An adaptive sampling and domain learning strategy for multivariate function approximation on unknown domains

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Abstract

Many problems arising in computational science and engineering can be described in terms of approximating a smooth function of \( d \) variables, defined over an unknown domain of interest \( \Omega \subset \mathbb{R}^d \), from sample data. Here both the underlying dimensionality of the problem (in the case \( d \gg 1 \)) as well as the lack of domain knowledge—with \( \Omega \) potentially irregular and/or disconnected—are confounding factors for sampling-based methods. Na"ive approaches for such problems often lead to wasted samples and inefficient approximation schemes. For example, uniform sampling can result in upwards of 20% wasted samples in some problems considered herein. In applications such as surrogate model construction in computational uncertainty quantification (UQ), the high cost of computing samples necessitates a more efficient sampling procedure. Over the last several years methods for computing such approximations from sample data have been studied in the case of irregular domains, and the advantages of computing sampling measures depending on an approximation space \( P \) of \( \text{dim}(P) = N \) have been shown. More specifically, such approaches confer advantages such as stability and well-conditioning, with an asymptotically optimal sample complexity scaling \( \mathcal{O}(N \log(N)) \). The recently-proposed adaptive sampling for general domains (ASGD) strategy is one such technique to construct these sampling measures. The main contribution of this paper is a procedure to improve upon the ASGD approach by adaptively updating the sampling measure in the case of unknown domains. We achieve this by first introducing a general domain adaptivity strategy (GDAS), which computes an approximation of the function and domain of interest from the sample points. Second, we propose an adaptive sampling strategy, termed adaptive sampling for unknown domains (ASUD), which generates sampling measures over a domain that may not be known in advance, based on the ideas introduced in the ASGD approach. We then derive (weighted) least squares and augmented least squares techniques for polynomial approximation on unknown domains. We present numerical experiments demonstrating the efficacy of the adaptive sampling techniques with least squares-based polynomial approximation schemes. Our results show that the ASUD approach can reduce the computational cost by as much as 50% when compared with uniform sampling for such problems.

1 Introduction

In this work, we consider the problem of approximating a smooth, multivariate function \( f : \Omega \to \mathbb{R} \) over a domain of interest \( \Omega \subset \mathbb{R}^d \) in \( d \geq 1 \) dimensions that is unknown a priori and may be irregular and/or disconnected. Throughout, we assume that \( \Omega \) is a subset of a known domain \( D \subset \mathbb{R}^d \), and that for any point in \( y \in D \) we have access to a black-box that evaluates the function \( f \). Given
input $\mathbf{y} \in D$, this black box either returns the value $f(\mathbf{y}) \in \mathbb{R}$, or, if $f$ is undefined at $\mathbf{y}$, returns some form of exit flag, in which case we formally write $f(\mathbf{y}) = +\infty$. Further, we assume that there is a known function $Q : \mathbb{R} \cup \{\infty\} \rightarrow \{0, 1\}$ that characterizes the domain of interest $\Omega$ through evaluations of $f$. In other words, we may write

$$\Omega = \{\mathbf{y} \in D : Q(f(\mathbf{y})) = 1\},$$

(1.1)

where, in particular, $Q(+\infty) = 0$. Typical examples we consider include the case

$$\Omega = \{\mathbf{y} \in D : f(\mathbf{y}) < \infty\},$$

i.e. where $\Omega$ is precisely the domain within $D$ in which $f$ is defined, or

$$\Omega = \{\mathbf{y} \in D : 0 \leq f(\mathbf{y}) < \infty\},$$

(1.2)

in which case $\Omega$ is the domain of interest in which $f$ is nonnegative. Note that both of these are examples of the general form

$$\Omega = \{\mathbf{y} \in D : a \leq f(\mathbf{y}) < b\},$$

(1.3)

for constants $-\infty < a < b \leq \infty$.

Our work is motivated by applications in Uncertainty Quantification (UQ). For this reason, we focus on three main challenges: first, the curse of dimensionality, since $d$ is often much larger than one in practice; second, computing pointwise evaluations of $f$ via the black box is expensive, and; third, the domain of interest $\Omega$ is unknown in advance, only accessible through evaluating $f$ (see (1.1)) and is generally irregular.

