Polling Set Construction and Worst-Case Complexity for Direct Search under Polyhedral Convex Constraints

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Abstract

Direct search is one of the most popular derivative-free optimization paradigms, that relies on exploring the variable space using polling directions. To analyze and implement direct search, one typically relies on positive spanning sets. This concept is somewhat decorrelated from interpolation-based sets used in model-based algorithms, another class of derivative-free optimization methods. This discrepancy is even more pronounced for constrained problems, where recent advances in the interpolation-based setting have produced a unified picture that is still lacking in the direct-search case.

In this paper, we introduce a new theoretical underpinning for direct-search methods, that can be defined for general convex constraints and lead to complexity guarantees, as in the model-based setting. By focusing on polyhedral convex constraints, we are able to construct polling sets that meet our new theoretical requirements. In particular, our polling sets necessarily include directions outside of the approximate tangent cone, giving theoretical justification to existing practical heuristics which incorporate this idea. Our numerical results confirm that adding these extra directions significantly improves practical performance.

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1 Introduction

Optimization problems that arise in practice commonly feature black-box, computationally expensive, or noisy objectives [2]. As a result, standard derivative-based algorithms cannot be used to tackle these problems, but derivative-free optimization (DFO) methods form a useful alternative [3, 9, 26]. Among DFO methods, *direct search* schemes are quite popular because of their simplicity of description and analysis [14, 24], and have given rise to efficient practical techniques [4]. Each iteration of a direct-search methods builds a finite *polling set* of (feasible) points near the current iterate. The quality of polling sets is instrumental to obtaining convergence guarantees for direct-search algorithms. In particular, when the problem is unconstrained, convergence is ensured by using *positive spanning sets* (PSSs), that span the variable space through nonnegative linear combinations, as polling sets. Moreover, by ensuring those sets have good enough *cosine measure*, worst-case complexity results can be established [39]. Although using random directions has recently gained popularity as a scalable alternative to positive spanning sets [19, 37], the use of the latter remains necessary to guarantee deterministic convergence.

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Choosing polling sets in presence of constraints is a significant challenge, as the feasible set geometry must be taken in account. To the best of our knowledge, and despite recent global convergence results on this topic [23], there is no direct-search technique equipped with complexity guarantees for convexly constrained problems. Nevertheless, a number of approaches have been developed to tackle the linearly constrained case [1, 5, 24, 25, 29], with bound constraints being the subject of dedicated investigation [6, 28, 30]. In the bound-constrained setting, using coordinate directions and their negative as polling sets gives rise to feasible iterate methods with convergence guarantees [28, 30]. This approach can be extended to general linear inequality constraints, by requiring polling sets to generate approximate tangent cones defined by nearby constraints, using nonnegative linear combinations as in the case of PSSs [25, 29]. Since approximate tangent cones can only be described using finite generators when they are polyhedral (e.g. [38, Theorem 2.8.8]), this approach does not extend to the convexly constrained case. Still, these polling choices not only lead to global convergence results, but also allow for a worst-case complexity analysis the in presence of general linear constraints [20]. However, in practice, the performance of these algorithms is greatly improved by searching along directions defined by the constraint normals [27]. Thus, even though the concept of PSS has been used successfully to obtain theoretically sound direct-search techniques in the linearly constrained setting, the practical implementations of these methods has yet to be fully understood.

Meanwhile, another class of DFO algorithms termed model-based algorithms, proceeds by building models of the objective function, that can then be minimized (typically over a trust region) in order to produce a candidate for the next function evaluation [9]. Model-based DFO methods consider interpolation sets at which function values are available to construct such models [35]. Provided those sets satisfy a geometric quality condition termed Λ-poisedness, the resulting algorithms can be endowed with complexity analysis in both unconstrained and convexly constrained settings [21, 35]. Unlike in direct-search methods, the use of approximate tangent cones is not required in model-based DFO, and thus the notion of Λ-poisedness readily extends to the convex setting [36]. Overall, despite both model-based and direct-search schemes being developed with geometrical insights, the connection between polling directions and interpolation sets remains underexplored.

In this paper, we introduce the notion of Λ-positive spanning sets (Λ-PSS), a novel property for polling sets in direct search inspired by Λ-poisedness in model-based derivative-free methods. In the unconstrained setting, our definition is similar to that of positive spanning sets, and leads to comparable complexity guarantees. For linearly constrained problems, our Λ-PSS theory relies on using polling directions lying outside of approximate tangent cones, thus departing from existing theory, but not standard practice. In fact, our explicit constructions of Λ-PSS provide a theoretical grounding for popular implementations [20, 27]. More broadly, our numerical experiments demonstrate that using generators of approximate tangent cones and their negatives (a valid Λ-PSS construction) outperforms both classical approaches with theoretical guarantees, that only rely on approximate tangent cones, and standard practice, which leverages active constraint normals.

The rest of this paper is organized as follows. Section 2 provides background material on direct-search methods for smooth unconstrained and linear inequality constrained problems. Section 3 introduces a new approach for measuring the quality of polling sets, which is then used in Section 4 to revisit complexity guarantees for direct search on both unconstrained and (polyhedral) convex constrained problems. Section 5 provides detailed constructions for polling sets in presence of explicit linear constraints. The numerical performance of this approach is showcased in Section 6.

Notation Throughout the paper, we use $\|\cdot\|$ to be the Euclidean norm of vectors and operator 2-norm (i.e. largest singular value) of matrices. Given a matrix $\boldsymbol{A}$, we denote its Moore-Penrose pseudoinverse as $\boldsymbol{A}^\dagger$ and the set of its column vectors by $\mathrm{col}(\boldsymbol{A})$. Given a cone $K \subseteq \mathbb{R}^n$, we denote its polar cone as $K^\circ := \{\boldsymbol{y} \in \mathbb{R}^n : \boldsymbol{y}^T\boldsymbol{x} \leq 0,\ \forall \boldsymbol{x} \in K\}$. For $\boldsymbol{x} \in \mathbb{R}^n$ and $\alpha > 0$ we define $B(\boldsymbol{x}, \alpha) := \{\boldsymbol{y} \in \mathbb{R}^n : \|\boldsymbol{y} - \boldsymbol{x}\| \leq \alpha\}$ to be the closed ball of radius α centered at $\boldsymbol{x}$. Finally, the projection onto a convex set S will be denoted by $\mathrm{proj}_S[\boldsymbol{v}]$.

Algorithm 1 Basic direct-search method for (2.1).

Inputs: $\boldsymbol{x}_0 \in \Omega$, $\alpha_{\max} > 0$, $\alpha_0 \in (0, \alpha_{\max}]$, $\sigma > 0$, $0 < \gamma_{\text{dec}} < 1 < \gamma_{\text{inc}}$.

for $k = 0, 1, 2, \ldots$ **do**

Compute a polling set $\mathcal{D}_k \subset \mathbb{R}^n$.

If there exists $\boldsymbol{d}_k \in \mathcal{D}_k$ such that $\boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k \in \Omega$ and

$$f(\boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k) < f(\boldsymbol{x}_k) - \frac{\sigma}{2}\alpha_k^2, \tag{2.3}$$

set $\boldsymbol{x}_{k+1} := \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$ and $\alpha_{k+1} := \min\{\gamma_{\text{inc}}\alpha_k, \alpha_{\max}\}$ ("successful iteration").

Otherwise, set $\boldsymbol{x}_{k+1} := \boldsymbol{x}_k$ and $\alpha_{k+1} := \gamma_{\text{dec}}\alpha_k$ ("unsuccessful iteration").

end for

2 Linearly constrained problems and direct search

In this paper, we study direct-search methods applied to solving problems of the form

$$\min_{\boldsymbol{x} \in \Omega} f(\boldsymbol{x}), \tag{2.1}$$

where we assume that f is smooth and Ω is a polyhedral set, in the sense of the following two assumptions.

Assumption 2.1. The objective function f (2.1) is C^1, its gradient ∇f is L-Lipschitz continuous for some $L > 0$, and f is bounded below on Ω by f_{low}.

Assumption 2.2. The feasible set Ω is a a polyhedral convex set with nonempty interior. Moreover, it admits a description of the form

$$\Omega = \{\boldsymbol{x} \in \mathbb{R}^n : \boldsymbol{a}_i^T \boldsymbol{x} \leq b_i, \ \forall i = 1, \ldots, m\}. \tag{2.2}$$

Note that the description (2.2) covers the unconstrained setting ($m = 1$, $\boldsymbol{a}_1 = \boldsymbol{0}$ and $b_1 = 0$), but that Ω cannot be a proper subspace of $\mathbb{R}^n$. Linear equality constraints, that define linear subspaces, can however be accounted for by other techniques closer to the unconstrained setting [20], and are not the focus of this paper.

The rest of this section describes existing results on direct-search schemes applied to problem (2.1). In particular, we recall existing complexity results in the unconstrained and linearly constrained setting, that leverage the concept of positive spanning set (PSS).

2.1 Direct-search algorithm

Algorithm 1 describes a generic direct-search framework for solving problem (2.1). The method starts with a feasible point and explores the space along directions that preserve feasibility. At every iteration, a finite set of p polling directions $\mathcal{D}_k \subset \mathbb{R}^n$ is selected, and the function value is queried at $\boldsymbol{x}_k + \alpha_k \boldsymbol{d}$ for $\boldsymbol{d} \in \mathcal{D}_k$, where $\boldsymbol{x}_k$ is the current iterate and α_k is a dynamically updated stepsize. If a polled point with sufficiently small objective value is found, then this becomes the new iterate and the stepsize is usually increased. Otherwise, the iterate does not change and the stepsize is reduced.

Algorithm 1 relies on a sufficient decrease condition (2.3) to accept trial points, which is necessary to obtain complexity guarantees [14, 39]. However, our condition departs from standard choices in that it does not involve $\|\boldsymbol{d}_k\|$. Removing the norm dependency turns out to be critical for our new polling set technique, as will be shown in Section 4.

2.2 Positive spanning sets and the unconstrained case

In this section, we focus on the unconstrained case, i.e. problem (2.1) with $\Omega = \mathbb{R}^n$. In this setting, convergence of Algorithm 1 can be guaranteed by ensuring that every polling set $\mathcal{D}_k$ contains at least one descent direction, i.e. a direction making an acute angle with the negative gradient. When $\mathcal{D}_k$ is chosen as a *positive spanning set* (for $\mathbb{R}^n$), this property is ensured without access to derivative information.

Definition 2.3. A set $\{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a positive spanning set (PSS) for $\mathbb{R}^n$ if, for any $\boldsymbol{v} \in \mathbb{R}^n$, there exist constants $c_1, \ldots, c_p \geq 0$ such that $\boldsymbol{v} = \sum_{i=1}^p c_i \boldsymbol{d}_i$.

Lemma 2.4 (Theorem 3.1, [10])**.** *The set $\mathcal{D} := \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a PSS for $\mathbb{R}^n$ if and only if*

$$\min_{\boldsymbol{v} \neq \boldsymbol{0}} \max_{\boldsymbol{d} \in \mathcal{D}} \boldsymbol{d}^T \boldsymbol{v} > 0. \tag{2.4}$$

It follows from Lemma 2.4 that a set of (nonzero) vectors $\mathcal{D}$ is a PSS if and only if $\mathrm{cm}(\mathcal{D}) > 0$, where $\mathrm{cm}(\mathcal{D})$ is the *cosine measure* of $\mathcal{D}$ defined by

$$\mathrm{cm}(\mathcal{D}) := \min_{\boldsymbol{v} \neq \boldsymbol{0}} \max_{\substack{\boldsymbol{d} \in \mathcal{D} \\ \boldsymbol{d} \neq \boldsymbol{0}}} \frac{\boldsymbol{d}^T \boldsymbol{v}}{\|\boldsymbol{d}\| \, \|\boldsymbol{v}\|}. \tag{2.5}$$

Assuming that the sequence $\{\mathrm{cm}(\mathcal{D}_k)\}$ is uniformly bounded away from zero leads to both convergence and complexity guarantees [14, 39].

Assumption 2.5. At every iteration of Algorithm 1, the set $\mathcal{D}_k$ satisfies $\mathrm{cm}(\mathcal{D}_k) \geq \kappa$, and $d_{\min} \leq \|\boldsymbol{d}\| \leq d_{\max}$ for all $\boldsymbol{d} \in \mathcal{D}_k$, for some $\kappa > 0$ and $d_{\max} \geq d_{\min} > 0$ independent of k. Moreover, $\mathcal{D}_k$ has at most p vectors, where p is a positive integer value.

Theorem 2.6. *Suppose Assumptions 2.1 and 2.5 hold. Then Algorithm 1 achieves $\|\nabla f(\boldsymbol{x}_k)\| \leq \epsilon$ after at most $\mathcal{O}(\kappa^{-2}\epsilon^{-2})$ iterations, or $\mathcal{O}(p\kappa^{-2}\epsilon^{-2})$ objective evaluations. Hence* $\liminf_{k\to\infty} \|\nabla f(\boldsymbol{x}_k)\| = 0$.

A canonical choice for $\mathcal{D}_k$ is the set of positive and negative coordinate vectors, $\mathcal{D}_k = \{\pm\boldsymbol{e}_1, \ldots, \pm\boldsymbol{e}_n\}$, which satisfies Assumption 2.5 with $\kappa = 1/\sqrt{n}$ and $d_{\min} = d_{\max} = 1$. Using this polling set at every iteration yields complexity guarantees in $\mathcal{O}(n\epsilon^{-2})$ iterations and $\mathcal{O}(n^2\epsilon^{-2})$ objective evaluations, that are optimal for direct search in terms of dependencies on n [12].

