Penalty methods in constrained optimization

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PENALTY METHODS IN CONSTRAINED OPTIMIZATION

Master Thesis

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I dedicate this master thesis to my family. Thank you for your endless love and support. I would like to sincerely thank my advisor, Assoc. Prof. Dr. Sc. Marko Vrdoljak for his guidance through this study. Also, a special feeling of gratitude to my friends who made this journey easier.

Contents

Chapter 1

Introduction

The Latin word *optimum* means *the best*. Therefore, optimization is the art of determining the best among a number of different alternatives. Maximization and minimization problems have been studied and solved since the beginning of the mathematical analysis, but modern optimization theory started around 1948 with George Dantzig who introduced and popularized the concept of linear programming and proposed a solution algorithm [7]. Constrained optimization is one of the most used mathematical concepts for modelling real-world problems. Problems of that type often appear in different areas of science, such as structural engineering, protein folding and machine learning. Also, making any kind of business decision typically involves using optimization, i.e., when maximizing profit or minimizing loss. But, despite their widespread usage, constrained problems may be extremely difficult to solve. On the contrary, there is a wide variety of algorithms which solve unconstrained problems easily and efficiently. This leads to an idea of rewriting a constrained problem as unconstrained one. While solving a constrained nonlinear minimization problem in which we can not eliminate the constraints easily, it is very important to balance the aims of reducing the objective function and staying inside the feasible region. The basic idea of a penalty function is a combination of the objective function and a penalty parameter which controls constraints violations by penalizing them. Penalty methods offer a simple and straightforward method for handling constrained problems. Also, they are especially interesting because, to be able to overcome possible slow convergence, all aspects of optimization theory are brought into play.

1.1   A Brief Introduction to Optimization

First of all, some useful details for further consideration and development of the theory will be described. As stated earlier, our strategy for solving a constrained problem is to solve a sequence of unconstrained ones. The next step is to present important results

related to constrained as well as unconstrained optimization from [7]. We start with the basic definitions about functions and then state important results connected to constrained optimization. There are two types of optimization, constrained and unconstrained. An unconstrained optimization problem is to minimize function $f(\mathbf{x})$ without any constraints on $\mathbf{x}$.

Definition 1.1.1. *A point $\bar{\mathbf{x}} \in X$ is a local minimum point of the function $f : X \to \bar{\mathbb{R}}$ if there exists an open ball $B = B(\bar{\mathbf{x}}; r)$ with center at $\bar{\mathbf{x}}$ such that $f(x) \geq f(\bar{\mathbf{x}})$ for all $x \in X \cap B$. The point is a global minimum point if $f(x) \geq f(\bar{\mathbf{x}})$ for all $x \in X$.*

Definition 1.1.2. *A subset $X \subseteq \mathbb{R}^n$ is called convex if the segment $[x, y] \subseteq X$, for any $x, y \in X$.*

Definition 1.1.3. *Let $f : X \to \bar{\mathbb{R}}$ be a function with a domain $X \subseteq \mathbb{R}^n$. The set $epi f = \{(x, t) \in X \times \mathbb{R} \mid f(x) \leq t\}$ is called the epigraph of the function.*

Definition 1.1.4. *A function $f : X \to \bar{\mathbb{R}}$ is called convex if its domain X and epigraph $epi f$ are convex sets.*

Theorem 1.1.5. *A function $f : X \to \bar{\mathbb{R}}$ with a convex domain is convex if and only if*

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y),$$

for all points $x, y \in X$ and all numbers $\lambda \in [0, 1]$.

Theorem 1.1.6. *Suppose that the function $f : X \to \bar{\mathbb{R}}$ is convex and that $\bar{\mathbf{x}}$ is its local minimum point. Then $\bar{\mathbf{x}}$ is a global minimum point. The minimum point is unique if f is strictly convex.*

Theorem 1.1.7. *Suppose $f : X \to \mathbb{R}$ is a differentiable convex function. Then $\bar{\mathbf{x}} \in X$ is a global minimum point if and only if $Df(\bar{\mathbf{x}}) = 0$.*

The theorem above uses the gradient vector whose components are the first partials of f. Therefore, it is called the first-order condition. Necessary and sufficient conditions can also be stated in terms of the Hessian matrix $\mathbf{H}$ whose elements are the second partials of f. Hence, they are called the second-order conditions.

Definition 1.1.8. *A symmetric real matrix $\mathbf{M}$ is said to be positive definite if $x^T M x > 0$ for all $x \in \mathbb{R}^n$.*

Theorem 1.1.9. *Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable at $\bar{\mathbf{x}}$. If $\nabla f(\bar{\mathbf{x}}) = 0$ and $\mathbf{H}(\bar{\mathbf{x}})$ is positive definite, then $\bar{\mathbf{x}}$ is a strict local minimum.*

The goal of constrained optimization is to find a point that minimizes the objective function among all points which satisfy the constraints. If the objective function and the set of constraints are determined by a set of linear equations and inequalities, the problem is referred to as a linear programming problem. However, we are especially interested in nonlinear programming where, on the contrary, the objective function or some or all of the constraints are not linear. That problem can be formulated as:

$$
\begin{aligned}
&\underset{x}{\text{minimize}} && f(\mathbf{x}) \\
&\text{subject to} && g_i(x) \le 0, \quad i = 1, \ldots, m \\
& && h_j(x) = 0, \quad j = 1, \ldots, l \\
& && \mathbf{x} \in \mathbb{R}^n
\end{aligned}
\tag{P}
$$

where $f : \mathbb{R}^n \to \mathbb{R}$, $g_i : \mathbb{R}^n \to \mathbb{R}$, $h_j : \mathbb{R}^n \to \mathbb{R}$.

Definition 1.1.10. *Any vector $\mathbf{x}$ that satisfies the constraints is called a feasible solution. The set of all feasible vectors $\Omega = \{\mathbf{x} \in \mathbb{R}^n : h(\mathbf{x}) = 0, g(\mathbf{x}) \le 0\}$ is called the feasible region.*

Definition 1.1.11. *The minimization problem* (P) *is called convex if the constraint set Ω is convex, the objective function f is convex, the constraint functions g_i are convex for $i = 1, \ldots, m$ and the constraint functions h_j are affine for $j = 1, \ldots, l$.*

Definition 1.1.12. *A point $\bar{\mathbf{x}}$ satisfying the constraint $h(\bar{\mathbf{x}}) = 0$ is said to be a regular point of the constraint if the gradient vectors $\nabla h_1(\bar{\mathbf{x}}), \ldots, \nabla h_l(\bar{\mathbf{x}})$ are linearly independent.*

Definition 1.1.13. *Let $f : X \to \bar{\mathbb{R}}$ be a convex function defined on a subset X of $\mathbb{R}^n$. A vector $\xi \in \mathbb{R}^n$ is called a subgradient of f at the point $a \in X$ if the inequality*

$$
f(x) \ge f(a) + \xi^t(x - a)
$$

holds true for all $x \in X$. The set of all subgradients of f at a is called the subdifferential of f and is denoted by $\delta f(a)$.

Definition 1.1.14. *The problem* (P) *satisfies Slater's condition if there is a feasible point $\bar{\mathbf{x}}$ in the relative interior of Ω, i.e., such that $g_i(\bar{\mathbf{x}}) < 0$ for each non-affine constraint function g_i.*

Definition 1.1.15. *Function $L : \Omega \times \mathbb{R}^m \times \mathbb{R}^l \to \bar{\mathbb{R}}$, defined by*

$$
L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i g_i(x) + \sum_{j=1}^{l} v_j h_j(x)
\tag{1.1}
$$

is called the Lagrangian function of the minimization problem (P) *and the variables $u_1, \ldots, u_m$, $v_1, \ldots, v_l$ are called the Lagrangian multipliers.*

Theorem 1.1.16 (The Karush-Kuhn-Tucker Theorem)**.** *Let the minimization problem* (P) *be a convex problem and suppose that the objective and constraint functions are differentiable at the feasible point* $\bar{\mathbf{x}}$*. Also, let* $I = \{i : g_i(\bar{\mathbf{x}}) = 0\}$*.*

  (i) *If there exist scalars* $\bar{u}_i \geq 0$*, for* $i \in I$ *and* $\bar{v}_j$ *for* $j = 1, \dots, l$ *that satisfy the KKT-condition*

$$\begin{cases} \nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \bar{u}_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\bar{\mathbf{x}}) = 0. \\ \bar{u}_i g_i(\bar{\mathbf{x}}) = 0 \quad \text{for } i = 1, \dots, m. \end{cases}$$

  then $\bar{\mathbf{x}}$ *is an optimal solution to the problem* (P)*.*

  (ii) *If Slater's condition is fulfilled,* $\bar{\mathbf{x}}$ *is an optimal solution and* $\nabla g_i(\bar{\mathbf{x}})$*,* $i \in I$ *and* $\nabla h_j(\bar{\mathbf{x}})$*,* $j = 1, \dots, l$ *are linearly independent then there exist unique scalars* $\bar{u}_i$ *for* $i \in I$ *and* $\bar{v}_j$ *for* $j = 1, \dots, l$ *that satisfy KKT-condition.*

Theorem 1.1.17 (Karush-Kuhn-Tucker Second-Order Necessary Conditions)**.** *Consider the minimization problem* (P) *where the objective function and constraints are all twice differentiable, X a nonempty and open set in* $\mathbb{R}^n$*. Let* $\bar{\mathbf{x}}$ *be a local minimum for* (P) *and* $I = \{i : g_i(\bar{\mathbf{x}}) = 0\}$*. Denote the Hessian of Lagrangian function at* $\bar{\mathbf{x}}$ *with associated multipliers* $\bar{u}$*,* $\bar{v}$ *by:*

$$\nabla_{\bar{\mathbf{x}}}^2 L(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{v}}) = \nabla^2 f(\bar{\mathbf{x}}) + \sum_{i \in I} \bar{u}_i \nabla^2 g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla^2 h_j(\bar{\mathbf{x}})$$

$\nabla^2 f(\bar{\mathbf{x}})$*,* $\nabla^2 g_i(\bar{\mathbf{x}})$ *for* $i \in I$ *and* $\nabla^2 h_j(\bar{\mathbf{x}})$ *for* $j = 1, \dots, l$ *are the Hessians of the corresponding functions at* $\bar{\mathbf{x}}$*. Let us assume that* $\nabla g_i(\bar{\mathbf{x}})$*,* $i \in I$ *and* $\nabla h_j(\bar{\mathbf{x}})$*,* $j = 1, \dots, l$ *are linearly independent. It follows that* $\bar{\mathbf{x}}$ *is a KKT point with Lagrangian multipliers* $\bar{u} \geq 0$ *and* $\bar{v}$ *associated with the inequality and equality constraints, respectively. In addition,* $\mathbf{d}^t \nabla^2 L(\bar{\mathbf{x}}) \mathbf{d} \geq 0$*, for any* $\mathbf{d} \in C = \{\mathbf{d} \neq 0 : \nabla g_i(\bar{\mathbf{x}})^t \mathbf{d} = 0 \text{ for } i \in I^+, \nabla g_i(\bar{\mathbf{x}})^t \mathbf{d} \leq 0 \text{ for } i \in I^0, \nabla h_j(\bar{\mathbf{x}})^t \mathbf{d} = 0 \text{ for } j = 1, \dots, l\}$*, where* $I^0 = \{i \in I, \bar{u}_i = 0\}$ *and* $I^+ = \{i \in I : \bar{u}_i > 0\}$*.*

Theorem 1.1.18 (Karush-Kuhn-Tucker Second-Order Sufficient Conditions)**.** *Consider the minimization problem* (P) *where the objective function and constraints are all twice differentiable, X a nonempty and open set in* $\mathbb{R}^n$*. Let* $\bar{\mathbf{x}}$ *be a KKT point for* (P) *with Lagrangian multipliers* $\bar{u}$ *and* $\bar{v}$ *associated with the inequality and equality constraints. Denote* I*,* I^+*,* I^0*, the Hessian of Lagrangian function* $\nabla^2 L(\bar{\mathbf{x}})$ *and the cone C as in the Theorem 1.1.17. If* $\mathbf{d}^t \nabla^2 L(\bar{\mathbf{x}}) \mathbf{d} > 0$ *for all* $\mathbf{d} \in C$*,* $\bar{\mathbf{x}}$ *is a strict local minimum for minimization problem* (P)*.*

Chapter 2

Concept of Penalty Functions

2.1 Penalty Function Definition

As already mentioned, the goal is to approximate a constrained minimization problem by a sequence of problems that are easier to solve. For that purpose we will introduce penalty function. The basic idea is to place constraints into the objective function via a penalty parameter which assigns a high cost to infeasible points. Consider the following problem:

$$\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & h(\mathbf{x}) = 0
\end{aligned} \tag{EQ}$$

Suppose that we can rewrite the previous problem as:

$$\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) + \mu h^2(\mathbf{x}) \\
\text{subject to} \quad & \mathbf{x} \in \mathbb{R}^n,
\end{aligned} \tag{2.1}$$

where μ is a large number.

Intuitively, it can easily be imagined that an optimal solution of (2.1) has to have $h^2(\mathbf{x})$, as well as $h(\mathbf{x})$, close to zero. If that is not the case, a large penalty would be incurred. However, the penalty $\mu h(\mathbf{x})^2$ is not always appropriate. It depends on the type of the constraint. Now consider the following problem:

$$\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & g(\mathbf{x}) \leq 0
\end{aligned} \tag{NEQ}$$

It is obvious that, in the case of using the form $f(\mathbf{x}) + \mu g(\mathbf{x})^2$, the penalty would be incurred whether $g(\mathbf{x}) < 0$ or $g(\mathbf{x}) > 0$. But, we do not need penalty for feasible points. That is why

we formulate the belonging unconstrained problem as follows:

$$\underset{x}{\text{minimize}} \quad f(\mathbf{x}) + \mu \max\{0, g(\mathbf{x})\}$$
$$\text{subject to} \quad \mathbf{x} \in \mathbb{R}^n \tag{2.2}$$

When **x** is a feasible point, no penalty is incurred. On the other hand, any point **x** for which $g(\mathbf{x})$ is greater than zero is penalized. For general constrained optimization problem (P) a suitable penalty function must incur a positive penalty for infeasible points and no penalty for feasible ones.

