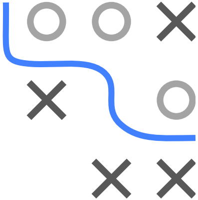
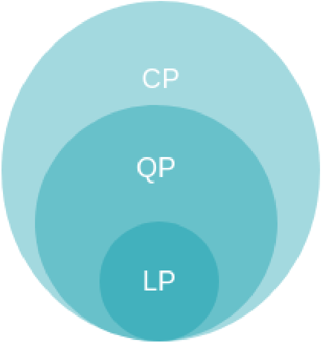
Optimization in Machine Learning



Optimization Problems
Constrained problems



Learning goals

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

CONSTRAINED OPTIMIZATION PROBLEM

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

- **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**

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

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

Equivalent formulation:

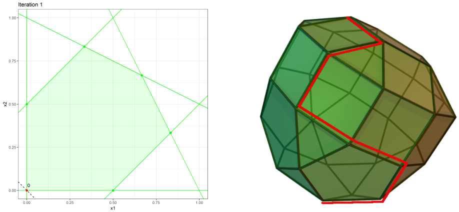
$$\begin{aligned} \min \quad & f(\mathbf{x}) & \\ \text{such that} \quad & g_i(\mathbf{x}) \leq 0 & \text{for } i = 1, \ldots, k \\ & h_j(\mathbf{x}) = 0 & \text{for } j = 1, \ldots, l. \end{aligned}$$

LINEAR PROGRAM (LP)

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

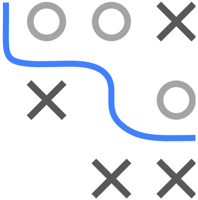
$$\begin{aligned} \min_{\mathbf{x}\in\mathbb{R}^d} \quad & \boldsymbol{c}^\top \mathbf{x} \\ \text{s.t.} \quad & \boldsymbol{A}\mathbf{x} \geq \boldsymbol{b} \\ & \mathbf{x} \geq 0 \end{aligned}$$

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



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

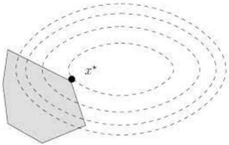
QUADRATIC PROGRAM (QP)



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

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

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



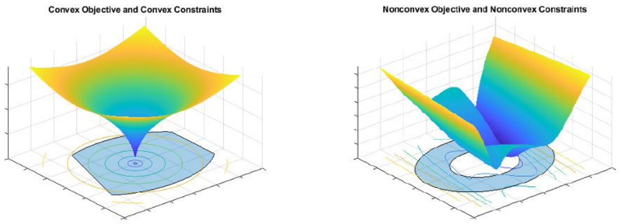
Visualization of quadratic objective (dashed) over linear constraints (grey). Source: Ma, Signal Processing Optimization Techniques, 2015.

CONVEX PROGRAM (CP)

- f convex, convex inequality constraints, linear equality constraints. Standard form:

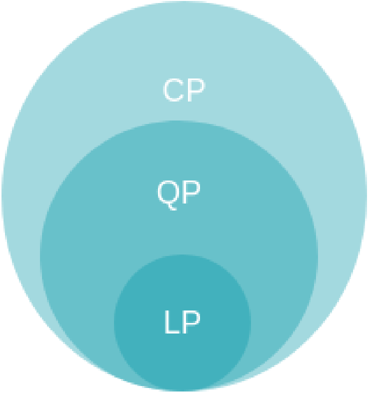
$$\begin{aligned} \min_{\mathbf{x}\in\mathbb{R}^d} \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & g_i(\mathbf{x}) \leq 0, i = 1, ..., k \\ & \boldsymbol{A}\mathbf{x} = \boldsymbol{b} \end{aligned}$$

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



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

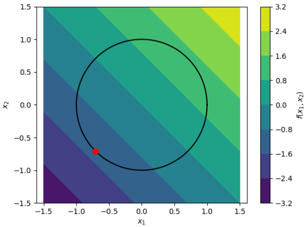
FURTHER TYPES



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

EXAMPLE 1: UNIT CIRCLE

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



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 $\mathbf{x} = (x_1, ..., x_k)$, x_j being the number of balls drawn in color j, is:

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

The parameters p_j are subject to the following constraints:

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

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

EXAMPLE 2: MAXIMUM LIKELIHOOD / 2

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

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

f, g, h are smooth.
Convex program: convex$^{(*)}$ objective + box/linear constraints).

