DS-GA 1003: Machine Learning

Lecture 4: Convex Optimization and SVMs

Slides adapted from material from David Rosenberg.

Outline

Convexity Primer

Convex Optimization

Convex Optimization: Duality

Constraint Qualification & Complementary Slackness

SVM Optimization Problem

SVM Dual Optimization

Strong Duality applied to SVM

Why Convex Optimization?

Motivation

Historically

Linear programs (linear objectives & constraints) were the focus.

Nonlinear programs: some easy, some hard.

Early 2000s

Main distinction is between convex and non-convex problems.

Convex problems are the ones we know how to solve efficiently.

2010+

Many people begin to understand optimization / estimation / approximation error tradeoffs.

Accepted stochastic methods often faster to get good results (especially on "big data").

These days: nobody's scared of non-convex problems – SGD works well enough on problems of interest (i.e. neural networks).

Classification Losses

Convexity

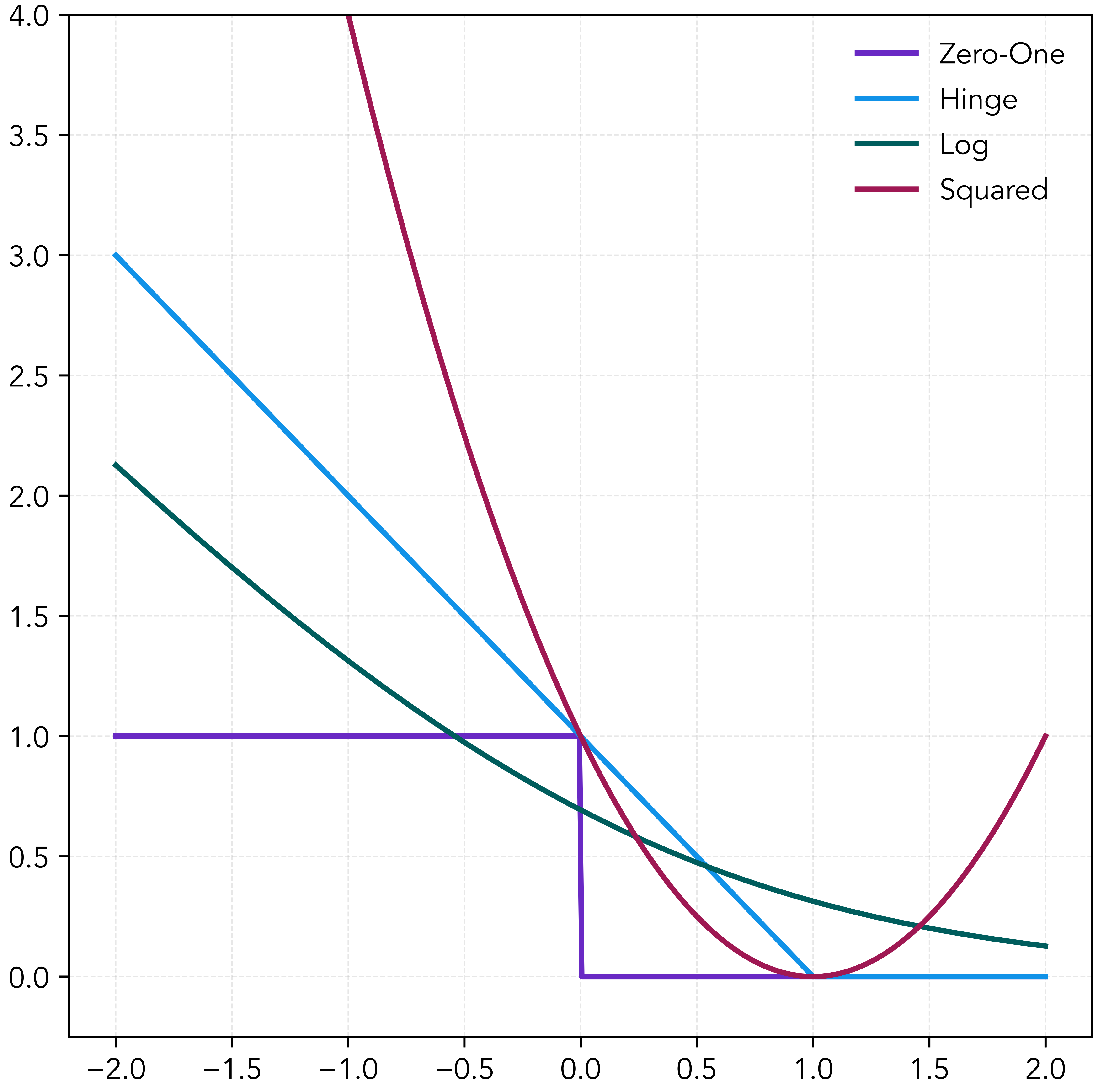
All of these losses have a property in common: **convexity**.

$$\ell_{\text{hinge}}(m) := \max(1 - m, 0)$$

$$\ell_{\text{perc}}(m) := \max(-m, 0)$$

$$\ell_{\log}(m) := \log(1 + e^{-m})$$

$$\ell_{\text{square}}(m) := (1 - m)^2$$



Gradient Descent Guarantee

Convex, Smooth Functions

Recall: Convex functions are the functions where gradient descent is *guaranteed* to converge.

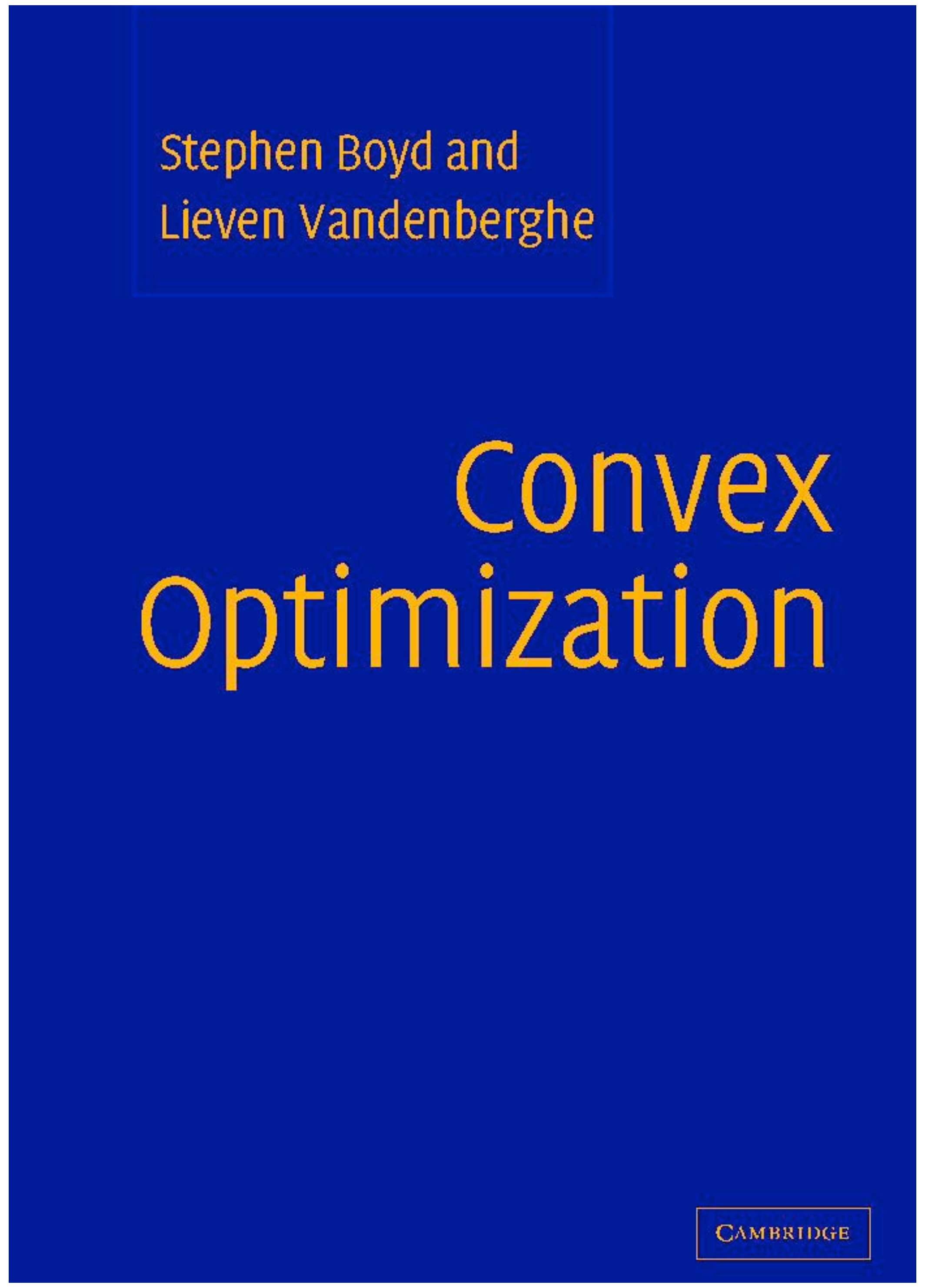
Theorem (GD on Convex, Smooth Functions). If $F : \mathbb{R}^d \to \mathbb{R}$ is convex, differentiable, and L -smooth, then gradient descent with $\eta \leq 1/L$ converges:

$$F(w^{(T)}) - F(w*) \leq \frac{\|w^{(0)} - w*\|^2}{2\eta T} \text{ after } T \text{ steps.}$$

Convex Opt. Reference

Boyd & Vandenberghe (2004)

Standard, comprehensive reference for convex optimization is Boyd & Vandenberghe (2004).



Notation

From Boyd & Vandenberghe

$f : \mathbb{R}^d \to \mathbb{R}$ means that f maps from some *subset* of $\mathbb{R}^d$.

Write $\mathbf{dom}\, f \subset \mathbb{R}^d$, where $\mathbf{dom}\, f$ is the domain of f.

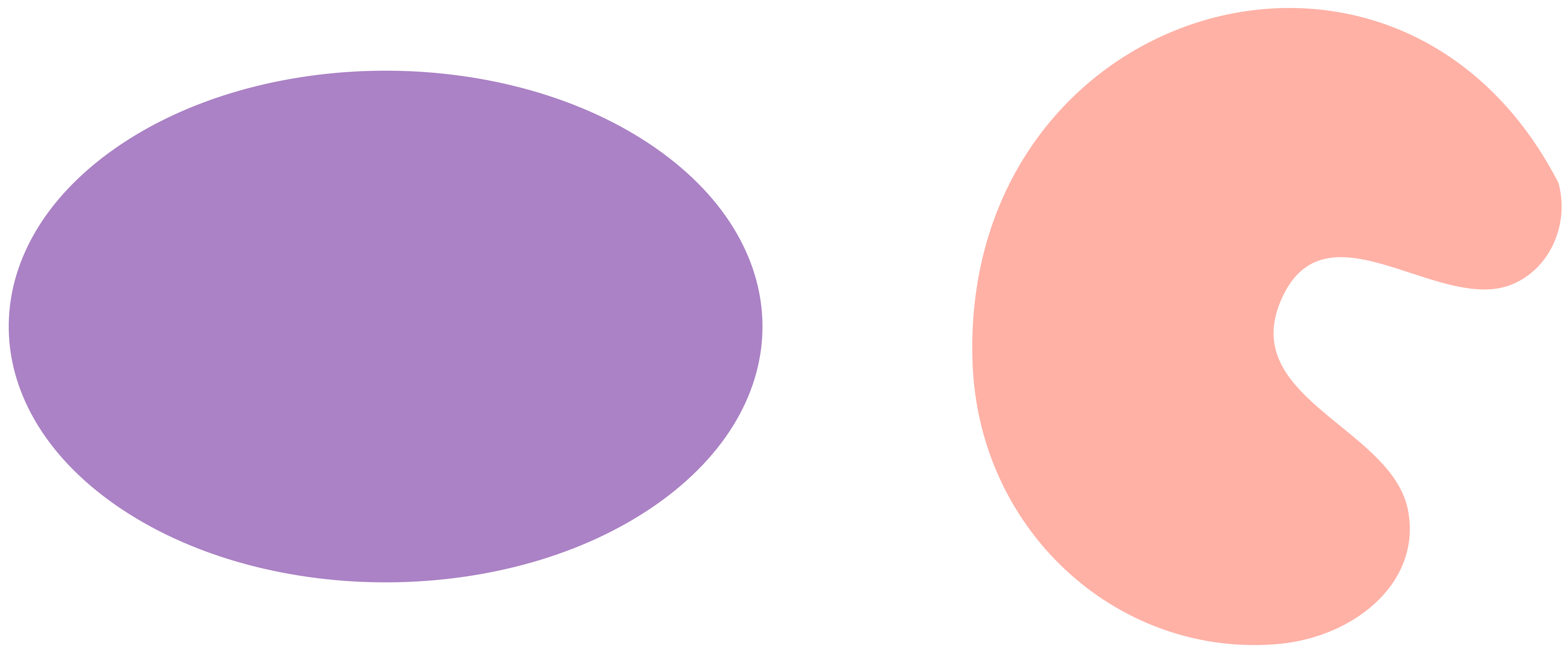
Convex Sets

Definition

A set C is convex if for any $x_1, x_2 \in C$ and any θ with $0 \leq \theta \leq 1$ we have

$$\theta x_1 + (1 - \theta) x_2 \in C.$$

"All line segments between points in the set are in the set."



