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Abstract
In this paper, we are concerned with minimization problems over the unit simplex. Here, we propose the use of an active-set estimate that enables us to define an algorithmic framework where the variables estimated active and those estimated non-active are updated separately at each iteration. In particular, we consider different variants of the Frank-Wolfe direction to be combined with the proposed active-set strategy, proving the convergence of the algorithm for each of them. Then, we focus on the problem of minimizing a function over the ℓ₁-ball, showing how our algorithmic framework can be efficiently adapted to this problem. Preliminary numerical results show the benefits of the proposed active-set estimate.

Keywords. Active-set methods. Frank-Wolfe. Unit simplex. ℓ₁-ball.

AMS subject classifications. 65K05. 90C06. 90C30.
1 Introduction

We focus on the following minimization problem:

$$\min_x f(x)$$

$$\sum_{i=1}^{n} x_i = 1$$

$$x_i \geq 0, \quad i = 1, \ldots, n,$$

where $f \in C^1(\mathbb{R}^n)$. Throughout the paper, we also make the assumption that $\nabla f(x)$ is Lipschitz continuous on the feasible set.

We remark that every minimization problem where the feasible region is a polytope can be rewritten as a minimization problem over the unit simplex. In fact, let us consider a problem of the form:

$$\min_x h(x)$$

$$x \in D,$$

where $h: \mathbb{R}^n \to \mathbb{R}$ and $D$ is the convex hull of $\{v_1, \ldots, v_m\}$, with $v_i \in \mathbb{R}^n, i = 1, \ldots, m$. It follows that every feasible point $x$ can be expressed as a convex combination of $v_1, \ldots, v_m$, that is, there exist $\alpha_1, \ldots, \alpha_m$ such that

$$x = \sum_{i=1}^{m} \alpha_i v_i,$$

$$\sum_{i=1}^{m} \alpha_i = 1,$$

$$\alpha_i \geq 0, \quad i = 1, \ldots, m.$$

By introducing the matrix $V = [v_1 \ldots v_m] \in \mathbb{R}^{n \times m}$, we can then rewrite the problem as

$$\min_{\alpha} f(\alpha)$$

$$\sum_{i=1}^{m} \alpha_i = 1$$

$$\alpha_i \geq 0, \quad i = 1, \ldots, m,$$

where

$$f(\alpha) = h(V \alpha).$$

An interesting example into this context is given by the minimization of a function over the $\ell_1$-ball:

$$\min_{x \in \mathbb{R}^n} h(x)$$

$$\|x\|_1 \leq \tau,$$
with \( \tau > 0 \). Indeed, the feasible set of this problem is the convex hull of \( \{ \pm \tau e_1, \ldots, \pm \tau e_n \} \). Hence, using the reasoning considered above, we obtain again a minimization problem whose feasible set is the unit simplex in \( \mathbb{R}^{2n} \). As to be shown in Section 5, this particular problem has interesting properties that enables us not to double the number of variables.

The rest of the paper is organized as follows. In Section 1, we introduce the minimization problem over the unit simplex. In Section 2, we describe our active-set estimate. In Section 3, we present our algorithmic framework. In Section 4, we carry out the convergence analysis of the algorithm for different choices of the search direction. In Section 5, we show how our algorithm can be easily extended to minimization problems over the \( \ell_1 \)-ball. In Section 6, we provide some preliminary numerical results. Finally, in Section 7, we draw some conclusions.

Hereinafter, we indicate with \( \| \cdot \| \) the Euclidean norm. Given a vector \( v \in \mathbb{R}^n \) and an index set \( I \subseteq \{1, \ldots, n\} \), we denote with \( v_I \) the subvector with components \( v_i, i \in I \). We indicate with \( e_i \) the \( i \)-th unit vector (all components are 0 except for the \( i \)-th component, which is 1) and with \( e \in \mathbb{R}^n \) the \( n \)-dimensional vector with all components equal to 1. Given a set of vectors \( D = \{ v_1, \ldots, v_m \} \subseteq \mathbb{R}^n \), we indicate with \( \text{conv}(D) \) the convex hull of \( D \). Finally, the open ball with center \( x \) and radius \( \rho > 0 \) is denoted by \( B(x, \rho) \).

## 2 Active-set estimate

Using an active-set strategy to solve a constrained problem can be crucial from both a computational and theoretical point of view. In this section, we present an active-set estimate technique for problem (1), pointing out its theoretical properties.

First, we provide the definition of stationary point for problem (1).

**Definition 1.** A feasible point \( x^* \) of problem (1) is a stationary point if and only if it satisfies the following first order necessary optimality conditions:

\[
\nabla f(x^*) - \lambda^* e - \mu^* = 0, \tag{2}
\]

\[
(\mu^*)^T x^* = 0, \tag{3}
\]

\[
\mu^* \geq 0. \tag{4}
\]

where \( \lambda^* \in \mathbb{R} \) and \( \mu^* \in \mathbb{R}^n \) are the KKT multipliers.

Now, we can define the active-set for a stationary point \( x^* \) as the subset of zero-components of \( x^* \). In particular, we provide the following definition.

**Definition 2.** Let \( x^* \in \mathbb{R}^n \) be a stationary point of problem (1). We define as active-set the following set:

\[
\bar{A}(x^*) = \{ i \in \{1, \ldots, n\} : x^*_i = 0 \}. \tag{5}
\]

We further define the non-active set \( \bar{N}(x^*) \) as the complementary set of \( \bar{A}(x^*) \):

\[
\bar{N}(x^*) = \{1, \ldots, n\} \setminus \bar{A}(x^*) = \{ i \in \{1, \ldots, n\} : x^*_i > 0 \}. \tag{6}
\]
Here, the active-set estimate is computed by following the approach proposed in [3, 4], which requires proper approximation of the KKT multipliers. The latter are obtained by means of multiplier functions.

In particular, let us describe how to compute the multiplier functions \( \lambda: \mathbb{R}^n \to \mathbb{R} \) and \( \mu: \mathbb{R}^n \to \mathbb{R}^n \). Given a stationary point \( x^* \) of (1), let \( (\lambda^*, \mu^*) \) be the KKT multipliers associated to \( x^* \). By (2), we have

\[
\mu^* = \nabla f(x^*) - \lambda^* e,
\]

then, multiplying by \( x^* \) and taking into account complementarity condition (3), we get

\[
0 = (\mu^*)^T x^* = (\nabla f(x^*) - \lambda^* e)^T x^*.
\]

From the feasibility of \( x^* \), we obtain the following expression for the multipliers:

\[
\lambda^* = \nabla f(x^*)^T x^*, \quad \mu^* = \nabla f(x^*) - \lambda^* e.
\]

From (7)–(8), we can introduce the following two multiplier functions:

\[
\lambda(x) = \nabla f(x)^T x, \quad \mu_i(x) = \nabla_i f(x) - \lambda(x), \quad i = 1, \ldots, n.
\]

Now, for every feasible point \( x \), we define the active-set estimate \( A(x) \) and the non-active set estimate \( N(x) \) as

\[
A(x) = \{i: x_i = 0, \mu_i(x) > 0\} \subseteq \bar{A}(x^*) \subseteq \tilde{A}(x^*), \quad N(x) = \{i: x_i > \epsilon \mu_i(x)\} \subseteq \tilde{N}(x^*),
\]

where \( \epsilon \) is a positive scalar.

By adapting the results shown in [4], we can state the following theorem.

**Theorem 1.** If \((x^*, \lambda^*, \mu^*)\) satisfies KKT conditions for problem (1), then there exists a neighborhood \( \mathcal{B}(x^*, \rho) \) such that, for each \( x \) in this neighborhood, we have

\[
\{i: x_i^* = 0, \mu_i(x^*) > 0\} \subseteq A(x) \subseteq \bar{A}(x^*).
\]

Furthermore, if strict complementarity holds, then

\[
\{i: x_i^* = 0, \mu_i(x^*) > 0\} = A(x) = \bar{A}(x^*),
\]

for each \( x \in \mathcal{B}(x^*, \rho) \).

### 2.1 Characterization of stationary points

In this subsection, we provide a characterization of stationary points based on the proposed active-set estimate. First, we need the following proposition to state necessary and sufficient conditions for stationarity.
Proposition 1. Let \( x^* \) be a feasible point of problem (1). Then, \( x^* \) is a stationary point if and only if

\[
\min_{i=1,\ldots,n} \{ \nabla_i f(x^*) \} = \max_{j \in \tilde{N}(x^*)} \{ \nabla_j f(x^*) \},
\]

(13)

Proof. First, we prove necessary. From KKT conditions (2)–(4), we can write

\[
\nabla f(x^*) - \lambda^* e = \mu^* \geq 0.
\]

(14)

From (3), we have that \( \mu_j^* = 0 \) for every index \( j \in \tilde{N}(x^*) \). It follows that

\[
\nabla_j f(x^*) = \lambda^*, \quad \forall j \in \tilde{N}(x^*).
\]

The above relation, combined with (14), implies that

\[
\nabla_i f(x^*) \geq \lambda^* = \max_{j \in \tilde{N}(x^*)} \{ \nabla_j f(x^*) \}, \quad \forall i = 1,\ldots,n,
\]

and then (13) holds.

Now, assume that (13) is satisfied. It follows that

\[
\min_{j \in \tilde{N}(x^*)} \{ \nabla_j f(x^*) \} \geq \max_{j \in \tilde{N}(x^*)} \{ \nabla_j f(x^*) \},
\]

implying that all \( \nabla_j f(x^*) \), with \( j \in \tilde{N}(x^*) \), have the same value. Therefore, there exists a scalar \( \lambda^* \) such that

\[
\nabla_j f(x^*) = \lambda^*, \quad \forall j \in \tilde{N}(x^*).
\]

(15)

From (13) and (15), there exist \( \mu_1^*,\ldots,\mu_n^* \in \mathbb{R} \) such that

\[
\nabla_i f(x^*) - \lambda^* = \mu_i^* \geq 0, \quad i = 1,\ldots,n,
\]

\[
\mu_j^* = 0, \quad j \in \tilde{N}(x^*).
\]

Then, conditions (2)–(4) hold.

Moreover, from the previous proposition, we can easily state the following corollary.

Corollary 1. Let \( x^* \) be a feasible point of problem (1). Then, \( x^* \) is a stationary point if and only if there exists a scalar \( \xi \) such that

\[
\nabla_j f(x^*) = \xi, \quad \forall j \in \tilde{N}(x^*),
\]

\[
\nabla_i f(x^*) \geq \xi, \quad \forall i \in \tilde{A}(x^*).
\]

Proof. The proof follows from that of Proposition 1, observing that for every index \( j \in \tilde{N}(x^*) \), we have that \( \nabla_j f(x^*) = \lambda^* \), where \( \lambda^* \) is the KKT multiplier appearing in (2)–(4).

The following two propositions show how our active-set estimate can be used to characterize stationary points.

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Proposition 2. Given a feasible point $\bar{x}$ of problem (1), assume that

$$\{i \in A(\bar{x}): \bar{x}_i > 0\} = \emptyset.$$  

Then, $\bar{x}$ is a stationary point of problem (1) if only if

$$\min_{i \in N(\bar{x})} \{\nabla_i f(\bar{x})\} = \max_{j \in N(\bar{x})} \{\nabla_j f(\bar{x})\}.$$  

Proof. First, we observe that, under the hypothesis (16), we have that

$$\{j \in N(\bar{x}): \bar{x}_j > 0\} = \{j \in \{1, \ldots, n\}: \bar{x}_j > 0\}.$$  

Let us assume that (17) holds. Then,

$$\nabla_j f(\bar{x}) = \bar{\xi}, \quad j \in N(\bar{x}), \; \bar{x}_j > 0.$$  

Recalling (11)–(12), and using (18) and (19), for every index $i \in A(\bar{x})$ we can write

$$0 = \bar{x}_i \leq \epsilon (\nabla_i f(\bar{x}) - \nabla f(\bar{x})^T \bar{x}) = \epsilon (\nabla_i f(\bar{x}) - \sum_{\bar{x}_j > 0} \nabla_j f(\bar{x}) \bar{x}_j)$$

$$\quad = \epsilon (\nabla_i f(\bar{x}) - \bar{\xi} e^T \bar{x}) = \epsilon (\nabla_i f(\bar{x}) - \bar{\xi}).$$

Thus, we have

$$\nabla_i f(\bar{x}) \geq \bar{\xi}, \quad \forall i \in A(\bar{x}).$$

It follows that (13) holds.

