Instance-Dependent Bounds for Zeroth-order Lipschitz Optimization with Error Certificates

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Abstract

We study the problem of zeroth-order (black-box) optimization of a Lipschitz function f defined on a compact subset $\mathcal{X}$ of $\mathbb{R}^d$, with the additional constraint that algorithms must certify the accuracy of their recommendations. We characterize the optimal number of evaluations of any Lipschitz function f to find and certify an approximate maximizer of f at accuracy ε. Under a weak assumption on $\mathcal{X}$, this optimal sample complexity is shown to be nearly proportional to the integral $\int_{\mathcal{X}} \mathrm{d}\boldsymbol{x}/(\max(f) - f(\boldsymbol{x}) + \varepsilon)^d$. This result, which was only (and partially) known in dimension $d = 1$, solves an open problem dating back to 1991. In terms of techniques, our upper bound relies on a slightly improved analysis of the DOO algorithm that we adapt to the certified setting and then link to the above integral. Our instance-dependent lower bound differs from traditional worst-case lower bounds in the Lipschitz setting and relies on a local worst-case analysis that could likely prove useful for other learning tasks.

1 Introduction

The problem of optimizing a black-box function f with as few evaluations of f as possible arises in many scientific and industrial fields such as computer experiments (Jones et al., 1998; Richet et al., 2013) or automatic selection of hyperparameters in machine learning (Bergstra et al., 2011). For safety-critical applications, e.g., in aircraft or nuclear engineering, using sample-efficient methods is not enough. *Certifying* the accuracy of the output of the optimization method can be a crucial additional requirement (Vanaret et al., 2013). As a concrete example, Azzimonti et al. (2021) describe a black-box function in nuclear engineering whose output is a k-effective multiplication factor, for which a higher value corresponds to a higher nuclear hazard. Certifying the optimization error is a way to certify the worst-case k-effective factor, which may be required by safety authorities.

In this paper, we formally study the problem of finding and certifying an ε-approximate maximizer of a Lipschitz function f of d variables and characterize the optimal number of evaluations of any such function f to achieve this goal. We start by formally defining the setting.

1.1 Setting: Zeroth-order Lipschitz Optimization with Error Certificates

Let $f\colon \mathcal{X} \to \mathbb{R}$ be a function on a compact non-empty subset $\mathcal{X}$ of $\mathbb{R}^d$ and $\boldsymbol{x}^\star \in \mathcal{X}$ a maximizer.

Lipschitz assumption. We assume that f is Lipschitz with respect to a norm $\|\cdot\|$, that is, there exists $L \geq 0$ such that $\big|f(\boldsymbol{x}) - f(\boldsymbol{y})\big| \leq L\,\|\boldsymbol{x} - \boldsymbol{y}\|$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{X}$. Furthermore, we assume such a Lipschitz bound L to be known. Even though the smallest Lipschitz constant $\mathrm{Lip}(f) := \min\{L' \geq 0 : f \text{ is } L'\text{-Lipschitz}\}$ is well defined mathematically, it is rarely known exactly in practical black-box problems. As a theoretical curiosity, we will briefly discuss the case

$L = \mathrm{Lip}(f)$ (i.e., when the best Lipschitz constant of the unknown black-box function f is known exactly) in Section 4, but for most of our results, we will make the following more realistic assumption.

Assumption 1. *For some known Lipschitz constant L, the function $f\colon \mathcal{X} \to \mathbb{R}$ belongs to*

$$\mathcal{F}_L := \big\{ g\colon \mathcal{X} \to \mathbb{R} \mid g \text{ is Lipschitz and } \mathrm{Lip}(g) < L \big\} \,. \tag{1}$$

The Lipschitzness of f implies the weaker property that $f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) \leq L \, \|\boldsymbol{x}^\star - \boldsymbol{x}\|$ for all $\boldsymbol{x} \in \mathcal{X}$, sometimes referred to as *Lipschitzness around a maximizer* $\boldsymbol{x}^\star \in \mathcal{X}$. Although this is not the focus of our work, we will mention when our results hold under this weaker assumption.

Online learning protocol. We study the case in which f is black-box, i.e., except for the *a priori* knowledge of L, we can only access f by sequentially querying its values at a sequence $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \in \mathcal{X}$ of points of our choice. At every round $n \geq 1$, the query point $\boldsymbol{x}_n$ can be chosen as a deterministic function of the values $f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_{n-1})$ observed so far. At the end of round n, using all the values $f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n)$, the learner outputs two quantities:

- a recommendation $\boldsymbol{x}_n^\star \in \mathcal{X}$, with the goal of minimizing the *optimization error* (a.k.a. *simple regret*): $\max(f) - f(\boldsymbol{x}_n^\star)$;
- an *error certificate* $\xi_n \geq 0$, with the constraint to correctly upper bound the optimization error for any L-Lipschitz function $f\colon \mathcal{X} \to \mathbb{R}$, i.e., so that $\max(f) - f(\boldsymbol{x}_n^\star) \leq \xi_n$.

We call *certified algorithm* any algorithm for choosing such a sequence $(\boldsymbol{x}_n, \boldsymbol{x}_n^\star, \xi_n)_{n \geq 1}$.

Our goal is to quantify the smallest number of evaluations of f that certified algorithms need in order to find and certify an approximate maximizer of f at accuracy ε. This objective motivates the following definition. For any accuracy $\varepsilon > 0$, we define the *sample complexity* of a certified algorithm A for an L-Lipschitz function f as

$$\sigma(A, f, \varepsilon) := \inf\big\{ n \geq 1 : \xi_n \leq \varepsilon \big\} \in \{1, 2, \ldots\} \cup \{+\infty\} \,. \tag{2}$$

This corresponds to the first time when we can stop the algorithm while being sure to have an ε-optimal recommendation $\boldsymbol{x}_n^\star$.

1.2 Main Contributions and Outline of the Paper

The main result of this paper is a tight characterization (up to a $\log$ factor) of the optimal sample complexity of certified algorithms in any dimension $d \geq 1$, solving a three-decade old open problem raised by Hansen et al. (1991). More precisely, we prove the following instance-dependent upper and lower bounds, which we later state formally in Theorem 3 of Section 4 (see also discussions therein, as well as Propositions 2 and 3 for the limit case $L = \mathrm{Lip}(f)$).

Theorem (Informal statement)**.** *Under a mild geometric assumption on $\mathcal{X}$, there exists a computationally tractable algorithm A (e.g.,* c.DOO*, Algorithm 1) such that, for some constant $C > 0$, any Lipschitz function $f \in \mathcal{F}_L$ (see* (1)*) and any accuracy ε,*

$$\sigma(A, f, \varepsilon) \leq C \int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} \,, \tag{3}$$

while any certified algorithm A' must satisfy, for all $f \in \mathcal{F}_L$ and $c \approx (1 - \mathrm{Lip}(f)/L)^d / \log(1/\varepsilon)$,

$$c \int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} \leq \sigma(A', f, \varepsilon) \,. \tag{4}$$

In particular, this result extends to any dimension $d \geq 1$ the upper bound proportional to $\int_0^1 \mathrm{d}x / (f(x^\star) - f(x) + \varepsilon)$ that Hansen et al. (1991) derived in dimension $d = 1$ using arguments specific to the geometry of the real line.

Detailed contributions and outline of the paper. We make the following contributions.

- As a warmup, we show in Section 2 how to add error certificates to the DOO algorithm (well-known in the more classical zeroth-order Lipschitz optimization setting *without* error certificates, see Perevozchikov 1990; Munos 2011). We then upper bound its sample complexity by the quantity $S_{\mathrm{C}}(f, \varepsilon)$ defined in (5) below. This bound matches a recent bound derived by Bouttier et al. (2020) for a computationally much more expensive algorithm. In passing, we also slightly improve the packing arguments that Munos (2011) used in the non-certified setting.
- In Section 3 we show that, under a mild geometric assumption on $\mathcal{X}$, the complexity measure $S_{\mathrm{C}}(f, \varepsilon)$ is actually proportional to the compact integral $\int_{\mathcal{X}} \mathrm{d}\boldsymbol{x} / \big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d$, which implies (3) above. This extends the bound of Hansen et al. (1991) ($d = 1$) to any dimension d.
- Finally, in Section 4, we prove the instance-dependent lower bound (4), which differs from traditional worst-case lower bounds in the Lipschitz setting. Our proof relies on a *local* worst-case analysis that could likely prove useful for other learning tasks.

Some of the proofs are deferred to the Supplementary Material, where we also recall useful results on packing and covering numbers (Section A), as well as provide a slightly improved sample complexity bound on the DOO algorithm in the more classical non-certified setting (Section E).

Limitations and open problems. There are some interesting directions that would be worth investigating in the future but we did not cover in this paper, such as noisy observations (see, e.g, Bubeck et al. 2011; Kleinberg et al. 2019) or adaptivity to smoothness (e.g., Munos 2011; Bartlett et al. 2019; we consider L-Lipschitz functions f with L known, although our lower bound suggests that no adaptivity could be possible for certified algorithms). Finally, even if the results of Section 2 could be easily extended to pseudo-metric spaces as in Munos (2014) and related works, our other results are finite-dimensional and exploit the normed space structure.

1.3 Related Works

We detail below some connections with the global optimization and the bandit optimization literatures.

Zeroth-order Lipschitz optimization with error certificates. The problem of optimizing a function with error certificates has been studied in different settings over the past decades. For instance, in convex optimization, an example of error certificate is given by the *duality gap* between primal and dual feasible points (see, e.g., Boyd and Vandenberghe 2004).

In our setting, namely, global zeroth-order Lipschitz optimization with error certificates, most of the attention seems to have been on the very natural (yet computationally expensive) algorithm introduced by Piyavskii (1972) and Shubert (1972).[1] In dimension $d = 1$, Hansen et al. (1991) proved that its sample complexity $\sigma(\mathrm{PS}, f, \varepsilon)$ for L-Lipschitz functions $f\colon [0,1] \to \mathbb{R}$ is at most proportional to the integral $\int_0^1 \big(f(x^\star) - f(x) + \varepsilon\big)^{-1} \mathrm{d}x$, and left the question of extending the results to arbitrary dimensions open, stating that the task of "*Extending the results of this paper to the multivariate case appears to be difficult*". Recently, writing $\mathcal{X}_\varepsilon := \{\boldsymbol{x} \in \mathcal{X} : \max(f) - f(\boldsymbol{x}) \le \varepsilon\}$ for the set of ε-optimal points, $\mathcal{X}_{(a,b]} := \{\boldsymbol{x} \in \mathcal{X} : a < \max(f) - f(\boldsymbol{x}) \le b\}$ for the set of points in between a and b optimal, and $\mathcal{N}(E, r)$ for the packing number of a set E at scale r (see Section 1.4), Bouttier et al. (2020, Theorem 2) proved a bound valid in any dimension $d \ge 1$ roughly of this form:

$$S_{\mathrm{C}}(f, \varepsilon) := \mathcal{N}\left(\mathcal{X}_\varepsilon, \frac{\varepsilon}{L}\right) + \sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k, \varepsilon_{k-1}]}, \frac{\varepsilon_k}{L}\right) , \tag{5}$$

where the number of terms in the sum is $m_\varepsilon := \big\lceil \log_2(\varepsilon_0/\varepsilon) \big\rceil$ (with $\varepsilon_0 := L \sup_{\boldsymbol{x},\boldsymbol{y} \in \mathcal{X}} \|\boldsymbol{x} - \boldsymbol{y}\|$) and the associated scales are given by $\varepsilon_{m_\varepsilon} := \varepsilon$ and $\varepsilon_k := \varepsilon_0 2^{-k}$ for all $k \in \{0, 1, \dots, m_\varepsilon - 1\}$.

[1] For the interested reader who is unfamiliar with this classic algorithm, we added some details in Section D.2 of the Supplementary Material.

The equivalence we prove in Section 3 between $S_{\mathrm{C}}(f,\varepsilon)$ and $\int_{\mathcal{X}} \mathrm{d}\boldsymbol{x}/(f(\boldsymbol{x}^\star)-f(\boldsymbol{x})+\varepsilon)^d$ solves in particular the question left open by Hansen et al. (1991). The upper bound we prove for the certified DOO algorithm in Section 2 also indicates that the bound $S_{\mathrm{C}}(f,\varepsilon)$ and the equivalent integral bound can be achieved with a computationally much more tractable algorithm. Indeed, the Piyavskii-Shubert algorithm requires at every step n to solve an inner global Lipschitz optimization problem close to the computation of a Voronoi diagram (see discussion in Bouttier et al. 2020, Section 1.1), hence a running time believed to grow as $n^{\Omega(d)}$ after n function evaluations. On the contrary, as detailed in Remark 1 (Section 2), the running time of our certified version of the DOO algorithm is only of the order of $n\log(n)$ after n of evaluations of f.