2.3 Linearly constrained case

We now turn to the linearly constrained setting. Under Assumptions 2.1 and 2.2, first-order stationarity can be assessed using the following measure [7, 21]:

$$\pi(\boldsymbol{x}) := \left| \min_{\substack{\boldsymbol{x}+\boldsymbol{v} \in \Omega \\ \|\boldsymbol{v}\| \leq 1}} \nabla f(\boldsymbol{x})^T \boldsymbol{v} \right|, \qquad \forall \boldsymbol{x} \in \Omega. \tag{2.6}$$

Indeed, we always have $\pi(\boldsymbol{x}) \geq 0$, and $\pi(\boldsymbol{x}) = 0$ if and only if $\boldsymbol{x}$ is first-order critical for (2.1) [8, Theorem 12.1.6]. Moreover, since Ω is assumed to be closed, the problem (2.6) always has a solution. Letting $\boldsymbol{v}^*(\boldsymbol{x})$ denote such a solution, it follows that

$$\pi(\boldsymbol{x}) = -\nabla f(\boldsymbol{x})^T \boldsymbol{v}^*(\boldsymbol{x}), \quad \boldsymbol{x} + \boldsymbol{v}^*(\boldsymbol{x}) \in \Omega, \quad \|\boldsymbol{v}^*(\boldsymbol{x})\| \leq 1. \tag{2.7}$$

Deriving convergence guarantees for Algorithm 1 requires to relate the polling sets to the stationarity measure (2.6). To this end, one must rely on more than positive spanning sets, and use directions that conform to the geometry of nearby constraints. More precisely, given a feasible point $\boldsymbol{x} \in \Omega$ and tolerance $\alpha \geq 0$, we define the *nearly active* constraints at $\boldsymbol{x}$ to be those whose boundaries are within distance α of $\boldsymbol{x}$, i.e.

$$I(\boldsymbol{x}, \alpha) := \{i \in \{1, \ldots, m\} : b_i - \alpha\|\boldsymbol{a}_i\|^2 \leq \boldsymbol{a}_i^T \boldsymbol{x}\}, \tag{2.8}$$

noting that we always have $\boldsymbol{a}_i^T \boldsymbol{x} \leq b_i$ for all i since $\boldsymbol{x}$ is feasible. The approximate normal cone of Ω at $\boldsymbol{x}$ is then defined as

$$N_\Omega(\boldsymbol{x}, \alpha) := \mathrm{cone}(\{\boldsymbol{a}_i : i \in I(\boldsymbol{x}, \alpha)\}), \tag{2.9}$$

while the approximate tangent cone is the polar of $N_\Omega(\boldsymbol{x}, \alpha)$, i.e. $T_\Omega(\boldsymbol{x}, \alpha) := N_\Omega(\boldsymbol{x}, \alpha)^\circ$. When $\alpha = 0$, these cones coincide with the usual tangent and normal cones from constrained optimization [33, Section 12.2].

To guarantee convergence of Algorithm 1, it suffices to use polling sets that contain generators of tangent cones at every iteration. Complexity results are obtained assuming sufficient quality of those sets, in the sense of an extension of the cosine measure to the linearly constrained case [20, 25].

Assumption 2.7. At every iteration of Algorithm 1, the set $\mathcal{D}_k$ consists of unit vectors, and satisfies

$$\mathrm{cm}_{T_\Omega(\boldsymbol{x}_k, \alpha_k)}(\mathcal{D}_k) := \inf_{\substack{\boldsymbol{v} \in \mathbb{R}^n \\ \mathrm{proj}_{T_\Omega(\boldsymbol{x}_k, \alpha_k)}(\boldsymbol{v}) \neq \boldsymbol{0}}} \max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{\boldsymbol{d}^T \boldsymbol{v}}{\|\boldsymbol{d}\| \, \|\mathrm{proj}_{T_\Omega(\boldsymbol{x}_k, \alpha_k)}(\boldsymbol{v})\|} \geq \kappa$$

for some $\kappa > 0$.

Note that the use of unit vectors was made for simplicity in Gratton et al. [20], and that the theory can on principle be extended to allow for uniform bounds on the direction norms, as in Assumption 2.5. A key contribution of this paper is to allow for the minimum direction norm to vary with the iteration (and the stepsize).

Note also that $\mathrm{cm}_{T_\Omega(\boldsymbol{x}_k, \alpha_k)}(\mathcal{D}_k) \geq \kappa > 0$ implies that $\mathcal{D}_k$ contains a set of generators for the approximate tangent cone. Since the only finitely generated cones are polyhedral [38, Theorem 2.8.8], this strategy cannot be extended to general convex sets using polling sets of finite cardinality. In the linearly constrained setting, however, the reasoning from the unconstrained case leads to both convergence and complexity results [20, 25].

Theorem 2.8. *Let Assumptions 2.1, 2.2 and 2.7 hold. Suppose further that the gradient of f is bounded on Ω. Then, Algorithm 1 achieves $\pi(\boldsymbol{x}_k) \leq \epsilon$ after at most $\mathcal{O}(\kappa^{-2}\epsilon^{-2})$ iterations, or $\mathcal{O}(p\kappa^{-2}\epsilon^{-2})$ objective evaluations. Hence $\liminf_{k\to\infty} \pi(\boldsymbol{x}_k) = 0$.*

Quantifying the value of p and κ for arbitrary linear constraints is challenging in general. However, when the set Ω consists only of bound constraints, both approximate normal and tangent cones are generated by coordinate vectors and their negatives. Letting $\mathcal{D}_k$ be the subset of $\{\pm \boldsymbol{e}_i\}$ that are feasible for the stepsize α_k guarantees that Assumption 2.7 holds with $\kappa = 1/\sqrt{n}$, as in the unconstrained setting. One then obtains complexity bounds of $\mathcal{O}(n\epsilon^{-2})$ iterations and $\mathcal{O}(n^2\epsilon^{-2})$ objective evaluations, thus matching the unconstrained case [20]. We will revisit the bound-constrained setting in Section 5.1.

3 Λ-Positive Spanning Sets

In this section, we introduce an alternative to the cosine measure for assessing the quality of a polling set, inspired by model-based derivative-free optimization. We illustrate this concept for both unconstrained and bound-constrained optimization, deferring the general case to Section 5.

3.1 Motivation: Linear Interpolation

In model-based optimization, local polynomial approximations to the objective f are constructed by interpolation to known function values, and replace Taylor-like approximations inside trust-region methods [35]. The simplest formulation consists in building a linear interpolant for f: given a base point $\boldsymbol{x}$ and points $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$ near $\boldsymbol{x}$, we find a linear (model) function $m : \mathbb{R}^n \to \mathbb{R}$ such that

$$f(\boldsymbol{y}_i) \approx m(\boldsymbol{y}_i) := f(\boldsymbol{x}) + \boldsymbol{g}^T(\boldsymbol{y}_i - \boldsymbol{x}), \qquad i = 1, \ldots, n, \tag{3.1}$$

by solving the $n \times n$ linear system

$$\begin{bmatrix} \boldsymbol{d}_1^T \\ \vdots \\ \boldsymbol{d}_n^T \end{bmatrix} \boldsymbol{g} = \begin{bmatrix} f(\boldsymbol{y}_1) - f(\boldsymbol{x}) \\ \vdots \\ f(\boldsymbol{y}_n) - f(\boldsymbol{x}) \end{bmatrix}, \tag{3.2}$$

where $\boldsymbol{d}_i := \boldsymbol{y}_i - \boldsymbol{x}$ for $i = 1, \ldots, n$. The vector $\boldsymbol{g}$ is also known as a simplex gradient for f, and can be used to define algorithmic steps [34].

Although the matrix in (3.2) is invertible if and only if the vectors $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_n$ span $\mathbb{R}^n$ in the sense of Definition 2.3, the quality of the model is not defined according to the cosine measure of this set in model-based DFO. Rather, the quality of the model (3.1) relates to how well it can approximate the associated Taylor series for f [35, Lemma 5.1]. Under Assumption 2.1, for any interpolation point $\boldsymbol{y}_i$, we have [35, Lemma 5.2]:

$$\begin{aligned} |(\boldsymbol{g} - \nabla f(\boldsymbol{x}))^T(\boldsymbol{y}_i - \boldsymbol{x})| &= |m(\boldsymbol{y}_i) - f(\boldsymbol{x}) - \nabla f(\boldsymbol{x})^T(\boldsymbol{y}_i - \boldsymbol{x})|, \\ &= |f(\boldsymbol{y}_i) - f(\boldsymbol{x}) - \nabla f(\boldsymbol{x})^T(\boldsymbol{y}_i - \boldsymbol{x})|, \\ &\leq \frac{L}{2}\|\boldsymbol{y}_i - \boldsymbol{x}\|^2 = \frac{L}{2}\|\boldsymbol{d}_i\|^2. \end{aligned}$$

Now consider another point $\boldsymbol{y}$ near $\boldsymbol{x}$. If the vectors $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_n$ span $\mathbb{R}^n$, then there exist constants $c_1(\boldsymbol{y}), \ldots, c_n(\boldsymbol{y}) \in \mathbb{R}$ such that

$$\boldsymbol{y} - \boldsymbol{x} = \sum_{i=1}^{n} c_i(\boldsymbol{y})\boldsymbol{d}_i,$$

and so we may compute

$$|m(\boldsymbol{y}) - f(\boldsymbol{x}) - \nabla f(\boldsymbol{x})^T(\boldsymbol{y} - \boldsymbol{x})| = |(\boldsymbol{g} - \nabla f(\boldsymbol{x}))^T(\boldsymbol{y} - \boldsymbol{x})| \leq \frac{L}{2}\left(\max_i \|\boldsymbol{d}_i\|^2\right)\sum_{i=1}^{n} |c_i(\boldsymbol{y})|.$$

In model-based DFO, the points $\boldsymbol{y}_i$s are usually close to $\boldsymbol{x}$, typically within a trust region as a ball centered at $\boldsymbol{x}$ [9]. The quality of the interpolation set is then measured by the quantity $\sum_{i=1}^{n} |c_i(\boldsymbol{y})|$, where the values $c_i(\boldsymbol{y})$ correspond to the Lagrange polynomials for the interpolation points, evaluated at $\boldsymbol{y}$. An upper bound $\Lambda > 0$ on the quantity $\sum_{i=1}^{n} |c_i(\boldsymbol{y})|$ is called a Λ-poisedness constant for the interpolation set. In the next section, we adapt this concept to positive spanning sets.

3.2 Λ-Positive Spanning Sets

We now propose an alternate characterization of a positive spanning set, inspired by the results of Section 3.1. Unlike the classical definition of a PSS, Definition 3.1 below assesses the quality of a set within a ball.

Definition 3.1. Let $\boldsymbol{x} \in \mathbb{R}^n$, $\alpha > 0$ and $\Lambda > 0$. A set $\{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a Λ-positive spanning set (Λ-PSS) for $B(\boldsymbol{x}, \alpha)$ if, for any $\boldsymbol{v} \in B(\boldsymbol{0}, \alpha)$, there exists $\boldsymbol{c}(\boldsymbol{v}) \in \mathbb{R}^p$ with $\boldsymbol{c}(\boldsymbol{v}) \geq \boldsymbol{0}$ such that

$$\boldsymbol{v} = \sum_{i=1}^{p} c_i(\boldsymbol{v})\boldsymbol{d}_i \quad \text{and} \quad \|\boldsymbol{c}(\boldsymbol{v})\|_1 = \sum_{i=1}^{p} c_i(\boldsymbol{v}) \leq \Lambda. \tag{3.3}$$

Definition 3.1 is a stronger requirement than the positive spanning set property of Definition 2.3. As shown below, bounding the coefficients $c_i(\boldsymbol{v})$ tightens the notion of a PSS in the same way than bounding the cosine measure from below.

Lemma 3.2. *Let $\boldsymbol{x} \in \mathbb{R}^n$, $d_{\max} > 0$ and $\alpha > 0$. If $\mathcal{D} := \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a Λ-PSS for $B(\boldsymbol{x}, \alpha)$ and $\|\boldsymbol{d}_i\| \leq d_{\max}\alpha$ for all $i = 1 \ldots, p$, then $\mathrm{cm}(\mathcal{D}) \geq \kappa$ with $\kappa := \frac{1}{d_{\max}\Lambda}$.*

Proof. To find a contradiction, suppose that $\mathrm{cm}(\mathcal{D}) < \kappa$. Then, there exists $\boldsymbol{v} \neq \boldsymbol{0}$ such that $\boldsymbol{v}^T\boldsymbol{d}_i < \kappa\|\boldsymbol{v}\| \cdot \|\boldsymbol{d}_i\|$ for all $i = 1, \ldots, p$. Now consider $\hat{\boldsymbol{v}} := \frac{\alpha}{\|\boldsymbol{v}\|}\boldsymbol{v}$, so that $\|\hat{\boldsymbol{v}}\| = \alpha$. Since $\mathcal{D}$ is a Λ-PSS for $B(\boldsymbol{x}, \alpha)$, we can write $\hat{\boldsymbol{v}} = \sum_{i=1}^p c_i\boldsymbol{d}_i$ for some $c_i \geq 0$ and $\sum_{i=1}^p c_i \leq \Lambda$ (we omit the dependency on $\hat{\boldsymbol{v}}$ for simplicity). Thus,

$$\alpha^2 = \hat{\boldsymbol{v}}^T\hat{\boldsymbol{v}} = \sum_{i=1}^p c_i\boldsymbol{d}_i^T\hat{\boldsymbol{v}} = \frac{\alpha}{\|\boldsymbol{v}\|}\sum_{i=1}^p c_i\boldsymbol{d}_i^T\boldsymbol{v} < \frac{\alpha}{\|\boldsymbol{v}\|}\sum_{i=1}^p c_i\kappa\|\boldsymbol{v}\|\,\|\boldsymbol{d}_i\| \leq \alpha^2\kappa\Lambda d_{\max} = \alpha^2, \qquad (3.4)$$

where the last equality follows by definition of κ, and we have a contradiction. ☐

Lemma 3.3. *Let $\boldsymbol{x} \in \mathbb{R}^n$ and $\alpha > 0$. If $\mathcal{D} := \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a PSS such that $\mathrm{cm}(\mathcal{D}) \geq \kappa > 0$ and $\|\boldsymbol{d}_i\| \geq d_{\min}\alpha$ for all $i = 1, \ldots, p$, then $\mathcal{D}$ is a Λ-PSS for $B(\boldsymbol{x}, \alpha)$ with $\Lambda := \frac{1}{d_{\min}\kappa}$.*

Proof. To find a contradiction, suppose that $\mathcal{D}$ is not a Λ-PSS for $B(\boldsymbol{x}, \alpha)$. Then, there exists a nonzero $\boldsymbol{v} \in B(\boldsymbol{0}, \alpha)$ such that any decomposition of the form $\boldsymbol{v} = \sum_{i=1}^p c_i\boldsymbol{d}_i$ with $c_i \geq 0$ requires $\sum_{i=1}^p c_i > \Lambda$. Letting $D \in \mathbb{R}^{n\times p}$ have i-th column $\boldsymbol{d}_i$ and $\boldsymbol{e}$ denote the vector of all ones, it follows that the linear system

$$D\boldsymbol{c} = \boldsymbol{v}, \qquad \boldsymbol{c}^T\boldsymbol{e} + b = \Lambda, \qquad \text{and} \qquad \boldsymbol{c} \geq \boldsymbol{0},\ b \geq 0, \qquad (3.5)$$

has no solution. By Farkas' lemma (e.g. [33, Lemma 12.4]), if (3.5) has no solution, there must exist $\boldsymbol{y}_1 \in \mathbb{R}^n$ and $y_2 \in \mathbb{R}$ such that

$$D^T\boldsymbol{y}_1 + y_2\boldsymbol{e} \geq \boldsymbol{0}, \qquad y_2 \geq 0, \qquad \text{and} \qquad \boldsymbol{v}^T\boldsymbol{y}_1 + \Lambda y_2 < 0. \qquad (3.6)$$