### 1.1 Motivations

Our primary motivation is surrogate model construction in UQ, in which case $f$ is some unknown quantity of interest, $\mathbf{y}$ represents the parameters in the model and the black box is typically some large computer code that evaluates $f$, e.g., a numerical PDE solver. Such problems are often high dimensional, since models usually involve many parameters, and samples are expensive to compute, since they typically involve expensive computer simulations, (see, e.g., [29, 31] for introductions to UQ, as well as [3]).

It is standard in surrogate model problems to assume that $D$ is a tensor-product domain, e.g. the unit hypercube $[-1, 1]^d$, and then to perform Monte Carlo sampling over $D$. That is, the sample points $\mathbf{y}_1, \mathbf{y}_2, \ldots$ are drawn randomly and independently from an underlying probability distribution on $D$, such as the uniform or Chebyshev distribution. However, in practice the situation often arises where $f$ represents some physical quantity (mass, pressure, and so forth) which may be known to be nonnegative (e.g. $\Omega$ as in (1.2)) or bounded between finite minimum and maximum values (e.g. $\Omega$ as in (1.3)), in which case, the model has no physical interpretation outside of $\Omega$. In other cases, the model may simply not be well defined over the whole of $D$, e.g. in the context of a PDE model, if certain parameter values lead to an ill-posed PDE system. In general, though, there may be no straightforward way to determine $\Omega$ without first evaluating $f$. This makes Monte Carlo sampling wasteful, since any sample that returns a value $Q(f(\mathbf{y}_i)) = 0$ (in the general setting (1.1)) is simply rejected. Indeed, one expects roughly $\text{meas}(D \setminus \Omega) / \text{meas}(D)$ of the evaluations $f(\mathbf{y}_1), f(\mathbf{y}_2), \ldots$ to return such a value (here $\text{meas}$ is the measure of a set with respect to the probability measure) thus wasting a constant proportion of the samples. In practical situations, it is not uncommon for 15% to 20% of the samples to be wasted in this way [26, 28].

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Note that this problem is related to the problem of dependent random variables in surrogate model construction \[13, 17, 19, 30\]. It is also related to the problem of hidden constraints in surrogate optimization \[9, 18, 20, 26\].

In this paper we introduce a new procedure for approximating a function \( f \) efficiently over an unknown domain of interest. Our approach is based on an adaptive sampling procedure, termed Adaptive Sampling for Unknown Domains (ASUD), that improves on function approximation strategies based on Monte Carlo sampling. It does so by iteratively learning an approximation to the domain of interest \( \Omega \), and then using this information to adaptively define new sampling distributions from which subsequent sample points are drawn.

### 1.2 Adaptive Sampling for General Domains (ASGD)

Our approach is based on recent work on adaptive sampling for irregular domains. In \[4\], the first two authors introduced a method for function approximation – that we henceforth refer to as Adaptive Sampling for General Domains (ASGD) – over arbitrary, but known domains \( \Omega \) (similar approaches have also been developed in \[12, 25\]). The essence of this method is a (weighted) least-squares procedure in an arbitrary finite-dimensional space \( P \), typically a polynomial space, of dimension \( \text{dim}(P) = N \). It first replaces \( \Omega \) by a fine grid of \( K \gg N \) points. Next, it defines certain discrete sampling measures over the grid, related to the Christoffel function of \( P \), from which the samples are drawn randomly and independently. As was shown in \[4\], this method has provably near-optimal sample complexity, with the number of samples \( M \) required for a quasi-best approximation \( \tilde{f} \in P \) to \( f \) scaling like \( N \log(N) \). To make this procedure adaptive, one first considers a sequence of nested subspaces \( P_1 \subset P_2 \subset \ldots \) of dimensions \( \text{dim}(P_k) = N_k, \ k = 1, 2, \ldots \). Then, following an approach introduced in \[23\], one generates a sequence of sampling measures so that at the \((k + 1)\)th step a total of \( M_{k+1} - M_k \) new samples are drawn and combined with the existing \( M_k \) samples, giving a total of \( M_{k+1} \) samples. As shown in \[4\], if the subspaces are nested and the measures defined in a suitable way, a sequence of quasi-best approximations \( \tilde{f}_k \in P_k \) is obtained from a near-optimal sample complexity, i.e. \( M_k \asymp N_k \log(N_k) \) for each \( k \). Note that alternative adaptive schemes are also possible; see, e.g., \[8\].