Connections with the bandit optimization literature: upper bounds. Our work is also strongly connected to the bandit optimization literature, in which multiple authors studied the global Lipschitz optimization problem with zeroth-order (or *bandit*) feedback, either with perfect (deterministic) or noisy (stochastic) observations. In the deterministic setting considered here, these papers show that though the number $(L/\varepsilon)^d$ of evaluations associated to a naive grid search is optimal for worst-case Lipschitz functions (e.g., Thm 1.1.2 by Nesterov 2003), sequential algorithms can approximately optimize more benign functions with a much smaller number of evaluations. Examples of algorithms with such guarantees in the deterministic setting are the branch-and-bound algorithm by Perevozchikov (1990), the DOO algorithm by Munos (2011) or the LIPO algorithm by Malherbe and Vayatis (2017). Examples of algorithms in the stochastic setting are the HOO algorithm by Bubeck et al. (2011) or the (generic yet computationally challenging) Zooming algorithm by Kleinberg et al. (2008, 2019). More examples and references can be found in the textbooks by Munos (2014) and Slivkins (2019).

Note however that, except for the work of Bouttier et al. (2020) mentioned earlier, these bandit optimization papers did not address the problem of *certifying* the accuracy of the recommendations $\boldsymbol{x}_n^\star$. Indeed, all bounds are related to a more classical notion of sample complexity, namely, the minimum number of queries made by an algorithm A before outputting ε-optimal recommendations only:

$$\zeta(A,f,\varepsilon) := \inf\{n \geq 1 : \boldsymbol{x}_n^\star \in \mathcal{X}_\varepsilon\} \in \{1,2,\ldots\} \cup \{+\infty\}\,. \tag{6}$$

Though $\zeta(A,f,\varepsilon)$ is always upper bounded by $\sigma(A,f,\varepsilon)$ defined in (2), these two quantities can differ significantly, as shown by the simple example of constant functions f, for which $\zeta(A,f,\varepsilon)=1$ but $\sigma(A,f,\varepsilon)\approx(L/\varepsilon)^d$ since the only way to *certify* that the output is ε-optimal is essentially to perform a grid-search with step-size roughly ε/L, so as to be sure there is no hidden bump of height more than ε. At a high level, the more "constant" a function is, the easier it is to recommend an ε-optimal point, but the harder it is to certify that such recommendation is actually a good recommendation. See the Supplementary Material (Section E) for a comparison of bounds.

Despite this important difference, the bandit viewpoint (using packing numbers instead of more specific one-dimensional arguments) is key to obtain our multi-dimensional integral characterization.

Comparison with existing lower bounds. Several worst-case (minimax) lower bounds were derived in the bandit Lipschitz optimization setting. When rewritten in terms of the accuracy ε and translated into our deterministic setting, the lower bounds of Horn (2006) (when $d^\star = d/2$) and of Bubeck et al. (2011) (for any $d^\star$) are of the form $\inf_A \sup_{f\in\mathcal{G}_{d^\star}} \zeta(A,f,\varepsilon) \geq \psi_{d^\star}(\varepsilon)$, where $\mathcal{G}_{d^\star}$ is the subset of L-Lipschitz functions with near-optimality dimension at most $d^\star$.

On the contrary, our instance-dependent lower bound (4) quantifies the minimum number of evaluations to certify an ε-optimal point *for each function* $f \in \mathcal{F}_L$. Our proof relies on a *local* worst-case analysis in the same spirit as for distribution-dependent lower bounds in stochastic multi-armed bandits (see, e.g., Theorem 16.2 in Lattimore and Szepesvári 2020), yet for continuous instead of finite action sets. We believe this lower bound technique should prove useful for other learning tasks.

1.4 Recurring Notation

This short section contains a summary of all the notation that we use in the paper and can be used by the reader for easy referencing. We denote the set of positive integers $\{1,2,\ldots\}$ by $\mathbb{N}^*$ and let $\mathbb{N} := \mathbb{N}^* \cup \{0\}$. For all $n \in \mathbb{N}^*$, we denote by $[n]$ the set of the first n integers $\{1,\ldots,n\}$. We denote the Lebesgue measure of a (Lebesgue-measurable)

set E by $\mathrm{vol}(E)$ and refer to it simply as its *volume*. For all $\rho > 0$ and $\boldsymbol{x} \in \mathbb{R}^d$, we denote by $B_\rho(\boldsymbol{x})$ the closed ball with radius ρ centered at $\boldsymbol{x}$, with respect to the arbitrary norm $\|\cdot\|$ that is fixed throughout the paper. We also write B_ρ for the ball with radius ρ centered at the origin and denote by v_ρ its volume.

$\mathrm{Lip}(f)$ denotes the smallest Lipschitz constant of our target L-Lipschitz function $f\colon \mathcal{X} \to \mathbb{R}$. The set of its ε-optimal points is denoted by $\mathcal{X}_\varepsilon := \{\boldsymbol{x} \in \mathcal{X} : \max(f) - f(\boldsymbol{x}) \le \varepsilon\}$, its complement (i.e., the set of *ε-suboptimal points*) by $\mathcal{X}_\varepsilon^c$, and for all $0 \le a < b$, the $(a, b]$-*layer* (i.e., the set of points that are b-optimal but a-suboptimal) by $\mathcal{X}_{(a,b]} := \mathcal{X}_a^c \cap \mathcal{X}_b = \big\{\boldsymbol{x} \in \mathcal{X} : a < f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) \le b\big\}$. Since f is L-Lipschitz, every point in $\mathcal{X}$ is ε_0-optimal, with ε_0 defined by $\varepsilon_0 := L \max_{\boldsymbol{x},\boldsymbol{y}\in\mathcal{X}} \|\boldsymbol{x} - \boldsymbol{y}\|$. In other words, $\mathcal{X}_{\varepsilon_0} = \mathcal{X}$. For this reason, without loss of generality, we will only consider values of accuracy ε smaller than or equal to ε_0.

For any bounded set $E \subset \mathbb{R}^d$ and all $r > 0$, the *r-packing number* of E is the largest cardinality of an r-packing of E, that is, $\mathcal{N}(E, r) := \sup\big\{k \in \mathbb{N}^* : \exists \boldsymbol{x}_1, \dots, \boldsymbol{x}_k \in E, \min_{i\neq j} \|\boldsymbol{x}_i - \boldsymbol{x}_j\| > r\big\}$ if E is nonempty, zero otherwise; the *r-covering number* of E is the smallest cardinality of an r-covering of E, i.e., $\mathcal{M}(E, r) := \min\big\{k \in \mathbb{N}^* : \exists \boldsymbol{x}_1, \dots, \boldsymbol{x}_k \in \mathbb{R}^d, \forall \boldsymbol{x} \in E, \exists i \in [k], \|\boldsymbol{x} - \boldsymbol{x}_i\| \le r\big\}$ if E is nonempty, zero otherwise. Well-known and useful properties of packing (and covering) numbers are recalled in Section A of the Supplementary Material.

2 Warmup: Certified DOO Has Sample Complexity $S_{\mathrm{C}}(f, \varepsilon)$

In this section, we start by adapting the well-known DOO algorithm (Perevozchikov, 1990; Munos, 2011) to the certified setting. We then bound its sample complexity by the quantity $S_{\mathrm{C}}(f, \varepsilon)$ defined in Eq. (5). In passing, we slightly improve the packing arguments used by Munos (2011) in the non-certified setting (Supplementary Material, Section E). In Section 4, we will prove that this rate is optimal (up to logarithmic factors) for certified algorithms.

The certified DOO algorithm (c.DOO, Algorithm 1) is defined for a fixed $K \in \mathbb{N}^\star$, by an infinite sequence of subsets of $\mathcal{X}$ of the form $(X_{h,i})_{h\in\mathbb{N}, i=0,\dots,K^h-1}$, called *cells*. For each $h \in \mathbb{N}$, the cells $X_{h,0}, \dots, X_{h,K^h-1}$ are non-empty, pairwise disjoint, and their union contains $\mathcal{X}$. The sequence $(X_{h,i})_{h\in\mathbb{N}, i=0,\dots,K^h-1}$ is associated with a K-ary tree in the following way. For any $h \in \mathbb{N}$ and $j \in \{0, \dots, K^h - 1\}$, there exist K distinct $i_1, \dots, i_K \in \{0, \dots, K^{h+1} - 1\}$ such that $X_{h+1,i_1}, \dots, X_{h+1,i_K}$ form a partition of $X_{h,j}$. We call $(h + 1, i_1), \dots, (h + 1, i_K)$ the *children* of (h, j). To each cell $X_{h,i}$ ($h \in \mathbb{N}$, $i \in \{0, \dots, K^h - 1\}$) is associated a *representative* $\boldsymbol{x}_{h,i} \in X_{h,i}$, which can be thought of as the "center" of the cell. We assume that feasible cells have feasible representatives, i.e., that $X_{h,i} \cap \mathcal{X} \neq \varnothing$ implies $\boldsymbol{x}_{h,i} \in \mathcal{X}$. The two following assumptions prescribe a sufficiently good behavior of the sequences of cells and representatives.

Assumption 2. *There exist two positive constants $\delta \in (0, 1)$ and $R > 0$ such that, for any cell $X_{h,i}$ ($h \in \mathbb{N}$, $i = 0, \dots, K^h - 1$) and all $\boldsymbol{u}, \boldsymbol{v} \in X_{h,i}$, it holds that $\|\boldsymbol{u} - \boldsymbol{v}\| \le R\delta^h$.*

Assumption 3. *There exists $\nu > 0$ such that, with δ as in Assumption 2, for any $h \in \mathbb{N}$, $i = 0, \dots, K^h - 1$, $h' \in \mathbb{N}$, $i' = 0, \dots, K^{h'} - 1$, with $(h, i) \neq (h', i')$, $\|\boldsymbol{x}_{h,i} - \boldsymbol{x}_{h',i'}\| \ge \nu\delta^{\max(h,h')}$.*

The classic Assumption 2 is simply stating that diameters of cells decrease geometrically with the depth of the tree. Assumption 3, which is key for our improved analysis, is slightly stronger than the corresponding one in Munos (2011), yet very easy to satisfy. Indeed, one can prove that for any compact $\mathcal{X}$, it is always possible to find a sequence of cells and representatives satisfying Assumptions 2 and 3. For instance, if $\mathcal{X}$ is the unit hypercube $[0, 1]^d$ and $\|\cdot\|$ is the supremum norm $\|\cdot\|_\infty$, we can define cells by bisection, letting $K = 2^d$, $X_{h,i}$ be a hypercube of edge-length 2^{-h}, and $\boldsymbol{x}_{h,i}$ be its center (for $h \in \mathbb{N}$ and $i = 0, \dots, 2^{dh} - 1$). In this case, Assumptions 2 and 3 are satisfied with $R = 1$ and $\delta = \nu = 1/2$.

Our certified version of the DOO algorithm (c.DOO, Algorithm 1) maintains a set of indices of *active* cells $\mathcal{L}_n$ throughout rounds n. During each iteration k, it selects the index of the most promising active cell $(h^\star, i^\star)$ (Line 5) and splits it into its K children $\mathcal{L}_+$ (Line 6). Then, it sequentially picks the representatives of the cells corresponding to each of these children (Line 10), observes the value of the target function f at these points (Line 11), recommends the point with the highest observed value of f (Line 12), and outputs a certificate $\xi_n = \big(f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star}\big) - f(\boldsymbol{x}_n^\star)$ (Line 13) that is the difference between an upper bound on f and the currently recommended value $f(\boldsymbol{x}_n^\star)$. In the meantime, all children in $\mathcal{L}_+$ are added to the set of active indices $\mathcal{L}_n$ (Line 9), and the current iteration is concluded by removing $(h^\star, i^\star)$ from $\mathcal{L}_n$ (Line 14), now that it has been replaced by its refinement $\mathcal{L}_+$.