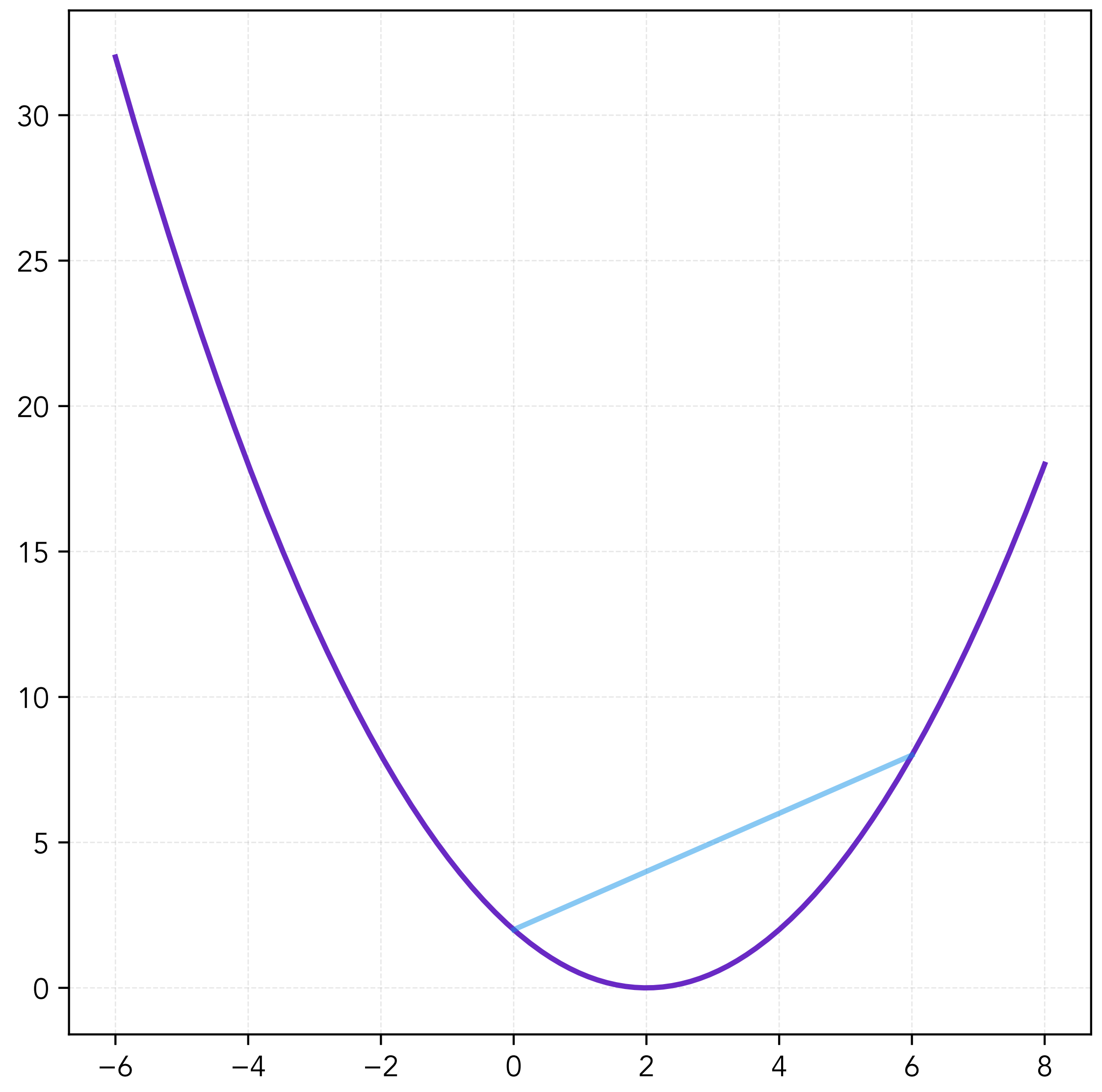
Convex Functions

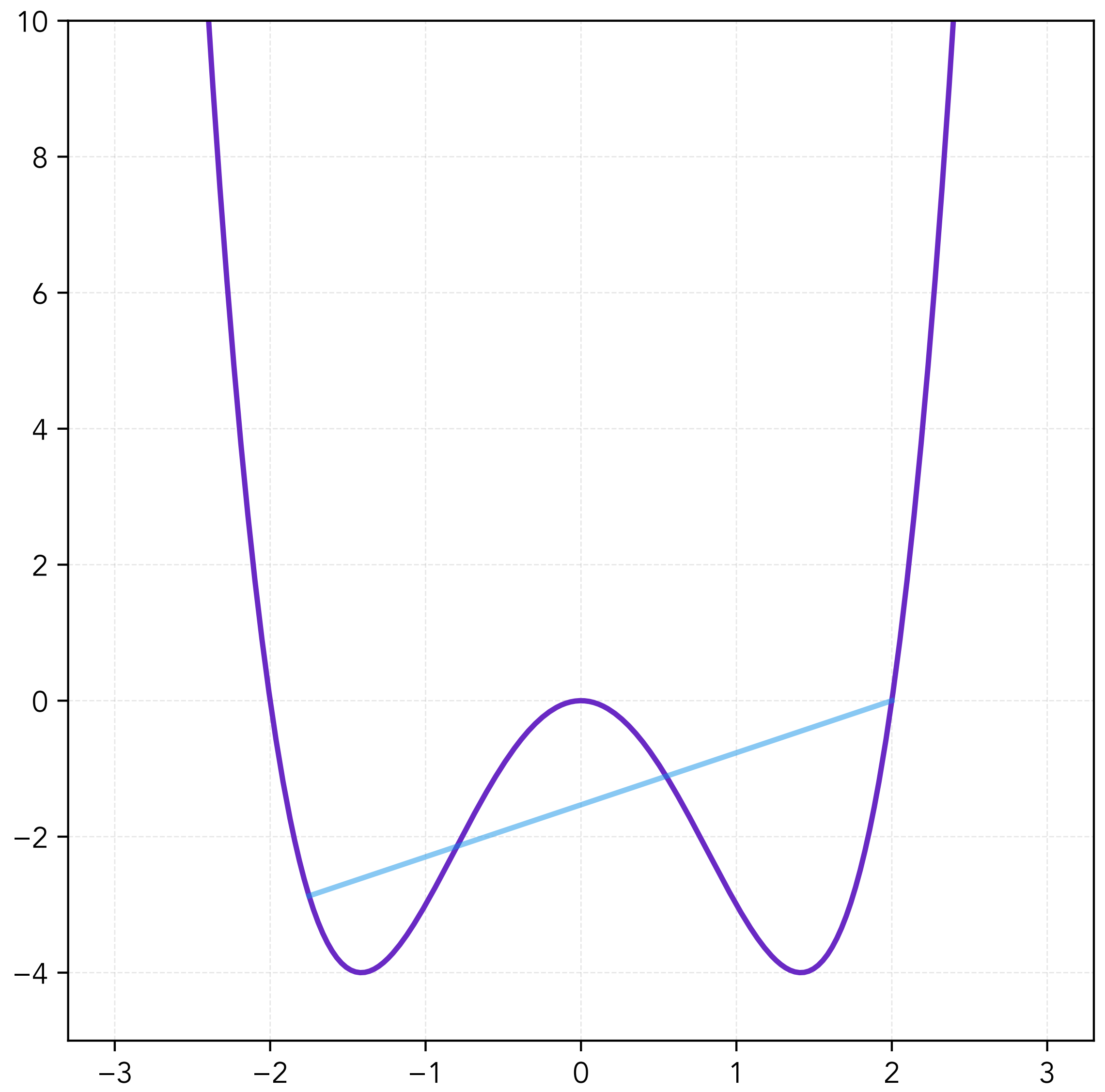
Definition

A function $f : \mathbb{R}^d \to \mathbb{R}$ is <u>convex</u> if $\mathrm{dom}\, f$ is a convex set and if for all $x, y \in \mathrm{dom}\, f$ and $0 \leq \theta \leq 1$:

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y).$$

"All secant lines lie above the function."





Convex Functions

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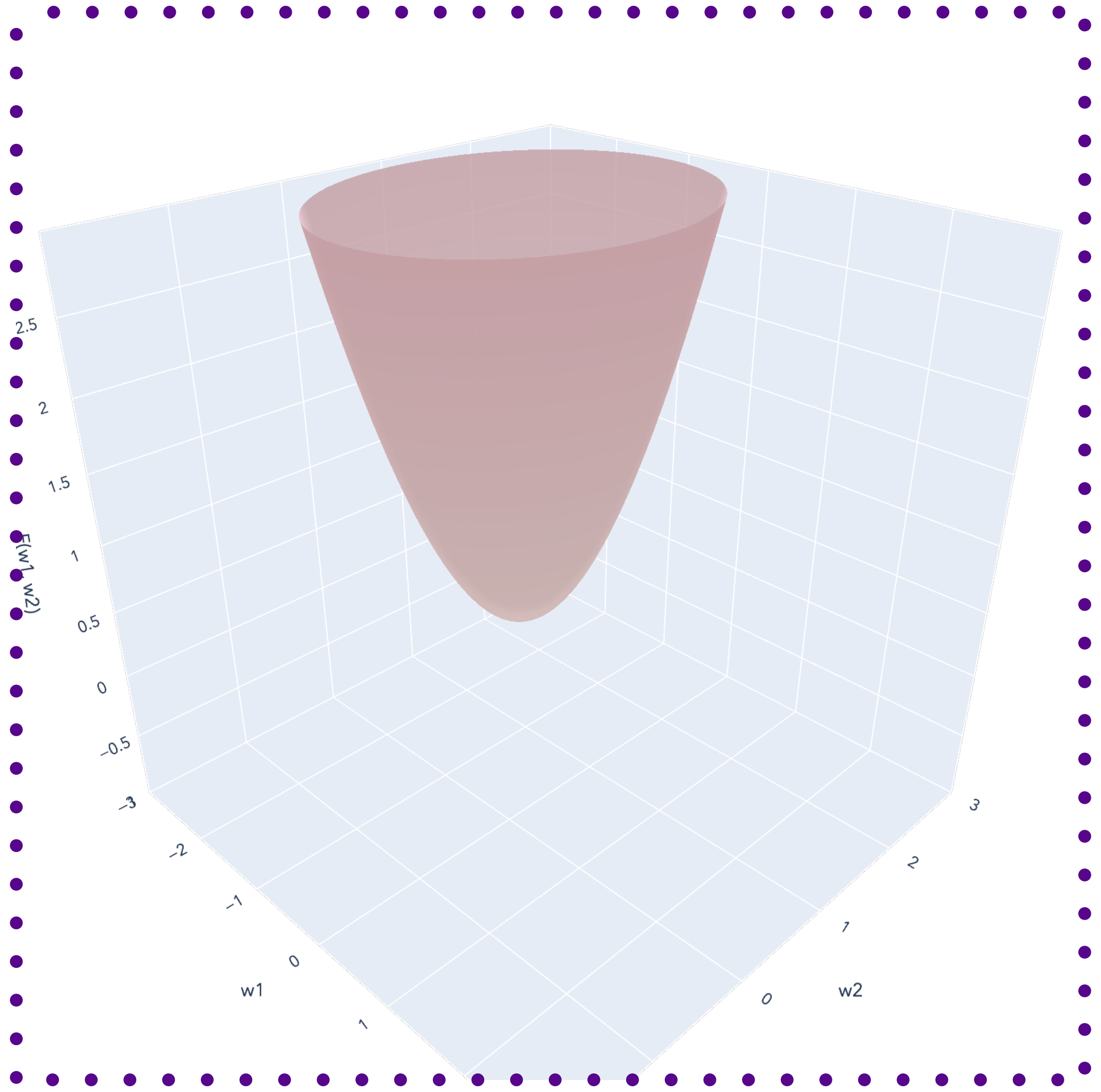
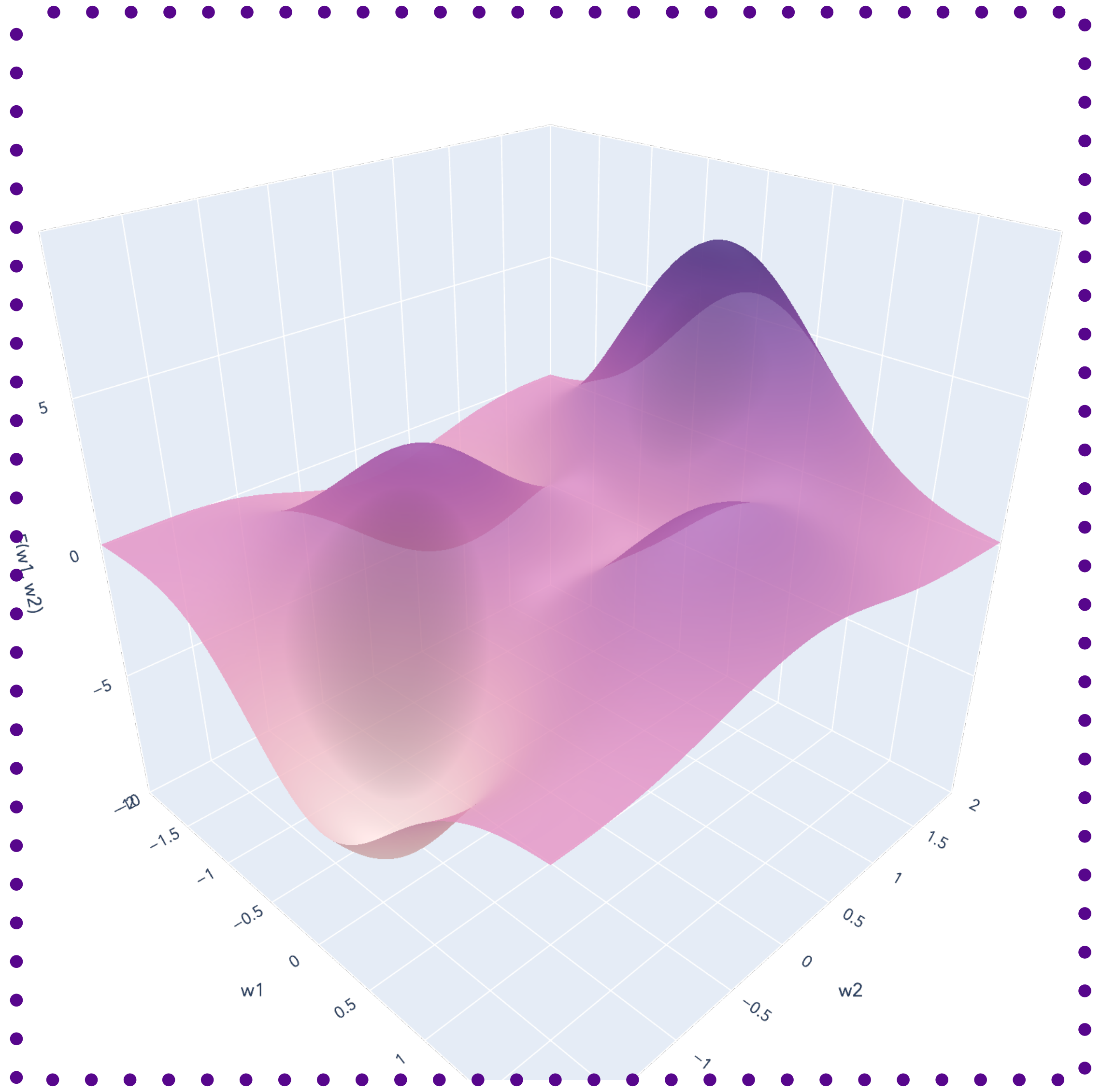