Now, let us assume that $\bar{x}$ is a stationary point, that is,

$$\min_{i=1, \ldots, n} \{\nabla_i f(\bar{x})\} = \max_{j=1, \ldots, n} \{\nabla_j f(\bar{x})\}.$$  

(20)

It is easy to see that the following relations hold:

$$\min_{i=1, \ldots, n} \{\nabla_i f(\bar{x})\} \leq \min_{j \in N(\bar{x})} \{\nabla_j f(\bar{x})\} \leq \max_{j \in N(\bar{x})} \{\nabla_j f(\bar{x})\} \leq \max_{j=1, \ldots, n} \{\nabla_j f(\bar{x})\}.$$  

From (20), it follows that (17) holds. \qed

Proposition 3. Given a feasible point $\bar{x}$ of problem (1), assume that

$$\min_{i \in N(\bar{x})} \{\nabla_i f(\bar{x})\} = \max_{j \in N(\bar{x})} \{\nabla_j f(\bar{x})\}.$$  

Then, $\bar{x}$ is a stationary point of problem (1) if only if

$$\{i \in A(\bar{x}): \bar{x}_i > 0\} = \emptyset.$$  

(22)
Proof. First, from (21) we observe that
\[ \nabla_j f(\bar{x}) = \bar{\xi}, \quad j \in N(\bar{x}), \quad \bar{x}_j > 0. \]
(23)

Now, let us assume that (22) holds. Recalling (11)–(12), and using (23), for every index \( i \in A(\bar{x}) \) we can write
\[
0 = \bar{x}_i \leq \epsilon (\nabla_i f(\bar{x}) - \nabla f(\bar{x})^T \bar{x}) = \epsilon \left( \nabla_i f(\bar{x}) - \sum_{x_j > 0} \nabla_j f(\bar{x}) \bar{x}_j \right)
= \epsilon (\nabla_i f(\bar{x}) - \bar{\xi}^T x) = \epsilon (\nabla_i f(\bar{x}) - \bar{\xi}).
\]

Thus, we have
\[ \nabla_i f(\bar{x}) \geq \bar{\xi}, \quad \forall i \in A(\bar{x}). \]

It follows that (13) holds.

Now, let us assume that \( \bar{x} \) is a stationary point. From Corollary 1, we have that
\[ \nabla_j f(\bar{x}) = \bar{\xi}, \quad j \in N(\bar{x}). \]

By contradiction, we assume that there exists \( i \in A(\bar{x}) \) such that \( \bar{x}_i > 0 \). It follows that
\[
0 < \bar{x}_i \leq \epsilon (\nabla_i f(\bar{x}) - \nabla f(\bar{x})^T \bar{x}) = \epsilon \left( \nabla_i f(\bar{x}) - \sum_{x_j > 0} \nabla_j f(\bar{x}) \bar{x}_j \right)
= \epsilon (\nabla_i f(\bar{x}) - \bar{\xi}^T x) = \epsilon (\nabla_i f(\bar{x}) - \bar{\xi})
\]
and then
\[ \nabla_i f(\bar{x}) > \bar{\xi}, \]
thus contradicting (13). \( \square \)

2.2 Descent property of the active-set

In this subsection, we show how, given a feasible point \( x \), we can obtain a sufficient decrease in the objective function by setting the estimated active variables to zero.

In particular, our approach takes inspiration from the one proposed in [1] for box-constrained problems, where a decrease in the objective function was obtained by setting the estimated active variables to the bounds. Here, differently from the box-constrained case, we have a linear constraint, imposing that all variables sum up to 1. Therefore, in order to maintain feasibility, at least one non-active variable must be updated as well.

In particular, let us define the following index set:
\[ J(x) = \left\{ j : \quad j \in \text{Argmin}_{i=1,\ldots,n} \{ \nabla_i f(x) \} \right\}. \]
(24)

As to be shown, after setting the estimated active variables to zero, we can guarantee that the objective function decreases and that the new point is still feasible by suitably updating only one variable \( x_j \), with \( j \) chosen in \( N(x) \cap J(x) \).

First, we need to prove that \( N(x) \cap J(x) \) is non-empty for every feasible point \( x \). This is stated in the following proposition.
Proposition 4. For every feasible point $x$ of problem (1), we have

$$N(x) \cap J(x) \neq \emptyset.$$  

Proof. We distinguish two different cases.

(1) $|J(x)| = n$. For every $j \in J(x)$, we have

$$\nabla f(x)^T x = \nabla_j f(x)e^T x = \nabla_j f(x),$$  

(25)

Exploiting the feasibility of $x$, we can choose an index $\nu \in J(x)$ such that $x_\nu > 0$ and, recalling definition of multipliers (9) and equation (25), we can write

$$\mu_\nu(x) = \nabla_\nu f(x) - \lambda = \nabla_\nu f(x) - \nabla f(x)^T x = \nabla_\nu f(x) - \nabla_\nu f(x) = 0 < x_\nu.$$  

Since $x_\nu > 0$ and $\mu_\nu(x) = 0$, we have that $x_\nu > \epsilon \mu_\nu(x)$ and then $\nu \in N(x)$.

(2) $|J(x)| < n$. We consider two subcases.

- We first assume that for every $h$ such that $\nabla_h f(x) > \nabla_j f(x)$, $j \in J(x)$, we have $x_h = 0$. It follows that

$$\sum_{j \in J(x)} x_j = 1$$

and, reasoning as in the previous case, we get that (25) holds for all $j \in J(x)$. Using the fact that $x$ is a feasible solution for problem (1), we can choose an index $\nu \in J(x)$ such that $x_\nu > 0$ and, recalling definition of multipliers (9) and equation (25), we can write

$$\mu_\nu(x) = \nabla_\nu f(x) - \lambda = \nabla_\nu f(x) - \nabla f(x)^T x = \nabla_\nu f(x) - \nabla_\nu f(x) = 0 < x_\nu.$$  

Since $x_\nu > 0$ and $\mu_\nu(x) = 0$, we have that $x_\nu > \epsilon \mu_\nu(x)$ and then $\nu \in N(x)$.

- Now we consider the case when there exists $h$ such that $\nabla_h f(x) > \nabla_j f(x)$, $j \in J(x)$, and $x_h > 0$. It follows that

$$\nabla f(x)^T x > \nabla_j f(x)e^T x = \nabla_j f(x).$$

Choosing $\nu = j$, for any $j \in J(x)$, and reasoning as before, we can write

$$\mu_\nu(x) = \nabla_\nu f(x) - \lambda = \nabla_\nu f(x) - \nabla f(x)^T x < \nabla_\nu f(x) - \nabla_\nu f(x) = 0 \leq x_\nu.$$  

Since $x_\nu \geq 0$ and $\mu_\nu(x) < 0$, we have that $x_\nu > \epsilon \mu_\nu(x)$ and then $\nu \in N(x)$. 

$$\square$$

Remark 1. Proposition 4 implies that for every feasible point $x$, the set $N(x)$ is non-empty.

Before stating the main result of this section, we need an assumption on the parameter $\epsilon$ appearing in the definition of the active-set.
**Assumption 1.** Assume that the parameter $\epsilon$ appearing in the estimates (11)–(12) satisfies the following conditions:

$$0 < \epsilon \leq \frac{1}{2Ln},$$

where $L$ is the Lipschitz constant of $\nabla f(x)$ over the unit simplex.

Now, we are ready to state the main theoretical result of this section.

**Proposition 5.** Let Assumption 1 hold. Given a feasible point $x$ of problem (1), let $j \in N(x) \cap J(x)$ and $I = \{1, \ldots, n\} \setminus \{j\}$. Let $\hat{A}(x)$ be a set of indices such that $\hat{A}(x) \subseteq A(x)$. Let $\tilde{x}$ be the feasible point defined as follows:

$$\tilde{x}_i = \begin{cases} 0, & i \in \hat{A}(x), \\ x_i, & i \in I \setminus \hat{A}(x), \\ x_i + \sum_{h \in \hat{A}(x)} x_h, & i = j. \end{cases}$$

Then,

$$f(\tilde{x}) - f(x) \leq -L\|\tilde{x} - x\|^2,$$

where $L$ is the Lipschitz constant of $\nabla f(x)$ over the unit simplex.

**Proof.** We first define the following set

$$\hat{A} = \hat{A}(x).$$

Using the mean value theorem, we can write:

$$f(\tilde{x}) = f(x) + \nabla f(w)^T(\tilde{x} - x),$$

where $w = x + \xi(\tilde{x} - x)$, $\xi \in (0, 1)$.

From the Lipschitz continuity of the gradient, we have that

$$f(\tilde{x}) = f(x) + \nabla f(x)^T(\tilde{x} - x) + \left[\nabla f(w) - \nabla f(x)\right]^T(\tilde{x} - x)$$
$$\leq f(x) + \nabla f(x)^T(\tilde{x} - x) + \left\|\nabla f(w) - \nabla f(x)\right\|\|\tilde{x} - x\|$$
$$\leq f(x) + \nabla f(x)^T(\tilde{x} - x) + L\|\tilde{x} - x\|^2$$

and, by adding and removing $L\|\tilde{x} - x\|^2$, we get

$$f(\tilde{x}) \leq f(x) + \nabla f(x)^T(\tilde{x} - x) + 2L\|\tilde{x} - x\|^2 - L\|\tilde{x} - x\|^2.$$

(27)

In order to prove the proposition, we need to show that

$$\nabla f(x)^T(\tilde{x} - x) + 2L\|\tilde{x} - x\|^2 \leq 0.$$

(28)
From the definition of the components $\tilde{x}_i$, $i = 1, \ldots, n$, we can write

$$\tilde{x}_i - x_i = \begin{cases} -x_i, & i \in \hat{A}, \\ 0, & i \in I \setminus \hat{A}, \\ \sum_{h \in \hat{A}} x_h, & i = j, \end{cases}$$

so that

$$\|\tilde{x} - x\|^2 = \sum_{i \in \hat{A}} (x_i)^2 + \left(\sum_{i \in \hat{A}} x_i\right)^2 \leq \sum_{i \in \hat{A}} (x_i)^2 + |\hat{A}| \sum_{i \in \hat{A}} (x_i)^2 = (|\hat{A}| + 1) x_{\hat{A}}^T x_{\hat{A}}$$

(29)

and

$$\nabla f(x)^T (\tilde{x} - x) = -\nabla f(x)^T x_{\hat{A}} + \nabla f(x) \sum_{i \in \hat{A}} x_i = x_{\hat{A}}^T \left( \nabla f(x) e_{\hat{A}} - \nabla f(x) \right).$$

(30)

From the definition of the index $j$, we have that $\nabla_i f(x) \geq \nabla_j f(x)$ for all $i \in \{1, \ldots, n\}$. Then, we can write

$$\sum_{i=1}^{n} \nabla_i f(x) x_i \geq \sum_{i=1}^{n} \nabla_j f(x) x_i = \nabla_j f(x) \sum_{i=1}^{n} x_i = \nabla_j f(x).$$

(31)

Recalling the active-set estimation, we have that

$$x_i \leq \epsilon \left( \nabla_i f(x) - \sum_{i=1}^{n} \nabla_i f(x) x_i \right) \leq \epsilon \left( \nabla_i f(x) - \nabla_j f(x) \right), \quad \forall i \in \hat{A},$$

(32)

where the last inequality follows from (31). Using (29) and (32), we can write

$$\|\tilde{x} - x\|^2 \leq \epsilon (|\hat{A}| + 1) x_{\hat{A}}^T \left( \nabla f(x) - \nabla_j f(x) e_{\hat{A}} \right).$$

(33)

From (30) and (33), we get

$$\nabla f(x)^T (\tilde{x} - x) + 2L\|\tilde{x} - x\|^2 \leq x_{\hat{A}}^T \left[ \nabla f(x) e_{\hat{A}} - \nabla f(x) \right] +$$

$$+ 2L(|\hat{A}| + 1) \epsilon x_{\hat{A}}^T \left( \nabla f(x) - \nabla f(x) e_{\hat{A}} \right)$$

$$= [2L(|\hat{A}| + 1) \epsilon - 1] x_{\hat{A}}^T \left( \nabla f(x) - \nabla f(x) e_{\hat{A}} \right)$$

$$\leq (2L \epsilon - 1) x_{\hat{A}}^T \left( \nabla f(x) - \nabla f(x) e_{\hat{A}} \right),$$

where the last inequality follows from the non-negativity of $x_{\hat{A}}^T \left( \nabla f(x) - \nabla f(x) e_{\hat{A}} \right)$ (implied by (33)) and from the fact that $|\hat{A}| \leq n - 1$ (implied by Proposition 4). Then, inequality (28) follows from the assumption we made on $\epsilon$. \qed
3 Algorithmic framework

In this section, we describe an algorithmic framework to minimize a function over the unit simplex, called Active-Set framework for optimization over the Simplex (AS-SIMPLEX).