Algorithm 1: Certified DOO (c.DOO)

input: $\mathcal{X}$, L, K, δ, R, cells $(X_{h,i})_{h\in\mathbb{N},i=0,\dots,K^h-1}$, representatives $(\boldsymbol{x}_{h,i})_{h\in\mathbb{N},i=0,\dots,K^h-1}$
initialization: let $n \leftarrow 1$ and $\mathcal{L}_1 \leftarrow \{(0,0)\}$
1 pick the first query point $\boldsymbol{x}_1 \leftarrow \boldsymbol{x}_{0,0}$
2 observe the value $f(\boldsymbol{x}_1)$
3 output recommendation $\boldsymbol{x}_1^\star \leftarrow \boldsymbol{x}_1$ and error certificate $\xi_1 \leftarrow LR$
4 **for** *iteration* $k = 1, 2, \dots$ **do**
5 let $(h^\star, i^\star) \in \operatorname{argmax}_{(h,i)\in\mathcal{L}_n} \{f(\boldsymbol{x}_{h,i}) + LR\delta^h\}$ `// ties broken arbitrarily`
6 let $\mathcal{L}_+$ be the set of the K children of $(h^\star, i^\star)$
7 **for each** *child* $(h^\star+1, j) \in \mathcal{L}_+$ *of* $(h^\star, i^\star)$ **do**
8 **if** $X_{h^\star+1,j} \cap \mathcal{X} \neq \varnothing$ **then**
9 let $n \leftarrow n+1$ and $\mathcal{L}_n \leftarrow \mathcal{L}_{n-1} \cup \{(h^\star+1, j)\}$
10 pick the next query point $\boldsymbol{x}_n \leftarrow \boldsymbol{x}_{h^\star+1,j}$
11 observe the value $f(\boldsymbol{x}_n)$
12 output a recommendation $\boldsymbol{x}_n^\star \in \operatorname{argmax}_{\boldsymbol{x}\in\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_n\}} f(\boldsymbol{x})$
13 output the error certificate $\xi_n \leftarrow f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star} - f(\boldsymbol{x}_n^\star)$
14 remove $(h^\star, i^\star)$ from $\mathcal{L}_n$

Remark 1. *The running-time of* c.DOO *(ignoring the cost of calling the function f) is driven by the computation of the recommendation $\boldsymbol{x}_n^\star \in \operatorname{argmax}_{\boldsymbol{x}\in\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_n\}} f(\boldsymbol{x})$ (Line 12) and the search of the index of the most promising active cell $(h^\star, i^\star) \in \operatorname{argmax}_{(h,i)\in\mathcal{L}_n} \{f(\boldsymbol{x}_{h,i}) + LR\delta^h\}$ (Line 5). The recommendation $\boldsymbol{x}_n^\star$ can be computed sequentially in constant time (by comparing the new value $f(\boldsymbol{x}_n)$ with the current maximum). In Line 5, the leaf $(h^\star, i^\star)$ to be split at iteration k can be computed sequentially in logarithmic time (using a max-heap structure). Therefore, the running time of* c.DOO *is of order $n\log(n)$ in the number n of evaluations of the function f.*

The next proposition shows that the sample complexity of the certified DOO algorithm is upper bounded (up to constants) by the instance-dependent quantity $S_{\mathrm{C}}(f,\varepsilon)$ introduced in Eq. (5).

Proposition 1. *If Assumptions 2 and 3 hold, then Algorithm 1 is a certified algorithm and letting $a := 1 + K\big(\mathbf{1}_{\nu/R\geq 1} + \mathbf{1}_{\nu/R<1}(4R/\nu)^d\big)$, its sample complexity satisfies, for all Lipschitz functions $f \in \mathcal{F}_L$ and any accuracy $\varepsilon \in (0, \varepsilon_0]$,*

$$\sigma(\text{c.DOO}, f, \varepsilon) \leq a S_{\mathrm{C}}(f,\varepsilon)\ .$$

The proof is postponed to Section B of the Supplementary Material and shares some arguments with those of Perevozchikov (1990) and Munos (2011), originally written for the non-certified setting. The key change is to partition the values of f, instead of its domain $\mathcal{X}$ at any depth h of the tree (see Munos 2011), when counting the representatives selected at all levels. The idea of using layers $\mathcal{X}_{(\varepsilon_i,\ \varepsilon_{i-1}]}$ was already present in Kleinberg et al. (2008, 2019) and Bouttier et al. (2020) for more computationally challenging algorithms (see discussion in Section 1.3).

3 Characterization of $S_{\mathrm{C}}(f,\varepsilon)$

Earlier, we mentioned that the quantity $S_{\mathrm{C}}(f,\varepsilon)$ introduced in Eq. (5) upper bounds the sample complexity of several certified algorithms, such as c.DOO or Piyavskii-Shubert. In this section, we provide a characterization of this quantity in terms of a much cleaner and compact integral expression.

This result is inspired by Hansen et al. (1991), that in dimension $d = 1$, derive an elegant bound on the sample complexity $\sigma(\text{PS}, f, \varepsilon)$ of the certified Piyavskii-Shubert algorithm for any Lipschitz function f and accuracy ε. They proved that $\sigma(\text{PS}, f, \varepsilon)$ is upper bounded by $\int_0^1 \mathrm{d}x/(f(x^\star) - f(x) + \varepsilon)$ up to constants. However, the authors rely heavily on the one-dimensional assumption and the specific form of the Piyavskii-Shubert algorithm in this setting, stating that the task of "*Extending the results of this paper to the multivariate case appears to be difficult*". In this section, we show an equivalence between $S_{\mathrm{C}}(f,\varepsilon)$ and this type of integral bound in any dimension d. Putting this

together with a recent result of Bouttier et al. (2020) (which proves that up to constants, $\sigma(\mathrm{PS}, f, \varepsilon) \leq S_{\mathrm{C}}(f, \varepsilon)$) solves the long-standing problem raised by Hansen et al. (1991) three decades ago.

To tame the wild spectrum of shapes that compact subsets may have, we will assume that $\mathcal{X}$ satisfies the following mild geometric assumption. At a high level, it says that a constant fraction of each (sufficiently small) ball centered at a point in $\mathcal{X}$ is included in $\mathcal{X}$. This removes sets containing isolated points or cuspidal corners and includes most domains that are typically used, such as non-degenerate polytopes, ellipsoids, finite unions of them, etc. This natural assumption is weaker than the classic rolling ball assumption from the statistics literature (Cuevas et al., 2012; Walther, 1997) and has already been proved useful in the past (Hu et al., 2020).

Assumption 4. *There exist two constants $r_0 > 0, \gamma \in (0, 1]$ such that, for any $\boldsymbol{x} \in \mathcal{X}$ and all $r \in (0, r_0)$, $\mathrm{vol}\big(B_r(\boldsymbol{x}) \cap \mathcal{X}\big) \geq \gamma v_r$.*

We can now state the main result of this section. Its proof relies on some additional technical results that are deferred to the Supplementary Material.

Theorem 1. *For any Lipschitz function $f \in \mathcal{F}_L$, if Assumption 4 holds with $r_0 > \varepsilon_0/2L, \gamma \in (0, 1]$,[2] then there exist $c, C > 0$ (e.g., $c := 1/v_{1/L}$ and $C := 1/(\gamma v_{1/128L})$) such that, for all $\varepsilon \in (0, \varepsilon_0]$,*

$$c \int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} \leq S_{\mathrm{C}}(f, \varepsilon) \leq C \int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} \,.$$

Proof. Fix any $\varepsilon \in (0, \varepsilon_0]$ and recall that $m_\varepsilon := \big\lceil \log_2(\varepsilon_0/\varepsilon) \big\rceil$, $\varepsilon_{m_\varepsilon} := \varepsilon$, and for all $k \leq m_\varepsilon - 1$, $\varepsilon_k := \varepsilon_0 2^{-k}$. Partition the domain of integration $\mathcal{X}$ into the following $m_\varepsilon + 1$ sets: the set of ε-optimal points $\mathcal{X}_\varepsilon$ and the m_ε layers $\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}$, for $k \in [m_\varepsilon]$. We begin by proving the first inequality:

$$\begin{aligned}
\int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} &\leq \frac{\mathrm{vol}(\mathcal{X}_\varepsilon)}{\varepsilon^d} + \sum_{k=1}^{m_\varepsilon} \frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\big)}{(\varepsilon_k + \varepsilon)^d} \\
&\leq \frac{\mathcal{M}\big(\mathcal{X}_\varepsilon,\, \frac{\varepsilon}{L}\big) \cdot v_1 \big(\frac{\varepsilon}{L}\big)^d}{\varepsilon^d} + \sum_{k=1}^{m_\varepsilon} \frac{\mathcal{M}\big(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\big) \cdot v_1 \big(\frac{\varepsilon_k}{L}\big)^d}{\varepsilon_k^d} \\
&\leq \frac{v_1}{L^d} \left(\mathcal{N}\left(\mathcal{X}_\varepsilon,\, \frac{\varepsilon}{L}\right) + \sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right) \right) \,,
\end{aligned}$$

where the first inequality follows by lower bounding $f(\boldsymbol{x}^\star) - f$ with its infimum on the partition, the second one by dropping $\varepsilon > 0$ from the second denominator and upper bounding the volume of a set with the volume of the balls of a smallest ε_k/L-cover, and the last one by the fact that covering numbers are always smaller than packing numbers (we recall this known result in the Supplementary Material, Lemma 1, Eq. (8)). This proves the first part of the theorem.

For the second one, we have

$$\begin{aligned}
\int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\big(f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) + \varepsilon\big)^d} &\geq \frac{\mathrm{vol}(\mathcal{X}_\varepsilon)}{(\varepsilon + \varepsilon)^d} + \sum_{k=1}^{m_\varepsilon} \frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\big)}{(\varepsilon_{k-1} + \varepsilon)^d} \\
&\geq \frac{1}{2^d} \frac{\mathrm{vol}(\mathcal{X}_\varepsilon)}{\varepsilon^d} + \frac{1}{4^d} \sum_{k=1}^{m_\varepsilon} \frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\big)}{\varepsilon_k^d} \geq \frac{1}{32^d} \left(\frac{\mathrm{vol}(\mathcal{X}_{2\varepsilon})}{\varepsilon^d} + \sum_{k=1}^{m_\varepsilon} \frac{\mathrm{vol}\left(\mathcal{X}_{\left(\frac{1}{2}\varepsilon_k,\, 2\varepsilon_{k-1}\right]}\right)}{\varepsilon_{k-1}^d} \right) \\
&\geq \frac{\mathcal{N}\left(\mathcal{X}_\varepsilon,\, \frac{\varepsilon}{L}\right) \mathrm{vol}\left(\frac{\varepsilon}{2L} B_1\right)}{(32\,\varepsilon)^d/\gamma} + \sum_{k=1}^{m_\varepsilon} \frac{\mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right) \mathrm{vol}\left(\frac{\varepsilon_k}{2L} B_1\right)}{(32\,\varepsilon_{k-1})^d/\gamma} \\
&\geq \gamma v_{1/64L} \mathcal{N}\left(\mathcal{X}_\varepsilon,\, \frac{\varepsilon}{L}\right) + \gamma v_{1/128L} \sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right) \,,
\end{aligned}$$

[2] We actually prove a stronger result. The first inequality holds more generally for any f that is L-Lipschitz around a maximizer and Lebesgue-measurable, and does not require $\mathcal{X}$ to satisfy Assumption 4.

where the first inequality follows by upper bounding $f(\boldsymbol{x}^\star) - f$ with its supremum on the partition, the second one by $\varepsilon \leq \varepsilon_{k-1}$ (for all $k \in [m_\varepsilon + 1]$) and $\varepsilon_{k-1} \leq 2\varepsilon_k$ (for all $k \in [m_\varepsilon]$), the third one by lower bounding the sum of disjoint layers with that of overlapping ones (proved in the Supplementary Material, Lemma 3), and the fourth one by the elementary inclusions $\mathcal{X}_{2\varepsilon} \supseteq \mathcal{X}_{\frac{3}{2}\varepsilon}$ and $\mathcal{X}_{\left(\frac{1}{2}\varepsilon_k,\, 2\varepsilon_{k-1}\right]} \supseteq \mathcal{X}_{\left(\frac{1}{2}\varepsilon_k,\, \frac{3}{2}\varepsilon_{k-1}\right]}$ (for all $k \in [m_\varepsilon]$) followed by a relationship between packing numbers and volumes (proved in the Supplementary Material, Proposition 4) that holds under Assumption 4. □

4 Optimality of $S_{\mathrm{C}}(f, \varepsilon)$

We begin this section by proving an f-dependent lower bound on the sample complexity of certified algorithms that matches the upper bound $S_{\mathrm{C}}(f, \varepsilon)$ on the sample complexity of the c.DOO algorithm (Proposition 1), up to a $\log(1/\varepsilon)$ term.

The proof of this result differs from those of traditional worst-case lower bounds. The idea is to build a *local* worst-case analysis, introducing a weaker notion of sample complexity τ that is smaller than $\sigma(A, f, \varepsilon)$. Then we further lower bound this quantity by finding adversarial perturbations of the target function f with the following opposing properties. First, these perturbations have to be similar enough to f so that running A on them would return the same recommendations for sufficiently many rounds. Second, they have to be different enough from f so that enough rounds have to pass before being able to certify sub-ε accuracy. We recall that $m_\varepsilon := \lceil \log_2(\varepsilon_0/\varepsilon) \rceil$.

Theorem 2. *The sample complexity of any certified algorithm A satisfies*

$$\sigma(A, f, \varepsilon) > \frac{c}{1 + m_\varepsilon} S_{\mathrm{C}}(f, \varepsilon)$$

for any Lipschitz function $f \in \mathcal{F}_L$ and all $\varepsilon \in (0, \varepsilon_0]$, where $c := 2^{-2}\big(2^{-7}\big(1 - \mathrm{Lip}(f)/L\big)\big)^d$.

