

Numerical Optimization - Sheet 4

If you are a student in mathematics please solve the exercises with no tag and the ones with the tag **Mathematics**. If you are a data science student please solve the problems with no tag and those with the tag **Data Science**. Submissions with tags other than your subject count as bonus points. The tag **Programming** marks programming exercises.

Ex 1

(2 Points)

Let $x \in \mathbb{R}^2$. Use the necessary and sufficient conditions for optimality to solve

$$\begin{aligned} \min_x \quad & x_1 + x_2 \\ \text{s.t.} \quad & x_1^2 + x_2^2 = 2. \end{aligned}$$

Solution 1:

Due to $\mathcal{L} = x_1 + x_2 + \lambda(x_1^2 + x_2^2 - 2)$ and $\nabla_x \mathcal{L} = (1 + \lambda 2x_1, 1 + \lambda 2x_2)$ we obtain from the KKT-conditions

$$\begin{aligned} 1 + \lambda 2x_1 &= 0 \\ 1 + \lambda 2x_2 &= 0. \end{aligned}$$

The constraints yield

$$x_1^2 + x_2^2 = 2.$$

Therefore

$$x_1 = x_2 = -\frac{1}{2\lambda}$$

and an application of the constraints imply

$$\lambda = \pm \frac{1}{2}.$$

As

$$\nabla^2 \mathcal{L} = \begin{bmatrix} 2\lambda & 0 \\ 0 & 2\lambda \end{bmatrix}$$

is positive definite only if $\lambda = \frac{1}{2}$, we obtain the solution

$$\hat{x} = (-1, -1).$$

Ex 2

(4 Points)

Find a local minimum of the problems.

- (i) Let $c > 0$ be fixed.

$$\begin{aligned} \min_{r,h \in \mathbb{R}} \quad & r^2 + rh \\ \text{s.t.} \quad & \pi r^2 h = c \\ & r \geq 0. \end{aligned}$$

- (ii)

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & \frac{1}{2} x^\top \begin{bmatrix} 4 & 6 \\ 6 & 9 \end{bmatrix} x - x^\top \begin{pmatrix} 14 \\ 21 \end{pmatrix} \\ \text{s.t.} \quad & [1, -2] x = 0. \end{aligned}$$

Solution 2:

- (i) The constraints yield that $r \neq 0$. We can therefore substitute

$$\frac{c}{\pi r^2} = h.$$

So we rewrite the problem

$$\begin{aligned} \min_{r,h \in \mathbb{R}} \quad & r^2 + rh \\ \text{s.t.} \quad & \pi r^2 h = c \\ & r \geq 0. \end{aligned}$$

as

$$\begin{aligned} \min_{r \in \mathbb{R}} \quad & r^2 + \frac{c}{\pi r} =: f(r) \\ \text{s.t.} \quad & r \geq 0. \end{aligned}$$

We now search a stationary point r^* of f and check whether it fulfills the constraints $r^* \geq 0$ in a second step. The necessary condition

$$f'(r^*) = 2r^* - \frac{c}{\pi r^{*2}} = 0,$$

gives

$$r^* = \left(\frac{c}{\pi 2} \right)^{\frac{1}{3}} \geq 0,$$

which also fulfills $r^* \geq 0$. The constraints in the original problem finally show that

$$h^* = \left(\frac{2c^2}{\pi^2} \right)^{\frac{1}{3}}.$$

- (ii)

$$\mathcal{L}(x, \lambda) = \frac{1}{2} x^\top \begin{bmatrix} 4 & 6 \\ 6 & 9 \end{bmatrix} x - x^\top \begin{pmatrix} 14 \\ 21 \end{pmatrix} - \lambda \begin{pmatrix} 1 \\ -2 \end{pmatrix}^\top x$$

1. Order Conditions

We obtain the KKT Conditions

$$4x_1 + 6x_2 - 14 - \lambda = 0 \quad (1)$$

$$6x_1 + 9x_2 - 21 + \lambda 2 = 0 \quad (2)$$

If we subtract $\frac{2}{3}(1)$ from (2) we obtain $\lambda = 0$. The rows in the Hessian of the objective are linearly dependent.

Constraints

The constraints yield $x_1 = 2x_2$. Therefore (1) yields

$$8x_2 + 6x_2 = 14 \Rightarrow x_2 = 1$$

Which implies $x_1 = 2$.

2. Order Sufficient Cond. We now fix the vector $\tilde{x} = (1, 2)$ of which we know that $\text{span}(\tilde{x}) = \ker(C)$ as $\ker(C)$ is 1-dimensional and we find that

$$\tilde{x}^\top \begin{bmatrix} 4 & 6 \\ 6 & 9 \end{bmatrix} \tilde{x} = 64 > 0.$$

So the 2. derivative of the objective is positive definite on the kernel of the constraints and the above solution is a strict local minimum.