Definition 2.1.1. *A suitable penalty function α for the problem* (P) *is defined by*

$$\alpha(\mathbf{x}) = \sum_{i=1}^{m} \phi(g_i(\mathbf{x})) + \sum_{j=1}^{l} \psi(h_j(\mathbf{x})), \tag{2.3}$$

where ϕ and ψ are continuous functions and satisfy the following:

1. *$\phi(\mathbf{x}') = 0$ if $\mathbf{x}' \leq 0$ and $\phi(\mathbf{x}') > 0$ if $\mathbf{x}' > 0$*

2. *$\psi(\mathbf{x}') = 0$ if $\mathbf{x}' = 0$ and $\psi(\mathbf{x}') > 0$ if $\mathbf{x}' \neq 0$*

The penalty function α is typically of the form:

$$\alpha(\mathbf{x}) = \sum_{i=1}^{m} [\max\{0, g_i(\mathbf{x})\}]^p + \sum_{j=1}^{l} |h_j(\mathbf{x})|^p.$$

Example 2.1.2. Consider the following problem:

$$\underset{x}{\text{minimize}} \quad -x$$
$$\text{subject to} \quad x + 3 \leq 0 \tag{2.4}$$

We notice that the constraint is of the form $g(x) \leq 0$, where $g(x) = x + 3$. Thus, $\alpha(x) = [\max\{0, x + 3\}]^2$. The minimum of $f + \mu\alpha$ occurs at the point $1/(2\mu) - 3$. If we let $\mu \to \infty$, $1/(2\mu) - 3 \to \bar{x} = -3$, which is the minimizing point of the original constrained problem. The figure below illustrates this example for two different values of μ.
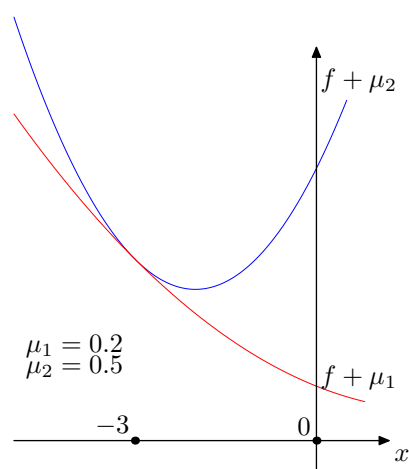
Figure 2.1: The minimum of $f + \mu\alpha$ approaches -3 as μ is getting larger

Example 2.1.3. Now, consider the minimization problem with the equality constraint.

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & 2x_1^2 + 2x_2^2 \\ \text{subject to} \quad & x_1 + x_2 - 2 = 0 \end{aligned} \tag{2.5}$$

After solving the previous problem with classical methods, we get $x = y = 1$ and the objective value 4. Now, consider the equivalent penalty problem.

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & 2x_1^2 + 2x_2^2 + \mu(x_1 + x_2 - 2)^2 \\ \text{subject to} \quad & (x_1, x_2) \in \mathbb{R}^2 \end{aligned} \tag{2.6}$$

Suppose that μ is a very large number. The objective function is convex, regardless of the parameter μ. From the Theorem 1.1.7, in order to find a minimum point, we calculate the following:

$$\begin{aligned} 2x_1 + \mu(x_1 + x_2 - 2) &= 0 \\ 2x_2 + \mu(x_1 + x_2 - 2) &= 0. \end{aligned} \tag{2.7}$$

We get $x_1 = x_2 = \mu/(\mu + 1)$. Obviously, by choosing μ large enough, we approach the optimal solution.

2.2 Interpretation of Penalty Function

2.2.1 The Primal Function

Firstly, the function that gives the optimal value of the objective function for diverse values of the right-hand side is defined.

Definition 2.2.1. *Consider the problem* (EQ). *The corresponding primal value function is defined in a neighborhood of 0 as*

$$v(\varepsilon) = min\{f(\mathbf{x}) : h(\mathbf{x}) = \varepsilon\}$$

The existence of $v(\varepsilon)$, as well as $\nabla v(\varepsilon) = -\mathbf{v}^t$, where $\mathbf{v}$ is Lagrangian multiplier vector associated with a local solution $\mathbf{x}^*$, follows directly from the Sensitivity theorem stated below. The proof can be found in [8].

Theorem 2.2.2 (Sensitivity Theorem). *Let $f, h \in C^2$ and consider the problem:*

$$\begin{aligned} \underset{x}{minimize} \quad & f(\mathbf{x}) \\ subject\ to \quad & h(\mathbf{x}) = \varepsilon \end{aligned} \tag{2.8}$$

Suppose that for $\varepsilon = \mathbf{0}$ there exists a local solution $\mathbf{x}^*$ that is a regular point and that, together with its associated Lagrangian multiplier vector $\mathbf{v}$, satisfies the second-order sufficiency conditions for a strict local minimum. Then for every $\varepsilon \in \mathbf{X}^l$ in a region containing $\mathbf{0}$ there is an $\mathbf{x}(\varepsilon)$ such that $\mathbf{x}(\mathbf{0}) = \mathbf{x}^*$ and such that $\mathbf{x}(\varepsilon)$ is a local minimum of (2.8) Furthermore,

$$\nabla_\varepsilon f(\mathbf{x}(\varepsilon))\big|_{\varepsilon=0} = -\mathbf{v}^t$$

Note the following relations:

$$\begin{aligned} min\left\{f(\mathbf{x}) + \mu \sum_{j=1}^{l} h_j^2(\mathbf{x})\right\} &= \min_{x,\varepsilon}\{f(\mathbf{x}) + \mu \|\varepsilon\|^2 : h(\mathbf{x}) = \varepsilon\} \\ &= \min_\varepsilon\{\mu \|\varepsilon\|^2 + v(\varepsilon)\} \end{aligned} \tag{2.9}$$

Geometric interpretation of the primal function is illustrated in the Figure 2.2. The value of primal function, the lowest curve, at $\varepsilon = 0$ is the value of the original constrained problem. Above it are penalty function for various values of μ. The minimum value of the penalty problem is, according to (2.9), the minimum point of this curve. We see that, as penalty parameter μ increases, this curve becomes convex near 0, even if $v(\varepsilon)$ is not convex.

2.2.2 Geometric Interpretation

Now consider the following minimization problem to illustrate the idea behind penalty functions geometrically.

$$\begin{aligned} \underset{x}{minimize} \quad & 2x_1^2 + 2x_2^2 \\ subject\ to \quad & x_1 + x_2 - 2 = \varepsilon \end{aligned} \tag{2.10}$$
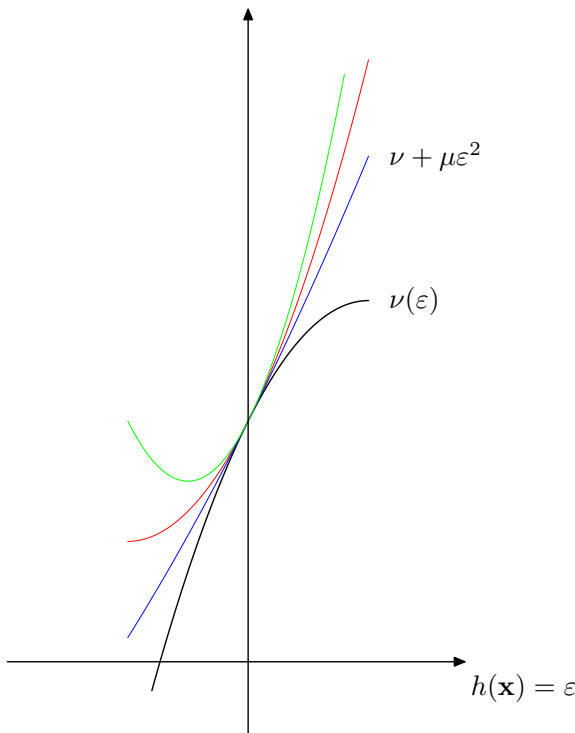
Figure 2.2: Geometric interpretation of the primal function with associated penalty functions

First we substitute x_2 by $x_2 = 2 + \varepsilon - x_1$ and get the objective function of form $2x_1^2 + 2(2 + \varepsilon - x_1)^2$. Then we find the optimum by calculating the derivative and equating it to zero. Hence, $4x_1 - 4(2 + \varepsilon - x_1) = 0$. For any ε, the optimal solution is given by $x_1 = x_2 = 1 + \varepsilon/2$ with objective value $v(\varepsilon) = (2 + \varepsilon)^2$. Obviously, given any point (x_1, x_2) in $\mathbb{R}^2$ that satisfies the constraint $h(\mathbf{x}) = \varepsilon$, its objective value lies between $(2+\varepsilon)^2$ and ∞. Consider the penalty problem to minimize $f(\mathbf{x}) + \mu h^2(\mathbf{x})$ where $\mathbf{x} \in \mathbb{R}^2$, $\mu > 0$ fixed. We want to minimize the term $f + \mu h^2$, so the parabola $f + \mu h^2 = k$ needs to be moved downward until it becomes tangential to the shaded set. Therefore, for μ, the optimal value of the penalty problem is the intercept of the parabola on the f-axis. The set $\{(h(\mathbf{x}), f(\mathbf{x})) : \mathbf{x} \in \mathbb{R}^2\}$ is illustrated in the Figure 2.3. The lower envelope of this set is given by the parabola $(2 + h)^2$, which is actually equal to $(2 + \varepsilon)^2 = v(\varepsilon)$. The set of feasible points to the primal problem is the shaded set above $v(\varepsilon)$. Also, $\mu' > \mu$ and points A, B, C denote the optimal solution to the primal problem, penalty problem with parameter μ and μ', respectively. Notice that optimal solution to the penalty problem with larger penalty parameter μ' is closer to the optimal solution than one with smaller penalty parameter μ. Therefore, as μ increases, the parabola of the penalty function becomes steeper and the point of tangency comes closer to the optimal solution of the original problem.
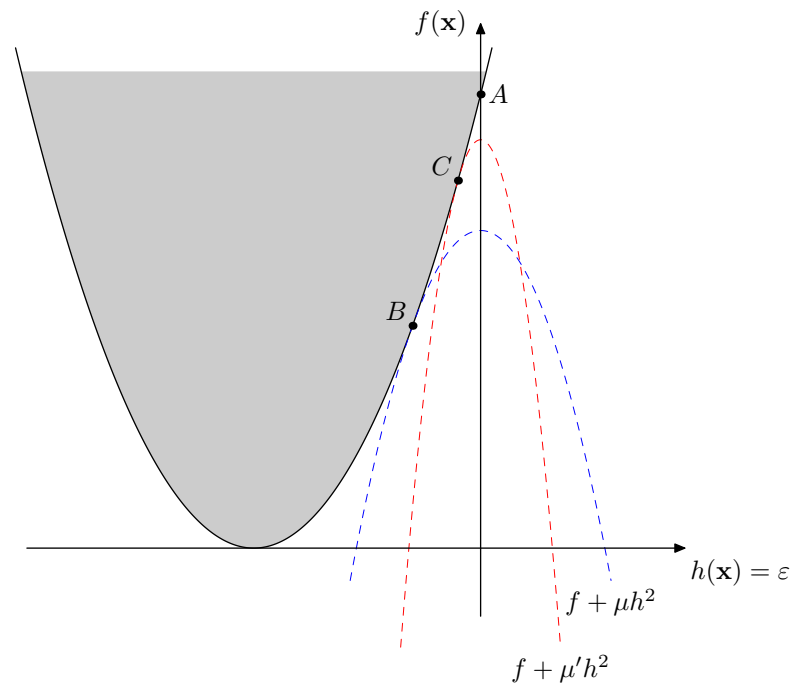
Figure 2.3: Geometric interpretation of the convex example

Remark 2.2.3. *When it comes to a nonconvex case, we know that Lagrangian dual approach would fail in finding an optimal solution because of a duality gap. Penalty functions, using a nonlinear support, can get arbitrarily close to an optimum if a large penalty parameter μ is used. This is illustrated in the Figure 2.4. Point A denotes an optimal solution to the primal problem while point B is an optimal solution to the penalty problem with parameter μ and C is an optimal objective value of the Lagrangian dual problem.*

Figure 2.4: Geometric interpretation of the nonconvex example

Chapter 3

Exterior Penalty Function Method

3.1 Important Results

Let α be a function defined as in the Definition 2.1.1. The basic approach in the penalty method is to find

$$\sup_{\mu} \quad \theta(\mu)$$
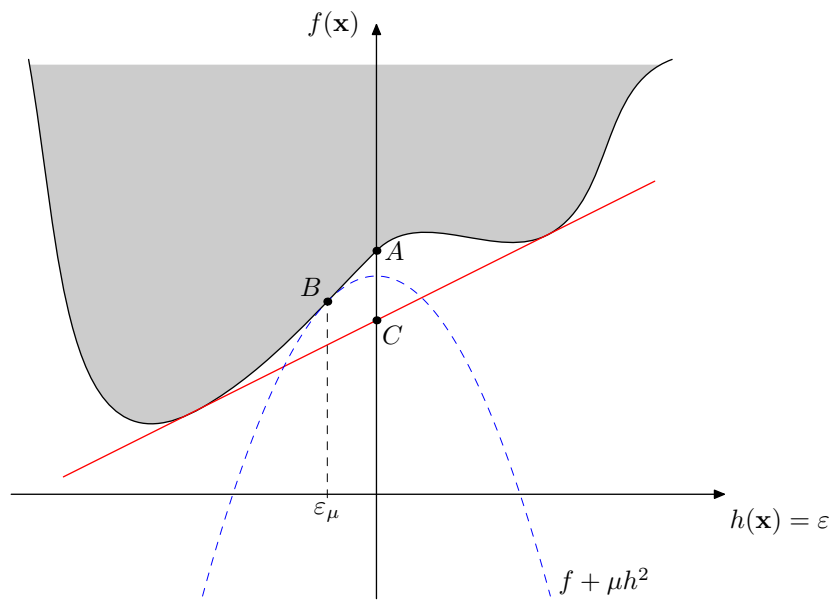$$\text{subject to} \quad \mu \geq 0, \tag{3.1}$$

where $\theta(\mu) = \inf\{f(\mathbf{x}) + \mu\alpha(\mathbf{x}) : \mathbf{x} \in X\}$.