The proposed approach exploits the active-set strategy described in the previous section and it is based on performing two minimization steps at each iteration: one for updating the estimated active variables and one for updating the estimated non-active variables.

In particular, let $x^k$ be the point produced at a generic iteration $k$ and assume that we have computed the active and non-active set estimates $A(x^k), N(x^k)$. Then,

- first, we get a reduction in the objective function by generating the feasible point $\tilde{x}^k$, obtained by setting $x_{A(x^k)}$ to zero and updating the variable $x_j^k, j \in J(x^k)$, as indicated in Proposition 5, being $J(x^k)$ the index set defined as in (24);
- afterwards, we compute the next iterate $x^{k+1}$ by moving the estimated non-active variables along a suitable search direction.

The formal scheme of the proposed algorithmic framework is reported in Algorithm 1.

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**Algorithm 1**

**Active-Set framework for optimization over the Simplex (AS-SIMPLEX)**

1. Choose a feasible point $x^0$
2. For $k = 0, 1, \ldots$
   3. If $x^k$ is a stationary point, then STOP
   
   **Active-Set Estimation:**
   4. Compute $A^k := A(x^k)$ and $N^k := N(x^k)$
   
   **Minimization procedure over $A^k$:**
   5. Compute $J^k := J(x^k)$, choose $j \in N^k \cap J^k$ and define $\tilde{N}^k = N^k \setminus \{j\}$
   6. Set $\tilde{x}_{A^k}^k = 0$, $\tilde{x}_{N^k}^k = x_{N^k}^k$ and $\tilde{x}_j^k = x_j^k + \sum_{h \in A^k} x_h^k$
   
   **Minimization procedure over $N^k$:**
   7. Set $d_{A^k}^k = 0$
   8. Compute a feasible direction $d_{N^k}^k$ in $\tilde{x}^k$ and a maximum stepsize $\alpha_{\text{max}}^k$
   9. If $\nabla f(\tilde{x}^k)^T d^k < 0$ then
      10. Compute a stepsize $\alpha^k \in (0, \alpha_{\text{max}}^k]$ by means of the Armijo line search (Algorithm 2)
   
   Else
   11. Set $\alpha^k = 0$
   12. End if
   13. Set $x^{k+1} = \tilde{x}^k + \alpha^k d^k$
14. End for
Algorithm 2 Armijo line search within Algorithm 1

0 Choose $\delta \in (0, 1)$, $\gamma \in (0, \frac{1}{2})$
1 Choose initial stepsize $\alpha \in (0, \alpha_{\text{max}}]$
2 While $f(\tilde{x}^k + \alpha \bar{d}^k) > f(\tilde{x}^k) + \gamma \alpha \nabla f(\tilde{x}^k)^T \bar{d}^k$
3 Set $\alpha = \delta \alpha$
4 End while

Remark 2. In Algorithm 1, we allow for directions $d^k$ such that $\nabla f(\tilde{x}^k)^T d^k = 0$. This is due to the fact that only the estimated non-active variables are updated by moving $\tilde{x}^k$ along $d^k$ (since $d_{A_k}^k = 0$). But, at a generic iteration $k$, it can happen that all the estimated non-active variables satisfy stationarity conditions over $N^k$, and then, $d^k = 0$.

Now, we describe some possible choices of the search directions $d^k$ to be used in Algorithm 1. In particular, we consider different Frank-Wolfe (FW) type directions. For the sake of completeness, in the next subsection we preliminarily recall the classical Frank-Wolfe method and some of its variants.

3.1 The Frank-Wolfe method and its variants

The Frank-Wolfe method [6] (also known as conditional gradient method) is a popular algorithm to solve constrained problems of the following form:

$$\min f(x)$$

$$x \in D,$$  (34)

where $f: \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function and $D$ is a compact convex set.

At every iteration, the Frank-Wolfe method computes a feasible search direction by minimizing a linear approximation of the objective function. Then, a stepsize is chosen by the Armijo line search. The method is reported in Algorithm 3.

Algorithm 3 Frank-Wolfe method to solve problem (34)

0 Choose $x^0 \in D$
1 For $k = 0, 1, \ldots$
2 If $x^k$ is a stationary point, then STOP
3 Compute $y^k \in \text{Argmin}_{x \in D} \{\nabla f(x^k)^T (x - x^k)\}$ and set $d^k = y^k - x^k$
4 Set $\alpha_{\text{max}} = 1$ and compute $\alpha^k$ by the Armijo line search (Algorithm 4)
5 Set $x^{k+1} = x^k + \alpha^k d^k$
6 Set $k = k + 1$
7 End while

It can be proved that, if $x^k$ is non-stationary, then a descent direction $d^k$ is produced at every iteration $k$. Moreover, the convexity of $D$ implies that $x^k + \alpha d^k \in D$ for all $\alpha \in (0, 1]$.

A key point in the Frank-Wolfe method is the computation of the search direction $d^k$, because it requires to minimize the linear function $\nabla f(x^k)^T (x - x^k)$ over the feasible set $D$.  

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Algorithm 4 Armijo line search within the Frank-Wolfe method

0 Given $\gamma \in (0, 1)$, $\delta \in (0, 1)$, $\alpha_{\text{max}}^k > 0$
1 Set $\alpha = \alpha_{\text{max}}$
2 While $f(x^k + \alpha d^k) > f(x^k) + \gamma \alpha \nabla f(x^k)^T d^k$
3 Set $\alpha = \delta \alpha$
4 End while
5 Set $\alpha^k = \alpha$

Algorithm 5 Frank-Wolfe method to solve problem (1)

0 Choose a feasible point $x^0$
1 For $k = 0, 1, \ldots$
2 If $x^k$ is a stationary point, then STOP
3 Compute $\hat{i} \in \text{Argmin}_{h=1,\ldots,n} \{\nabla_h f(x^k)\}$ and set $d^k = e_{\hat{i}} - x^k$
4 Set $\alpha_{\text{max}}^k = 1$ and compute $\alpha^k$ by the Armijo line search (Algorithm 4)
5 Set $x^{k+1} = x^k + \alpha^k d^k$
6 Set $k = k + 1$
7 End for

If $D$ is a polyhedron, this means solving a linear problem at every iteration, which can be made efficiently. Moreover, since $x^k$ is fixed, we can simply write $y^k \in \text{Argmin}_{x \in D} \{\nabla f(x^k)^T x\}$.

The Frank-Wolfe method converges to points satisfying first-order optimality conditions. For what concerns the convergence rate, assuming that $D$ is a polytope, that the objective function is strongly convex on $D$ and that $\nabla f(x)$ is Lipschitz continuous on $D$, we have that the sequence $\{f(x^k)\}$ converges to the optimal value $f(x^*)$ linearly if the optimal solution $x^*$ lies in the relative interior of the feasible set [7]. Otherwise, the convergence rate is sublinear, due to the zigzagging effect. To guarantee a linear convergence rate also when the solution lies on the boundary of the feasible set, some variants of the Frank-Wolfe algorithm were proposed in the literature [8] (described below).

Now, let us analyze the property of the Frank-Wolfe algorithm when applied to solve problem (1). Computing the vector $y^k$ at Step 3 is extremely simple, as the feasible set is a polytope and, from known results on linear programming, there exists a vertex of the feasible set which minimizes the function $\nabla f(x^k)^T x$.

Moreover, the set of vertices of the unit simplex is $\{e_1, \ldots, e_n\}$ and, for every $x = e_h$, $h = 1, \ldots, n$, we have that $\nabla f(x^k)^T x = \nabla_h f(x^k)$. Consequently, we can set $y^k = e_i$, where $i \in \text{Argmin}_{h=1,\ldots,n} \{\nabla_h f(x^k)\}$.

For the sake of completeness, we report in Algorithm 5 the Frank-Wolfe method to solve problem (1).

As mentioned above, some variants of the Frank-Wolfe method were studied in the literature. Here, two versions are considered: the Away-Step Frank-Wolfe method (AFW) [13, 7] and the Pairwise Frank-Wolfe method (PFW)[10]. In particular, we only focus on minimization problems over the unit simplex, but the considerations that will be presented
Algorithm 6 Away-Step Frank-Wolfe method to solve problem (1)

0 Choose a feasible point $x^0$
1 For $k = 0, 1, \ldots$
2 If $x^k$ is a stationary point, then STOP
3 Compute $\hat{i} \in \text{Argmin}_{h=1,\ldots,n}\{\nabla_h f(x^k)\}$ and set $d^{FW} = e_i - x^k$
4 Compute $\hat{j} \in \text{Argmax}_{h: x^k_h > 0}\{\nabla_h f(x^k)\}$ and set $d^A = x^k - e_j$
5 If $\nabla f(x^k)^T d^{FW} \leq \nabla f(x^k)^T d^A$ then
6 Set $d^k = d^{FW}$ and $\alpha_{\text{max}}^k = 1$
7 Else
8 Set $d^k = d^A$ and $\alpha_{\text{max}}^k = \frac{x^k_j}{1 - x^k_j}$
9 End if
10 Compute $\alpha^k$ by the Armijo line search (Algorithm 4)
11 Set $x^{k+1} = x^k + \alpha^k d^k$
12 Set $k = k + 1$
13 End for

below can be easily extended to minimization problems over a polytope.

The distinguishing feature of the AFW method is to compute, at every iteration $k$, two potential search directions: the first one is the Frank-Wolfe direction described above, which will be referred to as $d^{FW}$; and the second one is the so called Away-Step direction $d^A$. The search direction $d^{AFW}$ employed by the algorithm is the one, between $d^{FW}$ and $d^A$, that minimizes $\nabla f(x^k)^T d$.

In particular, $d^A$ is computed as $d^A = x^k - e_j$, where $e_j$ is the vertex that maximizes $\nabla f(x^k)^T e_h = \nabla_h f(x^k)$ with respect to the vertices $e_h$ such that $x^k_h > 0$. In other words, $j \in \text{Argmax}_{h: x^k_h > 0}\{\nabla_h f(x^k)\}$.

We observe that, if the search direction selected by the algorithm is $d^{AFW} = d^A$ (i.e., if $\nabla f(x^k)^T d^A < \nabla f(x^k)^T d^{FW}$), then we have to set a proper value $\alpha_{\text{max}}^k$ in the line search procedure, in order to produce feasible points. It is easy to verify that the largest acceptable step length for the Away-Step direction $d^A$ is equal to $\frac{x^k_j}{1 - x^k_j}$, where $j \in \text{Argmax}_{h: x^k_h > 0}\{\nabla_h f(x^k)\}$.

We report in Algorithm 6 the Away-Step Frank-Wolfe algorithm to solve problem (1).

Now, we briefly examine the PFW method. At every iteration $k$, the method employs the Pairwise Frank-Wolfe direction $d^{PFW}$, computed as $d^{PFW} = d^{FW} + d^A = e_i - e_j$, where $i \in \text{Argmin}_{h=1,\ldots,n}\{\nabla_h f(x^k)\}$ and $j \in \text{Argmax}_{h: x^k_h > 0}\{\nabla_h f(x^k)\}$. When employing this search direction, it is easy to verify that the largest step length that guarantees feasibility is equal to $x^k_j$.