Proof. Fix any $f \in \mathcal{F}_L$ and an accuracy $\varepsilon \in (0, \varepsilon_0]$. We begin by defining the tightest error certificate that a certified algorithm A could return based on its first n observations of f. Formally,

$$\mathrm{err}_n(A) := \sup\big\{\max(g) - g(\boldsymbol{x}_n^\star) : g \text{ is } L\text{-Lipschitz and } f(\boldsymbol{x}) = g(\boldsymbol{x}) \text{ for all } x \in \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}\big\}$$

where $\boldsymbol{x}_i = \boldsymbol{x}_i(A, f)$ and $\boldsymbol{x}_i^\star = \boldsymbol{x}_i^\star(A, f)$ are the query and recommendation points chosen by A at time i when run on f (to lighten the notation, we omit the explicit dependencies on A and f of $\boldsymbol{x}_i$ and $\boldsymbol{x}_i^\star$). In particular, $\max(f) - f(\boldsymbol{x}_n^\star) \leq \mathrm{err}_n(A)$. Based on this quantity, we define a corresponding notion of optimal sample complexity τ as the smallest number of rounds n that the best certified algorithm A' needs in order to guarantee that $\mathrm{err}_n(A') \leq \varepsilon$. Formally,

$$\tau := \min\big\{n \in \mathbb{N}^* : \inf_{A'}\big(\mathrm{err}_n(A')\big) \leq \varepsilon\big\}\,, \tag{7}$$

where the infimum is over all certified algorithms A'. It is immediate to prove that τ is finite, by considering an algorithm that queries a dense sequence of points (independently of the observed function values) and outputs a recommendation that maximizes the observed values.

Crucially, τ lower bounds the sample complexity $\sigma(A, f, \varepsilon)$ of any certified algorithm A. At a high level, this makes intuitive sense because τ guarantees a weaker property: that the best certificate of the best algorithm is small, while $\sigma(A, f, \varepsilon)$ controls the certificate of the specific algorithm A. We defer a formal proof of this statement to the Supplementary Material, Section D.1. Since $\sigma(A, f, \varepsilon) \geq \tau$, to prove the theorem it is sufficient to show that

$$\tau > \frac{c}{1 + m_\varepsilon} S_{\mathrm{C}}(f, \varepsilon)\,.$$

Let $K := 16L/\big(L - \mathrm{Lip}(f)\big)$. If $S_{\mathrm{C}}(f, \varepsilon)/(1 + m_\varepsilon) < 3(8K)^d$, then $\tau \geq 1 > 3/4 > cS_{\mathrm{C}}(f, \varepsilon)/(1 + m_\varepsilon)$. Assume from now on that $S_{\mathrm{C}}(f, \varepsilon)/(1 + m_\varepsilon) \geq 3(8K)^d$.

The idea now is to upper bound the sum of $1 + m_\varepsilon$ packing numbers that define $S_{\mathrm{C}}(f, \varepsilon)$ in (5) with the largest one multiplied by $1 + m_\varepsilon$. This way, $S_{\mathrm{C}}(f, \varepsilon)/(1 + m_\varepsilon)$ can be controlled by (an upper bound of) the largest summand in

$S_{\mathrm{C}}(f,\varepsilon)$. Let $\tilde{\varepsilon}$ be the scale achieving the maximum in (5), that is

$$\tilde{\varepsilon} = \begin{cases} \varepsilon\,, & \text{if } \mathcal{N}\left(\mathcal{X}_\varepsilon,\ \frac{\varepsilon}{L}\right) \geq \max_{i\in\{1,\dots,m_\varepsilon\}} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\ \varepsilon_{i-1}]},\ \frac{\varepsilon_i}{L}\right)\,, \\ \varepsilon_{i^\star-1}\,, & \text{otherwise, where } i^\star \in \operatorname{argmax}_{i\in\{1,\dots,m_\varepsilon\}} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\ \varepsilon_{i-1}]},\ \frac{\varepsilon_i}{L}\right)\,. \end{cases}$$

Since $\mathcal{N}\left(\mathcal{X}_\varepsilon,\ \varepsilon/L\right) \leq \mathcal{N}\left(\mathcal{X}_\varepsilon,\ \varepsilon/2L\right)$ and $\mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\ \varepsilon_{i-1}]},\ \varepsilon_i/L\right) \leq \mathcal{N}\left(\mathcal{X}_{\ \varepsilon_{i-1}},\ \varepsilon_{i-1}/2L\right)$, we then have $S_{\mathrm{C}}(f,\varepsilon) \leq (m_\varepsilon+1)\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ \tilde{\varepsilon}/2L\right)$. Let now $n \leq cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$. We then have $n \leq c\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ \tilde{\varepsilon}/2L\right)$. From a known property of packing numbers (Supplementary Material, Lemma 2),

$$\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ \frac{K\tilde{\varepsilon}}{L}\right) \geq \left(\frac{1}{8K}\right)^d \mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ \frac{\tilde{\varepsilon}}{2L}\right) \geq \left(\frac{1}{8K}\right)^d \frac{S_{\mathrm{C}}(f,\varepsilon)}{m_\varepsilon+1} \geq 3\,,$$

by our initial assumption. Then we have $n \leq c(8K)^d\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ K\tilde{\varepsilon}/L\right)$. Since $c(8K)^d = 1/4$, we thus obtain $n \leq \mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ K\tilde{\varepsilon}/L\right) - 2$.

Consider a certified algorithm A for L-Lipschitz functions. Fix a $(K\tilde{\varepsilon}/L)$-packing $\tilde{\boldsymbol{x}}_1,\dots,\tilde{\boldsymbol{x}}_N$ of $\mathcal{X}_{\tilde{\varepsilon}}$ with cardinality $N = \mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\ K\tilde{\varepsilon}/L\right)$. Then the open balls of centers $\tilde{\boldsymbol{x}}_1,\dots,\tilde{\boldsymbol{x}}_N$ and radius $K\tilde{\varepsilon}/2L$ are disjoint and two of them, with centers, say, $\tilde{\boldsymbol{x}}_1$ and $\tilde{\boldsymbol{x}}_2$, do not contain any of the points $\boldsymbol{x}_1,\dots,\boldsymbol{x}_n$ queried by A when it is run on f. Let, for $\boldsymbol{x}\in\mathcal{X}$,

$$g_{\tilde{\varepsilon}}(\boldsymbol{x}) := \left(8\tilde{\varepsilon} - \tfrac{16L}{K}\left\|\boldsymbol{x}-\tilde{\boldsymbol{x}}_1\right\|\right)\mathbb{I}\left\{\boldsymbol{x}\in\mathcal{X}\cap B_{K\tilde{\varepsilon}/2L}(\tilde{\boldsymbol{x}}_1)\right\}\,.$$

Then $g_{\tilde{\varepsilon}}(x)$ is $16L/K = L - \mathrm{Lip}(f)$ Lipschitz. Hence $f+g_{\tilde{\varepsilon}}$ and $f-g_{\tilde{\varepsilon}}$ are L-Lipschitz. Note that f, $f+g_{\tilde{\varepsilon}}$ and $f-g_{\tilde{\varepsilon}}$ coincide on the points $\boldsymbol{x}_1,\dots,\boldsymbol{x}_n$ that A queries when it is run on f. As a consequence, A queries the same points and returns the same recommendation $\boldsymbol{x}_n^\star$ when it is run on any of the three functions f, $f+g_{\tilde{\varepsilon}}$, and $f-g_{\tilde{\varepsilon}}$.

Consider first the case $\boldsymbol{x}_n^\star \in B(\tilde{\boldsymbol{x}}_1, K\tilde{\varepsilon}/4L)$. Then, we have, by definition of $g_{\tilde{\varepsilon}}$ and the fact that $\tilde{\boldsymbol{x}}_2 \in \mathcal{X}_{\tilde{\varepsilon}}$, $f(\tilde{\boldsymbol{x}}_2) - g_{\tilde{\varepsilon}}(\tilde{\boldsymbol{x}}_2) - f(\boldsymbol{x}_n^\star) + g_{\tilde{\varepsilon}}(\boldsymbol{x}_n^\star) \geq -\tilde{\varepsilon} + 8\tilde{\varepsilon} - \frac{16L}{K}\frac{K\tilde{\varepsilon}}{4L} = 3\tilde{\varepsilon}$.

Now consider the case $\boldsymbol{x}_n^\star \notin B(\tilde{\boldsymbol{x}}_1, K\tilde{\varepsilon}/4L)$. Then, we have, by definition of $g_{\tilde{\varepsilon}}$ and the fact that $\tilde{\boldsymbol{x}}_1 \in \mathcal{X}_{\tilde{\varepsilon}}$, $f(\tilde{\boldsymbol{x}}_1) + g_{\tilde{\varepsilon}}(\tilde{\boldsymbol{x}}_1) - f(\boldsymbol{x}_n^\star) - g_{\tilde{\varepsilon}}(\boldsymbol{x}_n^\star) \geq -\tilde{\varepsilon} + 8\tilde{\varepsilon} - 8\tilde{\varepsilon} + \frac{16L}{K}\frac{K\tilde{\varepsilon}}{4L} = 3\tilde{\varepsilon}$.

Therefore, in both cases $\mathrm{err}_n(A) \geq 3\tilde{\varepsilon} > \varepsilon$. Repeating the same construction from any other certified algorithm A', we obtain that $\inf_{A'}\left(\mathrm{err}_n(A')\right) > \varepsilon$. Since this has been shown for any $n \leq cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$, by definition of τ we can conclude that $\tau > cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$. □

Putting together Proposition 1 and Theorem 2 shows that the sample complexity of c.DOO applied to any Lipschitz function $f\in\mathcal{F}_L$ is of order $S_{\mathrm{C}}(f,\varepsilon)$ and no certified algorithm A can do better, *not even if A knows f exactly*. This is a striking difference with the classical non-certified setting in which the best algorithm for each fixed function f has trivially sample complexity 1. In particular, for non-pathological sets $\mathcal{X}$, combining Proposition 1 and Theorem 2 with Theorem 1 gives the following compact characterization of the optimal sample complexity of certified algorithms.

Theorem 3. *Let $L>0$ and suppose that Assumption 4 holds with $r_0 > \varepsilon_0/2L$. Then, there exist two constants $c', C > 0$ such that, for all Lipschitz functions $f\in\mathcal{F}_L$ and any accuracy $\varepsilon\in(0,\varepsilon_0]$, letting $c := c'(1-\mathrm{Lip}(f)/L)^d/(1+\log(\varepsilon_0/\varepsilon))$, the optimal sample complexity of any certified algorithm A satisfies*

$$c\int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\left(f(\boldsymbol{x}^\star)-f(\boldsymbol{x})+\varepsilon\right)^d} \leq \inf_A \sigma(A,f,\varepsilon) \leq \sigma(\text{c.DOO},f,\varepsilon) \leq C\int_{\mathcal{X}} \frac{\mathrm{d}\boldsymbol{x}}{\left(f(\boldsymbol{x}^\star)-f(\boldsymbol{x})+\varepsilon\right)^d}\,.$$

For the sake of completeness, we conclude the section by briefly discussing the boundary case in which $L = \mathrm{Lip}(f)$, i.e., when the best Lipschitz constant of the target function is known exactly by the algorithm. As we mentioned earlier, this case is not of great relevance in practice, as one can hardly think of a scenario in which f is unknown but the learner has somehow perfect knowledge of its smallest Lipschitz constant $\mathrm{Lip}(f)$. It could, however, be of some theoretical interest.

The dependence of the sample complexity on $1 - L/\mathrm{Lip}(f)$ in Theorem 2 suggests that the problem becomes easier the closer L gets to $\mathrm{Lip}(f)$, and, when $L = \mathrm{Lip}(f)$, constant sample complexity could be achieved. The next result gives some formal evidence for this intuition in dimension $d\geq 2$.

Proposition 2. *Let $d\geq 2$, $\mathcal{X} := B_1$, and $\|\cdot\|$ be a norm. The certified Piyavskii-Shubert algorithm* PS *with initial guess $\boldsymbol{x}_1 := \mathbf{0}$ is a certified algorithm satisfying, for the L-Lipschitz function $f := L\|\cdot\|$ and any $\varepsilon\in(0,\varepsilon_0)$, $\sigma(\mathrm{PS},f,\varepsilon) = 2 \ll c/\varepsilon^{d-1} \leq S_{\mathrm{C}}(f,\varepsilon)$, for some constant $c>0$.*

For a full proof and a refresher on the PS algorithm, see Section D.2 of the Supplementary Material. The next result shows that, surprisingly, the sample complexity in dimension $d = 1$ behaves differently. In this case, $S_{\mathrm{C}}(f, \varepsilon)$ remains a lower bound even when $L = \mathrm{Lip}(f)$. More precisely, the following proposition holds. Its proof is deferred to Section D.3 of the Supplementary Material.

Proposition 3. *If $d = 1$, let $c = 2^{-8}/3$. Then, the sample complexity of any certified algorithm A satisfies, for any L-Lipschitz function f and all $\varepsilon \in (0, \varepsilon_0]$, $\sigma(A, f, \varepsilon) > cS_{\mathrm{C}}(f, \varepsilon)/(1 + m_\varepsilon)$.*

5 Conclusions

In this paper, we studied the sample complexity of certified zeroth-order Lipschitz optimization. We first showed that the sample complexity of the computationally tractable c.DOO algorithm scales with the quantity $S_{\mathrm{C}}(f, \varepsilon)$ introduced in Eq. (5) (Proposition 1). We then characterized this quantity in terms of the compact integral expression $\int_{\mathcal{X}} \mathrm{d}\boldsymbol{x}/(\max(f) - f(\boldsymbol{x}) + \varepsilon)^d$ (Theorem 1), solving as a corollary a long-standing open problem in Hansen et al. (1991). Finally we proved an instance-dependent lower bound (Theorem 2) showing that this integral characterizes (up to $\log$ factors) the optimal sample complexity of certified zeroth-order Lipschitz optimization in any dimensions $d \geq 1$ whenever the smallest Lipschitz constant of f is not known exactly by the algorithm (Theorem 3).