Before stating the main theorem, we need the following lemma from [10]. Consider the problem (P).

Lemma 3.1.1. *Suppose that $f, g_1, \ldots, g_m, h_1, \ldots, h_l$ are continuous functions on $\mathbb{R}^n$ and let $X \subseteq \mathbb{R}^n$, $X \neq \emptyset$. Let α be a function on $\mathbb{R}^n$ defined in (2.1.1) and suppose that for every μ, there is an $x_\mu \in X$ such that $\theta(\mu) = f(\mathbf{x}_\mu) + \mu\alpha(\mathbf{x}_\mu)$. Then, the following statements are true:*

1) $\inf\{f(\mathbf{x}) : \mathbf{x} \in X, g(\mathbf{x}) \leq 0, h(\mathbf{x}) = 0\} \geq \sup_{\mu \geq 0} \theta(\mu)$, where $\theta(\mu) = \inf\{f(\mathbf{x}) + \mu\alpha(\mathbf{x}) : \mathbf{x} \in X\}$ and where g is the vector function whose components are $g_1, \ldots, g_m$ and h is the vector function whose components are $h_1, \ldots, h_l$.

2) $f(\mathbf{x}_\mu)$ is a non-decreasing function of $\mu \geq 0$, $\theta(\mu)$ is a non-decreasing function of μ and $\alpha(\mathbf{x}_\mu)$ is a non-increasing function of μ.

Proof. Let $\mathbf{x} \in X$ such that $g(\mathbf{x}) \leq 0$ and $h(\mathbf{x}) = 0$. Therefore, $\alpha(\mathbf{x}) = 0$ because $\mathbf{x}$ satisfies the constraints. Let $\mu \geq 0$. From

$$f(\mathbf{x}) = f(\mathbf{x}) + \mu\alpha(\mathbf{x}) \geq \inf\{f(\mathbf{y}) + \mu\alpha(\mathbf{y}) : \mathbf{y} \in X\} = \theta(\mu). \tag{3.2}$$

follows the first statement.

Now, let $\lambda < \mu$. By the definition of $\theta(\lambda)$ and $\theta(\mu)$, we have:

$$f(\mathbf{x}_\mu) + \lambda\alpha(\mathbf{x}_\mu) \geq f(\mathbf{x}_\lambda) + \lambda\alpha(\mathbf{x}_\lambda) \tag{3.3}$$

$$f(\mathbf{x}_\lambda) + \mu\alpha(\mathbf{x}_\lambda) \geq f(\mathbf{x}_\mu) + \mu\alpha(\mathbf{x}_\mu) \tag{3.4}$$

By adding the previous two inequalities, we get:

$$(\mu - \lambda)(\alpha(\mathbf{x}_\lambda) - \alpha(\mathbf{x}_\mu)) \geq 0. \tag{3.5}$$

We assumed $\mu > \lambda$, so is $\alpha(\mathbf{x}_\lambda) \geq \alpha(\mathbf{x}_\mu)$. It follows from (3.3) that $f(\mathbf{x}_\mu) \geq f(\mathbf{x}_\lambda)$, for $\lambda \geq 0$. If we add and subtract $\mu\alpha(\mathbf{x}_\mu)$ to the left-hand side, we get

$$f(\mathbf{x}_\mu) + \mu\alpha(\mathbf{x}_\mu) + (\lambda - \mu)\alpha(\mathbf{x}_\mu) \geq \theta(\lambda). \tag{3.6}$$

It implies that $\theta(\mu) \geq \theta(\lambda)$ because $\mu > \lambda$ and $\alpha(\mathbf{x}_\mu) \geq 0$. This establishes the second statement. □

The following theorem from [10] says that finding the infimum of the primal problem (P) is equivalent to finding the supremum of $\theta(\mu)$. It justifies the use of the penalty functions for solving constrained problems.

Theorem 3.1.2. *Consider the problem* (P), *where* $f, g_1, \ldots, g_m, h_1, \ldots, h_l$ *are continuous functions on* $\mathbb{R}^n$ *and* $X \subseteq \mathbb{R}^n$, $X \neq \emptyset$. *Suppose that the problem has a feasible solution and let* α *be a continuous function given by the Definition* 2.1.1. *Furthermore, suppose that for every* μ *there exists a solution* $\mathbf{x}_\mu \in X$ *to the problem of minimization* $f(\mathbf{x}) + \mu\alpha(\mathbf{x})$ *subject to* $\mathbf{x} \in X$ *and that* $\{x_\mu\}$ *is contained in a compact subset of* X. *Then*

$$\inf\{f(\mathbf{x}) : \mathbf{x} \in X, g(\mathbf{x}) \leq 0, h(\mathbf{x}) = 0\} = \sup_{\mu \geq 0} \theta(\mu) = \lim_{\mu \to \infty} \theta(\mu),$$

where $\theta(\mu) = \inf\{f(\mathbf{x}) + \mu\alpha(\mathbf{x}) : \mathbf{x} \in X\} = f(\mathbf{x}_\mu) + \mu\alpha(\mathbf{x}_\mu)$. *Furthermore, the limit* $\bar{\mathbf{x}}$ *of any convergent subsequence of* $\{\mathbf{x}_\mu\}$ *is an optimal solution to the original problem and* $\mu\alpha(\mathbf{x}_\mu) \to 0$ *as* $\mu \to \infty$.

Proof. From the second statement of the Lemma 3.1.1, $\theta(\mu)$ is monotone. That implies that $\sup_{\mu \geq 0} \theta(\mu) = \lim_{\mu \to \infty} \theta(\mu)$.

Firstly, let us show that $\alpha(\mathbf{x}_\mu) \to 0$ as $\mu \to \infty$. Let $\mathbf{y}$ be a feasible point and $\varepsilon > 0$. Also, let $\mathbf{x}_1$ be an optimal solution to the minimization problem of $f(\mathbf{x}) + \mu\alpha(\mathbf{x})$ subject to $\mathbf{x} \in X$ for $\mu = 1$. If $\mu \geq (1/\varepsilon)|f(\mathbf{y}) - f(\mathbf{x}_1)| + 2$, then, from the Lemma 3.1.1 2), follows that $f(\mathbf{x}_\mu) \geq f(\mathbf{x}_1)$.

We now show that $\alpha(\mathbf{x}_\mu) \leq \varepsilon$. By contradiction, suppose $\alpha(\mathbf{x}_\mu) > \varepsilon$. Again, from the Lemma 3.1.1 1), we get:

$$\inf\{f(\mathbf{x}) : g(\mathbf{x}) \leq 0, h(\mathbf{x}) = 0, \mathbf{x} \in X\} \geq \theta(\mu) = f(\mathbf{x}_\mu) + \mu\alpha(\mathbf{x}_\mu) \geq f(\mathbf{x}_1) + \mu\alpha(\mathbf{x}_\mu)$$
$$> f(\mathbf{x}_1) + |f(\mathbf{y}) - f(\mathbf{x}_1)| + 2\varepsilon > f(\mathbf{y}).$$

However, it is a contradiction to the fact $\mathbf{y}$ is a feasible point. Therefore, $\alpha(\mathbf{x}_\mu) \leq \varepsilon$, for any $\mu \geq (1/\varepsilon)|f(\mathbf{y}) - f(\mathbf{x}_1)| + 2$. It follows that $\alpha(\mathbf{x}_\mu) \to 0$ as $\mu \to \infty$.

Let $\{\mathbf{x}_{\mu_k}\}$ be any convergent subsequence of $\{\mathbf{x}_\mu\}$ and $\bar{\mathbf{x}}$ its limit. Then

$$\sup_{\mu \geq 0} \theta(\mu) \geq \theta(\mu_k) = f(\mathbf{x}_{\mu_k}) + \mu_k\alpha(\mathbf{x}_{\mu_k}) \geq f(\mathbf{x}_{\mu_k}). \tag{3.7}$$

Since $\mathbf{x}_{\mu_k} \to \bar{\mathbf{x}}$ and f is a continuous function, (3.7) implies that

$$\sup_{\mu \geq 0} \theta(\mu) \geq f(\bar{\mathbf{x}}). \tag{3.8}$$

Because $\alpha(\mathbf{x}_\mu) \to 0$ when $\mu \to \infty$, $\alpha(\bar{\mathbf{x}}) = 0$. In other words, $\bar{\mathbf{x}}$ is a feasible solution to (P). From (3.8) and the Lemma (3.1.1) 1), it follows that $\bar{\mathbf{x}}$ is an optimal solution and $\sup_{\mu \geq 0} \theta(\mu) = f(\bar{\mathbf{x}})$. Notice that $\mu\alpha(\mathbf{x}_\mu) = \theta(\mu) - f(\mathbf{x}_\mu)$. When $\mu \to \infty$, both $\theta(\mu)$ and $f(\mathbf{x}_\mu)$ approach $f(\bar{\mathbf{x}})$. Therefore, $\mu\alpha(\mathbf{x}_\mu) \to 0$. $\square$

Now, it is obvious that as μ takes higher values, the approximation becomes more accurate.

Remark 3.1.3. *If $\alpha(\mathbf{x}_\mu) = 0$ for some μ, then $\mathbf{x}_\mu$ is an optimal solution to the problem.*

3.2 Karush-Kuhn-Tucker Multipliers at Optimality

Consider the problem (P). Suppose that the penalty function α is defined by (2.1.1). In addition to that definition, suppose that ϕ and ψ are continuously differentiable with $\phi'(y) > 0$, for any $y > 0$ and $\phi'(y) = 0$, for any $y \leq 0$. Furthermore, suppose that for every μ there exists a solution $\mathbf{x}_\mu \in \mathbb{R}^n$ to the problem of minimization $f(\mathbf{x}) + \mu\alpha(\mathbf{x})$ subject to $\mathbf{x} \in \mathbb{R}^n$ and that $\{x_\mu\}$ is contained in a compact subset of $\mathbb{R}^n$ (Theorem 3.1.2). Because x_μ is the solution to the minimization problem, the gradient of the objective function must vanish at that point. Hence,

$$\nabla f(\mathbf{x}_\mu) + \sum_{i=1}^m \mu\phi'(g_i(\mathbf{x}_\mu))\nabla g_i(\mathbf{x}_\mu) + \sum_{j=1}^l \mu\psi'(h_j(\mathbf{x}_\mu))\nabla h_j(\mathbf{x}_\mu) = 0, \quad \forall\mu \tag{3.9}$$

Let $\bar{\mathbf{x}}$ be a limit point of the sequence $\{\mathbf{x}_\mu\}$. Also, assume that $\{\mathbf{x}_\mu\} \to \bar{\mathbf{x}}$. Label $I = \{i : g_i(\bar{\mathbf{x}}) = 0\}$. I is the set of inequality constraints that bind at $\bar{\mathbf{x}}$. From the Theorem 3.1.2

and the fact that $g_i(\bar{\mathbf{x}}) < 0$, for any $i \notin I$, it follows that $g_i(\mathbf{x}_\mu) < 0$ for μ sufficiently large. Therefore, $\mathbf{x}_\mu$ is a feasible point and $\mu\phi'(g_i(\mathbf{x}_\mu)) = 0$. Hence, for all μ large enough, we can rewrite (3.9) as follows:

$$\nabla f(\mathbf{x}_\mu) + \sum_{i \in I} (\mathbf{u}_\mu)_i \nabla g_i(\mathbf{x}_\mu) + \sum_{j=1}^{l} (\mathbf{v}_\mu)_j \nabla h_j(\mathbf{x}_\mu) = 0, \tag{3.10}$$

where

$$(\mathbf{u}_\mu)_i = \mu\phi'(g_i(\mathbf{x}_\mu)) \geq 0, \forall i \in I \text{ and } (\mathbf{v}_\mu)_j = \mu\psi'(h_j(\mathbf{x}_\mu)), \forall j = 1, \ldots, l. \tag{3.11}$$

Now, assume that $\bar{\mathbf{x}}$ is a regular solution as defined in the Theorem 1.1.16. Then there exist unique Lagrangian multipliers $\bar{u}_i \geq 0$, $i \in I$ and $\bar{v}_j$, $j = 1, \ldots, l$ such that:

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \bar{u}_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\bar{\mathbf{x}}) = 0. \tag{3.12}$$

From continuous differentiabillity of g, h, ϕ, ψ and $\{\mathbf{x}_\mu\} \to \bar{\mathbf{x}}$ where $\bar{\mathbf{x}}$ is a regular point, what follows is that $(u_\mu)_i \to \bar{u}_i$, for any $i \in I$ and $(v_\mu)_j \to \bar{v}_j$, for any $j = 1, \ldots, l$. Therefore, for all μ large enough, the multipliers from (3.11) can be used in order to estimate the Karush-Kuhn-Tucker multipliers at optimality. The following example from [10] illustrates the discussion above.

Example 3.2.1. Let us suppose that the penalty function α is given by

$$\alpha(\mathbf{x}) = \sum_{i=1}^{m} [\max\{0, g_i(\mathbf{x})\}]^2 + \sum_{j=1}^{l} h_j^2(\mathbf{x}).$$

Then, $\phi'(y) = 2\max\{0, y\}$, $\psi'(y) = 2y$. From (3.11) we see that $(u_\mu)_i = 2\mu\max\{0, g_i(\mathbf{x}_\mu)\}$, for any $i \in I$ and $(v_\mu)_j = 2\mu h_j(\mathbf{x}_\mu)$, for any $j = 1, \ldots, l$. Notice that if $\bar{u}_i > 0$ for some $i \in I$ then $(u_\mu)_i$ is also greater than 0 for μ large enough. Hence, $g_i(\mathbf{x}_\mu)$ is greater than 0. That means that the constraint $g_i(\mathbf{x}) \leq 0$ is violated all the way to $\bar{\mathbf{x}}$ and in the accumulation point, $g_i(\bar{\mathbf{x}}) = 0$.