### 1.3 Contributions

In this work, we extend the ASGD method to tackle the significantly more challenging scenario where the domain of interest \( \Omega \) is unknown in advance. Our main contribution is the introduction of the aforementioned ASUD procedure. This method is in turn based on a general strategy for function approximation and domain learning, which we term General Domain Adaptivity Strategy (GDAS). Similar to previous works (see, e.g., \[12, 4, 25\]) the approximation is computed via a (weighted) least-squares procedure. However, we consider two different formulations of this procedure, termed ASUD-LS (ASUD-least squares) and ASUD-ALS (ASUD-augmented least squares). We discuss the relative merits of each procedure. Specifically, the latter can offer better domain learning in practice, at the price of worse function approximation when the function is badly behaved (e.g. singular) outside of the domain of interest.

We present a series of numerical experiments to demonstrate the benefits of ASUD on different problems. In these experiments, we observe significant benefits of ASUD over Monte Carlo (MC) sampling, both in terms of approximating the function and learning the domain. Even in the best cases, MC sampling requires at least 50% more samples to achieve a similar error to ASUD. In other cases, it may also fail to achieve the same accuracy. On the other hand, while MC sampling wastes a significant proportion of the samples, the ASUD procedure is asymptotically optimal in
terms of its samples. That is to say, the proportion of rejected samples tends to zero as the number of iterations increases. In fact, the performance of ASUD is very similar to ASGD, which requires a priori domain knowledge. The GitHub repository can be found in https://www.github.com/JMcardenas/Adaptive-sampling-and-domain-learning.

1.4 Outline

The outline of the remainder of this paper is as follows. We commence in §2 by introducing GDAS. Next, in §3 we first review ASGD and then introduce ASUD. In §4 we then introduce the two approximation methods studied: (weighted) least squares and augmented (weighted) least squares. In §5 we present a series of numerical experiments comparing the various methods. Then in §6 we discuss a number of theoretical considerations. Finally, we conclude in §7 with some open problems and topics for future work.

2 General Domain Adaptivity Strategy (GDAS)

In this section, we describe the GDAS procedure on which the methods developed later are based.

2.1 Setup

As noted above, we consider a domain \(D \subseteq \mathbb{R}^d\), an unknown black box function \(f : D \rightarrow \mathbb{R} \cup \{+\infty\}\) and a known function \(Q : \mathbb{R} \cup \{+\infty\} \rightarrow \{0, 1\}\) with \(Q(+\infty) = 0\) that characterizes an unknown domain of interest \(\Omega \subseteq D\) as

\[\Omega = \{y \in D : Q(f(y)) = 1\}.\]  \hspace{1cm} (2.1)

Following the approach of [4, 25, 12], our first step is to discretize the domain \(D\). As shown in these works, discretizing the domain allows for the construction of optimal sampling measures in the setting of possibly irregular domains. To this end, we assume that there is a finite grid of points \(Z \subset D\) and a discrete probability measure \(\tau\) supported on \(Z\). Normally, \(\tau\) is taken to be the discrete uniform measure over \(Z\). Throughout the paper, we assume samples \(y_1, y_2, \ldots\) are drawn randomly according to certain distributions that are supported on \(Z\). We write \(\tilde{\mu}_i\) for the measure supported on \(Z\) from which the \(i\)th sample \(y_i\) is drawn.