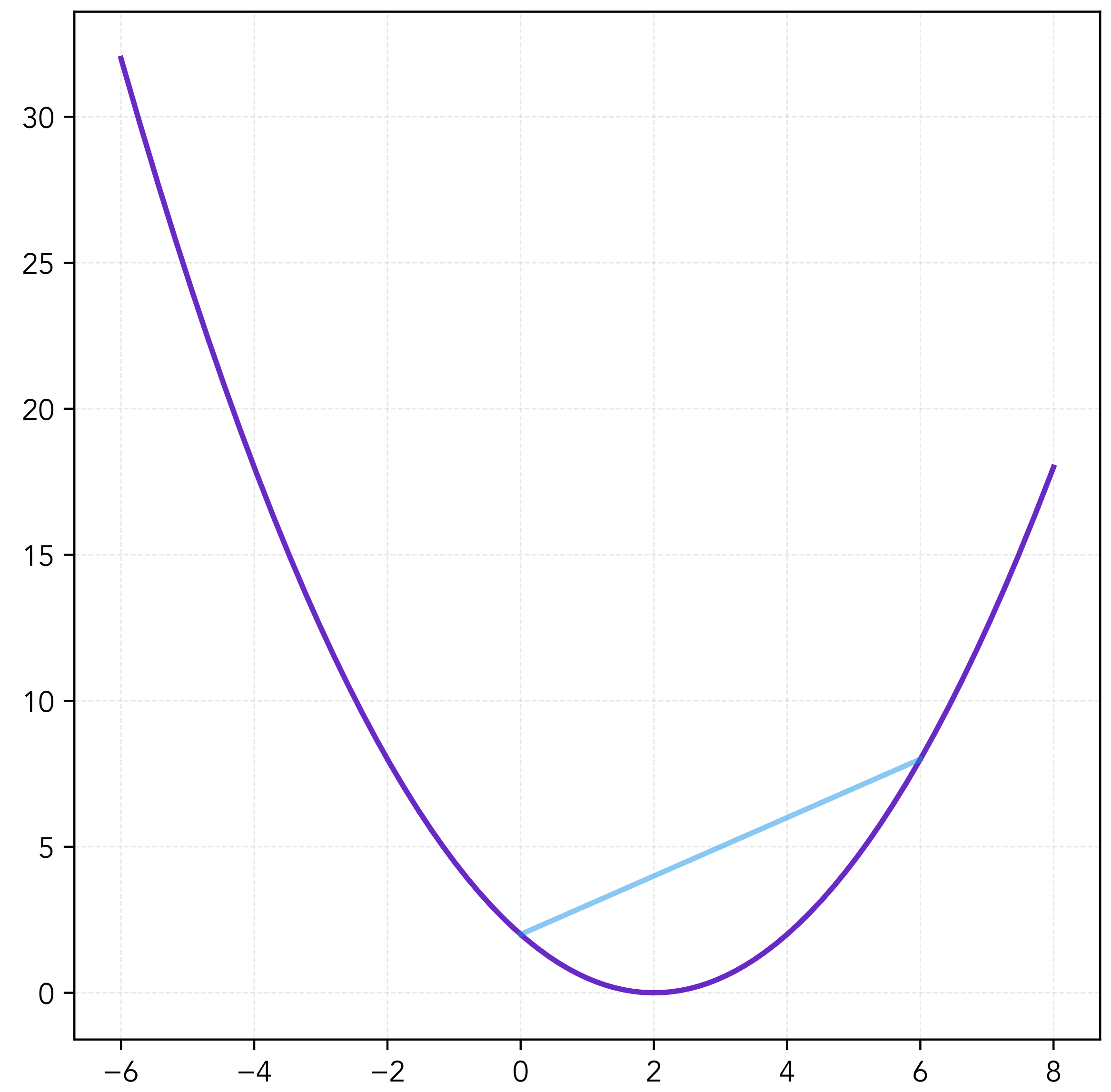


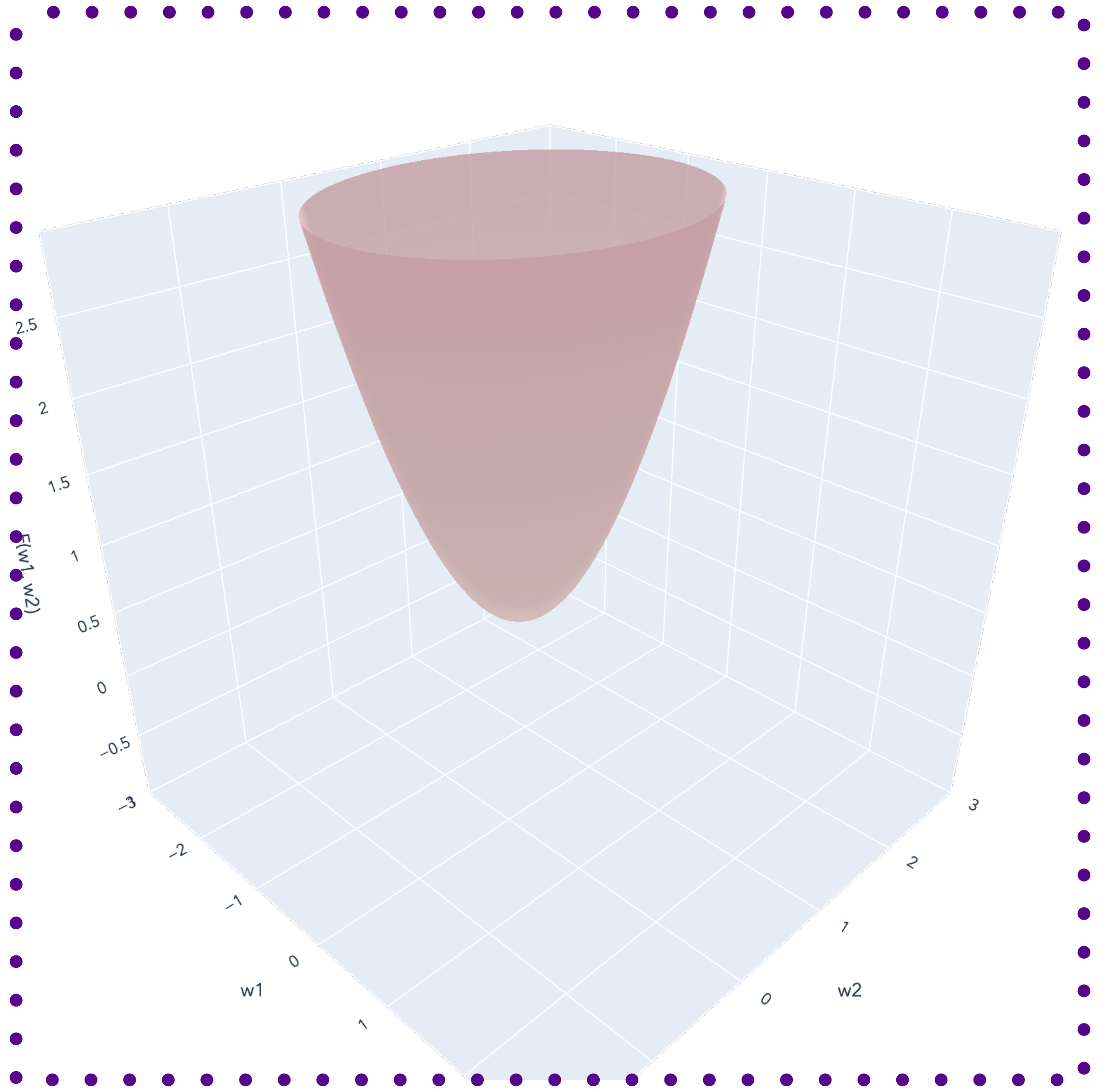
Strictly Convex Functions

Definition

$f : \mathbb{R}^d \to \mathbb{R}$ is strictly convex if $\mathrm{dom}\, f$ is a convex set and if for all $x, y \in \mathrm{dom}\, f$ and $0 \leq \theta \leq 1$:

$$f(\theta x + (1-\theta)y) < \theta f(x) + (1-\theta)f(y).$$





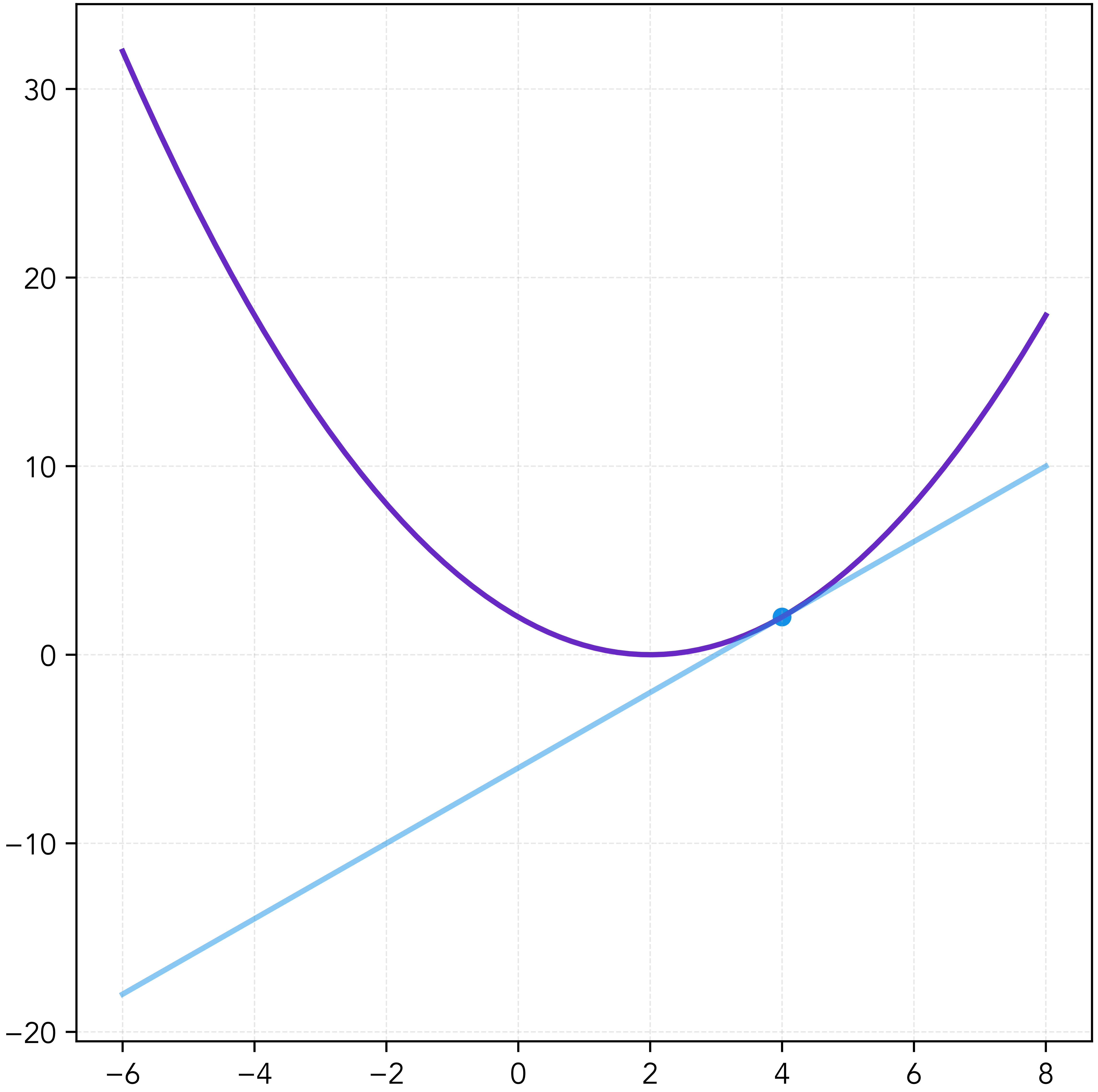
Convex Functions

First-order Condition

A *differentiable* function $f : \mathbb{R}^d \to \mathbb{R}$ is a convex if, for any $x, y \in \mathbb{R}^d$:

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x)\,.$$

Tangent at any x lies *below* the function.



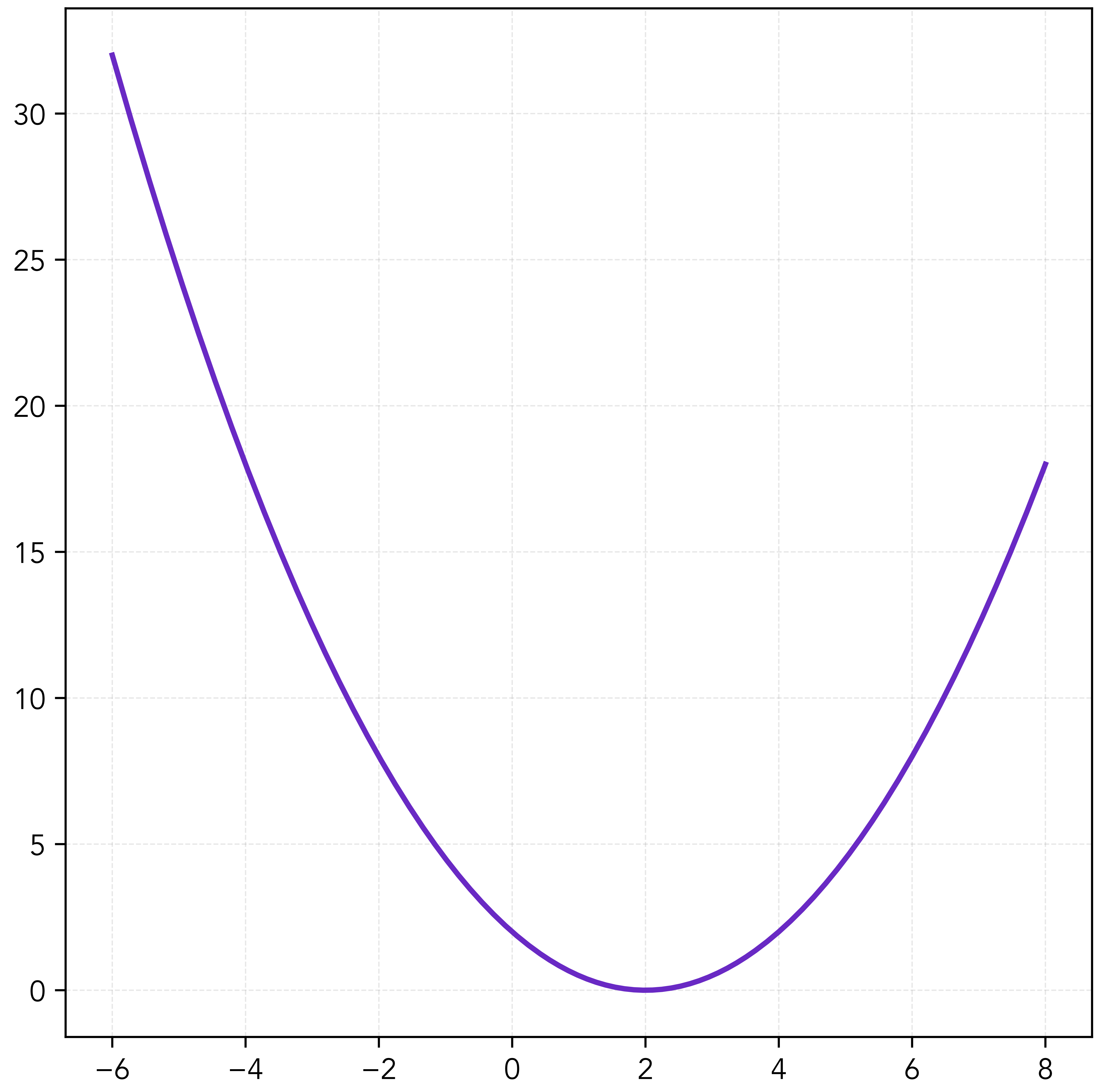
Convex Functions

Second-order Condition

A *twice-differentiable* function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if, for any $x \in \mathbb{R}^d$, the Hessian $\nabla^2 f(x)$ is positive semidefinite:

$$d^\top \nabla^2 f(x) d \geq 0 \text{ for all } d \in \mathbb{R}^d.$$

The function has a nonnegative "second derivative."



Common Convex Functions

Examples

Affine functions. $x \mapsto ax + b$ is both convex and concave on $\mathbb{R}$ for all $a, b \in \mathbb{R}$.

Powers. $x \mapsto \quad x^{\,p}$ for $p \geq 1$ is convex on $\mathbb{R}$.

Exponentials. $x \mapsto e^{ax}$ is convex on $\mathbb{R}$ for all $a \in \mathbb{R}$.

Logarithm. $x \mapsto \log x$ is concave for all $x \geq 0$.

Norms. All norms on $\mathbb{R}^d$ are convex (e.g. $\|x\|_1$ and $\|x\|_2$).

Maximum. $(x_1, \ldots, x_d) \mapsto \max\{x_1, \ldots, x_d\}$ is convex on $\mathbb{R}^d$.

Closure of Convex Functions

The "Algebra" of Convex Functions

We can also combine convex functions with operations that preserve convexity:

Nonnegative linear combination. If $f_1, \ldots, f_n$ convex, then $g(x) := \lambda_1 f_1(x) + \ldots + \lambda_n f_n(x)$ is convex.

Extends to infinite sums and integrals.

Pre-composition with affine function. If f is convex, so is $f(Ax + b)$.

Maximum. If $f_1, \ldots, f_n$ are convex, then $g(x) := \max\{f_1(x), \ldots, f_n(x)\}$ is convex.

Extends to pointwise supremum.

See *Boyd and Vandenberghe* Section 3.2 for comprehensive reference.

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Convex Optimization: Duality

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Strong Duality applied to SVM

Convex Optimization

Standard Form

$$
\begin{aligned}
\min_{x \in \mathbb{R}^d} \quad & f_0(x) \\
\text{s.t.} \quad & f_i(x) \leq 0, \quad i = 1, \ldots, m, \\
& h_j(x) = 0, \quad j = 1, \ldots, k\,.
\end{aligned}
$$

where $x \in \mathbb{R}^d$ are the optimization/decision variables and f_0 is the objective function.

Convex Optimization

Terminology: Feasibility

$$\begin{aligned} \min_{x \in \mathbb{R}^d} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad i = 1, \ldots, m, \\ & h_j(x) = 0, \quad j = 1, \ldots, k\,. \end{aligned}$$

The set of points satisfying the constraints is called the feasible set.

A point x in the feasible set is called a feasible point.

If x is feasible and $f_i(x) = 0$, then we say the equality constraint $f_i(x) \leq 0$ is active at x.

Convex Optimization

Terminology: Optimality

$$\begin{aligned} \min_{x \in \mathbb{R}^d} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad i = 1,\ldots,m, \\ & h_j(x) = 0, \quad j = 1,\ldots,k\,. \end{aligned}$$

The optimal value p^* of the problem is defined as:

$$p^* = \min\{f_0(x) : x \text{ satisfies all constraints}\}.$$

x^* is an optimal point (or a solution) if x^* is feasible and $f_0(x^*) = p^*$.

Convex Optimization

Equality Constraints

$$h(x) = 0 \iff h(x) \geq 0 \text{ AND } h(x) \leq 0.$$

Any equality-constrained problem

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & h(x) = 0 \end{aligned}$$

can be rewritten as:

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & h(x) \leq 0 \\ \text{s.t.} \quad & -h(x) \leq 0 \end{aligned}$$

So without loss off generality, we will only consider **inequality-constrained** optimization problems.

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Lagrangian

Definition

General (inequality-constrained) optimization problem:

$$\begin{aligned} \min_{x \in \mathbb{R}^d} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad i = 1, \ldots, m \end{aligned}$$

The Lagrangian for this optimization problem is:

$$L(x, \lambda) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x).$$

The λ_i are called the Lagrange multipliers (or dual variables).

Lagrangian

Encoding Constraints

Maximizing over the Lagrangian gives back encoding of objective and constraints:

$$\max_{\lambda \geq 0} L(x, \lambda) = \max_{\lambda \geq 0} \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right)$$

$$= \begin{cases} f_0(x) & \text{when } f_i(x) \leq 0 \text{ for all } i \\ \infty & \text{otherwise} \end{cases}$$

Equivalent **primal form** of the optimization problem:

$$p^* = \min_{x} \max_{\lambda \geq 0} L(x, \lambda).$$

Lagrangian

Primal and Dual

Original optimization problem in primal form:

$$p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda)$$

The Lagrangian dual problem comes from "swapping the $\min$ and the $\max$":

$$d^* = \max_{\lambda \geq 0} \min_x L(x, \lambda)$$

$p^* \geq d^*$ for *any* optimization problem (this is called weak duality).

Weak Max-Min Inequality

Theorem

Theorem (Weak Duality). For any $f : W \times Z \to \mathbb{R}$, we have:

$$\max_{z \in Z} \min_{w \in W} f(w, z) \leq \min_{w \in W} \max_{z \in Z} f(w, z).$$

Proof. For any $w_0 \in W$ and $z_0 \in Z$, by definition of $\min$ and $\max$:

$$\min_{w \in W} f(w, z_0) \leq f(w_0, z_0) \leq \max_{z \in Z} f(w_0, z).$$

Sine $\min_{w \in W} f(w, z_0) \leq \max_{z \in Z} f(w_0, z)$ for all w_0 and z_0, we must also have:

$$\max_{z_0 \in Z} \min_{w \in W} f(w, z_0) \leq \min_{w_0 \in W} \max_{z \in Z} f(w_0, z).$$

Weak Duality

Duality Gap

For any optimization problem, the weak max-min inequality implies weak duality:

$$
\begin{aligned}
p^* &= \min_{x} \max_{\lambda \geq 0} \left[f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right] \\
&\geq \max_{\lambda \geq 0} \min_{x} \left[f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right] = d^*
\end{aligned}
$$

The difference $p^* - d^*$ is called the duality gap.