Remark 3.2.2. *As seen in the previous example, the optimal points $\{\mathbf{x}_\mu\}$ do not satisfy the constraints, but for μ large enough, the points converge to optimal solution from outside the feasible region. This defines the name exterior penalty function method.*

3.3 Computational Difficulties

As already mentioned, by choosing μ large enough, the solution to the penalty problem can be made arbitrarily close to an optimal solution. Naturally, we inquire about the degree of the difficulty in solving those kind of problems. When a very large μ is chosen, it might incur some computational difficulties related to ill-conditioning.

Consider the equality constrained problem (EQ). Let $F(\mathbf{x}) = f(\mathbf{x}) + \mu\alpha(\mathbf{x})$ be the penalized objective function, where $\alpha(\mathbf{x}) = \sum_{j=1}^{l} \psi[h_j(\mathbf{x})]$. Also, ψ is assumed to be twice differentiable. It follows:

$$
\nabla F(\mathbf{x}) = \nabla f(\mathbf{x}) + \mu \sum_{j=1}^{l} \psi'[h_j(\mathbf{x})]\nabla h_j(\mathbf{x})
$$

$$
\nabla^2 F(\mathbf{x}) = \left[\nabla^2 f(\mathbf{x}) + \sum_{j=1}^{l} \mu\psi'[h_j(\mathbf{x})]\nabla^2 h_j(\mathbf{x}) \right] + \mu \sum_{j=1}^{l} \psi''[h_j(\mathbf{x})]\nabla h_j(\mathbf{x})\nabla h_j(\mathbf{x})^t,
$$

(3.13)

where ∇, ∇^2 denote the gradient and the Hessian operators, respectively, and ψ', ψ'' the first and the second derivatives of ψ.

The degree of difficulty depends on eigenvalue structure of $\nabla^2 F$. Let us analyse the eigenstructure of (3.13) as $\mu \to \infty$, and, under the conditions of Theorem 3.1.2, as $\mathbf{x} = \mathbf{x}_\mu \to \bar{\mathbf{x}}$. If $\bar{\mathbf{x}}$ is a regular solution, it follows that $\mu\psi'[h_j(\mathbf{x}_\mu)] \to \bar{\mathbf{v}}_j$, the optimal Lagrangian multiplier associated with jth constraint. Hence, the term inside the brackets approaches the Hessian of the Lagrangian function $L(\mathbf{x}) = f(\mathbf{x}) + \sum_{j=1}^{l} \bar{v}_j h_j(\mathbf{x})$. Suppose that $\psi(y) = y^2$, then the second term is equal to 2μ times a matrix that approaches $\sum_{j=1}^{l} \nabla h_j(\bar{\mathbf{x}})\nabla h_j(\bar{\mathbf{x}})^t$, a matrix of rank l. It can then be shown that as $\mu \to \infty$, we have $\mathbf{x} = \mathbf{x}_\mu \to \bar{\mathbf{x}}$ and $\nabla^2 F$ has l eigenvalues that approach infinity. To conclude, for high values of penalty parameter μ the corresponding optimization problem can easily become ill-conditioned. In that case, more importance is placed on feasibility and most of the procedures for solving unconstrained optimization problems will move quickly to a feasible point. Despite the fact that the point might be far from the optimum point, premature termination could occur. Hence, usual methods as steepest descent method stumble upon significant difficulties if the penalty parameter is very large and the starting point is not near an optimal solution.

Example 3.3.1. Consider the same problem as in the Example 2.1.3. Hessian of $F(\mathbf{x}) = 2x_1^2 + 2x_2^2 + \mu(x_1 + x_2 - 2)^2$ is given by

$$
\nabla^2 F(\mathbf{x}) = \begin{bmatrix} 4 + 2\mu & 2\mu \\ 2\mu & 4 + 2\mu \end{bmatrix}.
$$

The eigenvalues of the matrix are $\lambda_1 = 4$ and $\lambda_2 = 4(1 + \mu)$ with the corresponding eigenvectors $(-1, 1)^t$ and $(1, 1)^t$. When $\mu \to \infty$, also $\lambda_2 \to \infty$. Therefore, the condition number

of $\nabla^2 F$ approaches ∞ as $\mu \to \infty$. For a very large value of penalty parameter μ, the steepest descent method would zigzag to the optimum if we do not choose a convenient starting point.

3.4 Algorithm

- **Initialization Step** Let $\varepsilon > 0$ be a termination scalar. Choose a starting point $\mathbf{x}_1$, a penalty parameter $\mu_1 > 0$, and a scalar $\delta > 1$. Let $k = 1$.

- **Main Step**

  1. Starting with $\mathbf{x}_k$, solve:

  $$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(\mathbf{x}) + \mu_k \alpha(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in X \end{aligned}$$

  Let $\mathbf{x}_{k+1}$ be an optimal solution and go to Step 2.

  2. If $\alpha(\mathbf{x}_{k+1}) < \varepsilon$, stop. Otherwise, let $\mu_{k+1} = \delta\mu_k$, replace k by $k + 1$ and return to Step 1.

Chapter 4

Exact Penalty Methods

From the previous sections, it can been seen that, in order to get an optimal solution, we need to make the penalty parameter μ infinitely large. However, by changing the origin of the penalty term, we can recover an optimal solution for finite μ. Those kind of functions are known as exact penalty functions. With these functions it is not necessary to solve an infinite sequence of penalty problems in order to obtain an optimum.

4.1 The l_1 Exact Penalty Function

Firstly, we introduce the absolute value or l_1 penalty function. It is the simplest exact penalty function in which constraint violations are penalized by weighted l_1 terms. But, a new difficulty is its non-smoothness. Therefore, many techniques for smooth optimization can not be used. Throughout this chapter, given a penalty parameter $\mu > 0$, we shall consider the following problem:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \\
& h_j(x) = 0, \quad j = 1, \ldots, l
\end{aligned}
\tag{4.1}
$$

Then, the l_1 objective function is given by:

$$
F_E(\mathbf{x}) = f(\mathbf{x}) + \mu \left[\sum_{i=1}^{m} \max\{0, g_i(\mathbf{x})\} + \sum_{j=1}^{l} |h_j(\mathbf{x})| \right]
\tag{4.2}
$$

The following result from [10] presents conditions under which there exists a finite value of penalty parameter μ that will recover an optimum solution to (P) via the minimization of (4.2).

Theorem 4.1.1. *Consider the problem* (4.1). *Let* $\bar{\mathbf{x}}$ *be a KKT point with Lagrangian multipliers* $\bar{u}_i$, $i \in I$ *and* $\bar{v}_j$, $j = 1, \ldots, l$ *associated with the inequality and the equality constraints, respectively, where* $I = \{i \in \{1, \ldots, m\} : g_i(\bar{\mathbf{x}}) = 0\}$ *is the index set of active inequality constraints. Furthermore, suppose that* f *and* g_i, $i \in I$ *are convex functions and that* h_j, $j = \ldots, l$ *are affine functions. Then, for* $\mu \geq \max\{\bar{u}_i, i \in I, |\bar{v}_j|, j = 1, \ldots, l\}$, $\bar{\mathbf{x}}$ *also minimizes the exact* l_1 *penalized objective function* F_E *defined by* (4.2).

Proof. As assumed, $\bar{\mathbf{x}}$ is a KKT point for problem (4.1). Thus, it is feasible to (4.1) and satisfies

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \bar{u}_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\bar{\mathbf{x}}) = 0, \quad \bar{u}_i \geq 0, \forall i \in I \tag{4.3}$$

Problem of minimizing $F_E(\mathbf{x})$ over $\mathbf{x} \in \mathbb{R}^n$, for any $\mu \geq 0$, can be reformulated as follows:

$$
\begin{aligned}
\text{minimize} \quad & f(\mathbf{x}) + \mu \left[\sum_{i=1}^{m} \mathbf{y}_i + \sum_{j=1}^{l} \mathbf{z}_j \right] \\
\text{subject to} \quad & y_i \geq g_i(\mathbf{x}), y_i \geq 0 && \forall i = 1, \ldots, m \\
& z_j \geq h_j(\mathbf{x}), z_j \geq -h_j(\mathbf{x}) && \forall j = 1, \ldots, l.
\end{aligned}
\tag{4.4}
$$

That follows easily by noticing that for any $\mathbf{x} \in \mathbb{R}^n$, the maximum value of the problem (4.4) is obtained by taking $y_i = \max\{0, g_i(\mathbf{x})\}$, for $i = 1, \ldots, m$ and $z_j = |h_j(\mathbf{x})|$, for $j = 1, \ldots, l$.

Note that of the inequalities $y_i \geq g_i(\mathbf{x})$, $i = 1, \ldots, m$, only those where $i \in I$ are binding, while all the other inequalities in (4.4) are binding at $(\bar{\mathbf{x}}, \bar{\mathbf{y}}, \bar{\mathbf{z}})$. In order to $(\bar{\mathbf{x}}, \bar{\mathbf{y}}, \bar{\mathbf{z}})$ be a KKT point for (4.4), we must find Lagrangian multipliers u_i^+, u_i^-, $i = 1, \ldots, m$ and v_j^+, v_j^-, $j = 1, \ldots, l$, associated with the constraints in (4.4) so that:

$$
\begin{aligned}
\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} u_i^+ \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} (v_j^+ - v_j^-) \nabla h_j(\bar{\mathbf{x}}) &= 0 \\
\mu - u_i^+ - u_i^- &= 0 \quad \forall i = 1, \ldots, m \\
\mu - v_j^+ - v_j^- &= 0 \quad \forall j = 1, \ldots, l \\
(u_i^+, u_i^-) &\geq 0 \quad \forall i = 1, \ldots, m \\
(v_j^+, v_j^-) &\geq 0 \quad \forall j = 1, \ldots, l \\
u_i^+ &= 0 \quad \forall i \notin I.
\end{aligned}
$$

From $\mu \geq \max\{\bar{u}_i, i \in I, |\bar{v}_j|, j = 1, \ldots, l\}$ follows that $u_i^+ = \bar{u}_i$, $\forall i \in I$, $u_i^+ = 0$, $\forall i \notin I$, $u_i^- = \mu - u_i^+$, $\forall i = 1, \ldots, m$, $v_j^+ = (\mu + \bar{v}_j)/2$ and $v_j^- = (\mu - \bar{v}_j)/2$, $\forall j = 1, \ldots, l$ satisfy the KKT conditions. From the Theorem 1.1.16, it follows that $(\bar{\mathbf{x}}, \bar{\mathbf{y}}, \bar{\mathbf{z}})$ solves the equivalent problem. Therefore, $\bar{\mathbf{x}}$ minimizes F_E. $\square$

Example 4.1.2. Once again, let us consider the following problem:

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & 2x_1^2 + 2x_2^2 \\ \text{subject to} \quad & x_1 + x_2 - 2 = 0 \end{aligned} \tag{4.5}$$

From before, it is known that optimum lies at $\bar{\mathbf{x}} = (1, 1)$. The associated Lagrangian multiplier in the KKT conditions is $\bar{v} = -4\bar{x}_1 = -4\bar{x}_2 = -4$. Consider the exact penalty function $F_E = (2x_1^2 + 2x_2^2) + \mu|x_1 + x_2 - 2|$. If $\mu = 0$, it is minimized at $(0, 0)$. On the other hand, if $\mu > 0$, minimizing $F_E(\bar{\mathbf{x}})$ is equivalent to:

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & 2x_1^2 + 2x_2^2 + \mu z \\ \text{subject to} \quad & z \geq x_1 + x_2 - 2 \\ & z \geq -x_1 - x_2 + 2 \end{aligned}$$

From the KKT conditions, it follows that $4x_1 + (v^+ - v^-) = 0$, $4x_2 + (v^+ - v^-) = 0$. $\mu = v^+ + v^-$, $v^+(z - x_1 - x_2 + 2) = v^-(z + x_1 + x_2 - 2) = 0$. Also, $z = |x_1 + x_2 - 2|$.

- If $x_1 + x_2 < 2$, then $z = -x_1 - x_2 + 2$ and $v^+ = 0$, $v^- = \mu$, $x_1 = x_2 = \mu/4$ where $\bar{\mathbf{x}}$ is a KKT point and $\mu < 4$.

- If $x_1 + x_2 = 2$, then $z = 0$, $x_1 = x_2 = 1 = (v^- - v^+)/4$, therefore, $v^- = (\mu + 4)/2$, $v^+ = (\mu - 4)/2$ and $\bar{\mathbf{x}}$ is a KKT point where $\mu \geq 4$.

- If $x_1 + x_2 > 2$, then $z = x_1 + x_2 - 2$, $v^- = 0$, $x_1 = x_2 = -v^+/4$, $v^+ = \mu$. It follows that $2x_1 + 2x_2 = -\mu > 4$ which is a contradiction to the assumption that $\mu \geq 0$.

Therefore, the minimum of F_E occurs at the point $(\mu/4, \mu/4)$ for $\mu < 4$. For all $\mu \geq 4$, the optimum is the same as the optimum of the original problem, $(1, 1)$.