The grid \(Z\) and measure \(\tau\) serve two purposes. First, \(Z\) is used to perform the key computations: namely, adaptively generating the discrete sampling measures in the algorithm. Second, \(\tau\) – or more precisely its normalized restriction to \(\Omega\), which we denote by \(\tilde{\tau}\) – is the measure with respect to which we evaluate the error of the approximation. To be precise, if \(\tilde{f}\) is an approximation to \(f\), we compute the error

\[E(f) = \frac{\|f - \tilde{f}\|_{L^2(\Omega, \tilde{\tau})}}{\|f\|_{L^2(\Omega, \tilde{\tau})}}, \quad d\tilde{\tau}(y) := \frac{d\Omega(y)}{\int_\Omega d\tau(y)} d\tau(y).\]

Our objective is to approximate \(f\) over the unknown domain \(\Omega\) as accurately as possible (with respect to this error measure) from as few samples as possible. Hence, we assume throughout that \(Z_\Omega := Z \cap \Omega\) is sufficiently fine so as to represent \(\Omega\) well. Loosely speaking, by this we mean that if an approximation \(\tilde{f}\) approximates \(f\) well on \(Z_\Omega\) then it also approximates \(f\) well on \(\Omega\) itself. This raises the question of how fine the grid \(Z\) should be in practice. We will not discuss this issue, although we note that theoretical estimates are available in many cases – in particular, when the grid is generated via Monte Carlo sampling. See [7, 12] for further discussion on this topic.
2.2 GDAS

Given $Z$ and $\tau$, we first define sampling numbers $0 = M_0 < M_1 < M_2 < \ldots$, where $M_l$ is the number of number of samples of $f$ from $\Omega$ used in the $l$th step. The $l = 1$ step of the GDAS strategy now proceeds as follows:

(a) We first construct sampling measures $\mu_1, \ldots, \mu_{M_1}$ supported on $Z_0$.

(b) Next, for each $i = 1, \ldots, M_1$, we draw a point $y_i$ randomly according to $\mu_i$ and evaluate $f(y_i)$. If $Q(f(y_i)) = 1$ then we accept $y_i$ and write $y_i = y$. Otherwise, we reject it, draw a new point $y$ and repeat until we obtain $Q(f(y)) = 1$. Having done this for each $i = 1, \ldots, M_1$ and obtained the sample points $S_1 = \{y_i\}_{i=1}^{M_1}$, we write $F_1 \geq M_1$ for the total number of evaluations of $f$ used and let $R_1 = \{u_i\}_{i=1}^{T_1}$ be the rejected points, where $T_1 = F_1 - M_1$.

(c) Next, we compute an approximation $\tilde{f}_1$ to $f$ from the values $\{f(y_i)\}_{i=1}^{M_1}$, and potentially also using the rejected values $\{f(u_i)\}_{i=1}^{T_1}$ (if finite).

(d) We then compute the domain approximation

$$Z_1 = \{z \in Z : Q(\tilde{f}_1(z)) = 1\} \cup \{y_i\}_{i=1}^{M_1} \cup S_1 \setminus R_1$$

using the function $Q$ applied to the approximation $\tilde{f}_1$. We explicitly include the sample points $S_1 = \{y_i\}_{i=1}^{M_1}$ and exclude the rejected points $R_1 = \{u_i\}_{i=1}^{T_1}$.

Note that one may choose the initial measures simply as the discrete measure over $Z$, i.e. $\mu_1 = \ldots = \mu_{M_1} = \tau$. This is common in surrogate model construction. However, as we explain in Section 3.2 one may also consider other approaches.

Having completed the $l = 1$ step, the $l$th step of GDAS, $l \geq 2$, proceeds as follows:

(a) We use the domain approximation $Z_{l-1}$ to construct sampling measures $\mu_{M_{l-1}+1}, \ldots, \mu_{M_l}$ supported on $Z_{l-1}$.

(b) For each $i = M_{l-1} + 1, \ldots, M_l$, we proceed as in (a) above, drawing $y_i$ using a combination of $\mu_i$ and rejection sampling according to $Q(f(y))$. We write $G_l \geq M_l - M_{l-1}$ for the total number of function evaluations in doing this, so that $F_l = F_{l-1} + G_l$ is the total number of function evaluations used up to and including the $l$th step. We also let $S_l = \{y_i\}_{i=1}^{M_l}$ be the set of all sample points and $R_l = \{u_i\}_{i=1}^{T_l}$ be the set of all rejected points, where $T_l = F_l - M_l$.

(c) We compute an approximation $\tilde{f}_l$ to $f$ from the values $\{f(y_i)\}_{i=1}^{M_l}$, and potentially also using the rejected values $\{f(u_i)\}_{i=1}^{T_l}$ (if these values are finite).