Since $\Lambda > 0$, the last two inequalities in (3.6) imply that $\boldsymbol{y}_1 \neq \boldsymbol{0}$. Hence, because $\mathrm{cm}(\mathcal{D}) \geq \kappa$, there is at least one i such that $\boldsymbol{d}_i^T(-\boldsymbol{y}_1) \geq \kappa\|\boldsymbol{y}_1\|\|\boldsymbol{d}_i\|$. Using that the i-th row of $D^T\boldsymbol{y}_1 + y_2\boldsymbol{e}$ is $\boldsymbol{d}_i^T\boldsymbol{y}_1 + y_2$, we obtain that $y_2 \geq \kappa\|\boldsymbol{y}_1\|\|\boldsymbol{d}_i\| \geq \kappa d_{\min}\alpha\|\boldsymbol{y}_1\|$, and thus

$$\boldsymbol{v}^T\boldsymbol{y}_1 < -\Lambda y_2 \leq -\Lambda\kappa d_{\min}\alpha\|\boldsymbol{y}_1\| = -\alpha\|\boldsymbol{y}_1\|. \qquad (3.7)$$

On the other hand, the Cauchy-Schwarz inequality gives $\boldsymbol{v}^T\boldsymbol{y}_1 \geq -\|\boldsymbol{v}\|\,\|\boldsymbol{y}_1\| \geq -\alpha\|\boldsymbol{y}_1\|$, which contradicts (3.7). ☐

Although the notion of Λ-PSS can be identified with requirements on the cosine measure, a key difference is that cosine measure is scale-invariant, whereas the constant Λ depends on the built-in scale α. When directions are scaled to length α, being a Λ-PSS corresponds to having a cosine measure of at least $\kappa = \Lambda^{-1}$ (with Definition 2.3 corresponding to the limit case $\Lambda \to \infty$). The following example illustrates this property.

Example 3.4. Given any $\alpha > 0$, the set $\mathcal{D} = \{\pm\alpha\boldsymbol{e}_1, \ldots, \pm\alpha\boldsymbol{e}_n\}$ is a PSS with $\mathrm{cm}(\mathcal{D}) = \frac{1}{\sqrt{n}}$. Moreover, by Lemma 3.3, for any $\boldsymbol{x} \in \mathbb{R}^n$, $\mathcal{D}$ is a $\sqrt{n}$-PSS for $B(\boldsymbol{x}, \alpha)$.

The interest of considering Λ-PSSs lies in allowing directions with arbitrarily small norm without jeopardizing theoretical guarantees of direct search. In the next section, we will show that complexity guarantees can be derived using Λ-PSSs in lieu of standard PSSs with bounded cosine measure.

4 Complexity of direct search using Λ-PSSs

In this section, we revisit the worst-case complexity of direct search by assuming that polling directions form Λ-PSSs. We first analyze the unconstrained case (Section 4.1), then move to the main focus of this paper, i.e. the polyhedral convex case (Section 4.2).

Algorithm 2 Alternative direct-search method for (2.1).

Inputs: $\boldsymbol{x}_0 \in \Omega$, $\alpha_{\max} > 0$, $\alpha_0 \in (0, \alpha_{\max}]$, $\sigma > 0$, $0 < \gamma_{\text{dec}} < 1 < \gamma_{\text{inc}}$.

for $k = 0, 1, 2, \ldots$ **do**

Compute a finite polling set $\mathcal{D}_k \subset \mathbb{R}^n$.

If there exists $\boldsymbol{d}_k \in \mathcal{D}_k$ such that $\boldsymbol{x}_k + \boldsymbol{d}_k \in \Omega$ and

$$f(\boldsymbol{x}_k + \boldsymbol{d}_k) < f(\boldsymbol{x}_k) - \frac{\sigma}{2}\alpha_k^2, \tag{4.1}$$

set $\boldsymbol{x}_{k+1} := \boldsymbol{x}_k + \boldsymbol{d}_k$ and $\alpha_{k+1} := \min\{\gamma_{\text{inc}}\alpha_k, \alpha_{\max}\}$ ("successful").

Otherwise, set $\boldsymbol{x}_{k+1} := \boldsymbol{x}_k$ and $\alpha_{k+1} := \gamma_{\text{dec}}\alpha_k$ ("unsuccessful").

end for

4.1 Unconstrained case

In order to analyze direct search based on Λ-PSSs, we adapt the basic framework of Algorithm 1 so that polling directions are defined using the current stepsize. The resulting method is given in Algorithm 2, and merely differs from Algorithm 1 in the implicit use of α_k to scale the directions upon computation.

Our analysis will rely on the following key assumption on the polling sets. We again emphasize that the directions in $\mathcal{D}_k$ are scaled according to α_k, unlike in classical direct-search schemes.

Assumption 4.1. At each iteration, the polling set $\mathcal{D}_k$ is a Λ-PSS for $B(\boldsymbol{x}_k, \alpha_k)$, and $\|\boldsymbol{d}\| \le d_{\max}\alpha_k$ for all $\boldsymbol{d} \in \mathcal{D}_k$, where $\Lambda > 0$ and $d_{\max} > 0$.

Under Assumption 4.1, one can relate the stepsize with the gradient norm, akin to classical direct-search theory.

Lemma 4.2. *Suppose that we run Algorithm 2 to solve* (2.1) *with* $\Omega = \mathbb{R}^n$ *under Assumptions 2.1 and 4.1. If* $\|\nabla f(\boldsymbol{x}_k)\| \neq \boldsymbol{0}$ *and* $\alpha_k < \frac{2\|\nabla f(\boldsymbol{x}_k)\|}{(Ld_{\max}^2+\sigma)\Lambda}$*, then iteration* k *is successful.*

Proof. To find a contradiction, suppose iteration k is unsuccessful. By Assumption 2.1, it follows that

$$-\frac{\sigma}{2}\alpha_k^2 \le f(\boldsymbol{x}_k + \boldsymbol{d}) - f(\boldsymbol{x}_k) \le \boldsymbol{d}^T\nabla f(\boldsymbol{x}_k) + \frac{L}{2}\|\boldsymbol{d}\|^2 \le \boldsymbol{d}^T\nabla f(\boldsymbol{x}_k) + \frac{L}{2}d_{\max}^2\alpha_k^2,$$

for all $\boldsymbol{d} \in \mathcal{D}_k$. Since $\alpha_k > 0$, this rearranges to

$$-\frac{Ld_{\max}^2 + \sigma}{2}\,\alpha_k^2 \le \boldsymbol{d}^T\nabla f(\boldsymbol{x}_k), \tag{4.2}$$

for all $\boldsymbol{d} \in \mathcal{D}_k$.

Define now $\boldsymbol{v}_k := -\frac{\alpha_k}{\|\nabla f(\boldsymbol{x}_k)\|}\nabla f(\boldsymbol{x}_k)$ so that $\|\boldsymbol{v}_k\| \le \alpha_k$ and $\alpha_k\|\nabla f(\boldsymbol{x}_k)\| = -\boldsymbol{v}_k^T\nabla f(\boldsymbol{x}_k)$. Since $\mathcal{D}_k = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\}$ is a Λ-PSS for $B(\boldsymbol{x}_k, \alpha_k)$, we may write $\boldsymbol{v}_k = \sum_{i=1}^p c_i\boldsymbol{d}_i$ for some constants $c_i \ge 0$ with $\sum_{i=1}^p c_i \le \Lambda$. Using (4.2), we then obtain

$$\begin{aligned}\|\nabla f(\boldsymbol{x}_k)\| = -\frac{1}{\alpha_k}\boldsymbol{v}_k^T\nabla f(\boldsymbol{x}_k) = -\frac{1}{\alpha_k}\sum_{i=1}^p c_i\boldsymbol{d}_i^T\nabla f(\boldsymbol{x}_k), &\le \frac{Ld_{\max}^2 + \sigma}{2}\,\alpha_k\sum_{i=1}^p c_i, \\ &\le \frac{Ld_{\max}^2 + \sigma}{2}\,\alpha_k\Lambda,\end{aligned}$$

which contradicts our assumption that $\alpha_k < \frac{2\|\nabla f(\boldsymbol{x}_k)\|}{(Ld_{\max}^2+\sigma)\Lambda}$. □

Equipped with Lemma 4.2, we can derive a worst-case complexity bound for Algorithm 2. Although the proof is identical to that of a direct-search method based on PSSs, we provide it below for sake of completeness.

Theorem 4.3. *Suppose that we run Algorithm 2 to solve* (2.1) *with* $\Omega = \mathbb{R}^n$ *under Assumptions 2.1 and 4.1. Then, for any* $\epsilon > 0$, $\|\nabla f(\boldsymbol{x}_k)\| \le \epsilon$ *occurs for the first time after at most*

$$\left(1 + \frac{\log(\gamma_{\text{inc}})}{\log(\gamma_{\text{dec}}^{-1})}\right) \left\lceil \frac{2[f(\boldsymbol{x}_0) - f_{\text{low}}]}{\sigma \alpha_{\min}^2} \right\rceil + \frac{\log(\alpha_0/\alpha_{\min})}{\log(\gamma_{\text{dec}}^{-1})} \tag{4.3}$$

iterations, where

$$\alpha_{\min} := \gamma_{\text{dec}} \frac{2\epsilon}{(Ld_{\max}^2 + \sigma)\Lambda}. \tag{4.4}$$

Proof. Suppose that $\min_{k=0,\dots,K-1} \|\nabla f(\boldsymbol{x}_k)\| > \epsilon$. Lemma 4.2 then implies that any iteration k such that $\alpha_k < \frac{2\epsilon}{(Ld_{\max}^2+\sigma)\Lambda}$ is successful, and results in an increase of α_k. Combining this observation with the update rules on α_k, we find that $\alpha_k \ge \alpha_{\min}$ for every $k = 0, \dots, K-1$, where $\alpha_{\min}$ is given by (4.4).

Let $\mathcal{S} = \{k \le K-1 : \text{iteration } k \text{ is successful}\}$ and $\mathcal{U} = \{k \le K-1 : \text{iteration } k \text{ is unsuccessful}\}$. On one hand, summing (4.1) over $k \in \mathcal{S}$ gives

$$f(\boldsymbol{x}_0) - f_{\text{low}} \ge \sum_{k\in\mathcal{S}} f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \ge \frac{\sigma}{2}\alpha_{\min}^2 |\mathcal{S}|,$$

hence

$$|\mathcal{S}| \le \frac{2[f(\boldsymbol{x}_0) - f_{\text{low}}]}{\sigma \alpha_{\min}^2}. \tag{4.5}$$

On the other hand, the updating rules on α_k give

$$\alpha_{\min} \le \alpha_k \le \alpha_0 \gamma_{\text{inc}}^{|\mathcal{S}|} \gamma_{\text{dec}}^{|\mathcal{U}|},$$

from which we bound the number of unsuccessful iterations as follows:

$$|\mathcal{U}| \le \frac{1}{\log(\gamma_{\text{dec}}^{-1})} \left[\log\left(\frac{\alpha_0}{\alpha_{\min}}\right) + |\mathcal{S}| \log \gamma_{\text{inc}}\right]. \tag{4.6}$$

Putting (4.5) and (4.6) together, we arrive at

$$\begin{aligned} K = |\mathcal{S}| + |\mathcal{U}| &\le \left(1 + \frac{\log(\gamma_{\text{inc}})}{\log(\gamma_{\text{dec}}^{-1})}\right) |\mathcal{S}| + \frac{\log(\alpha_0/\alpha_{\min})}{\log(\gamma_{\text{dec}}^{-1})}, \\ &\le \left(1 + \frac{\log(\gamma_{\text{inc}})}{\log(\gamma_{\text{dec}}^{-1})}\right) \left\lceil \frac{2[f(\boldsymbol{x}_0) - f_{\text{low}}]}{\gamma \alpha_{\min}^2} \right\rceil + \frac{\log(\alpha_0/\alpha_{\min})}{\log(\gamma_{\text{dec}}^{-1})}, \end{aligned}$$

and we get the desired result. □

The complexity bound (4.3) is $\mathcal{O}(\Lambda^2\epsilon^{-2})$, and implies that a $\mathcal{O}(p\Lambda^2\epsilon^{-2})$ bound on objective evaluations holds assuming polling sets have at most p vectors. Using $\kappa \sim \frac{1}{\Lambda}$ from Lemma 3.2, we recover the standard complexity bounds of $\mathcal{O}(\kappa^{-2}\epsilon^{-2})$ iterations and $\mathcal{O}(p\kappa^{-2}\epsilon^{-2})$ evaluations stated in Theorem 2.6.

4.2 Polyhedral convex-constrained case

In this section, we return to the generic case of a constrained set Ω satisfying Assumption 2.2. Note that the analysis below applies to any convex constraint set with nonempty interior, even though the algorithm is only implementable using finite polling sets when Ω is polyhedral.

To establish complexity guarantees for Algorithm 2 in this setting, we introduce the following constrained version of the Λ-PSS property.

Definition 4.4. Consider a point $\boldsymbol{x} \in \Omega$ and radius $\alpha > 0$, and a constant $\Lambda \ge 0$. A polling set $\{\boldsymbol{d}_1, \dots, \boldsymbol{d}_p\} \subset \mathbb{R}^n$ is a Λ-*positive spanning set* (Λ-PSS) for $B(\boldsymbol{x}, \alpha) \cap \Omega$ if $\boldsymbol{x} + \boldsymbol{d}_i \in \Omega$ for all $i = 1, \dots, p$ and, for any $\boldsymbol{v} \in \mathbb{R}^n$ with $\boldsymbol{x} + \boldsymbol{v} \in \Omega$ and $\|\boldsymbol{v}\| \le \alpha$, there exists $\boldsymbol{c}(\boldsymbol{v}) \in \mathbb{R}^p$ with $c_i(\boldsymbol{v}) \ge 0$ such that $\boldsymbol{v} = \sum_{i=1}^p c_i(\boldsymbol{v})\boldsymbol{d}_i$, and $\|\boldsymbol{c}(\boldsymbol{v})\|_1 \le \Lambda$.