We report in Algorithm 7 the Pairwise Frank-Wolfe method to solve problem (1).

We notice that only two variables are updated by the PFW method at every iteration. It is also worth mentioning that such a framework is employed in some popular algorithmic schemes for training Support Vector Machines [9, 11].
Algorithm 7 Pairwise Frank-Wolfe method to solve problem (1)

0 Choose a feasible point $x^0$
1 For $k = 0, 1, \ldots$
2 If $x^k$ is a stationary point, then STOP
3 Compute $i \in \operatorname{Argmin}_{h=1,\ldots,n} \{ \nabla_h f(x^k) \}$
4 Compute $j \in \operatorname{Argmax}_{h: x^k_h > 0} \{ \nabla_h f(x^k) \}$
5 Set $d^A = e_i - e_j$ and $\alpha_{\text{max}}^k = x_j^k$
6 Compute $\alpha^k$ by the Armijo line search (Algorithm 4)
7 Set $x^{k+1} = x^k + \alpha^k d^k$
8 Set $k = k + 1$
9 End for

Finally, an in-depth analysis on the convergence rate of Frank-Wolfe variants for minimization problems over a polytope can be found in [8].

3.2 Combining FW variants with the active-set strategy

According to Step 7–8 of Algorithm 1, at every iteration $k$ we have to compute a search direction $d^k$ such that

\[
\begin{align*}
&d^k_{\text{A}} = 0, \\
&\nabla f(\tilde{x}^k)^T d^k = \nabla_{N^k} f(\tilde{x}^k)^T d^k_{N^k} \leq 0.
\end{align*}
\]

Recalling Remark 2, the above conditions in practice imply that only the estimated non-active variables are moved along $d^k_{N^k}$, provided that $\tilde{x}^k$ does not satisfy stationarity conditions over $N^k$.

In this subsection, we focus on the case where $d^k_{N^k}$ is either the Frank-Wolfe direction, or one of its variants. Then, at the iteration $k$, two feasible directions $d^k_{N^k}$ can be computed (in the subspace $N^k$):

- the Frank-Wolfe direction
  \[
  d^\text{FW}_{N^k} = e_i - \tilde{x}^k_{N^k}, \quad i \in \operatorname{Argmin}_{i \in N^k} \{ \nabla_i f(\tilde{x}^k) \};
  \] (35)

- the Away-Step direction
  \[
  d^\text{A}_{N^k} = \tilde{x}^k_{N^k} - e_j, \quad j \in \operatorname{Argmax}_{j \in N^k_0} \{ \nabla_j f(\tilde{x}^k) \},
  \] (36)

where $N^k_0 = \{ j \in N^k: \tilde{x}^k_j > 0 \}$.

So, we can compute the final search direction $d^k$ according to one of the following three rules:
(FW) rule: $d_{Nk}^k$ is chosen as the Frank-Wolfe direction, that is,

$$
\begin{align*}
    d_{Ak}^k &= 0, \\
    d_{Nk}^k &= d_{Nk}^{FW}.
\end{align*}
$$

In this case, we simply write

$$
    d^k = d_{Nk}^{FW}.
$$

(AFW) rule: $d_{Nk}^k$ is chosen as the Away-Step Frank-Wolfe direction, that is,

$$
\begin{align*}
    d_{Ak}^k &= 0, \\
    d_{Nk}^k &= d_{Nk}^{AFW} =
    \begin{cases}
        d_{Nk}^{FW}, & \text{if } \nabla_{Nk} f (\tilde{x}^k) \trans d_{Nk}^{FW} \leq \nabla_{Nk} f (\tilde{x}^k) \trans d_{Ak}^k, \\
        d_{Nk}^{A}, & \text{otherwise}.
    \end{cases}
\end{align*}
$$

In this case, we simply write

$$
    d^k = d_{Nk}^{AFW}.
$$

(PFW) rule: $d_{Nk}^k$ is chosen as the Pairwise Frank-Wolfe direction, that is,

$$
\begin{align*}
    d_{Ak}^k &= 0, \\
    d_{Nk}^k &= d_{Nk}^{PFW} = d_{Nk}^{FW} + d_{Ak}^k = e_i - e_j,
\end{align*}
$$

where $i$ and $j$ are defined as in (35) and (36), respectively. In this case, we simply write

$$
    d^k = d_{Nk}^{PFW}.
$$

The following lemma claims that all the above three search directions are non-ascent directions.

**Lemma 1.** Let $\tilde{x}^k$ be a feasible point generated by AS-SIMPLEX (Step 6) at iteration $k$. Let $d^k$ be a search direction computed according to one among (FW), (AFW) and (PFW) rule. Then,

$$
\nabla f(\tilde{x}^k) \trans d^k \leq 0.
$$

**Proof.** First, we consider $d^k = d_{Nk}^{FW}$. We can write

$$
\nabla f(\tilde{x}^k) \trans d^k = -\nabla f(\tilde{x}^k) \trans \tilde{x} + \nabla f(\tilde{x}^k),
$$

where $i$ is defined as in (35). Since $\tilde{x}_{Ak}^k = 0$, we also have that $\nabla f(\tilde{x}^k) \trans \tilde{x}^k = \sum_{h \in N^k} \nabla h f(\tilde{x}^k)^{\trans} \tilde{x}_h^k$. Consequently, we obtain

$$
\nabla f(\tilde{x}^k) \trans d^k \leq -\nabla_i f(\tilde{x}^k) \sum_{h \in N^k} \tilde{x}_h^k + \nabla_i f(\tilde{x}^k) = 0,
$$

where the first inequality follows from the definition of $i$ and the feasibility of $\tilde{x}^k$ and the last equality follows from the fact that $\tilde{x}_{Ak}^k = 0$. 

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Now, we consider $d^k = d^{A_{FW}}$. As we have already shown that the assertion holds when $d^k_{N_k} = d^{FW}_{N_k}$, we only have to prove that $\nabla f(\tilde{x}^k)^T d^k \leq 0$ when $d^k_{N_k} = d^{A}_{N_k}$. In this case, we can write
\[
\nabla f(\tilde{x}^k)^T d^k = \nabla f(\tilde{x}^k)^T \tilde{x}^k - \nabla_j f(\tilde{x}^k),
\]
where $j$ is defined as in (36). Reasoning as before, since $\tilde{x}_{A^k} = 0$, we have that $\nabla f(\tilde{x}^k)^T \tilde{x}^k = \sum_{h \in N_k} \nabla_h f(\tilde{x}^k) \tilde{x}_h^k$. Consequently, we obtain
\[
\nabla f(\tilde{x}^k)^T d^k \leq \nabla_j f(\tilde{x}^k) \sum_{h \in N_k} \tilde{x}_h^k - \nabla_j f(\tilde{x}^k) = 0,
\]
where the first inequality follows from the definition of $j$ and the feasibility of $\tilde{x}^k$ and the last equality follows from the fact that $\tilde{x}_{A^k} = 0$.

Finally, it is easy to see that the assertion is true when $d^k = d^{PFW}$ as well, since $d^{PFW} = d^{FW} + d^{A_{FW}}$. 

In the next lemma, we show that at every point $\tilde{x}^k$ produced by $\text{AS-SIMPLEX}$, the directional derivative along $d^{PFW}$ is not larger than the directional derivative along $d^{A_{FW}}$. This fact will play a crucial role for proving the convergence of the algorithm for all the considered variants of the Frank-Wolfe direction.

**Lemma 2.** Let $\tilde{x}^k$ be a feasible point generated by $\text{AS-SIMPLEX}$ at iteration $k$. Then,
\[
\nabla f(\tilde{x}^k)^T d^{PFW} \leq \nabla f(\tilde{x}^k)^T d^{A_{FW}}.
\]

**Proof.** In the following, we indicate with $i$ and $j$ the indices defined as in (35)–(36), respectively. Exploiting the feasibility of $\tilde{x}^k$, and the fact that $\tilde{x}_{A^k} = 0$, we can write
\[
\nabla f(\tilde{x}^k)^T d^{FW} = \nabla_i f(\tilde{x}^k) - \nabla f(\tilde{x}^k)^T \tilde{x}^k = \nabla_i f(\tilde{x}^k) - \sum_{h \in N_k} \nabla_h f(\tilde{x}^k) \tilde{x}_h^k
\]
\[
\geq \nabla_i f(\tilde{x}^k) - \nabla_j f(\tilde{x}^k) \sum_{h \in N_k} \tilde{x}_h^k = \nabla_i f(\tilde{x}^k) - \nabla_j f(\tilde{x}^k)
\]
\[
= \nabla f(\tilde{x}^k)^T d^{PFW}.
\]

Similarly, we have that
\[
\nabla f(\tilde{x}^k)^T d^{A} = \nabla f(\tilde{x}^k)^T \tilde{x}^k - \nabla_j f(\tilde{x}^k) = \sum_{h \in N_k} \nabla_h f(\tilde{x}^k) \tilde{x}_h^k - \nabla_j f(\tilde{x}^k)
\]
\[
\geq \nabla_i f(\tilde{x}^k) \sum_{h \in N_k} \tilde{x}_h^k - \nabla_j f(\tilde{x}^k) = \nabla_i f(\tilde{x}^k) - \nabla_j f(\tilde{x}^k)
\]
\[
= \nabla f(\tilde{x}^k)^T d^{PFW}.
\]

From the above relations, we get
\[
\nabla f(\tilde{x}^k)^T d^{PFW} \leq \min\{\nabla f(\tilde{x}^k)^T d^{FW}, \nabla f(\tilde{x}^k)^T d^{A}\} = \nabla f(\tilde{x}^k)^T d^{A_{FW}}.
\]
3.3 Computation of the stepsize

Now, we can show the convergence results of the line search procedure for all the considered variants of the Frank-Wolfe direction, which will enable us to prove the global convergence of AS-SIMPLEX.

Depending on the direction $d_k$ used in the line search procedure, the maximum stepsize $\alpha_k^{\text{max}}$ is set as follows:

(i) Frank-Wolfe direction: $\alpha_k^{\text{max}} = 1$;

(ii) Away-Step Frank-Wolfe direction:

- if $d_{N_k}^{\text{FW}} = d_{N_k}^{\text{FW}}$, then $\alpha_k^{\text{max}} = 1$;
- if $d_{N_k}^{\text{FW}} = d_{N_k}^{\text{AW}}$, then $\alpha_k^{\text{max}} = \tilde{x}_j^k / (1 - \tilde{x}_j^k)$ where $\hat{j}$ is the index defined as in (36);

(iii) Pairwise direction: $\alpha_k^{\text{max}} = \tilde{x}_j^k$, where $\hat{j}$ is the index defined as in (36).

It is easy to verify that, for every considered search direction $d_k$, this choice guarantees that $\tilde{x}_k^k + \alpha d_k$ is feasible for all $\alpha \in (0, \alpha_k^{\text{max}}]$.

Now, we prove a theorem that follows from classical results on the Armijo line search. It guarantees that $\|\tilde{x}_k - x_k\|$ converges to zero and that the sequence of the directional derivatives along the search direction converges to zero as well, for all the considered search directions.

**Theorem 2.** Let Assumption 1 hold. Let $\{x^k\}$, $\{\tilde{x}^k\}$ and $\{d^k\}$ be the sequences produced by AS-SIMPLEX, where $d^k$ is computed at Step 7–8 according to one among (FW), (AFW) and (PFW) rule. If AS-SIMPLEX does not terminate in a finite number of iterations, then

$$\lim_{k \to \infty} \|\tilde{x}_k - x_k\| = 0,$$

$$\lim_{k \to \infty} \nabla f(\tilde{x}^k)^T d_k = 0.$$  

**Proof.** First, we observe that, from standard results on the Armijo line search, Algorithm 2 computes $\alpha_k$ in a finite number of steps at every iteration $k$ for which $\nabla f(\tilde{x}_k)^T d_k < 0$.