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Instance-Dependent Bounds for Zeroth-order Lipschitz Optimization with Error Certificates

Supplementary Material

A Useful Results on Packing and Covering

For the sake of completeness, we recall the definitions of packing and covering numbers, as well as some known useful results.

Definition 1. *Fix any norm $\|\cdot\|$. For any non-empty and bounded subset E of $\mathbb{R}^d$ and all $r > 0$,*

- *the* r-packing number *of E is the largest cardinality of an r-packing of E, i.e.,*

$$\mathcal{N}(E, r) := \sup\big\{k \in \mathbb{N}^* : \exists \boldsymbol{x}_1, \dots, \boldsymbol{x}_k \in E, \min_{i \neq j} \|\boldsymbol{x}_i - \boldsymbol{x}_j\| > r\big\} ;$$

- *the* r-covering number *of E is the smallest cardinality of an r-covering of E, i.e.,*

$$\mathcal{M}(E, r) := \min\big\{k \in \mathbb{N}^* : \exists \boldsymbol{x}_1, \dots, \boldsymbol{x}_k \in \mathbb{R}^d, \forall \boldsymbol{x} \in E, \exists i \in [k], \|\boldsymbol{x} - \boldsymbol{x}_i\| \leq r\big\} .$$

We also define $\mathcal{N}(\varnothing, r) = \mathcal{M}(\varnothing, r) = 0$ for all $r > 0$.

Covering numbers and packing numbers are closely related. In particular, the following well-known inequalities hold—see, e.g., (Wainwright, 2019, Lemmas 5.5 and 5.7, with permuted notation of $\mathcal{M}$ and $\mathcal{N}$).[4]

Lemma 1. *Fix any norm $\|\cdot\|$. For any bounded set $E \subset \mathbb{R}^d$ and all $r > 0$,*

$$\mathcal{N}(E, 2r) \leq \mathcal{M}(E, r) \leq \mathcal{N}(E, r) . \tag{8}$$

Furthermore, for any $\delta > 0$ and all $r > 0$,

$$\mathcal{M}\left(B_\delta, r\right) \leq \left(1 + 2\frac{\delta}{r}\mathbb{I}_{r<\delta}\right)^d . \tag{9}$$

We now state a known lemma about packing numbers at different scales. This is the go-to result for rescaling packing numbers.

Lemma 2. *Fix any norm $\|\cdot\|$. For any bounded $E \subset \mathbb{R}^d$ and all $0 < r_1 < r_2 < \infty$, we have*

$$\mathcal{N}\left(E, r_1\right) \leq \left(4\frac{r_2}{r_1}\right)^d \mathcal{N}\left(E, r_2\right) .$$

Proof. Fix any bounded $E \subset \mathbb{R}^d$ and $0 < r_1 < r_2 < \infty$. Consider an r_1-packing $F = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_{N_1}\}$ of E with cardinality $N_1 = \mathcal{N}\left(E, r_1\right)$. Consider then the following iterative procedure. Let $F_0 = F$ and initialize $k = 1$. While F_{k-1} is non-empty, let $\boldsymbol{y}_k$ be any point in F_{k-1}, let F_k be obtained from F_{k-1} by removing the points at $\|\cdot\|$-distance less or equal to r_2 from $\boldsymbol{y}_k$ (including $\boldsymbol{y}_k$ itself), and increase k by one. Then this procedure yields an r_2-packing of E with cardinality equal to the number of steps (the final value k_{fin} of k). At each step k, the balls with radius $r_1/2$ centered at points that are removed at this step are included in the ball with radius $2r_2$ centered at $\boldsymbol{y}_k$. By a volume argument, then, the number of removed points at each step is smaller than or equal to $v_{2r_2}/v_{r_1/2} = (4r_2/r_1)^d$. Hence the total number of steps k_{fin} is greater than or equal to $\mathcal{N}\left(E, r_1\right)(r_1/4r_2)^d$. This concludes the proof since $\mathcal{N}\left(E, r_2\right)$ is greater than or equal to the total number of steps k_{fin}. □

[4] The definition of r-covering number of a subset E of $\mathbb{R}^d$ implied by (Wainwright, 2019, Definition 5.1) is slightly stronger than the one used in our paper, because elements $x_1, \dots, x_N$ of r-covers belong to E rather than just $\mathbb{R}^d$. Even if we do not need it for our analysis, Inequality (9) holds also in this stronger sense.

B Missing Proofs of Section 2

In Section 2, we introduced a certified version of the DOO algorithm. To prove Proposition 1, we adapt and slightly improve (see Remark 2) some of the arguments in Munos (2011), showing that the sample complexity of c.DOO is upper bounded (up to constants) by $S_{\mathrm{C}}(f, \varepsilon)$, defined in Eq. (5).

Proof of Proposition 1. Recall that f is an L-Lipschitz function with a global maximizer $\boldsymbol{x}^\star$.

Let us first show that Algorithm 1 is indeed a certified algorithm, that is, $f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_n) \leq \xi_n$ for all $n \geq 1$. Note that $f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_1) \leq LR = \xi_1$, since f is L-Lipschitz and R bounds the diameter of $X_{0,0} \supset \mathcal{X}$. So, take any $n \geq 2$. Consider the state of the algorithm after exactly n evaluations of f. Let $(h^\star, i^\star)$ correspond to the last time that Line 5 was reached and let m be the total number of evaluations of f made up to that time ($m \leq n$). Then the error certificate is $\xi_n = f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star} - f(\boldsymbol{x}_n^\star)$. By induction, it is straightforward to show that the union of the cells in $\mathcal{L}_j$ contains $\mathcal{X}$ at all steps $j \in \mathbb{N}^\star$. Therefore, the global maximizer $\boldsymbol{x}^\star$ belongs to a cell $X_{\bar{h},\bar{i}}$ with $(\bar{h}, \bar{i}) \in \mathcal{L}_m$. We have, using first Line 5 and then Assumption 2 and that f is L-Lipschitz,

$$\begin{aligned} f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star} &\geq f(\boldsymbol{x}_{\bar{h},\bar{i}}) + LR\delta^{\bar{h}} \\ &\geq f(\boldsymbol{x}^\star) - LR\delta^{\bar{h}} + LR\delta^{\bar{h}} \\ &= f(\boldsymbol{x}^\star)\,. \end{aligned} \tag{10}$$

This shows $\xi_n \geq f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_n^\star)$. Hence Algorithm 1 is a certified algorithm.

We now show the upper bound on $\sigma(\text{c.DOO}, f, \varepsilon)$. Consider the infinite sequence $((h_\ell^\star, i_\ell^\star))_{\ell \in \mathbb{N}^*}$ of the leaves that are successively selected at Line 5 of Algorithm 1. For any leaf $(h, i) \in ((h_\ell^\star, i_\ell^\star))_{\ell \in \mathbb{N}^*}$, let $N_{h,i}$ be the number of evaluations of f made by Algorithm 1 until the leaf (h, i) is selected at Line 5. Define then the stopping time

$$I_\varepsilon = \inf\left\{ \ell \in \mathbb{N}^*; f(\boldsymbol{x}_{h_\ell^\star,i_\ell^\star}) + LR\delta^{h_\ell^\star} \leq \max_{i \in [N_{h_\ell^\star,i_\ell^\star}]} f(\boldsymbol{x}_i) + \varepsilon \right\}$$

which corresponds to the first iteration when the event

$$f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star} \leq \max_{i \in [N_{h^\star,i^\star}]} f(\boldsymbol{x}_i) + \varepsilon \tag{11}$$

holds at Line 5. Consider the N-th evaluation of f with $N = N_{h_{I_\varepsilon}^\star, i_{I_\varepsilon}^\star} + 1$, that is, the first evaluation of f after the event (11) holds for the first time. Then we have, from (11) with $(h^\star, i^\star) = (h_{I_\varepsilon}^\star, i_{I_\varepsilon}^\star)$,

$$f(\boldsymbol{x}_{h^\star,i^\star}) + LR\delta^{h^\star} \leq \max_{i \in [N_{h^\star,i^\star}]} f(\boldsymbol{x}_i) + \varepsilon \leq \max_{i \in [N]} f(\boldsymbol{x}_i) + \varepsilon,$$

and thus $\xi_N \leq \varepsilon$. Since by definition $\sigma(\text{c.DOO}, f, \varepsilon) = \min\{n \in \mathbb{N}^* : \xi_n \leq \varepsilon\}$, we have

$$\sigma(\text{c.DOO}, f, \varepsilon) \leq N = N_{h_{I_\varepsilon}^\star, i_{I_\varepsilon}^\star} + 1 \leq 2 + K(I_\varepsilon - 1)\,. \tag{12}$$

We now bound $I_\varepsilon - 1$ from above. Assume without loss of generality that $I_\varepsilon - 1 \geq 1$ and consider the sequence $(h_1^\star, i_1^\star), \ldots, (h_{I_\varepsilon-1}^\star, i_{I_\varepsilon-1}^\star)$ corresponding to the first $I_\varepsilon - 1$ times the DOO algorithm went through Line 5. Let $\mathcal{E}_\varepsilon$ be the corresponding finite set $\{\boldsymbol{x}_{h_1^\star,i_1^\star}, \ldots, \boldsymbol{x}_{h_{I_\varepsilon-1}^\star,i_{I_\varepsilon-1}^\star}\}$. Recall that $\varepsilon_{m_\varepsilon} := \varepsilon$ and $\varepsilon_i := \varepsilon_0 2^{-i}$ for $i < m_\varepsilon$, with $\varepsilon_0 := L \max_{\boldsymbol{x},\boldsymbol{y} \in \mathcal{X}} \|\boldsymbol{x} - \boldsymbol{y}\|$. Recall also that $\mathcal{X}_\varepsilon := \{\boldsymbol{x} \in \mathcal{X} : \max(f) - f(\boldsymbol{x}) \leq \varepsilon\}$ and for all $0 \leq a < b$, $\mathcal{X}_{(a,b]} := \{\boldsymbol{x} \in \mathcal{X} : a < f(\boldsymbol{x}^\star) - f(\boldsymbol{x}) \leq b\}$. Since any $\boldsymbol{x} \in \mathcal{X}$ is ε_0-optimal, then it either belongs to $\mathcal{X}_\varepsilon$ or one of the layers $\mathcal{X}_{(\varepsilon_i, \varepsilon_{i-1}]}$. Thus we have $\mathcal{E}_\varepsilon \subset \mathcal{X}_\varepsilon \bigcup \left(\bigcup_{i=1}^{m_\varepsilon} \mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}\right)$, so that

$$I_\varepsilon - 1 = \mathrm{card}(\mathcal{E}_\varepsilon) \leq \mathrm{card}\left(\mathcal{E}_\varepsilon \cap \mathcal{X}_\varepsilon\right) + \sum_{i=1}^{m_\varepsilon} \mathrm{card}\left(\mathcal{E}_\varepsilon \cap \mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}\right)\,. \tag{13}$$

Let $N_{\varepsilon,m_\varepsilon+1}$ be the cardinality of $\mathcal{E}_\varepsilon \cap \mathcal{X}_\varepsilon$. For $i = 1, \ldots, m_\varepsilon$, let $N_{\varepsilon,i}$ be the cardinality of $\mathcal{E}_\varepsilon \cap \mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}$.