For *convex problems*, we often have strong duality: $p^* = d^*$.

Dual Function

Definition

The Lagrangian dual problem:

$$d^* = \max_{\lambda \geq 0} \min_x L(x, \lambda).$$

The Lagrangian dual function (or just dual function) is:

$$g(\lambda) = \min_x L(x, \lambda) = \min_x \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right).$$

The dual function may take on the value $-\infty$ (one example: $f_0(x) = x$).

The dual function is always **concave** (it is pointwise minimum of affine functions).

Dual Function

Best Lower Bound

$$g(\lambda) = \min_x L(x, \lambda) = \min_x \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right)$$

In terms of the Lagrange dual function, we can write weak duality as:

$$p^* \geq \max_{\lambda \geq 0} g(\lambda) = d^*.$$

$$p^* \geq g(\lambda) \text{ for all } \lambda \geq 0.$$

So any λ with $\lambda \geq 0$ in dual function gives a **lower bound** on the optimal solution.

Dual Function

Best Lower Bound

Weak duality: $p^* \geq \max_{\lambda \geq 0} g(\lambda) = d^*$

The Lagrange dual problem is a search for the best lower bound on p^*:

$$\begin{aligned} \max \quad & g(\lambda) \\ \text{s.t.} \quad & \lambda \geq 0 \end{aligned}$$

λ is dual feasible if $\lambda \geq 0$ and $g(\lambda) > -\infty$ and dual optimal if, in addition, $g(\lambda) = d^*$.

Lagrange dual problem often easier to solve (simpler constraints) and can reveal structure.

d^* can be used as stopping criterion for primal optimization.

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Strong Duality

Convex Optimization

A convex optimization problem is a (possibly constrained) optimization problem

$$\begin{aligned} \min_{x \in \mathbb{R}^d} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad i = 1, \ldots, m \end{aligned}$$

where $f_0, f_1, \ldots, f_m$ are all **convex functions.**

Strong Duality

Convex Optimization

For convex optimization problems, we *usually* have strong duality, but not always:

$$\begin{aligned} \min_{x,y} \quad & e^{-x} \\ \text{s.t.} \quad & x^2/y \le 0 \\ & y > 0 \end{aligned}$$

The additional conditions needed for strong duality are called **constraint qualifications**.

Constraint Qualification

Slater's Conditions

When is $p^* = d^*$ (strong duality) for *convex optimization*?

Roughly: the problem must be **strictly** feasible (there is *some* solution).

Qualifications when problem domain $\mathcal{D} = \bigcap_{i=0}^{m} \operatorname{dom} f_i \subseteq \mathbb{R}^d$ is an open set:

Strict feasibility is sufficient (there exists x such that $f_i(x) < 0$ for all $i = 1,\ldots,m$).

For affine inequality constraints, finding x such that $f_i(x) \leq 0$ is sufficient.

If $\mathcal{D}$ is not open, see notes in B&V Section 5.2.3, pg. 226.

Complementary Slackness

Definition

If **strong duality** holds, we get an interesting relationship between:

Optimal Lagrange multiplier λ_i^* and

The ith constraint at the optimum: $f_i(x^*)$.

The relationship is called complementary slackness:

$$\lambda_i^* f_i(x^*) = 0$$

Always have Lagrange multiplier is zero **or** constraint is active at optimum **or** both.

Complementary Slackness

"Sandwich Proof"

Assume strong duality: $p^* = d^*$. Let x^* be primal optimal and let λ^* be dual optimal. Then:

$$
\begin{aligned}
f_0(x^*) = g(\lambda^*) &= \min_x L(x, \lambda^*) \\
&\leq L(x^*, \lambda^*) \\
&= f_0(x^*) + \sum_{i=1}^{m} \underbrace{\lambda_i^* f_i(x^*)}_{\leq 0} \\
&\leq f_0(x^*)
\end{aligned}
$$

Each term in the sum $\sum_{i=1}^{m} \lambda_i^* f_i(x^*)$ must actually be 0. That is, $\lambda_i^* f_i(x_i^*) = 0$ for $i = 1, \ldots, m$.

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Classification

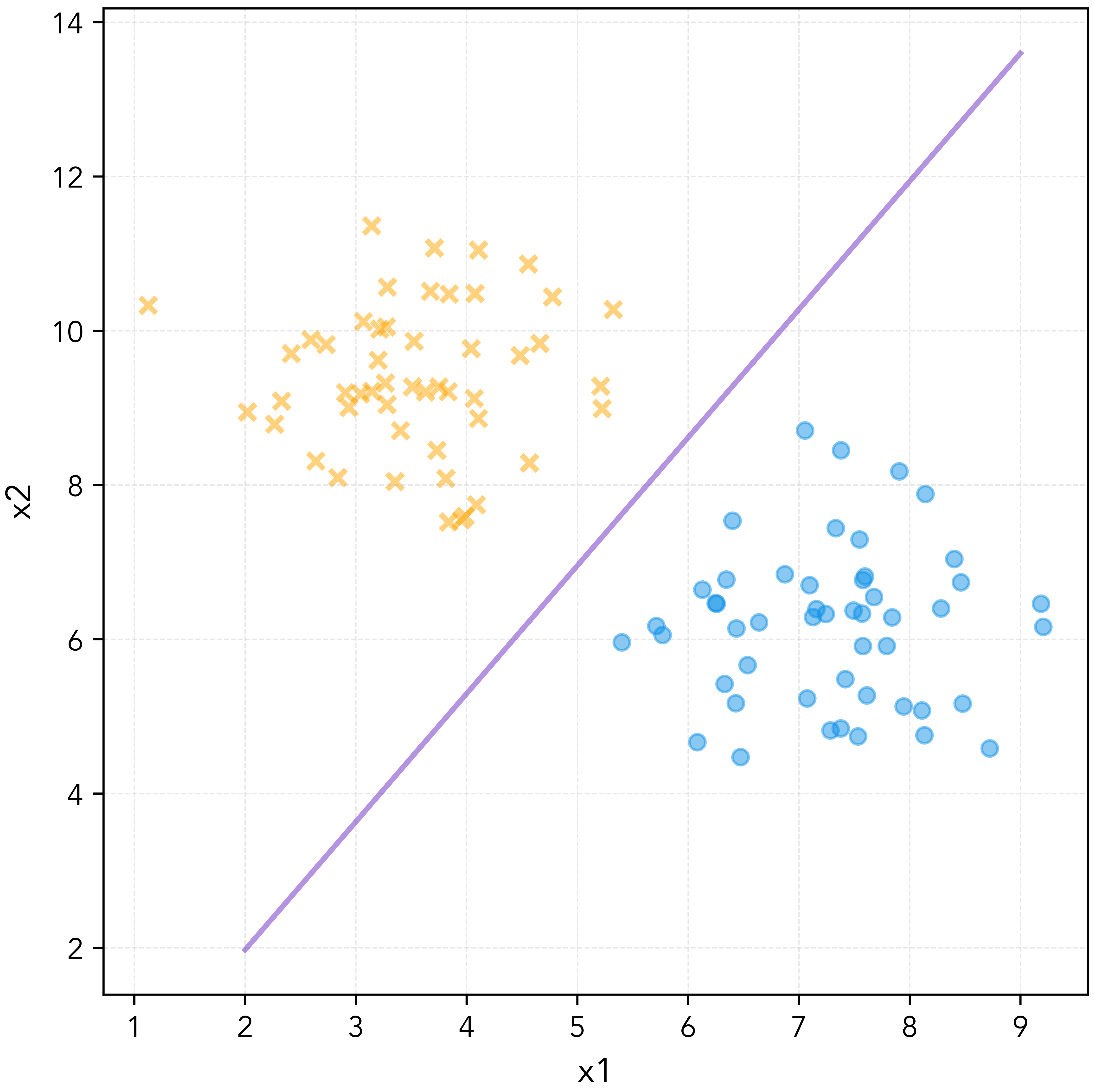
Geometric Picture

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \{-1,1\}$

Outcome space: $\mathcal{Y} = \{-1,1\}$

We will focus on methods that induce
linear decision boundaries (hyperplanes).



Classification

Problem Instance

Input space: $\mathcal{X} = \mathbb{R}^d$

Action space: $\mathcal{A} = \mathbb{R}$

Outcome space: $\mathcal{Y} = \{-1,1\}$

For a **linear** function $f(x) = w^\top x$, the semantics typically are:

$$w^\top x > 0 \implies \text{Predict } 1$$

$$w^\top x < 0 \implies \text{Predict } -1$$

Margin

Definition

The margin for a predicted score $\hat{y}$ and the true class $y \in \{-1,1\}$ is $y\hat{y}$.

With a score function $f : \mathcal{X} \to \mathbb{R}$, the margin is $yf(x)$.

If y and $\hat{y}$ are the same sign, prediction is **correct** and margin is **positive**.

If y and $\hat{y}$ have different sign, prediction is **incorrect** and margin is **negative**.

We want to find f that **maximizes** the margin.

Many classification losses only depend on the margin (margin-based losses).

Classification Losses

Convexity

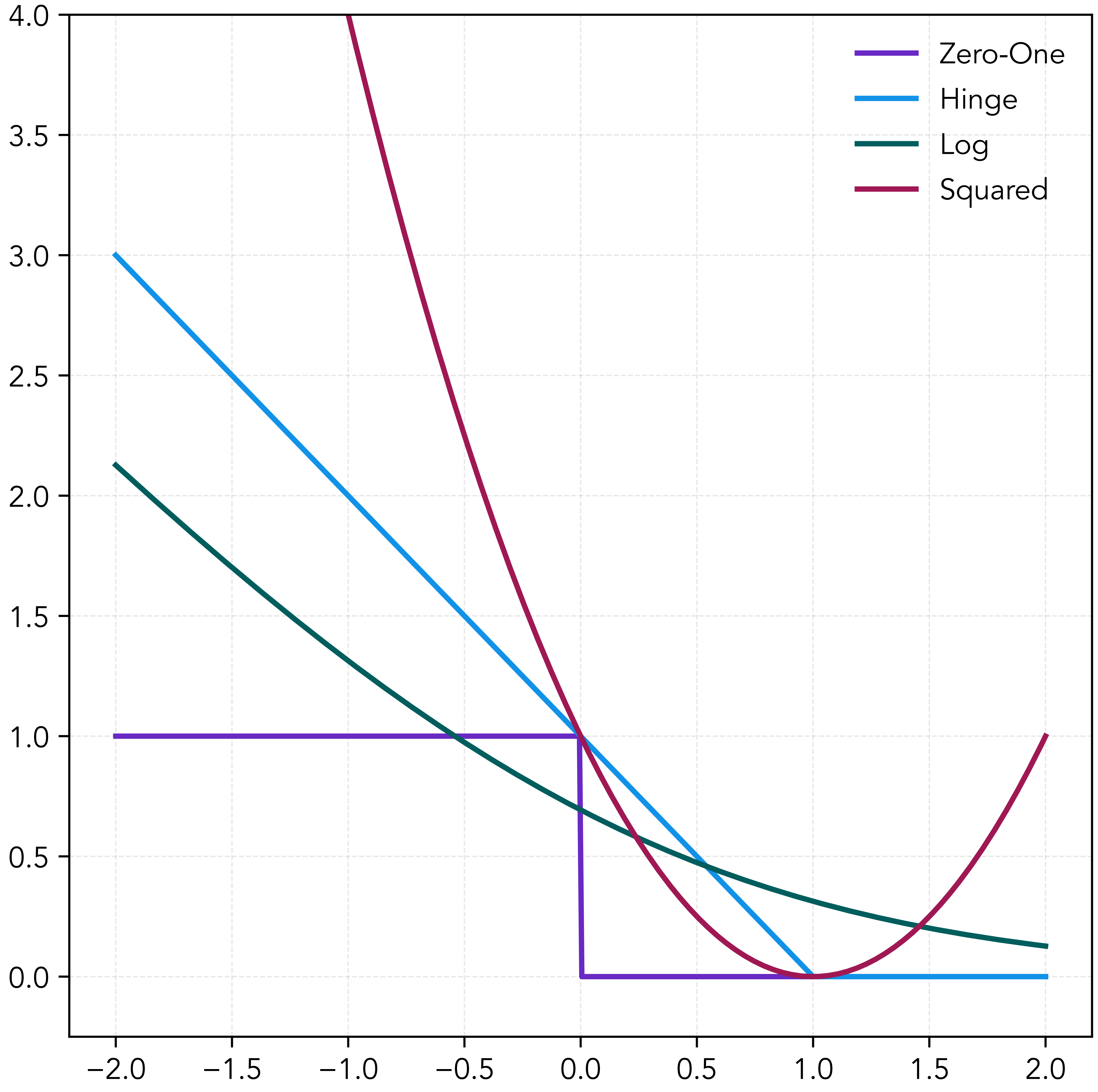
All of these losses have a property in common: **convexity**.

