An Adaptive Sampling Algorithm for Level-set Approximation

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Problem Statement

Let $D \subset\subset \mathbb{R}^d$ be a d-dimensional domain with compact closure and a sufficiently smooth boundary. We are interested in approximating the zero level set of a function f,

$$\mathcal{L}_0 := \{\mathrm{x} \in \overline{D} \ : \ f(x) := \mathrm{E}[\, \tilde{f}_\ell(\mathrm{x})\,] = 0\}$$

for some random function(s), $\tilde{f}_\ell : D \to \mathbb{R}$, which can be evaluated pointwise with cost M_ℓ.

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$$\tilde{f}_\ell(\mathrm{x}) = \frac{1}{M_\ell} \sum_{i=1}^{M_\ell} f^{(i)}(x).$$

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In general, we assume the bound, e.g., $\beta = 1/2$,

$$\sup_{\mathrm{x} \in \overline{D}} \mathbb{E}\left[\left(f(\mathrm{x}) - \tilde{f}_\ell(\mathrm{x})\right)^p\right]^{1/p} \le \sigma M_\ell^{-\beta}.$$

When $\sigma = 0$, we have access to direct evaluation of $f(x)$ at cost $\mathcal{O}(1)$.

Assumption on f

We will use the following assumption: There exist some $\delta_0, \rho_0 > 0$ such that for all $0 < b < \delta_0$ we have

$$\mu(\{x \in \overline{D} : |f(x)| \leq b\}) \leq \rho_0 b$$

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This would follow by assuming that f is Lipschitz continuous, using the compactness of $\overline{D}$ which imply that the level set $\mathcal{L}_0 = \{x \in \overline{D} : f(x) = 0\}$ is a $(d-1)$-rectifiable set.

Functional approximation

Similar to[1], our method is cell-based.

- For a fixed N, select N points in a cell $\square$, say $\mathrm{x}_1^\square, \ldots, \mathrm{x}_N^\square$, deterministically,
- evaluate the approximations $\tilde{f}_\ell(\mathrm{x}_1^\square), \ldots, \tilde{f}_\ell(\mathrm{x}_N^\square)$. Denote the vector $P^\square \tilde{f}_\ell = (\tilde{f}_\ell(\mathrm{x}_i^\square))_{i=1}^N$
- Obtain an approximate function $T^\square P^\square \tilde{f}_\ell = \hat{f}_\ell^\square$ via a known approximation (or interpolation) scheme, T, on the N samples in $\square$.
- Compute the union of zero level-sets of $\{\hat{f}_\ell^\square\}_\square$.

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Notation summary:

- $f(\cdot)$ is the exact expectation.
- $\tilde{f}_\ell(\cdot)$ is the point approximation, evaluated on $\{x_i^\square\}_{i=1}^N$, e.g., each using M_ℓ samples.
- $\hat{f}_\ell^\square(\cdot)$ is the functional approximation/interpolation on cell $\square$.

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Approximation error

For any $\ell \in \mathbb{N} \cup \{0\}$ a uniform refinement of $\overline{D}$ into a collection of uniform cells, U_ℓ, each with size $h_\ell \propto 2^{-\ell}$, satisfies

$$\left(\sum_{\square \in U_\ell} \int_\square \left| f(x) - (T^\square P^\square f)(x) \right|^p \mathrm{d}\mu(x) \right)^{1/p} \leq c\, h_\ell^\alpha$$

for some (unknown) constant $c > 0$ and and some known rate $\alpha > 0$ associated with our chosen approximation method.