Now, we prove (37). From the instructions of the algorithm and Proposition 5, we can write

$$f(x^{k+1}) \leq f(\tilde{x}^k) \leq f(x^k) - L \|\tilde{x}^k - x^k\|^2.$$  

From the continuity of the objective function and the compactness of the feasible set, it follows that

$$\lim_{k \to \infty} [f(x^{k+1}) - f(x^k)] = 0.$$  

The above relation, combined with (39), proves (37).

To prove (38), we consider separately the iterations in which $\nabla f(\tilde{x}^k)^T d_k < 0$ from those in which $\nabla f(\tilde{x}^k)^T d_k = 0$. Namely, we identify two iteration index subsets $H, K \subseteq \{1, 2, \ldots \}$, such that:

- $\nabla f(\tilde{x}^k)^T d_k < 0$, for all $k \in K;$
• $H = \{1, 2, \ldots \} \setminus K$.

By assumption, the algorithm does not terminate in a finite number of iterations, and then, at least one of the above sets is infinite. Since we are interested in the asymptotic behavior of the sequence produced by \texttt{AS-SIMPLEX}, we assume without loss of generality that both $H$ and $K$ are infinite sets.

From the instructions of the algorithm, it is straightforward to verify that

$$
\lim_{k \to \infty, k \in H} \nabla f(\hat{x}^k)^T d^k = 0.
$$

Therefore, we limit our analysis to consider the subsequence $\{x^k\}_K$. For all $k \in K$, since $\nabla f(\hat{x}^k)^T d^k < 0$, the line search procedure computes a value $\alpha^k \in (0, 1]$ in a finite number of iterations, such that

$$
f(x^{k+1}) \leq f(\hat{x}^k) + \gamma \alpha^k \nabla f(\hat{x}^k)^T d^k, \quad \forall k \in K,
$$
or equivalently,

$$
f(\hat{x}^k) - f(x^{k+1}) \geq \gamma \alpha^k |\nabla f(\hat{x}^k)^T d^k|, \quad \forall k \in K,
$$

From (37) and (40), we get that the left-hand side of the above inequality converges to zero, hence

$$
\lim_{k \to \infty} \alpha^k |\nabla f(\hat{x}^k)^T d^k| = 0. \quad (41)
$$

Now, proceeding by contradiction, we assume that (38) does not hold. From the compactness of the feasible set, $\{x^k\}_K$ attains limit points. Let $\bar{x}$ be any limit point of $\{x^k\}_K$. Using (37), since $\{x^k\}, \{\hat{x}^k\}$ and $\{d^k\}$ are bounded, and taking into account that $A^k$ and $N^k$ are subsets of a finite set of indices, without loss of generality we redefine $\{x^k\}_K$ the subsequence such that

$$
\lim_{k \to \infty, k \in K} x^k = \lim_{k \to \infty, k \in K} \hat{x}^k = \bar{x}, \quad (42)
$$

and

$$
A^k = \hat{A}, \quad N^k = \hat{N}, \quad \forall k \in K, \quad (43)
$$
$$
\lim_{k \to \infty, k \in K} d^k = \hat{d}. \quad (44)
$$

As we have assumed that (38) does not hold, then the above relations, combined with the continuity of the gradient, imply that

$$
\lim_{k \to \infty, k \in K} \nabla f(\hat{x}^k)^T d^k = \nabla f(\hat{x})^T \hat{d} = -\eta < 0. \quad (45)
$$

We first prove that, if (45) holds, then $M > 0$ exists such that

$$
\alpha^k_{\max} \geq M, \quad \forall k \in K. \quad (46)
$$

By contradiction, let us assume that an infinite subset of $K$ (that we denote with $K$ for simplicity) exists such that

$$
\lim_{k \to \infty, k \in K} \alpha^k_{\max} = 0. \quad (47)
$$

We distinguish three different cases, depending on the strategy used for computing the direction $d^k$ at Step 7–8 in Algorithm 1:
• Case (FW): it is easy to see that we get a contradiction since \( \alpha_{\text{max}}^k \) has a constant value equal to 1.

• Case (AFW): recalling the definition of \( d_{\text{AFW}} \), the case we need to analyze is the one where we get an infinite subsequence of Away-Step directions in \( N_k \). So, we assume that an infinite subset \( \tilde{K} \subseteq K \) exists such that

\[
d_{N_k}^k = d_{N_k}^A, \quad \forall k \in \tilde{K}.
\]

We have that \( \alpha_{\text{max}}^k = \frac{\tilde{x}_j^k}{1 - \tilde{x}_j^k} \), for all \( k \in \tilde{K} \), where \( j \) is the index computed according to (36). Since the number of indices in \( \tilde{N} \) is finite, we can consider a further subsequence (that we denote with \( \tilde{K} \) for simplicity), where the index \( j \) is fixed. Taking into account (47), it is easy to see that

\[
\lim_{k \to \infty, k \in \tilde{K}} \tilde{x}_j^k = 0.
\]  

Now, from (45), (48) and the continuity of \( \nabla f(x) \), it follows that an index \( \tilde{k} \in \tilde{K} \) exists such that, for all \( k \geq \tilde{k}, k \in \tilde{K} \), we have that

\[
\nabla f(\tilde{x}^k) d^k = \nabla f(\tilde{x}^k) (\tilde{x}^k - e_j) \leq -\frac{\eta}{2},
\]

\[
\tilde{x}_j^k \leq \frac{\eta}{2}.
\]

Therefore, we obtain

\[
\tilde{x}_j^k \leq \epsilon \nabla f(x^k) (e_j - \tilde{x}_j^k), \quad \forall k \geq \tilde{k}, k \in \tilde{K}.
\]

Recalling (11), this implies that \( j \in \hat{A} \) and, considering the definition of \( j \) in (36), we get a contradiction.

• Case (PFW): in this case \( \alpha_{\text{max}}^k = \tilde{x}_j^k \) and the contradiction follows from the same reasoning done above for (AFW).

So, (46) holds.

Now, from (41) and (45), we get

\[
\lim_{k \to \infty, k \in K} \alpha^k = 0.
\]  

Taking into account (46), it follows that a value \( \bar{k} \in K \) exists such that

\[
\alpha^k < \alpha_{\text{max}}^k, \quad \forall k \geq \bar{k}, k \in K.
\]

In other words, for \( k \geq \bar{k}, k \in K \), the stepsize \( \alpha^k \) cannot be set equal to the maximum stepsize and, taking into account the line search procedure, we can write

\[
f\left(\tilde{x}^k + \frac{\alpha^k}{\delta} d^k\right) > f(\tilde{x}^k) + \gamma \frac{\alpha^k}{\delta} \nabla f(\tilde{x}^k)^T d^k, \quad \forall k \geq \bar{k}, k \in K.
\]
We can apply the mean value theorem and we have that $\xi_k \in (0, 1)$ exists such that
\[
\begin{align*}
  f(\tilde{x}^k + \frac{\alpha_k}{\delta}d^k) &= f(\tilde{x}^k) + \frac{\alpha_k}{\delta} \nabla f(\tilde{x}^k + \xi_k \frac{\alpha_k}{\delta} d^k) T d^k, \quad \forall k \geq \bar{k}, k \in K. \tag{51}
\end{align*}
\]
By substituting (51) within (50), we have
\[
\begin{align*}
  \nabla f(\tilde{x}^k + \xi_k \frac{\alpha_k}{\delta} d^k) T d^k > \gamma \nabla f(\tilde{x}^k) T d^k. \tag{52}
\end{align*}
\]
From (49), (37), and exploiting the fact that $\{\xi_k\}$ and $\{d_k\}$ are bounded, we also get
\[
\begin{align*}
  \lim_{k \to \infty, k \in K} \tilde{x}^k + \xi_k \frac{\alpha_k}{\delta} d^k = \lim_{k \to \infty, k \in K} \tilde{x}^k = \bar{x}. \tag{53}
\end{align*}
\]
Finally, from (45), (52) and (53), we obtain
\[
-\eta = \nabla f(\bar{x}) T \bar{d} \geq \gamma \nabla f(\bar{x}) T \bar{d} = -\gamma \eta,
\]
which is a contradiction, since we set $\gamma < 1$ in AS–SIMPLEX.

4 Global convergence analysis

In this section, we prove the global convergence of AS–SIMPLEX to stationary points, for every considered choice of the direction $d^k$.

Remark 3. From Proposition 2 and 3, it follows that Algorithm 1 is well defined by employing any direction $d^k$ among $d^{FW}$, $d^{AFW}$ and $d^{PFW}$, in the sense that a new point $x^{k+1}$ is computed if and only if $x^k$ is non-stationary.

Theorem 3. Let Assumption 1 hold and let $\{x^k\}$ be the sequence of points produced by AS–SIMPLEX. Let us assume that the search direction $d^k$ is computed according to one among (FW), (AFW) and (PFW) rule.

Then, either an integer $\bar{k} \geq 0$ exists such that $x^\bar{k}$ is a stationary point for problem (1), or the sequence $\{x^k\}$ is infinite and every limit point $x^*$ of the sequence is a stationary point for problem (1).

Proof. First, we consider the case where $d^k$ is computed according to (FW) rule, that is, $d^k = d^{FW}$. Then, we will prove the remaining two cases.

Let $\{x^k\}$ be the sequence produced by Algorithm 1 and let us assume that a stationary point is not produced in a finite number of iterations. Since the feasible set is compact, then the sequence $\{x^k\}$ attains a limit point $x^*$ and, recalling (37) of Theorem 2, there exists $K \subseteq \mathbb{N}$ such that
\[
\begin{align*}
  \lim_{k \to \infty, k \in K} x^k &= \lim_{k \to \infty, k \in K} \tilde{x}^k = x^*. \tag{54}
\end{align*}
\]
Let $\Phi_i(x)$ be the continuous function defined as
\[
\Phi_i(x) = \max\{0, -\nabla f(x)^T (e_i - x)\},
\]
for $i = 1, \ldots, n$. The function $\Phi_i(x)$ is non-negative and continuous. Therefore, it follows that
\[
\begin{align*}
  \Phi_i(x) &= \max\{0, -\nabla f(x)^T (e_i - x)\} \geq 0, \quad \forall x \in \mathbb{R}^n.
\end{align*}
\]
that measures the violation of the optimality conditions for a variable \( x_i, i = 1, \ldots, n \).

By contradiction, we assume that \( x^* \) is not a stationary point, so that an index \( \nu \in \{1, \ldots, n\} \) exists such that

\[
|\Phi_\nu(x^*)| > 0. \tag{55}
\]

Taking into account that the number of possible different choices of \( A^k \) and \( N^k \) is finite, we can find a subset of iteration indices \( \bar{K} \subseteq K \) such that \( A^k = \hat{A} \) and \( N^k = \hat{N} \) for all \( k \in \bar{K} \).

First, suppose that \( \nu \in \hat{A} \). Then, by definition, we can write

\[
0 \leq x^k_\nu \leq \epsilon \nabla f(x^k)^T(e_\nu - x^k),
\]

so that

\[
\Phi_\nu(x^k) = \max\{0, -\nabla f(x^k)^T(e_\nu - x^k)\} = 0,
\]

for all \( k \in \bar{K} \). Thus, from (54) and the continuity of the function \( \Phi_i(\cdot) \), we get a contradiction with (55).