Note that the arguments leading to (10) imply that for $\boldsymbol{x}_{h,j} \in \mathcal{E}_\varepsilon$,

$$\boldsymbol{x}_{h,j} \in \mathcal{X}_{LR\delta^h}\,. \tag{14}$$

Consider two distinct $\boldsymbol{x}_{h,j}, \boldsymbol{x}_{h',j'} \in \mathcal{E}_\varepsilon \cap \mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}$. Then, from Assumption 3 and (14), we obtain

$$||\boldsymbol{x}_{h,j} - \boldsymbol{x}_{h',j'}|| \geq \nu\delta^{\max(h,h')} > \frac{\nu\varepsilon_i}{LR}\,.$$

Hence, by definition of packing numbers, we have

$$N_{\varepsilon,i} \leq \mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}, \frac{\nu\varepsilon_i}{LR}\right).$$

Using now Lemma 2 (Section A), we obtain

$$N_{\varepsilon,i} \leq \left(\mathbf{1}_{\nu/R\geq 1} + \mathbf{1}_{\nu/R<1}\left(\frac{4R}{\nu}\right)^d\right)\mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\, \varepsilon_{i-1}]}, \frac{\varepsilon_i}{L}\right). \tag{15}$$

Let now $\boldsymbol{x}_{h_\ell^\star,i_\ell^\star} \in \mathcal{E}_\varepsilon \cap \mathcal{X}_\varepsilon$, with $\ell \in \{1,\dots,I_\varepsilon - 1\}$. The leaf $(h_\ell^\star, i_\ell^\star)$ was selected when the algorithm went through Line 5 for the ℓ-th time. By definition of I_ε, the event (11) does not hold when $(h^\star, i^\star) = (h_\ell^\star, i_\ell^\star)$ and thus

$$f(\boldsymbol{x}_{h_\ell^\star,i_\ell^\star}) + LR\delta^{h_\ell^\star} > \max_{i\in[N_{h_\ell^\star,i_\ell^\star}]} f(\boldsymbol{x}_i) + \varepsilon \geq f(\boldsymbol{x}_{h_\ell^\star,i_\ell^\star}) + \varepsilon\,.$$

This implies that $LR\delta^{h_\ell^\star} > \varepsilon$ and thus

$$\delta^{h_\ell^\star} > \frac{\varepsilon}{LR}\,.$$

Now consider two distinct $\boldsymbol{x}_{h,j}, \boldsymbol{x}_{h',j'} \in \mathcal{E}_\varepsilon \cap \mathcal{X}_\varepsilon$. Then, from Assumption 3, we obtain

$$||\boldsymbol{x}_{h,j} - \boldsymbol{x}_{h',j'}|| \geq \nu\delta^{\max(h,h')} > \frac{\nu\varepsilon}{LR}\,.$$

Hence, we have

$$N_{\varepsilon,m_\varepsilon+1} \leq \mathcal{N}\left(\mathcal{X}_\varepsilon, \frac{\nu\varepsilon}{LR}\right).$$

Using now Lemma 2 (Section A), we obtain

$$N_{\varepsilon,m_\varepsilon+1} \leq \left(\mathbf{1}_{\nu/R\geq 1} + \mathbf{1}_{\nu/R<1}\left(\frac{4R}{\nu}\right)^d\right)\mathcal{N}\left(\mathcal{X}_\varepsilon, \frac{\varepsilon}{L}\right).$$

Combining (12) and (13) with (15) and the last inequality concludes the proof. □

Remark 2. *The analysis of the DOO algorithm in Munos (2011, Theorem 1) does not address the certified setting. The previous proof adapts this analysis to the certified setting and, in passing, slightly improves some of the arguments. Indeed, when counting the cell representatives that are selected, Munos (2011, Theorem 1) partitions the domain $\mathcal{X}$ at any depth h of the tree, yielding bounds involving packing numbers of the form $\mathcal{N}\left(\mathcal{X}_{\varepsilon_{k-1}}, \frac{\varepsilon_k}{L}\right)$, $k = 1,\dots,m_\varepsilon$. In contrast we partition the values of f, yielding bounds involving the smaller packing numbers $\mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\varepsilon_{k-1}]}, \frac{\varepsilon_k}{L}\right)$, $k = 1,\dots,m_\varepsilon$ (and $\mathcal{N}\left(\mathcal{X}_\varepsilon, \frac{\varepsilon}{L}\right)$ that is specific to the certified setting). This improvement also enables us to slightly refine the bound of Munos (2011, Theorem 1) in the non-certified setting, see Remark 4 in Section E. We also refer to this remark for more details on the two partitions just discussed.*

Remark 3. *The bound of Proposition 1, based on Eq.* (5)*, is built by partitioning $[0,\varepsilon_0]$ into the $m_\varepsilon + 1$ sets $[0,\varepsilon], (\varepsilon,\varepsilon_{m_\varepsilon-1}], (\varepsilon_{m_\varepsilon-1},\varepsilon_{m_\varepsilon-2}], \dots, (\varepsilon_1,\varepsilon_0]$ whose lengths are sequentially doubled (except from $[0,\varepsilon]$ to $(\varepsilon,\varepsilon_{m_\varepsilon-1}]$ and from $(\varepsilon,\varepsilon_{m_\varepsilon-1}]$ to $(\varepsilon_{m_\varepsilon-1},\varepsilon_{m_\varepsilon-2}]$). As can be seen from the proof of Proposition 1, more general bounds could be obtained, based on more general partitions of $[0,\varepsilon_0]$. The benefits of the present partition are the following. First, except for $[0,\varepsilon]$, it considers sets whose upper values are no more than twice the lower values, which controls the magnitude of their corresponding packing numbers in Eq.* (5)*, at scale the lower values. Second, the number of sets in the partition is logarithmic in $1/\varepsilon$ which controls the sum in Eq.* (5)*. Finally, the upper bound is then tight up to a logarithmic factor for functions $f \in \mathcal{F}_L$, as proved in Section 4. Note also that the same generalization could be applied in the non-certified setting, see Section E.*

C Missing Proofs of Section 3

We now prove a result on the sum of volumes of overlapping layers that is used in the proof of Theorem 1.

Lemma 3. *If f is L-Lipschitz, fix $\varepsilon > 0$ and recall that $m_\varepsilon := \lceil \log_2(\varepsilon_0/\varepsilon) \rceil$, $\varepsilon_{m_\varepsilon} := \varepsilon$, and for all $k \leq m_\varepsilon - 1$, $\varepsilon_k =: \varepsilon_0 2^{-k}$. Then, there exist $c, C > 0$ (e.g., $c = 1/5$ and $C := 2 \cdot 16^d$) such that, for all $\varepsilon \in (0, \varepsilon_0]$,*

$$\frac{\mathrm{vol}\big(\mathcal{X}_{2\varepsilon}\big)}{\varepsilon^d} + \sum_{k=1}^{m} \frac{\mathrm{vol}\left(\mathcal{X}_{(\frac{1}{2}\varepsilon_k,\, 2\varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} \leq 8^d \left(\frac{\mathrm{vol}(\mathcal{X}_\varepsilon)}{\varepsilon^d} + \sum_{i=1}^{m} \frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\big)}{\varepsilon_{k-1}^d} \right) .$$

Proof. To avoid clutter, we denote m_ε simply by m. The left hand side can be upper bounded by

$$\begin{aligned}
&\frac{\mathrm{vol}\big(\mathcal{X}_\varepsilon\big) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_m,\, \varepsilon_{m-1}]}\big) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-1},\, \varepsilon_{m-2}]}\big)}{\varepsilon^d} \\
&\qquad + \sum_{k=1}^{m-2} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_{k+1},\, \varepsilon_k]}\right) + \mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right) \mathrm{vol}\left(\mathcal{X}_{(\varepsilon_{k-1},\, \varepsilon_{k-2}]}\right)}{\varepsilon_{k-1}^d} \\
&\qquad + \frac{\mathrm{vol}\left(\mathcal{X}_\varepsilon\right) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_m,\, \varepsilon_{m-1}]}\big) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-1},\, \varepsilon_{m-2}]}\big) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-2},\, \varepsilon_{m-3}]}\big)}{\varepsilon_{m-2}^d} \\
&\qquad + \frac{\mathrm{vol}\left(\mathcal{X}_\varepsilon\right) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_m,\, \varepsilon_{m-1}]}\big) + \mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-1},\, \varepsilon_{m-2}]}\big)}{\varepsilon_{m-1}^d} \\
&\leq 3\frac{\mathrm{vol}\big(\mathcal{X}_\varepsilon\big)}{\varepsilon^d} + (2^d+2)\frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_m,\, \varepsilon_{m-1}]}\big)}{\varepsilon_{m-1}^d} + (4^d+2^d+1)\frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-1},\, \varepsilon_{m-2}]}\big)}{\varepsilon_{m-2}^d} \\
&\qquad + \frac{1}{2^d}\sum_{k=2}^{m-1} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} + \sum_{k=1}^{m-2} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} + 2^d \sum_{k=1}^{m-3} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} \\
&= 3\frac{\mathrm{vol}\big(\mathcal{X}_\varepsilon\big)}{\varepsilon^d} + \frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_m,\, \varepsilon_{m-1}]}\big)}{\varepsilon_{m-1}^d} + 4^d\frac{\mathrm{vol}\big(\mathcal{X}_{(\varepsilon_{m-1},\, \varepsilon_{m-2}]}\big)}{\varepsilon_{m-2}^d} \\
&\qquad + \frac{1}{2^d}\sum_{k=2}^{m-1} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} + \sum_{k=1}^{m} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d} + 2^d \sum_{k=1}^{m} \frac{\mathrm{vol}\left(\mathcal{X}_{(\varepsilon_k,\, \varepsilon_{k-1}]}\right)}{\varepsilon_{k-1}^d}
\end{aligned}$$

where we applied several times the definition of the ε_k's, the inequality follows by $1/\varepsilon^d + 1/\varepsilon_{m-1}^d + 1/\varepsilon_{m-2}^d \leq \min\big\{3(1/\varepsilon^d),\ (2^d+2)(1/\varepsilon_{m-1}^d),\ (4^d+2^d+1)(1/\varepsilon_{m-2}^d)\big\}$, and the proof is concluded observing that $\max(3, 1, 4^d) = 4^d$ and $4^d + 1/2^d + 1 + 2^d \leq 8^d$. ☐

We denote by $A + B$ the Minkowski sum of two sets A, B and for any set A and all $\lambda \in \mathbb{R}$, we let $\lambda A := \{\lambda \boldsymbol{a} : \boldsymbol{a} \in A\}$.

Proposition 4. *If f is L-Lipschitz and $\mathcal{X}$ satisfies Assumption 4 with $r_0 > 0, \gamma \in (0, 1]$, then, for all $0 < w < u < 2Lr_0$,*

$$\mathcal{N}\left(\mathcal{X}_u,\ \frac{u}{L}\right) \leq \frac{1}{\gamma}\frac{\mathrm{vol}\big(\mathcal{X}_{(3/2)u}\big)}{\mathrm{vol}\left(\frac{u}{2L}B_1\right)} \qquad \textit{and} \qquad \mathcal{N}\left(\mathcal{X}_{(w,u]},\ \frac{w}{L}\right) \leq \frac{1}{\gamma}\frac{\mathrm{vol}\big(\mathcal{X}_{(w/2,\,3u/2]}\big)}{\mathrm{vol}\left(\frac{w}{2L}B_1\right)} .$$

Proof. Fix any $u > w > 0$. Let $\eta_1 := \frac{u}{L}$, $\eta_2 := \frac{w}{L}$, $E_1 := \mathcal{X}$, $E_2 := \mathcal{X}_w^c$, and $i \in [2]$. Note that for any $\eta > 0$ and $A, E \subset \mathbb{R}^d$, the balls of radius $\eta/2$ centered at the elements of an η-packing of A intersected with E are all disjoint and included in $(A + B_{\eta/2}) \cap E$. Thus, $\mathcal{N}\left(\mathcal{X}_u \cap E_i,\ \eta_i\right) \leq \mathrm{vol}\big((\mathcal{X}_u \cap E_i + B_{\eta_i/2}) \cap \mathcal{X}\big)/\mathrm{vol}(B_{\eta_i/2} \cap \mathcal{X})$. To lower bound the denominator, simply apply Assumption 4 to obtain $\mathrm{vol}\big(B_{\eta_i/2}(\boldsymbol{x}) \cap \mathcal{X}\big) \geq \gamma\,\mathrm{vol}(B_{\eta_i/2})$. To upper bound the numerator, take an arbitrary point $\boldsymbol{x}_i \in (\mathcal{X}_u \cap E_i + B_{\eta_i/2}) \cap \mathcal{X}$. By definition of Minkowski sum, there exists $\boldsymbol{x}_i' \in \mathcal{X}_u \cap E_i$ such that $\|\boldsymbol{x}_i - \boldsymbol{x}_i'\| \leq \eta_i/2$. Hence $f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_i) \leq f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_i') + \big|f(\boldsymbol{x}_i') - f(\boldsymbol{x}_i)\big| \leq u + L(\eta_i/2) \leq (3/2)u$. This implies that $\boldsymbol{x}_i \in \mathcal{X}_{(3/2)u}$, which proves the first inequality. For the second one, note that $\boldsymbol{x}_2$ satisfies $f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_2) \geq f(\boldsymbol{x}^\star) - f(\boldsymbol{x}_2') - \big|f(\boldsymbol{x}_2') - f(\boldsymbol{x}_2)\big| \geq w - L(\eta_2/2) = (1/2)w$. ☐

D Missing Proofs of Section 4

In this section we provide all missing details and proofs from Section 4.

