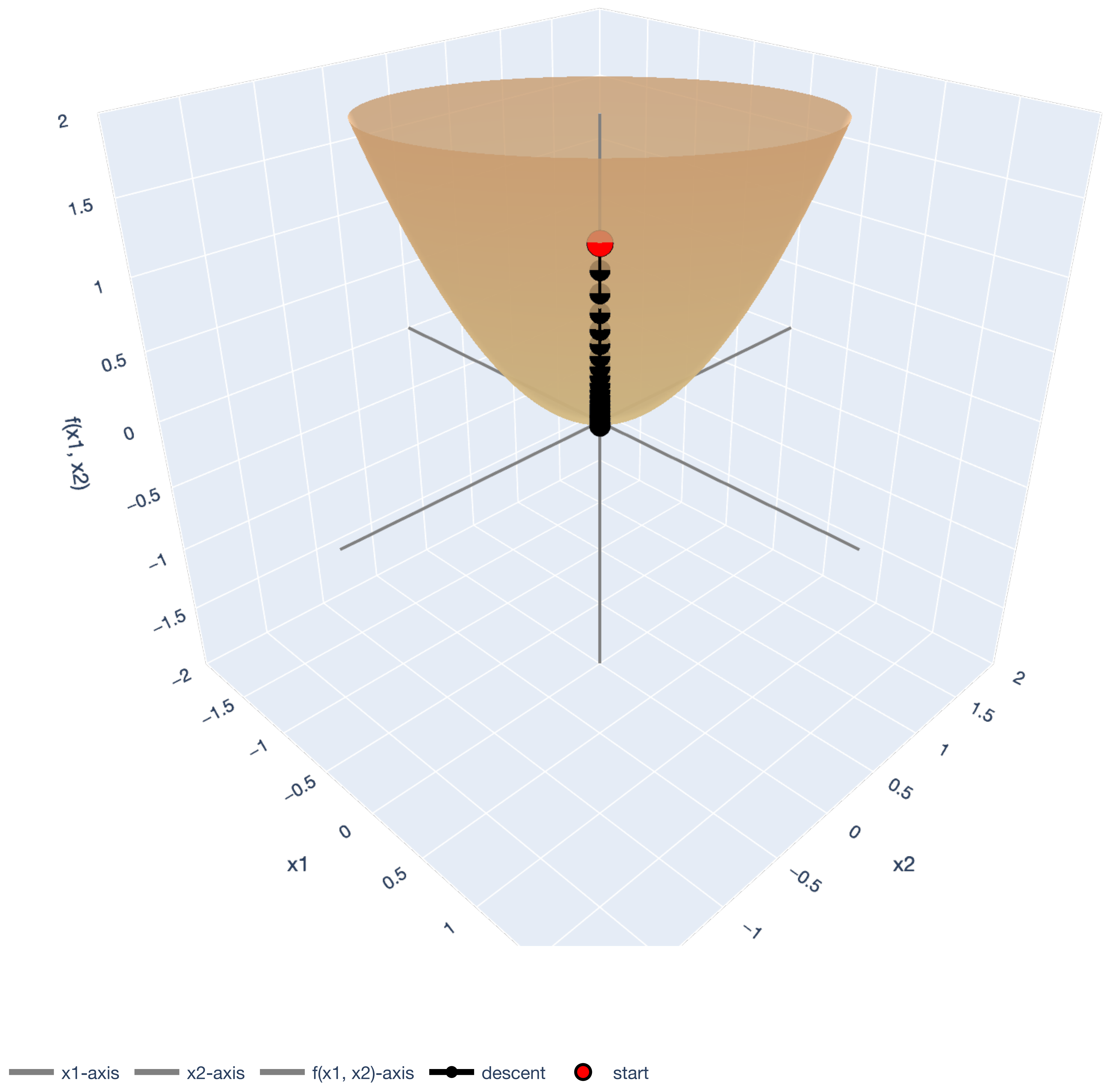




Lesson Overview

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 $\mathscr{C} \subseteq \mathbb{R}^d$:

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

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.***

$\mathscr{C} \subseteq \mathbb{R}^n$ is the ***constraint/feasible set.***

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$\mathbf{x}^*$ 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 $f(\mathbf{x}^*)$.

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

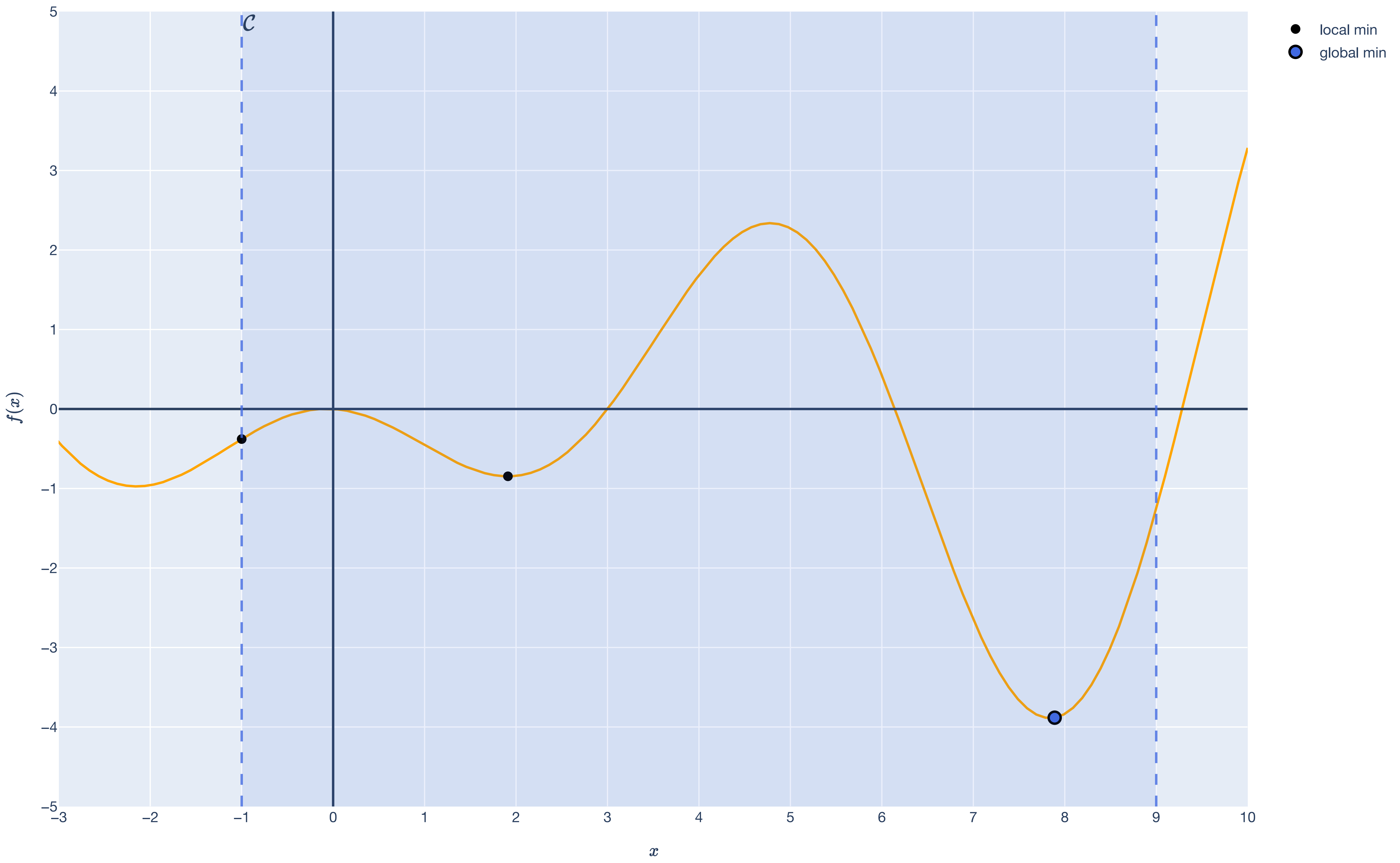
Note: to maximize $f(\mathbf{x})$, just minimize $-f(\mathbf{x})$. So we'll only focus on *minimization* problems.

Motivation

Optimization in single-variable calculus

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

Intermediary goal: Find the *local minima.*



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***.

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

$\preceq$ 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.

There are three recipes we know:

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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Cost (including labor): $3

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Cost (including labor): $2

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

Cost (including labor): $1

$\Longrightarrow$

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

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$\Longrightarrow$

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 ($d = 3$, $n = 7$)

Linear program:

$$
\begin{aligned}
\text{minimize} \quad & 3x_1 + 2x_2 + x_3 \\
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& x_1 + x_2 \leq 300 \\
& x_1 \geq 0 \\
& x_2 \geq 0 \\
& x_3 \geq 0
\end{aligned}
$$

$$\Longrightarrow$$

LP in matrix form:

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

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

Regression
Setup

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

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}.$$

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:

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

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

To find $\hat{\mathbf{w}}$, we follow the *principle of least squares.*

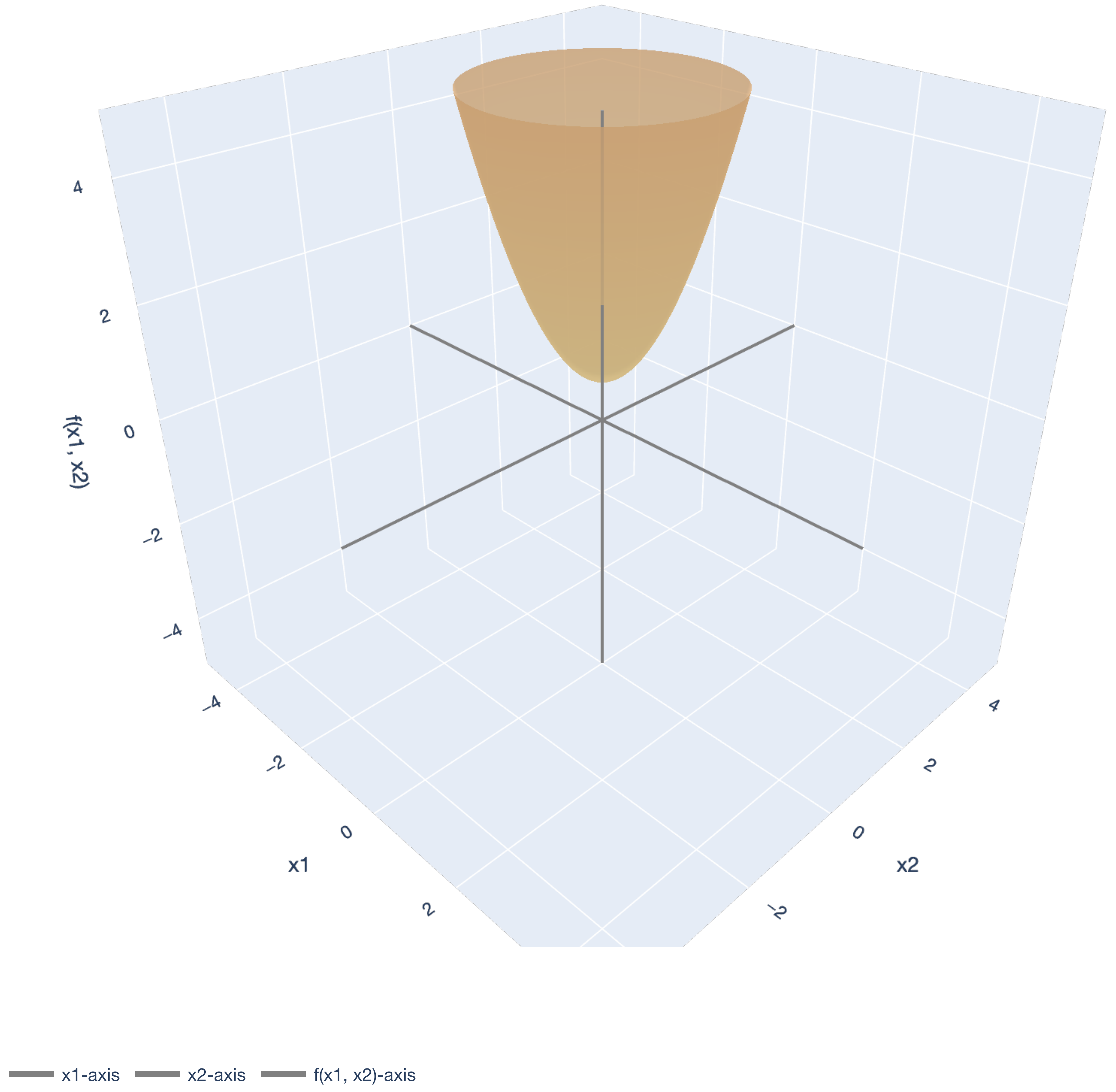
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

Least Squares

Optimization Problem

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$ be fixed. Let $\mathbf{w} \in \mathbb{R}^d$ be the decision variables.

$$\begin{aligned} \underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} \quad & \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \\ \text{subject to} \quad & \mathbf{w} \in \mathbb{R}^d \end{aligned}$$



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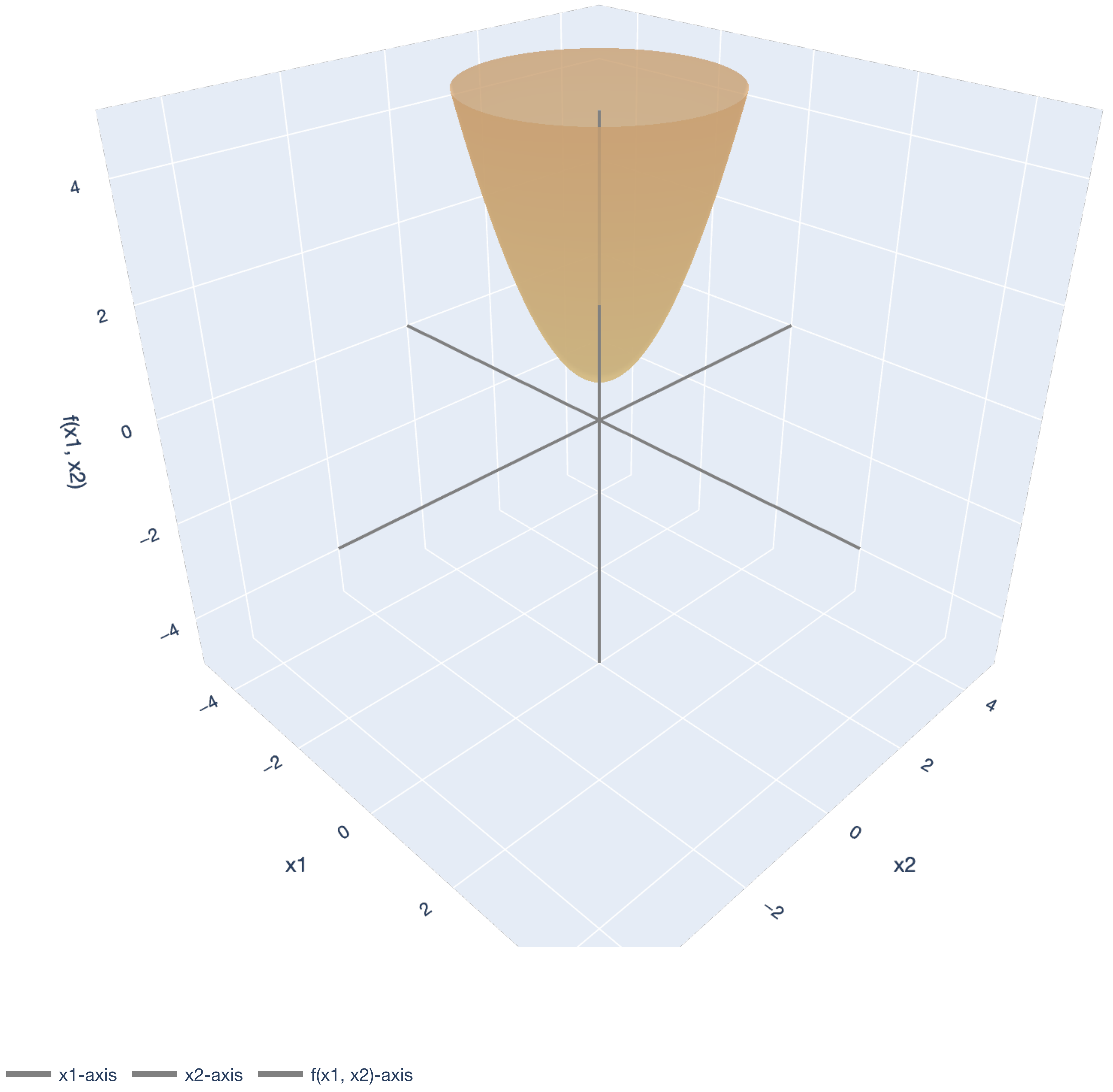
How to find the minimizer?



Least Squares

OLS Theorem

Theorem (Ordinary Least Squares). 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:

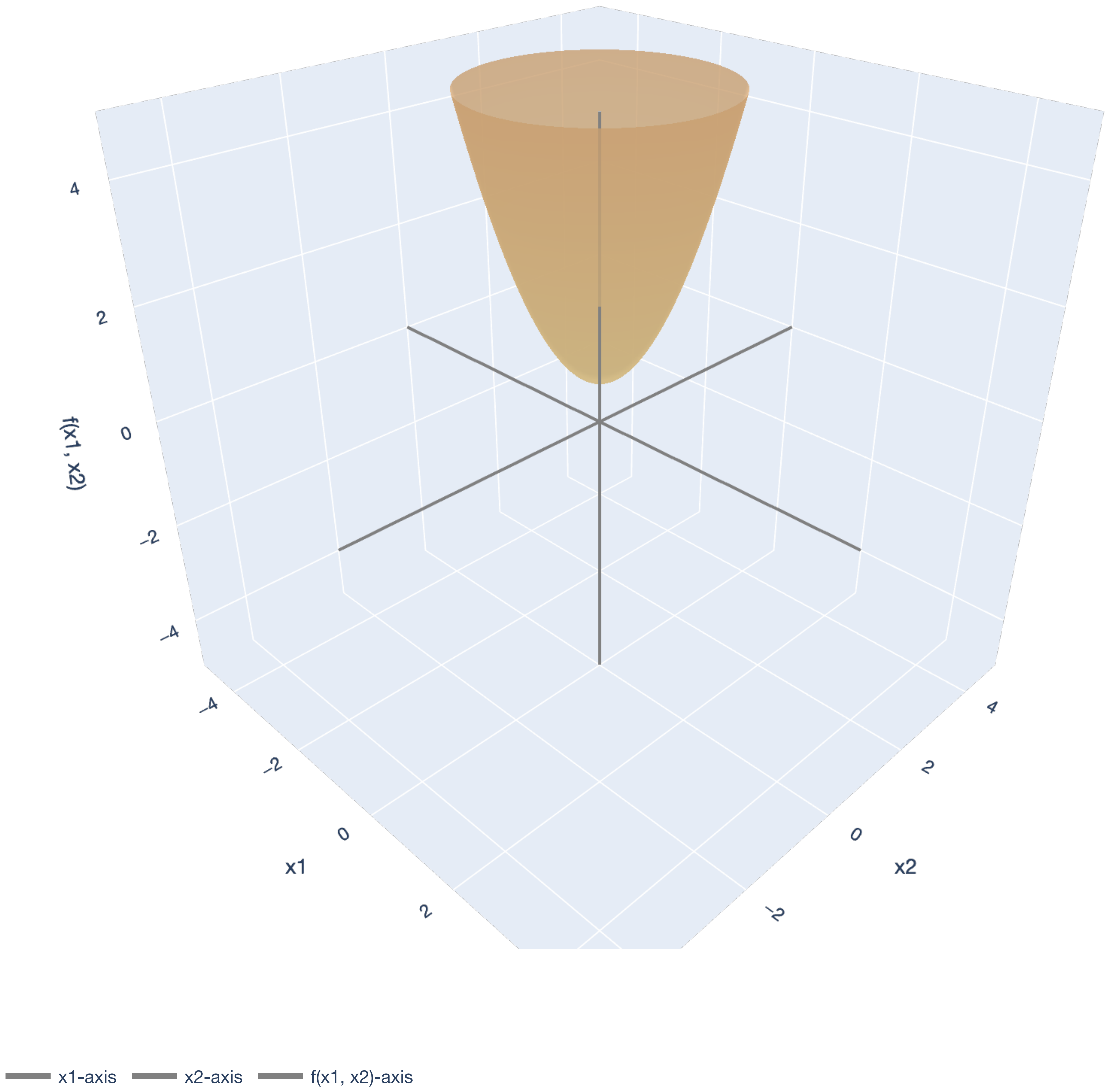
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

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 (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." Take the gradient.

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

Set it equal to $\mathbf{0}$.