Unlike Definition 3.1 above, Definition 4.4 makes explicit use of the point $\boldsymbol{x}$ to guarantee feasibility of all directions, as well as to restrict the Λ-PSS property to feasible vectors $\boldsymbol{v}$ within $B(\mathbf{0}, \alpha)$. We will thus analyze Algorithm 2 under the following assumption.

Assumption 4.5. At each iteration of Algorithm 2, the polling set $\mathcal{D}_k$ is a Λ-PSS for $B(\boldsymbol{x}_k, \alpha_k) \cap \Omega$, and $\|\boldsymbol{d}\| \leq d_{\max}\alpha_k$ for all $\boldsymbol{d} \in \mathcal{D}_k$, where $\Lambda > 0$ and $d_{\max} > 0$.

Under Assumption 4.5, Algorithm 2 produces only feasible iterates and trial points. As a result, our analysis will focus on bounding the number of iterations and evaluations necessary to achieve $\pi(\boldsymbol{x}_k) \leq \epsilon$, as in Section 2.3. We follow the same reasoning than in the unconstrained setting.

Lemma 4.6. *Consider the kth iteration of Algorithm 2 under Assumptions 2.1, 2.2 and 4.5. If* $\pi(\boldsymbol{x}_k) \neq 0$ *and* $\alpha_k < \min\left(\frac{2\pi(\boldsymbol{x}_k)}{(Ld_{\max}^2+\sigma)\Lambda}, 1\right)$, *then iteration k is successful.*

Proof. To find a contradiction, suppose iteration k is unsuccessful. By the same reasoning as in the unconstrained case (Lemma 4.2), it follows that

$$-\frac{Ld_{\max}^2 + \sigma}{2}\,\alpha_k^2 \leq \boldsymbol{d}^T \nabla f(\boldsymbol{x}_k), \tag{4.7}$$

for all $\boldsymbol{d} \in \mathcal{D}_k$.

Defining $\boldsymbol{v}_k := \boldsymbol{v}^*(\boldsymbol{x}_k)$ as in (2.7), we have $\pi(\boldsymbol{x}_k) = -\nabla f(\boldsymbol{x}_k)^T \boldsymbol{v}_k$ with $\boldsymbol{x}_k + \boldsymbol{v}_k \in \Omega$ and $\|\boldsymbol{v}_k\| \leq 1$. Moreover, since $\pi(\boldsymbol{x}_k) \neq 0$ by assumption, we also have $\boldsymbol{v}_k \neq \mathbf{0}$.

Let $\hat{\boldsymbol{v}}_k := \alpha_k \boldsymbol{v}_k$, so $\|\hat{\boldsymbol{v}}_k\| \leq \alpha_k$ and $\boldsymbol{x}_k + \hat{\boldsymbol{v}}_k \in \Omega$ by convexity of Ω (recall that $\alpha_k < 1$). From Assumption 4.5, we may write $\hat{\boldsymbol{v}}_k = \sum_{i=1}^p c_i \boldsymbol{d}_i$ for constants $c_i \geq 0$ with $\sum_{i=1}^p c_i \leq \Lambda$. Using (4.7), we get

$$\pi(\boldsymbol{x}_k) = -\boldsymbol{v}_k^T \nabla f(\boldsymbol{x}_k) = -\frac{1}{\alpha_k}\hat{\boldsymbol{v}}_k^T \nabla f(\boldsymbol{x}_k) = \frac{1}{\alpha_k}\sum_{i=1}^p c_i \boldsymbol{d}_i^T \nabla f(\boldsymbol{x}_k) \leq \frac{Ld_{\max}^2 + \sigma}{2}\,\alpha_k \Lambda,$$

which contradicts $\alpha_k < \frac{2\pi(\boldsymbol{x}_k)}{(Ld_{\max}^2+\sigma)\Lambda}$. ☐

Theorem 4.7. *Suppose that we run Algorithm 2 to solve* (2.1) *under Assumptions 2.1, 2.2 and 4.5. Then, for any* $\epsilon > 0$, $\pi(\boldsymbol{x}_k) \leq \epsilon$ *occurs for the first time after at most*

$$\left(1 + \frac{\log(\gamma_{\text{inc}})}{\log(\gamma_{\text{dec}}^{-1})}\right)\left\lceil \frac{2[f(\boldsymbol{x}_0) - f_{\text{low}}]}{\gamma \hat{\alpha}_{\min}^2} \right\rceil + \frac{\log(\alpha_0/\hat{\alpha}_{\min})}{\log(\gamma_{\text{dec}}^{-1})} \tag{4.8}$$

iterations, where

$$\hat{\alpha}_{\min} := \gamma_{\text{dec}} \min\left(\frac{2\epsilon}{(Ld_{\max}^2 + \sigma)\Lambda}, 1\right). \tag{4.9}$$

Proof. Suppose that $\min_{k=0,\ldots,K-1} \pi(\boldsymbol{x}_k) > \epsilon$. From Lemma 4.6, we know that any iteration k such that $\alpha_k < \min(\frac{2\epsilon}{(Ld_{\max}^2+\sigma)\Lambda}, 1)$ is successful, and leads to an increase in α_k. Hence for all iterations $k = 0, \ldots, K-1$, we must have $\alpha_k \geq \hat{\alpha}_{\min}$ with $\hat{\alpha}_{\min}$ defined in (4.9).

The remainder of the proof is identical to that of Theorem 4.3. ☐

As in the unconstrained case, the complexity bound (4.8) simplifies to $\mathcal{O}(\Lambda^2\epsilon^{-2})$ iterations for small ϵ, and yields a bound of $\mathcal{O}(p\Lambda^2\epsilon^{-2})$ objective evaluations when the polling sets have p vectors. The dependency on ϵ is the same than other DFO and derivative-based methods applied to convex-constrained problems [7, 21]. In the next section, we investigate the dependency on n through Λ and p by explicit construction of Λ-PSS.

5 Constructing a Λ-PSS with explicit linear constraints

We now describe the generation of Λ-PSSs when the constraint set Ω is given by (2.2) and satisfies Assumption 2.2. We first consider the case of bound constraints, then extend our approach to the general case.

5.1 Bound Constraints

Suppose first that the feasible set is given by

$$\Omega = \{\boldsymbol{x} \in \mathbb{R}^n : \boldsymbol{x}^L \leq \boldsymbol{x} \leq \boldsymbol{x}^U\}, \tag{5.1}$$

where $x_i^L < x_i^U$, $i = 1, \ldots, n$. In this setting , given a (feasible) point $\boldsymbol{x}$ and a stepsize $\alpha > 0$, the approximate tangent cone is generated by positive and negative coordinate directions $\pm \boldsymbol{e}_i$ such that $\boldsymbol{x} \pm \alpha \boldsymbol{e}_i \in \Omega$, while the approximate normal cone is generated by the remaining positive and negative coordinate directions. Using these vectors as $\mathcal{D}$ guarantees that $\mathrm{cm}_{T_\Omega(\boldsymbol{x},\alpha)}(\mathcal{D}) \geq \frac{1}{\sqrt{n}}$ [20].

To define a Λ-PSS for the same pair ($\boldsymbol{x}$,α), we scale all positive and negative directions to ensure feasibility, i.e. we consider

$$\mathcal{D} = \cup_{i=1}^n \{-\alpha_{-i}\boldsymbol{e}_i, \alpha_i \boldsymbol{e}_i\}, \tag{5.2}$$

where the scalings $\alpha_{\pm i}$ are given by

$$\alpha_{-i} := \min(\alpha, x_i - x_i^L) \qquad \text{and} \qquad \alpha_i := \min(\alpha, x_i^U - x_i). \tag{5.3}$$

Note that all the scaling values (5.3) lie in $[0, \alpha]$ since $\boldsymbol{x} \in \Omega$. Importantly, the value $\alpha_{\pm i} = 0$ is allowed, and amounts to discarding the corresponding direction (note that $\alpha_i + \alpha_{-i} > 0$ since $x_i^L < x_i^U$). The next result quantifies the quality of the set (5.2).

Theorem 5.1. *Let Ω be given by* (5.1)*. Given any $\boldsymbol{x} \in \Omega$ and $\alpha > 0$, the set defined by* (5.2) *is a Λ-PSS for $B(\boldsymbol{x}, \alpha) \cap \Omega$ with*

$$\Lambda \;=\; \min\left[n, \frac{\sqrt{n}\alpha}{\min\left\{\alpha, \min_{x_i \neq x_i^L} x_i - x_i^L, \min_{x_i \neq x_i^U} x_i^U - x_i\right\}}\right]. \tag{5.4}$$

Proof. The definition of $\alpha_{\pm i}$ in (5.3) ensures that $\boldsymbol{x} + \boldsymbol{d} \in \Omega$ for any $\boldsymbol{d} \in \mathcal{D}$.

Consider now any vector $\boldsymbol{v} \in \mathbb{R}^n$ such that $\boldsymbol{x} + \boldsymbol{v} \in \Omega$ and $\|\boldsymbol{v}\| \leq \alpha$. We have $\boldsymbol{v} = \sum_{i=1}^n v_i^+ \boldsymbol{e}_i + v_i^-(-\boldsymbol{e}_i)$ where $v_i^+ = \max(\boldsymbol{v}_i, 0)$ and $v_i^- = \max(-v_i, 0)$ are the positive and negative parts of $\boldsymbol{v}_i$, respectively. We can then write $\boldsymbol{v}$ in terms of the polling directions (5.2) as

$$\boldsymbol{v} = \sum_{i=1}^n c_i(\alpha_i \boldsymbol{e}_i) + c_{-i}(-\alpha_{-i}\boldsymbol{e}_i), \tag{5.5}$$

where $c_i = v_i^+/\alpha_i$ when $\alpha_i > 0$ and $c_i = 0$ otherwise, and $c_{-i} = v_i^-/\alpha_{-i}$ when $\alpha_{-i} > 0$ and $c_{-i} = 0$ otherwise. To obtain the desired result, we will bound each $c_i + c_{-i}$ separately, noting that the bound can be refined if $v_i = 0$ for any i, given that this implies $c_i = c_{-i} = 0$.

Suppose first that $\alpha_i > 0$ and $\alpha_{-i} = 0$. In that case, we have $v_i^+ = v_i = |v_i|$ and

$$c_i + c_{-i} = c_i = \frac{v_i^+}{\alpha_i} = \frac{|v_i|}{\min(\alpha, x_i^U - x_i)} \tag{5.6}$$

where $\alpha_i > 0$ guarantees that $x_i < x_i^U$. From $\|v\| \leq \alpha$, we get that $|v_i| \leq \alpha$, while $\boldsymbol{x} + \boldsymbol{v} \in \Omega$ ensures that $|v_i| = v_i^+ \leq x_i^U - x_i$. It follows that $c_i \leq 1$.

Suppose now that $\alpha_i = 0$ and $\alpha_{-i} > 0$. The same argument than above leads to

$$c_i + c_{-i} = c_{-i} = \frac{v_i^-}{\alpha_{-i}} = \frac{|v_i|}{\min(\alpha, x_i - x_i^L)}, \tag{5.7}$$

where again the properties of $\boldsymbol{v}$ guarantee that $c_{-i} \leq 1$.

Finally, suppose that $\alpha_i > 0$ and $\alpha_{-i} > 0$. In that case,

$$c_i + c_{-i} = \frac{v_i^+}{\alpha_i} + \frac{v_i^-}{\alpha_{-i}} = \frac{v_i^+}{\min(\alpha, x_i^U - x_i)} + \frac{v_i^-}{\min(\alpha, x_i - x_i^L)} \leq \frac{|v_i|}{\min(\alpha, x_i - x_i^L, x_i^U - x_i)} \leq 1. \tag{5.8}$$

Combining (5.6), (5.7) and (5.8), we arrive at

$$c_i + c_{-i} \leq \frac{|v_i|}{\min(\alpha, \delta_i)}, \qquad \delta_i := \begin{cases} x_i - x_i^L & \text{if } x_i = x_i^U \\ x_i^U - x_i & \text{if } x_i = x_i^L \\ \min(x_i - x_i^L, x_i^U - x_i) & \text{otherwise,} \end{cases} \tag{5.9}$$

and the right-hand side of (5.9) is smaller than 1. Summing (5.9) over all indices i and using that $\|\boldsymbol{v}\|_1 \leq \sqrt{n}\|\boldsymbol{v}\| \leq \sqrt{n}\alpha$, we obtain

$$\sum_{i=1}^{n}(c_i + c_{-i}) \leq \sum_{i=1}^{n} \frac{|v_i|}{\min(\alpha, \delta_i)} \leq \frac{1}{\min(\alpha, \min_i \delta_i)}\|\boldsymbol{v}\|_1 \leq \frac{\sqrt{n}\alpha}{\min(\alpha, \min_i \delta_i)}. \tag{5.10}$$

Finally, using that $c_i + c_{-i} \leq 1$ for every i ensures that $\sum_{i=1}^{n}(c_i + c_{-i}) \leq n$, which together with (5.10) gives (5.4). □

The formula (5.4) reduces $\Lambda = \sqrt{n}$ when no constraints are approximately active for $(\boldsymbol{x}, \alpha)$ (or when the problem is unconstrained), which matches the cosine measure of tangent cone generators in both the unconstrained and bound-constrained setting, where $\kappa = \frac{1}{\sqrt{n}}$ [20]. In the general setting, however, we have $\sqrt{n} \leq \Lambda \leq n$, and the upper bound is attained when n linearly independent bound constraints are approximately active, which can occur near an extreme point. This increase in Λ seems unavoidable when using directions beyond tangent cone generators, but affects our complexity guarantees. Still, our polling set choice provides a richer description of the feasible region, and can lead to faster convergence, as illustrated by Example 5.2 and our numerical results in Section 6.

Example 5.2. Suppose we have the simple 1D minimization problem

$$\min_{x \in \mathbb{R}} -x, \quad \text{s.t.} \quad x \leq 1.1, \tag{5.11}$$

with solution $x^* = 1.1$, and consider running Algorithm 2 with either $\mathcal{D}_k$ taken as generators of the approximate tangent cone (per [20]), or as (5.2). For demonstration purposes, we take $x_0 = 0$, $\alpha_0 = 1$, the standard values $\gamma_{\text{dec}} = 0.5$ and $\gamma_{\text{inc}} = 2$, and assume $\gamma < 1$ so that all positive steps are successful in the analysis below.