D.1 Missing details in the Proof of Theorem 2

We claimed that the quantity τ introduced in Eq. (7) lower bounds the sample complexity $\sigma(A, f, \varepsilon)$ of any certified algorithm A. To prove this formally, fix an arbitrary certified algorithm A, let $N = \sigma(A, f, \varepsilon)$, and assume by contradiction that $N < \tau$. Then we have $\mathrm{err}_N(A) \geq \inf_{A'}\big(\mathrm{err}_N(A')\big) > \varepsilon$ by definition of τ. This means that there exists an L-Lipschitz function g, coinciding with f on $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$ and such that $\max(g) - \boldsymbol{x}_N^\star > \varepsilon$. Now, since $\boldsymbol{x}_i$, $\boldsymbol{x}_i^\star$, and ξ_i are deterministic functions of the previous observations $f(\boldsymbol{x}_1) = g(\boldsymbol{x}_1), \dots, f(\boldsymbol{x}_{i-1}) = g(\boldsymbol{x}_{i-1})$ (for all $i = 1, \dots, N$), running A on either f or g returns the same $\boldsymbol{x}_i$, $\boldsymbol{x}_i^\star$, and ξ_i (for all $i = 1, \dots, N$). Thus we have that $\sigma(A, g, \varepsilon) = \sigma(A, f, \varepsilon) = N$. This, together with the fact that A is a certified algorithm, implies that $\varepsilon < \max(g) - \boldsymbol{x}_N^\star \leq \xi_N \leq \varepsilon$, which yields a contradiction. □

D.2 The Piyavskii-Shubert Algorithm and Proof of Proposition 2

The Piyavskii-Shubert Algorithm. In this section, we recall the definition of the certified Piyavskii-Shubert algorithm (Algorithm 2, Piyavskii 1972; Shubert 1972) and we show that if $\mathrm{Lip}(f) = L$ (i.e., if the best Lipschitz constant of f is known exactly by the algorithm) the sample complexity can be constant in dimension $d \geq 2$ (Proposition 2).

Algorithm 2: Certified Piyavskii-Shubert algorithm (PS)

input: Lipschitz constant $L > 0$, norm $\|\cdot\|$, initial guess $\boldsymbol{x}_1 \in \mathcal{X}$
for $i = 1, 2, \dots$ **do**
  pick the next query point $\boldsymbol{x}_i$
  observe the value $f(\boldsymbol{x}_i)$
  output the recommendation $\boldsymbol{x}_i^\star \leftarrow \mathrm{argmax}_{\boldsymbol{x} \in \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_i\}} f(\boldsymbol{x})$
  output the error certificate $\xi_i = \widehat{f}_i^\star - f_i^\star$, where $\widehat{f}_i(\cdot) \leftarrow \min_{j \in [i]} \big\{ f(\boldsymbol{x}_j) + L \|\boldsymbol{x}_j - (\cdot)\| \big\}$,
  $\widehat{f}_i^\star \leftarrow \max_{\boldsymbol{x} \in \mathcal{X}} \widehat{f}_i(\boldsymbol{x})$, $f_i^\star \leftarrow \max_{j \in [i]} f(\boldsymbol{x}_j)$, and let $\boldsymbol{x}_{i+1} \in \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{X}} \widehat{f}_i(\boldsymbol{x})$

Proof of Proposition 2. Fix any $\varepsilon \in (0, \varepsilon_0)$ and any L-Lipschitz function f. Since f is L-Lipschitz, then $\max_{\boldsymbol{x} \in \mathcal{X}} \widehat{f}_i(\boldsymbol{x}) \geq \max_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x})$ for all $i \in \mathbb{N}^*$. Hence $\max_{\boldsymbol{x} \in \mathcal{X}} f(x) - f(\boldsymbol{x}_i^\star) \leq \max_{\boldsymbol{x} \in \mathcal{X}} \widehat{f}_i(\boldsymbol{x}) - f_i^\star = \xi_i$. This shows that the certified Piyavskii-Shubert algorithm is indeed a certified algorithm. Then, if $f := L \|\cdot\|$ and $\boldsymbol{x}_1 := \mathbf{0}$, we have that $\widehat{f}_1 = f$, $\xi_1 = L$, and $\boldsymbol{x}_2$ belongs to the the unit sphere, i.e., $\boldsymbol{x}_2$ is a maximizer of f. Since $\widehat{f}_2 = f$, we have that $\xi_2 = 0$, hence $\sigma(\mathrm{PS}, f, \varepsilon) = 2$. Finally, by definition (5), we have $S_{\mathrm{C}}(f, \varepsilon) \geq \mathcal{N}(\mathrm{argmax}_{\mathcal{X}} f, \varepsilon / L)$. Since $\mathrm{argmax}_{\mathcal{X}} f$ is the unit sphere, there exists a constant c, only depending on d, $\|\cdot\|$ and L, such that $S_{\mathrm{C}}(f, \varepsilon) \geq c / \varepsilon^{d-1}$. □

We give some intuition on Proposition 2. Consider a function f that has Lipschitz constant exactly L, and a pair of points in $\mathcal{X}$ whose respective values of f are maximally distant, that is the difference of values of f is exactly L times the norm of the input difference. This configuration provides strong information on the value of the global maximum of f, as is illustrated in the proof of Proposition 2. Another interpretation is that when f has Lipschitz constant exactly L, there is less flexibility for the L-Lipschitz function g that yields the maximal optimization error in $\mathrm{err}_n(A)$ (introduced in the proof of Theorem 2).

D.3 Proof of Proposition 3

Let f be an arbitrary L-Lipschitz function. Let $K = 8$. As for the proof of Theorem 2, it is sufficient to show that $\tau > c S_{\mathrm{C}}(f, \varepsilon) / (1 + m_\varepsilon)$, with τ defined in (7). If $c S_{\mathrm{C}}(f, \varepsilon) / (1 + m_\varepsilon) < 1$, then the result follows by $\tau \geq 1$. Consider then from now on that $c S_{\mathrm{C}}(f, \varepsilon) / (1 + m_\varepsilon) \geq 1$.

Defining $\tilde{\varepsilon}$ as in the proof of Theorem 2, one can prove similarly that $cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon) \leq c\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, \tilde{\varepsilon}/2L\right)$. From Lemma 2,

$$\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, \frac{K\tilde{\varepsilon}}{L}\right) \geq \frac{1}{8K}\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, \frac{\tilde{\varepsilon}}{2L}\right) \geq \frac{1}{8K}\frac{S_{\mathrm{C}}(f,\varepsilon)}{m_\varepsilon+1} \geq 12\;,$$

because $c = 1/96K$ and $cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon) \geq 1$. Let now $n \leq cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$. Then we have $n \leq c(8K)\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, K\tilde{\varepsilon}/L\right)$. Thus, by $c(8K) = 1/12$, $n \leq \mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, K\tilde{\varepsilon}/L\right)/12$, and $\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, K\tilde{\varepsilon}/L\right) \geq 12$, we have

$$n \leq \left\lfloor \frac{\mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon}},\, \frac{K\tilde{\varepsilon}}{L}\right)}{2} \right\rfloor - 4\;. \tag{16}$$

Consider a certified algorithm A for L-Lipschitz functions. Let us consider a $K\tilde{\varepsilon}/L$ packing $\tilde{x}_1 < \tilde{x}_2 < \cdots < \tilde{x}_N$ of $\mathcal{X}_{\tilde{\varepsilon}}$ with $N = \mathcal{N}\left(\mathcal{X}_{\tilde{\varepsilon},\, K\tilde{\varepsilon}/L}\right)$. Consider the $\lfloor N/2 \rfloor - 1$ disjoint open segments $(\tilde{x}_1, \tilde{x}_3)$, $(\tilde{x}_3, \tilde{x}_5)$, …, $(\tilde{x}_{2\lfloor N/2 \rfloor - 3}$, $\tilde{x}_{2\lfloor N/2 \rfloor - 1})$. Then from (16) there exists $i \in \left\{1, 3, \ldots, 2\left\lfloor N/2 \right\rfloor - 3\right\}$ such that the segment $(\tilde{x}_i, \tilde{x}_{i+2})$ does not contain any of the points $x_1 = x_1(A,f), \ldots, x_n = x_n(A,f)$ that A queries when run on f. Assume that $\tilde{x}_{i+1} - \tilde{x}_i \leq \tilde{x}_{i+2} - \tilde{x}_{i+1}$ (the case $\tilde{x}_{i+1} - \tilde{x}_i > \tilde{x}_{i+2} - \tilde{x}_{i+1}$ can be treated analogously; we omit these straightforward details for the sake of conciseness). Consider the function $h_{+,\tilde{\varepsilon}} \colon \mathcal{X} \to \mathbb{R}$ defined by

$$h_{+,\tilde{\varepsilon}}(x) = \begin{cases} f(x) & \text{if } x \in \mathcal{X} \backslash [\tilde{x}_i, \tilde{x}_{i+2}] \\ f(\tilde{x}_i) + L(x - \tilde{x}_i) & \text{if } x \in \mathcal{X} \cap [\tilde{x}_i, \tilde{x}_{i+1}] \\ f(\tilde{x}_i) + L(\tilde{x}_{i+1} - \tilde{x}_i) + (x - \tilde{x}_{i+1})\frac{f(\tilde{x}_{i+2}) - f(\tilde{x}_i) - L(\tilde{x}_{i+1} - \tilde{x}_i)}{\tilde{x}_{i+2} - \tilde{x}_{i+1}} & \text{if } x \in \mathcal{X} \cap (\tilde{x}_{i+1}, \tilde{x}_{i+2}]\;. \end{cases}$$

We see that $h_{+,\tilde{\varepsilon}}$ is L-Lipschitz (since $\tilde{x}_{i+1} - \tilde{x}_i \leq \tilde{x}_{i+2} - \tilde{x}_{i+1}$). Furthermore, $h_{+,\tilde{\varepsilon}}$ coincides with f at all query points $x_1, \ldots, x_n$. Similarly, consider the function $h_{-,\tilde{\varepsilon}} \colon \mathcal{X} \to \mathbb{R}$ defined by

$$h_{-,\tilde{\varepsilon}}(x) = \begin{cases} f(x) & \text{if } x \in \mathcal{X} \backslash [\tilde{x}_i, \tilde{x}_{i+2}] \\ f(\tilde{x}_i) - L(x - \tilde{x}_i) & \text{if } x \in \mathcal{X} \cap [\tilde{x}_i, \tilde{x}_{i+1}] \\ f(\tilde{x}_i) - L(\tilde{x}_{i+1} - \tilde{x}_i) + (x - \tilde{x}_{i+1})\frac{f(\tilde{x}_{i+2}) - f(\tilde{x}_i) + L(\tilde{x}_{i+1} - \tilde{x}_i)}{\tilde{x}_{i+2} - \tilde{x}_{i+1}} & \text{if } x \in \mathcal{X} \cap (\tilde{x}_{i+1}, \tilde{x}_{i+2}]\;. \end{cases}$$

As before, $h_{-,\tilde{\varepsilon}}$ is L-Lipschitz and coincides with f on $x_1, \ldots, x_n$.

Let $x_n^\star = x_n^\star(A,f)$ be the recommendation of A at round n when run on f.

Case 1: $x_n^\star \in \mathcal{X} \backslash [\tilde{x}_i, \tilde{x}_{i+2}]$. Then, since $\tilde{x}_i \in \mathcal{X}_{\tilde{\varepsilon}}$ and $\tilde{x}_{i+1} - \tilde{x}_i \geq K\tilde{\varepsilon}/L$, we have

$$h_{+,\tilde{\varepsilon}}(\tilde{x}_{i+1}) - h_{+,\tilde{\varepsilon}}(x_n^\star) = f(\tilde{x}_i) + L(\tilde{x}_{i+1} - \tilde{x}_i) - f(x_n^\star) \geq -\tilde{\varepsilon} + L\frac{K\tilde{\varepsilon}}{L} = 7\tilde{\varepsilon}\;.$$

Case 2: $x_n^\star \in \mathcal{X} \cap \left[\tilde{x}_i, (\tilde{x}_i + \tilde{x}_{i+1})/2\right]$. Then, since $\tilde{x}_{i+1} - \tilde{x}_i \geq K\tilde{\varepsilon}/L$, we have

$$h_{+,\tilde{\varepsilon}}(\tilde{x}_{i+1}) - h_{+,\tilde{\varepsilon}}(x_n^\star) = f(\tilde{x}_i) + L(\tilde{x}_{i+1} - \tilde{x}_i) - f(\tilde{x}_i) - L(x_n^\star - \tilde{x}_i) \geq L\frac{\tilde{x}_{i+1} - \tilde{x}_i}{2} \geq 4\tilde{\varepsilon}\;.$$

Case 3: $x_n^\star \in \mathcal{X} \cap \left[(\tilde{x}_i + \tilde{x}_{i+1})/2, \tilde{x}_{i+1}\right]$. Then, since $\tilde{x}_{i+1} - \tilde{x}_i \geq K\tilde{\varepsilon}/L$, we have

$$h_{-,\tilde{\varepsilon}}(\tilde{x}_i) - h_{-,\tilde{\varepsilon}}(x_n^\star) = f(\tilde{x}_i) - f(\tilde{x}_i) + L(x_n^\star - \tilde{x}_i) \geq L\frac{\tilde{x}_{i+1} - \tilde{x}_i}{2} \geq 4\tilde{\varepsilon}\;.$$