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

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

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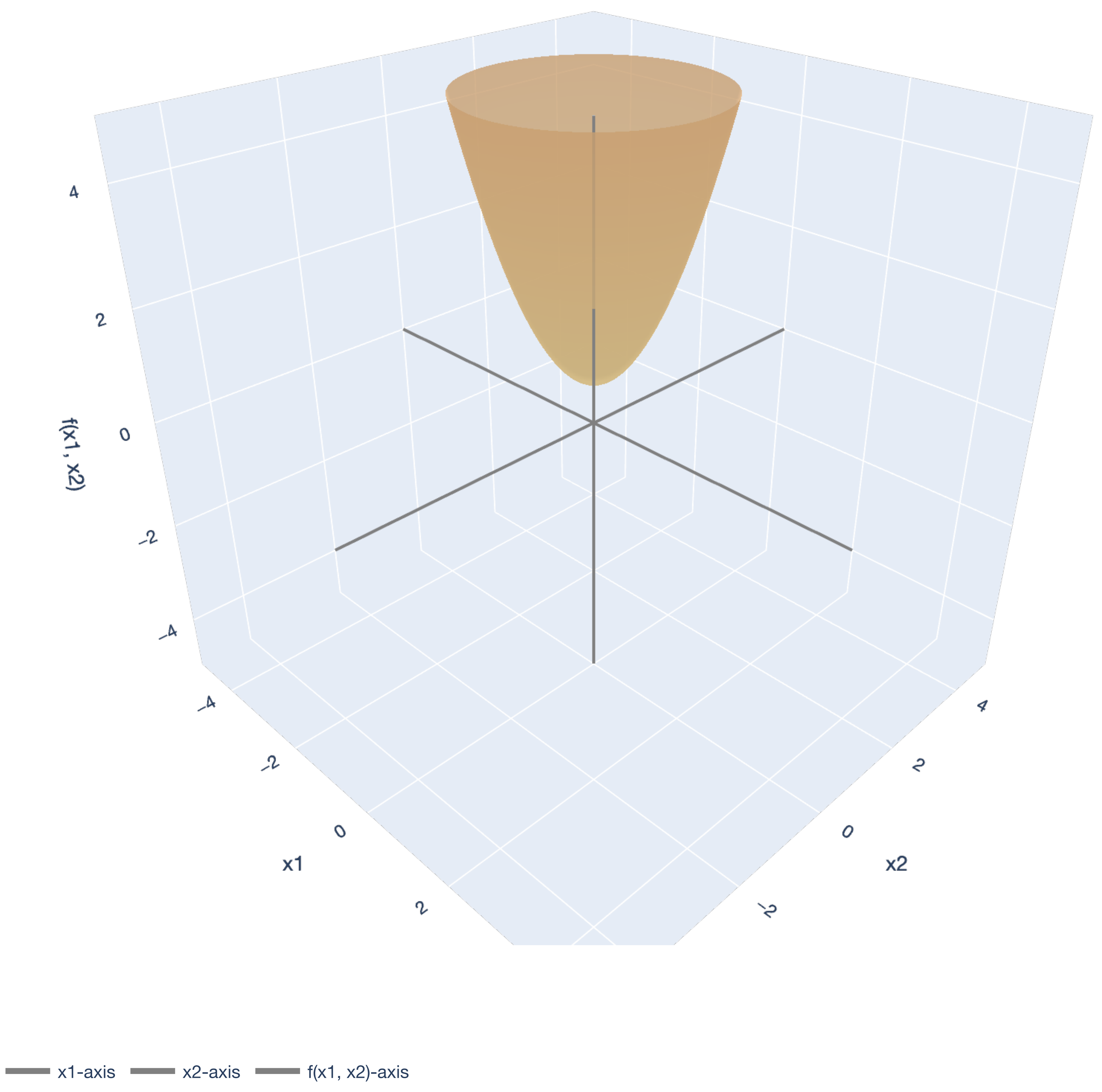

Least Squares

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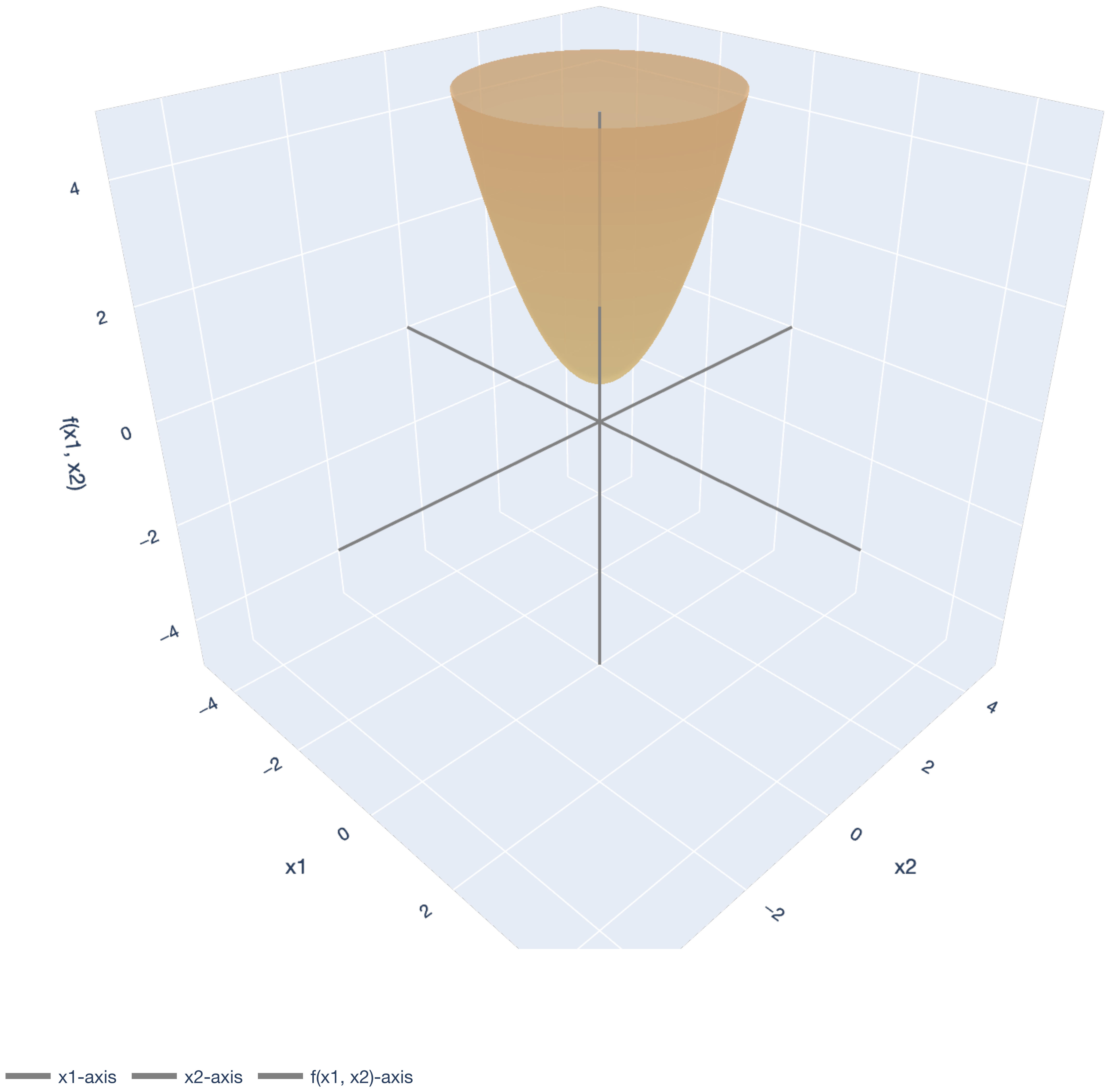
"Second derivative test." Take the *Hessian* of $f(\mathbf{w})$.

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

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

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



Least Squares

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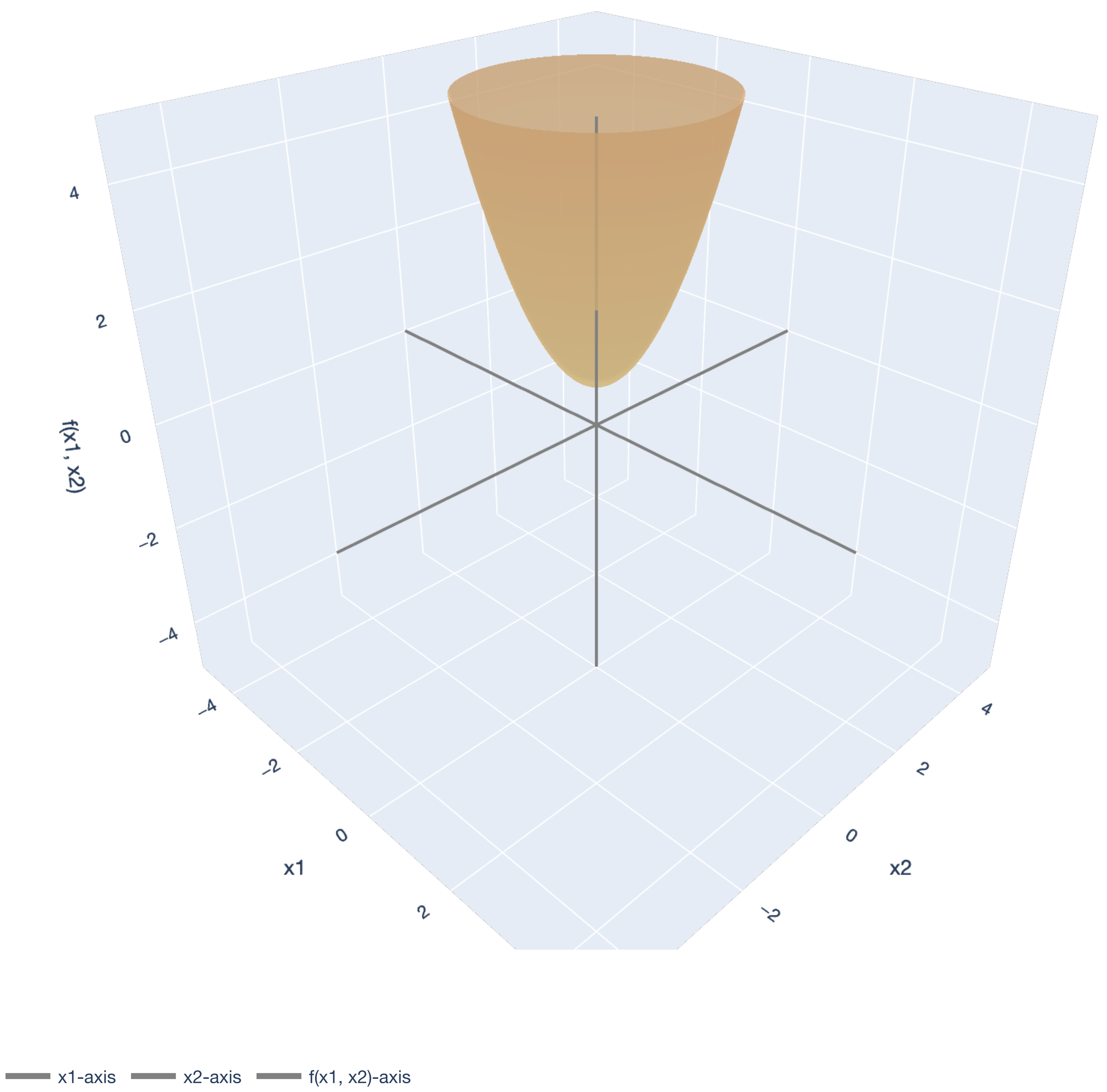


Local and global minima

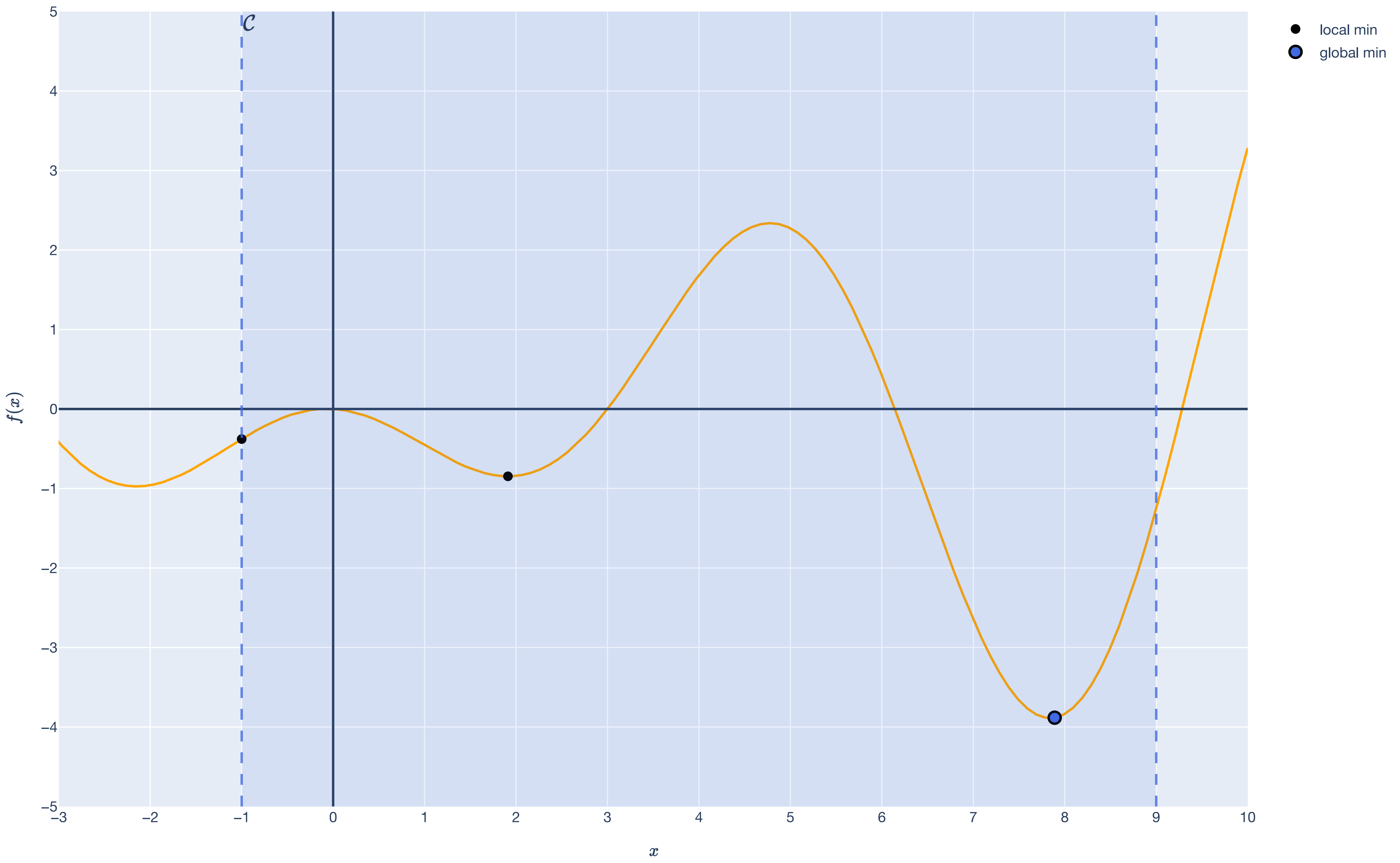
Definition of “locality” and different minima

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 an open ball/neighborhood

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

An open ball lets us approach $\mathbf{x}$ from all directions.

“Local” to a Point

Definition of the interior of a set

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

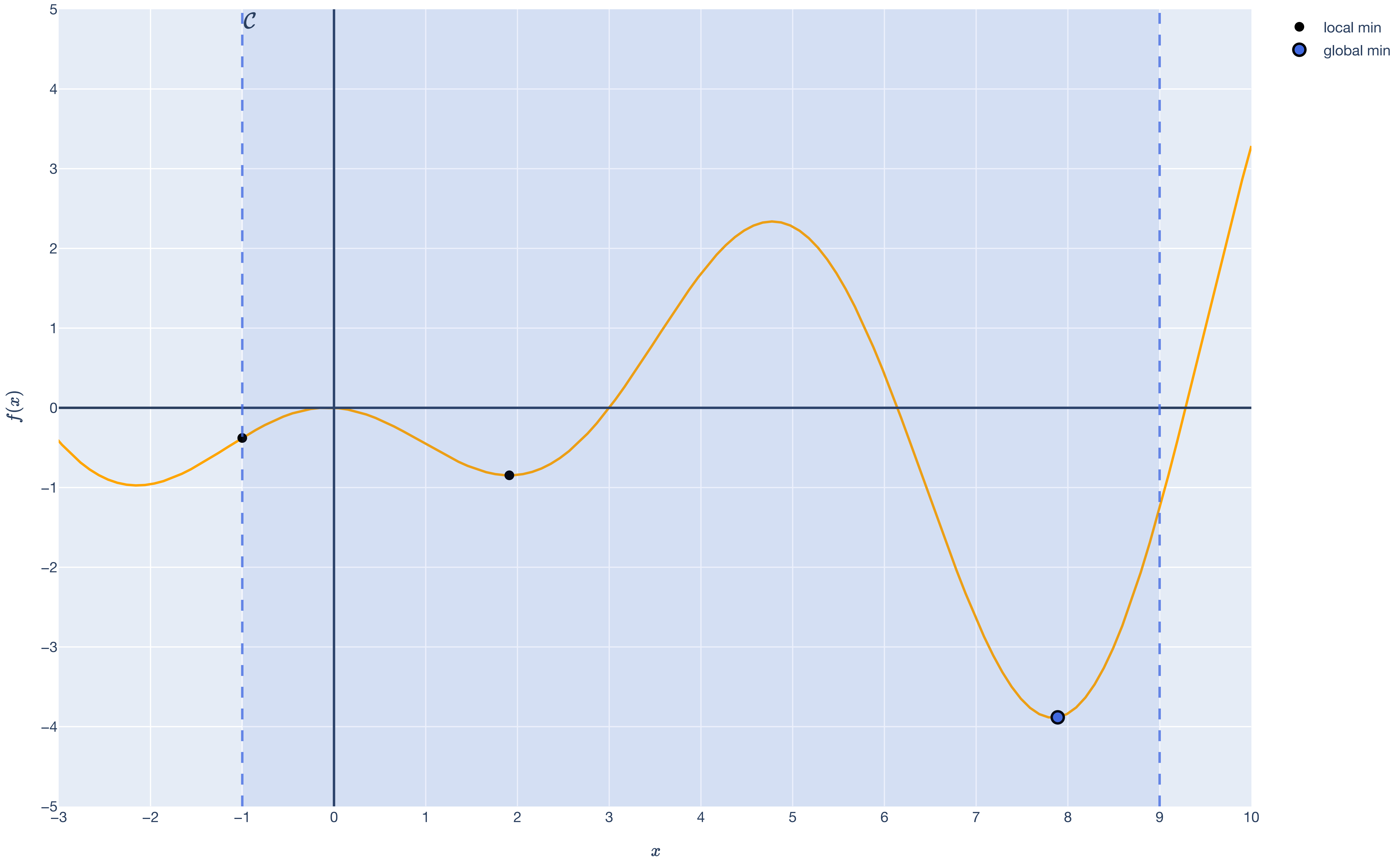
Let $S \subseteq \mathbb{R}^d$ be a set. A point $\mathbf{x} \in S$ is an ***interior point*** if there exists a neighborhood $B_\delta(\mathbf{x})$ around $\mathbf{x}$ such that $B_\delta(\mathbf{x}) \subset S$ (where $\subset$ is *proper subset*).

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

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

Types of Minima

Local and global minima



Types of Minima

Local and global minima

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

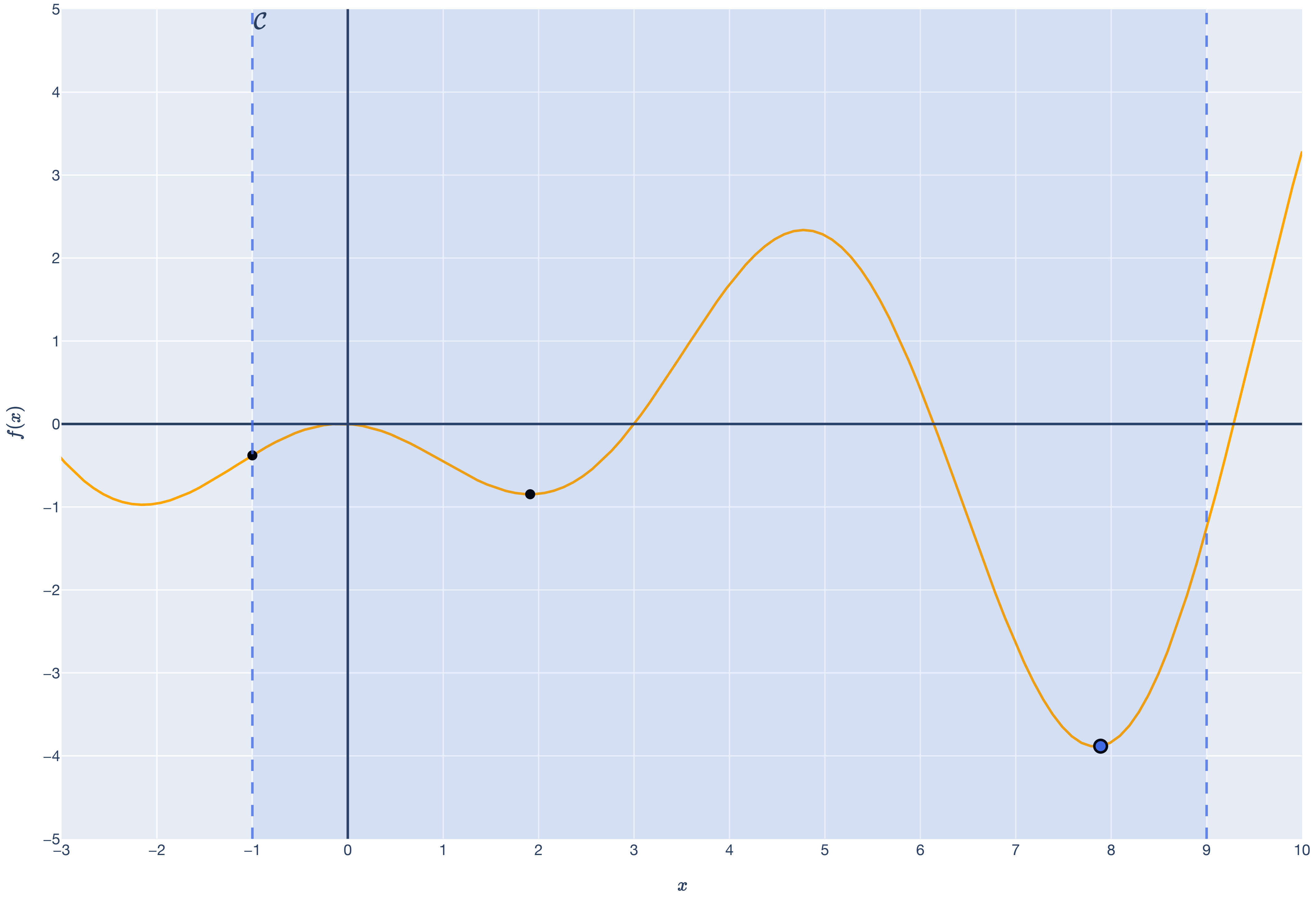
A point $\hat{\mathbf{x}} \in \mathscr{C}$ is a ***local minimum*** if there exists a neighborhood $B_\delta(\mathbf{x})$ around $\hat{\mathbf{x}}$ such that

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

We will also call this a ***constrained local minimum***.

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

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



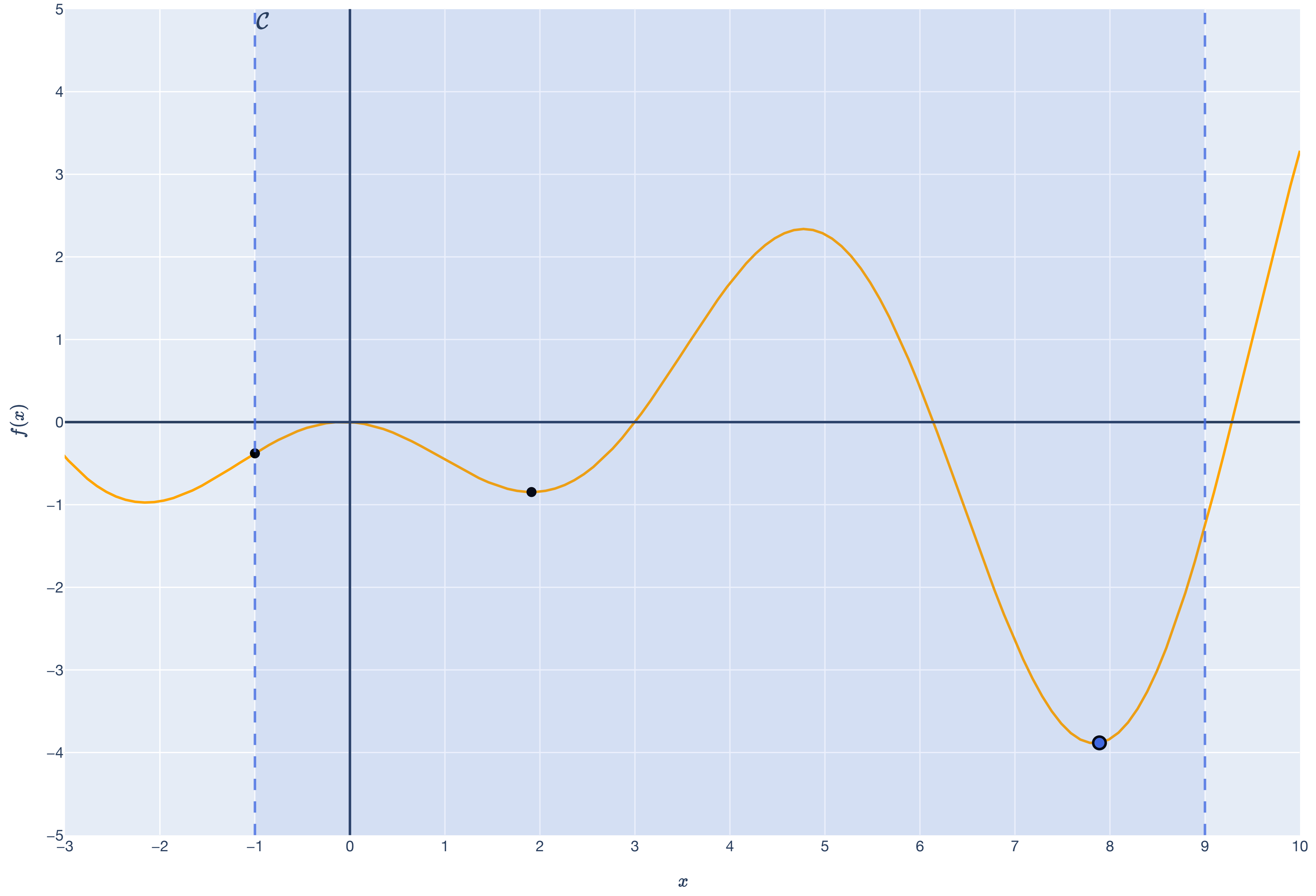
Types of Minima

Local and global minima

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

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

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



Types of Minima

Local and global minima

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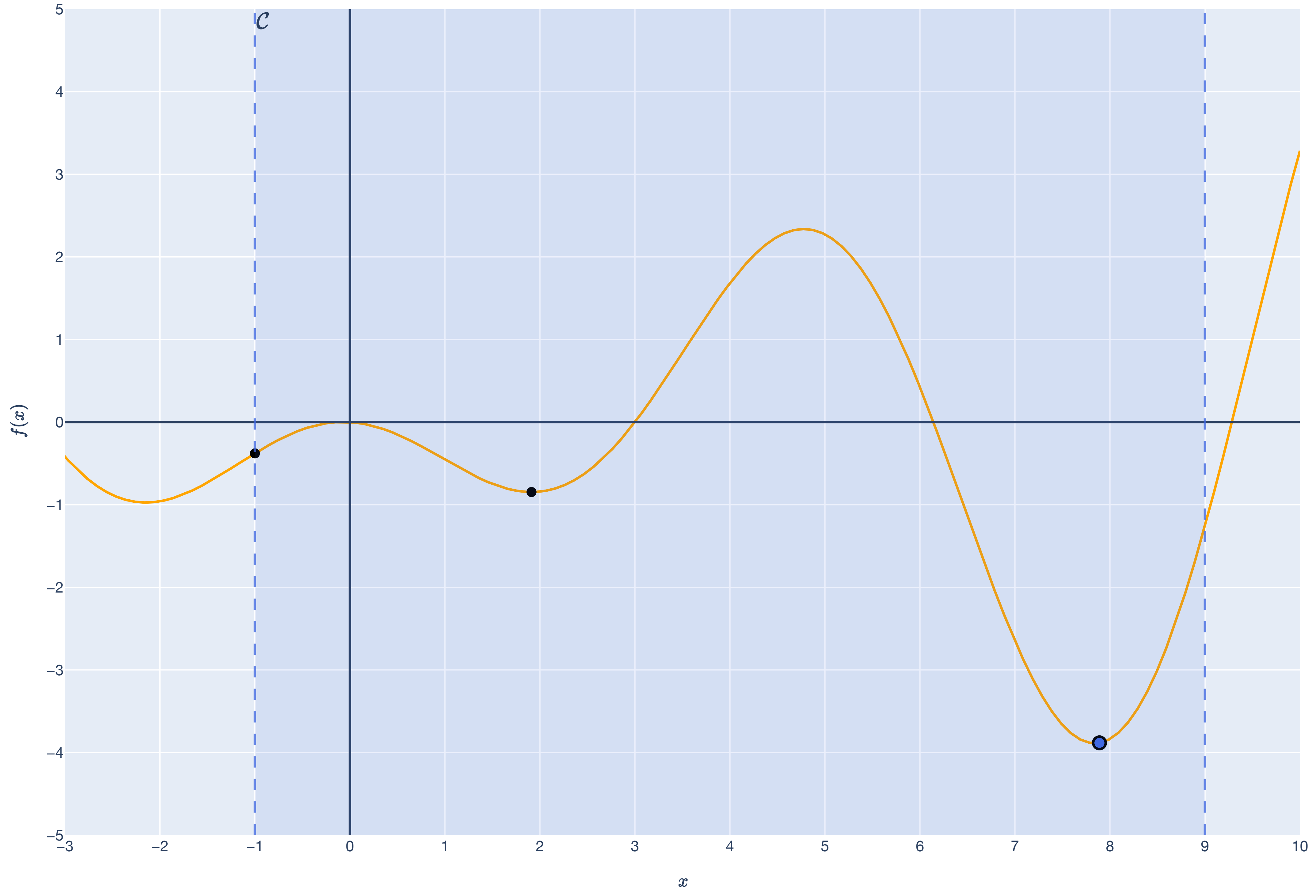
$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in B_\delta(\hat{\mathbf{x}}).$$

Unconstrained local minima are in the interior $\text{int}(\mathscr{C})$ of the constraint set.