Using just the approximate tangent cone, our initial polling set is $\mathcal{D}_0 = \{-1, 1\}$, which gives the successful step $x_1 = x_0 + 1 = 1$ and $\alpha_1 = 2$. Then, $\mathcal{D}_1 = \{-2\}$ and so the second iteration is unsuccessful. We continue having unsuccessful iterations until $\alpha_k \leq x^* - x_k$, and so $\mathcal{D}_k = \{-\alpha_k, \alpha_k\}$ and we get $x_{k+1} = x_k + \alpha_k$. Since α_k can only take integer powers of 2 (by choice of γ_{dec}, γ_{inc}), this first happens for $\alpha_6 = 2^{-4}$ with $x_7 = 1 + 2^{-4} = 1.0625$. After this, the next successful iteration comes from $\alpha_9 = 2^{-5}$ giving $x_{10} = 1 + 2^{-4} + 2^{-5} = 1.09375$. Continuing this way, our iterates x_k correspond to (truncated) binary fractions that under-approximate x^*. Since x^* has an infinite binary expansion, we converge linearly, but never actually reach x^* in finite time.

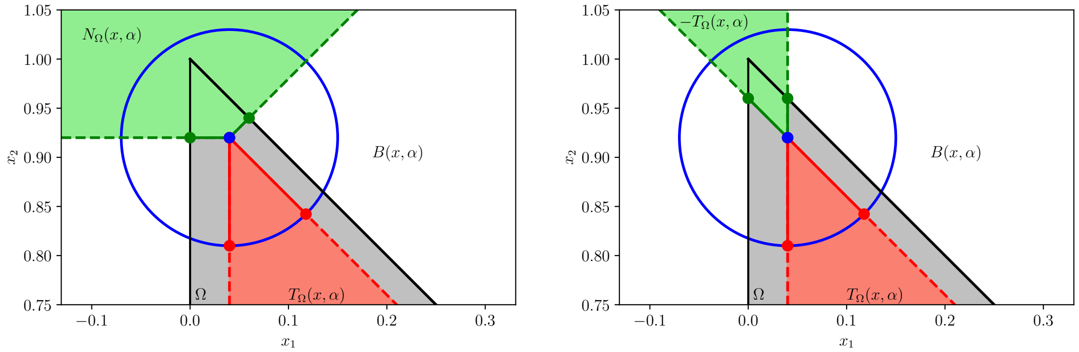
However, if we instead use (5.2), we get the same first iteration with $x_1 = 1$ and $\alpha_1 = 2$. Then, we have $\mathcal{D}_1 = \{-2, 0.1\}$ so that $x_2 = x_1 + 0.1 = x^*$ and we converge to the solution.

5.2 Independent Linear Inequality Constraints

We now come back to general polyhedral sets of the form (2.2) satisfying Assumption 2.2. Existing theory summarized in Section 2.3 shows that a polling set is of sufficient quality for a pair $(\boldsymbol{x}, \alpha) \in \Omega \times \mathbb{R}_{>0}$ provided it contains a set of generators for the approximate tangent cone $T_\Omega(\boldsymbol{x}, \alpha)$. The polar decomposition [32]

$$\boldsymbol{v} = \operatorname*{proj}_{T_\Omega(\boldsymbol{x},\alpha)}(\boldsymbol{v}) + \operatorname*{proj}_{N_\Omega(\boldsymbol{x},\alpha)}(\boldsymbol{v}), \qquad \forall \boldsymbol{v} \in \mathbb{R}^n,$$

suggests that generators from the approximate normal cone $N_\Omega(\boldsymbol{x}, \alpha)$ could provide additional directions when scaled appropriately. This strategy was found beneficial in direct-search implementations [27], even though it produces polling sets for which Assumption 2.7 does not hold (and thus theoretical guarantees are lost).



(a) Scaled generators of $N_\Omega(\boldsymbol{x},\alpha)$ *(b) Scaled generators of $-T_\Omega(\boldsymbol{x},\alpha)$*

Figure 1. Illustration of Example 5.3. A polling set is built by combining generators of $T_\Omega(\boldsymbol{x},\alpha)$ with scaled generators of $N_\Omega(\boldsymbol{x},\alpha)$ or $-T_\Omega(bx,\alpha)$.

One may naturally wonder whether the sets used in practice form Λ-PSSs. As shown by the example below, this is true but the constant Λ can be arbitrarily large, while we provide another Λ-PSS construction with bounded Λ.

Example 5.3. Consider $\Omega = \{\boldsymbol{x} \in \mathbb{R}^2 \mid x_1 \geq 0, x_1 + x_2 \leq 1\}$, and let $\boldsymbol{x} = [\epsilon_1, 1-\epsilon_2]^T$ with $\epsilon_1 < \epsilon_2 \ll 1$. Given a large enough $\alpha > 0$ such that the vertex $[0,1]^T \in B(\boldsymbol{x},\alpha)$, both constraints are nearly active at $\boldsymbol{x}$. Thus, the generators of $T_\Omega(\boldsymbol{x},\alpha)$ are $[0,-1]^T$ and $[1,-1]^T$, while the generators of $N_\Omega(\boldsymbol{x},\alpha)$ are $[-1,0]^T$ and $[1,1]^T$. Figure 1a shows a polling set built using those generators, namely

$$\mathcal{D} = \underbrace{\left\{\begin{bmatrix}0\\-\alpha\end{bmatrix}, \begin{bmatrix}\alpha/\sqrt{2}\\-\alpha/\sqrt{2}\end{bmatrix}\right\}}_{T_\Omega(\boldsymbol{x},\alpha)} \cup \underbrace{\left\{\begin{bmatrix}-\epsilon_1\\0\end{bmatrix}, \begin{bmatrix}(\epsilon_2-\epsilon_1)/2\\(\epsilon_2-\epsilon_1)/2\end{bmatrix}\right\}}_{N_\Omega(\boldsymbol{x},\alpha)}. \tag{5.12}$$

Those vectors form a Λ-PSS in the sense of Definition 4.4. However, to represent the vector $\boldsymbol{v} = [-\epsilon_1, \epsilon_2]^T$ (i.e. $\boldsymbol{x}+\boldsymbol{v} = [1,1]^T$) as a positive linear combination of these generators, we must write

$$\boldsymbol{v} = \frac{\epsilon_1+\epsilon_2}{\epsilon_1}\begin{bmatrix}-\epsilon_1\\0\end{bmatrix} + \frac{2\epsilon_2}{\epsilon_2-\epsilon_1}\begin{bmatrix}(\epsilon_2-\epsilon_1)/2\\(\epsilon_2-\epsilon_1)/2\end{bmatrix}. \tag{5.13}$$

The positive linear combination coefficients in (5.13) grow arbitrarily large by taking ϵ_1 and ϵ_2 small enough (i.e. making $\boldsymbol{x}$ arbitrarily close to $[01]^T$). As a result, the value of Λ can be made arbitrarily large.

Figure 1b shows another polling set obtained by replacing the generators of $N_\Omega(\boldsymbol{x},\alpha)$ by that of $-T_\Omega(\boldsymbol{x},\alpha)$, with proper scaling to ensure feasibility. Mathematically, this set is

$$\mathcal{D}' = \underbrace{\left\{\begin{bmatrix}0\\-\alpha\end{bmatrix}, \begin{bmatrix}\alpha/\sqrt{2}\\-\alpha/\sqrt{2}\end{bmatrix}\right\}}_{T_\Omega(\boldsymbol{x},\alpha)} \cup \underbrace{\left\{\begin{bmatrix}0\\\epsilon_2-\epsilon_1\end{bmatrix}, \begin{bmatrix}-\epsilon_1\\\epsilon_1\end{bmatrix}\right\}}_{-T_\Omega(\boldsymbol{x},\alpha)}.$$

Now, for the same $\boldsymbol{v}$ than in (5.13), the positive linear combination with columns of $\mathcal{D}'$ is

$$\boldsymbol{v} = \begin{bmatrix}0\\\epsilon_2-\epsilon_1\end{bmatrix} + \begin{bmatrix}-\epsilon_1\\\epsilon_1\end{bmatrix}, \tag{5.14}$$

whose coefficients are uniformly bounded for all values of ϵ_1 and ϵ_2.

Motivated by Example 5.3, we propose to construct our polling set by taking the generators of $T_\Omega(\boldsymbol{x},\alpha)$ and their negatives, scaled to ensure feasibility. If the generators of $T_\Omega(\boldsymbol{x},\alpha)$ do not (linearly) span $\mathbb{R}^n$, then we will also need to include vectors that positively span the corresponding null space. We will prove that this construction yields a Λ-PSS (i.e. satisfies Assumption 4.5) in the case where $\{\boldsymbol{a}_i : i \in I(\boldsymbol{x}, \alpha)\}$ are linearly independent.

First, we state some characterizations of polar cones.

Lemma 5.4. *Let* $A = [\boldsymbol{a}_1 \ \cdots \ \boldsymbol{a}_q] \in \mathbb{R}^{n\times q}$ *and consider the cones*

$$K_1 := \{\boldsymbol{y} \in \mathbb{R}^n : \boldsymbol{a}_j^T \boldsymbol{y} \le 0, \ \forall j = 1, \ldots, q\}, \quad \text{and} \quad K_2 := \operatorname{cone}(\{\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q\}).$$

Then, the following properties hold:

(a) $K_1^\circ = K_2$ *and* $K_2^\circ = K_1$.

(b) If $q \le n$ *and* $\operatorname{rank}(A) = q$, *then*

$$K_1^\circ = \{\boldsymbol{y} \in \mathbb{R}^n : -A^\dagger \boldsymbol{y} \le \boldsymbol{0} \ \text{and} \ (I - AA^\dagger)\boldsymbol{y} = \boldsymbol{0}\},$$

where $A^\dagger = (A^T A)^{-1} A^T$.

(c) Given $B \in \mathbb{R}^{l\times n}$, *the polar of*

$$K_B := \{\boldsymbol{y} \in \mathbb{R}^n : \boldsymbol{a}_j^T \boldsymbol{y} \le 0, \ \forall j = 1, \ldots, p\} \cap \operatorname{nul}(B^T),$$

is given by

$$K_B^\circ = \{\boldsymbol{y} \in \mathbb{R}^n : \boldsymbol{y} = A\boldsymbol{\lambda} + B\boldsymbol{r}, \ \forall \boldsymbol{\lambda} \ge \boldsymbol{0} \ \text{and} \ \boldsymbol{r} \in \mathbb{R}^l\}.$$

Proof. Part (a) is [38, Eq. (2.8.3)–(2.8.4)]. Part (b) is [11, Theorem 4.2]. Part (c) is [11, Eq. (6)]. □

We will use Lemma 5.4 to characterize Λ-PSSs associated with $\boldsymbol{x} \in \Omega$ and $\alpha > 0$ under the following linear independence assumption.

Assumption 5.5. The set of nearly-active constraints $I(\boldsymbol{x}, \alpha)$ (2.8) has at most n vectors, and the vectors $\{\boldsymbol{a}_i : i \in I(\boldsymbol{x}, \alpha)\}$ are linearly independent.

Note that Assumption 5.5 holds whenever all $\boldsymbol{a}_i$s are linearly independent (in which case $m \le n$). Without loss of generality, and for simplicity, we assume that $I(\boldsymbol{x}, \alpha) = \{1, \ldots, q\}$ in the rest of this section.

Lemma 5.6. *Suppose* $\boldsymbol{x} \in \Omega$, $\alpha > 0$ *and Assumption 5.5 holds. Then a set of generators for* $T_{\Omega(\boldsymbol{x},\alpha)}$ *is the set of* $2n - q$ *vectors*

$$\{-(A^\dagger)^T \boldsymbol{e}_i : i = 1, \ldots, q\} \cup \{\pm \boldsymbol{u}_{q+1}, \ldots, \pm \boldsymbol{u}_n\},$$

where $A = [\boldsymbol{a}_1 \cdots \boldsymbol{a}_q] \in \mathbb{R}^{n\times q}$ *and* $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n \in \mathbb{R}^n$ *are the (orthonormal) left singular vectors of* A.

Proof. By definition of $N_\Omega(\boldsymbol{x}, \alpha)$ (2.9) and Lemma 5.4(a), we may write

$$T(\boldsymbol{x}, \alpha) = N(\boldsymbol{x}, \alpha)^\circ = \{\boldsymbol{y} \in \mathbb{R}^n : \boldsymbol{a}_i^T \boldsymbol{y} \le 0, \ i = 1, \ldots, q\},$$

recalling that we are assuming $I(\boldsymbol{x}, \alpha) = \{1, \ldots, q\}$s. Hence by Lemma 5.4(b),

$$N(\boldsymbol{x}, \alpha) = T(\boldsymbol{x}, \alpha)^\circ = \{\boldsymbol{y} \in \mathbb{R}^n : -A^\dagger \boldsymbol{y} \le \boldsymbol{0} \ \text{and} \ (I - AA^\dagger)\boldsymbol{y} = \boldsymbol{0}\}.$$

So, applying Lemma 5.4(c), a generating set for $T(\boldsymbol{x}, \alpha) = N(\boldsymbol{x}, \alpha)^\circ$ is the set of columns of $-(A^\dagger)^T$ together with any vectors that positively span $\operatorname{col}(I - AA^\dagger)$.

It remains to show that $\{\pm \boldsymbol{u}_{q+1}, \ldots, \pm \boldsymbol{u}_n\}$ positively spans $\operatorname{col}(I - AA^\dagger)$. Since $AA^\dagger$ is the orthogonal projector onto $\operatorname{col}(A)$, the matrix $I - AA^\dagger$ is the orthogonal projector onto $\operatorname{col}(A)^\perp$. Since $\operatorname{rank}(A) = q$ by Assumption 5.5, the left singular vectors $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_q\}$ form an orthonormal basis for $\operatorname{col}(A)$, and $\{\boldsymbol{u}_{q+1}, \ldots, \boldsymbol{u}_n\}$ is an orthonormal basis for $\operatorname{col}(A)^\perp$. Thus $\{\pm \boldsymbol{u}_{q+1}, \ldots, \pm \boldsymbol{u}_n\}$ positively span $\operatorname{col}(A)^\perp$, as claimed. □

Given Lemma 5.6, we consider the set of polling directions

$$\mathcal{D} = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_q\} \cup \{-\alpha_1 \boldsymbol{d}_1, \ldots, -\alpha_q \boldsymbol{d}_q\} \cup \{\pm\alpha \boldsymbol{u}_{q+1}, \ldots, \pm\alpha \boldsymbol{u}_n\}, \tag{5.15}$$

where $\boldsymbol{d}_i := \frac{\alpha}{\|\hat{\boldsymbol{d}}_i\|}\hat{\boldsymbol{d}}_i$ for $\hat{\boldsymbol{d}}_i := -(A^\dagger)^T \boldsymbol{e}_i$, the constants α_i are the largest value in $[0,1]$ so that $\boldsymbol{x} - \alpha_i \boldsymbol{d}_i \in \Omega$, and $\boldsymbol{u}_{q+1}, \ldots, \boldsymbol{u}_n$ are the last $n-q$ left singular vectors of A. Note that $\hat{\boldsymbol{d}}_i \neq \boldsymbol{0}$ since $\operatorname{rank}((A^\dagger)^T) = \operatorname{rank}(A) = q$.

