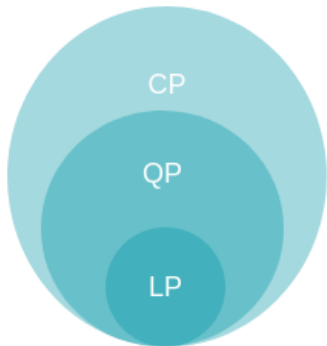


# Optimization in Machine Learning

## Optimization Problems

## Constrained problems



### Learning goals

- Definition
- LP, QP, CP
- Ridge and Lasso
- Soft-margin SVM

# CONSTRAINED OPTIMIZATION PROBLEM

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x}), \text{ with } f : \mathcal{S} \rightarrow \mathbb{R}.$$

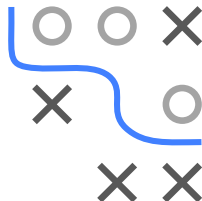
- **Constrained**, if domain  $\mathcal{S}$  is restricted:  $\mathcal{S} \subsetneq \mathbb{R}^d$ .
- **Convex** if  $f$  convex function and  $\mathcal{S}$  convex set
- Typically  $\mathcal{S}$  is defined via functions called **constraints**

$$\mathcal{S} := \{\mathbf{x} \in \mathbb{R}^d \mid g_i(\mathbf{x}) \leq 0, h_j(\mathbf{x}) = 0 \forall i, j\}, \text{ where}$$

- $g_i : \mathbb{R}^d \rightarrow \mathbb{R}, i = 1, \dots, k$  are called inequality constraints,
- $h_j : \mathbb{R}^d \rightarrow \mathbb{R}, j = 1, \dots, l$  are called equality constraints.

Equivalent formulation:

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{such that} & g_i(\mathbf{x}) \leq 0 \quad \text{for } i = 1, \dots, k \\ & h_j(\mathbf{x}) = 0 \quad \text{for } j = 1, \dots, l. \end{array}$$

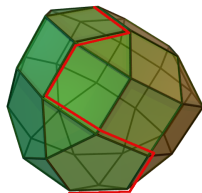
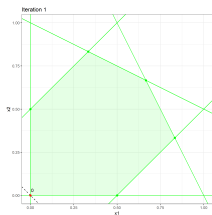


# LINEAR PROGRAM (LP)

- $f$  linear s.t. linear constraints. Standard form:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & \mathbf{Ax} \geq \mathbf{b} \\ & \mathbf{x} \geq 0 \end{aligned}$$

for  $\mathbf{c} \in \mathbb{R}^d$ ,  $\mathbf{A} \in \mathbb{R}^{k \times d}$  and  $\mathbf{b} \in \mathbb{R}^k$ .

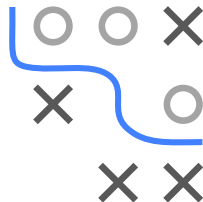


Visualization of constraints of 2D and 3D linear program (Source right figure: Wikipedia).

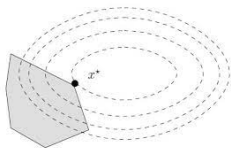
# QUADRATIC PROGRAM (QP)

- $f$  quadratic form s.t. linear constraints. Standard form:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & \frac{1}{2} \mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b}^\top \mathbf{x} + c \\ \text{s.t.} \quad & \mathbf{E} \mathbf{x} \leq \mathbf{f} \\ & \mathbf{G} \mathbf{x} = \mathbf{h} \end{aligned}$$



$$\mathbf{A} \in \mathbb{R}^{d \times d}, \mathbf{b} \in \mathbb{R}^d, c \in \mathbb{R}, \mathbf{E} \in \mathbb{R}^{k \times d}, \mathbf{f} \in \mathbb{R}^k, \mathbf{G} \in \mathbb{R}^{l \times d}, \mathbf{h} \in \mathbb{R}^l.$$



Visualization of quadratic objective (dashed) over linear constraints (grey). Source: Ma, Signal Processing Optimization Techniques, 2015.

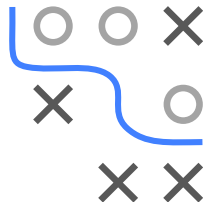
# CONVEX PROGRAM (CP)

- $f$  convex, convex inequality constraints, linear equality constraints.

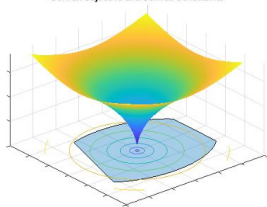
Standard form:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & g_i(\mathbf{x}) \leq 0, i = 1, \dots, k \\ & \mathbf{Ax} = \mathbf{b} \end{aligned}$$

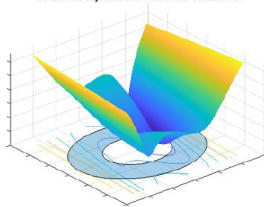
for  $\mathbf{A} \in \mathbb{R}^{l \times d}$  and  $\mathbf{b} \in \mathbb{R}^l$ .



