

# LIPO+: Frugal Global Optimization for Lipschitz Functions

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## ABSTRACT

In this paper, we propose simple yet effective empirical improvements to the algorithms of the LIPO family, introduced in [8], that we call LIPO+ and ADALIPO+. We compare our methods to the vanilla versions of the algorithms over standard benchmark functions and show that they converge significantly faster. Finally, we show that the LIPO family is very prone to the curse of dimensionality and tends quickly to Pure Random Search when the dimension increases. We give a proof for this, which is also formalized in Lean mathematical language. Source codes and a demo are provided online.

## KEYWORDS

global optimization, Lipschitz functions, frugal optimization, statistical analysis, numerical analysis.

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## 1 INTRODUCTION

Global optimization methods aim at finding the global maxima of a non-convex function, unknown a priori, over a compact set. This branch of applied mathematics has been extensively studied since it has countless impactful applications. Indeed, optimizing an unknown function is a common problem in many fields such as machine learning, physics, biology, etc. (e.g. [7, 12]). In this context, only local information about the function is available. Moreover, in many applications, the function is computationally expensive to evaluate. The goal of any global optimization algorithm is to find a precise estimate of the global maximum while minimizing the number of evaluations of the function. For instance, imagine a physical system for which a heavy computer program needs days to simulate possible future trajectories given an initialization and a set of parameters. In such a scenario, without a plan for frugal probing of the function it may be infeasible to optimize the behavior of such a system, with respect to its parameters.

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Several approaches have been proposed over the years. Some have theoretical guarantees (e.g. [6, 8, 13, 14]) while others are more heuristic (e.g. [4, 9, 11, 16]). Most are sequential, i.e. they use the information of the previous evaluations to decide where to evaluate the function next, and stochastic, i.e. they use a sampling process to explore the space. Recent results show that stochasticity is a key ingredient to achieve good performance (e.g. [1, 5, 17]).

In this short paper, we focus on the LIPO family of algorithms, namely the original LIPO algorithm and the adaptive variant ADALIPO, both introduced in [8]. This is a family of sequential stochastic optimization algorithms that assume the target is a Lipschitz function (see Eq. 1 and fig. 1a), which they exploit to ensure that algorithms' performance by theoretical guarantees. The Lipschitz assumption is common in many optimization frameworks, as it gives several tools to prove convergence rates of the algorithms, while being general enough to cover a wide range of functions. The contribution of this work is to propose two improved counterpart algorithms, called LIPO+ and ADALIPO+, by addressing certain practical limitations of the original versions and by introducing empirical modifications that work better in practice. Both the presented algorithms include a stopping criterion, while the adaptive variant is equipped with a decaying exploration rate. We compare the new algorithms to the vanilla versions on benchmark functions and validate their empirical performance. We show that the LIPO family of methods is very prone to the curse of dimensionality and tends quickly to Pure Random Search when the dimension increases. We give a proof for this and we also formalize it in Lean mathematical language [2], which ensures correctness and facilitates future reusability of theoretical results. Last but not least, our companion paper in [3] focuses on the reproducibility of this work, and makes available the pseudocodes, the implementation details, the source code of all the compared algorithms, and an online demo<sup>1</sup>.

## 2 LIPSCHITZ OPTIMIZATION

In this section, we briefly recall the LIPO and ADALIPO algorithms. For more details, we refer the reader to [8]. Note that we refer to the *maximization* of a function  $f : \mathcal{X} \rightarrow \mathbb{R}$ , yet this is only a convention since, due to the ordering property of real numbers, it is equivalent to *minimizing* its negative, i.e.  $\arg \max_x f(x) = \arg \min_x -f(x)$ .