We first confirm that our polling set (5.15) only comprises feasible points, and derive an explicit expression for the scaling factor α_i for the directions $-\boldsymbol{d}_i$.

Lemma 5.7. *Let Assumption 5.5 hold for $\boldsymbol{x} \in \Omega$ and $\alpha > 0$, and consider the polling set $\mathcal{D}$ defined by* (5.15)*. Then $\boldsymbol{x} + \boldsymbol{d} \in \Omega$ for $\boldsymbol{d} \in \mathcal{D}$, and*

$$\alpha_i = \min\left(\frac{\|\hat{\boldsymbol{d}}_i\| s_i}{\alpha}, 1\right), \tag{5.16}$$

for all $i = 1, \ldots, q$, where $s_i := b_i - \boldsymbol{a}_i^T \boldsymbol{x} \geq 0$ is the slack in the i-th constraint at $\boldsymbol{x}$.

Proof. We first note that $\|\boldsymbol{d}\| \leq \alpha$ for all $\boldsymbol{d} \in \mathcal{D}$ by construction. So, since $\boldsymbol{x} \in \Omega$, all points $\boldsymbol{x} + \boldsymbol{d}$ are feasible with respect to any constraints not in $I(\boldsymbol{x}, \alpha)$ (which is defined to be the set of constraints whose boundaries intersect $B(\boldsymbol{x}, \alpha)$). Hence we only need to consider feasibility with respect to the constraints $\boldsymbol{a}_j^T \boldsymbol{x} \leq b_j$ for $j = 1, \ldots, q$.

For all $i, j = 1, \ldots, q$, we observe

$$\boldsymbol{d}_i^T \boldsymbol{a}_j = -\frac{\alpha}{\|\hat{\boldsymbol{d}}_i\|}((A^\dagger)^T \boldsymbol{e}_i)^T \boldsymbol{a}_j = -\frac{\alpha}{\|\hat{\boldsymbol{d}}_i\|}\boldsymbol{e}_i^T A^\dagger A \boldsymbol{e}_j = \begin{cases} -\frac{\alpha}{\|\hat{\boldsymbol{d}}_i\|}, & i = j, \\ 0, & i \neq j, \end{cases} \tag{5.17}$$

where the last equality follows from $A^\dagger A = I$ (since A has full column rank, Assumption 5.5). Thus, for all $i, j = 1, \ldots, q$ we have $\boldsymbol{d}_i^T \boldsymbol{a}_j \leq 0$ and so

$$\boldsymbol{a}_j^T(\boldsymbol{x} + \boldsymbol{d}_i) \leq \boldsymbol{a}_j^T \boldsymbol{x} \leq b_j,$$

where the last inequality follows from $\boldsymbol{x} \in \Omega$. Hence $\boldsymbol{x} + \boldsymbol{d}_i \in \Omega$ for all $i = 1, \ldots, q$.

By construction of α_i, we automatically have $\boldsymbol{x} - \alpha_i \boldsymbol{d}_i \in \Omega$ for all $i = 1, \ldots, q$. In particular, this means that $\boldsymbol{a}_j^T(\boldsymbol{x} - \alpha_i \boldsymbol{d}_i) \leq b_j$, or

$$s_j = b_j - \boldsymbol{a}_j^T \boldsymbol{x} \geq -\alpha_i \boldsymbol{a}_j^T \boldsymbol{d}_i = \begin{cases} \frac{\alpha_i \alpha}{\|\hat{\boldsymbol{d}}_i\|}, & i = j, \\ 0, & i \neq j, \end{cases}$$

from (5.17). Hence, only the i-th constraint affects the feasibility of $\boldsymbol{x} - \alpha_i \boldsymbol{d}_i$, which gives us (5.16) (noting that $\alpha_i \leq 1$ by construction).

Lastly, since $\operatorname{col}(A) = \operatorname{span}(\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_q\})$ and $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n\}$ is an orthonormal set, each of the vectors $\boldsymbol{u}_{q+1}, \ldots, \boldsymbol{u}_n$ are orthogonal to all of $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q$, and so

$$\boldsymbol{a}_j^T(\boldsymbol{x} \pm \alpha \boldsymbol{u}_i) = \boldsymbol{a}_j^T \boldsymbol{x} \leq b_j,$$

for all $j = 1, \ldots, q$ and all $i = q+1, \ldots, n$. Hence $\boldsymbol{x} \pm \alpha \boldsymbol{u}_i \in \Omega$ for all $i = q+1, \ldots, n$. ☐

We now show that our polling set forms a Λ-PSS for $B(\boldsymbol{x}, \alpha) \cap \Omega$. Since $\|\boldsymbol{d}\| \leq \alpha$ for all $\boldsymbol{d} \in \mathcal{D}$, this implies that $\mathcal{D}$ satisfies Assumption 2.7 with $d_{\max} = 1$.

Theorem 5.8. *Let Assumption 5.5 hold for $\boldsymbol{x} \in \Omega$ and $\alpha > 0$, and consider the polling set $\mathcal{D}$ defined by* (5.15)*. Then $\mathcal{D}$ is a Λ-PSS for $B(\boldsymbol{x}, \alpha) \cap \Omega$ with*

$$\Lambda \; = \; q\kappa(A) + \sqrt{n-q}. \tag{5.18}$$

Proof. Notice first that Lemma 5.7 ensures $\boldsymbol{x}+\boldsymbol{d}\in\Omega$ for all $\boldsymbol{d}\in\mathcal{D}$.

Now, fix $\boldsymbol{v}\in\mathbb{R}^n$ with $\boldsymbol{x}+\boldsymbol{v}\in\Omega$ and $\|\boldsymbol{v}\|\le\alpha$. We write the orthogonal decomposition $\boldsymbol{v}=\boldsymbol{v}_1+\boldsymbol{v}_2$ where $\boldsymbol{v}_1=\operatorname{proj}_{\operatorname{col}(A)}(\boldsymbol{v})$ and $\boldsymbol{v}_2=\operatorname{proj}_{\operatorname{col}(A)^\perp}(\boldsymbol{v})$. Defining the slack variables s_j as in Lemma 5.7), it follows that $\boldsymbol{a}_j^T\boldsymbol{v}=\boldsymbol{a}_j^T\boldsymbol{v}_1\le s_j$ for all $j=1,\ldots,q$. Moreover, since $\|\boldsymbol{v}_1\|^2+\|\boldsymbol{v}_2\|^2=\|\boldsymbol{v}\|^2\le\alpha^2$, we have $\max\{\|\boldsymbol{v}_1\|,\|\boldsymbol{v}_2\|\}\le\alpha$.

We begin by consider $\boldsymbol{v}_2$. The definition of $\operatorname{col}(A)^\perp=\operatorname{span}(\{\boldsymbol{u}_{q+1},\ldots,\boldsymbol{u}_n\})$ gives

$$\boldsymbol{v}_2=\sum_{i=q+1}^{n}(\boldsymbol{v}_2^T\boldsymbol{u}_i)\boldsymbol{u}_i=\sum_{i=q+1}^{n}\frac{\boldsymbol{v}_2^T\boldsymbol{u}_i}{\alpha}\,\alpha\boldsymbol{u}_i=\sum_{i=q+1}^{n}\frac{|\boldsymbol{v}_2^T\boldsymbol{u}_i|}{\alpha}\,(\pm\alpha\boldsymbol{u}_i).$$

Since $|\boldsymbol{v}_2^T\boldsymbol{u}_i|\le\|\boldsymbol{v}_2\|\,\|\boldsymbol{u}_i\|\le\alpha$, we can therefore write

$$\boldsymbol{v}_2=\sum_{i=q+1}^{n}c_i(\alpha\boldsymbol{u}_i)+c_{-i}(-\alpha\boldsymbol{u}_i),$$

where $c_i=$ and c_{-i} are defined so the proof of Theorem 5.1. Since the vectors $\pm\boldsymbol{u}_i$ are feasible for α, applying the reasoning of Theorem 5.1 guarantees that

$$\sum_{i=q+1}^{n}(c_i+c_{-i})\le\sqrt{n-q}. \tag{5.19}$$

Consider now the vector $\boldsymbol{v}_1\in\operatorname{col}(A)=\operatorname{col}((A^\dagger)^T)$. Since the linear system $-(A^\dagger)^T\hat{\boldsymbol{c}}=\boldsymbol{v}_1$ is consistent, the vector $\hat{\boldsymbol{c}}=(-(A^\dagger)^T)^\dagger\boldsymbol{v}_1=-A^T\boldsymbol{v}_1\in\mathbb{R}^q$ is its minimal norm solution. It follows that

$$\boldsymbol{v}_1=\sum_{i=1}^{q}\hat{c}_i\hat{\boldsymbol{d}}_i=\sum_{i=1}^{q}c_i\boldsymbol{d}_i,\qquad\text{where}\quad c_i:=\frac{\hat{c}_i\|\hat{\boldsymbol{d}}_i\|}{\alpha}, \tag{5.20}$$

with $\hat{c}_i,c_i\in\mathbb{R}$, possibly negative. Since $\hat{c}_i=[A^T\boldsymbol{v}_1]_i$ and $\hat{\boldsymbol{d}}_i=-(A^\dagger)^T\boldsymbol{e}_i$, we have

$$|c_i|\le\frac{\|A^T\boldsymbol{v}_1\|_\infty\|(A^\dagger)^T\|}{\alpha}\le\frac{\|A^T\boldsymbol{v}_1\|\|(A^\dagger)^T\|}{\alpha}\le\kappa(A), \tag{5.21}$$

where the last inequality uses $\|\boldsymbol{v}_1\|\le\alpha$.

From above, we know that each of $\boldsymbol{u}_{q+1},\ldots,\boldsymbol{u}_n$ are orthogonal to all of $\boldsymbol{a}_1,\ldots,\boldsymbol{a}_q$, and so $\boldsymbol{v}_2$ is orthogonal to all of $\boldsymbol{a}_1,\ldots,\boldsymbol{a}_q$. Hence,

$$\boldsymbol{a}_j^T\boldsymbol{v}_1=\boldsymbol{a}_j^T\boldsymbol{v}\le s_j$$

for all $j=1,\ldots,q$. From (5.17) and (5.20), we get

$$s_j\ge\boldsymbol{a}_j^T\boldsymbol{v}_1=\sum_{i=1}^{q}c_i\boldsymbol{d}_i^T\boldsymbol{a}_j=-\frac{\alpha c_j}{\|\hat{\boldsymbol{d}}_j\|}, \tag{5.22}$$

for all $j=1,\ldots,q$. This implies that $c_i\ge0$ whenever $s_i=0$ (i.e. $\boldsymbol{x}$ lies on the boundary of the i-th constraint). Conversely, if $c_i<0$ then $s_i>0$ and so $\alpha_i>0$ from (5.16) (recalling that $\hat{\boldsymbol{d}}_i\neq\boldsymbol{0}$).

Since we do not know which (if any) c_i in (5.20) are non-negative, assume without loss of generality that $c_1,\ldots,c_k<0$ and $c_{k+1},\ldots,c_q\ge0$ for some $k\in\{0,\ldots,q\}$. In that case, $\alpha_1,\ldots,\alpha_k>0$, and so we can write

$$\boldsymbol{v}_1=\sum_{i=1}^{k}\frac{|c_i|}{\alpha_i}(-\alpha_i\boldsymbol{d}_i)+\sum_{i=k+1}^{q}|c_i|\boldsymbol{d}_i.$$

This expresses $\boldsymbol{v}_1$ as a non-negative combination of polling directions. We already have an upper bound on $|c_i|$ (5.21), so it remains to bound $|c_i|/\alpha_i$ for $i = 1, \ldots, k$. For any $i = 1, \ldots, k$, we use (5.17) to get

$$\boldsymbol{a}_i^T \boldsymbol{v}_1 = \frac{|c_i|}{\alpha_i}(-\alpha_i \boldsymbol{a}_i^T \boldsymbol{d}_i) = \frac{|c_i|}{\alpha_i} \cdot \frac{\alpha_i \alpha}{\|\hat{\boldsymbol{d}}_i\|} \quad \Leftrightarrow \quad \frac{|c_i|}{\alpha_i} = \frac{\boldsymbol{a}_i^T \boldsymbol{v}_1 \|\hat{\boldsymbol{d}}_i\|}{\alpha_i \alpha} \leq \frac{s_i \|\hat{\boldsymbol{d}}_i\|}{\alpha_i \alpha},$$

where the last inequality uses $\boldsymbol{a}_i^T \boldsymbol{v}_1 \leq s_i$ from (5.22). By definition of α_i in (5.16), it follows that

$$\frac{|c_i|}{\alpha_i} \leq \frac{s_i \|\hat{\boldsymbol{d}}_i\|}{\alpha_i \alpha} = 1 \quad \text{if } \alpha_i = \frac{s_i \|\hat{\boldsymbol{d}}_i\|}{\alpha} \qquad \text{and} \qquad \frac{|c_i|}{\alpha_i} = |c_i| \leq \kappa(A) \quad \text{if } \alpha_i = 1,$$

where the second inequality uses (5.21). Since $\kappa(A) \geq 1$ by definition, summing over $i = 1, \ldots, k$ yields

$$\sum_{i=1}^{k} \frac{|c_i|}{\alpha_i} \leq k\, \kappa(A). \tag{5.23}$$

Finally, for $i = k+1, \ldots, q$, using (5.21) gives

$$\sum_{i=k+1}^{q} |c_i| \leq (q-k)\kappa(A). \tag{5.24}$$

Overall, we have decomposed $\boldsymbol{v}$ into

$$\boldsymbol{v} = \boldsymbol{v}_1 + \boldsymbol{v}_2 = \sum_{i=1}^{k} \frac{|c_i|}{\alpha_i}(-\alpha_i \boldsymbol{d}_i) + \sum_{i=k+1}^{q} |c_i| \boldsymbol{d}_i + \sum_{i=q+1}^{n} \left[c_i(\alpha \boldsymbol{u}_i) + c_{-i}(-\alpha \boldsymbol{u}_i)\right],$$

where all coefficients are non-negative, and their sum is bounded by

$$\sum_{i=1}^{k} \frac{|c_i|}{\alpha_i} + \sum_{i=k+1}^{q} |c_i| + \sum_{i=q+1}^{n} (c_i + c_{-i}) \leq k\kappa(A) + (q-k)\kappa(A) + \sqrt{n-q} = q\kappa(A) + \sqrt{n-q},$$

which gives the value in (5.18). □

The above bound gives us a value of Λ depending on $A = [\boldsymbol{a}_1 \cdots \boldsymbol{a}_q]$, and so this value depends on the particular set of nearly active constraints, $I(\boldsymbol{x}, \alpha)$. In particular, when there are no active constraints ($q = 0$), we recover the unconstrained value $\Lambda = \sqrt{n}$. We now adjust the bound to make it completely independent of $\boldsymbol{x}$ and α.

