Stochastic Methods for Global Optimization

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Global optimization

Branch of mathematics who aim to find the global optima of an arbitrary function over a compact set. Also sometimes reffered as **non-convex op-timization**. This is a very hard problem and there is no general solution.

$$f: \Omega \subset \mathbb{R}^d o \mathbb{R}$$
 $x \in \underset{x \in \Omega}{\operatorname{argmin}} f(x),$

We focus on sequential and stochastic global optimization methods:

Algorithm 1: Sequential Stochastic Global Optimization Method

Input:

 $f:\Omega\to\mathbb{R}$, the objective function.

Output:

 \hat{x} , an approximation of a minimizer of f.

for i in 1...N do

 $x_i \sim d_{\theta}$ Sample a point w.r.t. a distribution d parametrized by θ . $\theta = F(x_1, ..., x_i, f(x_1), ..., f(x_i))$ Update θ using the previous points and their evaluations.

end for

return argmin $f(x_i)$

Return the best point found.

Lipschitz continuity commonly assumed to design consistent methods.

The need for randomness

- Emergence of deep learning \Rightarrow resurgence of nonsmooth Lipschitz optimization (nonsmooth components, e.g. ReLU)
- Recent negative results for deterministic methods [1]
- M. I. Jordan and others [2] raises this fundamental question:

What is the role of randomization in dimension-free nonsmooth nonconvex optimization?

Theorem (Necessity of randomness). For any $0 < \Delta$, $0 < \kappa$, $3 \le d$, $N \le d-2$, and any deterministic first-order algorithm \mathcal{A} , there exists a κ -Lipschitz function $f: \Omega \to \mathbb{R}$ such that $f(x_0) - \inf_{x \in \Omega} f(x) \le \Delta$ for which any of the N first iterates produced by \mathcal{A} applied to f is not a (δ, ε) -Goldstein stationary point of f, for any $\delta < \frac{\Delta}{\kappa}$ and $\varepsilon < \frac{\kappa}{252}$.

Randomness is necessary to achieve good performance on arbitrary Lipschitz functions.

Some stochastic methods

LIPO [3]

- Constructs upper bound and uses it to sample from an uniform distribution
- Adaptative version estimating the Lipschitz constant: Adalipo
- Both **consistent** over the class of Lipschitz functions

CMA-ES [4]

- Efficient method. Samples points from moving Gaussian distribution.
- Not consistent

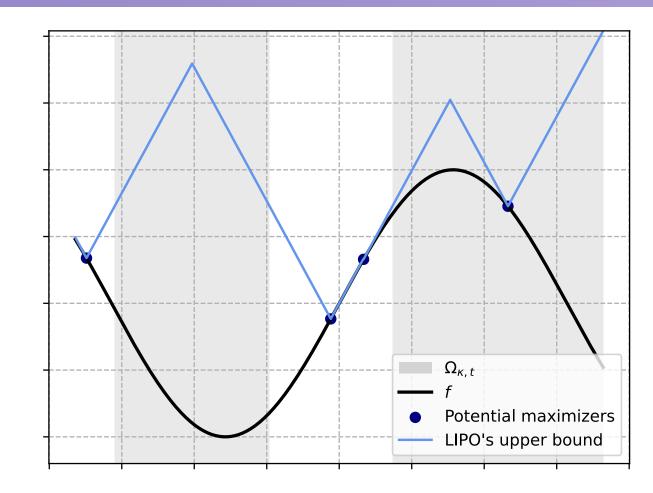


Figure 1: An example of upper bound constructed by LIPO. The set of point $\Omega_{\kappa,t}$ is the set of potential maximizers.