4.1.1 Geometric Interpretation

Let us consider the same example as in geometric interpretation illustrated in the Figure 2.3. The main difference is the fact that we want to minimize $f(\bar{\mathbf{x}}) + \mu|h(\mathbf{x})|$. As before, the contour $f + \mu|h(\mathbf{x})| = k$ needs to be moved downward until it becomes tangential to the shaded set. This is illustrated in the the Figure 4.1

The blue-colored graph represents a function $f + \mu|h|$ for $\mu < 4$ and the point B is the corresponding optimum. The red-colored one represents the same function for $\mu \geq 4$ and A denotes its optimum. It can be easily seen that for $\mu = 4$ (and for every $\mu > 4$), minimizing F_E is equivalent to minimizing the original problem.
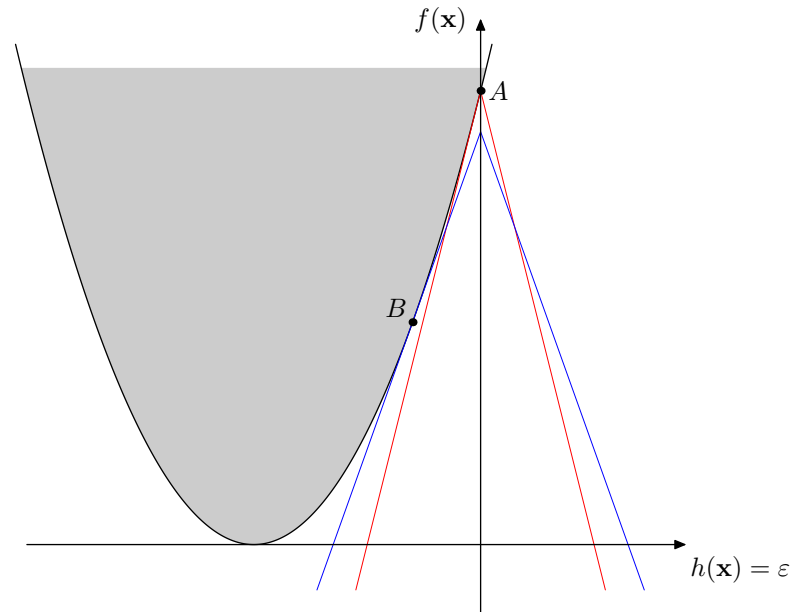
Figure 4.1: Geometric interpretation of the l_1 penalty function

4.2 Multiplier Penalty Functions

After examining the absolute value penalty function, we are motivated to construct an exact penalty function but, unlike the absolute, a differentiable one. The augmented Lagrangian penalty function enjoys that property. The area of Lagrangian multiplier methods for constrained optimization has undergone a radical transformation starting with the introduction of augmented Lagrangian functions and methods of multipliers in 1968 by Hestenes and Powell. The initial success of these methods in computational practice motivated further efforts at understanding and improving their properties. Firstly, we shall consider the problem (EQ). The main idea of the augmented Lagrangian penalty function (ALAG) is to add one more parameter to the penalty function. This suggests using the function

$$f(\mathbf{x}) + \mu \sum_{j=1}^{l} [h_j(\mathbf{x}) - \theta_j]^2 \tag{4.6}$$

The parameters θ_j correspond to shifts from 0 in constraint right-hand sides. Now, it becomes possible to recover an optimal solution without letting $\mu \to \infty$. It is more convenient to omit the constant term and rewrite (4.6) as:

$$F_{ALAG}(\mathbf{x}, \mathbf{v}) = f(\mathbf{x}) + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) + \mu \sum_{j=1}^{l} h_j^2(\mathbf{x}), \tag{4.7}$$

where $v_j = -2\mu\theta_j$, $\forall j = 1, \ldots, l$. There exists a corresponding optimum value of $\mathbf{v}$ for which $\bar{\mathbf{x}}$ minimizes $F_{ALAG}(\mathbf{x}, \mathbf{v})$. Note that if $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$ is a primal-dual KKT solution, then at $\mathbf{v} = \bar{\mathbf{v}}$, we have:

$$\nabla_x F_{ALAG}(\bar{\mathbf{x}}, \bar{\mathbf{v}}) = \left[\nabla f(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\bar{\mathbf{x}})\right] + 2\mu \sum_{j=1}^{l} h_j(\bar{\mathbf{x}}) \nabla h_j(\bar{\mathbf{x}}) = 0 \qquad (4.8)$$

for all μ. Now it is suitable to use $\mathbf{v}$ as the control parameter in a sequential minimization algorithm stated below.

 (i) Determine a sequence $\{\mathbf{v}_k\} \rightarrow \bar{\mathbf{v}}$.

 (ii) For every $\mathbf{v}_k$ find a local minimization solution, $\mathbf{x}(\mathbf{v}_k)$, to $F_{ALAG}(\mathbf{x}, \mathbf{v})$.

 (iii) Terminate when $h(\mathbf{x}(\mathbf{v}_k))$ is sufficiently small.

It is obvious that we only need to make μ large enough to recover a local minimizer. The name multiplier penalty function was motivated by the fact that (4.7) is a quadratic penalty function with additional multiplier term $\sum_{j=1}^{l} v_j h_j(\mathbf{x})$. Function (4.7) can be viewed as the usual quadratic penalty function where we want to minimize the following equivalent problem:

$$\text{minimize} \left\{ f(\mathbf{x}) + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) : h_j(\mathbf{x}) = 0, \forall j = 1, \ldots, l \right\}. \qquad (4.9)$$

Alternatively, (4.7) is the Lagrangian function in which the objective function is augmented by the term $\mu \sum_{j=1}^{l} h_j^2(\mathbf{x})$. Hence the term augmented Lagrangian function. Also, the problem below is equivalent to our original problem.

$$\text{minimize} \left\{ f(\mathbf{x}) + \mu \sum_{j=1}^{l} h_j^2(\mathbf{x}) : h_j(\mathbf{x}) = 0, \forall j = 1, \ldots, l \right\}. \qquad (4.10)$$

The result that $\bar{\mathbf{v}}$ is the optimum choice of the control parameter is expressed in the theorem below from [10].

Theorem 4.2.1. *Consider problem* (EQ). *If second order sufficient conditions hold true at KKT solution $\bar{\mathbf{x}}$ and $\bar{\mathbf{v}}$ (Theorem 1.1.18) then there exist a $\bar{\mu}$ such that for any $\mu \geq \bar{\mu}$, the augmented Lagrangian penalty function $F_{ALAG}(\cdot, \bar{\mathbf{v}})$ also achieves a strict local minimum at $\bar{\mathbf{x}}$. Specifically, if f is convex and h_j, $j = 1, \ldots, l$ are affine, then any minimizing solution $\bar{\mathbf{x}}$ for* (EQ) *also minimizes $F_{ALAG}(\cdot, \bar{\mathbf{v}})$, $\forall \mu \geq 0$.*

Proof. Firstly, observe that because $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$ is a KKT solution, we have

$$\nabla_x F_{ALAG}(\bar{\mathbf{x}}, \bar{\mathbf{v}}) = \left[\nabla f(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\bar{\mathbf{x}})\right] + 2\mu \sum_{j=1}^{l} h_j(\bar{\mathbf{x}}) \nabla h_j(\bar{\mathbf{x}}) = 0.$$

Let $H(\mathbf{x})$ denote the Hessian of $F_{ALAG}(\cdot, \bar{\mathbf{v}})$ at $\mathbf{x} = \bar{\mathbf{x}}$. It follows:

$$H(\bar{\mathbf{x}}) = \nabla^2 f(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \bar{v}_j \nabla^2 h_j(\bar{\mathbf{x}}) + 2\mu \sum_{j=1}^{l} [h_j(\bar{\mathbf{x}}) \nabla^2 h_j(\bar{\mathbf{x}}) + \nabla h_j(\bar{\mathbf{x}}) \nabla h_j(\bar{\mathbf{x}})^t]$$

$$= \nabla^2 L(\bar{\mathbf{x}}) + 2\mu \sum_{j=1}^{l} \nabla h_j(\bar{\mathbf{x}}) \nabla h_j(\bar{\mathbf{x}})^t, \tag{4.11}$$

where $\nabla^2 L(\bar{\mathbf{x}})$ denotes the Hessian of the Lagrangian function for (EQ). From the assumption that $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$ satisfies the second-order sufficiency conditions it follows that $\nabla^2 L(\bar{\mathbf{x}})$ is the positive definite matrix on the cone $C = \{\mathbf{d} \neq 0 : \nabla h_j(\bar{\mathbf{x}})^t \mathbf{d} = 0, \forall j = 1, \ldots, l\}$.

Suppose to the contrary that there does not exist a $\bar{\mu}$ such that $H(\bar{\mathbf{x}})$ is positive definite for all $\mu \geq \bar{\mu}$. Then, for any given $\mu_k = k$, $k = 1, 2, \ldots$ there exists a $\mathbf{d_k}$, such that $\|\mathbf{d_k}\| = 1$ and

$$\mathbf{d_k^t} H(\bar{\mathbf{x}}) \mathbf{d_k} = \mathbf{d_k^t} \nabla^2 L(\bar{\mathbf{x}}) \mathbf{d_k} + 2k \sum_{j=1}^{l} [\nabla h_j(\bar{\mathbf{x}})^t \mathbf{d_k}]^2 \leq 0. \tag{4.12}$$

Since $\|\mathbf{d}_k\| = 1$, $\forall k$, there exists a convergent subsequence for $\{d_k\}$ with an accumulation point $\bar{\mathbf{d}}$, $\|\bar{\mathbf{d}}\| = 1$. In order to (4.12) hold true for every k, we must have $\nabla h_j(\bar{\mathbf{x}})^t \bar{\mathbf{d}}$ equal to 0, $\forall j = 1, \ldots, l$. Obviously, $\bar{\mathbf{d}} \in C$. Now, because $\mathbf{d_k^t} \nabla^2 L(\bar{\mathbf{x}}) \mathbf{d_k} \leq 0$, $\forall k$, we also have $\bar{\mathbf{d}}^t \nabla^2 L(\bar{\mathbf{x}}) \bar{\mathbf{d}} \leq 0$. But, it is in contradiction to the second-order sufficiency conditions. Thus, $H(\bar{\mathbf{x}})$ is positive definite for all μ greater or equal to some value $\bar{\mu}$. By Theorem (1.1.9), $\bar{\mathbf{x}}$ is a strict local minimum for $F_{ALAG}(\cdot, \bar{\mathbf{v}})$.

Lastly, let f be a convex function, h_j, $j = 1, \ldots, l$ affine and $\bar{\mathbf{x}}$ optimal to (EQ). Then there exists a Lagrangian multiplier vector $\bar{\mathbf{v}}$ such that $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$ is a KKT solution. Again, $\nabla_x F_{ALAG}(\bar{\mathbf{x}}, \bar{\mathbf{v}}) = 0$. Also, $F_{ALAG}(\cdot, \bar{\mathbf{v}})$ is convex for all $\mu \geq 0$. Therefore, $\bar{\mathbf{x}}$ minimizes $F_{ALAG}(\cdot, \bar{\mathbf{v}})$, $\forall \mu \geq 0$. □

Example 4.2.2. Consider the same problem as in the Example 4.1.2. It follows that $\bar{\mathbf{x}} = (1, 1)$ with $\bar{\mathbf{v}} = -4$ is the unique KKT optimal point. Let us find out if the assumptions of the Theorem 4.2.1 are fulfilled. Firstly, from

$$F_{ALAG}(\bar{\mathbf{x}}, \bar{\mathbf{v}}) = (2x_1^2 + 2x_2^2) - 4(x_1 + x_2 - 2) + \mu(x_1 + x_2 - 2)^2$$

follows that F_{ALAG} is minimized at $\bar{\mathbf{x}} = (1, 1)$, for any $\mu \geq 0$. After that, we observe that $\nabla^2 L(\bar{\mathbf{x}})$ is positive definite, which implies that the second-order sufficiency conditions holds true at $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$. Consequently, both assertions from the Theorem 4.2.1 hold true.

The following example from [5] states that assumption of second-order sufficiency conditions is important and not easily relaxed.

Example 4.2.3. Consider the following problem:

$$\underset{x}{\text{minimize}} \quad x_1^4 + x_1 x_2$$
$$\text{subject to} \quad x_2 = 0 \tag{4.13}$$

Obviously, $\bar{\mathbf{x}} = 0$ solves the problem above with the unique Lagrangian multiplier $\bar{\mathbf{v}} = 0$. The second-order sufficiency conditions are not satisfied. Indeed,

$$\nabla^2 L(\bar{\mathbf{x}}) = \nabla^2 f(\mathbf{x}) = \begin{bmatrix} 0 & 1 \\ 1 & 2\mu \end{bmatrix}$$

is indefinite. We have $F_{ALAG}(\bar{\mathbf{x}}, \bar{\mathbf{v}}) = x_1^4 + x_1 x_2 + \mu x_2^2$.

$$\nabla F_{ALAG}(\mathbf{x}, \mathbf{v}) = \begin{bmatrix} 4x_1^3 + x_2 \\ x_1 + 2\mu x_2 \end{bmatrix}$$

For any $\mu > 0$, $\nabla F_{ALAG}(\mathbf{x}, \mathbf{v})$ vanishes at $\bar{\mathbf{x}} = 0$, but also at $\hat{\mathbf{x}} = (1/\sqrt{8\mu}, -1/(2\mu\sqrt{8\mu}))^t$. From

$$\nabla^2 F_{ALAG}(\mathbf{x}, \mathbf{v}) = \begin{bmatrix} 12x_1^2 & 1 \\ 1 & 2\mu \end{bmatrix}$$

we see that $\nabla^2 F_{ALAG}(\bar{\mathbf{x}}, \mathbf{v})$ is indefinite so $\bar{\mathbf{x}}$ is not a local minimizer. But, $\nabla^2 F_{ALAG}(\hat{\mathbf{x}}, \mathbf{v})$ is positive definite, and $\hat{\mathbf{x}}$ is the minimizer. Taking $\mu \to \infty$, $\hat{\mathbf{x}}$ approaches the optimum solution.