$$\ell_{\text{hinge}}(m) := \max(1 - m, 0)$$

$$\ell_{\text{perc}}(m) := \max(-m, 0)$$

$$\ell_{\log}(m) := \log(1 + e^{-m})$$

$$\ell_{\text{square}}(m) := (1 - m)^2$$



Classification Losses

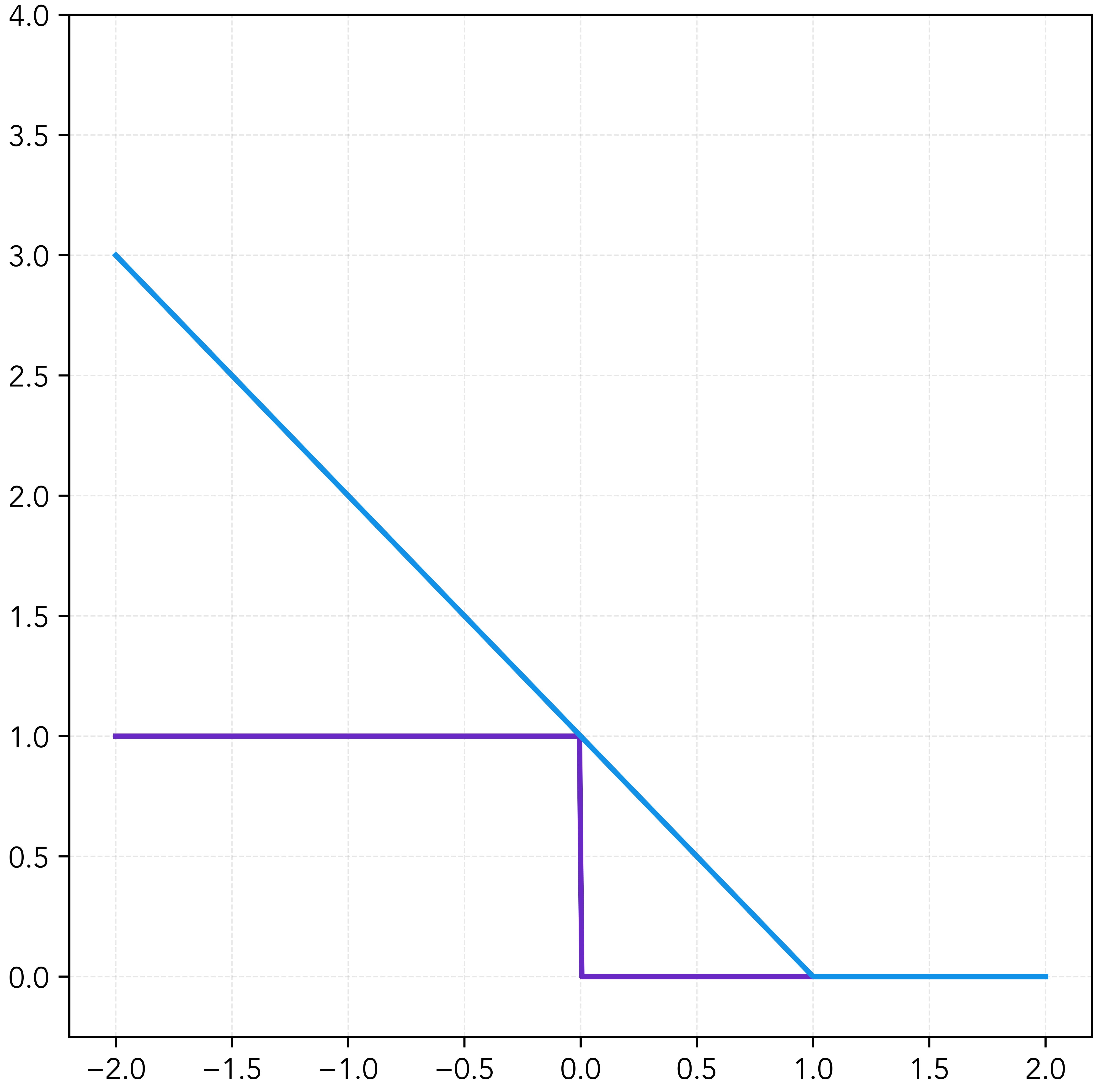
Hinge Loss

Margin: $m = \hat{y}y$

Hinge loss: $\ell_{\text{hinge}}(m) := \max(1 - m, 0)$

Hinge loss is **convex, upper bound** on zero-one loss.

Not differentiable at $m = 1$.



Hinge Loss

(Soft-Margin) Support Vector Machine

Hypothesis class: $\mathscr{H} = \{h_w(x) = w^\top x + b : w \in \mathbb{R}^d, b \in \mathbb{R}\}$

Loss: $\ell_{\text{hinge}}(m) = \max(1 - m, 0)$ (hinge loss)

Regularizer: ℓ_2

Empirical risk minimization:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} \max(1 - y^{(i)} h_w(x^{(i)}), 0) + \frac{C}{2} \|w\|_2^2$$

SVM Optimization Problem

Penalized ERM

Hypothesis class: $\mathscr{H} = \{h_w(x) = w^\top x + b : w \in \mathbb{R}^d, b \in \mathbb{R}\}$

Loss: $\ell_{\text{hinge}}(m) = \max(1 - m, 0)$ (hinge loss)

Regularizer: ℓ_2

Empirical risk minimization:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{C}{n} \sum_{i=1}^{n} \max(1 - y^{(i)}(w^\top x^{(i)} + b), 0) + \frac{1}{2}\|w\|_2^2$$

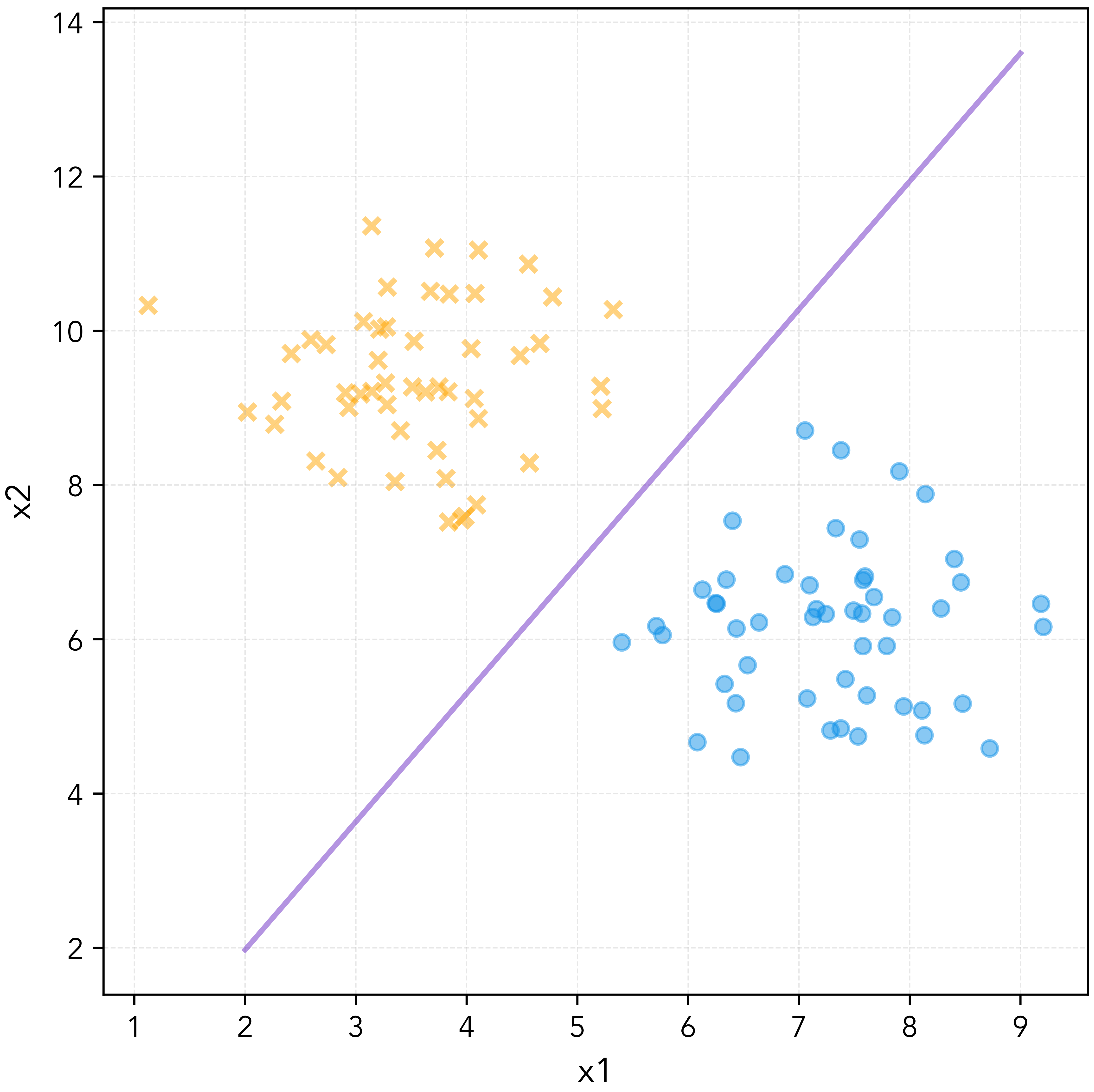
SVM Optimization

(Hyper)plane

The SVM hypothesis is the solution to:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{C}{n} \sum_{i=1}^{n} \max(1 - y^{(i)}(w^\top x^{(i)} + b), 0) + \frac{1}{2}\|w\|_2^2$$

The w and b define an affine (hyper)plane in $\mathbb{R}^d$.



SVM Optimization

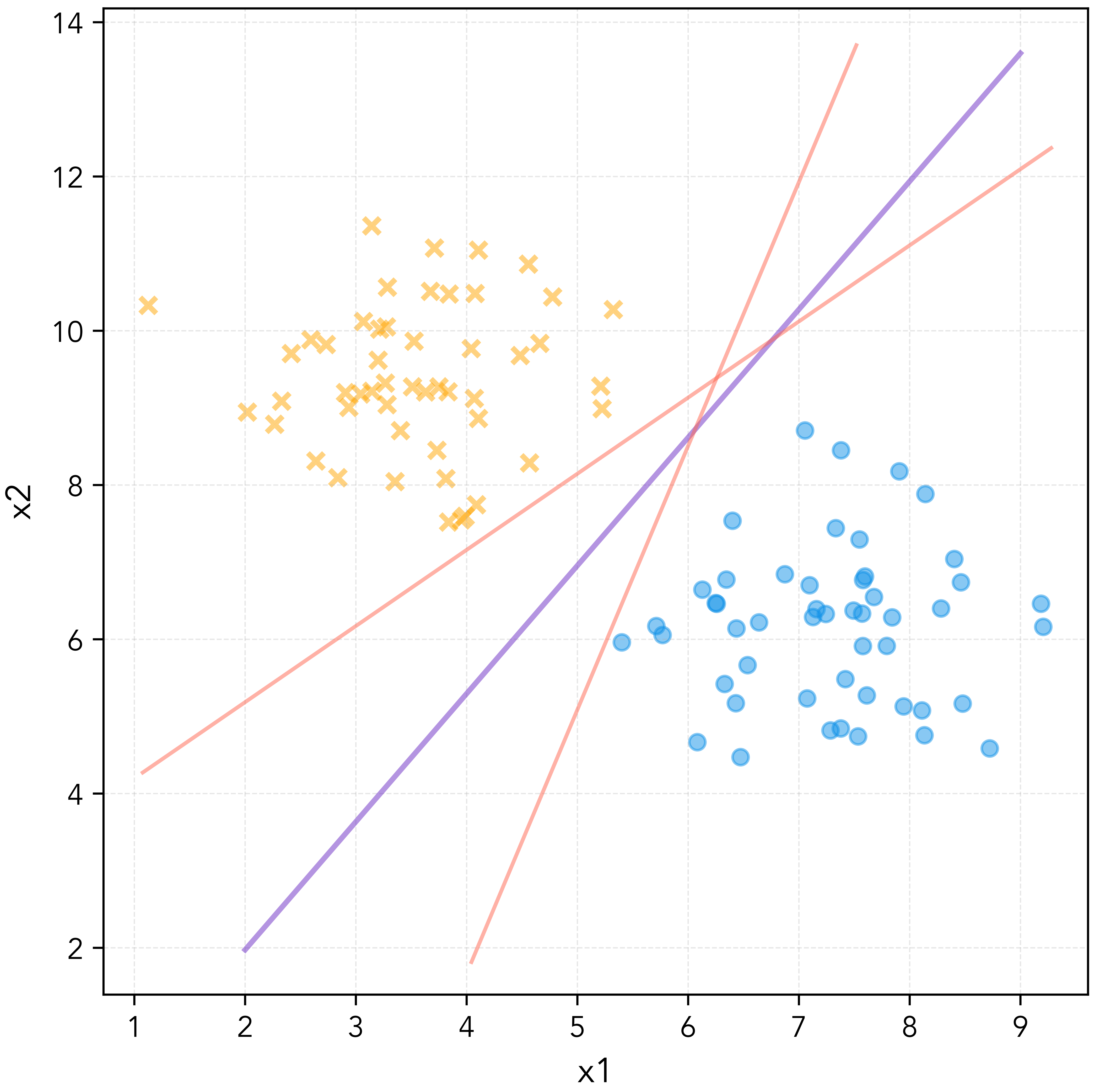
(Hyper)plane

The SVM hypothesis is the solution to:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{C}{n} \sum_{i=1}^{n} \max(1 - y^{(i)}(w^\top x^{(i)} + b), 0) + \frac{1}{2}\|w\|_2^2$$

The w and b define an affine (hyper)plane in $\mathbb{R}^d$.