(d) We compute the domain approximation

$$Z_l = \{z \in Z : Q(\tilde{f}_l(z)) = 1\} \cup S_l \setminus R_l.$$
Method 1. General Domain Adaptivity Strategy (GDAS)

**Inputs:** Finite grid $Z$, probability measure $\tau$ over $Z$, sampling numbers $0 = M_0 < M_1 < M_2 < \ldots$, function $Q$ as $Q_{\text{2.1}}$.

**Initialize:** Set $Z_0 = Z$, $F_0 = 0$, $S_1 = R_1 = \emptyset$.

$$\text{for } l = 1, 2, \ldots \text{ do}$$

Stage (a) Construct measures $\{\mu_i\}_{i=M_{l-1}+1}^{M_l}$ over $Z_{l-1}$.

Stage (b)

for $i = M_{l-1} + 1, \ldots, M_l$ do

Draw $y$ randomly and independently from $\mu_i$. If $Q(f(y)) = 0$ then add $y$ to $R_l$. Repeat until $Q(f(y)) = 1$ and then add $y$ to $S_l$.

end for

return Sample points $S_l = \{y_i\}_{i=1}^{M_l}$ and rejected points $R_l = \{u_i\}_{i=1}^{T_l}$, total number of function evaluations $F_l = F_{l-1} + G_l$, where $G_l$ is the number of evaluations of $f$ used in this stage, and $T_l = F_l - M_l$.

Stage (c) Compute an approximation $\tilde{f}_l$ to $f$ from the data $\{f(y_i)\}_{i=1}^{M_l}$, and potentially also using the rejected values $\{f(u_i)\}_{i=1}^{T_l}$.

Stage (d) Compute $Z_l = \{z \in Z : Q(\tilde{f}_l(z)) = 1\} \cup S_l \setminus R_l$.

Update $S_{l+1} = S_l$ and $R_{l+1} = R_l$.

end for

**Outputs:** The sequences of function approximations $\{\tilde{f}_l\}_{l \geq 1}$ and domain approximations $\{Z_l\}_{l \geq 1}$.

### 2.3 Discussion

Some remarks are in order. First, notice that this procedure produces sequences of approximations $\{\tilde{f}_l\}$ and $\{Z_l\}$ to both the function $f$ and the domain $\Omega$. We refer to the latter as domain learning. It is also adaptive, in that the domain estimate $Z_{l-1}$ is used in stage (a) to construct the new sampling measures.

Second, observe that the $l = 1$ step of GDAS is, in the case that the initial measures are taken as $\mu_1 = \ldots = \mu_{M_1} = \tau$, equivalent standard Monte Carlo sampling for surrogate model construction (albeit with a discrete measure). The samples $y_1, \ldots, y_{M_1}$ are drawn according to the initial measure $\tau$, combined with rejection sampling based on the value of $f(y)$. A substantial fraction of samples may therefore be rejected in this step. Or, in other words, the rejection rate $(F_1 - M_1)/F_1$ may be large. However, by adaptively learning $Z_l$, we hope that the overall rejection rate

\[
\frac{F_l - M_l}{F_l}
\]

decreases with increasing $l$. Ideally, it should decrease to zero as $l \to \infty$, meaning that asymptotically a vanishing proportion of samples are wasted. Later, in our numerical examples, we show that this situation does indeed occur in practice, i.e., the corresponding scheme is asymptotically optimal in the amount of samples wasted.

Third, notice that the point $y_i$ is computed by repeatedly drawing samples independently from $\mu_i$ and rejecting them if they fall outside $\Omega$. This means that $y_i \sim \mu_i$, where $\mu_i$ is the (normalized)
restriction of $\mu_i$ to $\Omega$, i.e.

$$d\tilde{\mu}_i(y) = \frac{I_{\Omega}(y) \, d\mu_i(y)}{\int_{\Omega} d\mu_i(y)}.$$  \hfill (2.2)

Since, by construction, the measure $\mu_i$ is supported on $Z_i$ for $i = M_l-1 + 1, \ldots, M_l$, the measure $\tilde{\mu}_i$ is supported on $Z_l \cap \Omega$.