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We also assume that $T^\square : \mathbb{R}^{N\times d} \to L^p(\square)$, for any $\ell \in \mathbb{N}$ and all $\square \in U_\ell$, is a bounded linear operator and

$$\sum_{\square \in U_\ell} \| T^\square \|_{\mathcal{L}(\mathbb{R}^N, L^p(\square))} \leq C_N$$

Approximation error

Under the previous assumptions, we have that,

$$\left(\sum_{\square \in U_\ell} \int_{\square} \mathrm{E}\left[\left| f(\mathrm{x}) - \hat{f}_\ell^{\square}(\mathrm{x}) \right|^p \right] d\mu(\mathrm{x}) \right)^{1/p} \leq c\, h_\ell^{\alpha} + \widetilde{C}_N M_\ell^{-\beta} \lesssim h_\ell^{\alpha},$$

for $M_\ell \sim h_\ell^{-\alpha/\beta}$.

Decision variable

Define[2]

$$\hat{\delta}_\ell^\square = \frac{\inf_{x \in \square} \left| \hat{f}_\ell^\square(x) \right|}{h_\ell^\alpha}$$

Instead of h_ℓ^α, we can also use a posteriori error estimates for sharper bounds and better constants.

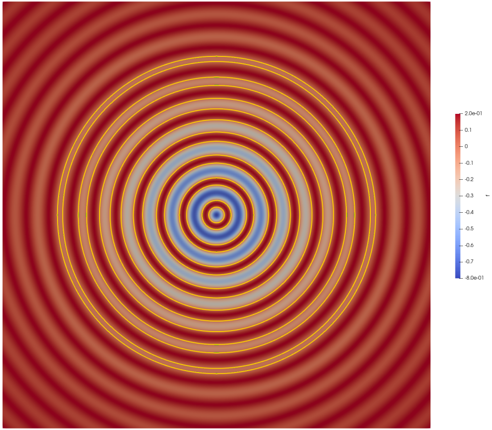
[2] Abdul-Lateef Haji-Ali et al. "Adaptive Multilevel Monte Carlo for probabilities". In: *SIAM Journal on Numerical Analysis* 60.4 (2022), pp. 2125–2149.

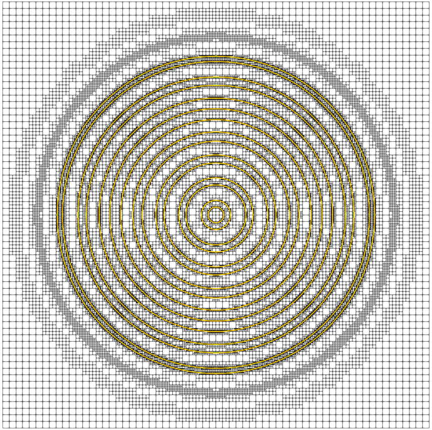
Adaptive Algorithm

Set $\mathcal{R}_0 = U_0$; ▷ Begin with a base uniform refinement
for $\ell \in \{0, \ldots, \theta - 1\}$ **do** ▷ θ is chosen to satisfy accuracy requirements
  for each cell $\square$ in $\mathcal{R}_\ell$ of size h_ℓ **do** ▷ Iterate over cells of the current level
    if $a_\ell = 0$ **then**
      Set $\hat{\delta}_\ell^\square = 0$ ▷ Always refine in this case
    else
      Evaluate $\tilde{f}_\ell$ at N points in $\square$; ▷ e.g. using $M_\ell \propto h_\ell^{-\alpha/\beta}$ samples
      Fit the cell-based estimate $\hat{f}_\ell^\square$ on the sampled values of $\tilde{f}_\ell$;
      Compute decision variable $\hat{\delta}_\ell^\square$;
    if $\hat{\delta}_\ell^\square \leq a_\ell$ **then**
      Refine $\square$ into multiple cells of size $h_{\ell+1}$, and add them to $\mathcal{R}_{\ell+1}$
    else
      Add $\square$ to $\mathcal{R}_{\ell+1}$;
Return the union of $\{\hat{f}_\theta^\square\}_{\square \in \mathcal{R}_\theta}$ zero level-sets. ▷ The final level-set estimate

An example: Drop-wave function

$$(1/5) - (1 + \cos(12\,\|x\|_2))/\left(\|x\|_2^2\,/\,2 + 2\right), \qquad x \in [-5, 5]^d.$$





