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,

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

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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for some random function(s), $\tilde{f}_\ell : D \to \mathbb{R}$, which can be evaluated pointwise with cost M_ℓ. For example, for each $x \in \overline{D}$, we can use iid samples $\{f^{(i)}(x)\}_{i=1}^{M_\ell}$,

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

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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 result: There exist some $\delta_0, \rho_0 > 0$ such that for all $0 < a < \delta_0$ we have

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

where μ is the d-dimensional Lebesgue measure.

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This follows by assuming that f is Lipschitz continuous, using the compactness of $\overline{D}$ and that the level set $\mathcal{L}_0 = \{x \in \overline{D} : f(x) = 0\}$ has Hausdorff dimension $k < d$, implying $\mathcal{L}_0$ is k-rectifiable.

Functional approximation

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 $P^\square \tilde{f}_\ell = (\tilde{f}_\ell(\mathrm{x}_i^\square))_{i=1}^N$
- to obtain an approximate function $I^\square P^\square \tilde{f}_\ell = \hat{f}_\ell^\square$ via a known approximation (or interpolation) scheme on the N samples in $\square$.
- Compute the union of zero level-sets of $\{\hat{f}_{\ell+k}^\square\}_\square$.

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Notation summary:

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

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

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

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 $I^{\square} : \mathbb{R}^{N \times d} \to L^p(\square)$, for all $\square$, is a bounded operator, i.e., for all $\square$ and any $f \in L^p(\square)$,

$$\| I^{\square} P^{\square} f \|_{L^p(\square)} \leq \| I^{\square} \|_{\mathcal{L}(\mathbb{R}^{N \times d}, L^p(\square))} \| P^{\square} f \|_{\ell^2} \leq C_N \| P^{\square} f \|_{\ell^2},$$

Under the previous assumptions, we have that,

$$
\begin{aligned}
&\left(\sum_{\square \in U_\ell} \int_{\square} \mathrm{E}\left[\left| f(\mathrm{x}) - \hat{f}_\ell^{\square}(\mathrm{x}) \right|^p \right] d\mu(\mathrm{x}) \right)^{1/p} \\
\leq &\left(\sum_{\square \in U_\ell} \int_{\square} \left| f(\mathrm{x}) - (I^{\square} P^{\square} f)(x) \right|^p d\mu(\mathrm{x}) \right)^{1/p} \\
&+ \left(\sum_{\square \in U_\ell} \int_{\square} \mathrm{E}[\, |(I^{\square} P^{\square} f)(x) - (I^{\square} P^{\square} \tilde{f}_\ell)(x)|^p \,] d\mu(\mathrm{x}) \right)^{1/p} \\
\leq &c\, h_\ell^{\alpha} + \left(\sum_{\square \in U_\ell} \| I^{\square} \|^p_{\mathcal{L}(\mathbb{R}^{N \times d}, L^p(\square))} \mathrm{E}[\, \| (P^{\square} f) - (P^{\square} \tilde{f}_\ell) \|^p_{\ell^2} \,] \right)^{1/p} \\
\leq &c\, h_\ell^{\alpha} + \widetilde{C}_N M_\ell^{-\beta} \lesssim h_\ell^{\alpha}, \qquad \text{for } M_\ell \sim h_\ell^{-\alpha/\beta}
\end{aligned}
$$

Decision variable

Define[1]

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

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

[1] 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

Require: the uniform grid U_ℓ to be refined, the constants α, β, d. A parameter $\theta > 0$, the number of points N to sample at in each cell, sequence $\{a_{\ell+k}\}_k$.

Set $R_\ell = U_\ell$

for $k = 0 \to \lfloor \theta\ell \rfloor$ **do**

  for each cell $\square_{\ell+k}$ in $R_{\ell+k}$ of size $h_{\ell+k}$ **do** ▷ Iterate over cells of the current level

    Evaluate $\tilde{f}_\ell$ at N points in $\square_{\ell+k}$. ▷ e.g., using $M_\ell \propto |\square_{\ell+k}|$ MC samples

    Fit estimate $\hat{f}_{\ell+k}^{\square_{\ell+k}}$ on sampled values $\tilde{f}_\ell$ and compute $\hat{\delta}_{\ell+k}$.