### 2.1 LIPO

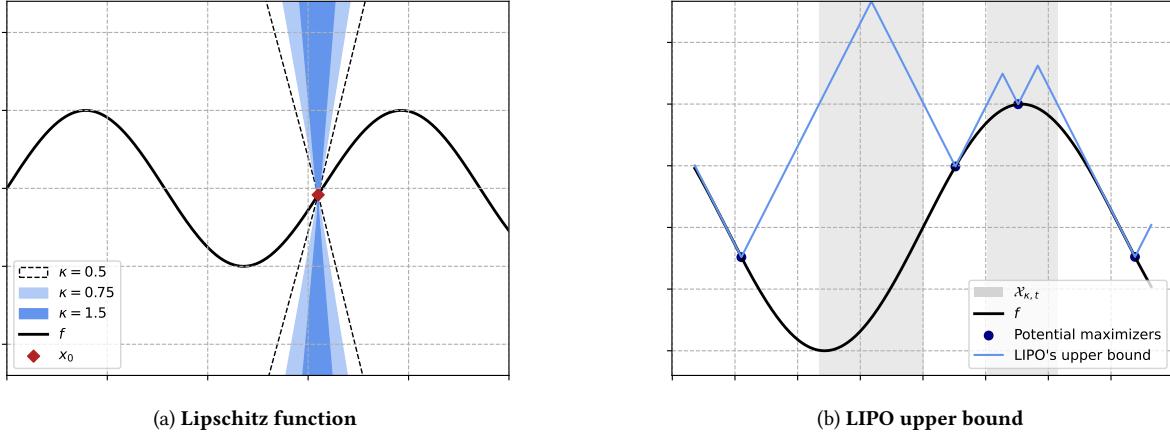
Formally, a function  $f$  is  $\kappa$ -Lipschitz in the domain  $\mathcal{X}$  when it holds:

$$\exists \kappa \geq 0, \quad |f(x) - f(x')| \leq \kappa \|x - x'\|_2 \quad \forall x, x' \in \mathcal{X} \subseteq \mathbb{R}^d. \quad (1)$$

where  $\kappa$  is the Lipschitz constant, and  $d$  denotes the number of dimensions of the space. LIPO is a sequential and stochastic method designed to optimize a  $\kappa$ -Lipschitz function  $f$  of known constant

<sup>1</sup>Source code: <https://github.com/gaetanserre/LIPO>

Demo: <https://ipolcore.ipol.im/demo/clientApp/demo.html?id=469>.



**Figure 1.** a) An example of a Lipschitz function ( $x \mapsto 0.5 \sin x$ ). The hourglass-shaped double cones are generated using a slope of  $\pm\kappa$ . As this function is 0.5-Lipschitz, the graph of the function is always outside of cones generated by a  $\kappa \geq 0.5$ . The bigger  $\kappa$ , the thinner are the cones. b) Example of an upper bound constructed by LIPO, given the potential maximizers  $(X_i)_{1 \leq i < t}$ .  $X_{\kappa,t}$  is the regions of the domain where the potential maximizers can be found at time  $t$ , and therefore the regions in which  $f$  is worth being probed. The upper bound (blue) is a piecewise linear function with slope coefficient in  $\{-\kappa, \kappa\}$  that passes through each potential maximizer.

$\kappa$ , over a domain  $\mathcal{X}$  that is compact and convex subset of  $\mathbb{R}^d$  with non-empty interior. Suppose  $(X_i)_{1 \leq i < t}$  is the sequence of the  $t - 1$  potential maximizers found so far. At each iteration, LIPO samples a candidate point  $x \in \mathcal{X}$  uniformly at random, and considers it as a potential maximizer iff:

$$\max_{1 \leq i < t} f(X_i) \leq \min_{1 \leq i < t} f(X_i) + \kappa \|x - X_i\|_2, \quad (2)$$

By making use of the  $\kappa$ -Lipschitz property of  $f$ , LIPO constructs the upper bound of the function at  $x$  appearing on the right-hand side of Eq. 2, and in this way checks the potential of the the candidate point before evaluating the function at it. The candidate is considered as a potential maximizer if the upper bound at  $X_t$  is greater than the function value at the best maximizer found so far. If the candidate is accepted, LIPO evaluates  $f$  at  $x$ , and the value is stored to compute Eq. 2 at the next iteration. The fact that  $f$  is  $\kappa$ -Lipschitz ensures that the upper bound is valid and thus no global maximizer is rejected. The algorithm is consistent because the region of potential maximizers tightens around the global maximizers as the number of evaluations increases. LIPO, as well as ADALIPO that we will see in the next subsection, are consistent over Lipschitz functions, with a convergence rate of at least  $O(t^{-1/d})$  (with high probability), where  $t$  is the number of actual function evaluations performed, or in other words the number of potential maximizers found. An example of the upper bound is given in fig. 1b. In a nutshell, LIPO maximizes  $f$  while minimizing the number of function evaluations by evaluating  $f$  only at candidates that are potential maximizers.

Note that, in what follows, the number of iterations of LIPO is denoted by  $t$ , i.e. the number of potential maximizers found so far and it should not be confused with the *the number of sampled candidates*. As we assume that  $f$  is costly, the number of time it is evaluated is a crucial measure to assess the performance of algorithms, and will be the only one used throughout this paper. The link between the number of samples and the number of potential maximizers is discussed in section 3.1.