Work definition

- Let $W_\ell^\square \propto M_\ell \propto h_\ell^{-\alpha/\beta}$ be the work required to approximate $\hat{f}_\ell^\square$ on $\square \in U_\ell$.
- Let $R(\square)$ be the collection of cells which result from a uniform refinement of the cell $\square$.
- Assuming that $|R(\square)| = 2^d$ for all $\square$, the work of such refinement at level ℓ is $2^d h_{\ell+1}^{-\alpha/\beta}$.
- We define the (random) work of our method by the recursive formula, starting from U_ϑ,

$$\sum_{\square_\vartheta \in U_\vartheta} W_\vartheta^{\square_\vartheta} := \sum_{\square_\vartheta \in U_\vartheta} h_\vartheta^{-\alpha/\beta} \mathbb{I}_{\hat{\delta}_\vartheta^{\square_\vartheta} \geq a_\vartheta} + \sum_{\square_\vartheta \in U_\vartheta} \mathbb{I}_{\hat{\delta}_\vartheta^{\square_\vartheta} < a_\vartheta} \sum_{\square_{\vartheta+1} \in R(\square_\vartheta)} W_{\vartheta+1}^{\square_{\vartheta+1}}$$

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$$\lesssim h_\vartheta^{-\alpha/\beta-d} + 2^d \sum_{\ell=\vartheta}^{\theta} h_\ell^{-\alpha/\beta} \left(\sum_{\square_\ell \in U_\ell} \mathbb{I}_{\hat{\delta}_\ell^{\square_\ell} < a_\ell} \right)$$

Bound on the number of cells (exact)

Recall: When f is Lipschitz continuous, there exist some $\delta_0, \rho_0 > 0$ such that for all $0 < b < \delta_0$ we have

$$\mu(\{x \in \overline{D} : |f(x)| \leq b\}) \leq \rho_0 b$$

where μ is the d-dimensional Lebesgue measure.
Let

$$\delta_\ell^{\square} = \frac{\inf_{x \in \square} |f(x)|}{h_\ell^\alpha}$$

A uniform grid, U_ℓ of $\overline{D}$ into $2^{d\ell}$ cells of size $h_\ell = h_0 2^{-\ell}$ satisfies for any $0 \leq a < h_\ell^{-\alpha}\delta_0 - L 2^{d/2} h_\ell^{1-\alpha}$,

$$\sum_{\square_\ell \in U_\ell} \mathbb{I}_{\delta_\ell^{\square_\ell} \leq a} \leq \sum_{\square_\ell \in U_\ell} \sup_{x \in \square_\ell} \mathbb{I}_{|f(x)| \leq a\, h_\ell^\alpha} \leq b\, h_\ell^{1-d} + c\, a\, h_\ell^{\alpha - d}$$

for some constants $b, c > 0$ independent of ℓ.

Bound on the number of cells (approximate)

A uniform grid, U_ℓ of $\overline{D}$ into $2^{\ell d}$ cells of size $h_\ell = h_0 2^{-\ell}$ satisfies for any $0 \le a < h_\ell^{-\alpha}\delta_0 - L 2^{d/2} h_\ell^{1-\alpha}$,

$$\sum_{\square_\ell \in U_\ell} \mathrm{E}[\, \mathbb{I}_{\hat{\delta}_\ell^{\square_\ell} \le a} \,] \le \sum_{\square_\ell \in U_\ell} \mathbb{E}\left[\sup_{x \in \square_\ell} \mathbb{I}_{|\hat{f}_\ell^{\square}(x)| \le a\, h_\ell^{\alpha}} \right]$$

$$\le c_1 h_\ell^{1-d} + c_2\, h_\ell^{\alpha\, 1_p - d} + c_3\, a\, h_\ell^{\alpha - d}$$

for some constants $c_1, c_2, c_3 > 0$ independent of ℓ.

