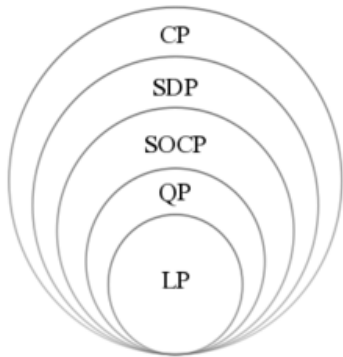


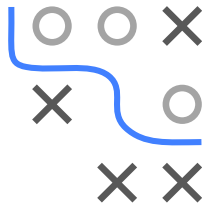
# Optimization in Machine Learning

## Constrained Optimization



### Learning goals

- Examples of constrained optimization in statistics and ML
- General definition
- Hierarchy of convex constrained problems



# CONSTRAINED OPTIMIZATION IN STATISTICS

## Example: Maximum Likelihood Estimation

For data  $(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)})$ , we want to find the maximum likelihood estimate

$$\max_{\theta} L(\theta) = \prod_{i=1}^n f(\mathbf{x}^{(i)}, \theta)$$

In some cases,  $\theta$  can only take **certain values**.

- If  $f$  is a Poisson distribution, we require the rate  $\lambda$  to be non-negative, i.e.  $\lambda \geq 0$



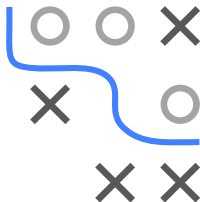
# CONSTRAINED OPTIMIZATION IN STATISTICS / 2

- If  $f$  is a multinomial distribution

$$f(x_1, \dots, x_p; n; \theta_1, \dots, \theta_p) = \begin{cases} \binom{n!}{x_1! \cdot x_2! \cdot \dots \cdot x_p!} \theta_1^{x_1} \cdot \dots \cdot \theta_p^{x_p} & \text{if } x_1 + \dots + x_p = n \\ 0 & \text{else} \end{cases}$$

The probabilities  $\theta_i$  must lie between 0 and 1 and add up to 1, i.e. we require

$$\begin{aligned} 0 \leq \theta_i \leq 1 & \quad \text{for all } i \\ \theta_1 + \dots + \theta_p &= 1. \end{aligned}$$



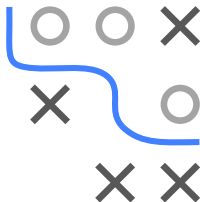
# CONSTRAINED OPTIMIZATION IN ML

- **Lasso regression:**

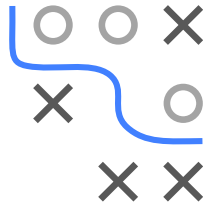
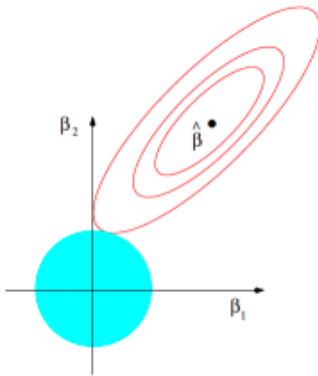
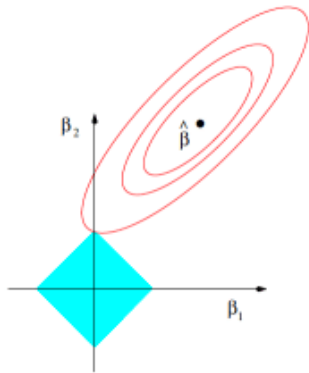
$$\begin{aligned} \min_{\beta \in \mathbb{R}^p} \quad & \frac{1}{n} \sum_{i=1}^n \left( y^{(i)} - \beta^T \mathbf{x}^{(i)} \right)^2 \\ \text{s.t.} \quad & \|\beta\|_1 \leq t \end{aligned}$$

- **Ridge regression:**

$$\begin{aligned} \min_{\beta \in \mathbb{R}^p} \quad & \frac{1}{n} \sum_{i=1}^n \left( y^{(i)} - \beta^T \mathbf{x}^{(i)} \right)^2 \\ \text{s.t.} \quad & \|\beta\|_2 \leq t \end{aligned}$$