## 2.2 Adapative LIPO

While LIPO is simple and efficient, the Lipschitz constant of  $f$  needs to be known. This information is not available in general. As a response to that issue, the ADALIPO variant [8] alternates stochastically between two states: a state of exploration, where all candidates get accepted, and a state of exploitation, where an estimation of the Lipschitz constant is used to reject candidates with the LIPO upper bound of Eq. 2. The Lipschitz constant at time  $t$  is estimated using the follow formula:

$$\hat{\kappa}_t \triangleq \inf \left\{ \kappa_{i \in \mathbb{Z}} : \max_{i \neq j} \frac{|f(X_i) - f(X_j)|}{\|X_i - X_j\|_2} \leq \kappa_i \right\},$$

where  $(\kappa_i)_{i \in \mathbb{Z}}$  can be any real-valued sequence. We use the sequence  $\kappa_i = (1 + \alpha)^i$ , with  $\alpha \triangleq 0.01$ , following the suggestion of [8]. Thus, one can compute the closed-form expression of  $\hat{\kappa}_t$ :

$$\hat{\kappa}_t = (1 + \alpha)^{i_t},$$

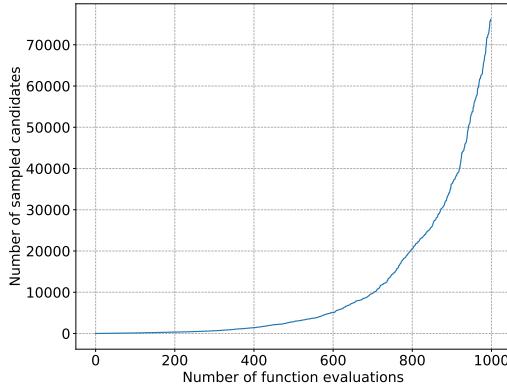
$$\text{where } i_t = \left\lceil \ln \left( \max_{i \neq j} \frac{|f(X_i) - f(X_j)|}{\|X_i - X_j\|_2} \right) \frac{1}{\ln(1 + \alpha)} \right\rceil.$$

This computation ensures that  $\kappa$  is not overestimated. Indeed, if there is  $i$  such that  $\kappa_i \leq \kappa \leq \kappa_{i+1}$ , then, at any time  $t$  it holds  $\hat{\kappa}_t \leq \kappa_{i+1}$  (see [8]). At each iteration, ADALIPO enters the exploration state with probability  $p$ , which is a fixed hyperparameter of the algorithm. By accepting any uniformly sampled candidates, the exploration state prevents the estimation of  $\kappa$  from being locally biased by the potential maximizers region. This behavior allows the method to be consistent over Lipschitz functions.

## 3 EMPIRICAL IMPROVEMENTS

### 3.1 Limitations of LIPO

The two main drawbacks of the approach of LIPO are: i) the calculation of the upper bound becomes computationally more expensive as  $t$  grows large, and ii) the uniform random sampling strategy



**Figure 2. Number of sampled candidates required by LIPO vs number of potential maximizers (i.e. evaluations of  $f$  on the  $x$ -axis) for the Rastrigin function. The number of function evaluations corresponds to the number of candidates that satisfy Eq. 2. It is evident that more and more candidates need to be sampled for finding the  $t$ -th potential maximizer as time  $t$  passes.**

across all the function domain  $X$ . The latter implies that, when the region of potential maximizers gets to be small (see the gray-shaded region  $X_{\kappa,t}$  in fig. 1b), the algorithm needs a long time before it finds a candidate in that region. fig. 2 demonstrates this phenomenon.

To address these issues, we present the LIPO+ and ADALIPO+ improved versions of the aforementioned algorithms, aiming at a better empirical performance. The first point of improvement is a stopping criterion, motivated by the discussion around fig. 2, that allows the algorithm to stop when the number of samples required to find a potential maximizer is growing *exponentially*. The second point of improvement concerns ADALIPO, where we introduce a *decaying probability* of entering the exploration state. This allows a faster convergence while restricting the approximation of the Lipschitz constant  $\kappa$  to the region of interest.