Here: $1_p = \frac{p}{p+1} \uparrow 1$.

Work bound

Therefore, the total expected work is bounded by

$$\sum_{\square_\vartheta \in U_\vartheta} \mathrm{E}[\, W_\vartheta^{\square_\vartheta} \,] \leq \; h_\vartheta^{-\alpha/\beta - d} + c_1\, 2^d \sum_{\ell=\vartheta}^{\theta} h_\ell^{1-\alpha/\beta-d} + c_2\, 2^d \sum_{\ell=\vartheta}^{\theta} h_\ell^{\alpha 1_p - \alpha/\beta - d}$$
$$+ c_3\, 2^d \sum_{\ell=\vartheta}^{\theta} a_\ell\, h_\ell^{\alpha - \alpha/\beta - d}$$

Assuming a geometric decrease of h_ℓ, and $\alpha 1_p \geq 1$, we take, for any $\vartheta, \theta \in \mathbb{N}$,

$$a_\ell \lesssim \begin{cases} 0 & k \leq \vartheta, \\ h_\ell^{1-\alpha} & k > \vartheta. \end{cases}$$

with $\vartheta\,(\frac{\alpha}{\beta} + d) \leq \; \theta(\frac{\alpha}{\beta} + d - 1)$, to have

$$\sum_{\square \in U_0} \mathbb{E}[W_0^\square] = \sum_{\square \in U_\vartheta} \mathbb{E}[W_\vartheta^\square] \lesssim N \left(h_\vartheta^{-(\alpha/\beta + d)} + c h_\theta^{-(\alpha/\beta + d - 1)} \right) \lesssim N h_\theta^{-(\alpha/\beta + d - 1)}$$

Error definition

Define the two sets

$$\mathcal{L}_{\text{in}} := \left\{ x \in \overline{D} \;\middle|\; f(x) \le 0 \right\}$$

$$\hat{\mathcal{L}}_{\text{in}}^{\ell,\square} := \left\{ x \in \square \;\middle|\; \hat{f}_\ell^{\square}(x) \le 0 \right\}; \qquad \hat{\mathcal{L}}_{\text{in}}^{\ell} := \bigcup_{\square_\ell \in U_\ell} \mathcal{L}_{\text{in}}^{\ell,\square_\ell}$$

and consider a metric of the accuracy of our level-set estimation based on the symmetric difference of the sets $\mathcal{L}_{\text{in}}$ and $\hat{\mathcal{L}}_{\text{in}}^{\ell}$, which we denote by $\mathcal{L}_{\text{in}} \,\Delta\, \hat{\mathcal{L}}_{\text{in}}^{\ell}$.

$$\Delta_\ell(x) := \mathbb{I}_{x \in \mathcal{L}_{\text{in}} \,\Delta\, \hat{\mathcal{L}}_{\text{in}}^{\ell}}$$

We define the error of our method starting from a uniform refinement U_ℓ by the recursive formula

$$\sum_{\square_\vartheta \in U_\vartheta} \mathrm{E}[\, E_\vartheta^{\square_\vartheta} \,] := \sum_{\square_\vartheta \in U_\vartheta} \int_{\square_\vartheta} \mathrm{E}\left[\mathbb{I}_{\hat{\delta}_\vartheta^{\square_\vartheta} \ge a_\vartheta} \Delta_\vartheta(x) \right] d\mu(x) + \sum_{\square_\vartheta \in U_\vartheta} \sum_{\square_{\vartheta+1} \in R(\square_\vartheta)} \mathrm{E}\left[\mathbb{I}_{\hat{\delta}_\vartheta^{\square_\vartheta} < a_\vartheta} E_{\vartheta+1}^{\square_{\vartheta+1}} \right]$$