On the other hand, *constrained local minima* can be on the “edge” of the constraint set.



Types of Minima

Which type of minima are each of these points?

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

constrained local:

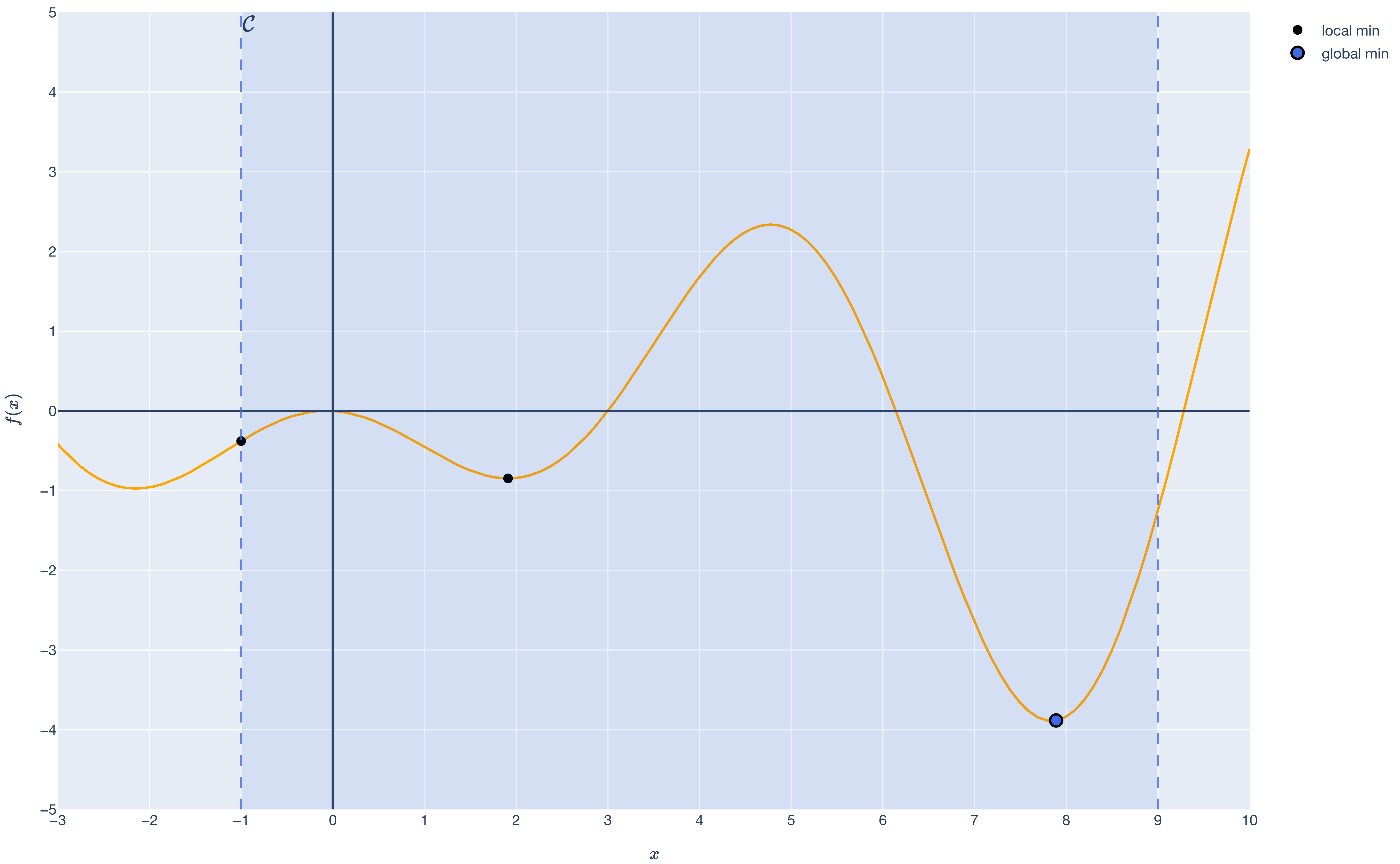
$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathscr{C} \cap B_\delta(\hat{\mathbf{x}})$$

unconstrained local:

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

global:

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

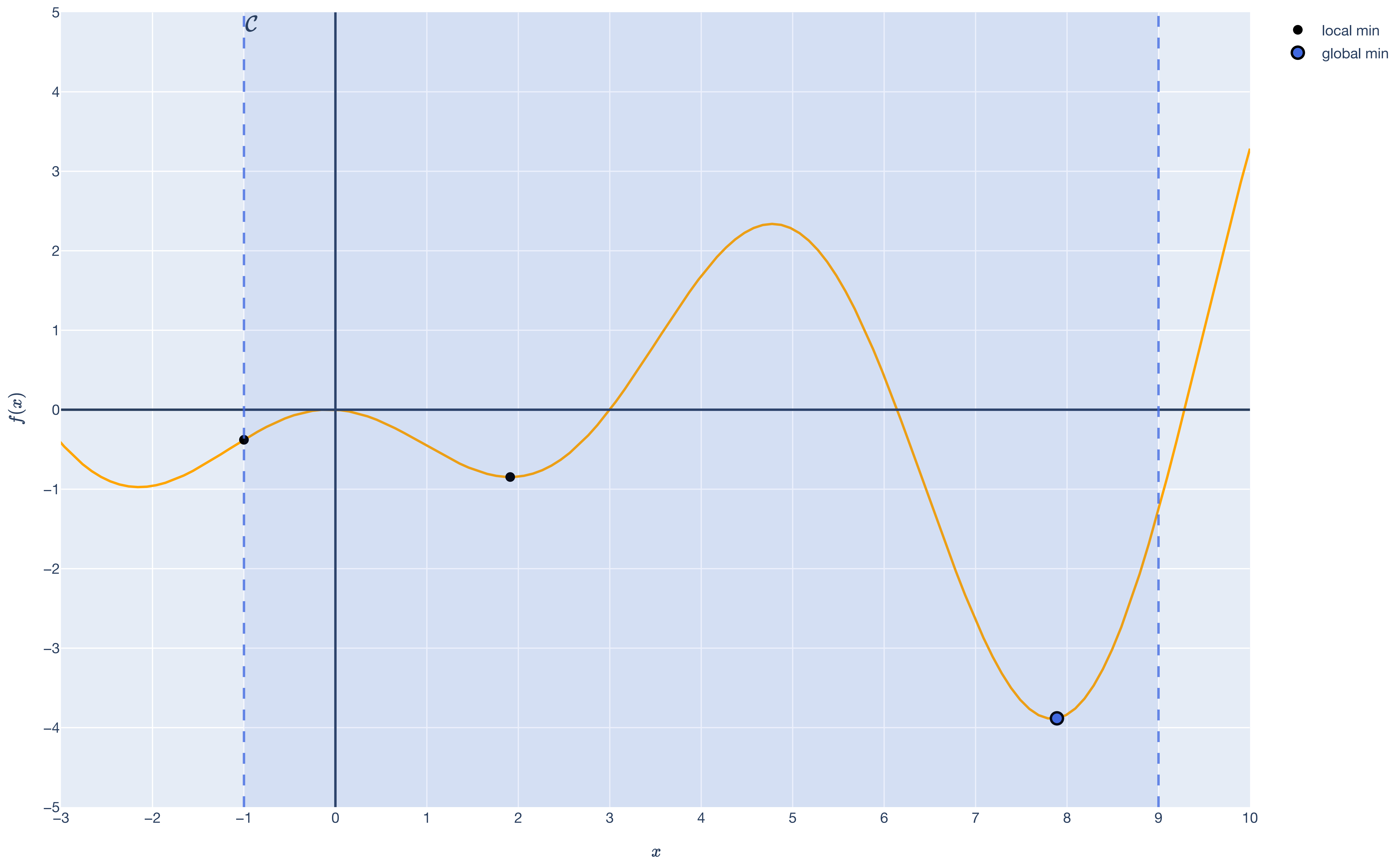


Types of Minima
Big picture

At the end of the day, 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 one of the *unconstrained local minima.*
>
> With $\mathscr{C}$, global minima may lie on the boundary of the constraint set.



Types of Minima
Big picture

At the end of the day, 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 one of the *unconstrained local minima.*
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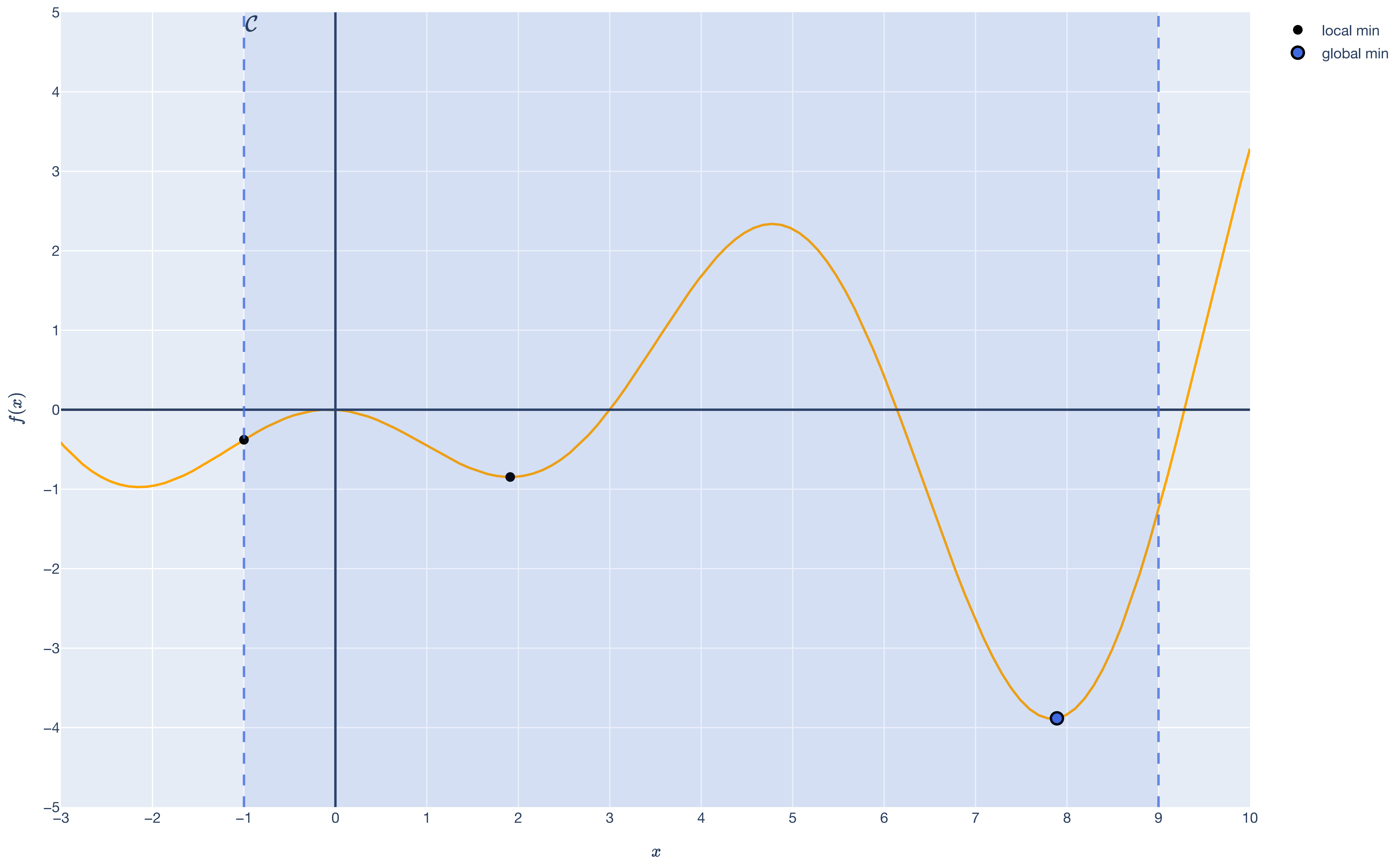
Strategy: Find all unconstrained and constrained local minima, then *test* for global minima.



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.

necessity: Your property cannot hold unless you assume this.

Example:

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

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

Unconstrained Minima

How do we find unconstrained minima?

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

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

From single-variable calculus:

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

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:*

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

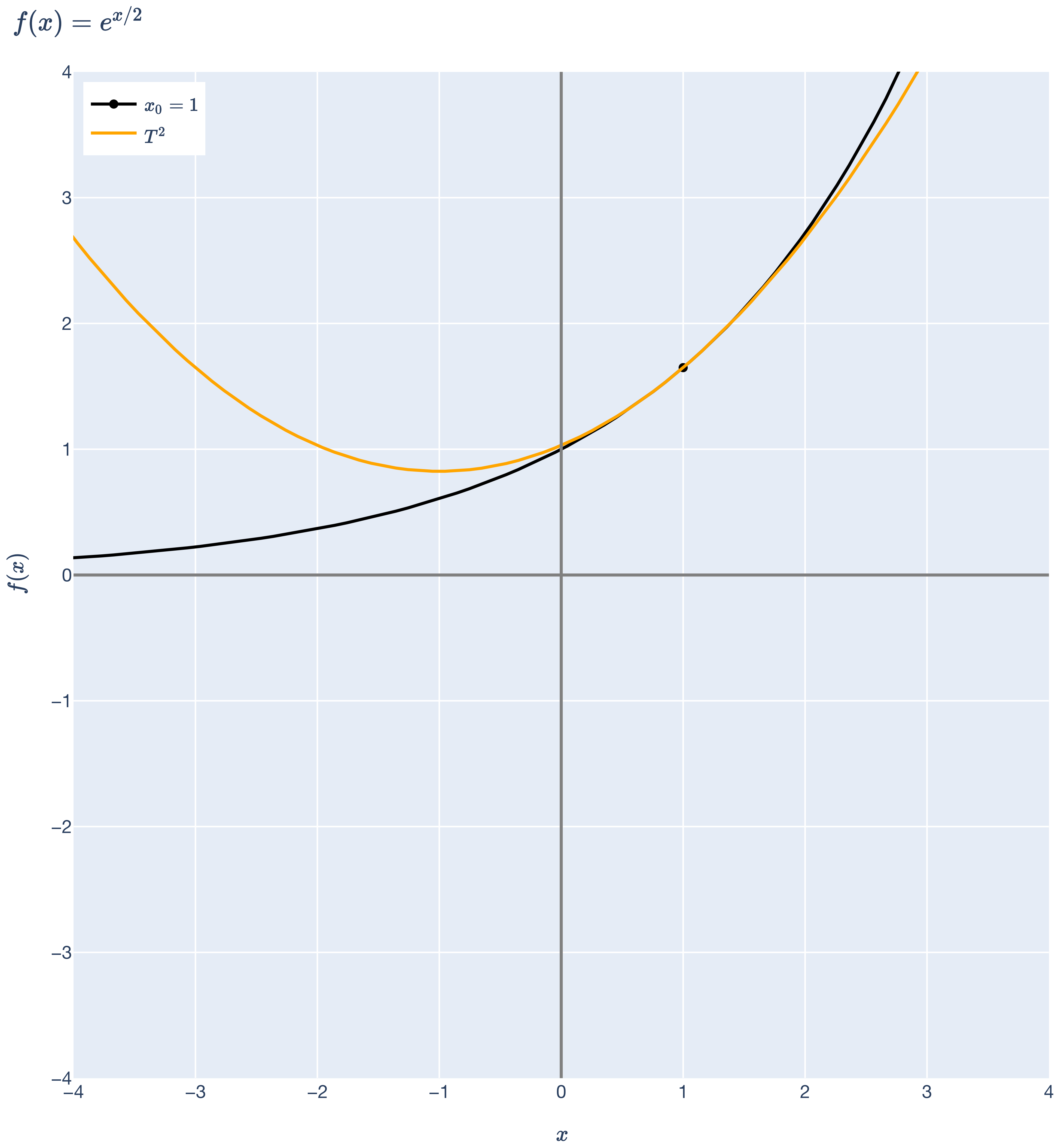
Second-order Taylor Approximation

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

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:*

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

Pretend that this function approximation is exact. Then…

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

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

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:*

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

Pretend that this function approximation is exact. Then…

What are the *necessary* conditions for x to be a minimum? $f'(x) = 0, f''(x) \geq 0.$

What are the *sufficient* conditions for x to be a minimum? $f'(x) = 0, f''(x) > 0.$