### 3.2 Stopping Criterion

As illustrated in fig. 2, the number of samples required to find a potential maximizer seems to grow exponentially whenever the region of potential maximizers is small: the uniform random sampling has a low probability of finding a candidate in that region. This effect is unavoidable and will eventually happen over time, but the number of previous potential maximizers needed for reaching this state is unknown and depends on both the function and its domain. As it is hard to select a fixed number of evaluations as a stopping criterion, we propose to stop the algorithm whenever the slope of the function represented in fig. 2 exceeds a given threshold  $\Delta$ . The slope is computed over a window of size  $w$ . A bigger  $\Delta$  value allows the algorithm to run longer, reaching to more precise final approximation.

### 3.3 Decaying Exploration Rate

As explained in section 2.2, the transition between the exploration and the exploitation state is controlled by a Bernoulli random variable of fixed parameter  $p$ :  $Y \sim \mathcal{B}(p)$ . By intuition and experience, we can assume that exploring a lot at the beginning of the process

is a good way to approximate correctly the Lipschitz constant  $\kappa$  first, and favor more and more the exploitation state as the number of evaluations increases. We propose to take  $p(t) = \min(1, \frac{1}{\ln(t)})$ , with the convention that  $p(1) = 1$ . As stated in section 2.2, the exploration state allows the estimation of  $\kappa$  to be unbiased. Our approach does not offer the same guarantee. Indeed, as the iterations increase, the probability of entering the exploration state decreases, and the estimation of  $\kappa$  will be restricted to the region of potential maximizers, and hence ADALIPO+ might highly underestimate the global  $\kappa$ . However, as the relative complement of this region w.r.t. to  $X$  is ignored by the algorithm, the estimation will be optimal over the current region of potential maximizers. We provide an illustration of the differences between the vanilla and our improved version in fig. 4.

## 4 EXPERIMENTS

In this section, we compare the vanilla LIPO algorithms to ours, LIPO+ and ADALIPO+. We set  $\Delta = 600$  and  $w = 5$ . We use standard benchmark functions used in global optimization literature [15]. Some have few local minima (e.g. the Sphere function) while others have many (e.g. the Rastrigin function). See fig. 3 for a visual representation of the functions. We set the dimension to  $d = 2$  for all functions. We run each algorithm 100 times on each function and report the results in table 1. The budget (maximum number of evaluations) depends on the function as some are easier to optimize than others. LIPO and ADALIPO exhaust the entire budget, while LIPO+ and ADALIPO+ may terminate earlier if the stopping criterion is met. One can see that, with significantly less evaluations, LIPO+ and ADALIPO+ compete with the original version.

In addition, we consider the AdALIPO+|ns variant of AdALIPO+ without using the stopping criterion defined in section 3.2. Same as the algorithms of the LIPO family, AdALIPO+|ns stops when the budget is exhausted. To compare the performance of AdALIPO+|ns to the original algorithms, we give them an infinite budget and stop them whenever the following condition is met:  $g(\theta) \leq \max_{1 \leq i < t} f(X_i)$ , where  $\theta \in [0, 1]$  a chosen threshold and

$$g(\theta) = \max_{x \in X} f(x) - \left( \max_{x \in X} f(x) - \int_X \frac{f(x)}{\lambda(X)} dx \right) (1 - \theta), \quad (3)$$

where  $\lambda$  is the standard Lebesgue measure that generalizes the notion of volume of any open set. This condition allows us to stop the algorithm whenever we consider it has reached close enough to the true maximum. The distance required is controlled by  $\theta$ : the closer to 1, the smaller the distance. We set  $\theta = 0.99$  for all the functions. The results are recorded in table 2. As one can see, AdALIPO+|ns significantly outperforms the original on this benchmark. It even succeeds to beat LIPO on almost every problem, while knowing less information on the function. It corroborates the fact our decaying exploration rate is a good strategy to improve the empirical performance of AdALIPO.

## 5 LIMITATIONS

A limitation of LIPO+ and AdALIPO+ is that the original proofs of consistency provided in [8] concerning the vanilla versions are not directly applicable. We do not provide any theoretical guarantees on the convergence of our methods. Since the consistency of the