Error expansion

Similar to the work, we arrive at

$$\sum_{\square_\vartheta \in U_\vartheta} \mathrm{E}[\, E_\vartheta^{\square_\vartheta} \,] \leq \sum_{k=\vartheta}^{\theta-1} \sum_{\square_\ell \in U_\ell} \int_{\square_\ell} \mathrm{E}\left[\mathbb{I}_{\hat{\delta}_\ell^{\square_\ell} \geq a_\ell} \Delta_\ell(x) \right] d\mu(x) + \sum_{\square_\theta \in U_\theta} \int_{\square_\theta} \mathrm{E}[\, \Delta_\theta(x) \,]\, d\mu(x)$$

Error analysis for uniform refinement

Under L^p bounds on the approximation error, we have that for any uniform refinement U_ℓ, for some constant c,

$$\sum_{\square_\theta \in U_\theta} \int_{\square_\theta} \mathrm{E}[\, \Delta_\theta(\mathrm{x}) \,] d\mu(\mathrm{x}) \leq \; c h_\theta^{\alpha 1_p}$$

$$\sum_{\square_\ell \in U_\ell} \int_{\square_\ell} \mathrm{E}\left[\mathbb{I}_{\hat{\delta}_\ell^{\square_\ell} \geq a_\ell} \Delta_\ell(x) \right] d\mu(\mathrm{x}) \leq \; c\, a_\ell^{-p}$$

Hence if $a_\ell = 0$ when $\ell \leq \vartheta$ and

$$\sum_{\ell=\vartheta}^{\theta-1} a_\ell^{-p} \leq c\, h_\theta^{\alpha\, 1_p}$$

we have

$$\sum_{\square_0 \in U_0} \mathrm{E}[\, E_0^{\square_0} \,] = \sum_{\square_\vartheta \in U_\vartheta} \mathrm{E}[\, E_\vartheta^{\square_\vartheta} \,] \leq c \sum_{\ell=\vartheta}^{\theta} a_k^{-p} + c\, h_\theta^{\alpha 1_p} \leq c'\, h_\theta^{\alpha 1_p}$$

An example

Adapted from[3], we consider a refinement criterion of the form

$$a_\ell = \begin{cases} 0 & \ell < \vartheta \\ c h_\ell^{\alpha 1_p/R - \alpha} h_\theta^{\alpha 1_p (R-1)/R} h_\vartheta^{-\alpha 1_p/R} & \ell \geq \vartheta \end{cases}$$

where the parameter $1 < R < \alpha 1_p$ determines the strictness of refinement (more strict as $R \to 1$).

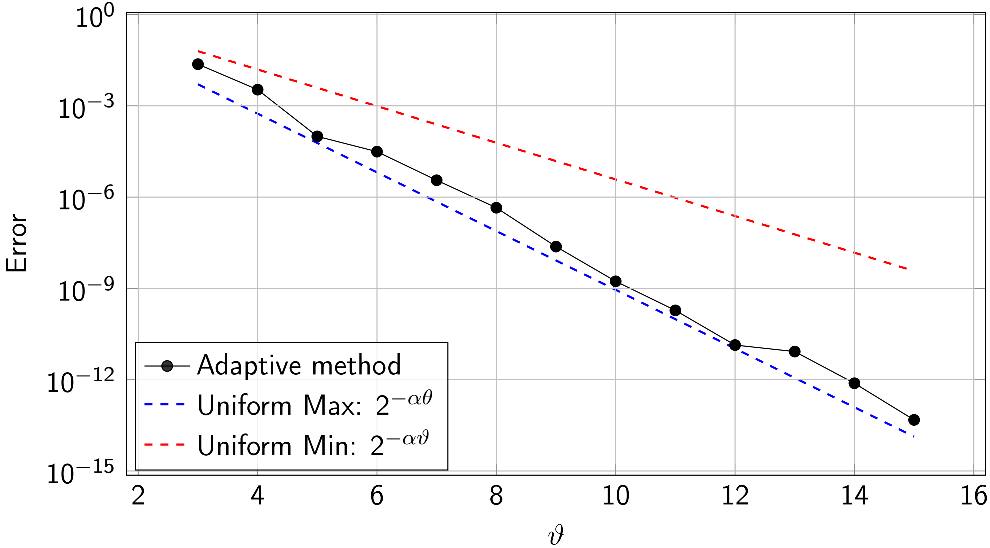
Set $\quad \vartheta = \left\lceil \theta \left(1 - \frac{1_p}{R} \right) \right\rceil, \quad$ and $\quad h_\theta = \mathcal{O}(\varepsilon^{-1/(\alpha 1_p)})$