Now, suppose that \( \nu \in \hat{N} \). We can choose an index \( \bar{\nu} \in \{1, \ldots, n\} \) and a further subset of iteration indices \( \hat{K} \subseteq \bar{K} \) such that

\[
\Phi_{\bar{\nu}}(\tilde{x}^k) = \max_{i \in \hat{N}}\{\Phi_i(\tilde{x}^k)\}, \quad \forall \, k \in \hat{K}.
\]

Hence,

\[
\Phi_{\bar{\nu}}(\tilde{x}^k) \geq \Phi_\nu(\tilde{x}^k) \geq 0, \quad \forall \, k \in \hat{K},
\]

which, by continuity of \( \Phi_i(\cdot) \), implies that

\[
\Phi_\nu(x^*) \geq \Phi_\nu(x^*) > 0. \tag{56}
\]

From the definition of \( \Phi_i(x) \) and \( \bar{\nu} \), for all \( k \in \hat{K} \) we can write

\[
\Phi_{\bar{\nu}}(\tilde{x}^k) = \max_{i \in \hat{N}}\{\max_{i \in \hat{N}}\{0, -\nabla f(\tilde{x}^k)^T(e_i - \tilde{x}^k)\}\}
\]

\[
= -\min_{i \in \hat{N}}\{\nabla f(\tilde{x}^k)^T(e_i - \tilde{x}^k)\}
\]

\[
= -\nabla f(\tilde{x}^k)^T d^{FW}. \tag{57}
\]

Since we are considering the case where \( d^k = d^{FW} \), from (54), (38) of Theorem 2 and the continuity of \( \Phi_i(\cdot) \), we have that

\[
0 = \lim_{k \to \infty} \nabla f(\tilde{x}^k)^T d^k = \lim_{k \to \infty} -\Phi_{\bar{\nu}}(\tilde{x}^k) = -\Phi_{\bar{\nu}}(x^*),
\]

which, combined with (56), implies that \( \Phi_{\bar{\nu}}(x^*) = 0 \), thus contradicting (55). Then, the assertion is proved for \( d^k = d^{FW} \).

Now, we consider together the cases where \( d^k = d^{AFW} \) and \( d^k = d^{PFW} \). In both cases, we can apply the same reasoning made before and we obtain (57) again. Recalling the definition of \( d^{AFW} \) and Lemma 2, we can write

\[
-\nabla f(\tilde{x}^k)^T d^k \geq -\nabla f(\tilde{x}^k)^T d^{FW} = \Phi_{\bar{\nu}}(\tilde{x}^k),
\]

22
for both $d^k = d^{AFW}$ and $d^k = d^{PFW}$. Consequently,

$$0 = \lim_{k \to \infty} \nabla f(\tilde{x}^k)^T d^k \leq \lim_{k \to \infty} -\Phi_\nu(\tilde{x}^k) = -\Phi_\nu(x^*),$$

which, combined with (56), implies that $\Phi_\nu(x^*) = 0$, thus contradicting (55). Then, the assertion is also proved for $d^k = d^{AFW}$ and $d^k = d^{PFW}$.

\[ \square \]

5 Extension to minimization problems over the $\ell_1$-ball

In this section, we focus on the following problem:

$$\min_{x \in \mathbb{R}^n} h(x)$$

$$\|x\|_1 \leq \tau,$$

with $h \in C^1(\mathbb{R}^n)$, $\nabla h(x)$ Lipschitz continuous on the feasible set and $\tau > 0$.

First, let us briefly analyze some theoretical properties concerning the equivalence between a minimization problem over a polytope and a minimization problem over the unit simplex. As mentioned in Section 1, we can rewrite as a minimization problem over the unit simplex every problem of the form

$$\min_{x \in D} h(x)$$

with $h: \mathbb{R}^n \to \mathbb{R}$ and $D$ is the convex hull of $m$ vectors. Namely,

$$D = \text{conv}\{v_1, \ldots, v_m\},$$

where $v_i \in \mathbb{R}^n$, $i = 1, \ldots, m$. Introducing the variable vector $\alpha \in \mathbb{R}^m$, we obtain the following equivalent problem:

$$\min_{\alpha} f(\alpha) = h(V\alpha)$$

$$\sum_{i=1}^n \alpha_i = 1$$

$$\alpha_i \geq 0, \quad i = 1, \ldots, n,$$

where $V = [v_1 \ldots v_n] \in \mathbb{R}^{n \times m}$. So, given a feasible point $\alpha$ of problem (60), we have that $x = V\alpha$ is a feasible point of problem (59). If $h(x)$ is continuously differentiable, we get the gradient of $f(\alpha)$ as

$$\nabla f(\alpha) = V^T \nabla h(V\alpha).$$

Moreover, the next proposition shows a correspondence between the solutions of (59) and those of (60).

**Proposition 6.** Let us consider problems (59) and (60). A point $\alpha^*$ is stationary for (60) if and only if the point the $x^* = V\alpha^*$ satisfies

$$\nabla h(x^*)^T (x - x^*) \geq 0, \quad \forall x \in D.$$
Proof. Let us denote the unitary simplex by $\Delta$. First, we prove that $\alpha^*$ satisfies KKT conditions for (60) if and only if

$$\nabla f(\alpha^*)^T (\alpha - \alpha^*) \geq 0. \quad (61)$$

Assuming that (61) holds, let $i$ be an index such that $x_i^* > 0$ and let $j$ be any index in $\{1, \ldots, n\}$, with $j \neq i$. Then, we can consider the point $\alpha$ such that $\alpha_i = 0$, $\alpha_j = \alpha_j^* + \alpha_i^*$ and $\alpha_h = \alpha_h^*$, $h \in \{1, \ldots, n\}$, $h \neq i, j$. It follows that $\nabla f(\alpha^*)^T (\alpha - \alpha^*) = |\nabla_i f(x^*) + \nabla_j f(x^*)| x_i^* \geq 0$, implying that $\nabla_j f(x^*) \geq \nabla_i f(x^*)$. So, using Proposition 1 with $x^*$ replaced by $\alpha^*$, it follows that $\alpha^*$ satisfies KKT conditions.

Now, assume that $\alpha^*$ satisfies KKT conditions (2)–(4) (with $x^*$ replaced by $\alpha^*$), with multipliers $\mu^* \in \mathbb{R}^n$ and $\lambda^* \in \mathbb{R}$. Exploiting Corollary 1, we have that

$$\nabla_j f(\alpha^*) = \lambda^*, \quad \forall j: \alpha_j^* > 0, \quad (62)$$

$$\nabla_i f(\alpha^*) \geq \lambda^*, \quad \forall i: \alpha_i^* > 0. \quad (63)$$

Moreover, using (7) (with $x^*$ replaced by $\alpha^*$), we also have that

$$\nabla f(\alpha^*)^T \alpha^* = \lambda^*. \quad (64)$$

From (62), (63) and (64), and exploiting the fact that $\alpha \in \Delta$, we obtain

$$\nabla f(\alpha^*)^T (\alpha - \alpha^*) = \sum_{i=1}^{n} \nabla_i f(\alpha^*) \alpha_i - \nabla f(\alpha^*)^T \alpha^* \geq \lambda^* \sum_{i=1}^{n} \alpha_i - \lambda^* = 0$$

and then (61) holds. Finally, since $x^* = V \alpha^*$, we can write

$$\nabla f(\alpha^*)^T (\alpha - \alpha^*) \geq 0, \quad \forall \alpha \in \Delta \iff \nabla h(V \alpha^*)^T (\alpha - \alpha^*) \geq 0, \quad \forall \alpha \in \Delta \iff \nabla h(V \alpha^*)^T [V(\alpha - \alpha^*)] \geq 0, \quad \forall \alpha \in \Delta \iff \nabla h(x^*)^T (x - x^*) \geq 0, \quad \forall x \in D.$$
We start by introducing the slack variable \( z \in \mathbb{R} \), in order to reformulate (58) as follows:

\[
\min_{x \in \mathbb{R}^n, z \in \mathbb{R}} \bar{h} \left( \begin{bmatrix} x \\ z \end{bmatrix} \right)
\]

\[
\|x\|_1 + z = \tau
\]

\[
z \geq 0,
\]

where \( \bar{h} : \mathbb{R}^{n+1} \to \mathbb{R} \) is defined such that \( \bar{h} \left( \begin{bmatrix} x \\ z \end{bmatrix} \right) = h(x) \), for every \( \begin{bmatrix} x \\ z \end{bmatrix} \in \mathbb{R}^{n+1} \).

Exploiting the fact that every feasible point of (65) can be expressed as a convex combination of the vertices, we can write the following equivalent problem:

\[
\min_{\alpha \in \mathbb{R}^{2n+1}} f(\alpha) = \bar{h}(M\alpha)
\]

\[
e^T \alpha = 1
\]

\[
\alpha \geq 0,
\]

by performing the following variable transformation:

\[
\begin{bmatrix} x \\ z \end{bmatrix} = M\alpha,
\]

where

\[
M = \tau \begin{bmatrix}
I & -I & 0 \\
0 & \ldots & 0 & 0 & \ldots & 0 & 1
\end{bmatrix} \in \mathbb{R}^{(n+1) \times (2n+1)}. \tag{67}
\]

Equivalently,

\[
x_i = \tau (\alpha_i - \alpha_{n+i}), \quad i = 1, \ldots, n,
\]

\[
z = \tau \alpha_{2n+1}. \tag{68}
\]

Now, we associate to every feasible point of (65) a particular point \( \alpha \in \mathbb{R}^{2n+1} \) that satisfies system (68):

\[
\alpha_i = \frac{1}{\tau} \max\{0, x_i\}, \quad i = 1, \ldots, n,
\]

\[
\alpha_{n+i} = \frac{1}{\tau} \max\{0, -x_i\}, \quad i = 1, \ldots, n,
\]

\[
\alpha_{2n+1} = \frac{1}{\tau} z. \tag{69}
\]

As mentioned above, we want to show that for every feasible point \( x \) of problem (58), there exists a correspondence between the estimated active variables \( x_i \) (i.e., those variables that are estimated to be zero at the stationary point) and the variables \( \alpha_i \) (obtained by (69)) that are estimated active for problem (66).

In particular, for every feasible point \( x \) of problem (58), we can build the following index sets:
A_{\ell_1}(x), which contains the indices of the estimated active variables;

- $N_{\ell_1}(x)$, which contains the indices of the estimated non-active variables.

Using (69), and recalling that $\alpha_i$ are nonnegative, it follows that

$$x_i = 0 \iff \alpha_i = \alpha_{n+i} = 0.$$ 

Then, we estimate $x_i$ active for (58) if both $\alpha_i$ and $\alpha_{n+i}$ are estimated active for (66). Consequently, we define $A_{\ell_1}(x)$ and $N_{\ell_1}(x)$ as follows:

$$A_{\ell_1}(x) = \{ i \in \{1, \ldots, n\} : i \in A(\alpha) \text{ and } (i + n) \in A(\alpha) \},$$

$$N_{\ell_1}(x) = \{ i \in \{1, \ldots, n\} : i \in N(\alpha) \text{ or } (i + n) \in N(\alpha) \}. \tag{71}$$

Now, we describe how to build the above index sets without explicitly dealing with (66). Let $x$ a feasible point of (58). We can easily set $z = \tau - \|x\|_1$ and then compute $\alpha$ by (69).