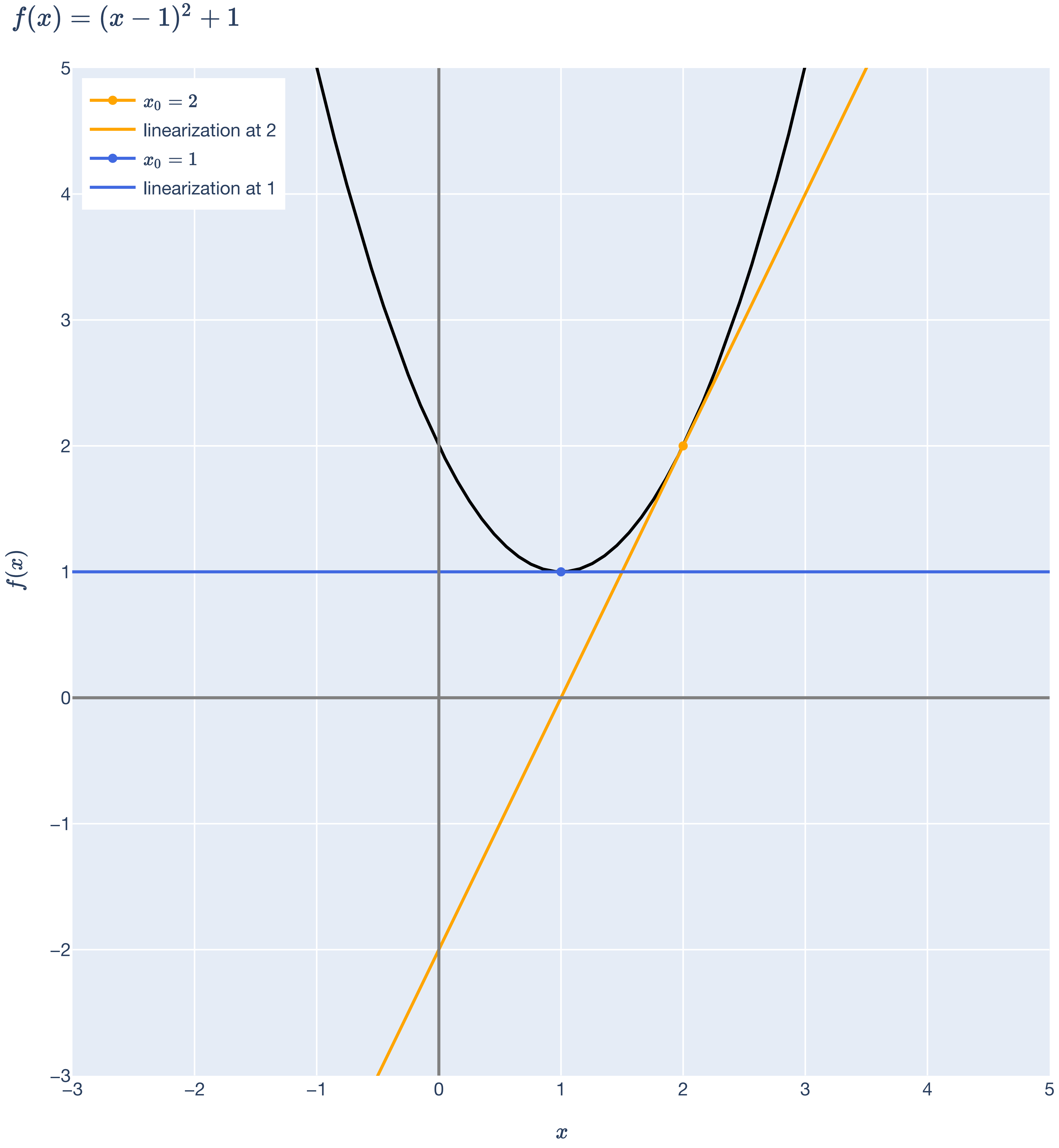
Unconstrained Minima

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



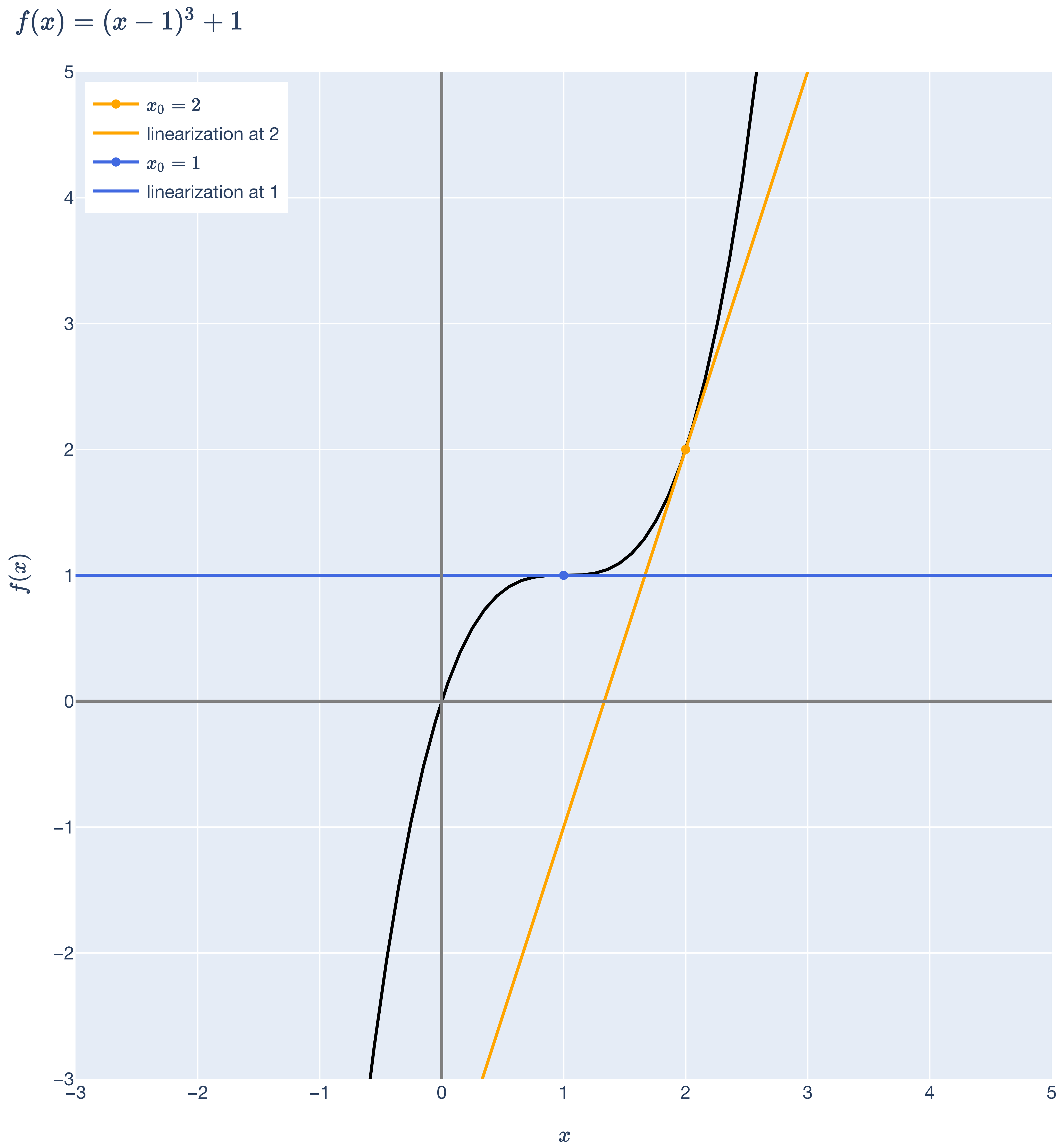
Unconstrained Minima

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

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



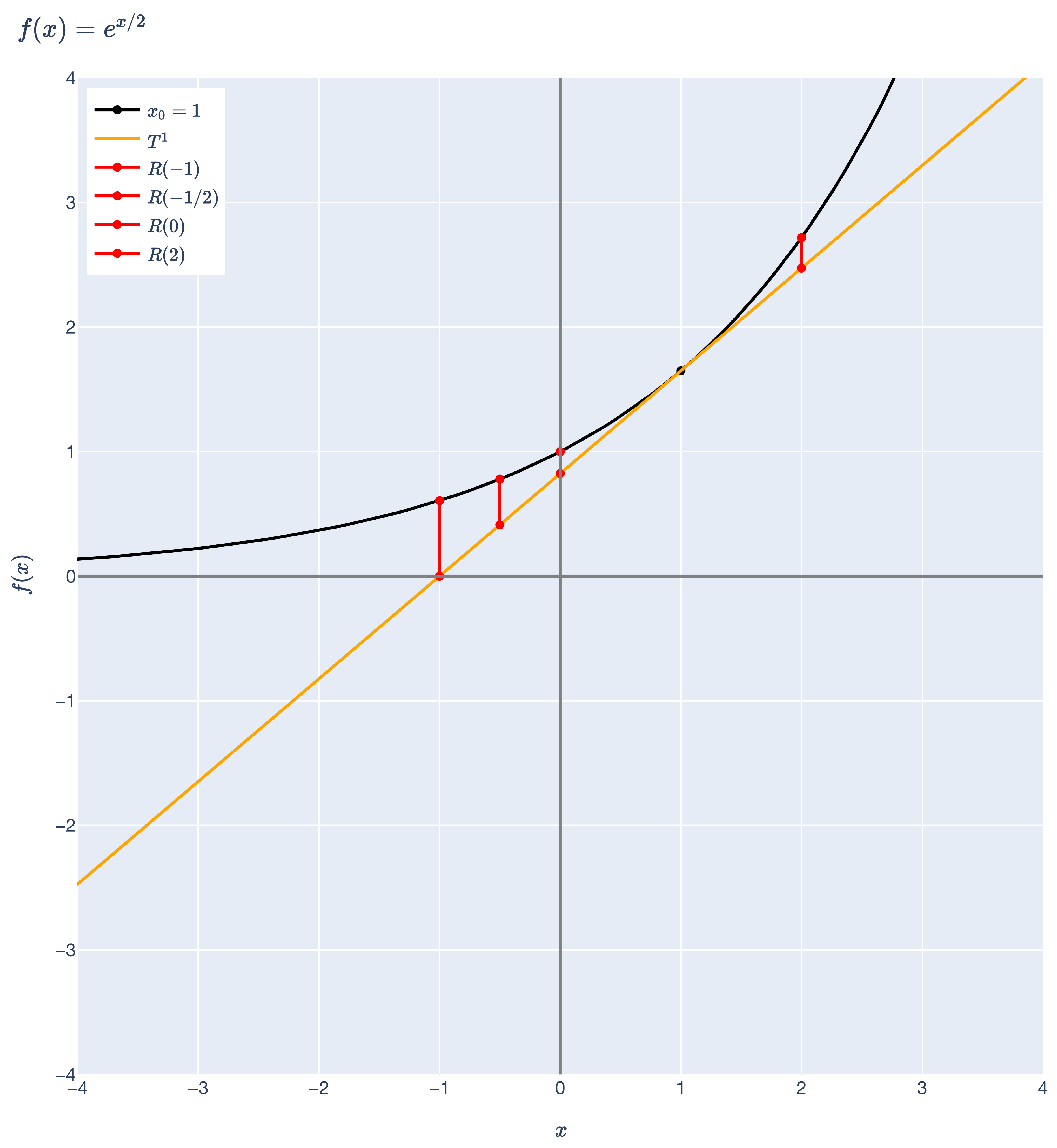
Remainder of Taylor Polynomial

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 $\mathbf{x}_0$).



Taylor's Theorem

Remainder Theorem 1: Peano's Form Taylor's Theorem

Theorem (2nd Order Taylor's Theorem: Peano's Form). Let $f : \mathbb{R}^d \to \mathbb{R}$ be a twice differentiable function at $\mathbf{x}_0$. Then, for every direction $\mathbf{d} \in \mathbb{R}^d$:

$$f(\mathbf{x}_0 + \mathbf{d}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{d} + \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}_0)\mathbf{d} + o(\|\mathbf{d}\|^2)\,.$$

The remainder is

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

and the claim is that $R^2(\mathbf{x}_0 + \mathbf{d}) = o(\|\mathbf{d}\|^2)$, meaning that $\lim_{\mathbf{d}\to\mathbf{0}} R^2(\mathbf{x}_0 + \mathbf{d})/\|\mathbf{d}\|^2 = 0$.

Taylor's Theorem

Remainder Theorem 1: Peano's Form Taylor's Theorem

What does $R^2(\mathbf{x}_0 + \mathbf{d}) = o(\|\mathbf{d}\|^2)$ mean?

For every $C > 0$, there exists a neighborhood $B_\delta(\mathbf{0})$ such that

$$R^2(\mathbf{x}_0 + \mathbf{d}) \;\; \leq C\|\mathbf{d}\|^2, \quad \forall \mathbf{d} \in B_\delta(\mathbf{0})\,.$$

We can make the remainder term as *small as we like* as long as $\|\mathbf{d}\|$ is sufficiently small ($\|\mathbf{d}\| < \delta$ does the trick).

Taylor’s Theorem

Remainder Theorem 1: Peano’s Form Taylor’s Theorem

What does $R^2(\mathbf{x}_0 + \mathbf{d}) = o(\|\mathbf{d}\|^2)$ mean?

Let $\mathbf{d} \in \mathbb{R}^d$ be a unit vector with $\|\mathbf{d}\| = 1$ and $\alpha > 0$ be a scalar, so:

$$o(\|\alpha\mathbf{d}\|^2) = o(\alpha^2).$$

Then, $R^2(\mathbf{x}_0 + \alpha\mathbf{d}) = o(\alpha^2)$ means:

$$\lim_{\alpha \to 0} \frac{R^2(\mathbf{x}_0 + \alpha\mathbf{d})}{\alpha^2} = 0$$

(the remainder goes to 0 *faster* than a quadratic).

Taylor's Theorem

Remainder Theorem 1: Peano's Form Taylor's Theorem

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

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

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

Unconstrained local minima

Necessary conditions

Least Squares

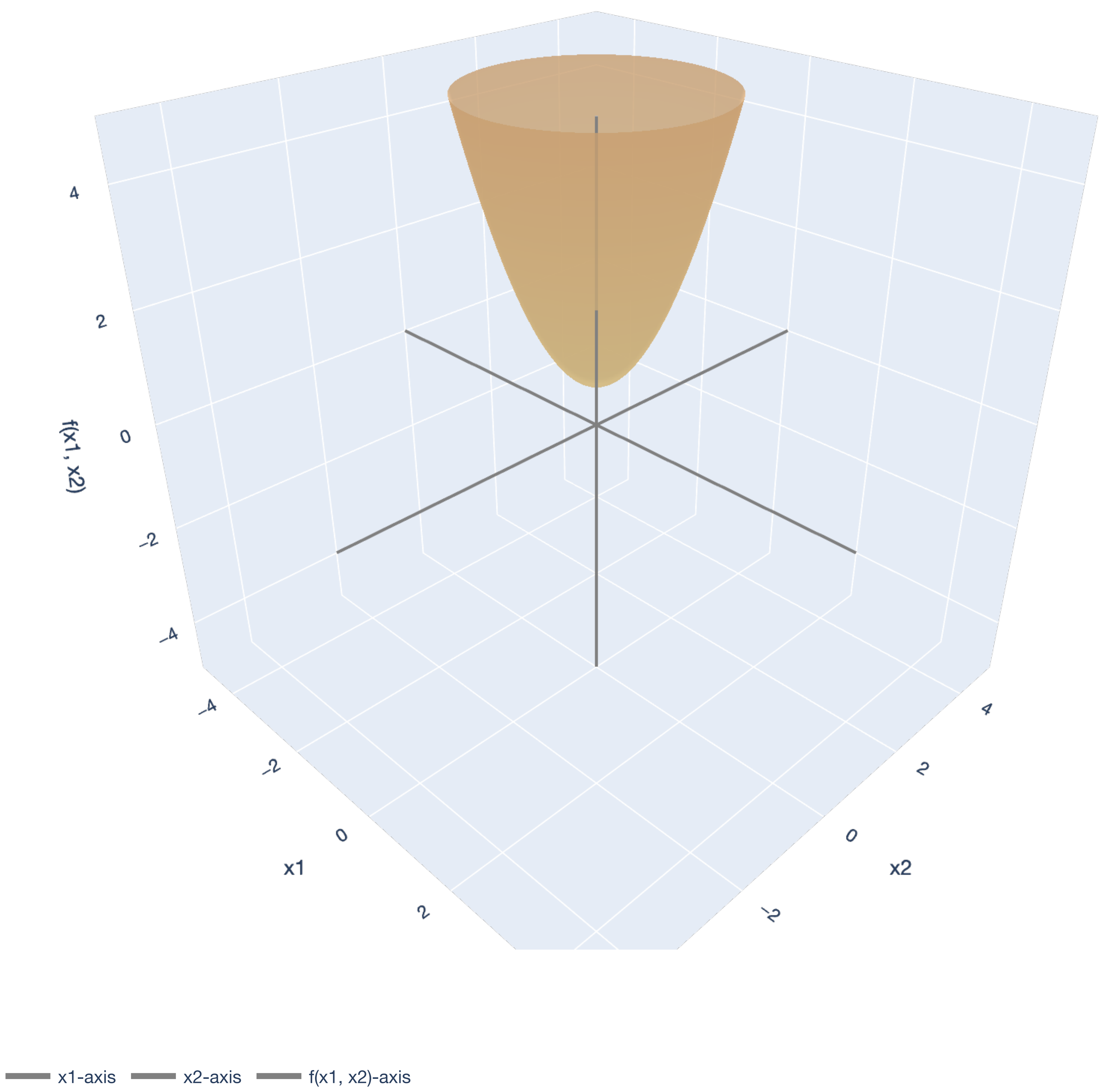
OLS Theorem

<u>**Proof (OLS).**</u>

"First derivative test." Take the gradient.

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

Set it equal to $\mathbf{0}$.



Least Squares

OLS Theorem

<u>**Proof (OLS).**</u>

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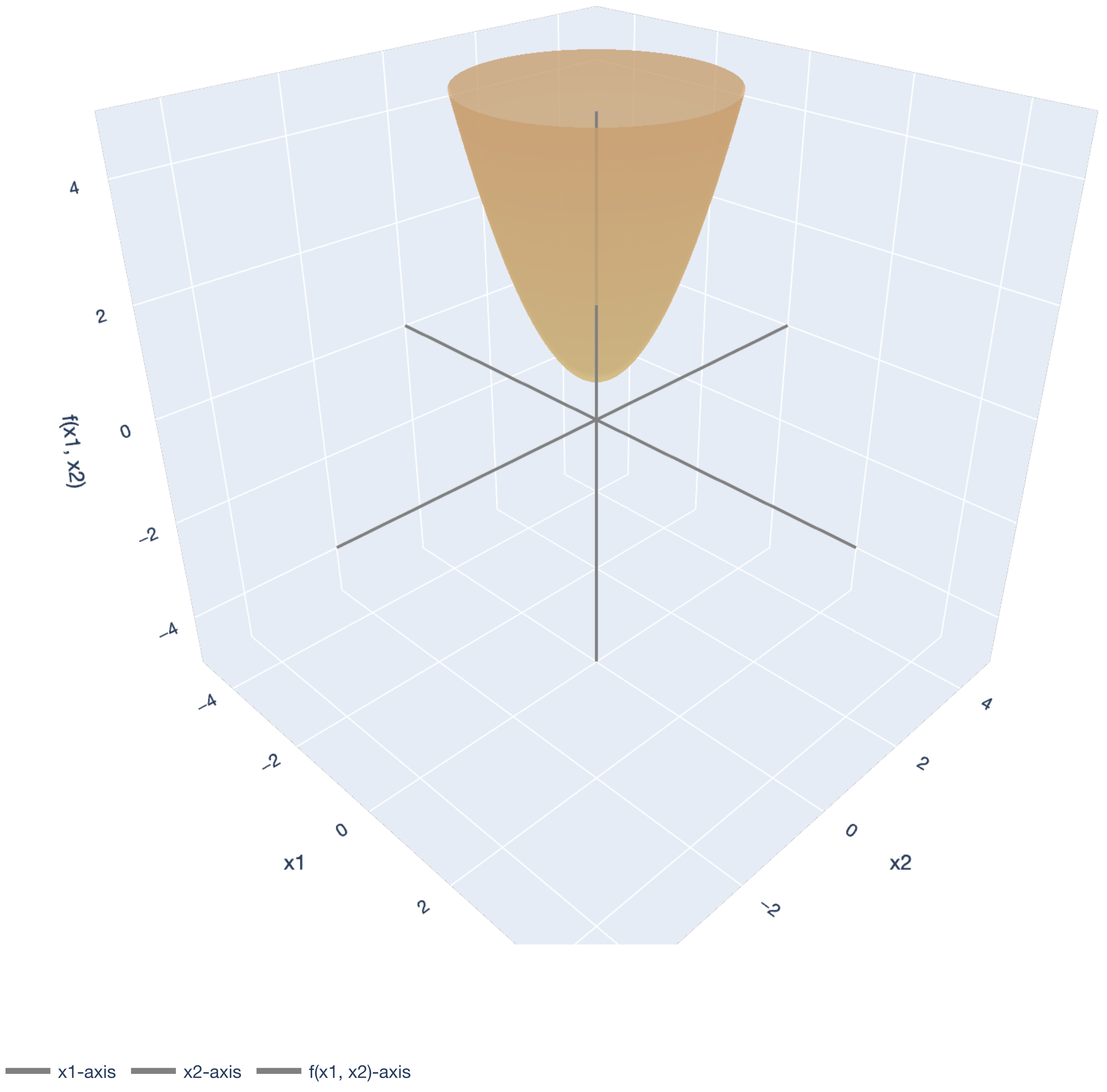
Set it equal to $\mathbf{0}$.

Why is this the right thing to do?



Taylor's Theorem

Remainder Theorem 1: Peano's Form Taylor's Theorem

For all intents and purposes,

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \frac{1}{2}f''(x_0)\delta^2 \text{ when } \delta \text{ is small enough.}$$

is analogous to:

$$f(\mathbf{x}_0 + \mathbf{d}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{d} + \frac{1}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}_0)\mathbf{d} \text{ when } \|\mathbf{d}\| \text{ is small enough.}$$

Unconstrained Minima

Necessary conditions

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

when δ is small enough.

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

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

Necessary conditions:

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

Necessary conditions:

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

Total Derivative

Review of definition

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a function and let $\mathbf{x}_0 \in \mathbb{R}^d$ be a point. If there exists a gradient vector $\nabla f(\mathbf{x}_0) \in \mathbb{R}^d$ such that

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

then f is ***differentiable*** *at* $\mathbf{x}_0$ and has the ***(total) derivative*** $\nabla f(\mathbf{x}_0)$.

Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum). Consider the optimization problem

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

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 necessary conditions

First order condition

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

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

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:

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

Proof of necessary conditions

First order condition

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

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

From Step 1,

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

$\mathbf{x}^*$ 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),

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

Proof of necessary conditions

First order condition

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

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

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 $\|\mathbf{d}\| = 1$.

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

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

$$\vdots$$

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

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

Proof of necessary conditions

Second order condition

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

Step 1: Use second-order Taylor's theorem with $\alpha\mathbf{d} \in \mathbb{R}^d$ with $\|\mathbf{d}\| = 1$.

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. By Taylor's Theorem (Peano's form):

$$
\begin{aligned}
f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*) &= \nabla f(\mathbf{x}^*)^\top(\alpha\mathbf{d}) + \frac{1}{2}(\alpha\mathbf{d})^\top \nabla^2 f(\mathbf{x}^*)(\alpha\mathbf{d}) + o(\|\alpha\mathbf{d}\|^2) \\
&= \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} + o(\alpha^2)
\end{aligned}
$$

Proof of necessary conditions

Second order condition

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

Step 2: Use first-order condition on difference $f(\mathbf{x}^* + \alpha\mathbf{d}) - f(\mathbf{x}^*)$.

From Step 1,

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

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

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

Proof of necessary conditions

Second order condition

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

Step 3: Take $\alpha \to 0$ to get rid of the little-oh terms.

From Step 3,

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

Recall that if $g = o(h)$, then $\lim_{\alpha \to 0} \frac{g(\alpha)}{h(\alpha)} = 0$.

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

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

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

Least Squares

OLS Theorem

Proof (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." Take the gradient.

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

Set it equal to $\mathbf{0}$.

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

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

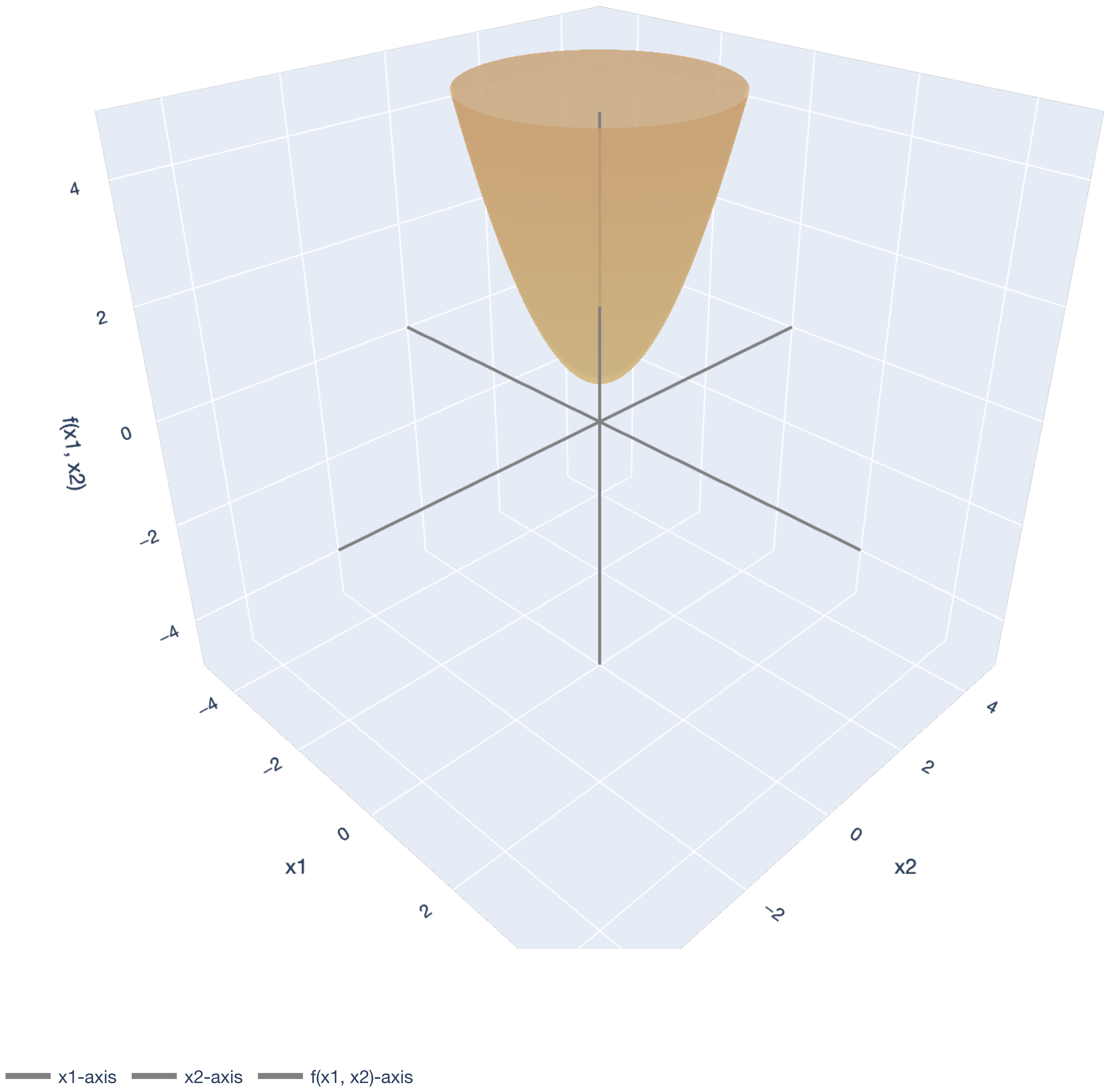
$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." Take the *Hessian* of $f(\mathbf{w})$.