Turns out this has nice geometric properties (max geometric margin)!



SVM Optimization Problem

Penalized ERM

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{C}{n} \sum_{i=1}^{n} \max(1 - y^{(i)}(w^\top x^{(i)} + b), 0) + \frac{1}{2}\|w\|_2^2$$

Unconstrained optimization problem (penalized ERM).

Not differentiable because of the max (right at the “hinge” of the hinge loss).

Can we re-formulate into a differentiable problem?

SVM Optimization

Constrained ERM

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{C}{n} \sum_{i=1}^{n} \max(1 - y^{(i)}(w^\top x^{(i)} + b),\ 0) + \frac{1}{2}\|w\|_2^2$$

is equivalent to:

$$\begin{aligned} \min_{w \in \mathbb{R}^d, b \in \mathbb{R}, \xi \in \mathbb{R}^n} \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n} \xi_i \\ \text{s.t.} \quad & \xi_i \geq \max\left(1 - y^{(i)}(w^\top x^{(i)} + b),\ 0\right) \end{aligned}$$

SVM Optimization

Constrained ERM

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n} \xi_i \\ \text{s.t.} \quad & \xi_i \geq \max\left(1 - y^{(i)}(w^\top x^{(i)} + b),\ 0\right) \end{aligned}$$

is equivalent to:

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n} \xi_i \\ \text{s.t.} \quad & \xi_i \geq 1 - y^{(i)}(w^\top x^{(i)} + b) \quad \text{for } i = 1,\ldots,n \\ & \xi_i \geq 0 \quad \text{for } i = 1,\ldots,n \end{aligned}$$

SVM Optimization

…is just convex optimization

The SVM optimization problem is equivalent to the **convex optimization problem**:

$$
\begin{aligned}
\min \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i \\
\text{s.t.} \quad & \left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \le 0 \quad \text{for } i = 1,\ldots,n \\
& -\xi_i \le 0 \quad \text{for } i = 1,\ldots,n
\end{aligned}
$$

Objective function is differentiable and convex.

$n + d + 1$ unknowns and $2n$ affine constraints.

Now a quadratic program that can be solved using any off-the-shelf QP solver!

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Lagrange Multipliers

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i \\ \text{s.t.} \quad & \left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \le 0 \quad \text{for } i = 1,\ldots,n \\ & -\xi_i \le 0 \quad \text{for } i = 1,\ldots,n \end{aligned}$$

Lagrange multiplier $\alpha_i \Longleftrightarrow$ Constraint $\left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \le 0.$

Lagrange multiplier $\lambda_i \Longleftrightarrow$ Constraint $-\xi_i \le 0.$

Lagrangian: $L(w, b, \xi, \alpha, \lambda) = \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(1 - y^{(i)}(w^\top x^{(i)} + b) - \xi_i\right) + \sum_{i=1}^{n}\lambda_i(-\xi_i)$

Dual SVM Problem

Weak Duality

$$L(w, b, \xi, \alpha, \lambda) = \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(1 - y^{(i)}(w^\top x^{(i)} + b) - \xi_i\right) + \sum_{i=1}^{n}\lambda_i(-\xi_i)$$

$$\iff L(w, b, \xi, \alpha, \lambda) = \frac{1}{2}w^\top w + \sum_{i=1}^{n}\xi_i\left(\frac{C}{n} - \alpha_i - \lambda_i\right) + \sum_{i=1}^{n}\alpha_i\left(1 - y^{(i)}\left(w^\top x^{(i)} + b\right)\right)$$

By **weak duality**: $p^* = \min_{w,\xi,b}\max_{\alpha,\lambda\geq 0} L(w, b, \xi, \alpha, \lambda) \geq \max_{\alpha,\lambda\geq 0}\min_{w,\alpha,b} L(w, b, \xi, \alpha, \lambda) = d^*$.

Do we have **strong duality**:

$$p^* = d^*?$$

Constraint Qualification

Slater's Conditions

When is $p^* = d^*$ (strong duality) for *convex optimization*?

Roughly: the problem must be **strictly** feasible (there is *some* solution).

Qualifications when problem domain $\mathcal{D} = \bigcap_{i=0}^{m} \mathrm{dom}\, f_i \subseteq \mathbb{R}^d$ is an open set:

Strict feasibility is sufficient (there exists x such that $f_i(x) < 0$ for all $i = 1,\ldots,m$).

For affine inequality constraints, finding x such that $f_i(x) \leq 0$ is sufficient.

If $\mathcal{D}$ is not open, see notes in B&V Section 5.2.3, pg. 226.

Checking Strong Duality

Slater's Condition

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i \\ \text{s.t.} \quad & \left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \le 0 \quad \text{for } i = 1,\ldots,n \\ & -\xi_i \le 0 \quad \text{for } i = 1,\ldots,n \end{aligned}$$

Convex problem + affine constraints $\Longrightarrow$ strong duality iff the problem is feasible.

Constraints are satisfied by $w = b = 0$ and $\xi_i = 1$ for $i = 1,\ldots,n$.

Therefore, we do have strong duality!

$$p^* = \min_{w,\xi,b} \max_{\alpha,\lambda \ge 0} L(w, b, \xi, \alpha, \lambda) = \max_{\alpha,\lambda \ge 0} \min_{w,\alpha,b} L(w, b, \xi, \alpha, \lambda) = d^*$$

Dual Function

Best Lower Bound

$$g(\lambda) = \min_x L(x, \lambda) = \min_x \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) \right)$$

In terms of the Lagrange dual function, we can write weak duality as:

$$p* \geq \max_{\lambda \geq 0} g(\lambda) = d*.$$

$$p* \geq g(\lambda) \text{ for all } \lambda \geq 0.$$

So any λ with $\lambda \geq 0$ in dual function gives a **lower bound** on the optimal solution.

Lagrangian Dual

How to find the Lagrangian dual?

Lagrangian dual is the $\min$ over primal variables of the Lagrangian:

$$\begin{aligned} g(\alpha, \lambda) &= \min_{w,b,\xi} L(w, b, \xi, \alpha, \lambda) \\ &= \min_{w,b,\xi} \left[\frac{1}{2} w^\top w + \sum_{i=1}^{n} \xi_i \left(\frac{C}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^{n} \alpha_i \left(1 - y^{(i)} \left(w^\top x^{(i)} + b \right) \right) \right] \end{aligned}$$

Taking the $\min$ of convex and differentiable function of w, b, ξ.

Quadratic in w and linear in ξ and b.

Thus, optimal point iff $\partial_w L = 0$, $\partial_b L = 0$, and $\partial_\xi L = 0$.

Lagrangian Dual

Taking derivatives

$$g(\alpha, \lambda) = \min_{w,b,\xi} L(w, b, \xi, \alpha, \lambda)$$

$$= \min_{w,b,\xi} \left[\frac{1}{2} w^\top w + \sum_{i=1}^{n} \xi_i \left(\frac{C}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^{n} \alpha_i \left(1 - y^{(i)} \left(w^\top x^{(i)} + b \right) \right) \right]$$

$$\partial_w L = 0 \iff w - \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} = 0 \iff w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)}$$

$$\partial_b L = 0 \iff -\sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \iff \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\partial_\xi L = 0 \iff \frac{C}{n} - \alpha_i - \lambda_i = 0 \iff \alpha_i + \lambda_i = \frac{C}{n}$$

Lagrangian Dual

Plugging back in to the dual

$$w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)}$$

$$\sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\alpha_i + \lambda_i = \frac{C}{n}$$

$$\begin{aligned} g(\alpha, \lambda) &= \min_{w,b,\xi} L(w, b, \xi, \alpha, \lambda) \\ &= \min_{w,b,\xi} \left[\frac{1}{2} w^\top w + \sum_{i=1}^{n} \xi_i \left(\frac{C}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^{n} \alpha_i \left(1 - y^{(i)} \left(w^\top x^{(i)} + b \right) \right) \right] \end{aligned}$$

Dual Optimization Problem

Maximum over the Lagrangian Dual

$$\max_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(j)})^\top x^{(i)}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\alpha_i \in \left[0, \frac{C}{n}\right] \quad \text{for } i = 1, \ldots, n$$

Given solution α^* to dual, the primal solution is $w^* = \sum_{i=1}^{n} \alpha_i^* y^{(i)} x^{(i)}$ (in the "span of the data")

Regularization parameter C controls the max weight put on each example: $\alpha_i^* \in \left[0, \frac{C}{n}\right]$.

SVM Optimization

Dual Optimization Problem

$$\max_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(j)})^\top x^{(i)}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\alpha_i \in \left[0, \frac{C}{n}\right] \quad \text{for } i = 1, \ldots, n$$

Quadratic objective with n unknowns and $n + 1$ constraints.

What other insights can we get from the dual formulation?

SVM Optimization

Primal and Dual

$$\min_{w,b,\xi} \quad \frac{1}{2}\|w\|^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad \left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \le 0 \quad \text{for } i = 1,\ldots,n$$

$$-\xi_i \le 0 \quad \text{for } i = 1,\ldots,n$$

$$\max_{\alpha} \quad \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(j)})^\top x^{(i)}$$