    if $\hat{\delta}_{\ell+k}^{\square_{\ell+k}} \leq a_{\ell+k}$ **then**

      Split $\square_{\ell+k}$ into cells each of size $h_{\ell+k+1}$, add them to $R_{\ell+k+1}$.

    else

      add $\square_{\ell+k}$ to $R_{\ell+k+1}$.

    end if

  end for

end for

Return the union of $\{\hat{f}_{\ell+k}^{\square}\}_{\square \in R_{\ell+\lfloor\theta\ell\rfloor}}$ zero level-sets ▷ Final level set estimate

Work definition

Let $W_\ell^\square \propto M_\ell \propto h_\ell^{-\alpha/\beta}$ be the work required to approximate $\hat{f}_\ell^{\square_\ell}$ on $\square_\ell \in U_\ell$.

Let $R(\square_\ell)$ be the collection of cells which result from a uniform refinement of the cell $\square_\ell$.

Assuming that $|R(\square_\ell)| = 2^d$ for all $\square_\ell$, the work of such refinement is $2^d h_{\ell+1}^{-\alpha/\beta}$.

Work definition

We define the (random) work of our method by the recursive formula

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

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&\leq 2^{d\ell} h_\ell^{-\alpha/\beta} + 2^d \Bigg[h_{\ell+1}^{-\alpha/\beta} \sum_{\square_\ell \in U_\ell} \mathbb{I}_{\hat{\delta}_\ell^{\square_\ell} < a_\ell} + h_{\ell+2}^{-\alpha/\beta} \sum_{\square_\ell \in U_\ell} \sum_{\square_{\ell+1} \in R(\square_\ell)} \mathbb{I}_{\hat{\delta}_{\ell+1}^{\square_{\ell+1}} < a_{\ell+1}} \\
&\qquad + \ldots + h_{\ell+\lfloor \theta\ell \rfloor}^{-\alpha/\beta} \sum_{\square_\ell \in U_\ell} \sum_{\square_{k+1} \in R(\square_k)} \cdots \sum_{\square_{\ell+\lfloor \theta\ell \rfloor - 1} \in R(\square_{\ell+\lfloor \theta\ell \rfloor - 1})} \mathbb{I}_{\hat{\delta}_{\ell+\lfloor \theta\ell \rfloor - 1}^{\square_{\ell+\lfloor \theta\ell \rfloor - 1}} < a_{\ell+\lfloor \theta\ell \rfloor - 1}} \Bigg] \\
&= 2^{d\ell} h_\ell^{-\alpha/\beta} + 2^d \sum_{k=1}^{\lfloor \theta\ell \rfloor} h_{\ell+k}^{-\alpha/\beta} \left(\sum_{\square_{\ell+k} \in U_{\ell+k}} \mathbb{I}_{\hat{\delta}_{\ell+k}^{\square_{\ell+k}} < a_{\ell+k}} \right)
\end{aligned}
$$

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 $0 < a < \delta_0$ we have

$$\mu(\{x \in \overline{D} : f(x) \le a\}) \le \rho_0 a$$

where μ is the d-dimensional Lebesgue measure.
Let

$$\delta_m^{\square_m} = \frac{\inf_{x \in \square_m} |f(x)|}{h_m^\alpha}$$

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

$$\sum_{\square_m \in U_m} \mathbb{I}_{\delta_m^{\square_m} \le a} \le \sum_{\square_m \in U_m} \sup_{x \in \square_m} \mathbb{I}_{|f(x)| \le a\, h_m^\alpha} \le b\, 2^{(d-1)m} + c\, a\, h_m^\alpha\, 2^{dm}$$

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

Bound on the number of cells (approximate)

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

$$\begin{aligned}
\sum_{\square_m \in U_m} \mathrm{E}[\,\mathbb{I}_{\hat{\delta}_m^{\square_m} \le a}\,] &\le \sum_{\square_m \in U_m} \mathbb{E}\left[\sup_{x \in \square_m} \mathbb{I}_{|\hat{f}_m^{\square}(x)| \le a\, h_m^{\alpha}}\right] \\
&\le c_1 2^{(d-1)m} + \left(c_2\, h_m^{\alpha\left(\frac{p}{p+1}\right)} + c_3\, a\, h_m^{\alpha} \right) 2^{dm}
\end{aligned}$$