Convex Objective and Convex Constraints

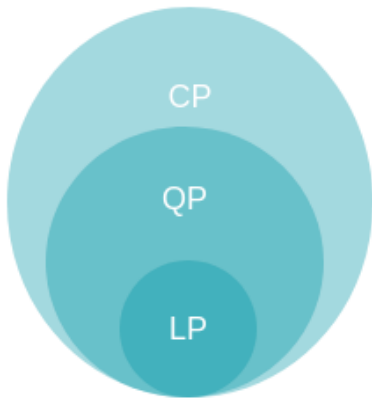


Nonconvex Objective and Nonconvex Constraints



Convex program (left) vs. nonconvex program (right). Source: Mathworks.

# FURTHER TYPES

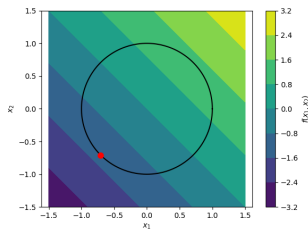


Quadratically constrained linear program (QCLP) and quadratically constrained quadratic program (QCQP).



# EXAMPLE 1: UNIT CIRCLE

$$\begin{array}{ll}\min & f(x_1, x_2) = x_1 + x_2 \\ \text{s.t.} & h(x_1, x_2) = x_1^2 + x_2^2 - 1 = 0\end{array}$$



$f, h$  smooth. Problem **not convex** ( $\mathcal{S}$  is not a convex set).

**Note:** If the constraint is replaced by  $g(x_1, x_2) = x_1^2 + x_2^2 - 1 \leq 0$ , the problem is a convex program, even a quadratically constrained linear program (QCLP).

## EXAMPLE 2: MAXIMUM LIKELIHOOD

**Experiment:** Draw  $m$  balls from a bag with balls of  $k$  different colors. Color  $j$  has a probability of  $p_j$  of being drawn.

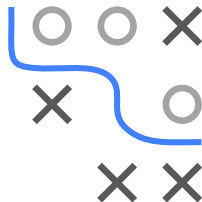
The probability to realize the outcome  $\mathbf{x} = (x_1, \dots, x_k)$ ,  $x_j$  being the number of balls drawn in color  $j$ , is:

$$f(\mathbf{x}, m, \mathbf{p}) = \begin{cases} \frac{m!}{x_1! \cdots x_k!} \cdot p_1^{x_1} \cdots p_k^{x_k} & \text{if } \sum_{i=1}^k x_i = m \\ 0 & \text{otherwise} \end{cases}$$

The parameters  $p_j$  are subject to the following constraints:

$$0 \leq p_j \leq 1 \quad \text{for all } i$$

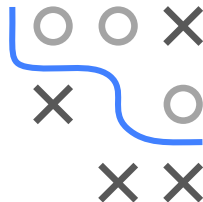
$$\sum_{j=1}^m p_j = 1.$$





## EXAMPLE 2: MAXIMUM LIKELIHOOD / 2

For a fixed  $m$  and a sample  $\mathcal{D} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)})$ , where  $\sum_{j=1}^k \mathbf{x}_j^{(i)} = m$  for all  $i = 1, \dots, n$ , the negative log-likelihood is:



$$\begin{aligned} -\ell(\mathbf{p}) &= -\log \left( \prod_{i=1}^n \frac{m!}{\mathbf{x}_1^{(i)}! \cdots \mathbf{x}_k^{(i)}!} \cdot p_1^{\mathbf{x}_1^{(i)}} \cdots p_k^{\mathbf{x}_k^{(i)}} \right) \\ &= \sum_{i=1}^n \left[ -\log(m!) + \sum_{j=1}^k \log(\mathbf{x}_j^{(i)}!) - \sum_{j=1}^k \mathbf{x}_j^{(i)} \log(p_j) \right] \\ &\propto -\sum_{i=1}^n \sum_{j=1}^k \mathbf{x}_j^{(i)} \log(p_j) \end{aligned}$$

$f, g, h$  are smooth.

**Convex program:** convex<sup>(\*)</sup> objective + box/linear constraints).

(<sup>\*</sup>): log is concave,  $-\log$  is convex, and the sum of convex functions is convex.

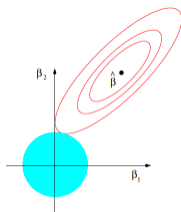
## EXAMPLE 3: RIDGE REGRESSION

Ridge regression can be formulated as regularized ERM:

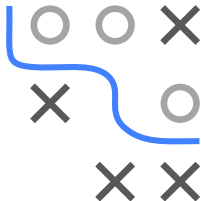
$$\hat{\theta}_{\text{Ridge}} = \arg \min_{\theta} \left\{ \sum_{i=1}^n \left( y^{(i)} - \theta^{\top} \mathbf{x} \right)^2 + \lambda \|\theta\|_2^2 \right\}$$

Equivalently it can be written as constrained optimization problem:

$$\begin{aligned} \min_{\theta} \quad & \sum_{i=1}^n \left( \theta^{\top} \mathbf{x}^{(i)} - y^{(i)} \right)^2 \\ \text{s.t.} \quad & \|\theta\|_2 \leq t \end{aligned}$$



$f, g$  smooth. **Convex program** (convex objective, quadratic constraint).