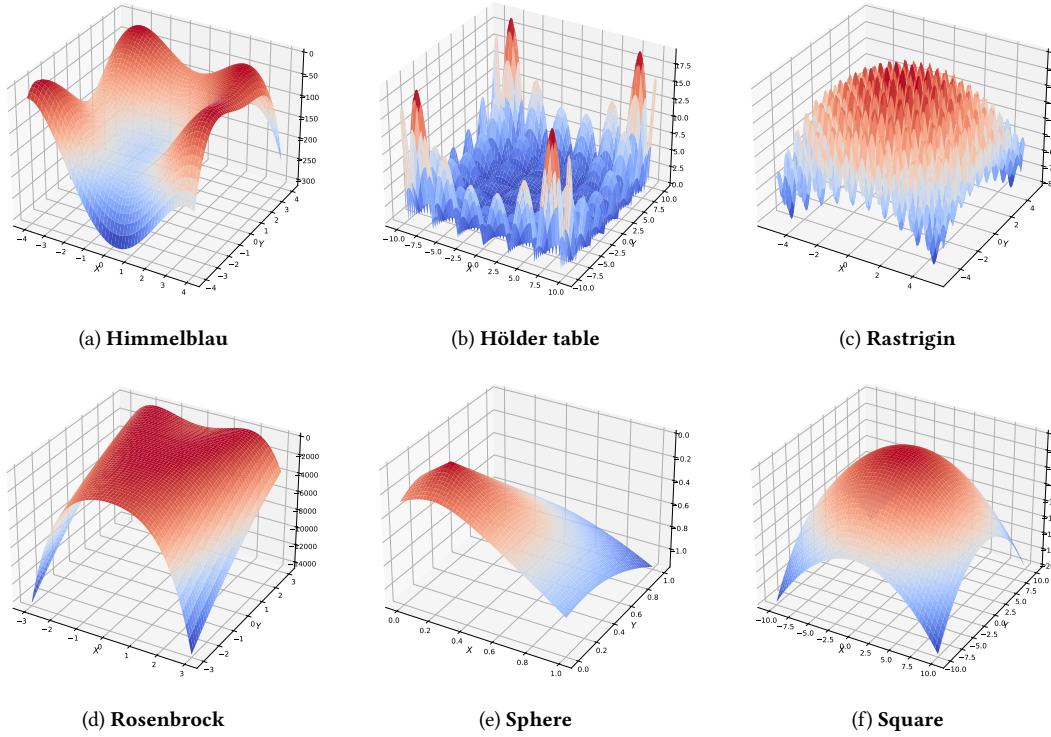


Figure 3. Graphs of the chosen benchmark functions in 2D.

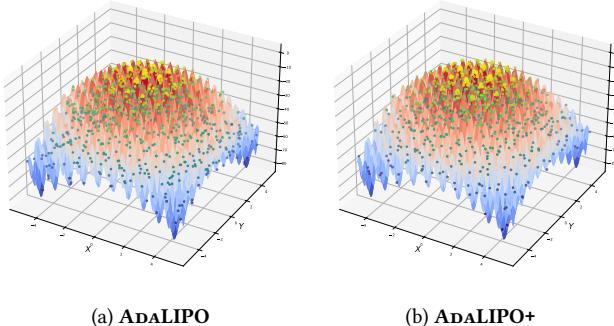


Figure 4. Visual understanding of the proposed improvements for ADALIPO on the Rastrigin function, which has several local minima. The color shades represent the function value, from blue (low) to red or yellow (high). Comparing to ADALIPO, the improved ADALIPO+ not only it tends to be more restricted over the region of higher interest (which can be seen with a higher number of evaluations at the center in yellow), but it also reduces the number of function evaluations (dots).

original algorithms is one of their key features of the LIPO family, this is a major drawback for the proposed improvements. Another limitation related to the curse of dimensionality is inherited from the vanilla approach. As the dimension increases, the volume of potential maximizers increases exponentially and thus, the probability

**Table 1.** Empirical results comparing the original algorithms and the proposed improved versions. # evals is the number of function evaluations (mean  $\pm$  std), and  $d_{\max}$  is the distance from the real maximum. One can see that, with significantly less evaluations, LIPO+ and ADALIPO+ compete with the original version in terms of distance to the real maximum.

	Hölder # evals	$d_{\max}$	Rastrigin # evals	$d_{\max}$	Sphere # evals	$d_{\max}$
LIPO	2000	0.0018	1000	0.0512	25	0.0306
LIPO+	1505 $\pm$ 104	0.0018	869 $\pm$ 34	0.1282	25	0.0320
ADALIPO	2000	0.003	1000	0.4106	25	0.0227
ADALIPO+	719 $\pm$ 457	0.023	753 $\pm$ 133	0.0569	20 $\pm$ 5	0.0063

**Table 2.** Empirical performance of our ADALIPO+|ns variant. The table shows the total number of function evaluations (mean  $\pm$  std) required to meet the condition stated in Eq. 3. ADALIPO+|ns outperforms LIPO and ADALIPO in almost all problems.