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

Work bound

Therefore, the total expected work is bounded by

$$\sum_{\square_\ell \in U_\ell} \mathrm{E}[\, W_\ell^{\square_\ell} \,] \le 2^{d\ell} h_\ell^{-\alpha/\beta} + c_1\, 2^d \sum_{k=0}^{\lfloor \theta\ell \rfloor} 2^{(d-1)(\ell+k)} h_{\ell+k}^{-\alpha/\beta} + c_2\, 2^d \sum_{k=0}^{\lfloor \theta\ell \rfloor} h_{\ell+k}^{\frac{\alpha p}{p+1}-\frac{\alpha}{\beta}} 2^{d(\ell+k)}$$
$$+ c_3\, 2^d \sum_{k=0}^{\lfloor \theta\ell \rfloor} a_{\ell+k}\, h_{\ell+k}^{\alpha-\alpha/\beta} 2^{d(\ell+k)}$$

Assuming a geometric decrease of h_ℓ, and $\alpha p/(p+1) \ge 1$, in order to have the desired bound for the work, we only require that

$$\sum_{k=0}^{\lfloor \theta\ell \rfloor} a_{\ell+k} h_{\ell+k}^{\alpha-\alpha/\beta} 2^{d(\ell+k)} \lesssim 2^\ell \sum_{k=0}^{\lfloor \theta\ell \rfloor} h_{\ell+k}^{-\frac{\alpha}{\beta}} 2^{(d-1)(\ell+k)},$$

which holds whenever

$$a_{\ell+k} \lesssim h_{\ell+k}^{-\alpha} 2^{-k}.$$

Error definition

We define the two sets

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

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

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

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

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

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

Error expansion

Similar to the work, we arrive at

$$\sum_{\square_\ell \in U_\ell} \mathrm{E}[\, E_\ell^{\square_\ell} \,] \leq \sum_{k=0}^{\lfloor\theta\ell\rfloor-1} \sum_{\square_\ell \in U_{\ell+k}} \int_{\square_{\ell+k}} \mathrm{E}\left[\mathbb{I}_{\hat{\delta}_\ell^{\square_{\ell+k}} \geq a_{\ell+k}} \Delta_{\ell+k}(x) \right] d\mu(x) + \sum_{\square_{\ell+\lfloor\theta\ell\rfloor} \in U_{\ell+\lfloor\theta\ell\rfloor}} \int_{\square_{\ell+\lfloor\theta\ell\rfloor}} \mathrm{E}\left[\, \Delta_{\ell+\lfloor\theta\ell\rfloor}(x) \,\right] d\mu(x)$$

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,

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

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

Hence

$$\sum_{\square_\ell \in U_\ell} \mathrm{E}[\, E_\ell^{\square_\ell} \,] \leq c \sum_{k=0}^{\lfloor \theta\ell \rfloor - 1} a_{\ell+k}^{-p} + c\, h_{\ell+\lfloor \theta\ell \rfloor}^{\alpha \frac{p}{p+1}}$$

Assuming that $a_{\ell+k}$ is geometrically increasing or decreasing in k, we can impose the condition

$$h_{\ell+\lfloor \theta\ell \rfloor}^{-\frac{\alpha}{p+1}} \lesssim a_{\ell+k}$$

for all $k \in \{0, \ldots, \lfloor \theta\ell \rfloor - 1\}$.

Analysis summary

Hence, we have the conditions

$$h_{\ell+\lfloor\theta\ell\rfloor}^{-\frac{\alpha}{p+1}} \lesssim a_{\ell+k} \lesssim h_{\ell+k}^{-\alpha} 2^{-k}.$$

for each $k \in \{0, \ldots, \lfloor\theta\ell\rfloor\}$ and all ℓ.
Under these conditions, we have the bounds on work and error of our method:

$$\text{Total work} = \sum_{\square_\ell \in U_\ell} \mathrm{E}[\, W_\ell^{\square_\ell} \,] \lesssim h_{\ell+\lfloor\theta\ell\rfloor}^{-\alpha/\beta} 2^{d\ell+(d-1)\lfloor\theta\ell\rfloor}$$

$$\text{Total error} = \sum_{\square_\ell \in U_\ell} \mathrm{E}[\, E_\ell^{\square_\ell} \,] \lesssim h_{\ell+\lfloor\theta\ell\rfloor}^{-\alpha\frac{p}{p+1}}$$