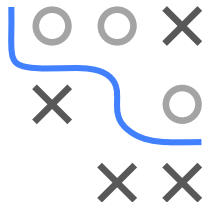
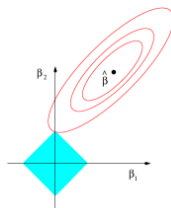
## EXAMPLE 4: LASSO REGRESSION

Lasso regression can be formulated as regularized ERM:

$$\hat{\theta}_{\text{Lasso}} = \arg \min_{\theta} \left\{ \sum_{i=1}^n \left( y^{(i)} - \theta^{\top} \mathbf{x} \right)^2 + \lambda \|\theta\|_1 \right\}$$

Equivalently it can be written as constrained optimization problem:

$$\begin{aligned} \min_{\theta} \quad & \sum_{i=1}^n \left( \theta^{\top} \mathbf{x}^{(i)} - y^{(i)} \right)^2 \\ \text{s.t.} \quad & \|\theta\|_1 \leq t \end{aligned}$$

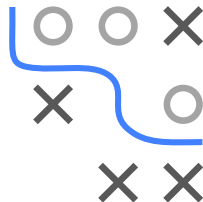


$f$  smooth,  $g$  **not smooth**. Still **convex program**.

# EXAMPLE 5: SUPPORT VECTOR MACHINES

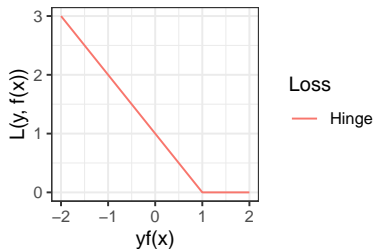
The SVM problem can be formulated in 3 equivalent ways: two primal, and one dual one (we will see later what "dual" means).

Here, we only discuss the nature of the optimization problems. A more thorough statistical derivation of SVMs is given in "Supervised learning".



**Formulation 1 (primal):** ERM with Hinge loss

$$\sum_{i=1}^n \max \left( 1 - y^{(i)} f^{(i)}, 0 \right) + \lambda \|\boldsymbol{\theta}\|_2^2, \quad f^{(i)} := \boldsymbol{\theta}^\top \mathbf{x}^{(i)}$$

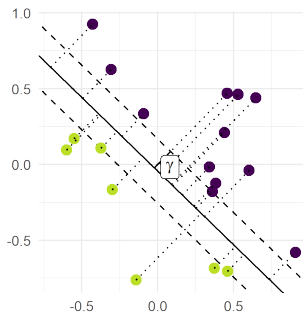


Unconstrained, convex problem  
with non-smooth objective

# EXAMPLE 5: SUPPORT VECTOR MACHINES / 2

## Formulation 2 (primal): Geometric formulation

- Find decision boundary which separates classes with **maximum** safety distance
- Distance to points closest to decision boundary (“safety margin  $\gamma$ ”) should be **maximized**

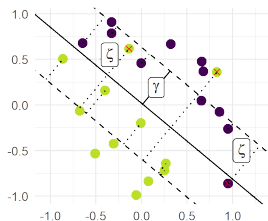




# EXAMPLE 5: SUPPORT VECTOR MACHINES

**Formulation 2 (primal):** Geometric formulation (soft constraints)

$$\begin{aligned} \min_{\theta, \theta_0, \zeta^{(i)}} \quad & \frac{1}{2} \|\theta\|^2 + c \sum_{i=1}^n \zeta^{(i)} \\ \text{s.t.} \quad & y^{(i)} \left( \langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0 \right) \geq 1 - \zeta^{(i)} \quad \forall i \in \{1, \dots, n\}, \\ \text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$



Maximize safety margin  $\gamma$ .

Margin violations are allowed,  
but are minimized.



The problem is a **QP**: Quadratic objective with linear constraints.

## EXAMPLE 5: SUPPORT VECTOR MACHINES

### Formulation 3 (dual): Dualizing the primal formulation

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle$$

$$\text{s.t.} \quad 0 \leq \alpha_i \leq C \quad \forall i \in \{1, \dots, n\}, \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0$$

*Matrix notation:*

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \alpha^\top \mathbf{1} - \frac{1}{2} \alpha^\top \text{diag}(\mathbf{y}) \mathbf{X}^\top \mathbf{X} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \quad \forall i \in \{1, \dots, n\}, \quad \alpha^\top \mathbf{y} = 0 \end{aligned}$$

**Kernelization:** Replace dot product between  $\mathbf{x}$ 's with  $\mathbf{K}_{ij} = k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ , where  $k(\cdot, \cdot)$  is a positive definite kernel function ( $\Rightarrow \mathbf{K}$  positive semi-definite).

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \alpha^\top \mathbf{1} - \frac{1}{2} \alpha^\top \text{diag}(\mathbf{y}) \mathbf{K} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \quad \forall i \in \{1, \dots, n\}, \quad \alpha^\top \mathbf{y} = 0 \end{aligned}$$

This is QP with a single affine equality constraint and  $n$  box constraints.