	LIPO	ADALIPO	ADALIPO+ ns
Himmelblau	100 $\pm$ 86	97 $\pm$ 77	65 $\pm$ 46
Hölder	508 $\pm$ 217	319 $\pm$ 201	228 $\pm$ 136
Rastrigin	670 $\pm$ 183	913 $\pm$ 297	616 $\pm$ 187
Rosenbrock	11 $\pm$ 10	12 $\pm$ 11	11 $\pm$ 10
Sphere	46 $\pm$ 10	28 $\pm$ 8	22 $\pm$ 6
Square	43 $\pm$ 22	62 $\pm$ 47	51 $\pm$ 36

of rejecting a point sampled uniformly in the domain decreases

accordingly. We provide the following upper bound for LIPO, which also holds for the other algorithms:

**THEOREM 5.1 (LIPO REJECTING PROBABILITY).** *For any  $\kappa$ -Lipschitz function  $f$ , let  $(X_i)_{1 \leq i \leq t}$  be the previous potential maximizers of LIPO at time  $t$ . For any  $x \in \mathcal{X}$ , let  $R(x, t)$  be the event of rejecting  $x$  at time  $t+1$ , i.e.*

$$R(x, t+1) = \max_{1 \leq i \leq t} f(X_i) < \min_{1 \leq i \leq t} f(X_i) + \kappa \|x - X_i\|_2.$$

We have the following upper bound:

$$\mathbb{P}(R(x, t+1)) \leq \frac{t\pi^{d/2}\Delta^d}{\kappa^d \Gamma(d/2+1)\lambda(\mathcal{X})},$$

where  $\Delta = \max_{x \in \mathcal{X}} f(x) - \min_{x \in \mathcal{X}} f(x) := \text{diam}(\mathcal{X})$  is the diameter of the domain,  $\lambda$  is the standard Lebesgue measure that generalizes the notion of volume of any open set, and  $\Gamma$  is the extended factorial function (i.e. the Gamma function) given by  $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$ .

**PROOF.** At time  $t$ , a candidate  $x \in \mathcal{X}$  is rejected iff it belongs to a ball within  $\mathcal{X}$ :

$$\min_{1 \leq i < t} f(X_i) + \kappa \|x - X_i\|_2 < \max_{1 \leq i < t} f(X_i).$$

Let  $j$  be in the argmin of the LHS of the above inequality. It is equivalent to

$$\begin{aligned} f(X_j) + \kappa \|x - X_j\|_2 &< \max_{1 \leq i < t} f(X_i) \\ \iff \kappa \|x - X_j\|_2 &< \max_{1 \leq i < t} f(X_i) - f(X_j) \\ \iff x \in B\left(X_j, \frac{\max_{1 \leq i < t} f(X_i) - f(X_j)}{\kappa}\right) \cap \mathcal{X} \\ &\subseteq B\left(X_j, \frac{\max_{1 \leq i < t} f(X_i) - f(X_j)}{\kappa}\right). \end{aligned}$$

As  $\text{diam}(f(\mathcal{X})) = \Delta$ , the volume of a ball of radius  $\frac{\Delta}{\kappa}$  is an upper bound on the volume that can be removed from the region of potential maximizers, for any sequence of iterations  $(X_i)_{1 \leq i < t}$ . Thus, at time  $t+1$ , at most the volume of  $t$  disjoint balls of radius  $\frac{\Delta}{\kappa}$  may have been removed. This leads to the following lower bound on the volume in which potential maximizers should be seek:

$$v_{t+1} \geq \lambda(\mathcal{X}) - \frac{t\pi^{d/2}\Delta^d}{\kappa^d \Gamma(d/2+1)}.$$

As LIPO samples candidates uniformly at random in  $\mathcal{X}$ , the probability of rejecting a candidate is bounded from above by the probability of sampling uniformly at a point in the union of the  $t$  disjoint balls:

$$\mathbb{P}(R(x, t+1)) \leq \frac{t\pi^{d/2}\Delta^d}{\kappa^d \Gamma(d/2+1)\lambda(\mathcal{X})}.$$

We provide a formalization of this proof in Lean [2] and its mathematical library Mathlib [10] in Appendix A. ■

This upper bound tends extremely quickly to 0 as the dimension increases. For instance, let us consider the function  $x \mapsto e^{\|x\|_2}$  over  $[-1, 1]^d$ , let  $C_d = \frac{\pi^{d/2}\Delta^d}{\kappa^d \Gamma(d/2+1)\lambda(\mathcal{X})}$ . Then,  $C_2 = 0.78$ ,  $C_5 = 0.16$ ,  $C_{10} = 0.002$ ,  $C_{50} = 1.5 \times 10^{-28}$ . This implies that LIPO and, by extension, the other algorithms, tend to Pure Random Search as the dimension increases, since they accept any candidate with a high probability.