Ex 3

(6 Points)

Let $C > 0$. Compute the Wolfe-Dual of the optimization problem

$$\begin{aligned} \min_{w, b, \xi} \quad & \frac{1}{2} \|w\|^2 + C \sum_{i=1}^m \xi_i \\ \text{s.t.} \quad & y_i(w^T x_i + b) \geq 1 - \xi_i, \forall i = 1, \dots, m \\ & \xi_i \geq 0, \forall i = 1, \dots, m. \end{aligned}$$

Solution 3:

The Lagrangian is given by

$$\mathcal{L}(w, b, \xi, \beta, \gamma) = \frac{1}{2} w^T w + C \sum_{i=1}^m \xi_i + \sum_{i=1}^m \beta_i (1 - \xi_i - y_i(w^T x_i + b)) - \sum_{i=1}^m \gamma_i \xi_i.$$

The constraints for the Wolfe dual are

$$\frac{\partial \mathcal{L}}{\partial w}(w) = w^T - \sum_{i=1}^m \beta_i y_i x_i^T = 0 \quad (3)$$

$$\frac{\partial \mathcal{L}}{\partial b}(b) = - \sum_{i=1}^m \beta_i y_i = 0 \quad (4)$$

$$\frac{\partial \mathcal{L}}{\partial \xi} = \mathbf{1}^T C - \beta^T - \gamma^T = 0 \quad (5)$$

$$\beta \geq 0, \gamma \geq 0. \quad (6)$$

The Wolfe dual is defined as

$$\begin{aligned} \max_{w, b, \xi, \beta, \gamma} \quad & \mathcal{L}(w, b, \xi, \beta, \gamma) \\ \text{s.t.} \quad & \nabla \mathcal{L}_{w, b, \xi} = 0 \\ & \beta, \gamma \geq 0. \end{aligned}$$

Substituting w and elimination of b, ξ and γ yield

$$\mathcal{L}(w, b, \xi, \beta, \gamma) = \frac{1}{2} w^T w + C \sum_{i=1}^m \xi_i + \sum_{i=1}^m \beta_i (1 - \xi_i - y_i (w^T x_i + b)) - \sum_{i=1}^m \gamma_i \xi_i \quad (\text{s. 1})$$

$$\begin{aligned} &= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + C \sum_{i=1}^m \xi_i + \sum_{i=1}^m \beta_i \left(1 - \xi_i - y_i \left(\sum_{j=1}^m \beta_j y_j x_j^T x_i + b \right) \right) - \sum_{i=1}^m \gamma_i \xi_i = \\ &= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + C \mathbf{1}^T \xi + \sum_{i=1}^m \beta_i - \beta^T \xi - \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j - \sum_{i=1}^m y_i \beta_i b - \gamma^T \xi = \\ &= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + C \mathbf{1}^T \xi - \beta^T \xi - \gamma^T \xi + \sum_{i=1}^m \beta_i - \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j - \sum_{i=1}^m y_i \beta_i b = \quad (\text{s. 2}) \end{aligned}$$

$$= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + C \mathbf{1}^T \xi - \beta^T \xi - \gamma^T \xi + \sum_{i=1}^m \beta_i - \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j = \quad (\text{s. 3})$$

$$= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + \sum_{i=1}^m \beta_i - \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j =$$

$$= -\frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j y_i y_j x_i^T x_j + \sum_{i=1}^m \beta_i.$$

Furthermore we obtain from (5) and (6) that

$$\begin{aligned} \mathbf{1}C - \beta &= \gamma \geq 0 \\ \Rightarrow 0 &\leq \beta \leq C. \end{aligned}$$

We are left with the variables β and y for which we copy the remaining constraints. Finally the Wolfe dual reduces to

$$\begin{aligned} &\max_{\beta} \sum_{i=1}^m \beta_i - \frac{1}{2} \sum_{i,j=1}^m \beta_i \beta_j x_i^T x_j y_i y_j \\ &\text{s.t.} \sum_{i=1}^m \beta_i y_i = 0 \\ &0 \leq \beta \leq C. \end{aligned}$$

Ex 4 Programming

(3 Points)

You find the iPython notebook `numopt_version02` in the folder Lecture 6 on Olat. Use this notebook as basis for the following exercise.

- (i) Consider the cell **chapter 2 SVM example code**. Uncomment the line which generates the "*not nicely separable points*" and fit a *linear* SVM using a hard and a soft margin. Fit a SVM with *rbf*-Kernel, again with hard and soft margin. Visualize your results with the code given in the notebook.
- (ii) The cell **chapter 3 3D pic for SVM illustration** visualizes the feature map

$$(x_1, x_2) \mapsto (x_1^2, x_2^2, \sqrt{2}x_1x_2).$$

The function `svm.SVC` allows user defined kernels. Determine and implement the corresponding kernel function and fit and visualize the model to the data of (i).

- (iii) Please comment on the result and the capabilities of the given kernel.