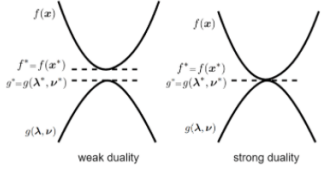
Optimization in Machine Learning

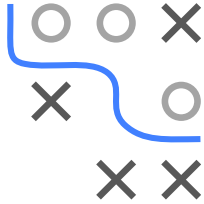
Nonlinear programs
Regularity Conditions



Learning goals

- KKT conditions
- Regularity conditions
- Examples

STATIONARY POINT OF THE LAGRANGIAN



When we introduced the Lagrangian $\mathcal{L}$ from a geometrical perspective for the equality constraint problem, we realized that the geometrical conditions for the optimum coincided with finding a stationary point of $\mathcal{L}$:

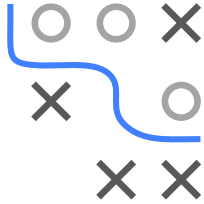
$$\begin{pmatrix} \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \beta) \\ \nabla_{\beta} \mathcal{L}(\mathbf{x}^*, \beta) \end{pmatrix} = \begin{pmatrix} \nabla f(\mathbf{x}^*) + \beta \nabla h(\mathbf{x}^*) \\ h(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

For this and the general Lagrangian, this leads to the following question.

Question: Is $\nabla L(\mathbf{x}, \alpha, \beta) = 0$ a **necessary / sufficient condition for the optimum**?

KKT CONDITIONS

In order to be able to formulate necessary and sufficient conditions for optimality, we need the **Karush-Kuhn-Tucker conditions** (KKT conditions).

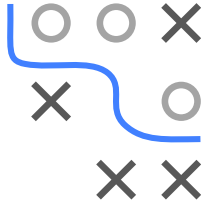


A triple $(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta})$ satisfies the KKT conditions if

- $\nabla_x L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = 0$ (stationarity)
- $g_i(\mathbf{x}) \leq 0, h_j(\mathbf{x}) = 0$ for all i, j (primal feasibility)
- $\boldsymbol{\alpha} \geq 0$ (dual feasibility)
- $\alpha_i g_i(\mathbf{x}) = 0$ for all i (complementary slackness)

KKT CONDITIONS / 2

Necessary condition for optimality:
Let $\mathbf{x}^*$ be a local minimum. If certain regularity conditions are fulfilled, there are $\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*$ such that $(\mathbf{x}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ fulfill the KKT conditions.

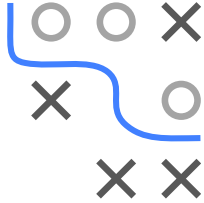


Under certain conditions, KKT conditions are also sufficient for optimality.

Sufficient condition for optimality:
Given a **convex problem** (f convex, $\mathcal{S}$ convex) and $(\mathbf{x}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ satisfies the KKT conditions. Then $\mathbf{x}^*$ is a global solution to the problem.

REGULARITY CONDITIONS

There are different regularity conditions (or constraint qualifications) that ensure that the KKT conditions apply (ACQ, LICQ, MFCQ, Slater condition, ...).

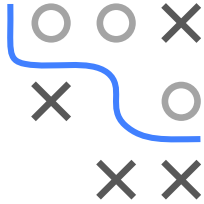


To be able to use the above results, at least one regularity condition must be examined to prove that the function behaves “regular”.

We do not go further into these regularity conditions here and refer to `https://docs.ufpr.br/~ademir.ribeiro/ensino/cm721/kkt.pdf`.