Fourth, notice that the grid $Z_l$ computed in (d) is constructed as the union of the points from $Z$ where $\tilde{f}_i$ returns the right value via $Q$ and the sample points $S_l = \{y_i\}_{i=1}^{M_l}$. The reason for defining $Z_l$ in this way is that the approximation $\tilde{f}_l$ will generally not be an interpolant of $f$ at the sample points. Hence one may have $Q(\tilde{f}_l(y_i)) = 0$ for some $i$, even though $Q(f(y_i)) = 1$ by construction. Therefore, to give the best estimate of $\Omega$, we include both sets of points in the definition of $Z_l$. In order to enhance the estimate of $\Omega$ further, the rejected points $R_l = \{u_i\}_{i=1}^{T_l}$ are also removed from $Z_l$, since we know they must lie outside of $\Omega$.

Finally, we note that the GDAS procedure does not specify how the approximations $\tilde{f}_l$ are computed, nor how the sampling measures $\mu_l$ are defined. This is the concern of the next two sections.

3 Adaptive Sampling for Unknown Domains (ASUD)

In this section, we describe how to generate the sampling measures, leading to the ASUD method. We divide this section into two parts. First, we recap how the sampling measures can be constructed when the domain is known. This is based on the ASGD method introduced in [4, 25]. With that in hand, we then introduce ASUD.

3.1 ASGD

Suppose that $\Omega$ is known, $Z = \{z_i\}_{i=1}^{K} \subset \Omega$ is a fine grid that represents $\Omega$ and $\tau$ is a probability measure that is supported on $Z$. Notice that since $\Omega$ is known in this case, we take $Z$ as a grid over $\Omega$ as opposed to $D$.

The basic idea behind ASGD is the following. Let $P \subset L^2(\Omega, \tau)$ be a finite-dimensional subspace of dimension $\dim(P) = N$ in which we expect that $f$ is well approximated. For example, if $f$ is smooth we may take $P$ to be a subspace of multivariate polynomials of a given maximum degree.
We also assume that $P$ satisfies the following assumption:

For any $y \in \text{supp}(\tau)$ there exists a $p \in P$ with $p(y) \neq 0$. \hfill (3.1)

Note that this assumption trivially holds whenever $P$ contains the constant function. This will always be the case in our numerical examples.

The goal of ASGD is to use the information about $\Omega$ and $P$ to devise sampling measures $\mu_1, \ldots, \mu_M$ – from which the $M$ sample points $y_1, \ldots, y_M$ are to be drawn randomly – for which a log-linear sample complexity $M \asymp N \log(N)$ is sufficient to stably represent elements of $P$ through their sample values. To be precise, we mean that for any $0 < \delta < 1$ there is a constant $c_\delta > 0$ such that

$$M \geq c_\delta N \log(N),$$

then, with high probability, when $M$ samples are drawn independently with $y_i \sim \mu_i$ for $i = 1, \ldots, M$ one has the equivalence

$$(1 - \delta)\|p\|^2_{L^2(\Omega, \tau)} \leq \frac{1}{M} \sum_{i=1}^{M} w(y_i) |p(y_i)|^2 \leq (1 + \delta)\|p\|^2_{L^2(\Omega, \tau)}\quad\forall p \in P,$$

over the subspace $P$ between the $L^2(\Omega, \tau)$-norm and a certain weighted discrete norm defined in terms of a positive weight function $w$.

**Remark 3.1** A particular consequence of this equivalence is that, if an approximation $\tilde{f}$ is computed as the (weighted) least-squares fit from the subspace $P$ based on the sample values $\{f(y_i)\}_{i=1}^{M}$, then $\tilde{f}$ is a quasi-best approximation to $f$ from $P$. Specifically, if (3.2) holds then the weighted least-squares approximation

$$\tilde{f} = \arg\min_{p \in P} \left\{ \frac{1}{M} \sum_{i=1}^{M} w(y_i) |f(y_i) - p(y_i)|^2 \right\},$$

(which is unique) of a function $f \in L^2(\Omega, \tau)$ satisfies

$$\|f - \tilde{f}\|_{L^2(\Omega, \tau)} \leq \inf_{p \in P} \left\{ \|f - p\|_{L^2(\Omega, \tau)} + c'_\delta \|f - p\|_{\text{disc}} \right\},$$

for some $c'_\delta > 0$ depending on $\delta$, where $\|g\|_{\text{disc}} = \sqrt{M^{-1} \sum_{i=1}^{M} w(y_i) |g(y_i)|^2}$.