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

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

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



Unconstrained local minima

Sufficient conditions

Least Squares

OLS Theorem

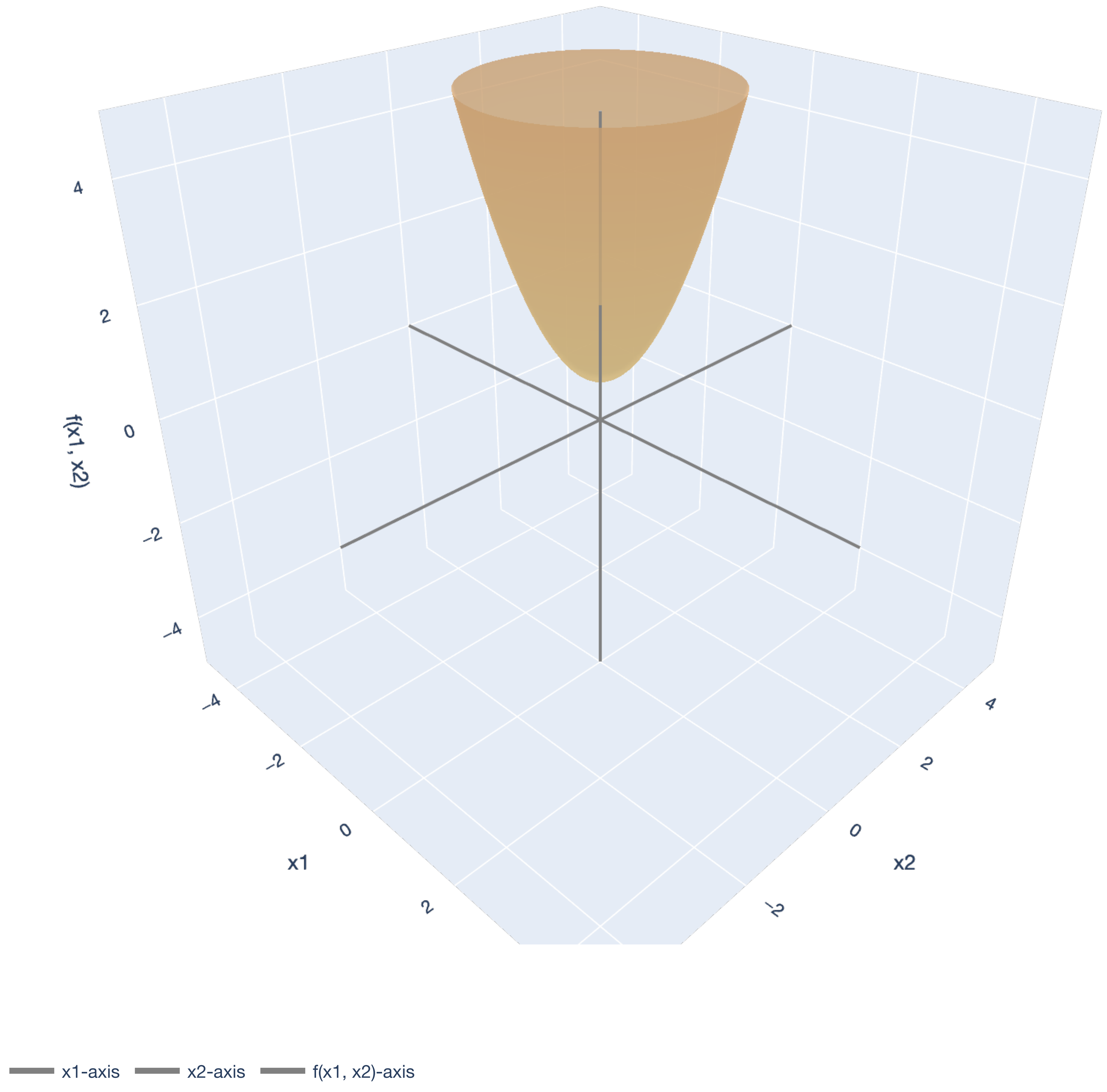
<u>Proof (OLS).</u>

"Second derivative test." Take the *Hessian* of $f(\mathbf{w})$.

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

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

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



Least Squares

OLS Theorem

<u>Proof (OLS).</u>

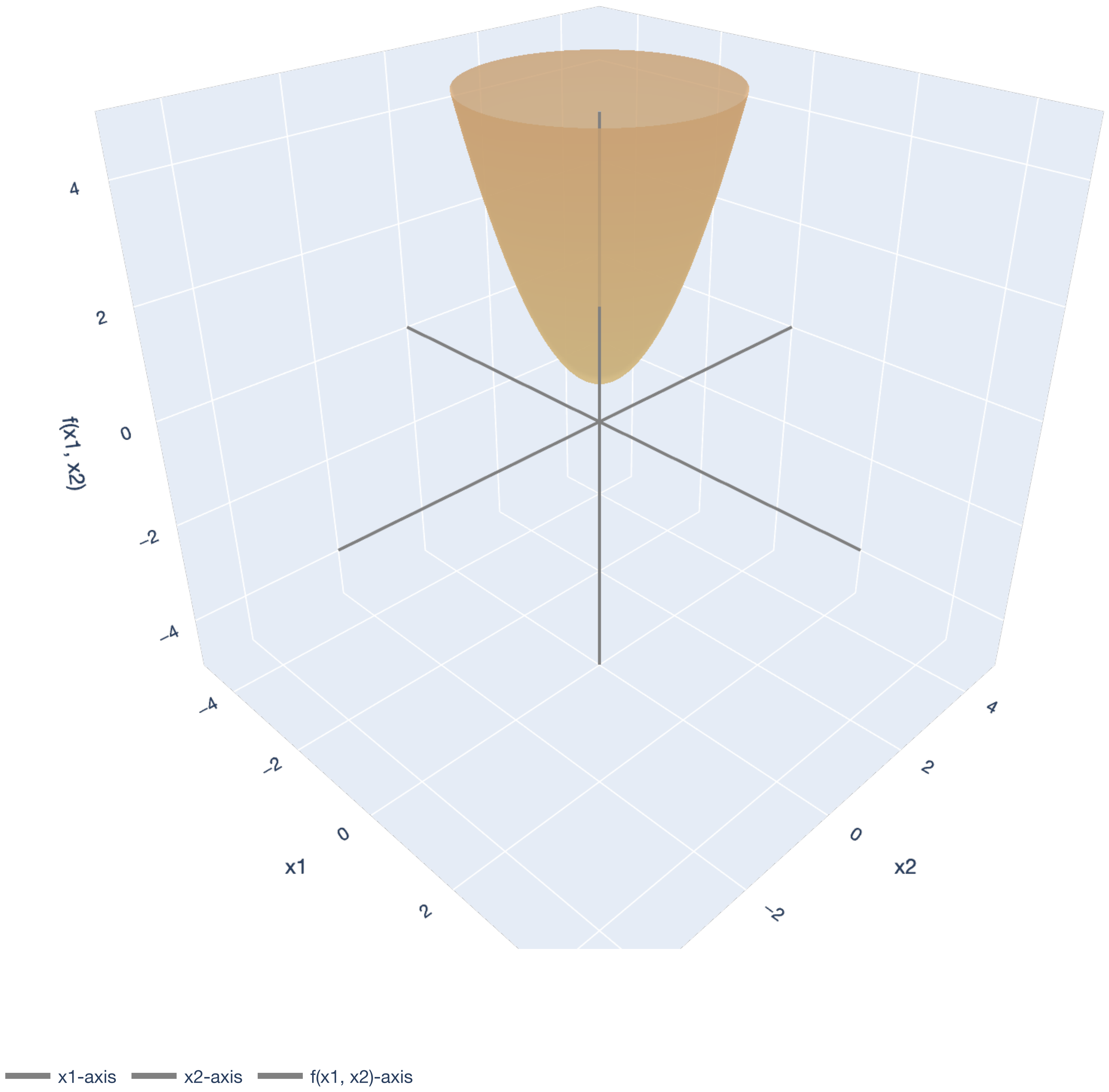
"Second derivative test." Take the *Hessian* of $f(\mathbf{w})$.

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

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

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

Why is this the right thing to do?



Unconstrained Minima

Sufficient conditions

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

when δ is small enough.

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

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

Sufficient conditions:

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

Sufficient 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).
Consider the optimization problem

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

Let $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$. If $f \in \mathscr{C}^2$ within a neighborhood $N_\delta(\mathbf{x}^*)$ of $\mathbf{x}^*$ 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 sufficient conditions

Second order condition

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

Step 1: Use second-order Taylor's theorem with $\alpha\mathbf{d} \in \mathbb{R}^d$ with $\|\mathbf{d}\| = 1$.

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. By Taylor's Theorem (Peano's form):

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

$$= \alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} + \frac{\alpha^2}{2}\mathbf{d}^\top \nabla^2 f(\mathbf{x}^*)\mathbf{d} + o(\alpha^2)$$

Proof of sufficient conditions

Second order condition

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

Step 2: $\nabla^2 f(\mathbf{x}^*)$ is positive definite, so its eigenvalues are all positive.

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

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

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 sufficient conditions

Second order condition

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

Step 3: We chose $\mathbf{d}$ arbitrarily, so the first-order term can be non-negative.

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

Because $\mathbf{d}$ is an arbitrary direction (could be negative or positive), $\alpha \nabla f(\mathbf{x}^*)^\top \mathbf{d} \geq 0$, and

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

Proof of sufficient conditions

Second order condition

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

Step 4: If α is small enough, then $o(\alpha^2)/\alpha^2$ can be as small as we like.

From Step 3,

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

For any $C > 0$, we can choose α small enough so $\left|\frac{o(\alpha^2)}{\alpha^2}\right| \leq C$.

Let's make $\left|\frac{o(\alpha^2)}{\alpha^2}\right|$ smaller than $C = \frac{\lambda}{4}$. Then, for any $\alpha > 0$ sufficiently small,

$$f(\mathbf{x}^* + \alpha\mathbf{d}) \geq f(\mathbf{x}^*) + \frac{\lambda}{4}\alpha^2 > f(\mathbf{x}^*).$$

Least Squares

OLS Theorem

Proof (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." Take the gradient.

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

Set it equal to $\mathbf{0}$.

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

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

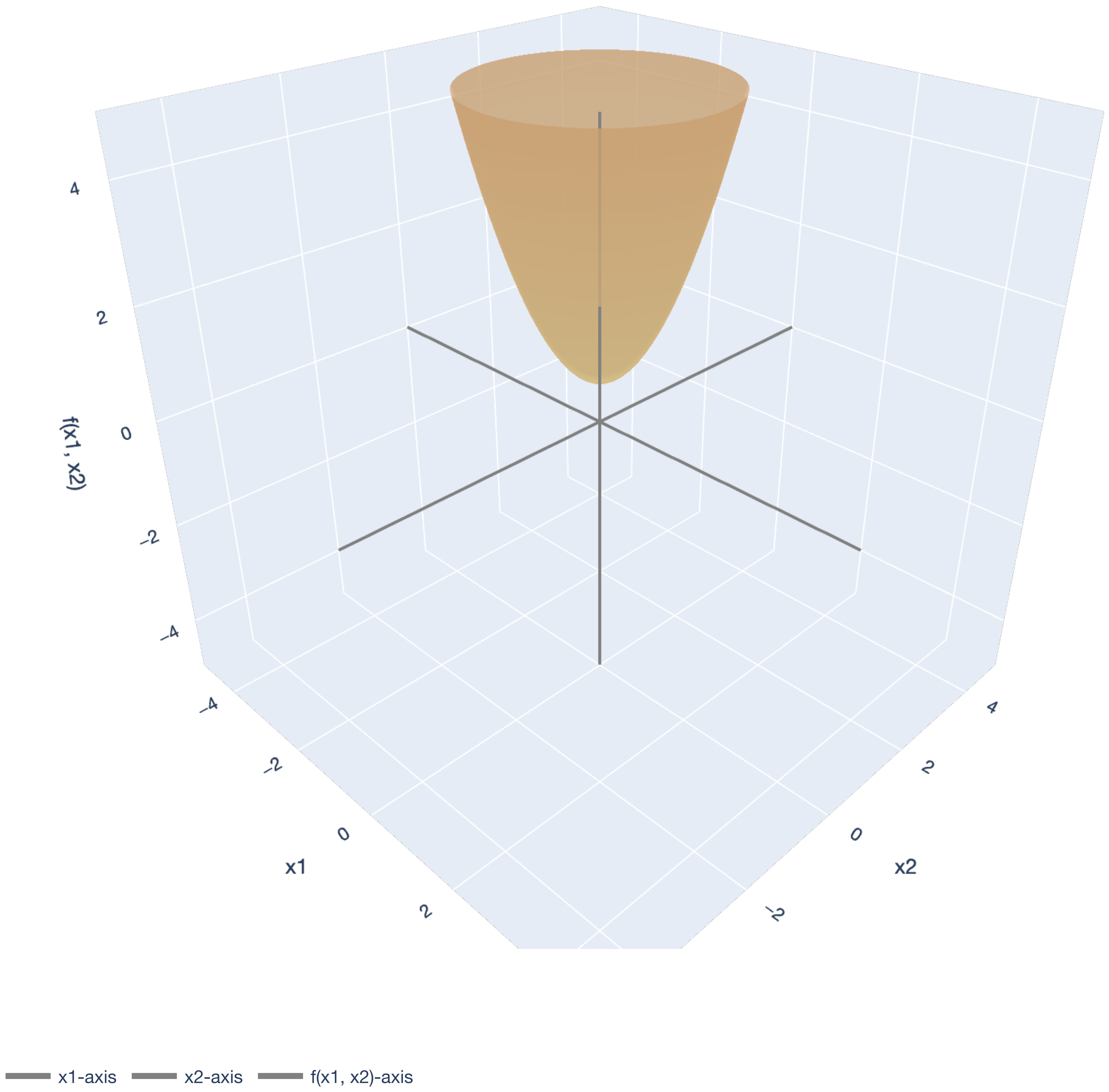
$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

"Second derivative test." Take the *Hessian* of $f(\mathbf{w})$.

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

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

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



Finding global minima

Introducing constraint sets

Types of Minima

Big picture

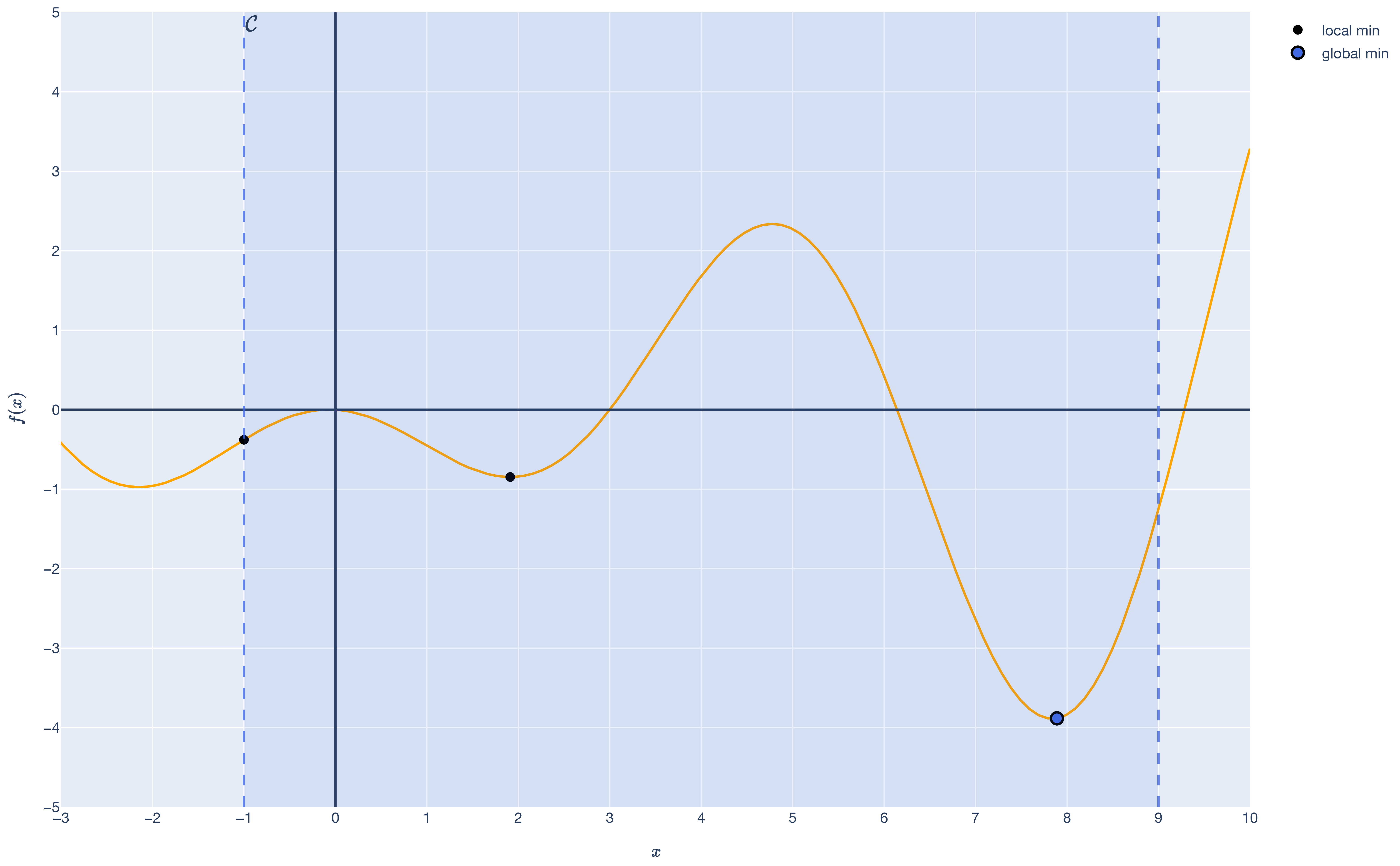
At the end of the day, we want to find ***global minima***.

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

Without $\mathscr{C}$, global minima are just one of the *unconstrained local minima.*

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

Strategy: Find all unconstrained and constrained local minima, then *test* for global minima.



Unconstrained Minima

Necessary conditions

Theorem (Necessary Conditions for Unconstrained Local Minimum). Consider the optimization problem

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

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 $\mathbf{v} \in \mathbb{R}^d$.

Note: *These necessary conditions only apply to* $\mathbf{x}^* \in \operatorname{int}(\mathscr{C})$*!*

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 the set of possible *unconstrained local minima* from the 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 $\mathbf{x} \in M \cup B$ and see which one is smallest.

Finding global minima

Using necessary conditions with constraints

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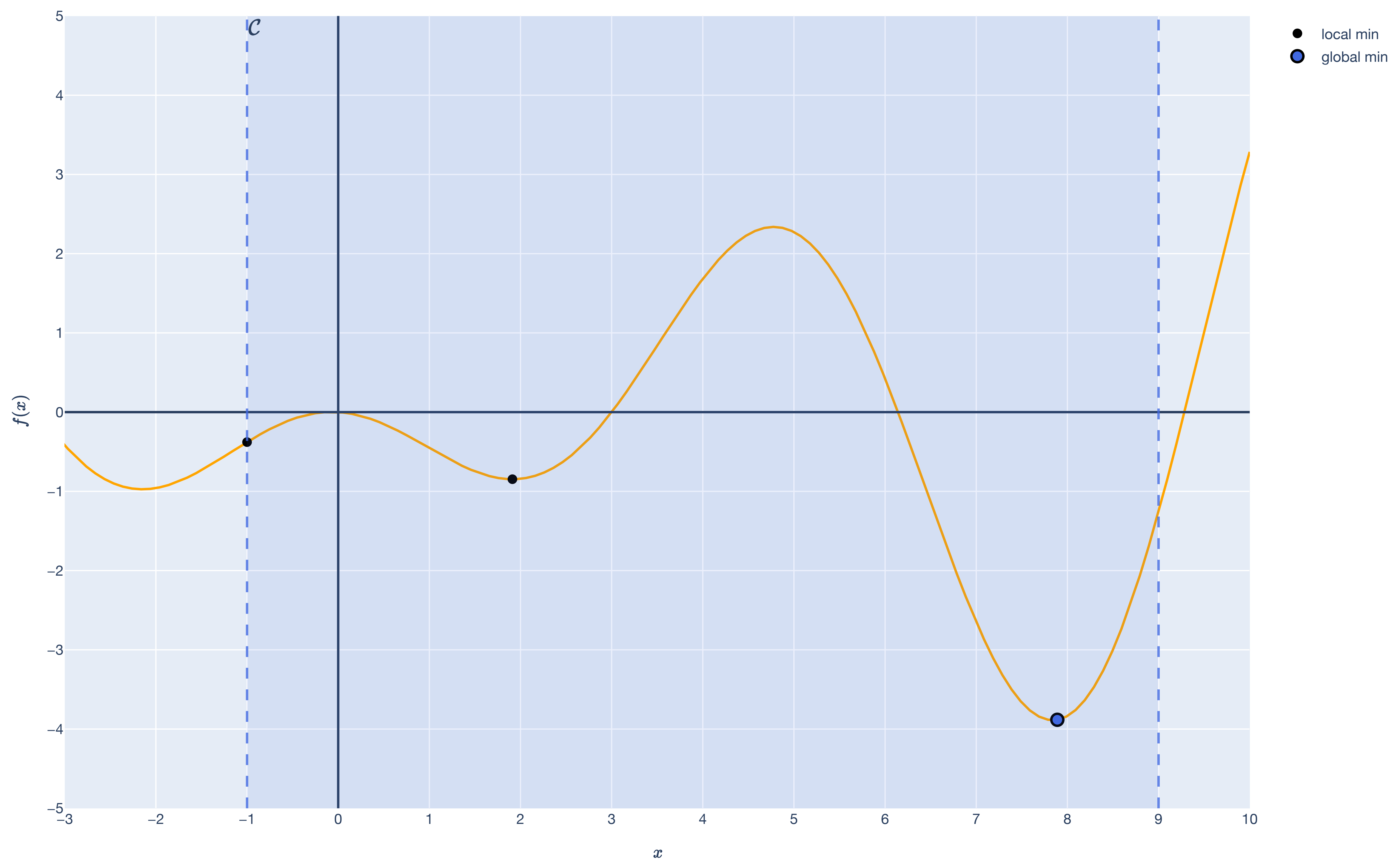

Finding global minima

Using necessary conditions without constraints

Necessary conditions for unconstrained local minima:

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

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

1. Find the set of possible *unconstrained local minima* from the first-order condition $M := \{\mathbf{x}^* \in \mathrm{int}(\mathscr{C}) : \nabla f(\mathbf{x}^*) = \mathbf{0}\} = \{\mathbf{x}^* \in \mathbb{R}^d : \nabla f(\mathbf{x}^*) = \mathbf{0}\}$.