Moreover, we can write

$$\nabla f(\alpha) = M^T \nabla \bar{h}(x) = M^T \begin{bmatrix} \nabla h(x) \\ 0 \end{bmatrix} = \tau \begin{bmatrix} \nabla_1 h(x) \\ \vdots \\ \nabla_n h(x) \\ -\nabla_1 h(x) \\ \vdots \\ -\nabla_n h(x) \\ 0 \end{bmatrix}, \tag{72}$$

and then

$$\nabla f(\alpha)^T \alpha = \begin{bmatrix} \nabla h(x)^T \\ 0 \end{bmatrix} M\alpha = \nabla h(x)^T x. \tag{73}$$

For each index $i = 1, \ldots, n$, we can distinguish two cases:

(i) $x_i \geq 0$. From (69), we have

$$\left\{ \begin{array}{l} \alpha_i = \frac{1}{\tau} x_i \geq 0, \\ \alpha_{n+i} = 0. \end{array} \right.$$ 

Recalling (11)–(12), and using (69), (72) and (73), we can write

$$i \in A(\alpha) \iff 0 \leq \frac{1}{\tau} x_i = \alpha_i \leq \epsilon \nabla f(\alpha)^T (e_i - \alpha)$$

$$= \epsilon (\nabla_i f(\alpha) - \nabla f(\alpha)^T \alpha)$$

$$= \epsilon (\tau \nabla_i h(x) - \nabla h(x)^T x)$$

$$= \epsilon \nabla h(x)^T (\tau e_i - x) \tag{74}$$

and

$$n + i \in A(\alpha) \iff -\frac{1}{\tau} x_i \leq 0 = \alpha_{n+i} \leq \epsilon \nabla f(\alpha)^T (e_{n+i} - \alpha)$$

$$= \epsilon (\nabla_{n+i} f(\alpha) - \nabla f(\alpha)^T \alpha)$$

$$= \epsilon (\tau \nabla_i h(x) - \nabla h(x)^T x)$$

$$= -\epsilon \nabla h(x)^T (\tau e_i + x). \tag{75}$$
(ii) $x_i < 0$. From (69), we have

$$
\begin{align*}
\alpha_i &= 0, \\
\alpha_{n+i} &= -\frac{1}{\tau} x_i > 0.
\end{align*}
$$

Similarly to the previous case, we can write

$$
\begin{align*}
i \in A(\alpha) &\iff \frac{1}{\tau} x_i < 0 = \alpha_i \leq \epsilon \nabla f(\alpha)^T (e_i - \alpha) \\
&= \epsilon (\nabla_i f(\alpha) - \nabla f(\alpha)^T \alpha) \\
&= \epsilon (\tau \nabla_i h(x) - \nabla h(x)^T x) \\
&= \epsilon \nabla h(x)^T (\tau e_i - x)
\end{align*}
$$

and

$$
\begin{align*}
(n + i) \in A(\alpha) &\iff 0 < -\frac{1}{\tau} x_i = \alpha_{n+i} \leq \epsilon \nabla f(\alpha)^T (e_{n+i} - \alpha) \\
&= \epsilon (\nabla_{n+i} f(\alpha) - \nabla f(\alpha)^T \alpha) \\
&= \epsilon (-\tau \nabla_i h(x) - \nabla h(x)^T x) \\
&= -\epsilon \nabla h(x)^T (\tau e_i + x).
\end{align*}
$$

From (74), (75), (76), (77), and recalling (70)–(71), we obtain

$$
\begin{align*}
A_{\ell_1}(x) &= \{i: \epsilon \tau \nabla h(x)^T (\tau e_i + x) \leq x_i \leq \epsilon \tau \nabla h(x)^T (\tau e_i - x)\}, \\
N_{\ell_1}(x) &= \{1, \ldots, n\} \setminus A_{\ell_1}(x).
\end{align*}
$$

Now, we show how the algorithmic framework described in the previous section can be easily adapted to problem (58), using the active and non-active estimates (78)–(79). We first need to define the following index set:

$$
J_{\ell_1}(x) = \left\{ j \in \{1, \ldots, n\} : j \in \text{Argmax}_{i=1,\ldots,n} \{ |\nabla_i h(x)| \} \right\}.
$$

We can show that for every non-stationary point $x$ of problem (58), the set $J_{\ell_1}(x) \cap N_{\ell_1}(x)$ is non-empty and we are able to get a sufficient reduction in the objective function by setting to zero the variables belonging to $A_{\ell_1}(x)$ and updating a variable $x_j$, with $j \in J_{\ell_1}(x) \cap N_{\ell_1}(x)$.

**Proposition 7.** Let $x$ be a feasible point of problem (58) and assume that $x$ is non-stationary. Then,

$$
N_{\ell_1}(x) \cap J_{\ell_1}(x) \neq \emptyset.
$$

**Proof.** Let $\alpha$ be the point given by (69). Considering problem (66), we can compute the active and non-active set estimates $A(\alpha), N(\alpha)$.

From (72), and exploiting the hypothesis that $x$ is non-stationary, it follows that

$$
\min_{i=1,\ldots,2n+1} \{ \nabla_i f(\alpha) \} < 0.
$$
In particular, this implies that

$$(2n + 1) \notin \text{Argmin} \{\nabla_i f(\alpha)\}.$$  

Hence, exploiting Proposition 4, there exists $\nu \in \{1, \ldots, 2n\}$ such that

$$\nu \in \text{Argmin}\{\nabla_i f(\alpha)\},$$  

$$\nu \in N(\alpha). \quad (81)$$

Recalling (72), we can rewrite (81) as

$$\nabla_\nu f(\alpha) \leq \min_{i=1,\ldots,n} \{\tau\nabla_1 h(x), \ldots, \tau\nabla_n h(x), -\tau\nabla_1 h(x), \ldots, -\tau\nabla_n h(x)\}, \quad (83)$$

that is,

$$-|\nabla_\nu f(\alpha)| \leq -\tau|\nabla_i h(x)|, \quad \forall i = 1, \ldots, n. \quad (84)$$

Now, we can define the index $j \in \{1, \ldots, n\}$ as

$$j = \begin{cases} \nu, & \text{if } \nu \in \{1, \ldots, n\}, \\ \nu - n, & \text{if } \nu \in \{n + 1, \ldots, 2n\}. \end{cases} \quad (85)$$

Using (72) again, we have

$$|\nabla_\nu f(\alpha)| = |\nabla_j f(\alpha)| = \tau|\nabla_j h(x)|.$$

The previous relation, combined with (84), implies that

$$j \in \text{Argmax} \{|\nabla_i h(x)|\}.$$  

Using (82) and (85), it follows that either $j \in N(\alpha)$, or $(j + n) \in N(\alpha)$. Recalling (71), it follows that

$$j \in N_{\ell_1}(x)$$

and then the assertion is proved. \hfill \Box

Now, we need an assumption on the parameter $\epsilon$ used in the active and non-active set estimates.

**Assumption 2.** Assume that the parameter $\epsilon$ appearing in the estimates (78)–(79) satisfies the following conditions:

$$0 < \epsilon \leq \frac{1}{4\tau^2 L(2n + 1)}, \quad (86)$$

where $L$ is the Lipschitz constant of $\nabla h(x)$ over the feasible set of (66).

We are ready to show how a sufficient decrease in the objective function of (58) can be obtained by setting the estimated active variables to zero and properly updating one estimated non-active variable.
Proposition 8. Let Assumption 2 hold. Given a feasible point \( x \) of problem (58), assume that \( x \) is non-stationary. Let \( j \in N_{\ell_1}(x) \cap J_{\ell_1}(x) \), \( I = \{1, \ldots, n\} \setminus \{j\} \) and let \( A_{\ell_1}(x) \) be a set of indices such that
\[
\hat{A}_{\ell_1}(x) \subseteq A_{\ell_1}(x).
\]
Let \( \tilde{x} \) be the feasible point defined as follows:
\[
\tilde{x}_i = \begin{cases} 
0, & i \in \hat{A}_{\ell_1}(x), \\
 x_i, & i \in I \setminus \hat{A}_{\ell_1}(x), \\
 x_i = x_i - \text{sgn}(\nabla_j h(x_j)) \sum_{h \in \hat{A}_{\ell_1}(x)} |x_h|, & i = j,
\end{cases}
\]
(87)
Then,
\[
h(\tilde{x}) - h(x) \leq -2\tau^2 L \|\tilde{x} - x\|^2.
\]
where \( L \) is the Lipschitz constant of \( \nabla h(x) \) over the feasible set of (58).

Proof. First, we show that \( \nabla f(\alpha) \) is Lipschitz continuous over the unit simplex with constant \( 2\tau^2 L \), where \( L \) is the Lipschitz constant of \( \nabla h(x) \) over the feasible region of (58). To prove it, let \( \bar{\alpha} \) and \( \hat{\alpha} \) be two feasible points of (66), and let \( \bar{x} \) and \( \hat{x} \) be the points obtained by applying (68) with \( \alpha = \bar{\alpha} \) and \( \alpha = \hat{\alpha} \), respectively. Taking into account (72), we have that
\[
\|\nabla f(\bar{\alpha}) - \nabla f(\hat{\alpha})\|^2 = \tau^2 \left\| \frac{\nabla h(\bar{x}) - \nabla h(\hat{x})}{\nabla h(\bar{x}) - \nabla h(\hat{x})} \right\|^2 = 2\tau^2 \|\nabla h(\bar{x}) - \nabla h(\hat{x})\|^2
\]
and then, exploiting the Lipschitz continuity of \( \nabla h(x) \), we obtain
\[
\|\nabla f(\bar{\alpha}) - \nabla f(\hat{\alpha})\| \leq \sqrt{2} \tau L \|\bar{x} - \hat{x}\|.
\]
(88)
Using (68), we get
\[
\|\bar{x} - \hat{x}\| \leq \|M\bar{\alpha} - M\hat{\alpha}\| \leq \|M\| \|\bar{\alpha} - \hat{\alpha}\|,
\]
(89)
where the first inequality is due to the presence of the slack variable \( z \) in (68). Exploiting known properties of real matrices, we can write
\[
\|M\|_2 \leq \sqrt{\left( \max_{1 \leq j \leq 2n+1} \left\{ \sum_{i=1}^{n+1} |M_{i,j}| \right\} \right) \left( \max_{1 \leq i \leq n+1} \left\{ \sum_{j=1}^{2n+1} |M_{i,j}| \right\} \right)} = \sqrt{2} \tau,
\]
where \( M_{i,j} \) is the entry of \( M \) in position \((i,j)\). Consequently, we have that
\[
\|\bar{x} - \hat{x}\| \leq \sqrt{2} \tau \|\bar{\alpha} - \hat{\alpha}\|.
\]
(90)
From (88) and (90), we get
\[
\|\nabla f(\bar{\alpha}) - \nabla f(\hat{\alpha})\| \leq 2\tau^2 L \|\bar{\alpha} - \hat{\alpha}\|,
\]
that is, \( 2\tau^2 L \) is the Lipschitz constant of \( \nabla f(\alpha) \) over the unit simplex.

Now, we show that the assertion is true. Let \( \alpha \) be the point given by (69) and let us consider the sets \( A(\alpha) \), \( N(\alpha) \) and \( J(\alpha) \). From (70), there exists \( \hat{A}(\alpha) \subseteq A(\alpha) \) such that
\[
i \in \hat{A}_{\ell_1}(x) \iff i, i + n \in \hat{A}(\alpha).
\]
We distinguish three cases:
(i) $\nabla_j h(x) = 0$. From (72) and the definition of $J_{\ell 1}(x)$, it follows that $\nabla h(x) = 0$, thus contradicting the hypothesis that $x$ is non-stationary. So, we can exclude this case from our analysis.

(ii) $\nabla_j h(x) < 0$. We first observe that, from (72), $j \neq 2n + 1$. Moreover, using (72) and the definition of $J_{\ell 1}(x)$, we can write

$$\tau \nabla h(x) \leq \tau \min \{\nabla_i h(x), -\nabla_i h(x)\} < -\tau \nabla h(x), \quad \forall i = 1, \ldots, n.$$ 

Exploiting again (72), and recalling the definition of $J(\alpha)$, the above relation implies that $j \in J(\alpha)$.

So, we can compute the vector $\tilde{\alpha}$ as

$$\tilde{\alpha}_i = \begin{cases} 0, & i \in \hat{A}(\alpha), \\ \alpha_i, & i \in \{1, \ldots, 2n + 1\} \setminus \{j\} \setminus \hat{A}(\alpha), \\ \alpha_i + \sum_{i \in \hat{A}(\alpha)} \alpha_i, & i = j. \end{cases}$$

Then, by applying (68), we obtain $\tilde{x}$ defined as in (87). In particular, let us observe that $\tilde{x}_j \geq x_j$ because $\tilde{\alpha}_j \geq \alpha_j$ and $\tilde{\alpha}_{j+n} = \alpha_{j+n}$.

Now, taking into account that $\nabla f(\alpha)$ is Lipschitz continuous over the unit simple with constant $2\tau^2 L$, the assumption we made on $\epsilon$ and the fact that problem (66) has $2n + 1$ variables, then the assertion follows from Proposition 5.

(iii) $\nabla_j h(x) > 0$. We can repeat the same reasons made for the previous case, with the difference that now we obtain $j + n \in J(\alpha)$.

So, we can compute the vector $\tilde{\alpha}$ as

$$\tilde{\alpha}_i = \begin{cases} 0, & i \in \hat{A}(\alpha), \\ \alpha_i, & i \in \{1, \ldots, 2n + 1\} \setminus \{j\} \setminus \hat{A}(\alpha), \\ \alpha_i + \sum_{i \in \hat{A}(\alpha)} \alpha_i, & i = j + n. \end{cases}$$

Applying (68), we obtain $\tilde{x}$ defined as in (87). In particular, we have that $\tilde{x}_j \leq x_j$, since $\tilde{\alpha}_j = \alpha_j$ and $\tilde{\alpha}_{j+n} \geq \alpha_{j+n}$.