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

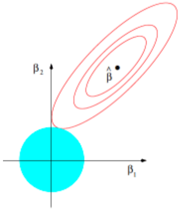
EXAMPLE 3: RIDGE REGRESSION

Ridge regression can be formulated as regularized ERM:

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

Equivalently it can be written as constrained optimization problem:

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



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

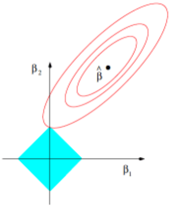
EXAMPLE 4: LASSO REGRESSION

Lasso regression can be formulated as regularized ERM:

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

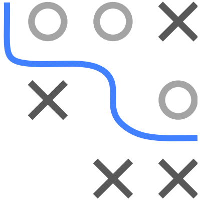
Equivalently it can be written as constrained optimization problem:

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



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

EXAMPLE 5: SUPPORT VECTOR MACHINES

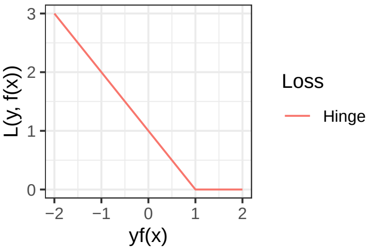


The SVM problem can be formulated in 3 equivalent ways: two primal, and one dual one (we will see later what "dual" means).

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

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

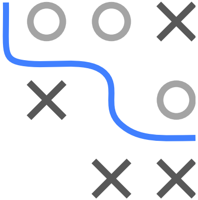


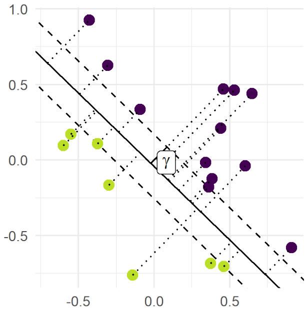
Unconstrained, convex problem with non-smooth objective

EXAMPLE 5: SUPPORT VECTOR MACHINES / 2

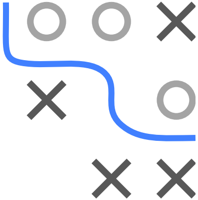
Formulation 2 (primal): Geometric formulation

- Find decision boundary which separates classes with **maximum** safety distance
- Distance to points closest to decision boundary ("safety margin γ") should be **maximized**





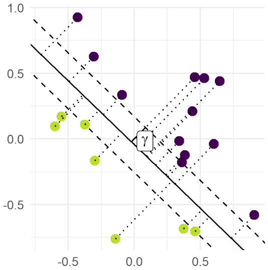
EXAMPLE 5: SUPPORT VECTOR MACHINES



Formulation 2 (primal): Geometric formulation

$$\min_{\boldsymbol{\theta}, \theta_0} \quad \frac{1}{2}\|\boldsymbol{\theta}\|^2$$

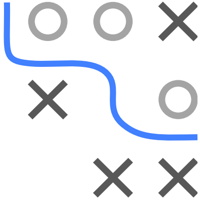
$$\text{s.t.} \quad y^{(i)}\left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0\right) \geq 1 \quad \forall i \in \{1, \ldots, n\}$$



Maximize safety margin γ. No point is allowed to violate safety margin constraint.

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

EXAMPLE 5: SUPPORT VECTOR MACHINES

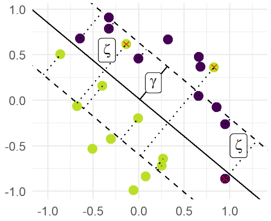


Formulation 2 (primal): Geometric formulation (soft constraints)

$$\min_{\boldsymbol{\theta},\boldsymbol{\theta}_0,\zeta^{(i)}} \quad \frac{1}{2}\|\boldsymbol{\theta}\|^2 + C\sum_{i=1}^{n}\zeta^{(i)}$$

$$\text{s.t.} \quad y^{(i)}\left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0\right) \geq 1 - \zeta^{(i)} \quad \forall\, i \in \{1, \dots, n\},$$

$$\text{and} \quad \zeta^{(i)} \geq 0 \quad \forall\, i \in \{1, \dots, n\}.$$

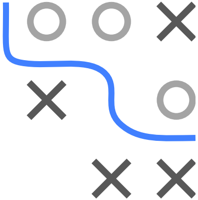


Maximize safety margin γ.

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

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

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

Matrix notation:

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^n} \quad \boldsymbol{\alpha}^\top\mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \operatorname{diag}(\boldsymbol{y})\,\mathbf{X}^\top\mathbf{X}\operatorname{diag}(\boldsymbol{y})\,\boldsymbol{\alpha}$$

$$\text{s.t.} \quad 0\leq\alpha_i\leq C \quad \forall\, i\in\{1,\ldots,n\}, \quad \boldsymbol{\alpha}^\top\boldsymbol{y} = 0$$

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

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^n} \quad \boldsymbol{\alpha}^\top\mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}\operatorname{diag}(\boldsymbol{y})\,\boldsymbol{K}\operatorname{diag}(\boldsymbol{y})\,\boldsymbol{\alpha}$$

$$\text{s.t.} \quad 0\leq\alpha_i\leq C \quad \forall\, i\in\{1,\ldots,n\}, \quad \boldsymbol{\alpha}^\top\boldsymbol{y} = 0$$

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