4.2.1 Geometric Interpretation

Firstly, let us assume that $\bar{\mathbf{x}}$ is a regular point and that $(\bar{\mathbf{x}}, \bar{\mathbf{v}})$ satisfies the second-order sufficiency conditions for a strict local minimum. From the Sensitivity theorem 2.2.2 follows that $\nabla v(0) = -\bar{\mathbf{v}}$ where $v(\varepsilon)$ is a primal function as defined as in (2.2.1). The augmented Lagrangian method looks for a minimum of $f(\mathbf{x}) + \bar{v}h(\mathbf{x}) + \mu h^2(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^2$. In other words, the goal is to find the smallest value of k for which $f + \bar{v}h + \mu h^2 = k$ has intersection with the epigraph of v. We can rewrite it as $f = -\mu(h + (\bar{v}/2\mu))^2 + (k + (\bar{v}^2/4\mu))$. That equation represents a parabola whose axis are shifted to $h = -\bar{v}^2/2\mu$, what makes it different from the interpretation in the Figure 2.3 where $h = 0$. This is illustrated in the figure below. It represents function $v(\varepsilon)$, as well as penalty functions $f + \bar{v}h + \mu h^2$ for two different values of μ. The point A represents an optimal solution to penalty problem for $\mu > 0$, while points B and C represent the x-axis of the vertex of parabolas. It is equal to

$-\bar{v}/(2\mu)$. Note that when k equals the optimal objective value for considered problem, i.e., $k = v(0)$, the parabola passes through $(0, v(0))$ and the tangent to the parabola has a slope that equals $-\bar{v}$. Thus, for any $\mu > 0$, the minimum of the augmented Lagrangian coincides with the optimal point to the considered problem.
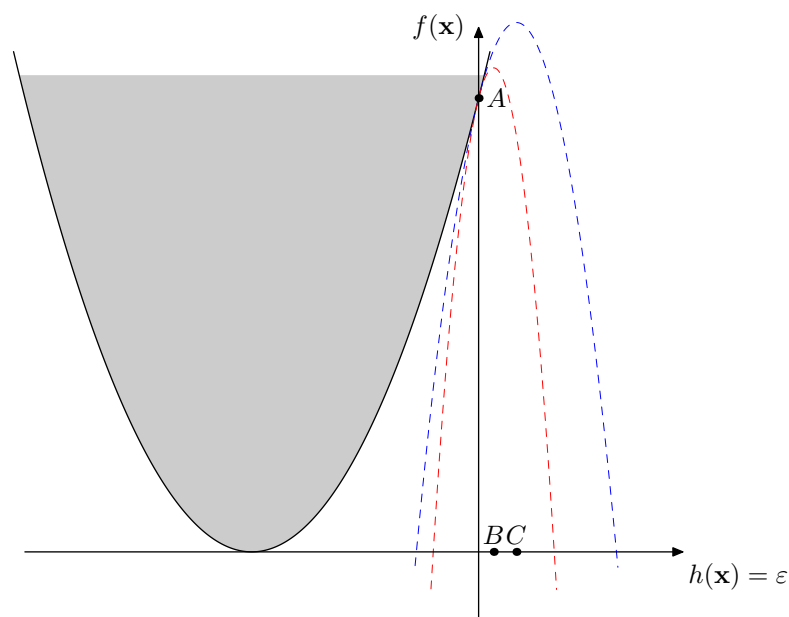

Figure 4.2: Geometric interpretation of the augmented Lagrangian penalty function

Note the following relations, for any v:

$$
\min_x \left\{ f(\mathbf{x}) + v^t h(\mathbf{x}) + \mu \|h(\mathbf{x})\|^2 \right\} = \min_{x,\varepsilon}\{f(\mathbf{x}) + v^t\varepsilon + \mu \|\varepsilon\|^2 : h(\mathbf{x}) = \varepsilon\}
$$
$$
= \min_\varepsilon \{v(\varepsilon) + v^t\varepsilon + \mu \|\varepsilon\|^2\}.
$$

(4.14)

When it comes to nonconvex case, when $\nabla v(0) = -\bar{\mathbf{v}}$, the above described situation happens only for μ large enough. Let us define $V(\varepsilon) = v(\varepsilon) + \bar{v}^t\varepsilon + \mu \|\varepsilon\|^2$ and let $v = \bar{v}$. When μ is large enough, V becomes convex function in the neighborhood of $\varepsilon = 0$ and $\nabla V(0) = \nabla v(0) + \bar{v} = 0$. Therefore, V has a strict local minimum at $\varepsilon = 0$. This is illustrated in the Figure 4.3.
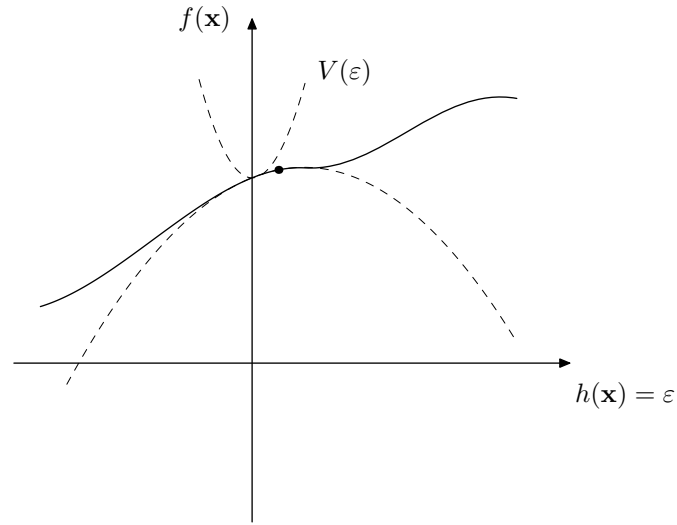
Figure 4.3: Geometric interpretation of the augmented Lagrangian penalty function, non-convex case

4.2.2 Algorithm

Consider the problem:

$$\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & h_j(\mathbf{x}) = 0, \quad j = 1, \dots, l
\end{aligned} \tag{4.15}$$

Let us, instead of one common parameter μ, assign each constraint h_j its own μ_j. Therefore,

$$F_{ALAG}(\mathbf{x}, \mathbf{v}) = f(\mathbf{x}) + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) + \sum_{j=1}^{l} \mu_j h_j^2(\mathbf{x}). \tag{4.16}$$

- **Initialization Step** Let $\mathbf{v} = \bar{\mathbf{v}}$ be an initial Lagrangian multiplier and let $\mu_1, \dots, \mu_l$ be some positive numbers, also let $\mathbf{x}_0$ be a null vector and $\text{VIOL}(\mathbf{x}_0) = \infty$, where $\text{VIOL}(\mathbf{x}) = \max\{|h_j(\mathbf{x})| : j = 1, \dots, l\}$. Put $k = 1$ and go to the inner loop.

- **Inner Loop Step** Let $\mathbf{x}_k$ denote the optimal solution to minimization problem of $F_{ALAG}(\mathbf{x}, \bar{\mathbf{v}})$. If $\text{VIOL}(\mathbf{x}_k) = 0$, stop. $\mathbf{x}_k$ is a KKT point. Also, we could stop the algorithm if $\text{VIOL}(\mathbf{x}_k)$ is less than some $\varepsilon > 0$. Else, if $\text{VIOL}(\mathbf{x}_k) \le (1/4)\text{VIOL}(\mathbf{x}_{k-1})$, go to the outer loop. But, if $\text{VIOL}(\mathbf{x}_k) > (1/4)\text{VIOL}(\mathbf{x}_{k-1})$, then for each constraint for which $|h_j(\mathbf{x})| > (1/4)\text{VIOL}(\mathbf{x}_{k-1})$, $j = 1, \dots, l$, multiply the penalty parameter μ_j by 10, $\mu_j = 10\mu_j$ and repeat the inner loop step.

- **Outer Loop Step** Let, $\forall j$, $(\bar{\mathbf{v}}_{new})_j = \bar{v}_j + 2\mu_j h_j(\mathbf{x}_k)$, $k = k + 1$ and return to the inner loop.

When it comes to solving the minimization problem in the inner loop, we can use $\mathbf{x}_{k-1}$ as a starting point and employ some of the methods for solving unconstrained minimization problems. Note that if $\text{VIOL}(\mathbf{x}_k) = 0$, then $\mathbf{x}_k$ is a feasible point and from

$$\nabla_x F_{ALAG}(\mathbf{x}_k, \bar{\mathbf{v}}) = \nabla f(\mathbf{x}_k) + \sum_{j=1}^{l} \bar{v}_j \nabla h_j(\mathbf{x}_k) + \sum_{j=1}^{l} 2\mu_j h_j(\mathbf{x}_k) \nabla h_j(\mathbf{x}_k) = 0, \qquad (4.17)$$

it follows that $\mathbf{x}_k$ is actually a KKT point. Whenever the VIOL measure is not improved by the factor $1/4$, the μ_j is multiplied by 10. We know that, from the Theorem 3.1.2, $h_j(\mathbf{x}_k) \to 0$ as $\mu_j \to \infty$, $\forall j = 1, \dots, l$. Because of that, when some $\varepsilon > 0$ is used, the outer loop of the algorithm will be visited after a finite number of iterations.

The previous argument is true in spite of updating a dual multiplier in the outer loop. Note that if we use the standard quadratic penalty function approach on the problem (4.9), the estimate of the Lagrangian multipliers is given by $2\mu_j h_j(\mathbf{x}_k)$, $\forall j = 1, \dots, l$. Equation in the outer loop gives an estimation for the Lagrangian multipliers associated with the constraints of the original problem because the fact that the Lagrangian multiplier for the original problem equals $\bar{\mathbf{v}}$ plus the Lagrangian multiplier vector for (4.9).

There exists an alternative Lagrangian duality-based interpretation of the update of $\bar{\mathbf{v}}$ in the outer loop when $\mu_j = \mu$, $\forall j = 1, \dots, l$. That leads to a procedure that has a better rate of convergence. The original problem is equivalent to the problem (4.10). At $\mathbf{v} = \bar{\mathbf{v}}$, the inner loop evaluates $\theta(\bar{\mathbf{v}}) = \min_x \{F_{ALAG}(\mathbf{x}, \bar{\mathbf{v}})\}$, determining an optimal solution $\mathbf{x}_k$. This yields $h(\mathbf{x}_k)$ as a subgradient (1.1.13) of θ at $\mathbf{v} = \bar{\mathbf{v}}$. The update of $\bar{\mathbf{v}}_{new}$ is actually a fixed-step-length subgradient direction-based iteration for the dual function.

Example 4.2.4. Once again, consider the same minimization problem as in the Example 4.1.2. Let us suppose that we start the multiplier method algorithm with some $\mathbf{v}$. We have $F_{ALAG}(\mathbf{x}, \mathbf{v}) = 2x_1^2 + 2x_2^2 + v(x_1 + x_2 - 2) + \mu(x_1 + x_2 - 2)^2$. The inner loop will evaluate $\theta(\mathbf{v}) = \min_x \{F_{ALAG}(\mathbf{x}, \mathbf{v})\}$. From solving $\nabla_x F_{ALAG}(\mathbf{x}, \mathbf{v}) = 0$, we get $x_1(v) = x_2(v) = (4\mu - v)/(4 + 4\mu)$. After that, we go to the outer loop which updates the Lagrangian multiplier, $\mathbf{v}_{new} = v + 2\mu(x_1(v) + x_2(v) - 2) = (2v - 8\mu)/(2 + 2\mu)$. Now, obviously, when $\mu \to \infty$, v_{new} approaches -4, which is the optimal Lagrangian multiplier value.

4.2.3 Inequality Constraints in the ALAG Penalty Function

Consider the following problem:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & g_i(\mathbf{x}) \leq 0 \quad i = 1, \ldots, m \\
& h_j(\mathbf{x}) = 0 \quad j = 1, \ldots, l
\end{aligned}
\tag{4.18}
$$

Note that now minimization problem consists of equality as well as inequality constraints. In order to incorporate the inequality constraints in the augmented Lagrangian penalty method and the method of multipliers, we write the inequalities as the equalities $g_i(\mathbf{x}) + s_i^2 = 0, \forall i = 1, \ldots, m$. Let us assume that there is $\bar{\mathbf{x}}$, a KKT point for the problem above, with optimal Lagrangian multipliers $\bar{v}_j$, $j = 1, \ldots, l$ and $\bar{u}_i$, $i = 1, \ldots, m$, associated with the equality and inequality constraints. Denote $I(\bar{\mathbf{x}}) = \{i : g_i(\bar{\mathbf{x}}) = 0\}$ as earlier. Suppose that $\bar{u}_i g_i(\bar{\mathbf{x}}) = 0, \forall i = 1, \ldots, m$ and $\bar{u}_i > 0, \forall i \in I(\bar{\mathbf{x}})$. Moreover, let $\nabla^2 L(\bar{\mathbf{x}})$ be positive definite over the cone $C = \{d \neq 0 : \nabla g_i(\bar{\mathbf{x}})^t d = 0, \forall i \in I(\bar{\mathbf{x}}), \nabla h_j(\bar{\mathbf{x}})^t d = 0, \forall j = 1, \ldots, l\}$. In other words, the second-order sufficiency condition holds true at $(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{v}})$. Now it follows that the conditions of the Theorem 4.2.1 are satisfied for the problem

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(\mathbf{x}) \\
\text{subject to} \quad & g_i(\mathbf{x}) + s_i^2 = 0, \quad i = 1, \ldots, m \\
& h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, l
\end{aligned}
\tag{4.19}
$$

at the solution $(\bar{\mathbf{x}}, \bar{\mathbf{s}}, \bar{\mathbf{u}}, \bar{\mathbf{v}})$ where $\bar{s}_i^2 = -g_i(\bar{\mathbf{x}}), \forall i = 1, \ldots, m$. Thus, at $(u, v) = (\bar{\mathbf{u}}, \bar{\mathbf{v}})$, $(\bar{\mathbf{x}}, \bar{\mathbf{s}})$ is a strict local minimizer for the augmented Lagrangian penalty function below, for sufficiently large penalty parameter μ:

$$
F_{ALAG}(\mathbf{x}, \mathbf{s}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \sum_{i=1}^{m} \mu_i(g_i(\mathbf{x}) + s_i^2) + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) + \mu \left[\sum_{i=1}^{m} (g_i(\mathbf{x}) + s_i^2)^2 + \sum_{j=1}^{l} h_j^2(\mathbf{x}) \right].
\tag{4.20}
$$