RIDGE REGRESSION

The following two formulas are common for ridge regression:



Formula 1:

$$\min_{\boldsymbol{\theta}} \quad f_\lambda(\boldsymbol{\theta}) := \|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda\|\boldsymbol{\theta}\|_2^2 \tag{1}$$

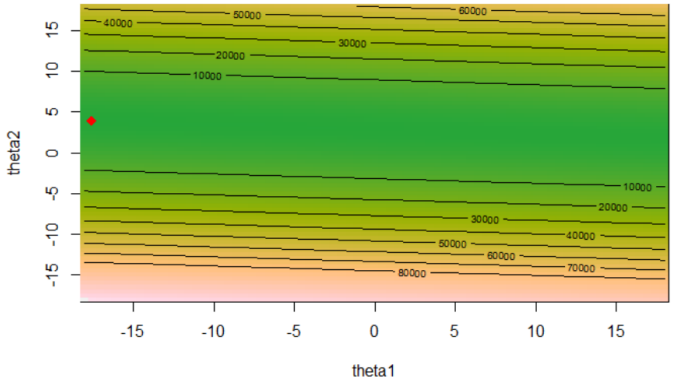
Formula 2:

$$\begin{aligned} \min_{\boldsymbol{\theta}} \quad & \|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 \\ \text{s.t.} \quad & \|\boldsymbol{\theta}\|_2^2 - t \leq 0 \end{aligned} \tag{2}$$

Why are these two formulas (for appropriate values t, λ) equivalent?

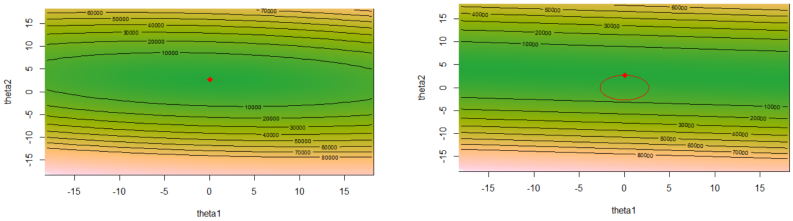
RIDGE REGRESSION / 2

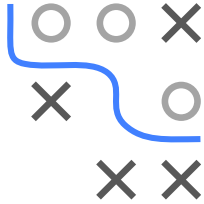
Visualization: see additional material



Quadratic-Loss for the `cars` dataset without penalty.

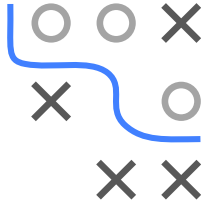
RIDGE REGRESSION / 3





Left: loss for Ridge regression with penalty term. Right: loss for ridge regression with corresponding constraint.

RIDGE REGRESSION / 4



First, consider (1). If $\boldsymbol{\theta}^*$ is our minimum, then the necessary condition applies.

$$\nabla f_\lambda(\boldsymbol{\theta}^*) = -2\boldsymbol{y}^T\mathbf{X} + 2(\boldsymbol{\theta}^*)^T\mathbf{X}^T\mathbf{X} + 2\lambda(\boldsymbol{\theta}^*)^T = 0.$$

We now show that we can find a t so that $\boldsymbol{\theta}^*$ is also solution for (2).

We calculate the Lagrange function of (2)

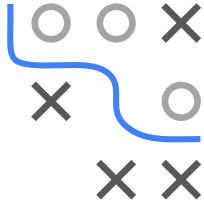
$$L(\boldsymbol{\theta}, \alpha) \quad = \quad \|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \alpha(\|\boldsymbol{\theta}\|_2^2 - t).$$

The first KKT condition (stationarity of the Lagrange function) is

$$\nabla_\theta L(\boldsymbol{\theta}, \alpha) = -2\boldsymbol{y}^T\mathbf{X} + 2\boldsymbol{\theta}^T\mathbf{X}^T\mathbf{X} + 2\alpha\boldsymbol{\theta}^T = 0.$$

Since we know from (1) that $\nabla f_\lambda(\boldsymbol{\theta}^*) = 0$, this condition is fulfilled if we set $\boldsymbol{\theta} = \boldsymbol{\theta}^*$ and $\alpha = \lambda$.

RIDGE REGRESSION / 5



However, complementary slackness must still apply for the KKT conditions.

$$\alpha(\|\boldsymbol{\theta}\|_2^2 - t) = 0$$

This is the case if we choose $t = \|\boldsymbol{\theta}^*\|^2$.

Vice versa it can be shown that a solution of (2) is a solution of (1) if we set $\lambda = \alpha$.