The refinement criteria

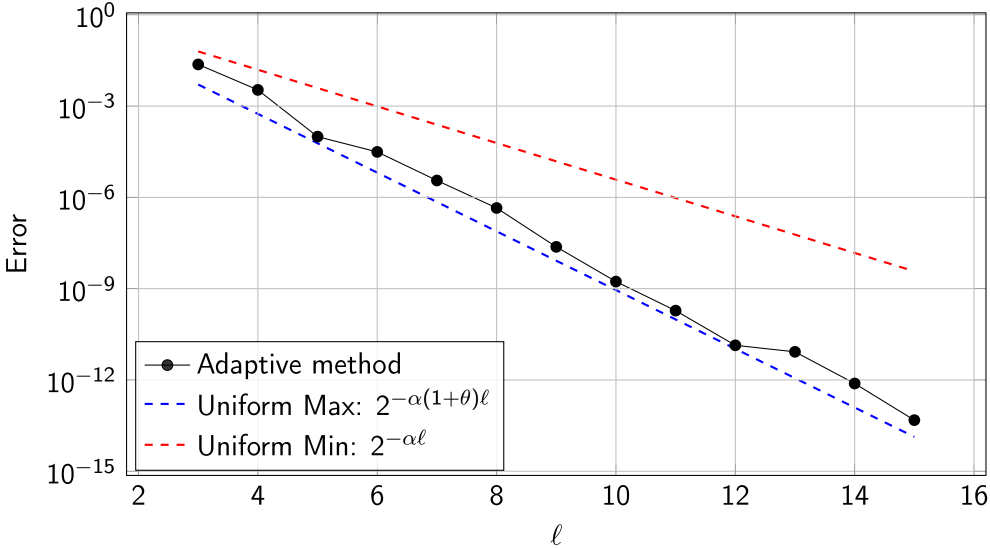
Adapted from[2], we consider a refinement criterion of the form

$$a_{\ell+k} = 2^{-(k+\theta\ell(R-1))(\alpha/\beta+d)/R} h_{\ell+k}^{-\alpha}$$

where the parameter R determines the strictness of refinement (more strict as $R \to 1$). In particular, this criteria satisfies the conditions above for $R > 1$ and $h_\ell \propto 2^{-\ell}$, given certain bounds on θ.

[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, 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



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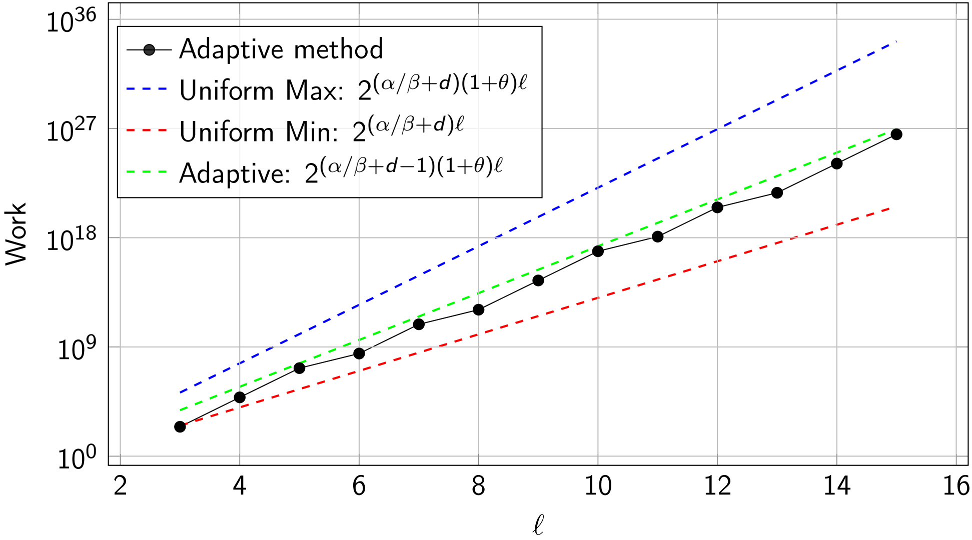

Conclusion

- 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 $\mathcal{L}_{\leq}$ is less than d and dim. of $\hat{\mathcal{L}}^{\ell}_{\leq}$ could be 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.