2. There are no boundary points!

3. The global minimum must be in the set M, so evaluate f on all $\mathbf{x} \in M$ and see which one is smallest.

Finding global minima

Using necessary conditions without constraints

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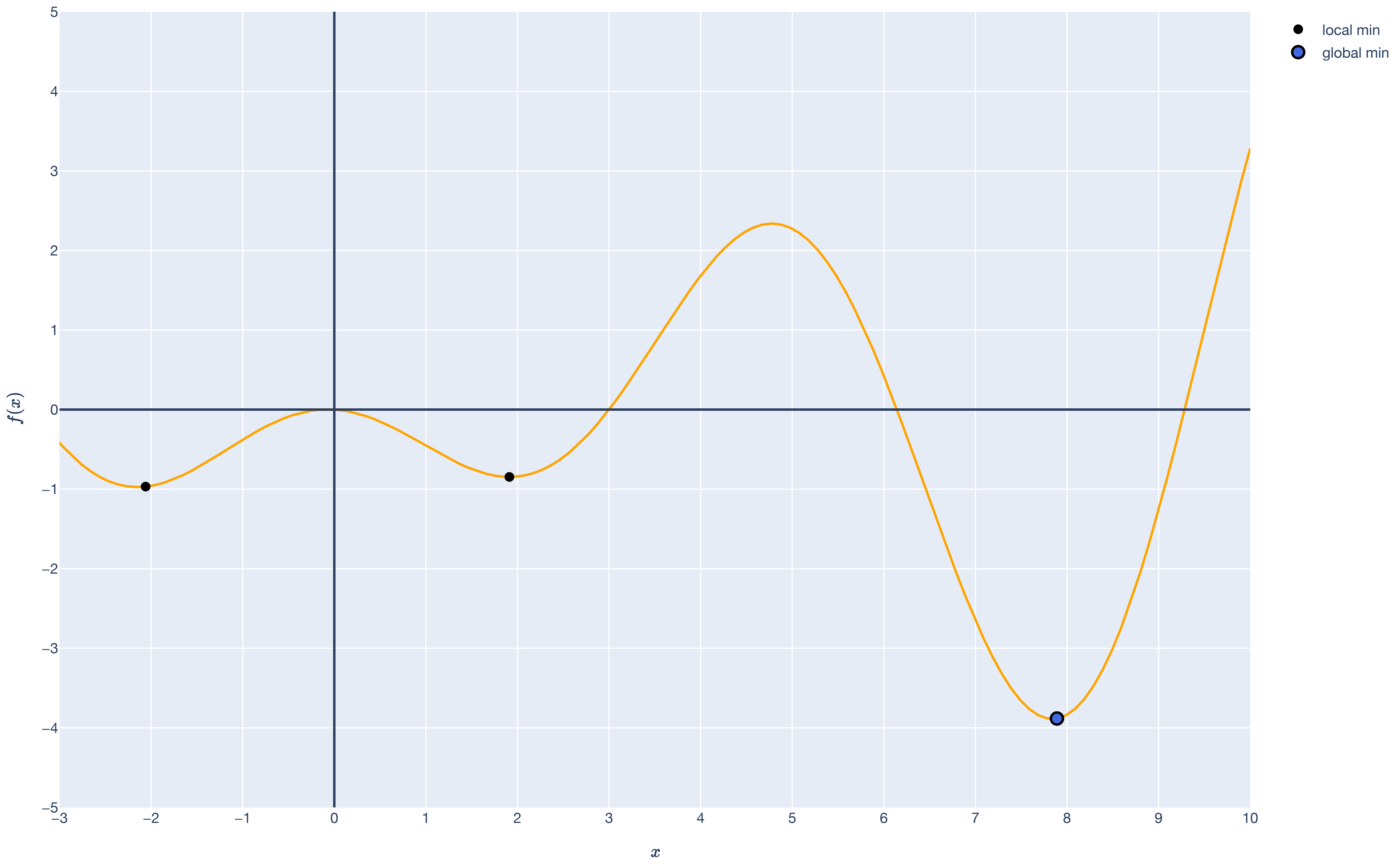


Unconstrained Minima

Example

Consider the one-dimensional optimization problem

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

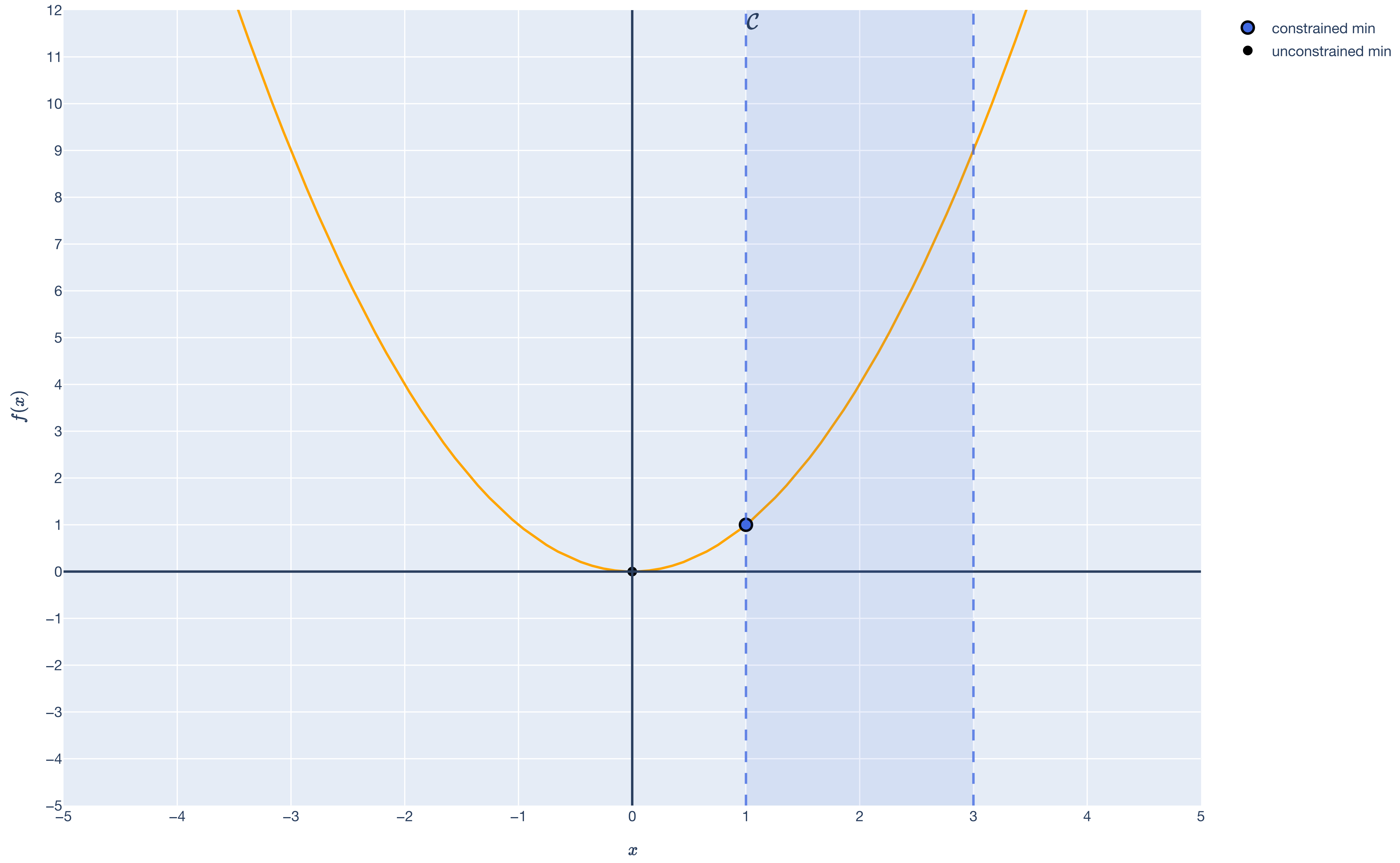
In general, this works for any one-dimensional problem where $f : \mathbb{R} \to \mathbb{R}$ is continuous on $\mathscr{C} = [a, b]$ and differentiable on $\operatorname{int}(\mathscr{C}) := (a, b)$.

Unconstrained Minima

Example

Consider the one-dimensional optimization problem

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



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Unconstrained Minima

Example: Why haven't we solved optimization?

Consider the two-dimensional optimization problem

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

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

This isn't feasible, so the question is:

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

Unconstrained Minima

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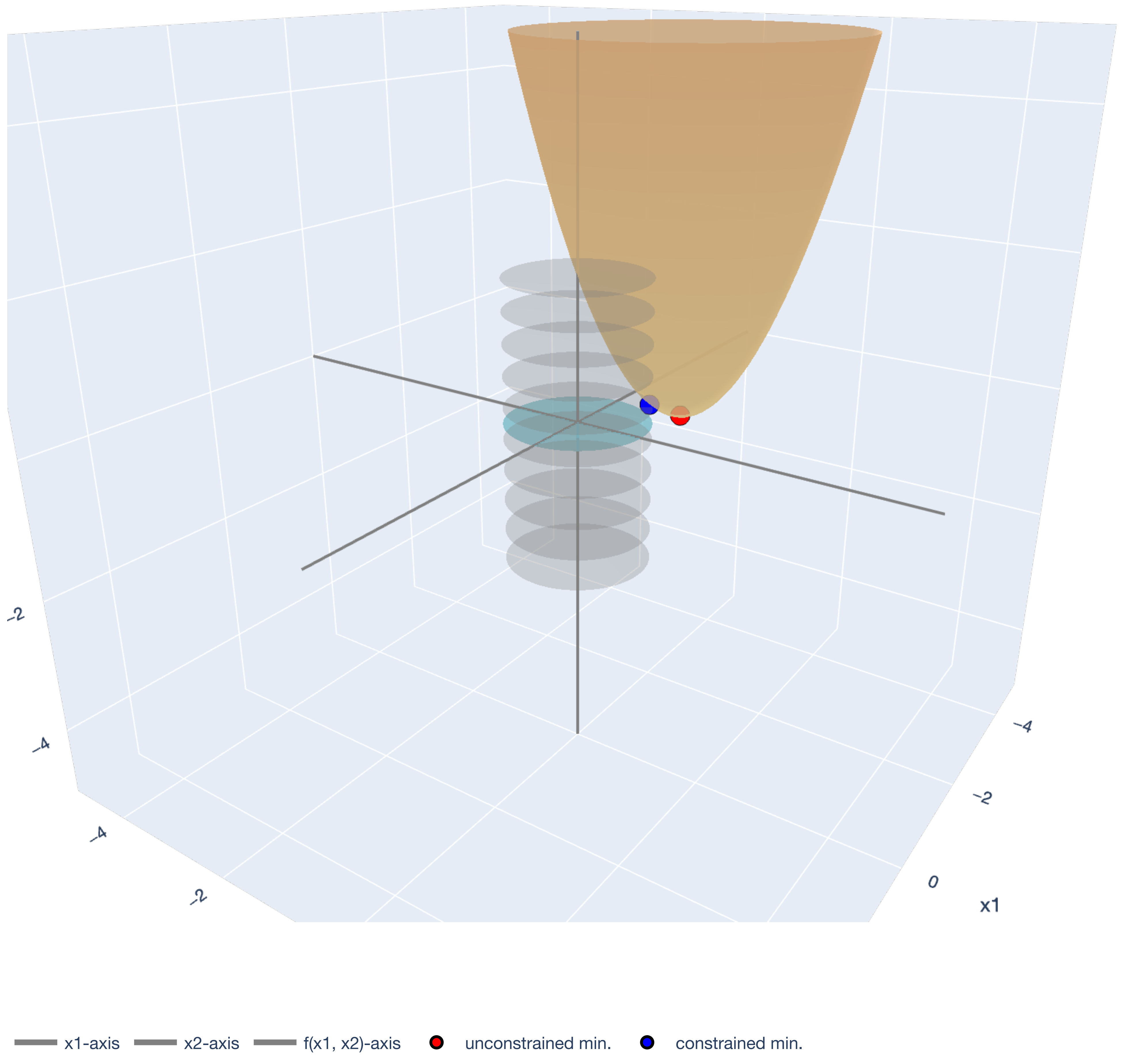


Constrained Minima

Equality Constraints and the Lagrangian

Constrained Minima

What can go wrong?

Recall the definitions of *(unconstrained) local minima* and *constrained local minima.*

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

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

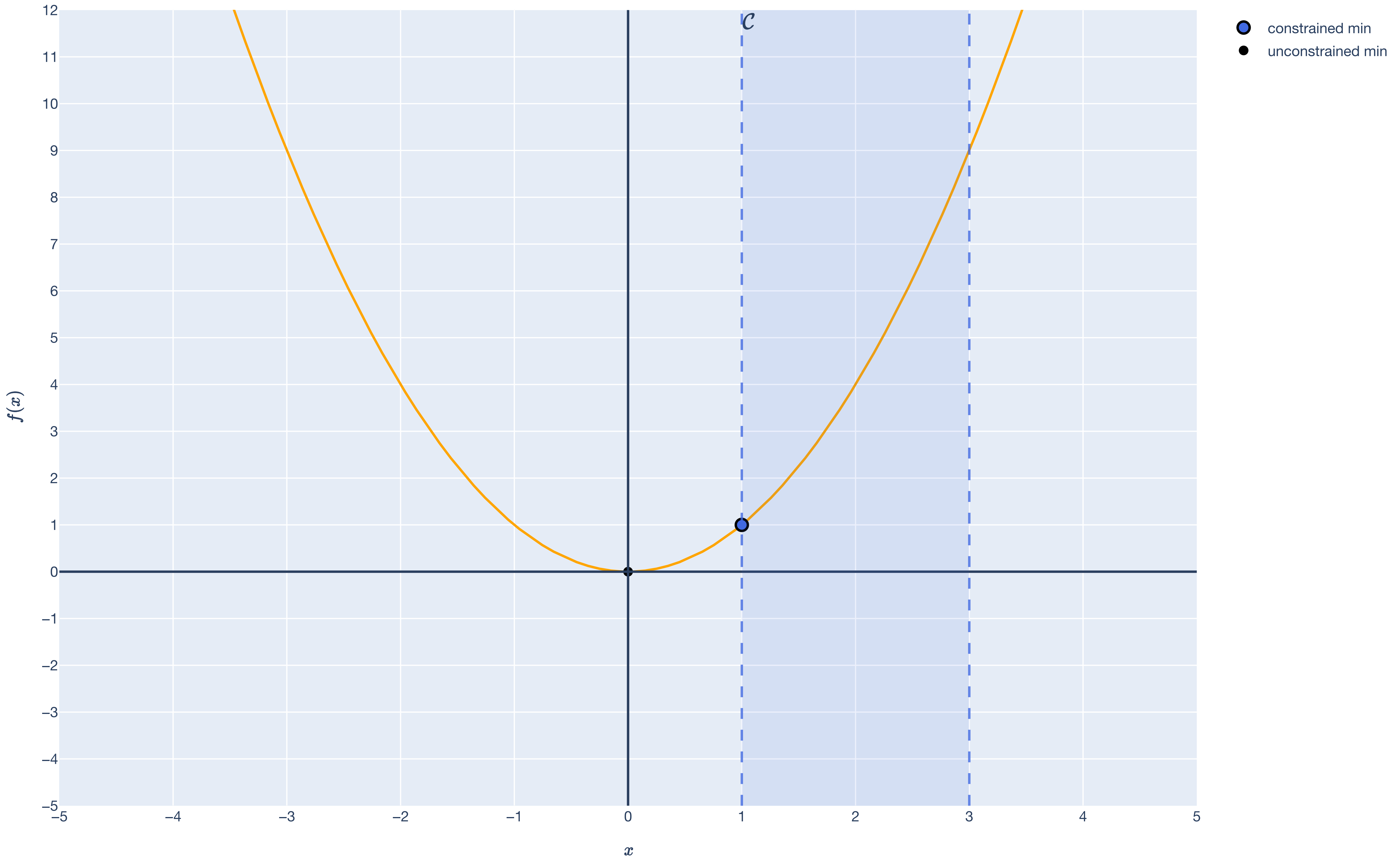
A point $\hat{\mathbf{x}} \in \mathscr{C}$ is a ***local minimum*** if there exists a neighborhood $B_\delta(\mathbf{x})$ around $\hat{\mathbf{x}}$ such that

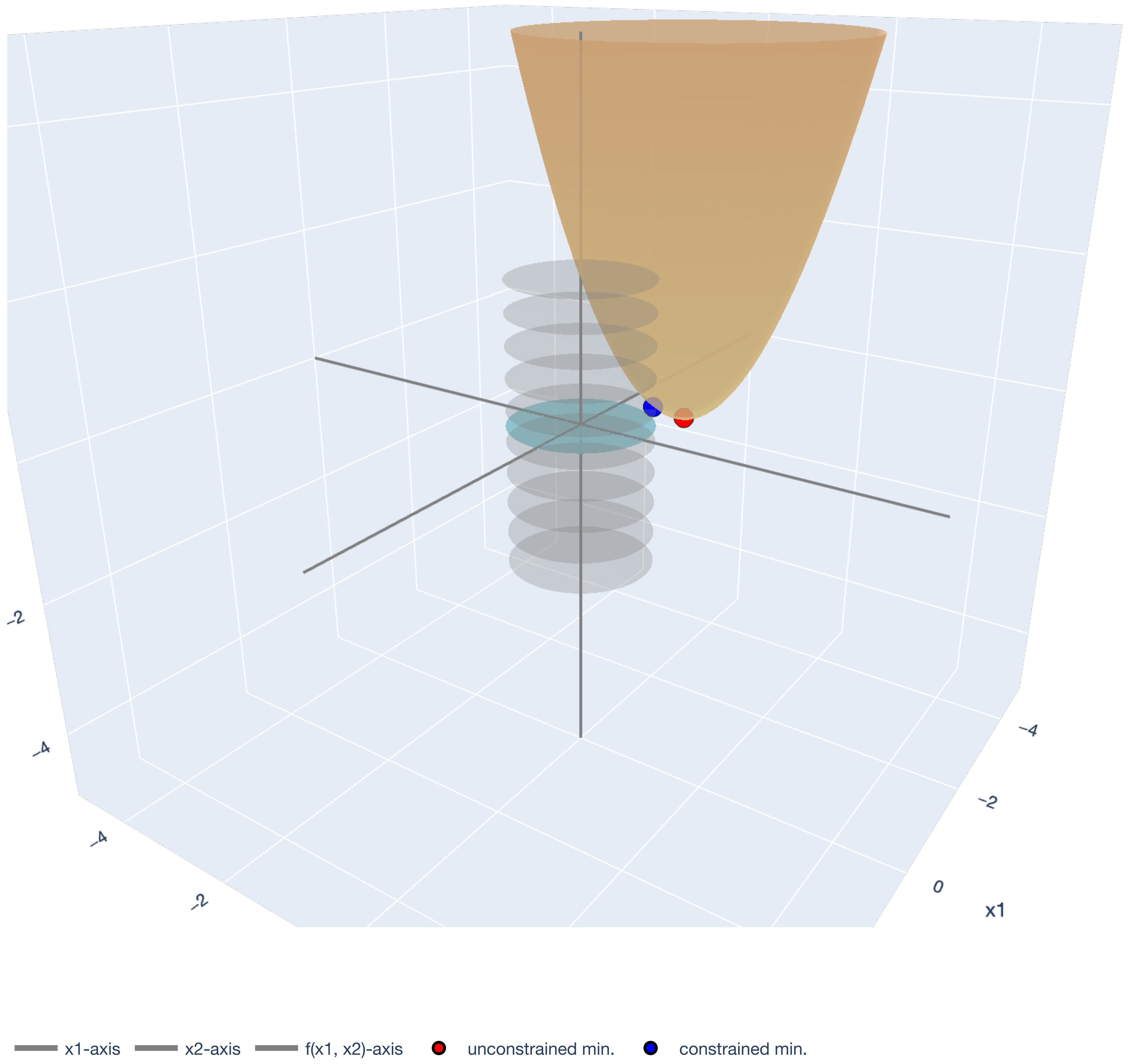
$$f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathscr{C} \cap B_\delta(\hat{\mathbf{x}}).$$

We also call this a ***constrained local minimum***.

Constrained Local Minima

Minimum values on the “edge of the constraint set”





Constrained Minima

Equality constrained optimization

An ***equality constrained minimization problem*** is an optimization problem defined by an objective function $f : \mathbb{R}^d \to \mathbb{R}$, decision variables $\mathbf{x} \in \mathbb{R}^d$, and constraints $h_1(\mathbf{x}), \ldots, h_m(\mathbf{x})$ from a $\mathscr{C}^1$ vector-valued function $\mathbf{h} : \mathbb{R}^d \to \mathbb{R}^m$, written as follows:

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

where $\mathbf{h}(\mathbf{x}) = (h_1(\mathbf{x}), \ldots, h_m(\mathbf{x}))$.

Constrained Minima

Equality constrained optimization

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

The $= 0$ constraint is WLOG:

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

Constrained Minima: Equality Constraints

Example: Maximum Volume Box

Consider the following optimization problem

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

Here, $\mathbf{x} \in \mathbb{R}^3$, the objective is $f(\mathbf{x}) = x_1x_2x_3$, and $h : \mathbb{R}^3 \to \mathbb{R}$ is just scalar-valued (one constraint) with $h(\mathbf{x}) = x_1x_2 + x_2x_3 + x_1x_3 - c/2$.

Constrained Minima: Equality Constraints

Idea

We will convert the *constrained* optimization problem into an *unconstrained* optimization problem and then use our tools for unconstrained optimization problems:

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

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

For an optimization problem with equality constraints

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

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

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

Notice that the function $L(\mathbf{x}, \lambda)$ is an *unconstrained* function.

Constrained Minima: Equality Constraints

Regularity Conditions

For an optimization problem with equality constraints,

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

a point $\mathbf{x} \in \mathbb{R}^n$ is a ***regular point*** if it is feasible and the gradients $\nabla h_1(\mathbf{x}), \ldots, \nabla h_m(\mathbf{x})$ are linearly independent.

This will be the (usually) easily checkable condition we need for a minimum in the Lagrangian. Another condition is that $h_1, \ldots, h_m$ are linear functions.

Constrained Minima: Equality Constraints

Lagrange Multiplier Theorem

Theorem (Lagrange Multiplier Theorem). 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 $\mathbf{d} \in \mathbb{R}^n$ such that $\nabla \mathbf{h}(\mathbf{x}^*)^\top \mathbf{d} = 0$, where $\nabla \mathbf{h}(\mathbf{x}^*) \in \mathbb{R}^{d \times m}$ is the Jacobian of $\mathbf{h}$ at $\mathbf{x}^*$.

Constrained Minima: Equality Constraints

How to remember the Lagrange multiplier theorem

The Lagrangian function is:

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

Remember the necessary conditions for local minima:

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

Applying the first-order necessary conditions for the Lagrangian, a 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: $\mathbf{h}(\mathbf{x}^*) = \mathbf{0}$.

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

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

$$\mathbf{d}^\top \nabla^2_{\mathbf{x},\mathbf{x}} L(\mathbf{x}^*, \lambda^*)\mathbf{d} > 0, \quad \forall \mathbf{d} \text{ such that } \nabla \mathbf{h}(\mathbf{x}^*)^\top \mathbf{d} = \mathbf{0}.$$

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

Constrained Minima: Equality Constraints

How do we use the Lagrangian?

Assuming that *a global minimum exists* and f and $\mathbf{h}$ are $\mathscr{C}^1$, let the Lagrangian be:

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

To find a global minimum…

1. Find the set $(\mathbf{x}^*, \lambda^*)$ satisfying the necessary conditions: $\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*) = 0$ and $\nabla_{\lambda} L(\mathbf{x}^*, \lambda^*) = 0$. This is just our usual first-order condition applied to $L(\,\cdot\,,\,\cdot\,)$!
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

Consider the following optimization problem

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

Constrained Minima

Inequality Constraints and the KKT Theorem

Constrained Minima

Inequality constrained optimization

An ***inequality constrained minimization problem*** with objective $f : \mathbb{R}^d \to \mathbb{R}$:

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

where $h_1(\mathbf{x}), \ldots, h_m(\mathbf{x})$ are $\mathscr{C}^1$ and $g_1(\mathbf{x}), \ldots, g_r(\mathbf{x})$ are $\mathscr{C}^1$.

Constrained Minima

Inequality constrained optimization

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

Main idea: 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

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

This means we get a new definition for a *regular point*…

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

For an optimization problem with equality *and* inequality constraints

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

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

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

Notice that the function $L(\mathbf{x}, \lambda, \mu)$ is an *unconstrained* function.

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem

Theorem (KKT Theorem). 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***).

If, in addition, $f(\cdot)$ and $h(\cdot)$ 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 $\nabla \mathbf{h}(\mathbf{x}^*)^\top \mathbf{d} = 0$, where $\nabla \mathbf{h}(\mathbf{x}^*) \in \mathbb{R}^{d \times m}$ is the Jacobian of $\mathbf{h}$ at $\mathbf{x}^*$.

Constrained Minima: Inequality Constraints

Karush-Kuhn-Tucker (KKT) Theorem

For the Lagrangian,

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

we can 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 $\nabla \mathbf{h}(\mathbf{x}^*)^\top \mathbf{d} = \mathbf{0}$ 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?