then the adaptive/non-adaptive algorithms have computational complexities

$$\mathcal{O}\left(\varepsilon^{-\left(\frac{1}{\beta} + \frac{d-1}{\alpha}\right)/1_p} \right) \quad \text{vs.} \quad \mathcal{O}\left(\varepsilon^{-\left(\frac{1}{\beta} + \frac{d}{\alpha}\right)/1_p} \right)$$

[3] Abdul-Lateef Haji-Ali et al. "Adaptive Multilevel Monte Carlo for probabilities". In: *SIAM Journal on Numerical Analysis* 60.4 (2022), pp. 2125–2149, Michael B Giles and Abdul-Lateef Haji-Ali. "Multilevel nested simulation for efficient risk estimation". In: *SIAM/ASA Journal on Uncertainty Quantification* 7.2 (2019), pp. 497–525.

Numerical results: A circle



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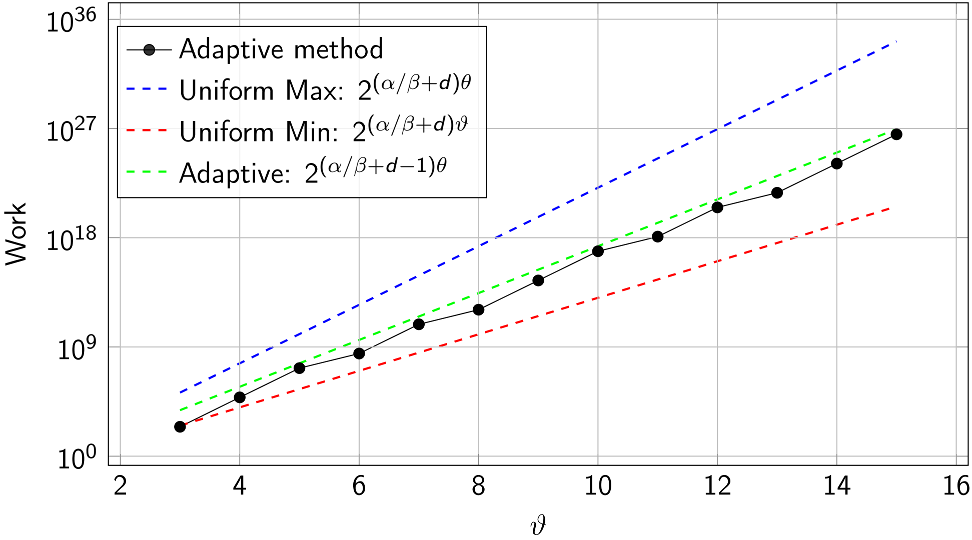

Conclusion

- A simple adaptive sampling algorithm for level-set approximation;
- The rate of growth of expected work involves, $d-1$, the dimension of the level-set, rather than d, the dimension of the ambient space.
- Rate of expected error decrease is of the same as when using uniform refinement.

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Next (current) steps:

- Consider level-sets of Hausdorff dimension less that $d-1$; work analysis is exactly the same, the error metric is more tricky (Hausdorff dim. of $\mathcal{L}_{\text{in}}$ and $\hat{\mathcal{L}}^{\ell}_{\text{in}}$ is less than d.).
- Use Sparse Grids as the base refinement rather than uniform refinement – to get dimension-independent convergence rates (in our results and in α). Requires sharper bounds on cell counting, and a method with dimension-independent refinement factor.