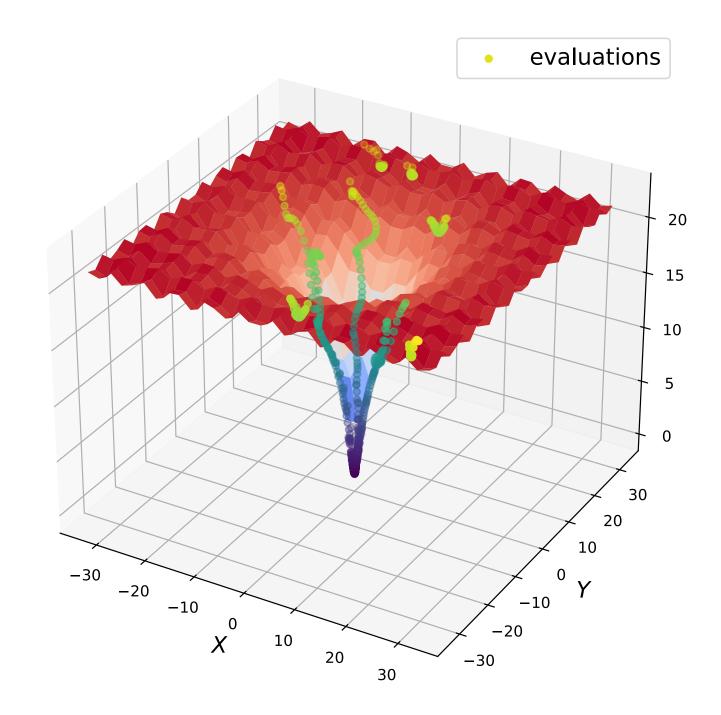


Figure 2: Movement of SBS' particles on the Ackley function.

Stein Boltzmann Sampling

- We propose the *Stein Boltzmann Sampling* method [5].
- Flow-based method. Samples from the Boltzmann distribution.
- Consistent over the class of Lipschitz functions
- Theory:
 - \hookrightarrow Multiple domains e.g. functional analysis, measure theory, flow theory

Theorem. Let k be a symmetric positive definite kernel, \mathcal{H} the associated RKHS, and μ a measure such that $\mu \ll \lambda$. The following integral operator is a mapping in \mathcal{H} :

$$T_k: L^2_{\mu(\Omega)} \to \mathcal{H}$$

$$f \mapsto \int_{\Omega} k(x, \cdot) f(x) \, \mathrm{d}\mu(x).$$

→ Some results formalized using Lean

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class RKHS {E F : Type*} [RCLike F] (H : Set (E → F))
[NormedAddCommGroup H] [InnerProductSpace F H] where
k : E → E → F
memb : ∀ (x : E), k x ∈ H
repro : ∀ (f : H), ∀ (x : E), f.1 x = inner f ⟨k x, memb x⟩
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- Easely adaptable for sampling in complex manifolds

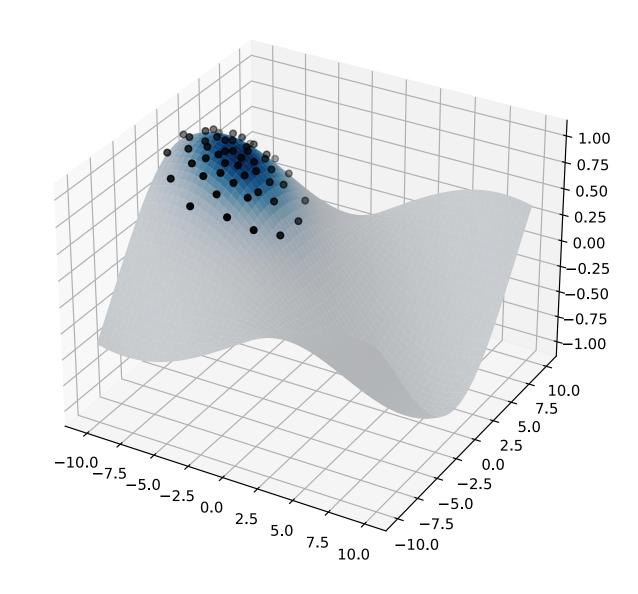


Figure 3: Sampling over a curve w.r.t. a Gaussian distribution using SVGD.

- [3] C. Malherbe and N. Vayatis, "Global Optimization of Lipschitz Functions," 2017.
- N. Hansen and A. Ostermeier, "Adapting arbitrary normal mutation distributions in evolution strategies: the covariance matrix adaptation," 1996.
- [5] G. Serré, A. Kalogeratos, and N. Vayatis, "Stein Boltzmann Sampling: A Variational Approach for Global Optimization." 2024.

^[1] G. Kornowski and O. Shamir, "Oracle complexity in nonsmooth nonconvex optimization," 2021.

^[2] M. I. Jordan and others, "Deterministic Nonsmooth Nonconvex Optimization." 2023.