## 6 CONCLUSION

In this paper, we proposed simple yet effective empirical improvements to the algorithms of the LIPO family, which we respectively call name LIPO+ and ADALIPO+. We showed experimentally that our methods converge significantly faster than the vanilla versions, and hence they are more suitable for frugal optimization problems over Lipschitz functions. Our methods ship two major limitations: the lack of theoretical guarantees compared to the original algorithms, while it inherits from them the a limitation related to the curse of dimensionality. For the latter, we provided an upper bound on the probability of rejecting a candidate for LIPO, which tends very quickly to 0 as the dimension increases.

## ACKNOWLEDGMENTS

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## REFERENCES

- [1] Damek Davis, Dmitriy Drusvyatskiy, Yin Tat Lee, Swati Padmanabhan, and Guanghao Ye. 2022. A gradient sampling method with complexity guarantees for Lipschitz functions in high and low dimensions. In *Proceedings of Advances in Neural Information Processing Systems*.
- [2] Leonardo de Moura and Sebastian Ullrich. 2021. The Lean 4 Theorem Prover and Programming Language. In *Automated Deduction – CADE 28*. Springer International Publishing.
- [3] Serré Gaétan, Beja-Battais Perceval, Chirrane Sophia, Kalogeratos Argyris, and Vayatis Nicolas. 2024. Implementation of Global Optimization Algorithms for Lipschitz Functions.
- [4] Nikolaus Hansen and Andreas Ostermeier. 1996. Adapting arbitrary normal mutation distributions in evolution strategies: the covariance matrix adaptation. In *Proceedings of the IEEE International Conference on Evolutionary Computation*.
- [5] Michael I. Jordan, Guy Kornowski, Tianyi Lin, Ohad Shamir, and Manolis Zampetakis. 2023. Deterministic Nonsmooth Nonconvex Optimization.
- [6] Scott Kirkpatrick, C Daniel Gelatt Jr, and Mario P Vecchi. 1983. Optimization by simulated annealing. *science* (1983).
- [7] Juyong Lee, In-Ho Lee, InSuk Joung, Jooyoung Lee, and Bernard R. Brooks. 2017. Finding multiple reaction pathways via global optimization of action. *Nature Communications* (2017).
- [8] Cédric Malherbe and Nicolas Vayatis. 2017. Global optimization of Lipschitz functions. In *Proceedings of the International Conference on Machine Learning*.
- [9] Ruben Martinez-Cantin. 2014. BayesOpt: A Bayesian Optimization Library for Nonlinear Optimization, Experimental Design and Bandits. *Journal of Machine Learning Research* (2014).
- [10] The mathlib Community. 2020. The Lean mathematical library. In *Proceedings of the ACM SIGPLAN International Conference on Certified Programs and Proofs*.
- [11] Seyedali Mirjalili and Andrew Lewis. 2016. The whale optimization algorithm. *Advances in engineering software* (2016).
- [12] János D Pintér. 1991. Global optimization in action. *Scientific American* (1991).
- [13] Alessandro Rudi, Ulysse Marteau-Ferey, and Francis Bach. 2024. Finding global minima via kernel approximations.
- [14] Gaétan Serré, Argyris Kalogeratos, and Nicolas Vayatis. 2024. Stein Boltzmann Sampling: A Variational Approach for Global Optimization. arXiv:2402.04689
- [15] S. Surjanovic and D. Bingham. 2022. Virtual Library of Simulation Experiments: Test Functions and Datasets. Retrieved from: <http://www.sfu.ca/~ssurjano>.
- [16] Jiankai Xue and Bo Shen. 2023. Dung beetle optimizer: A new meta-heuristic algorithm for global optimization.
- [17] Jingzhao Zhang, Hongzhou Lin, Stefanie Jegelka, Suvrit Sra, and Ali Jadbabaie. 2020. Complexity of Finding Stationary Points of Nonconvex Nonsmooth Functions. In *Proceedings of the International Conference on Machine Learning*.