Corollary 5.9. *Suppose the assumptions of Theorem 5.8 hold. Then, there exists a constant $C > 0$ depending only on the constraint vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_m$ (2.2) such that $\mathcal{D}$ is a Λ-PSS for $B(\boldsymbol{x}, \alpha) \cap \Omega$ where $\Lambda \leq nC$.*

Proof. For any $(\boldsymbol{x}, \alpha)$, we can apply Theorem 5.8 with a matrix $A_I = \{\boldsymbol{a}_i : i \in I\}$ to get

$$\Lambda = |I|\kappa(A_I) + \sqrt{n - |I|} \leq n\kappa(A_I),$$

where the second inequality comes from taking a maximum over $|I| \in \{0, \ldots, n\}$ with $\kappa(A_I) \geq 1$. Taking the maximum over the finitely many possibilities for I then yields the desired result. □

Since $\mathcal{D}$ has $2n$ vectors with $\Lambda = \mathcal{O}(n)$, Corollary 5.9 together with Theorem 4.7 imply that Algorithm 2 has a worst-case complexity of $\mathcal{O}(n^2\epsilon^{-2})$ iterations and $\mathcal{O}(n^3\epsilon^{-2})$ evaluations to achieve first-order optimality $\pi(\boldsymbol{x}_k) \leq \epsilon$. To the best of our knowledge, this is the first bound with quantifiable dependency on n for direct search with linear inequality constraints other than bounds.

5.3 Handling general linear constraints in practice

In the previous section, we provided explicit constructions for polling sets for bound-constrained problems and linearly constrained problems (2.2) satisfying Assumption 5.5. Assuming Asssumption 2.2 but not Assumption 5.5, we do not know of a polling set construction with guaranteed Λ-PSS properties. However, various algorithms exist for constructing a (minimal) set of generators for a general cone expressed as linear inequalities, such as the double description method [16]. In practice, we can use such a technique to construct a set of generators for $T_\Omega(\boldsymbol{x}, \alpha)$ for any set of linear inequality constraints.

To this end, a practical polling set construction method given $\boldsymbol{x} \in \Omega$ and $\alpha > 0$ consists in the following steps:

1. If $I(\boldsymbol{x}, \alpha) = \emptyset$, take $\mathcal{D} = \{\pm \boldsymbol{e}_1, \dots, \pm \boldsymbol{e}_n\}$ (as in the unconstrained case).
2. If Assumption 5.5 holds, take $\mathcal{D}$ as in (5.15).
3. Otherwise, construct a set of generators $\mathcal{G}$ for $T_\Omega(\boldsymbol{x}, \alpha)$.
   (a) If $\mathcal{G} \neq \emptyset$, set $\mathcal{D} = \{\frac{\alpha}{\|\boldsymbol{d}\|}\boldsymbol{d} : \boldsymbol{d} \in \mathcal{G}\} \cup \{-\alpha_d \boldsymbol{d} : \boldsymbol{d} \in \mathcal{G}\}$, where α_x is the largest value in $[0, \alpha]$ such that $\boldsymbol{x} - \alpha_d \boldsymbol{d} \in \Omega$;
   (b) Otherwise, if $\mathcal{G} = \emptyset$ (i.e. $T_\Omega(\boldsymbol{x}, \alpha) = \{\boldsymbol{0}\}$) then take $\mathcal{D}$ to be the generators of $N_\Omega(\boldsymbol{x}, \alpha)$. More precisely, set $\mathcal{D} = \{\alpha_i \boldsymbol{a}_i : i \in I(\boldsymbol{x}, \alpha)\}$, where $\alpha_i \geq 0$ is the largest value such that the polled point is feasible and in $B(\boldsymbol{x}, \alpha)$. Since $N_\Omega(\boldsymbol{x}, \alpha) = \mathbb{R}^n$ in this case, this set is a PSS for $\mathbb{R}^n$.
   (c) If $\text{span}(\mathcal{D}) \neq \mathbb{R}^n$ (linear span) for $\mathcal{D}$ from 3(a), then append to $\mathcal{D}$ a polling set for $\text{nul}(\mathcal{G}) \cap \Omega$ constructed recursively using this approach.

Although this approach is recursive (in the last step), it always terminates in finite time, since every recursive call operates on a proper subspace of its parent call. Note that if $\text{nul}(\mathcal{G})$ is one-dimensional, then we just take positive and negative steps (scaled to ensure feasibility and length at most α) along this one direction to complete the recursive step.

6 Numerical Experiments

In this section, we compare the strategy described in Section 5 with classical direct-search variants tailored to bound and linearly constrained problems. In addition to comparing these methods on a standard optimization benchmark, we also evaluate the quality of polling sets when generated as Λ-PSSs.

6.1 Implementation Details

Our implementation relies on the `directsearch` [37] Python package[1], which we augment with three different polling techniques to handle linear inequality constraints. More precisely, we implement Algorithm 2 with three choices of polling sets:

- Tangent generators: At iteration k, $\mathcal{D}_k$ is the set of generators of the tangent cone, scaled to have length α_k. If this set is empty (i.e. $T_\Omega(\boldsymbol{x}_k, \alpha_k) = \{\boldsymbol{0}\}$) then we use the scaled generators of the normal cone, as in step 3(b) of Section 5.3.
- Tangent and normal generators: At iteration k, $\mathcal{D}_k$ is the set of generators of the tangent cone, scaled to have length α_k, together with the nearly active constraints normals, scaled to be feasible and have length at most α_k (as in step 3(b) of Section 5.3). This follows the heuristic approach from Lewis et al. [27].
- Full Λ-PSS: the full polling set generation procedure described in Section 5.3. The extra 'negative directions' (i.e. $-\alpha_d \boldsymbol{d}$ for $\boldsymbol{d} \in \mathcal{G}$) are only polled after the directions in the tangent cone.

[1] `https://github.com/lindonroberts/directsearch`

All variants consider the same generators of the tangent cone, and the implementation always polls tangent directions first. We use opportunistic polling[2] and we replace the quantity $\frac{\sigma}{2}\alpha_k^2$ in (2.3) (resp. (4.1)) with the slightly modified quantity $\min(\epsilon, \epsilon\alpha_k^2)$ where $\epsilon = 10^{-5}$. We update α_k with $\gamma_{\text{dec}} = 0.5$, $\gamma_{\text{inc}} = 2$ and with α_k capped at $\alpha_{\max} = 10^3$. We terminate when $\alpha_k \le \alpha_{\min} = 10^{-6}$ or if a budget of $200(n+1)$ objective evaluations is reached for an n-dimensional problem. The initial stepsize was chosen as $\alpha_0 = \max(\alpha_{\min}, \max(0.1 \max(\|\boldsymbol{x}_0\|_\infty, 1), \alpha_{\max}))$.

For this implementation, we test the two polling set constructions on a collection of 122 problems from the CUTEst collection [18, 15]. These problems are mostly low-dimensional, with dimensions between 1 and 51. Bound constraints appear in 77 problems, while 45 problems possess general linear inequality constraints. This collection of test problems is based on the problems used for numerical experiments in Gratton et al. [20], and a full list of problems is given in Appendix A. Where the starting point $\boldsymbol{x}_0$ provided by CUTEst is not feasible, we replace it with $\text{proj}_\Omega(\boldsymbol{x}_0)$, to ensure the starting point is feasible.

6.2 Main Results

We report our comparison using data and performance profiles [31, 13]. Specifically, for each solver $\mathcal{S}$ and problem $\mathcal{P}$ we calculate the number of evaluations required for the problem to be 'solved' as

$$N(\mathcal{S}, \mathcal{P}, \tau) := \#\text{ obj. evals. to find } \boldsymbol{x} \in \Omega \text{ with } f(\boldsymbol{x}) \le f_{\min} + \tau(f(\boldsymbol{x}_0) - f_{\min}), \tag{6.1}$$

where $\tau \ll 1$ is an accuracy parameter, and $f_{\min}$ is the best (feasible) objective value found by any solver for the given problem. We define $N(\mathcal{S}, \mathcal{P}, \tau) = \infty$ (i.e. solver $\mathcal{S}$ never solved problem $\mathcal{P}$) if the solver never found a feasible point with sufficiently small objective value. Data profiles measure the proportion of problems $\mathcal{P}$ 'solved' by a solver $\mathcal{S}$ (in the sense of (6.1)) within a given number of evaluations $c(n+1)$ for some constant $c > 0$. Performance profiles measure the proportion of problems solved within some constant of the fastest solver for that problem, i.e. $N(\mathcal{S}, \mathcal{P}, \tau) \le c \min_{\mathcal{S}'} N(\mathcal{S}', \mathcal{P}, \tau)$ for some constant $c \ge 1$.

In Figure 2 we show data and performance profiles comparing the three methods for the full set of test problems. For both accuracy levels $\tau = 10^{-3}$ and $\tau = 10^{-6}$, we observe that only using generators of the tangent cone is the worst-performing variant. Adding nearly active constraint normals (per [27]) provides a good improvement, but using a full Λ-PSS (i.e. adding negative tangent cone generators) performs best. The benefit of Λ-PSS compared to tangent generators and normal directions is similar at both accuracy levels, but using only tangent directions is a relatively worse option when higher accuracy solutions are desired ($\tau = 10^{-6}$).

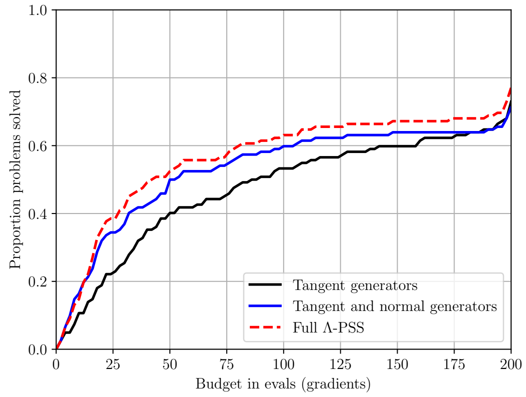
In Appendix B we provide the same results, but split separately into bound constrained and general linear inequality constrained problems. For bound-constrained problems, using either normal generators or a full Λ-PSS has essentially identical performance, which is somewhat expected from our construction. The benefit of using a Λ-PSS is much clearer for general linear inequality constrained problems, yielding a larger improvement over both alternative polling set constructions.

6.3 Estimating Λ-PSS Quality

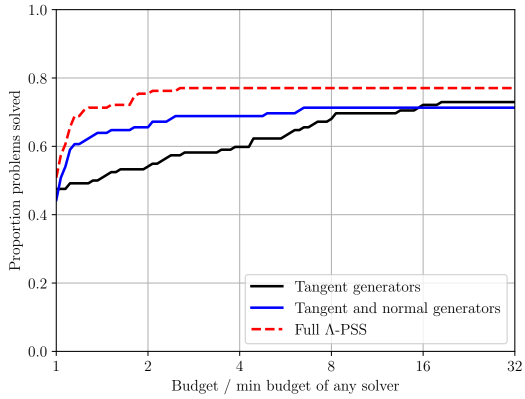
The "full Λ-PSS" polling set tested above is only proven to satisfy Definition 4.4 for general linear inequality constraints in the case of linearly independent tangent cone generators (Assumption 5.5). We now numerically assess the quality of the polling set formed via the approach in Section 5.3.

For all test problems with general linear inequality constraints, and all iterations of our numerical algorithm above, we estimate the value of Λ (in the sense of Definition 4.4) achieved

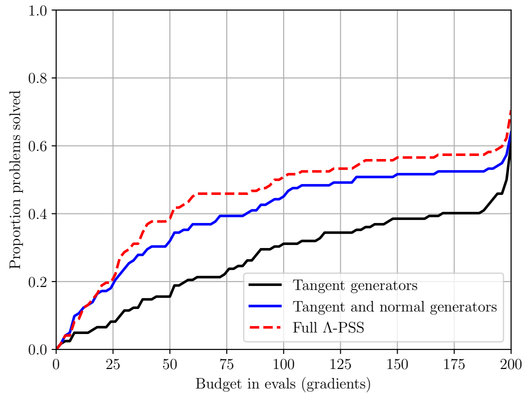
[2] That is, the first $\boldsymbol{d}_k \in \mathcal{D}_k$ satisfying the sufficient decrease condition is accepted.



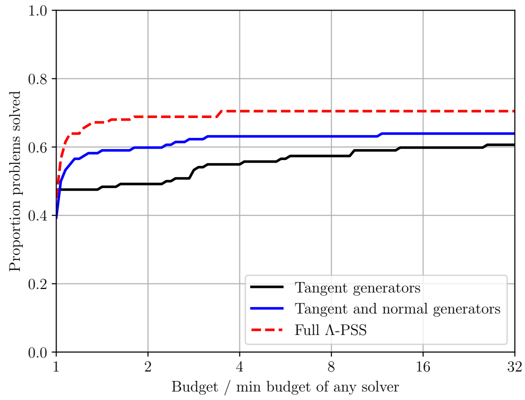
(a) Data profile, $\tau = 10^{-3}$



(b) Performance profile, $\tau = 10^{-3}$



(c) Data profile, $\tau = 10^{-6}$



(d) Performance profile, $\tau = 10^{-6}$

Figure 2. Data and performance profiles comparing polling set generation using only tangent cone generators compared to full Λ-PSS.

by the polling set in the current iteration, by solving

$$\Lambda = \max_{\boldsymbol{v}\in\mathbb{R}^n} \left\{ \min_{\boldsymbol{c}\in\mathbb{R}^p} \sum_{i=1}^{q} c_i \quad \text{s.t.} \quad \sum_{i=1}^{q} c_i \boldsymbol{d}_i = \boldsymbol{v},\ \boldsymbol{c} \geq \boldsymbol{0} \right\}, \tag{6.2a}$$

$$\text{s.t. } \boldsymbol{x}_k + \boldsymbol{v} \in \Omega,\ \|\boldsymbol{v}\| \leq \alpha_k, \tag{6.2b}$$

where $\mathcal{D}_k = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_q\}$ is the polling set at iteration k. We solve (6.2) using the default implementation of DIRECT provided in the SciPy library (based on [17]), with the objective value evaluated by solving the linear program for $\boldsymbol{c}$ using HiGHS [22].