In order to simplify the (4.20), let $\theta(\mathbf{u}, \mathbf{v})$ be the minimum of (4.20) for a given $\mu > 0$ and any set of Lagrangian multipliers $(\mathbf{u}, \mathbf{v})$. (4.20) is equivalent to:

$$
F_{ALAG}(\mathbf{x}, \mathbf{s}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \mu \sum_{i=1}^{m} \left[g_i(\mathbf{x}) + s_i^2 + \frac{u_i}{2\mu} \right]^2 - \sum_{i=1}^{m} \frac{u_i^2}{4\mu} + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) + \mu \sum_{j=1}^{l} h_j^2(\mathbf{x}).
\tag{4.21}
$$

By letting $s_i^2 = \max\{-(g_i(\mathbf{x}) + (u_i/2\mu)), 0\}$, we can easily minimize (4.21) over $(\mathbf{x}, \mathbf{s})$. Firstly, we minimize $(g_i(\mathbf{x}) + s_i^2 + (u_i/2\mu))$ over s_i in terms of $\mathbf{x}$, $\forall i = 1, \ldots, m$ and then minimize the whole expression over $\mathbf{x}$. Therefore,

$$\theta(\mathbf{u}, \mathbf{v}) = \min_x \left\{ f(\mathbf{x}) + \mu \sum_{i=1}^{m} \max^2 \left\{ g_i(\mathbf{x}) + \frac{u_i}{2\mu}, 0 \right\} - \sum_{i=1}^{m} \frac{u_i^2}{4\mu} + \sum_{j=1}^{l} v_j h_j(\mathbf{x}) + \mu \sum_{j=1}^{l} h_j^2(\mathbf{x}) \right\}$$

$$= \min_x \{ F_{ALAG}(\mathbf{x}, \mathbf{u}, \mathbf{v}) \}.$$

(4.22)

When it comes to the method of multipliers, the inner loop will evaluate $\theta(\mathbf{u}, \mathbf{v})$ and calculate $\mathrm{VIOL}(\mathbf{x}_k)$ and proceed as earlier. If $\mathbf{x}_k$ minimizes (4.22), the the subgradient component of $\theta(\mathbf{u}, \mathbf{v})$ corresponding to u_i at $(\bar{\mathbf{u}}, \bar{\mathbf{v}})$ is given by $2\mu \max\{g_i(\mathbf{x}_k) + (\bar{u}_i/2\mu), 0\}(1/2\mu) - (2\bar{u}_i/4\mu) = (-\bar{u}_i/2\mu) + \max\{g_i(\mathbf{x}_k) + (\bar{u}_i/2\mu), 0\}$. If we set the fixed step length of 2μ along this subgradient direction, in the outer loop step we get:

$$(\bar{u}_{new})_i = \bar{u}_i + \max\{2\mu g_i(\mathbf{x}_k), -\bar{u}_i\}, \quad \forall i = 1, \ldots, m. \tag{4.23}$$

As for the alternative, we can also revise u_i using an approximate second-order update scheme as for the case of the equality constrains.

Chapter 5

Application of Penalty Functions

5.1 Convex and Smooth Problem

By this point, we have elaborated all the important results about penalty functions. The next step is to check how well all of those methods approximate the exact solution. Consider the following minimization problem:

$$
\begin{aligned}
\underset{x_1, x_2}{\text{minimize}} \quad & (x_1 - 3)^2 + 2x_2^2 \\
\text{subject to} \quad & x_1 + x_2 = 4 \\
& (x_1 - x_2)^2 \leq 9.
\end{aligned}
\tag{5.1}
$$

The optimal solution lies at $\bar{x} = (\frac{7}{2}, \frac{1}{2})$ with objective function value $\frac{3}{4}$. The KKT multipliers at optimality are $v = -\frac{3}{2}$ and $u = \frac{1}{14} \approx 0.07$

As in developing theory behind penalty functions, first consider the following penalty function:

$$
\alpha(x_1, x_2) = (x_1 + x_2 - 4)^2 + \max\{0, (x_1 - x_2)^2 - 9\}^2
\tag{5.2}
$$

and define the violation of constraints as follows:

$$
\begin{aligned}
\text{violation}_1 &= |x_1 + x_2 - 4| \\
\text{violation}_2 &= \max\{0, (x_1 - x_2)^2 - 9\} \\
\text{violation} &= \max\{\text{violation}_1, \text{violation}_2\}
\end{aligned}
\tag{5.3}
$$

Therefore, our goal is to minimize:

$$
F(x_1, x_2) = (x_1 - 3)^2 + 2x_2^2 + \mu(x_1 + x_2 - 4)^2 + \mu \max\{0, (x_1 - x_2)^2 - 9\}^2.
\tag{5.4}
$$

As in the algorithm from (3.4), we set:

- a termination scalar $\varepsilon = 10^{-5}$

- a starting point $x_0 = (0, 0)$

- a penalty parameter $\mu_1 = 10$

- a scalar $\delta = 10$

In each iteration, we calculate the minimum of (5.4) depending on the current μ value. Every optimal solution is a starting point in the next iteration. The loop is stopped when violation is smaller than ε. All calculations are done in Python using scipy minimize function. It can be seen in the Table 5.1 that we are approaching the feasible region from

iteration	μ	x	objective value	violation
1	10	(3.46544586, 0.4648014)	0.648721	0.06975
2	100	(3.49631232, 0.49624341)	0.73884	0.00744
3	1000	(3.49962861, 0.49962167)	0.74887	0.00075
4	10000	(3.49996271, 0.49996202)	0.749887	7.527e-05
5	100000	(3.49999615, 0.49999608)	0.74999	7.77561e-06

Figure 5.1: Iterations and solutions in exterior penalty method

the outside and finally reach the point $(3.49999615, 0.49999608)$ which is still slightly infeasible but very close to the exact optimal solution. The objective value differs from the exact optimum objective value in 0.00001. In order to obtain the maximum permitted level of violation, μ has to be at least 100000.

```python
import math
import numpy as np
import pandas as pd
from scipy.optimize import minimize


def exterior(x):
    obj = (x[0]-3)**2+2*x[1]**2
    obj += mu*(x[0]+x[1]-4)**2
    obj += mu*max(0, (x[0]-x[1])**2-9)**2
    return obj

eps = 10**-5
mu = 10
delta = 10
x0 = np.zeros(2)
violence = np.zeros(2)
violence[0] = max(0, (x0[0]-x0[1])**2-9)
```

```
19  violence[1] = abs(x0[0]+x0[1]-4)
20  viol = max(violence)
21  i = 1
22  while (viol >= eps):
23      x0 = minimize(exterior, x0).x
24      violence[0] = max(0, (x0[0]-x0[1])**2-9)
25      violence[1] = abs(x0[0]+x0[1]-4)
26      viol = max(violence)
27      objective = (x0[0]-3)**2+2*x0[1]**2
28      vi = 2*mu*(x0[0]+x0[1]-4)
29      ui = 2*mu*max(0, (x0[0]-x0[1])**2-9)
30      print("{} -> mu= {}, x = {}, viol = {}, obj_value={}, exterior={}".
        format(i, mu, x0, viol, objective, exterior(x0)))
31      mu = mu*delta
32      i += 1
```

Listing 5.1: Python code for the exterior penalty function

Secondly, we want to examine the exact penalty functions. l_1 penalty function for the above given example is:

$$\alpha(x_1, x_2) = \max\{0, (x_1 - x_2)^2 - 9\} + |x_1 + x_2 - 4| \qquad (5.5)$$

So the original problem can be rewritten as:

$$\underset{x_1,x_2}{\text{minimize}} \quad (x_1 - 3)^2 + 2x_2^2 + \mu \max\{0, (x_1 - x_2)^2 - 9\} + \mu|x_1 + x_2 - 4| \qquad (5.6)$$

and violation calculations are as written in (5.3). Once again, we have set the termination scalar $\varepsilon = 10^{-5}$, the starting point $x_0 = (0, 0)$ and the scalar $\delta = 10$ and have done exactly as in the example above. But, because of dealing with non-differentiable penalty function, we use shgo minimization solver.

iteration	μ	x	objective value	violation
1	10	(3.4999967,4 0.50000326)	0.750003	6.37595e-09

Figure 5.2: Iterations and solutions in l_1 penalty method

Unlike the exterior penalty function, we have reached the end of the algorithm in just one iteration, for $\mu = 10$. The difference between the exact optimum objective value and objective value calculated by this method is 0.000003 which is less than the difference in the exterior method.

```
1  from shgo import shgo
2
```

```
 3 def l1(x):
 4     obj = (x[0]-3)**2+2*x[1]**2
 5     obj += mu*abs(x[0]+x[1]-4)
 6     obj += mu*max(0, (x[0]-x[1])**2-9)
 7     return obj
 8
 9
10 i = 1
11 eps = 10**-5
12 mu = 10
13 delta = 10
14 x0 = np.zeros(2)
15 violence = np.zeros(2)
16 violence[0] = abs(x0[0]+x0[1]-4)
17 violence[1] = max(0, (x0[0]-x0[1])**2-9)
18 viol = max(violence)
19 while (viol >= eps):
20     bounds = [(None, None), (None, None)]
21     x0 = shgo(l1, bounds).x
22     violence[0] = abs(x0[0]+x0[1]-4)
23     violence[1] = max(0, (x0[0]-x0[1])**2-9)
24     viol = max(violence)
25     objective = (x0[0]-3)**2+2*x0[1]**2
26     print("{} -> mu= {}, x = {}, viol = {}, obj_value ={}, l_1 ={}".format
       (i, mu, x0, viol, objective, l1(x0)))
27     mu = mu*delta
28     i += 1
```

Listing 5.2: Python code for the l_1 penalty function

Finally, let us consider the augmented Lagrangian penalty function

$$\alpha(x_1, x_2) = \max\left\{0, (x_1 - x_2)^2 - 9 + \frac{u}{2\mu}\right\}^2 - \frac{u^2}{4\mu^2} + \frac{1}{\mu}v(x_1 + x_2 - 4) + (x_1 + x_2 - 4)^2 \quad (5.7)$$

and find the minimum value of

$$F_{ALAG}(x_1, x_2) = (x_1-3)^2+2x_2^2+\mu \max\left\{0, (x_1 - x_2)^2 - 9 + \frac{u}{2\mu}\right\}^2 - \frac{u^2}{4\mu}+v(x_1+x_2-4)+\mu(x_1+x_2-4)^2,$$
$$(5.8)$$

where u and v are Lagrangian multipliers associated with the inequality and equality constraints, respectively.

We follow the algorithm from (4.2.2) and set:

- the initial Lagrangian multipliers, $v = 0$ and $u = 0$

- a termination scalar $\varepsilon = 10^{-5}$

- a initial solution $x_0 = (0, 0)$

- VIOL(x_0)=∞,

where violation is also defined in (5.3).

iteration	μ	x	objective value	violation
1	10	(3.46544586, 0.4648014)	0.64872	0.06975
2	10	(3.49758304 0.49753662)	0.74267	0.00488
3	10	(3.49983088, 0.49982763)	0.74949	0.00034
4	10	(3.49998817, 0.49998794)	0.74996	2.38932e-05
5	10	(3.49999917, 0.49999915)	0.749997	1.67562e-06

Figure 5.3: Iterations and solutions in multiplier penalty method

We see that the penalty parameter μ has not increased. Therefore, in every iteration violation was 4 times smaller than the previous one. In the final step, we get the optimal solution $\bar{\mathbf{x}} = (3.49999917, 0.49999915)$, corresponding Lagrangian multipliers $u = 0.083$ and $v = -1.5$ and objective value 0.749997. The difference from the actual objective value is only 0.000003.

```python
def alag(x):
    obj = (x[0]-3)**2+2*x[1]**2
    obj += mu*(x[0]+x[1]-4)**2 + v*(x[0]+x[1]-2)
    obj += mu*max((x[0]-x[1])**2-9 + (u/(2*mu)), 0)**2 - u**2/(4*mu)
    return obj


eps = 10**-5
mu = 10
delta = 10
x0 = np.zeros(2)
viol = math.inf
old_viol = viol
v = 0
u = 0
i = 1
while (viol >= eps):
    x0 = minimize(alag, x0).x
    violence[0] = abs(x0[0]+x0[1]-4)
    violence[1] = max(0, (x0[0]-x0[1])**2-9)
    viol = max(violence)
    objective = (x0[0]-3)**2+2*x0[1]**2
    print("{} -> mu= {}, x = {}, viol = {}, obj_value={}".format(i, mu,
    x0, viol, objective))
```

```
24    if (viol <= 1/4 * old_viol):
25        v = v + 2*mu*(x0[0]+x0[1]-4)
26        u = u + max(-u, 2*mu*((x0[0]-x0[1])**2-9))
27    else:
28        mu = mu*10
29    old_viol = viol
30    i += 1
```

Listing 5.3: Python code for the ALAG penalty function

5.2 Cardinality Constrained Portfolio

After showing that the method approximates the optimum very well when it comes to academic examples, it is natural to wonder if it solves real-world problems equally well. Let us consider the following portfolio problem:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & x^T Q x \\
\text{subject to} \quad & m^T x \geq \rho, \\
& e^T x \leq 1, \\
& 0 \leq x_i \leq u_i \quad \forall i = 1, \dots, n, \\
& \|x\|_0 \leq \chi,
\end{aligned}
\tag{5.9}
$$

where Q and m are the covariance matrix and mean of n possible assets, respectively and $e^T x \leq 1$ is a resource constraint. $\|x\|_0$ denotes the number of non-zero elements in **x**. It is a classical mean-variance portfolio selection model of Markowitz [9] with limits on the number of assets to be held in a portfolio, what makes it a mixed-integer problem. These requirements come from real-world practice. In general, a portfolio made up of a large number of assets with very small holdings is not desirable mainly because of transactions costs. Because of its wide usage, cardinality constrained portfolio optimization problem has lately been intensively studied, especially from the computational viewpoint. In general, mixed-integer optimization problems are very difficult to solve. While the classical Markowitz model is a convex quadratic programming problem with a polynomial complexity, the cardinality constrained problem is a NP-hard problem. Therefore, real-world cardinality constrained problems involving markets with less than a hundred assets have not yet been solved to optimality. This all being said motivates our attempt to solve the problem (5.9) using the penalty method. Firstly, from [3] follows that (5.9) can be refor-

mulated as

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & x^T Q x \\
\text{subject to} \quad & m^T x \geq \rho, \\
& e^T x \leq 1, \\
& 0 \leq x_i \leq u_i y_i \quad \forall i = 1, \dots, n, \\
& y_i \in \{0, 1\} \qquad \forall i = 1, \dots, n, \\
& e^T y \leq \chi.
\end{aligned}
\tag{5.10}
$$