From the previous results, we can define an algorithmic framework to solve problem (58), reported in Algorithm 8.

Also in this case, for every point $\tilde{x}^k$ generated at Step 6 of Algorithm 8, the search direction $d_k$ is computed in order to update only the estimated non-active variables, that is,

$$d_{A_k}^k = 0.$$
Algorithm 8 Active-Set framework for optimization over the $\ell_1$-Ball (AS-$\ell_1$-BALL)

1. Choose a feasible point $x^0$
2. For $k = 0, 1, \ldots$
3. If $x^k$ is a stationary point, then STOP

Active-Set Estimation:
4. Compute $A^k_{\ell_1} = A_{\ell_1}(x^k)$ and $N^k_{\ell_1} = N_{\ell_1}(x^k)$

Minimization step over $A^k_{\ell_1}$:
5. Compute $J^k_{\ell_1} = J_{\ell_1}(x^k)$, choose $j \in N^k_{\ell_1} \cap J^k_{\ell_1}$ and define $\tilde{N}^k_{\ell_1} = N^k_{\ell_1} \setminus \{j\}$
6. Set $\tilde{x}^k_{A_k} = 0$, $\tilde{x}^k_{\tilde{N}_k} = x^k_{\tilde{N}_k}$, $\tilde{x}^k_j = x^k_j - \text{sgn}(\nabla_j h(\tilde{x}^k_j)) \sum_{h \in A^k_{\ell_1}} |x^k_h|$

Minimization step over $N^k_{\ell_1}$:
7. Set $d^k_{A^k_{\ell_1}} = 0$
8. Compute a feasible direction $d^k_{N^k_{\ell_1}}$ in $\tilde{x}^k$ and a maximum stepsize $\alpha^k_{\text{max}}$
9. If $\nabla h(\tilde{x}^k)^T d^k < 0$ then
10. Compute a stepsize $\alpha^k \in (0, \alpha^k_{\text{max}}]$ by means of the Armijo line search (Algorithm 2)
11. Else
12. Set $\alpha^k = 0$
13. End if
14. Set $x^{k+1} = \tilde{x}^k + \alpha^k d^k$
15. End for

To compute $d^k_{N^k_{\ell_1}}$, we can employ either the standard Frank-Wolfe direction, or one of its variants. In particular, exploiting the relations between problem (58) and (66), we can easily compute, in the subspace $N^k_{\ell_1}$, every variant of the Frank-Wolfe direction that has been considered in Subsection 3.2.

For the sake of completeness, we describe how to compute such directions. At every iteration $k$, two feasible search directions $d^k_{N^k_{\ell_1}}$ can be computed (in the subspace $N^k_{\ell_1}$):

- the Frank-Wolfe direction
  \[
  d^k_{\text{FW}} = -\tau \text{sgn}(\nabla_i h(\tilde{x}^k)) e_i - \tilde{x}^k_{N^k_{\ell_1}}, \quad i = \text{Argmax}_{i \in N^k_{\ell_1}} \{|\nabla_i h(\tilde{x}^k)|\};
  \]

- the Away-Step direction
  \[
  d^k_{\text{A}} = \tilde{x}^k_{\tilde{N}_k} - \tau \text{sgn}(\nabla_j h(\tilde{x}^k)) e_j, \quad j = \text{Argmax}_{j \in N^k_{\ell_1}, \tilde{x}_j^k > 0} \{|\nabla_j h(\tilde{x}^k)|\}.
  \]

The final search direction $d^k$ can thus be computed according to one of the following three rules:
• (FW) rule: $d^k_{N_k}$ is chosen as the Frank-Wolfe direction, that is,

$$
\begin{align*}
&d^k_{A^k_{1'}} = 0, \\
&d^k_{N_k} = d^k_{N_k}.
\end{align*}
$$

In this case, we simply write

$$
d^k = d^k_{FW}.
$$

• (AFW) rule: $d^k_{N_k}$ is chosen as the Away-Step Frank-Wolfe direction, that is,

$$
\begin{align*}
&d^k_{A^k_{1'}} = 0, \\
&d^k_{N_k} = d^k_{AFW} = \begin{cases} \\
  d^k_{N_k}, & \text{if } \nabla_{N_k} h(\tilde{x}^k)^T d^k_{N_k} \leq \nabla_{N_k} h(\tilde{x}^k)^T d^k_{A^k_{1'}}, \\
  d^k_{A^k_{1'}}, & \text{otherwise.}
\end{cases}
\end{align*}
$$

In this case, we simply write

$$
d^k = d^k_{AFW}.
$$

• (PFW) rule: $d^k_{N_k}$ is chosen as the Pairwise Frank-Wolfe direction, that is,

$$
\begin{align*}
&d^k_{A^k_{1'}} = 0, \\
&d^k_{N_k} = d^k_{PFW} = d^k_{A^k_{1'}} + d^k_{N_k}.
\end{align*}
$$

In this case, we simply write

$$
d^k = d^k_{PFW}.
$$

Finally, exploiting the relations between problem (58) and problem (66), recalling Proposition 6 and 8, and taking into account how we compute $d^k$, we can state the convergence of $\text{AS-}\ell_1\text{-BALL}$ for every considered variant of the Frank-Wolfe direction, which follows from the convergence results of $\text{AS-SIMPLEX}$.

**Theorem 4.** Let Assumption 2 hold and let $\{x^k\}$ be the sequence of points produced by $\text{AS-}\ell_1\text{-BALL}$. Let us assume that the search direction $d^k$ is computed according to one among (FW), (AFW) and (PFW) rule.

Then, either an integer $\hat{k} \geq 0$ exists such that $\nabla h(x^k)^T (x - x^k) \geq 0$ for all $x: \|x\|_1 \leq \tau$, or the sequence $\{x^k\}$ is infinite and every limit point $x^*$ satisfies $\nabla h(x^*)^T (x - x^*) \geq 0$ for all $x: \|x\|_1 \leq \tau$.

### 6 Preliminary numerical results

In this section, we report some preliminary numerical results obtained by applying $\text{AS-}\ell_1\text{-BALL}$ on problems of the form:

$$
\min_{x \in \mathbb{R}^n} \frac{1}{2} \|Ax - b\|^2 \quad \text{subject to } \|x\|_1 \leq \tau,
$$

(91)
with $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^{m}$ and $\tau > 0$.

The testing problems were generating following the analysis suggested in [2, 12, 5]. In particular, several artificial signals were generated, with

- dimension $n \in \{2^{11}, 2^{12}, 2^{13}\}$;
- number of observations $m = n/4$;
- number of nonzeros $T = \text{round}(pm)$, with $\rho \in \{0.01, 0.03, 0.05, 0.07, 0.1\}$.

Matrix $A$ was obtained by generating a matrix with $m \times n$ independent and identically distributed elements from the Normal distribution $N(0, 1)$, and then normalizing the columns.

Once matrix $A$ has been built, the “true” signal $x^* \in \mathbb{R}^{n}$ was generated as a vector with all components equal to 0, except for $T$ randomly placed $\pm 1$ spikes. Vector $b$ was build as $Ax^* + \eta$, with $\eta$ drawn from a normal distribution with mean 0 and variance $10^{-3}$. Finally, we set $\tau = 1.1\|x^*\|_1$.

For each instance, we first run the Frank-Wolfe variants without using the active-set estimate, i.e., the Frank-Wolfe (FW), the Away-Step Frank-Wolfe (AFW) and the Pairwise Frank-Wolfe (PFW) method. Then, we run the corresponding active-set versions.

In particular, considering the framework reported in Algorithm 8, we call $\text{AS-FW-}\ell_1\text{-BALL}$, $\text{AS-AFW-}\ell_1\text{-BALL}$ and $\text{AS-PFW-}\ell_1\text{-BALL}$ the methods where the search direction $d^k$ is computed according to (FW), (AFW) and (PFW) rule, respectively.

All the considered algorithms employed the origin as starting point and they were terminated at the first iteration $k$ satisfying

$$\nabla h(x^k)^T x \geq -10^{-9}, \quad \forall x: \|x\|_1 \leq \tau,$$

where $h$ is the objective function of (91). Moreover, we arrested an algorithm when the number of iterations exceeded $200T$.

For what concerns the value of the parameter $\epsilon$ to use in the active-set estimate, generally it is not possible knowing an acceptable value a priori. Then, starting from the value $\epsilon = 1$, we employ the following updating rule: At every iteration $k$ we compute $\tilde{x}^k$ as indicated at Step 6 of Algorithm 8 and, if a sufficient decrease in the objective function is obtained, then we accept $\tilde{x}^k$ and we do not change the value of $\epsilon$. Otherwise, we do not accept $\tilde{x}^k$, we reduce $\epsilon$ and we estimate the active-set again, continuing until we get a sufficient decrease in the objective function.

All the codes were implemented in Matlab R2014b and the experiments were run on an Intel Xeon(R), CPU E5-1650 v2 3.50 GHz. For every fixed $n$ and $\rho$, the results have been averaged over 10 runs.

First, we analyze the effect of using the proposed active-set estimate in every Frank-Wolfe variant.

For what concerns FW, we actually do not observe significant differences when the active-set estimate is employed. Namely, $\text{AS-FW-}\ell_1\text{-BALL}$ and FW perform quite similarly.

Vice versa, for both AFW and PFW, the use of the active-set estimate leads to remarkable improvements. In particular, in Figure 1 we compare $\text{AS-AFW-}\ell_1\text{-BALL}$ with AFW, and in Figure 2 we compare $\text{AS-PFW-}\ell_1\text{-BALL}$ with PFW. In both figures, we plot the objective
function versus the computational time. It is clear that the objective function decreases much faster when the active-set estimate is employed, for every considered dimension $n$ and sparsity level $\rho$.

Finally, in Figure 3 we compare all the considered active-set variants, i.e., $\text{AS-FW-}\ell_1\text{-BALL}$, $\text{AS-AFW-}\ell_1\text{-BALL}$ and $\text{AS-PFW-}\ell_1\text{-BALL}$. Also in this figure, the objective function versus the computational time is plotted. We can easily see that both $\text{AS-AFW-}\ell_1\text{-BALL}$ and $\text{AS-PFW-}\ell_1\text{-BALL}$ significantly outperform $\text{AS-FW-}\ell_1\text{-BALL}$, confirming the theoretical results pointed out above. Moreover, $\text{AS-PFW-}\ell_1\text{-BALL}$ performs better than and $\text{AS-AFW-}\ell_1\text{-BALL}$ for all the considered problems, even if the difference becomes small when the problem dimension increases.

7 Conclusions

We have presented an algorithmic framework to solve minimization problems over the unit simplex. The proposed approach is based on the use of an active-set estimate to identify those variables that are equal to zero at the stationary point. This technique enables us to perform two steps at each iteration: first, we set the estimated active variables to zero and we update one estimated non-active variable, so that a new feasible point is generated and a sufficient decrease in the objective function is obtained. Then, we move the estimated non-active variables along a suitable search direction. The convergence of the algorithm has been proved when different variants of the Frank-Wolfe direction are employed.

Finally, we have considered the problem of minimizing a function over the $\ell_1$-ball. We have shown how our algorithmic framework can be adapted to this problem without any explicit variable transformation. Preliminary numerical result, obtained on some quadratic problems over the $\ell_1$-ball, have shown the effectiveness of the proposed active-set strategy.
Figure 1: Objective function vs CPU time (in seconds). Comparison between AS-AFW-ℓ₁-BALL and AFW. The y axis is in logarithmic scale.
Figure 2: Objective function vs CPU time (in seconds). Comparison between AS-PFW-$\ell_1$-BALL and PFW. The $y$ axis is in logarithmic scale.
Objective function vs CPU time (s) - Comparing active-set variants

Figure 3: Objective function vs CPU time (in seconds). Comparison between AS-FW-$\ell_1$-BALL, AS-AFW-$\ell_1$-BALL and AS-PFW-$\ell_1$-BALL. The $y$ axis is in logarithmic scale.
References