$$\text{s.t.} \quad \sum_{i=1}^{n}\alpha_i y^{(i)} = 0$$

$$\alpha_i \in \left[0, \frac{C}{n}\right] \quad \text{for } i = 1,\ldots,n$$

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Classification Losses

Hinge Loss

$$f^*(x) = x^\top w^* + b^*$$

Margin: $m = yf^*(x)$

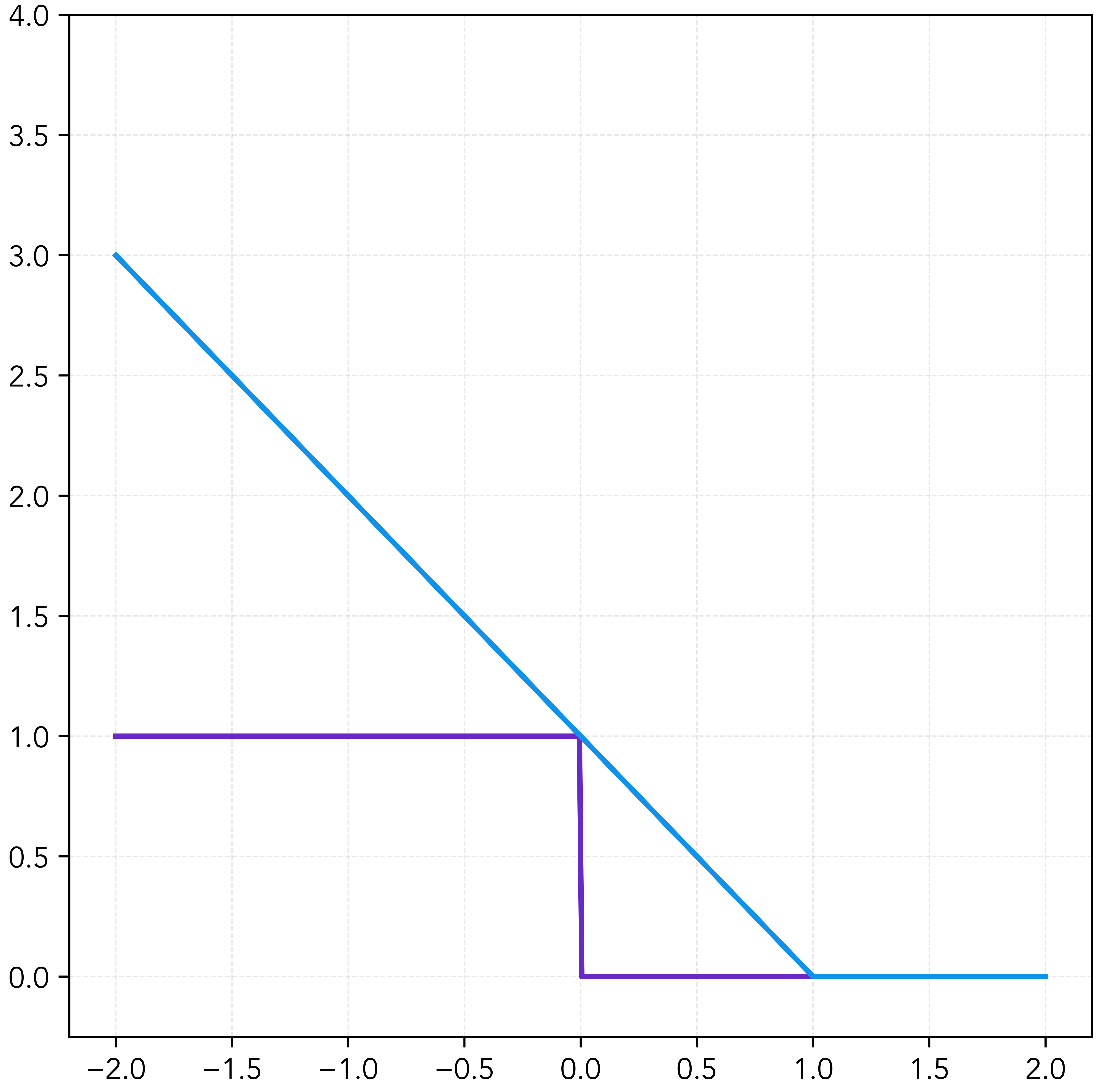
$$\ell_{\text{hinge}}(yf^*(x)) := \max(1 - yf^*(x), 0)$$

Incorrect: $yf^*(x) \leq 0.$

"Margin error": $yf^*(x) < 1.$

"On the margin": $yf^*(x) = 1$

"Good side of margin": $yf^*(x) > 1.$



Support Vectors

Relationship to margin

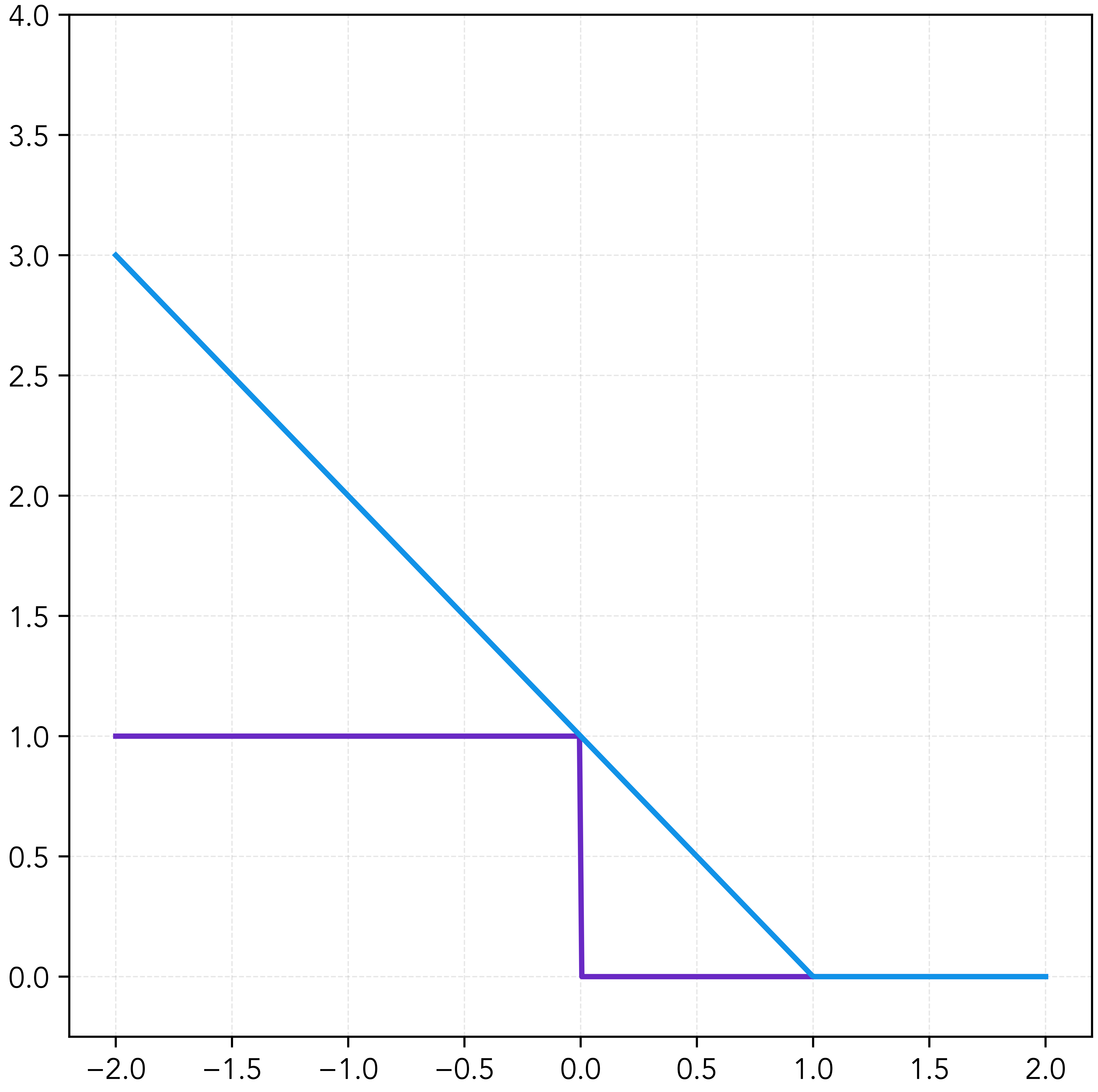
Slack variable $\xi_i^* = \max(1 - y^{(i)} f^*(x^{(i)}),\ 0)$ is the hinge loss on $(x^{(i)}, y^{(i)})$.

Suppose $\xi_i^* = 0$. Then, $y^{(i)} f^*(x^{(i)}) \geq 1$, i.e.

"On the margin" ($= 1$), or

"On the good side" (> 1).

$$\xi_i^* = 0 \iff y^{(i)} f^*(x^{(i)}) \geq 1$$



Complementary Slackness

Recall

If **strong duality** holds, we get an interesting relationship between:

Optimal Lagrange multiplier λ_i^* and

The ith constraint at the optimum: $f_i(x^*)$.

The relationship is called complementary slackness:

$$\lambda_i^* f_i(x^*) = 0$$

Always have Lagrange multiplier is zero **or** constraint is active at optimum **or** both.

Strong Duality

Complementary Slackness

Lagrange multiplier $\lambda_i \iff$ Constraint $-\xi_i \leq 0.$

Lagrange multiplier $\alpha_i \iff$ Constraint $\left(1 - y^{(i)}(w^\top x^{(i)} + b)\right) - \xi_i \leq 0.$

Recall first-order condition $\partial_{\xi_i} L = 0$ gave us $\lambda_i^* = \dfrac{C}{n} - \alpha_i^*$.

By strong duality, **complementary slackness**:

$$\lambda_i^* \xi_i^* = \left(\frac{C}{n} - \alpha_i^*\right) \xi_i^* = 0$$

$$\alpha_i^*(1 - y^{(i)} f^*(x^{(i)}) - \xi_i^*) = 0$$

Strong Duality

Complementary Slackness

$$\lambda_i^* \xi_i^* = \left(\frac{C}{n} - \alpha_i^* \right) \xi_i^* = 0$$

$$\alpha_i^* (1 - y^{(i)} f^*(x^{(i)}) - \xi_i^*) = 0$$

If $y^{(i)} f^*(x^{(i)}) > 1 \implies$ margin loss $\xi_i^* = 0$ so we get $\alpha_i^* = 0$.

If $y^{(i)} f^*(x^{(i)}) < 1 \implies$ margin loss $\xi_i^* > 0$ so $\alpha_i^* = \frac{C}{n}$.

If $\alpha_i^* = 0 \implies \xi_i^* = 0$, which implies no loss, so $y^{(i)} f^*(x^{(i)}) \geq 1$.

If $\alpha_i^* \in \left(0, \frac{C}{n}\right) \implies \xi_i^* = 0$, which implies $1 - y^{(i)} f^*(x^{(i)}) = 0$.

Strong Duality

Summary of Complementary Slackness

$$\alpha_i^* = 0 \implies y^{(i)} f^*(x^{(i)}) \geq 1$$

$$\alpha_i^* \in \left(0, \frac{C}{n}\right) \implies y^{(i)} f^*(x^{(i)}) = 1$$

$$\alpha_i^* = \frac{C}{n} \implies y^{(i)} f^*(x^{(i)}) \leq 1$$

$$y^{(i)} f^*(x^{(i)}) < 1 \implies \alpha_i^* = \frac{C}{n}$$

$$y^{(i)} f^*(x^{(i)}) = 1 \implies \alpha_i^* \in \left[0, \frac{C}{n}\right]$$

$$y^{(i)} f^*(x^{(i)}) > 1 \implies \alpha_i^* = 0$$

When $y^{(i)} f^*(x^{(i)}) > 1$ (*good side of margin*), we are guaranteed $\alpha_i^* = 0$.

When $y^{(i)} f^*(x^{(i)}) = 1$ (*exactly on margin*), we *could* have $\alpha_i^* = 0$ or $\alpha_i^* > 0$.

When $y^{(i)} f^*(x^{(i)}) < 1$ (*bad side of margin*), we are guaranteed $\alpha_i^* > 0$.

Strong Duality

Support Vector Interpretation

If α^* is a solution to the dual problem, the primal solution is:

$$w^* = \sum_{i=1}^{n} \alpha_i^* y^{(i)} x^{(i)} \quad \text{with } \alpha_i^* \in \left[0, \frac{C}{n}\right]$$

The $x^{(i)}$'s corresponding to $\alpha_i^* > 0$ are called **support vectors**.

By comp. slackness, correspond to points *on the margin* or *on bad side of margin*.

Few margin errors or "on the margin" examples $\Longrightarrow$ **sparsity in input examples**.

Strong Duality

Getting $b*$

$$\lambda_i^* \xi_i^* = \left(\frac{C}{n} - \alpha_i^*\right) \xi_i^* = 0$$

$$\alpha_i^*(1 - y^{(i)} f^*(x^{(i)}) - \xi_i^*) = 0$$

Suppose there's an i such that $\alpha_i^* \in \left(0, \frac{C}{n}\right)$.

$$\lambda_i^* \xi_i^* = \left(\frac{C}{n} - \alpha_i^*\right) \xi_i^* = 0 \Longrightarrow \xi_i^* = 0$$

$$\alpha_i^*(1 - y^{(i)} f^*(x^{(i)}) - \xi_i^*) = 0 \Longrightarrow y^{(i)}((x^{(i)})^\top w^* + b^*) = 1 \Longleftrightarrow (x^{(i)})^\top w^* + b^* = y^{(i)}$$

$$\Longleftrightarrow b^* = y^{(i)} - (x^{(i)})^\top w^*$$

Strong Duality

Getting b^*

Therefore, the optimal b is:

$$b^* = y^{(i)} - (x^{(i)})^\top w^*.$$

We get the same b^* for any choice of i with $\alpha_i^* \in \left(0, \frac{C}{n}\right)$.

If there are no $\alpha_i^* \in \left(0, \frac{C}{n}\right)$?

Then we have a **degenerate SVM training problem** ($w^* = 0$).

Dual Problem

Teaser for Kernelization

$$\max_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(j)})^\top x^{(i)}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\alpha_i \in \left[0, \frac{C}{n}\right] \quad \text{for } i = 1, \ldots, n$$

All dependence on inputs $x^{(i)}$ and $x^{(j)}$ is through the inner product $\langle x^{(j)}, x^{(i)} \rangle = (x^{(j)})^\top x^{(i)}$.

What if we replace $(x^{(j)})^\top x^{(i)}$ with some other inner product?

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