Also, we consider the standard relaxation of the mixed-integer problem:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & x^T Q x \\
\text{subject to} \quad & m^T x \geq \rho, \\
& e^T x \leq 1, \\
& 0 \leq x_i \leq u_i \qquad \forall i = 1, \dots, n, \\
& e^T y \geq n - \chi, \\
& x_i y_i = 0 \qquad \forall i = 1, \dots, n, \\
& 0 \leq y_i \leq 1 \qquad \forall i = 1, \dots, n,
\end{aligned}
\tag{5.11}
$$

To test our approach, we use the same data as in [6] but reduce the dimension to avoid memory issues. We take the first 15 rows from [2] and set the cardinality constraint to be 5. In order to compare the efficiency of the penalty method, we solved (5.10) directly using GUROBI via the provided Python interface. For more details about GUROBI see [1]. Because of dimension reduction, GUROBI has found the optimal point in every example. Our approach is based on the regularization problem below:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & x^T Q x \\
\text{subject to} \quad & m^T x \geq \rho, \\
& e^T x \leq 1, \\
& 0 \leq x_i \leq u_i \qquad \forall i = 1, \dots, n, \\
& e^T y \geq n - \chi, \\
& \phi(x_i, y_i; t) \leq 0 \quad \forall i = 1, \dots, n, \\
& \tilde{\phi}(x_i, y_i; t) \leq 0 \quad \forall i = 1, \dots, n, \\
& 0 \leq y_i \leq 1 \qquad \forall i = 1, \dots, n,
\end{aligned}
\tag{5.12}
$$

where function ϕ and $\tilde{\phi}$ are of the form:

$$
\phi(a, b; t) := \begin{cases} (a - t)(b - t) & \text{if } a + b \geq 2t, \\ -\frac{1}{2}[(a - t)^2 + (b - t)^2] & \text{if } a + b < 2t \end{cases}
\tag{5.13}
$$

$$\tilde{\phi}(a, b; t) := \begin{cases} (-a - t)(b - t) & \text{if } -a + b \ge 2t, \\ -\frac{1}{2}[(-a - t)^2 + (b - t)^2] & \text{if } -a + b < 2t \end{cases} \tag{5.14}$$

t is called the regularization parameter. It can be easily seen that $\forall t \ge 0$

$$\phi(a, b; t) \le 0 \iff a \le t \text{ or } b \le t \iff \min\{a, b\} \le t$$

as well as

$$\tilde{\phi}(a, b; t) \le 0 \iff -a \le t \text{ or } b \le t \iff \min\{-a, b\} \le t$$

(5.12) is solved iteratively, also using GUROBI, beginning with the regularization parameter $t = 1$ and decreasing it by 0.1 in every iteration. The algorithm would stop if the regularization parameter became too small, i.e., $t \le 10^{-10}$ or if the violation of the orthogonality conditions was sufficiently small, i.e., $\max_{i=1,\dots,n} |x_i y_i| \le 10^{-6}$. Convergence result of the regularization method can be found in [4]. Finally, we rewrite (5.12) using penalty functions as

$$\underset{x,y}{\text{minimize}} \quad x^T Q x + \mu \max\{0, e^T x - 1\}^2 + \mu \max\{0, \rho - m^T x\}^2 + \mu \max\{0, n - \chi - e^T y\}^2 +$$

$$\mu \sum_{i=1}^{n} \max\{0, \phi(x_i, y_i, t)\}^2 + \mu \sum_{i=1}^{n} \max\{0, \tilde{\phi}(x_i, y_i, t)\}^2 + \mu \sum_{i=1}^{n} \max\{0, x_i - u_i\}^2 +$$

$$\mu \sum_{i=1}^{n} \max\{0, -x_i\}^2 + \mu \sum_{i=1}^{n} \max\{0, -y_i\}^2 + \mu \sum_{i=1}^{n} \max\{0, y_i - 1\}^2 \tag{5.15}$$

where the penalty parameter μ is set to be $\mu = 1/t$.

	GUROBI	regularization	penalty method
orl200-005-a	45.31297	45.31297	45.29229
orl200-005-b	67.34859	67.34859	67.43854
orl200-05-a	32.41775	32.41775	32.40874
orl200-05-b	15.96268	15.96268	16.22719

Figure 5.4: Solutions of the cardinality constrained portfolio problem

From (5.4) can be seen that in every example solution of regularized portfolio problem is the same as the solution of original problem. Our approach approximates solutions very close to the optimal ones. Python codes for each of these methods are listed below.

```python
from gurobipy import *
import pandas as pd
import numpy as np

```

```python
5  size = 15
6  cardinality = 5
7  sigma = np.genfromtxt("orl200-005-a.mat", skip_header=1, dtype='int')
8  sigma = sigma[0:size, 0:size]
9  m = pd.read_csv("orl200-005-a.txt", sep=" ", index_col=False, skiprows
       =1, names=['mu_i', 'ignore'])
10 rho = np.genfromtxt("orl200-005-a.rho")
11 rho = rho.item()
12 m = m.iloc[0:size, 0]
13 bounds = pd.read_csv("orl200-005-a.bds", sep=" ", index_col=False, names
       =['l_i', 'u_i'])
14 bounds = bounds.transpose()
15 u_i = bounds.iloc[1, 0:size]
16 model = Model('portfolio')
17 vars_ = pd.Series(model.addVars(size))
18 y = pd.Series(model.addVars(size, vtype=GRB.BINARY))
19 vars_.start = np.zeros(size)
20 y.start = np.ones(size)
21 portfolio_risk = vars_.dot(sigma).dot(vars_)
22 model.setObjective(portfolio_risk, GRB.MINIMIZE)
23 model.addConstr(vars_.sum() <= 1, 'budget')
24 m = np.asarray(m)
25 model.addConstrs((0 <= vars_[i] for i in range(size)), 'nonnegative')
26 model.addConstrs((vars_[i] <= u_i[i]*y[i] for i in range(size)), 'u_i')
27 model.addConstr(y.sum() <= cardinality, 'cardinality')
28 portfolio_return = m.dot(vars_)
29 model.addConstr(rho <= m.dot(vars_), 'portf_return')
30 model.addConstrs((y[i] <= 1 for i in range(size)), 'interval')
31 model.addConstrs((0 <= y[i] for i in range(size)), 'interval2')
32 model.update()
33 model.optimize()
```

Listing 5.4: Python code for directly solving portfolio optimization problem using GUROBI

```python
1  t = 1
2  x_guess = np.zeros(size)
3  y_guess = np.ones(size)
4  cond = 1
5  while ((t >= 10**-10) & (cond > 10**-6)):
6      model = Model('portfolio')
7      vars_ = pd.Series(model.addVars(size))
8      y = pd.Series(model.addVars(size))
9      min1 = pd.Series(model.addVars(size))
10     min2 = pd.Series(model.addVars(size))
11     portfolio_risk = vars_.dot(sigma).dot(vars_)
12     model.setObjective(portfolio_risk, GRB.MINIMIZE)
13     model.addConstr(vars_.sum() <= 1, 'budget')
```

```
14    model.addConstrs(((y[i] <= 1) for i in range(size)), 'yL1')
15    model.addConstrs(((0 <= vars_[i]) for i in range(size)), 'u_i')
16    model.addConstrs(((vars_[i] <= u_i[i]) for i in range(size)), 'u_i')
17    model.addConstr(size-cardinality <= y.sum(), 'cardinality')
18    model.addConstr(rho <= m.dot(vars_), 'portf_return')
19    vars_.start = x_guess
20    y.start = y_guess
21    model.addConstrs((min1[i] == min_(vars_[i], y[i]) for i in range(
      size)), 'min1')
22    model.addConstrs((min1[i] <= t for i in range(size)), 'min1t')
23    model.update()
24    model.optimize()
25    x_guess = np.array([v.x for v in vars_])
26    y_guess = np.array([v.x for v in y])
27    t = t*0.01
28    cond = max(abs(np.multiply(x_guess, y_guess)))
```

Listing 5.5: Python code for solving regularized portfolio optimization problem using GUROBI

```
1  import math
2  from scipy.optimize import minimize
3
4
5  def phi(a, b, t):
6      if(a+b >= 2*t):
7          result = (a-t)*(b-t)
8      else:
9          result = -1/2*((a-t)**2+(b-t)**2)
10     return result
11
12
13 def phi_(a, b, t):
14     if(-a+b >= 2*t):
15         result = (-a-t)*(b-t)
16     else:
17         result = -1/2*((-a-t)**2+(b-t)**2)
18     return result
19
20
21 def objective(x):
22     obj = x[0:size].dot(sigma).dot(x[0:size])
23     obj += mu*max(0, x[0:size].sum()-1)**2
24     obj += mu*max(0, rho-m.dot(x[0:size]))**2
25     obj += mu*max(0, size-cardinality-x[size:size*2].sum())**2
26     for i in range(size):
27         obj += mu*max(0, x[i]-u_i[i])**2
28         obj += mu*max(0, -x[i])**2
```

```python
29          obj += mu*max(0, -x[i+size])**2
30          obj += mu*max(0, x[i+size]-1)**2
31          obj += mu*max(0, phi(x[i], x[i+size], t))**2
32          obj += mu*max(0, phi_(x[i], x[i+size], t))**2
33          obj += mu*max(0, -1/2*((-x[i]-t)**2+(x[i+size]-t)**2))**2
34      return obj
35
36  viol = math.inf
37  x0 = np.append(np.zeros(size), np.ones(size))
38  old_viol = viol
39  eps = 10**-10
40  cond = 1
41  it = 0
42  t = 1
43  while ((eps <= viol) & (t >= 10**-10)):
44      mu = 1/t
45      it += 1
46      x = minimize(objective, x0).x
47      violence = np.zeros(3+5*size)
48      violence[0] = max(0, x[0:size].sum()-1)
49      violence[1] = max(0, size-cardinality-x[size:size*2].sum())
50      violence[2] = max(0, rho-m.dot(x[0:size]))
51      for i in range(size):
52          violence[i+3] = max(0, phi(x[i], x[i+size], t))
53          violence[i+3] = max(0, phi_(x[i], x[i+size], t))
54          violence[(i+3)+size] = max(0, -x[i+size])
55          violence[(i+3)+2*size] = max(0, x[i+size]-1)
56          violence[(i+3)+3*size] = max(0, -x[i])
57          violence[(i+3)+4*size] = max(0, x[i]-u_i[i])
58      viol = max(violence)
59      print('{} -> {}'.format(it, x[0:size].dot(sigma).dot(x[0:size])))
60      x0 = x
61      t = t*0.1
```

Listing 5.6: Python code for solving portfolio optimization problem using penalty function

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Summary

This master thesis deals with penalty methods in constrained optimization. The approach is used to convert a constrained problem into an equivalent unconstrained problem. At the beginning, the most important definitions and results related to unconstrained, as well as constrained, optimization are presented. In the second chapter we begin with the basic definition of penalty function. Furthermore, the concept of the penalty function is elaborated and geometrically illustrated. In the next chapter, important result which justifies the use of the penalty function is stated and proven. Also, computational difficulties which motivate the next chapter are discussed. In the fourth chapter, exact penalty functions are presented. Finally, in the last chapter all the methods presented are applied on examples. Firstly, a simple convex optimization problem is solved by all of the methods and results are discussed. After that, cardinality constrained portfolio optimization problem is presented and solved with GUROBI and exterior penalty function method.

Sažetak

Ovaj rad bavi se s metodom kaznenih funkcija u uvjetnoj optimizaciji koja se koristi kako bi se problem uvjetne optimizacije ekvivalentno zapisao kao problem bezuvjetne optimizacije. Na početku rada navedene su najvažnije definicije i rezultati o bezuvjetnoj, kao i uvjetnoj, optimizaciji. U drugom poglavlju počinjemo s osnovnim definicijama o kaznenim funkcijama. Nadalje, prikazan je koncept kaznenih funkcija i njihova geometrijska interpretacija. U sljedećem poglavlju, naveden je i dokazan rezultat koji opravdava korištenje kaznenih funkcija u uvjetnoj optimizaciji. Također, opisane su računske složenosti koje su motivirale sljedeće poglavlje. U četvrtom poglavlju predstavljene su egzaktne kaznene funkcije. Na kraju rada nalazi se primjena opisanih metoda na jednostavnom konveksnom primjeru. Nakon toga, predstavljen je problem optimizacije portfelja s uvjetom kardinalnosti i riješen je pomoću GUROBI-ja i kaznene funkcije te su dobiveni rezultati uspoređeni.

Biography

I was born on June 13, 1995 in Našice, Croatia where I finished primary school 'OŠ Dore Pejačević' and mathematical grammar school 'SŠ Isidiora Kršnjavoga'. During my education, I realized that I was extremely good at solving mathematical problems and since then, my passion towards mathematics has been growing. I achieved a 100% score at Mathematics Matura Exam and enrolled into the Faculty of Science, Department of Mathematics at University of Zagreb in 2014. I earned my bachelor's degree in 2017 and immediately after that enrolled into the Master's Programme for Mathematical Statistics.

Životopis

Rođena sam 13. lipnja 1995. godine u Našicama gdje sam završila Osnovnu Školu Dore Pejačević i Prirodoslovno-matematičku gimnaziju Isidora Kršnjavoga. Tijekom svog obrazovanja, spoznala sam da sam izrazito dobra u rješavanju matematičkih problema i od tada moja strast prema matematici raste. Riješila sam višu razinu matematike na Državnoj maturi 100% i upisala Prirodoslovno-matematički fakultet u Zagrebu. Postala sam sveučilišni prvostupnik matematike 2014. godine i zatim upisala Diplomski studij Matematičke statistike na istom fakultetu.