The Sample Complexity of Level Set Approximation

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Problem, motivations, related work

Problem

Approximating $\{\boldsymbol{x} : f(\boldsymbol{x}) = a\} \subset [0,1]^d$

- $f : [0,1]^d \to \mathbb{R}$ unknown in some known smoothness class
- $a \in \mathbb{R}$ a fixed known threshold

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Determining parameters that result in a given outcome (computer experiments, uncertainty quantification, nuclear engineering, coastal flooding, etc.)

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Related work

- Gaussian process models: Chevalier et al. 2014 Technometrics, Azzimonti et al. 2020 Technometrics, Gotovos et al. 2013 IJCAI
- Global optimization algorithms: DOO, Munos 2011 NIPS, HOO, Bubeck et al. 2011 JMLR

Protocol and Objective

Online Protocol

For $n = 1, 2, \ldots$

1. pick the next query point $\boldsymbol{x}_n$
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Our Goal

Quantifying the sample complexity, i.e., smallest number of evaluations of f needed to

$$\{\boldsymbol{x} : f(\boldsymbol{x}) = a\} \subset S_n \subset \{\boldsymbol{x} : |f(\boldsymbol{x}) - a| \leq \varepsilon\}$$

for some error level $\varepsilon > 0$

A Hard Problem

Definition

The packing number of a non-empty set E is

$$\mathcal{N}(E,\varepsilon) := \sup\Big\{k \in \mathbb{N} : \exists\, \boldsymbol{x}_1,\ldots,\boldsymbol{x}_k \in E,\ \min_{i\neq j} \|\boldsymbol{x}_i - \boldsymbol{x}_j\|_\infty > \varepsilon\Big\}$$

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Theorem

If f is a non-constant continuous function, for any $\min(f) < a < \max(f)$,

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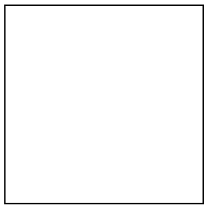
Not surprising, the level set is defined by a single equation in d unknowns

A General Solution

Bisect and Approximate (BA)



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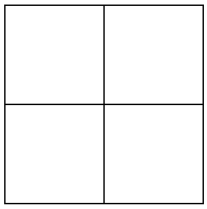
1. Bisect the current family of cells



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1. Bisect the current family of cells
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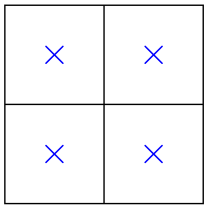

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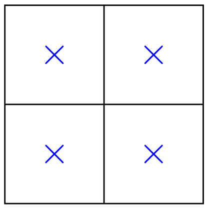

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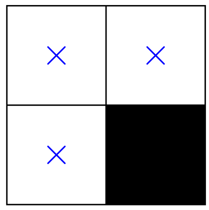
4. Remove a cell C if $|g_C(\boldsymbol{x}) - a|$ is large for all $\boldsymbol{x} \in C$



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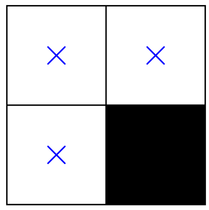

Theorem

If the g_C's are "accurate approximations" of f on the C's,

$$\text{sample complexity of BA} \lesssim \sum_{i=1}^{i(\varepsilon)} \mathcal{N}\Big(\{|f-a| \le c_i\}, d_i\Big)$$

where $i(\varepsilon) \approx \log(1/\varepsilon)$, $c_1 > c_2 > \dots$, $d_1 > d_2 > \dots$ depend on the g_C's and their error bounds

Consequence for γ-Hölder functions

γ-Hölder functions

f is γ-Hölder ($|f(\boldsymbol{x}) - f(\boldsymbol{y})| \leq c \, \|\boldsymbol{x} - \boldsymbol{y}\|^{\gamma}$, with $\gamma \in (0, 1]$)

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Local approximator for BAH

- For a cell C (hypercube), we query the center and take the local approximator g_C as constant
- The error of g_C on C is $\lesssim \mathrm{Diam}(C)^{\gamma}$

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Theorem (upper and lower bound)

The worst-case optimal sample complexity is attained by BAH and

$$\text{sample complexity of BAH} \lesssim \frac{1}{\varepsilon^{d/\gamma}}$$

For lower bound counter example functions are “flat + local bump” (classical)

Consequence for functions with γ_1-Hölder gradients

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- For a cell C (hypercube), we query the 2^d vertices and take the local approximator g_C as multilinear interpolating
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Convexity helps a little: $d \mapsto d - 1$

Theorem

When f has γ_1-Hölder gradient and is convex (+ quantitative conditions), then the worst-case optimal sample complexity is attained by BAG and

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Follows from geometric arguments on level sets of convex functions:

Theorem

If f is convex (+ quantitative conditions), there exists a constant $C^* > 0$ such that

$$\forall r \in (0,1)\ ,\ \mathcal{N}\Big(\{|f-a| \le r\},\ r\Big) \le C^* \left(\frac{1}{r}\right)^{d-1}$$

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