Assuming that *a global minimum exists* and f, $\mathbf{h}$, and $\mathbf{g}$ are $\mathscr{C}^1$, let the Lagrangian be:

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

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

Consider the following optimization problem over $\mathbf{x} \in \mathbb{R}^3$:

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

Least Squares Regression

Regularization and Ridge Regression

Regression
Setup

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

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}.$$

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

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": $\hat{\mathbf{w}} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

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

To find $\hat{\mathbf{w}}$, we follow the *principle of least squares.*

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

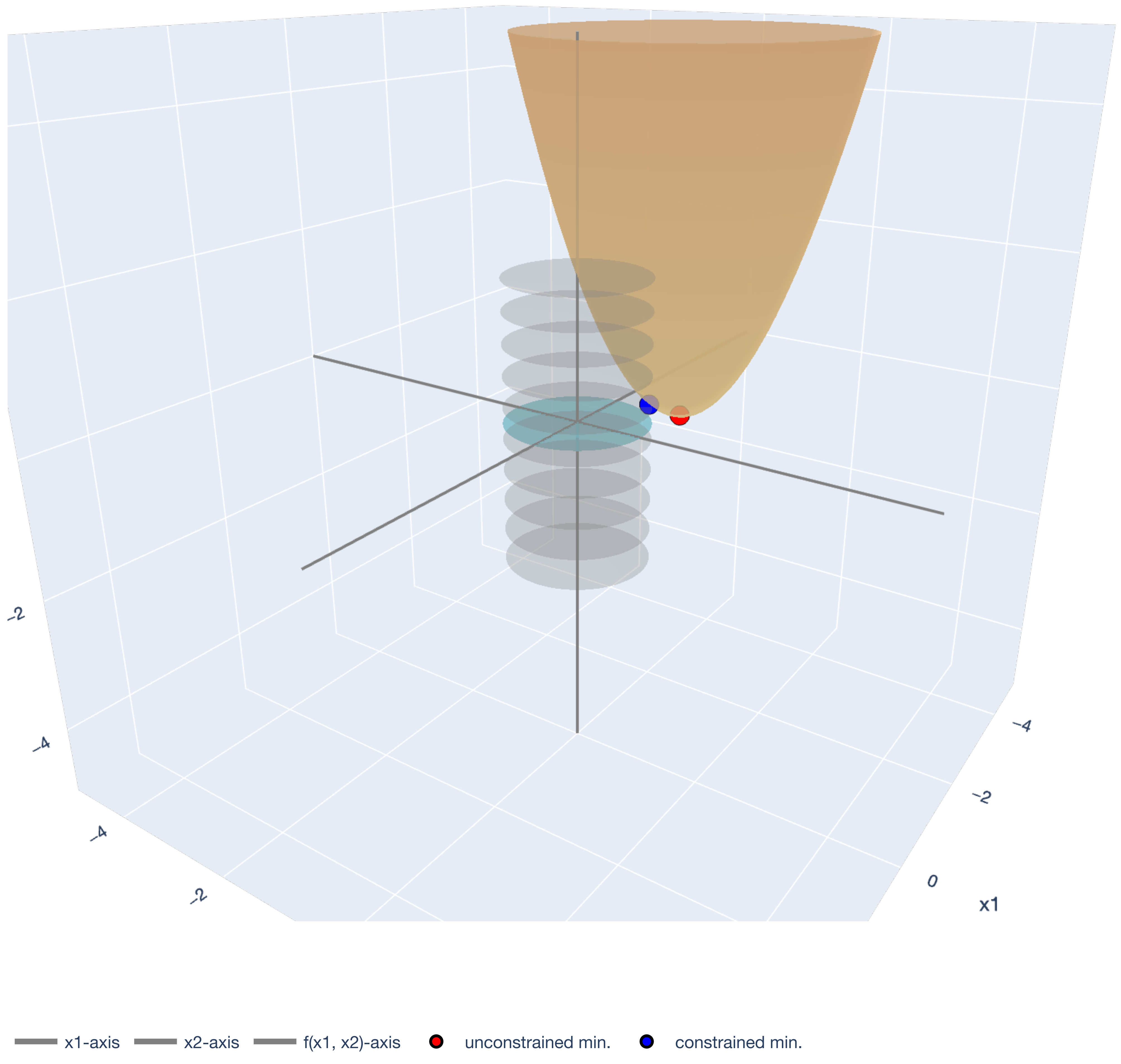
Regression

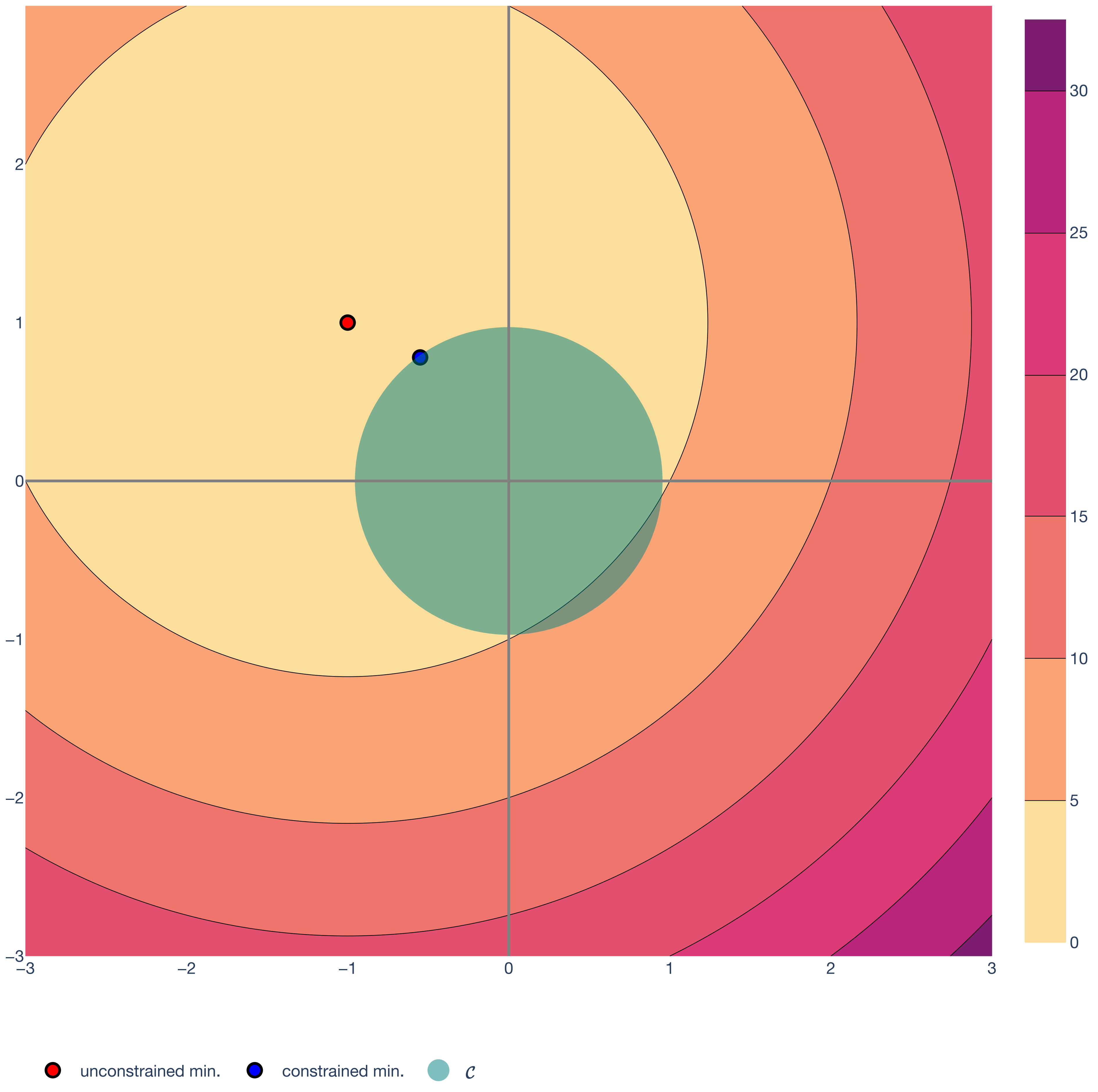
“Regularization” and keeping $\|\mathbf{w}\|$ small

One reasonable

Lesson Overview

Big Picture: Least Squares





Least Squares

Least norm exact solution

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

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

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

Least Squares

Least norm exact solution

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<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, $\hat{\mathbf{w}} = \mathbf{X}^{+}\mathbf{y} = \mathbf{V}\boldsymbol{\Sigma}^{+}\mathbf{U}^{\top}\mathbf{y}$ 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

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

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

Least Squares

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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 $\mathbf{X}\mathbf{w} - \mathbf{y} = \mathbf{0}$

Least Squares

Least norm exact solution

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

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

$$\implies \mathbf{w} = -\frac{1}{2}\mathbf{X}^\top\lambda \text{ and } \mathbf{X}\mathbf{w} = \mathbf{y}$$

Least Squares

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

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

Least Squares

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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

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Least Squares

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How about for the approximate solution to $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$?

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.***

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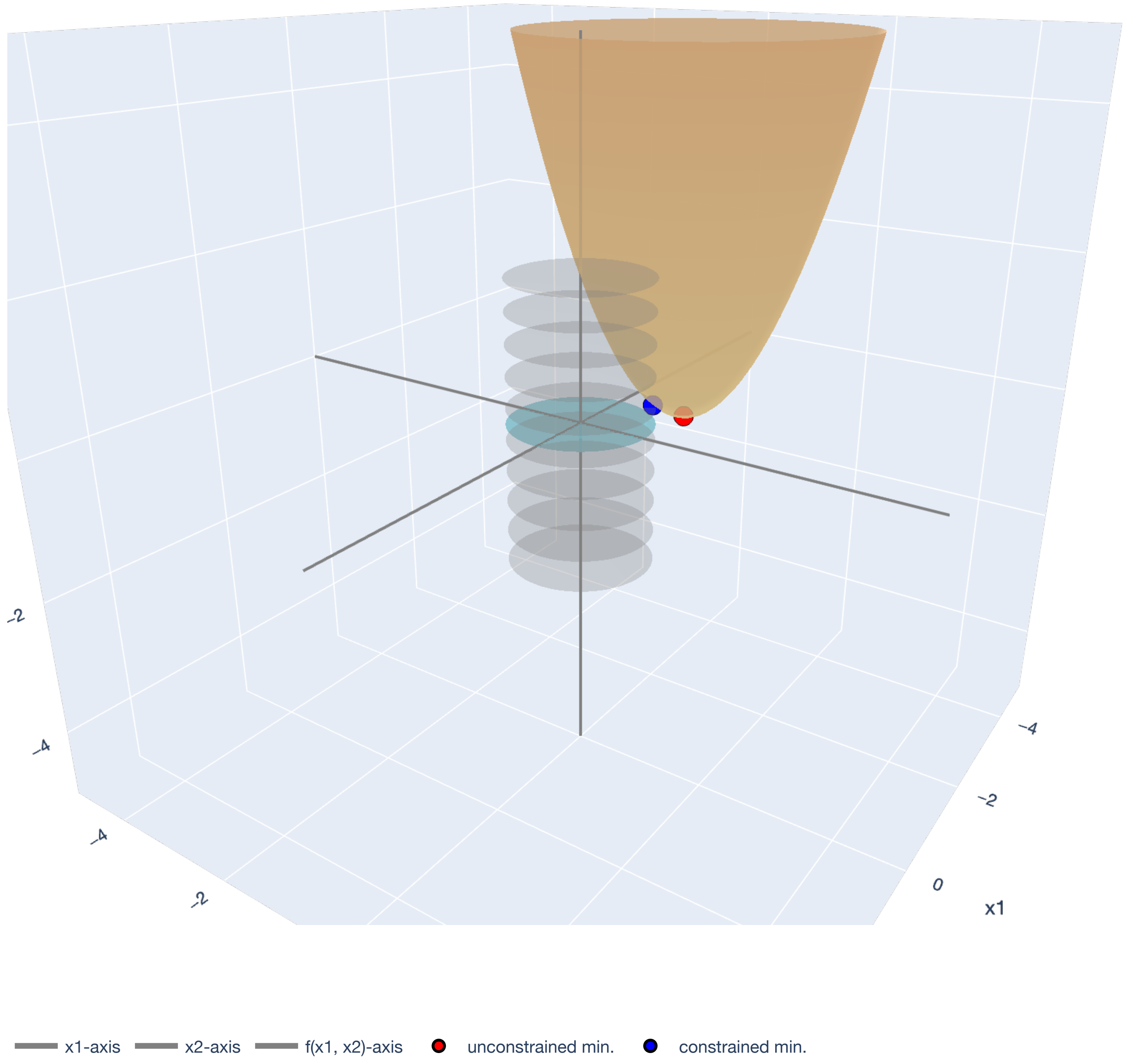

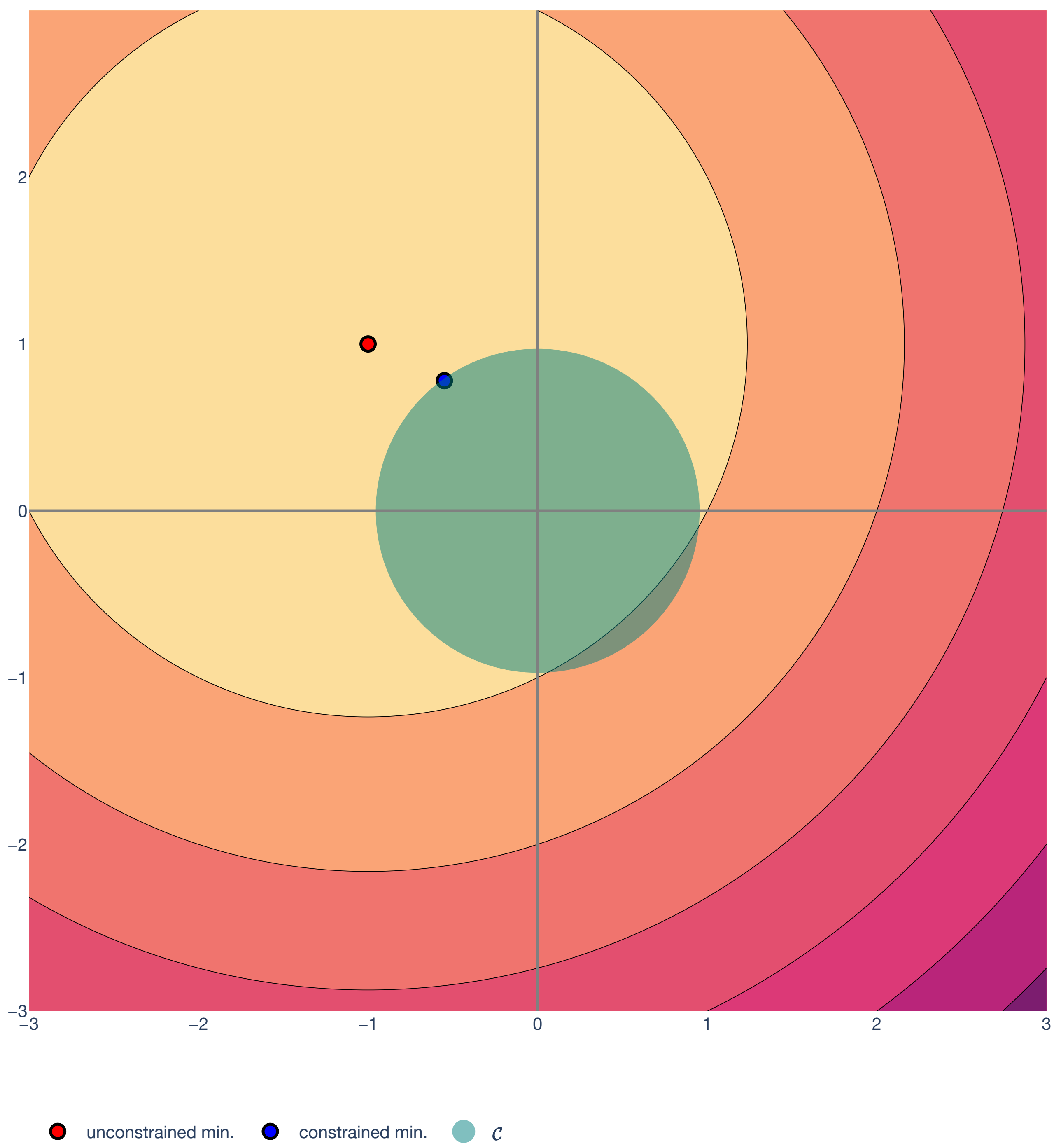

Least Squares

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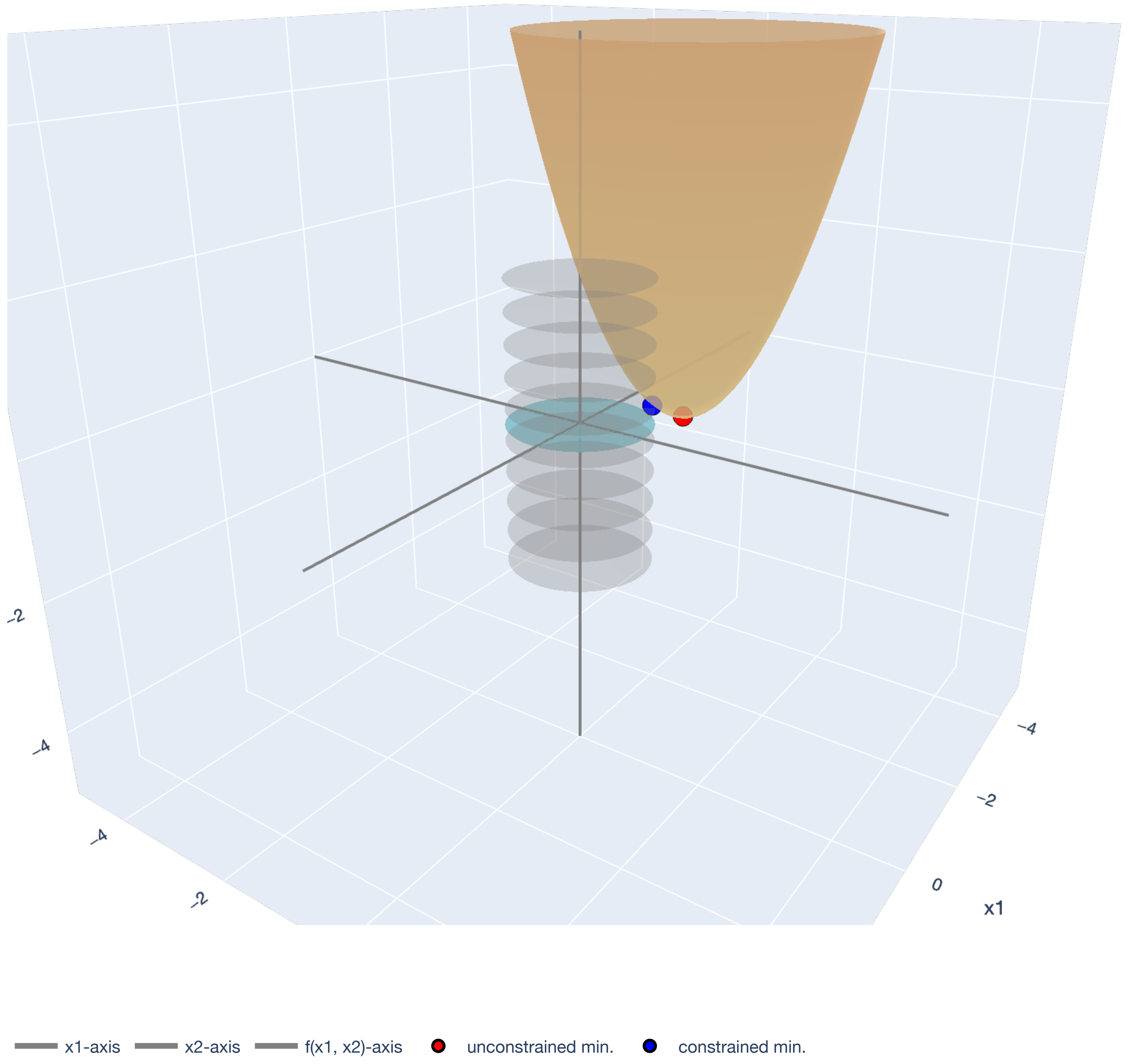

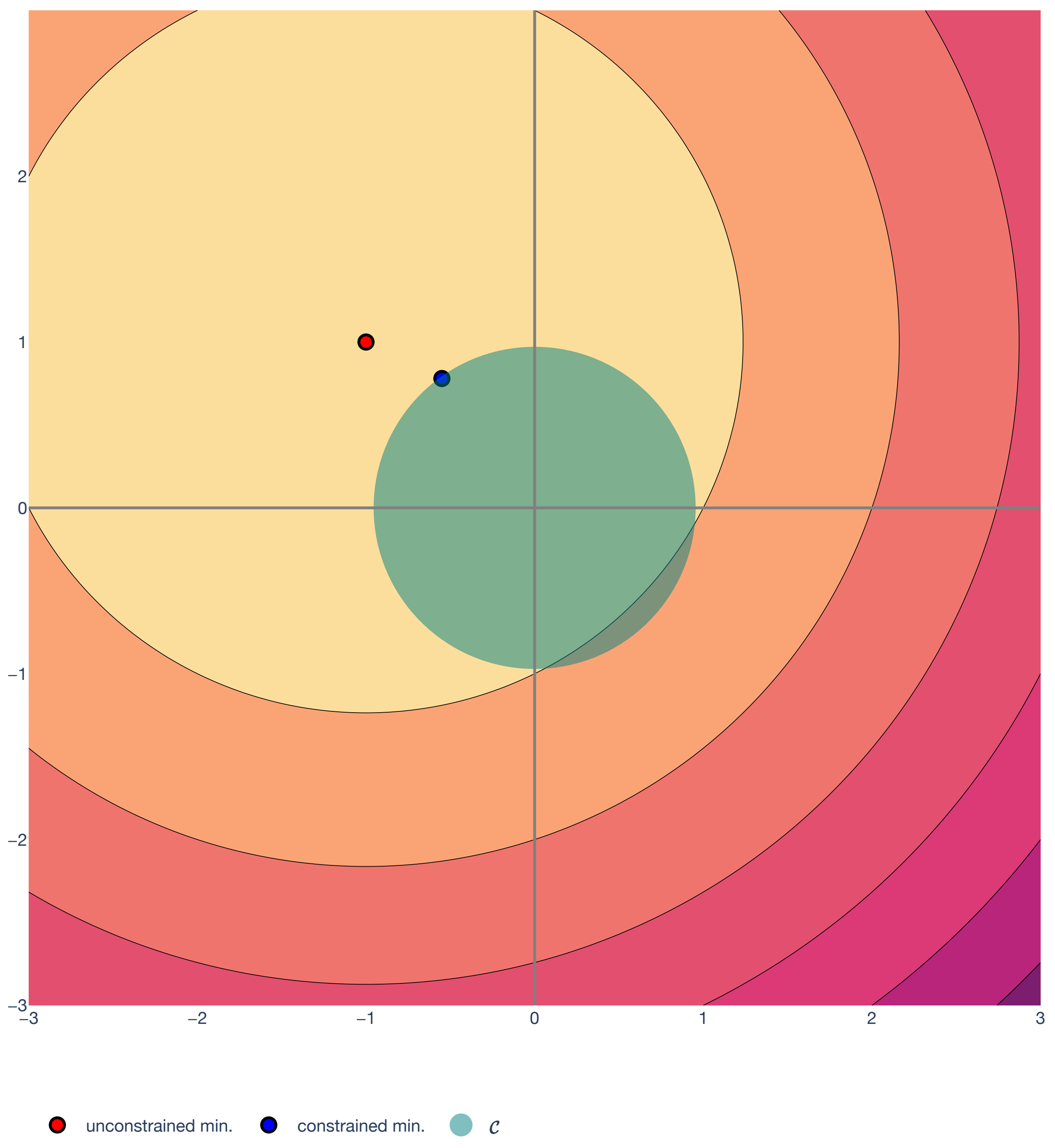

For bigger γ, bigger "constraint" ball!

Least Squares

Solving ridge regression

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

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

Least Squares

Solving ridge regression

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

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.

Least Squares

Solving ridge regression

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Proof. Let $\mathbf{v} \in \mathbb{R}^d$ be any vector.

$$\mathbf{v}^\top(\mathbf{A}+\gamma\mathbf{I})\mathbf{v} = \mathbf{v}^\top(\mathbf{A}\mathbf{v}+\gamma\mathbf{v}) = \mathbf{v}^\top\mathbf{A}\mathbf{v}+\gamma\mathbf{v}^\top\mathbf{v}$$

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

Least Squares

Solving ridge regression

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

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

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

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

Least Squares

Solving ridge regression

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

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

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

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

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

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

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

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

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!