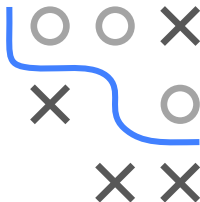
# CONSTRAINED OPTIMIZATION IN ML / 2



# CONSTRAINED OPTIMIZATION IN ML / 3

- Constrained Lasso regression:

$$\begin{aligned} \min_{\beta \in \mathbb{R}^p} \quad & \frac{1}{n} \sum_{i=1}^n \left( y^{(i)} - \beta^T \mathbf{x}^{(i)} \right)^2 \\ \text{s.t.} \quad & \|\beta\|_1 \leq t \\ & \mathbf{C}\beta \leq \mathbf{d} \\ & \mathbf{A}\beta = \mathbf{b}, \end{aligned}$$



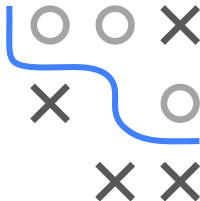
where the matrices  $\mathbf{A} \in \mathbb{R}^{l \times p}$  and  $\mathbf{C} \in \mathbb{R}^{k \times p}$  have full row rank.

This model includes many Lasso variants as special cases, e.g., the Generalized Lasso, (sparse) isotonic regression, log-contrast regression for compositional data, etc. (see, e.g., [Gaines et al., 2018](#)).

## CONSTRAINED OPTIMIZATION IN ML / 4

Remember the dual formulation of the SVM, which is a convex quadratic program with box constraints plus one linear constraint:

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$



# CONSTRAINED OPTIMIZATION

General definition of a **Constrained Optimization problem**:

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

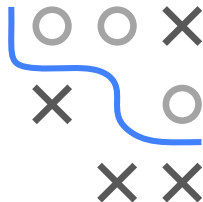
where

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

The set of inputs  $\mathbf{x}$  that fulfill the constraints, i.e.,

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

is known as the **feasible set**.

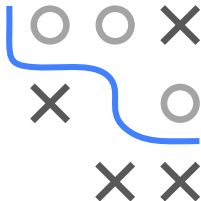
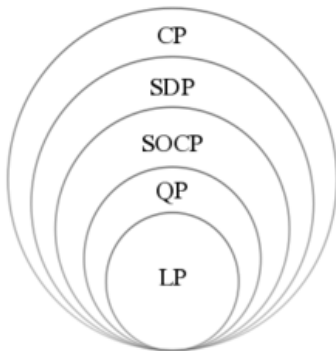




# CONSTRAINED CONVEX OPTIMIZATION

Special cases of constrained optimization problems are **convex programs**, with convex objective function  $f$ , convex inequality constraints  $g_i$ , and affine equality constraints  $h_j$  (i.e.  $h_j(\mathbf{x}) = \mathbf{A}_j^\top \mathbf{x} - \mathbf{b}_j$ ).

Convex programs can be categorized into



# CONSTRAINED CONVEX OPTIMIZATION / 2

- Linear program (LP): objective function  $f$  and all constraints  $g_i, h_j$  are linear functions
- Quadratic program (QP): objective function  $f$  is a quadratic form, i.e.

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{d}$$

for  $\mathbf{Q} \in \mathbb{R}^{d \times d}$ ,  $\mathbf{c} \in \mathbb{R}^d$ ,  $d \in \mathbb{R}$ , and constraints are linear.

as well as second-order cone programs (SOCP), semidefinite programs (SDP), and cone programs (CP).



# CONSTRAINED CONVEX OPTIMIZATION / 3

SOCs play a pivotal role in statistics and engineering and have been popularized in the seminal article by [Lobo et al., 1998](#).

In ML, SDPs are at the heart of, e.g., learning kernels from data (see, e.g., [Lanckriet et al., 2004](#)).

In general, this categorization of convex optimization problem classes helps in the design of specialized *optimization methods* that are tailored toward the specific type of convex optimization problem (keyword: disciplined convex programming [Grant et al., 2006](#)).