In Figure 3, we plot the distribution of estimated values of $\Lambda/\sqrt{n}$ (6.2) across all iterations of all test problems with general linear inequality constraints, split by the sub-method from Section 5.3 used to construct the polling set. We show $\Lambda/\sqrt{n}$ to normalize across problems of different dimensions, as this value is exactly 1 for unconstrained problems (with polling set $\{\pm\alpha_k\boldsymbol{e}_1, \ldots, \pm\alpha_k\boldsymbol{e}_n\}$).

In the 'unconstrained' and 'full rank' cases, we always see small values of $\Lambda = \mathcal{O}(\sqrt{n})$, which aligns with the theory from Sections 4.1 and 5 respectively, noting that $n \leq 15$ for all these test problems. For the other types of polling set constructions, the empirical values of Λ are small the vast majority of the time, but there are outliers for which Λ can become large. This conforms to our theory and further demonstrates that for the cases not covered by our theory, the practical polling set generation in Section 5.3 is suitable for most situations, but some degenerate cases may arise which require more careful polling set construction to ensure theoretical guarantees.

As an example, consider a situation in $\mathbb{R}^2$ where Ω is defined by the constraints $x_1, x_2 \geq 0$, $4x_1 + x_2 \leq 12$ and $3x_1 + 4x_2 \leq 12$, and we are at the base point $\boldsymbol{x} = [0.23, 2.55]^T$ with $\alpha = 3.4$.

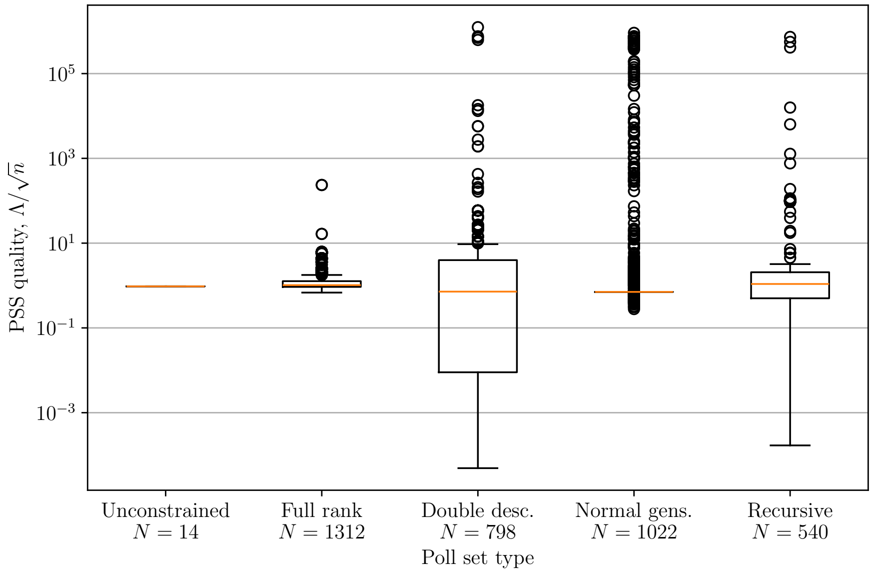


Figure 3. Distribution of estimated values $\Lambda/\sqrt{n}$ for polling sets in each iteration of each general linear inequality constrained test problem. Regarding the method in Section 5.3: "Unconstrained" is case 1, "Full rank" is case 2, "Double desc." is case 3(a), "Normal gens." is case 3(b), and "Recursive" is case 3(c). In case case, the value of N is how many iterations were in each case across all problems.

This is depicted in Figure 4. Here, $\boldsymbol{x}$ is far from the constraint $4x_1 + x_2 \leq 12$, but α is large enough that it is still nearly active. Hence $T_\Omega(\boldsymbol{x}, \alpha) = \{\boldsymbol{0}\}$ and $N_\Omega(\boldsymbol{x}, \alpha) = \mathbb{R}^2$. However, because $\boldsymbol{x}$ is very close to the top corner, the rightward-pointing outward normals both get scaled to very short lengths. This means that the effective Λ is very large, coming from points $\boldsymbol{x} + \boldsymbol{v}$ near the bottom-right corner of $B(\boldsymbol{x}, \alpha) \cap \Omega$. As $\boldsymbol{x}$ moves closer to the top corner of Ω, the effectively Λ grows.

7 Conclusion

We have introduced the concept of a Λ-PSS as an alternative to the commonly-used positive spanning sets for direct search. This allowed us to re-derive the existing theory for unconstrained direct search, but with a theoretical underpinning more aligned with model-based DFO, and

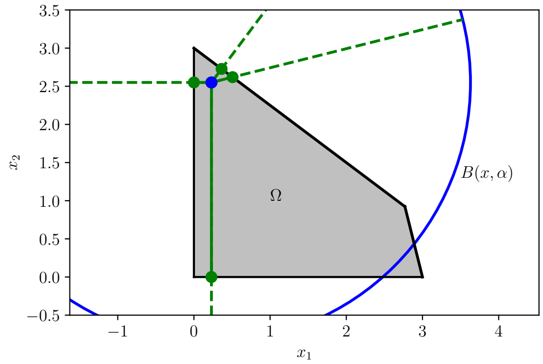


Figure 4. Example issue that can occur using generators of the normal cone as a polling set in case 3(b) of Section 5.3. Shaded region is Ω, blue circle is $B(\boldsymbol{x}, \alpha)$, marked points are $\boldsymbol{x}$ and the poll points based on scaled outward normals of nearly active constraints. All constraints are nearly active for this $\boldsymbol{x}$ and α.

which naturally generalizes to convex-constrained problems. We provided a global convergence and worst-case complexity analysis for general convex-constrained direct search, and specific constructions for polling set generation for bound and linear inequality constrained problems with theoretical guarantees and strong practical performance.

In presence of linearly dependent nearly active constraints (i.e. when Assumption 5.5 does not apply), our proposed construction does not guarantee the Λ-PSS property, despite exhibiting good practical performance. Further work is thus needed to provably build Λ-PSS in this setting. In addition, combining Λ-PSSs with probabilistic polling set construction [20] or polling in randomly generated subspaces [37] is a promising direction to improve the scalability and performance of these techniques.

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A List of Test Problems

Name (params)	n	NB	Name (params)	n	NB
ALLINIT	3	3	MAXLIKA	8	16
BQP1VAR	1	2	MCCORMCK ($N = 10$)	10	20
CAMEL6	2	4	MCCORMCK ($N = 50$)	50	100
CHEBYQAD ($N = 10$)	10	20	MDHOLE	2	1
CHEBYQAD ($N = 20$)	20	40	NCVXBQP1 ($N = 10$)	10	20
CHENHARK (*)	10	10	NCVXBQP1 ($N = 50$)	50	100
CVXBQP1 ($N = 10$)	10	20	NCVXBQP2 ($N = 10$)	10	20
CVXBQP1 ($N = 50$)	50	100	NCVXBQP2 ($N = 50$)	50	100
DEGDIAG ($N = 10$)	11	11	NCVXBQP3 ($N = 10$)	10	20
DEGDIAG ($N = 50$)	51	51	NCVXBQP3 ($N = 50$)	50	100
DEGTRID ($N = 10$)	11	11	NOBNDTOR ($Q = 2$)	4	4
DEGTRID ($N = 50$)	51	51	OBSTCLAE ($PX = 4$, $PY = 4$)	4	8
EG1	3	4	OBSTCLBL ($PX = 4$, $PY = 4$)	4	8
EXPLIN ($N = 12$, $M = 6$)	12	24	OSLBQP	8	11
EXPLIN2 ($N = 12$, $M = 6$)	12	24	PALMER1A	6	2
EXPQUAD ($N = 12$, $M = 6$)	12	12	PALMER2B	4	2
HARKERP2 ($N = 10$)	10	10	PALMER3E	8	1
HART6	6	12	PALMER4A	6	2
HATFLDA	4	4	PALMER5B	9	2
HATFLDB	4	5	PFIT1LS	3	1
HIMMELP1	2	4	POWELLBC ($P = 5$)	10	20
HS1	2	1	POWELLBC ($P = 10$)	20	40
HS110 ($N = 10$)	10	20	PROBPENL ($N = 10$)	10	20
HS110 ($N = 50$)	50	100	PROBPENL ($N = 50$)	50	100
HS2	2	1	PSPDOC	4	1
HS25	3	6	QRTQUAD ($N = 12$, $M = 6$)	12	24
HS3	2	1	S368 ($N = 8$)	8	16
HS38	4	8	S368 ($N = 50$)	50	100
HS3MOD	2	1	SCOND1LS ($N = 10$, $LN = 9$)	10	20
HS4	2	2	SCOND1LS ($N = 50$, $LN = 45$)	50	100
HS45	5	10	SIMBQP	2	2
HS5	2	4	SINEALI ($N = 10$)	10	20
JNLBRNG1 ($PT = 4$, $PY = 4$)	4	4	SINEALI ($N = 20$)	20	40
JNLBRNG2 ($PT = 4$, $PY = 4$)	4	4	SPECAN ($K = 3$)	9	18
JNLBRNGA ($PT = 4$, $PY = 4$)	4	4	TORSION1 ($Q = 2$)	4	8
JNLBRNGB ($PT = 4$, $PY = 4$)	4	4	TORSIONA ($Q = 2$)	4	8
KOEBHELB	3	2	WEEDS	3	4
LINVERSE ($N = 10$)	19	10	YFIT	3	1
LOGROS	2	2			

Table 1. List of 77 bound-constrained CUTEst problems used for numerical experiments. (parameters for CHENHARK are $N = 10$, $NFREE = 5$, $NDEGEN = 2$)*

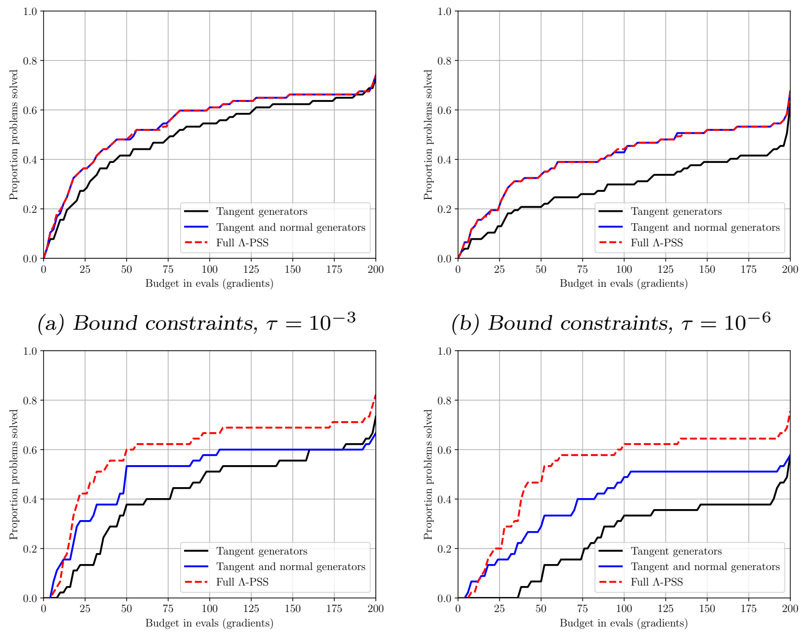
Name (params)	n	NB	LI	Name (params)	n	NB	LI
AVGASA	8	16	10	HS86	5	5	10
AVGASB	8	16	10	HUBFIT	2	1	1
BIGGSC4	4	8	13	LSQFIT	2	1	1
EQC	7	14	3	OET1	3	0	1002
EXPFITA	5	0	22	OET3	4	0	1002
EXPFITB	5	0	102	PENTAGON	6	0	15
EXPFITC	5	0	502	PT	2	0	501
HATFLDH	4	8	13	QC	7	14	4
HS105	8	16	1	QCNEW	7	14	3
HS118	15	30	29	S268	5	0	5
HS21	2	4	1	SIMPLLPA	2	2	2
HS21MOD	7	8	1	SIMPLLPB	2	2	3
HS24	2	2	3	SIPOW1	2	0	2000
HS268	5	0	5	SIPOW1M	2	0	2000
HS35	3	3	1	SIPOW2	2	0	2000
HS35I	3	6	1	SIPOW2M	2	0	2000
HS35MOD	2	2	1	SIPOW3	4	0	2000
HS36	3	6	1	SIPOW4	4	0	2000
HS37	3	6	2	STANCMIN	3	3	2
HS44	4	4	6	TFI2	3	0	101
HS44NEW	4	4	6	TFI3	3	0	101
HS76	4	4	3	ZECEVIC2	2	4	2
HS76I	4	8	3				

Table 2. List of 45 linear inequality constrained CUTEst problems used for numerical experiments.

Tables 1 and 2 contain lists of the 77 bound-constrained and 45 general linear inequality constrained CUTEst problems [18, 15] used for the numerical experiments in Section 6, based on the problems used in [20]. Any values in brackets after the problem name are the optional problem parameters used. The columns n, NB and LI are the problem dimension, number of (finite) bound constraints, and number of (finite) general linear inequality constraints for each problem respectively.

B Detailed Numerical Results

Here, we show the same numerical results as in Figure 2, but split separately into the 77 bound-constrained test problems and the 45 problems with general linear inequality constraints. For brevity, we only show data profiles.



(a) Bound constraints, $\tau = 10^{-3}$ *(b) Bound constraints, $\tau = 10^{-6}$*

(c) Linear ineq. constraints, $\tau = 10^{-3}$ *(d) Linear ineq. constraints, $\tau = 10^{-6}$*

Figure 5. Numerical results split by problem type.