## A FORMALIZATION OF THEOREM 5.1

Lean [2] is a programming language that facilitates the writing of mathematical proofs. The typechecker of Lean ensures that the proof is correct. The mathematical library Mathlib [10] provides a wide range of mathematical tools and theorems that can be used to prove other mathematical statements. We provide a formalization of the proof of theorem 5.1 in Lean using Mathlib. In this section, we

only provide the definition of the main objects and the statement of the main theorems. The complete code is available online<sup>2</sup>.

## A.1 Definitions

We first define the dimension of the space  $d$ , such that  $0 < d$ .

```
variable {d : ℕ} (hd : 0 < d)
```

We also need to define our search space  $X \subset \mathbb{R}^d$ . Note that it is not required to be compact, but only to be approximated by a measurable set, up to a null measure set.

```
variable {X : Set (EuclideanSpace ℝ (Fin d))} (null_measurable : NullMeasurableSet X)
```

This allows us to define the uniform measure over our space.

```
noncomputable def μ : Measure X := (volume X)^{-1} • volume
```

Then, we define the function to be optimized  $f : X \rightarrow \mathbb{R}$  where the sets of  $\arg \max$  and  $\arg \min$  of  $f$  are supposed to be non-empty.

```
variable (f : X → ℝ) (neamax : (argmax f).Nonempty) (neamin : (argmin f).Nonempty)
```

Note that this is a slightly more general framework than the one presented in the paper, where  $f$  is continuous and defined over a compact (which implies the properties of the above definition).

Next, for a given set of potential maximizers  $A$  and a Lipschitz constant  $\kappa$ , we define the event “*a candidate  $x$  is being rejected by LIPO*”.

```
def is_rejected {A : Finset X} (hA : A.Nonempty) (κ : ℝ) (x : X) := (A.image (fun y ↦ f y + κ * ‖x - y‖)).min' ≤ (image_nonempty hA) < (A.image f).max' (image_nonempty hA)
```

This allows us to define the set of all rejected candidates, given a set of potential maximizers  $A$  and a Lipschitz constant  $\kappa$ .

```
def rejected {A : Finset X} (hA : A.Nonempty) (κ : ℝ) := {x | is_rejected f hA κ x}
```

We define the diameter of the image of  $f$  as  $f(x) - f(y)$ , for any  $x \in \arg \max_{x \in A} f(x)$  and  $y \in \arg \min_{x \in A} f(x)$ .

```
noncomputable def diam {α β : Type*} [LE β] [HSub β β β] {f : α → β} (neamax : (argmax f).Nonempty) (neamin : (argmin f).Nonempty) := f.neamax.some - f.neamin.some
```

Finally, we define the volume of a ball of radius  $\frac{\text{diam}}{\kappa}$ .

```
noncomputable def measure_ball_diam (κ : ℝ) := (volume X)^{-1} * (ENNReal.ofReal (diam neamax neamin / κ) ^ d * ENNReal.ofReal (sqrt(Real.pi ^ d / ((d : ℝ) / 2 + 1).Gamma)))
```

## A.2 Theorems

We prove that, given a set of potential maximizers  $A$  and a Lipschitz constant  $\kappa$ , a candidate  $x$  is rejected by LIPO iff there exists a point  $x'$  in  $A$  such that  $x \in B\left(x', \frac{\max_{y \in A} f(y) - f(x')}{\kappa}\right)$ .

```
theorem reject_iff_ball {A : Finset X} (hA : A.Nonempty) {κ : ℝ} (hk : 0 < κ) (x : X) : is_rejected f hA κ x ↔ ∃ x' ∈ A, x ∈ ball x' (((A.image f).max' (image_ne hA) - f x') / κ)
```

This allows us to prove that the set of all rejected candidates is equal to the union indexed by  $A$  of balls defined as above.

```
theorem reject_iff_ball_set {A : Finset X} (hA : A.Nonempty) {κ : ℝ} (hk : 0 < κ) : rejected f hA κ = ⋃ x' ∈ A, ball x' (((A.image f).max' (image_ne hA) - f x') / κ)
```

Finally, using classical results on restricted measure, on the volume of balls in Euclidean space, and the fact that the diameter is bigger than any distance between two points in the image of  $f$ , we can prove theorem 5.1.

```
theorem measure_reject_le {A : Finset X} (hA : A.Nonempty) {κ : ℝ} (hk : 0 < κ) : μ (rejected f hA κ) ≤ A.card * measure_ball_diam f neamax neamin κ
```

<sup>2</sup>Source code: <https://github.com/gaetanserre/Lean-LIPO>.