Least Squares

Solving 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 $\hat{\mathbf{y}} \in \mathbb{R}^n$:

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

Least Squares

Solving ridge regression

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

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

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Theorem (OLS). 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 $\hat{\mathbf{y}} \in \mathbb{R}^n$:

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

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

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\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}$$

When $\epsilon \neq 0$, we have an error of $\hat{\mathbf{w}} - \mathbf{w}^* = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\epsilon$.

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

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

Error in Regression

Error using ridge regression

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

What happens when we use the ***ridge 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 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 $\epsilon \neq 0$, 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 $(\boldsymbol{\Lambda} + \gamma\mathbf{I})^{-1}$:

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

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, the ridge regression minimizer

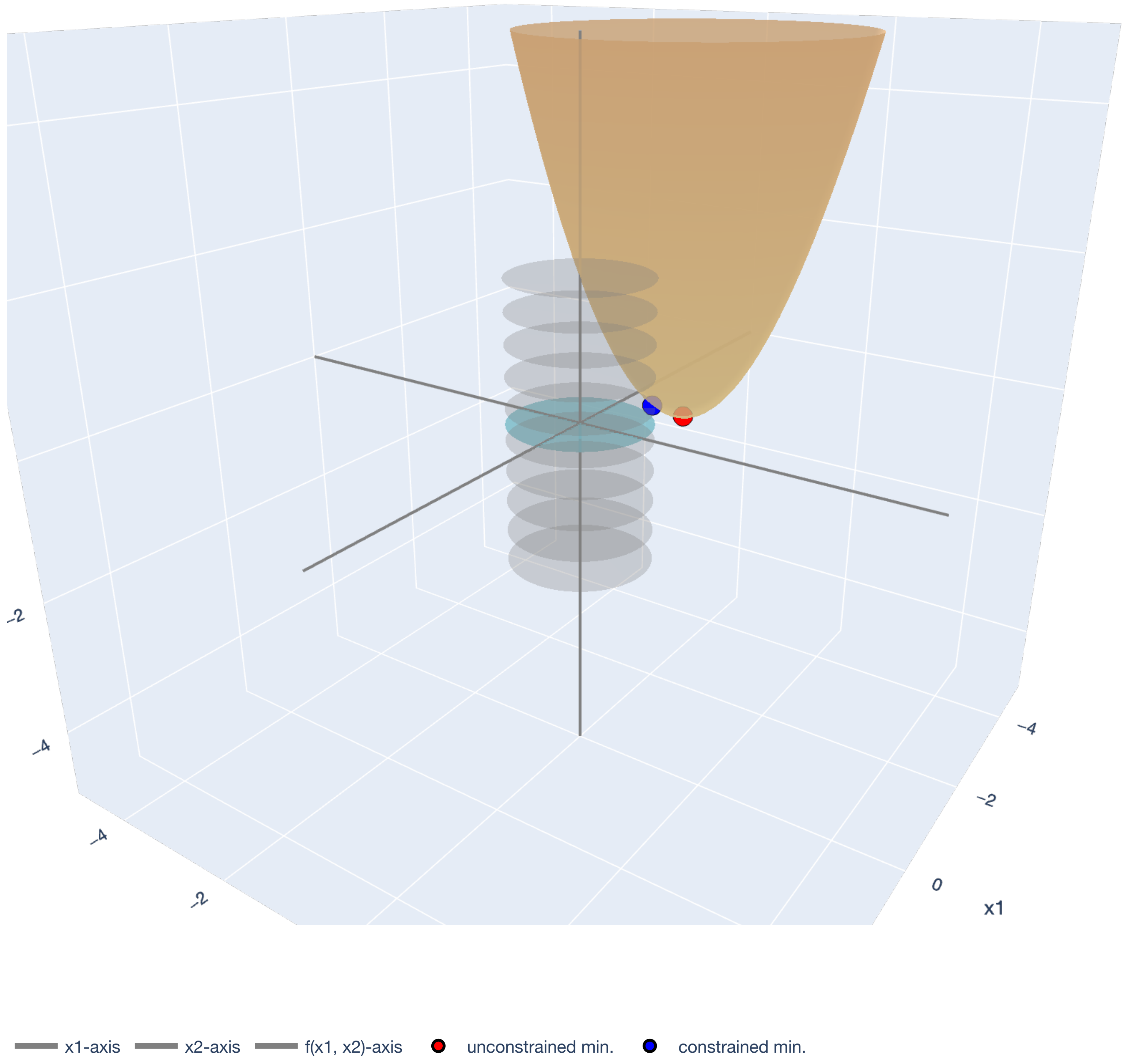
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \gamma \|\mathbf{w}\|^2$$

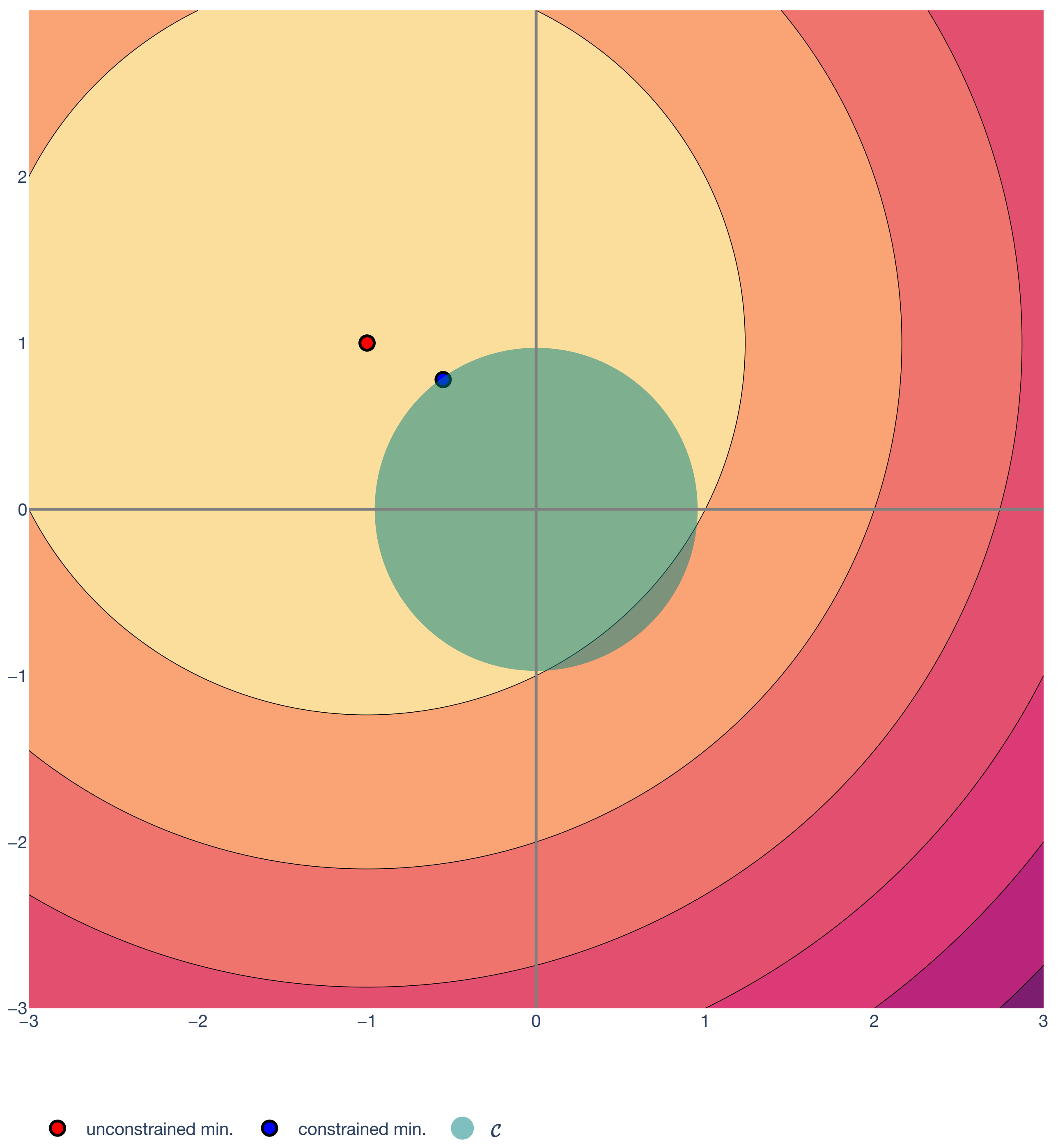
has the form:

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

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

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





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.

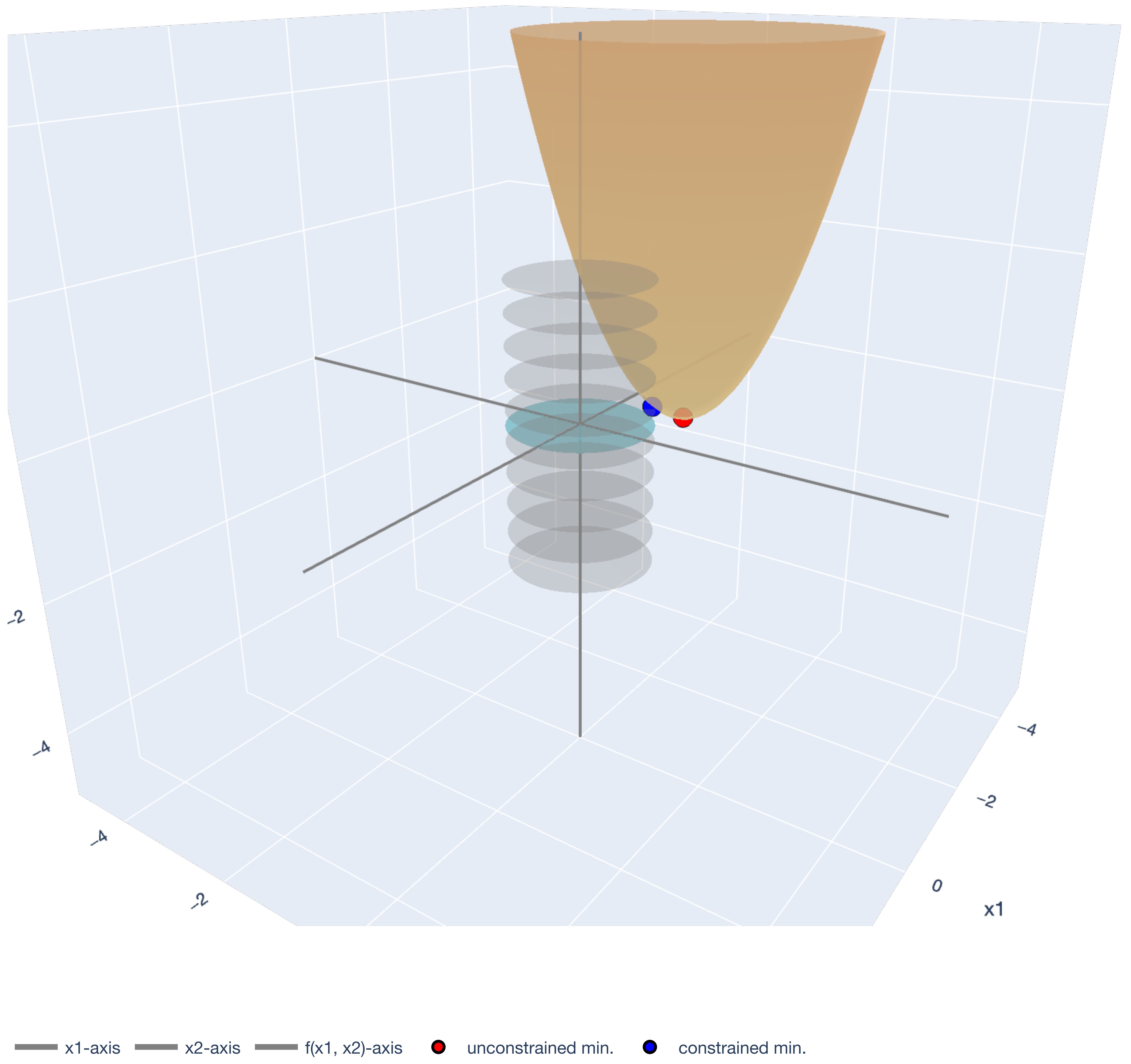
Unconstrained local optima. With no constraints, the standard tools of calculus give conditions for a point $\mathbf{x}^*$ to be optimal, at least to all points close to it.

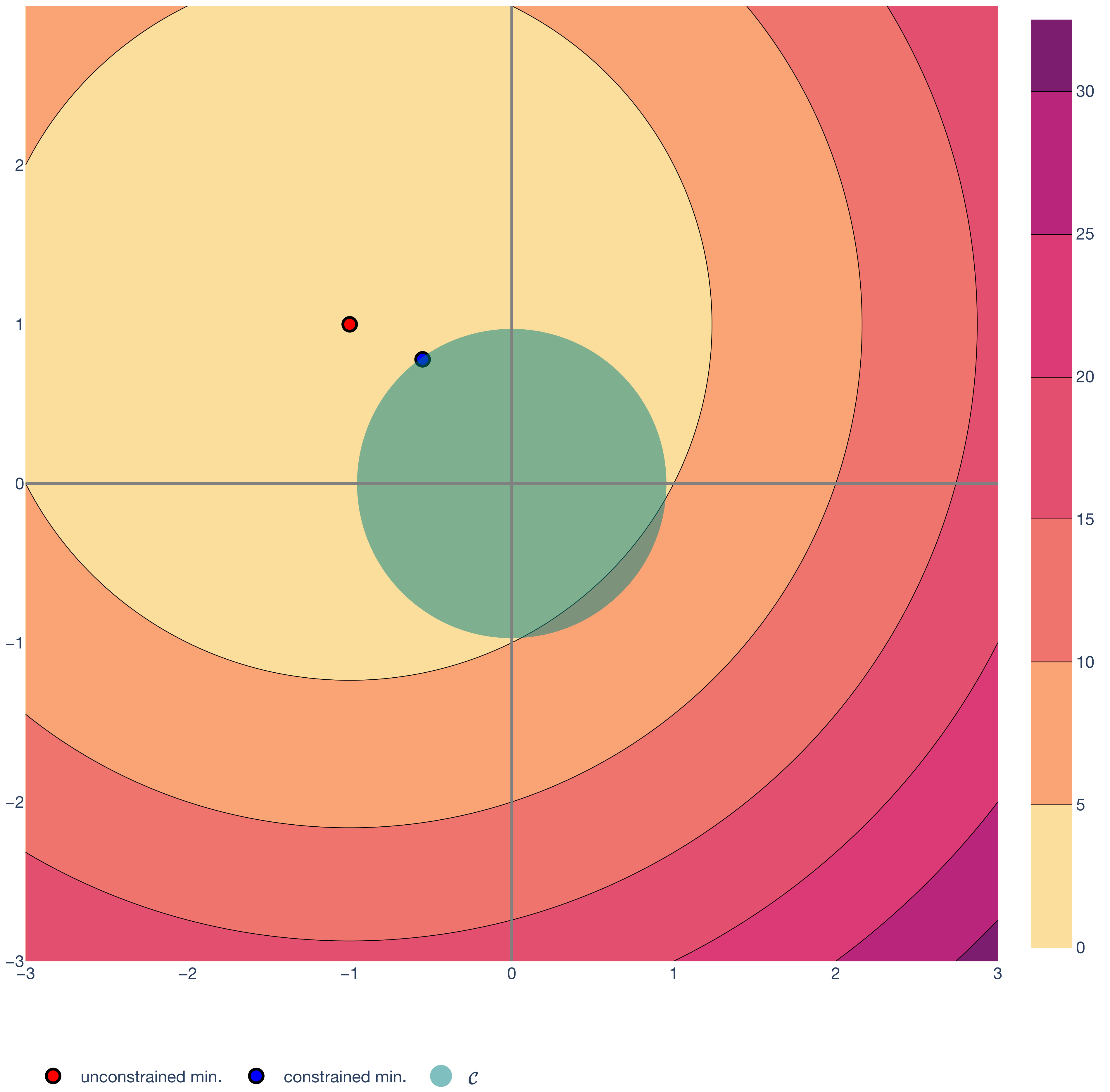
Constrained local optima (Lagrangian and KKT). When $\mathscr{C}$ is represented by inequalities and equalities, we can use the method of *Lagrange multipliers* and the *KKT Theorem* to "unconstrain" the problem.

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

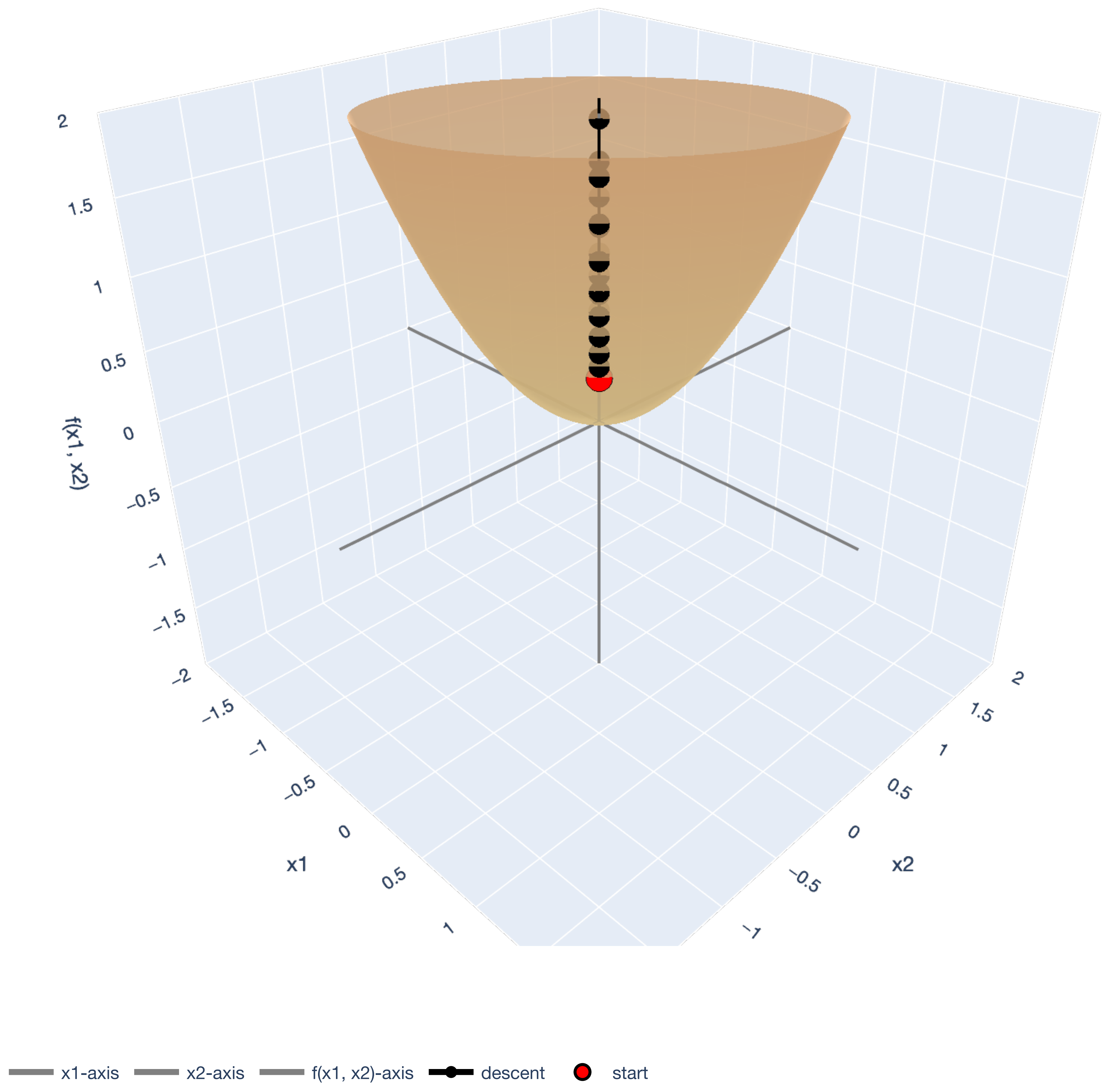
Big Picture: Least Squares

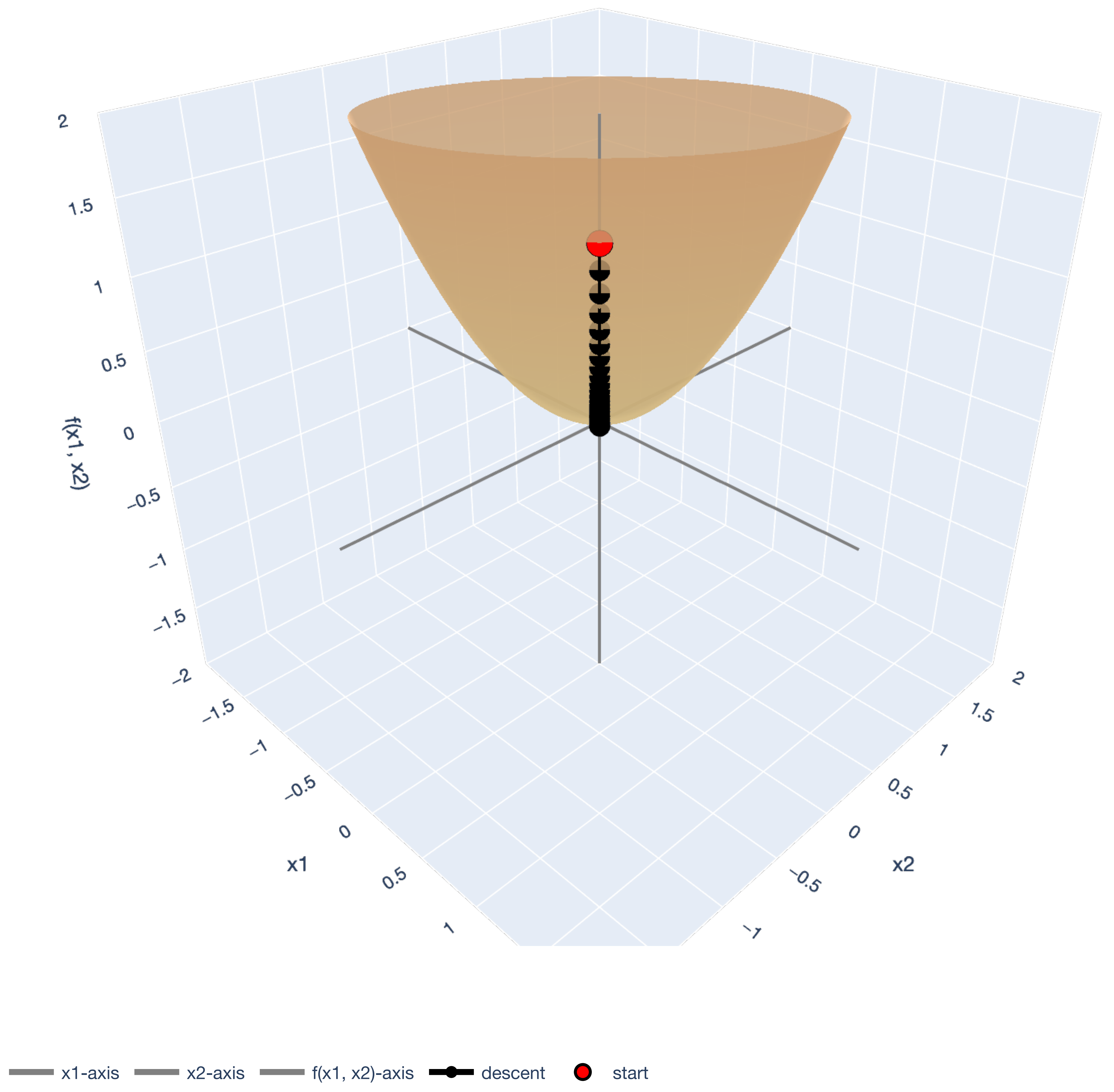




Lesson Overview

Big Picture: Gradient Descent





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