Case 4: $x_n^\star \in \mathcal{X} \cap \left[\tilde{x}_{i+1}, (\tilde{x}_{i+1} + \tilde{x}_{i+2})/2\right]$. Then, since $\tilde{x}_{i+1} - \tilde{x}_i \geq K\tilde{\varepsilon}/L$, since $\tilde{x}_i, \tilde{x}_{i+2} \in \mathcal{X}_{\tilde{\varepsilon}}$, and since $h_{-,\tilde{\varepsilon}}$ is linear increasing on $[\tilde{x}_{i+1}, \tilde{x}_{i+2}]$ with left value $f(\tilde{x}_i) - L(\tilde{x}_{i+1} - \tilde{x}_i)$ and right value $f(\tilde{x}_{i+2})$, we have

$$\begin{aligned} h_{-,\tilde{\varepsilon}}(\tilde{x}_i) - h_{-,\tilde{\varepsilon}}(x_n^\star) &\geq f(\tilde{x}_i) - \frac{f(\tilde{x}_i) - L(\tilde{x}_{i+1} - \tilde{x}_i) + f(\tilde{x}_{i+2})}{2} \\ &= \frac{f(\tilde{x}_i) - f(\tilde{x}_{i+2})}{2} + L\frac{\tilde{x}_{i+1} - \tilde{x}_i}{2} \geq -\frac{\tilde{\varepsilon}}{2} + \frac{K}{2}\tilde{\varepsilon} \geq 3\tilde{\varepsilon}\;. \end{aligned}$$

Case 5: $x_n^\star \in \mathcal{X} \cap \big[(\tilde{x}_{i+1}+\tilde{x}_{i+2})/2, \tilde{x}_{i+2}\big]$. Then, since $\tilde{x}_{i+1}-\tilde{x}_i \geq K\tilde{\varepsilon}/L$, since $\tilde{x}_i, \tilde{x}_{i+2} \in \mathcal{X}_{\tilde{\varepsilon}}$ and since $h_{+,\tilde{\varepsilon}}$ is linear decreasing on $[\tilde{x}_{i+1}, \tilde{x}_{i+2}]$ with left value $f(\tilde{x}_i)+L(\tilde{x}_{i+1}-\tilde{x}_i)$ and right value $f(\tilde{x}_{i+2})$, we have

$$\begin{aligned} h_{+,\tilde{\varepsilon}}(\tilde{x}_{i+1}) - h_{+,\tilde{\varepsilon}}(x_n^\star) &\geq f(\tilde{x}_i) + L(\tilde{x}_{i+1}-\tilde{x}_i) - \frac{f(\tilde{x}_i)+L(\tilde{x}_{i+1}-\tilde{x}_i)+f(\tilde{x}_{i+2})}{2} \\ &= \frac{f(\tilde{x}_i)-f(\tilde{x}_{i+2})}{2} + L\frac{\tilde{x}_{i+1}-\tilde{x}_i}{2} \geq -\frac{\tilde{\varepsilon}}{2} + \frac{K}{2}\tilde{\varepsilon} \geq 3\tilde{\varepsilon}\,. \end{aligned}$$

Putting all cases together and recalling the definition of $\mathrm{err}_n(A)$ in the proof of Theorem 2, we then obtain $\mathrm{err}_n(A) \geq 3\tilde{\varepsilon} > \varepsilon$. Being A arbitrary, this implies $\inf_{A'} \mathrm{err}_n(A') > \varepsilon$. Since this has been shown for any $n \leq cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$ we thus have $\tau > cS_{\mathrm{C}}(f,\varepsilon)/(1+m_\varepsilon)$. □

E Comparison with the classical non-certified setting

For the interested reader who is not familiar with DOO, in this section, we recall and analyze the classical non-certified version of this algorithm. As mentioned in Remark 2, our analysis is slightly tighter than that of Munos (2011), and serves as a better comparison for highlighting the differences between the certified and the non-certified settings (see Remark 5 below).

The difference between our certified version c.DOO and the classical non-certified DOO algorithm (denoted by nc.DOO below) is that the latter does not output any certificates $\xi_1, \xi_2, \ldots$. In other words, nc.DOO coincides with Algorithm 1 except for Lines 3 and 13. In particular, it outputs the same query points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots$ and recommendations $\boldsymbol{x}_1^\star, \boldsymbol{x}_2^\star, \ldots$ as c.DOO. The performance of this non-certified algorithm is classically measured by the non-certified sample complexity (6), i.e., the smallest number of queries needed before outputting an ε-optimal recommendation.

Proposition 5. *If Assumptions 2 and 3 hold, the non-certified sample complexity of the non-certified DOO algorithm* nc.DOO *satisfies, for all Lipschitz functions $f \in \mathcal{F}_L$[5] and any accuracy $\varepsilon \in (0, \varepsilon_0]$,*

$$\zeta(\mathrm{nc.DOO}, f, \varepsilon) \leq 1 + C\sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k, \varepsilon_{k-1}]}, \frac{\varepsilon_k}{L}\right)\,,$$

where $C = K\big(\mathbf{1}_{\nu/R\geq 1} + \mathbf{1}_{\nu/R<1}(4R/\nu)^d\big)$.

Proof. The proof of Proposition 1 (Section B), from the beginning to (10), implies that, for any $(h^\star, i^\star)$ in Line 5 of Algorithm 1,

$$f(\boldsymbol{x}_{h^\star,i^\star}) \in \mathcal{X}_{LR\delta^{h^\star}}\,. \tag{17}$$

The guarantee (17) is classical (e.g., Munos 2011).

We now proceed in a direction that is slightly different from the proof of Munos (2011, Theorem 1). Consider the first time at which the DOO algorithm reaches Line 5 with $f(\boldsymbol{x}_{h^\star,i^\star}) \geq f(\boldsymbol{x}^\star) - \varepsilon$. Then let I_ε be the number of times the DOO algorithm went through Line 5 strictly before that time, and denote by n_ε the total number of evaluations of f strictly before that same time. We have

$$n_\varepsilon \leq 1 + KI_\varepsilon\,.$$

Furthermore, after n_ε evaluations of f, we have, by definitions of the recommendation $\boldsymbol{x}_{n_\varepsilon}^\star$ and n_ε,

$$f(\boldsymbol{x}_{n_\varepsilon}^\star) = \max_{\boldsymbol{x}\in\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{n_\varepsilon}\}} f(\boldsymbol{x}) \geq f(\boldsymbol{x}_{h^\star,i^\star}) \geq f(\boldsymbol{x}^\star) - \varepsilon\,.$$

This inequality entails that the non-certified sample complexity of nc.DOO is bounded by n_ε and thus

$$\zeta(\mathrm{nc.DOO}, f, \varepsilon) \leq 1 + KI_\varepsilon. \tag{18}$$

We now bound I_ε from above, and assume without loss of generality that $I_\varepsilon \geq 1$. Consider now the sequence $(h_1^\star, i_1^\star), \ldots, (h_{I_\varepsilon}^\star, i_{I_\varepsilon}^\star)$ corresponding to the first I_ε times the DOO algorithm nc.DOO went through Line 5. Let $\mathcal{E}_\varepsilon$ be

[5] Our proof can be easily adapted to the weaker assumption that f is only L-Lipschitz around a maximizer.

the corresponding finite set $\{\boldsymbol{x}_{h_1^\star,i_1^\star},\dots,\boldsymbol{x}_{h_{I_\varepsilon}^\star,i_{I_\varepsilon}^\star}\}$ (a leaf can never be selected twice). By definition of I_ε, we have $\mathcal{E}_\varepsilon \subseteq \mathcal{X}_{(\varepsilon,\varepsilon_0]}$. Since $\varepsilon = \varepsilon_{m_\varepsilon} \leq \varepsilon_{m_\varepsilon-1} \leq \ldots \leq \varepsilon_0$, we have $\mathcal{E}_\varepsilon \subseteq \bigcup_{i=1}^{m_\varepsilon} \mathcal{X}_{(\varepsilon_i,\,\varepsilon_{i-1}]}$, so that the cardinality I_ε of $\mathcal{E}_\varepsilon$ satisfies

$$I_\varepsilon = \mathrm{card}(\mathcal{E}_\varepsilon) \leq \sum_{i=1}^{m_\varepsilon} \mathrm{card}\left(\mathcal{E}_\varepsilon \cap \mathcal{X}_{(\varepsilon_i,\,\varepsilon_{i-1}]}\right) \ . \tag{19}$$

Let $N_{\varepsilon,i}$ be the cardinality of $\mathcal{E}_\varepsilon \cap \mathcal{X}_{(\varepsilon_i,\,\varepsilon_{i-1}]}$. The same arguments as from (13) to (15) in the proof of Proposition 1 yield

$$N_{\varepsilon,i} \leq \left(\mathbf{1}_{\nu/R\geq 1} + \mathbf{1}_{\nu/R<1}\left(\frac{4R}{\nu}\right)^d\right) \mathcal{N}\left(\mathcal{X}_{(\varepsilon_i,\,\varepsilon_{i-1}]}, \frac{\varepsilon_i}{L}\right). \tag{20}$$

Combining the last inequality with (18) and (19) concludes the proof. □

Remark 4. *The analysis of the DOO algorithm in Munos (2011, Theorem 1) (non-certified version) yields a bound on the non-certified sample complexity* (6) *than can be expressed in the form* $1 + C\sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{\varepsilon_{k-1}},\, \frac{\varepsilon_k}{L}\right)$*, with a constant* C*. The corresponding proof relies on two main arguments. First, when a cell of the form* $(h^\star, i^\star)$*,* $i^\star \in \{0,\dots,K^{h^\star}-1\}$*, is selected in Line 5 of Algorithm 1, then the corresponding cell representative* $\boldsymbol{x}_{i^\star,h^\star}$ *is* $LR\delta^{h^\star}$*-optimal (we also use this argument). Second, as a consequence, for a given fixed value of* $h^\star$*, for the sequence of values of* $i^\star$ *that are selected in Line 5 of Algorithm 1, the corresponding cell representatives* $\boldsymbol{x}_{h^\star,i^\star}$ *form a packing of* $\mathcal{X}_{LR\delta^{h^\star}}$*.*

Our slight refinement in the proof of Proposition 5 stems from the observation that using a packing of $\mathcal{X}_{LR\delta^{h^\star}}$ *yields a suboptimal analysis, since the cell representatives* $\boldsymbol{x}_{h^\star,i^\star}$ *can be much better than* $LR\delta^{h^\star}$*-optimal. Hence, we proceed differently from Munos (2011), by first partitioning all the selected cell representatives (in Line 5 of Algorithm 1) according to their level of optimality as in* (19) *and then by exhibiting packings of the different layers of input points* $\mathcal{X}_{(\varepsilon,\varepsilon_{m_\varepsilon-1}]}, \mathcal{X}_{(\varepsilon_{m_\varepsilon-1},\varepsilon_{m_\varepsilon-2}]},\dots,\mathcal{X}_{(\varepsilon_1,\varepsilon_0]}$*. In a word, we partition the values of* f *instead of partitioning the input space when counting the representatives selected at all levels.*

Remark 5. *In the Introduction, below Eq.* (6)*, we mentioned the inherent difference between the sample complexity* $\sigma(A,f,\varepsilon)$ *in the certified setting and the more classical sample complexity* $\zeta(A,f,\varepsilon)$ *in the non-certified setting. We can now make our statements more formal.*

Our paper shows that in the certified setting, the sample complexity $\sigma(A,f,\varepsilon)$ *of an optimal algorithm* A *(e.g.,* $A = \mathrm{c.DOO}$*) is characterized by the quantity*

$$S_{\mathrm{C}}(f,\varepsilon) := \mathcal{N}\left(\mathcal{X}_\varepsilon, \frac{\varepsilon}{L}\right) + \sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right) \ .$$

In contrast, the previous proposition shows that in the non-certified setting the sample complexity $\zeta(\mathrm{nc.DOO}, f, \varepsilon)$ *of the* nc.DOO *algorithm is upper bounded (up to constants) by*

$$S_{\mathrm{NC}}(f,\varepsilon) := \sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right) \ .$$

The two expressions look remarkably alike but are subtly very different. In fact, the latter depends only on the "size" (i.e., the packing numbers) of suboptimal points. The former has an additional term measuring the size of near-optimal points. Now, note that the flatter a function is, the fewer suboptimal points there are. This implies that the sum $\sum_{k=1}^{m_\varepsilon} \mathcal{N}\left(\mathcal{X}_{(\varepsilon_k,\varepsilon_{k-1}]},\, \frac{\varepsilon_k}{L}\right)$ *becomes very small (hence, so does* $S_{\mathrm{NC}}(f,\varepsilon)$*), but in turn, the set of near-optimal points* $\mathcal{X}_\varepsilon$ *becomes large (hence, so does* $S_{\mathrm{C}}(f,\varepsilon)$*). For instance, in the extreme case of constant functions* f*, we have* $S_{\mathrm{NC}}(f,\varepsilon) = 0$ *but* $S_{\mathrm{C}}(f,\varepsilon) \approx (L/\varepsilon)^d$*. This fleshes out the fundamental difference between certified and non-certified optimization, giving formal evidence to the intuition that the more "constant" a function is, the easier it is to recommend an* ε*-optimal point, but the harder it is to certify that such recommendation is actually a good recommendation.*