The construction of such sampling measures is achieved via the *Christoffel function* of $P$. If $\{\phi_i\}_{i=1}^{N} \subset P$ is any orthonormal basis of $P$ in $H := L^2(\Omega, \tau)$, we define the normalized, reciprocal Christoffel function $K(P, H)$ as

$$K(P, H)(y) = \frac{1}{N} \sum_{i=1}^{N} |\phi_i(y)|^2,$$  

(3.4)

(the function $1/\sum_{i=1}^{N} |\phi_i(y)|^2$ is the Christoffel function of $P$ in $H$; see [27]). Note that $K(P, H)$ is strictly positive for each $y \in \text{supp}(\tau)$ if and only if (3.1) holds.

The idea of using the Christoffel function to construct the sampling measures was considered in [16] for total degree polynomial spaces, then later in [10] for arbitrary spaces. See [3, Sec. 5.5]
for an overview. As was shown in \cite{10}, a suitable choice of sampling measures is any collection \{\mu_i\}_{i=1}^M that satisfies
\begin{equation}
\frac{1}{M} \sum_{i=1}^M d\mu_i(y) = K(P,H)(y) \, d\tau(y) = \frac{1}{N} \sum_{i=1}^N |\phi_i(y)|^2 \, d\tau(y), \quad y \in \Omega. \tag{3.5}
\end{equation}

When chosen in this way, \eqref{eq:3.2} holds with the weight function given by \(w(y) = (K(P,H)(y))^{-1}\).

In practice, there are several ways to choose measures \(\mu_i\) that satisfy \eqref{eq:3.5}. One option is simply to set
\[ d\mu_i(y) = K(P,H)(y) \, d\tau(y), \quad i = 1, \ldots, M. \tag{3.6} \]

In other words, the first \(k\) points are drawn from a measure weighted by \(|\phi_1(y)|^2\), the next \(k\) points from a measure weighted by \(|\phi_2(y)|^2\), and so forth. The choice \eqref{eq:3.6} readily leads to an hierarchical scheme. Indeed, suppose the space \(P\) is enriched to a new space \(\tilde{P}\) of dimension \(\dim(\tilde{P}) := \tilde{N} \geq N\) with \(P \subseteq \tilde{P}\). Let
\[ \{\phi_1, \ldots, \phi_N, \phi_{N+1}, \ldots, \phi_{\tilde{N}}\} \subset L^2(\Omega, \tau), \]
be an orthonormal of \(\tilde{P}\), where \(\{\phi_i\}_{i=1}^N\) is the original orthonormal basis of \(P\). Consider a new sampling ratio \(\tilde{k} \in \mathbb{N}\), \(k \leq \tilde{k}\) and define \(M = \tilde{k} \tilde{N}\). Then we can retain the original \(M\) measures \(\mu_1, \ldots, \mu_M\) and define new measures \(\mu_{M+1}, \ldots, \mu_{\tilde{M}}\) by
\begin{align*}
&d\mu_i(y) = |\phi_j|^2 \, d\tau(y), \quad y \in \Omega, \quad (j-1)\tilde{k} < i \leq j\tilde{k}, \quad j = 1, \ldots, N, \\
&d\mu_i(y) = |\phi_j|^2 \, d\tau(y), \quad y \in \Omega, \quad (j-1)\tilde{k} < i \leq j\tilde{k}, \quad j = N + 1, \ldots, \tilde{N}.
\end{align*}

It is readily seen that the augmented set of measures \(\mu_1, \ldots, \mu_{\tilde{M}}\) satisfies the condition \eqref{eq:3.5} for the augmented space \(\tilde{P}\). However, since the first \(M\) measures remain unchanged, this means we can recycle the previously-drawn samples \(y_1, \ldots, y_M\) when constructing the subsequent approximation over \(\tilde{P}\), i.e. we only need to draw \(\tilde{M} - M\) new samples \(y_{M+1}, \ldots, y_{\tilde{M}}\) according to the new measures.

\textbf{Remark 3.2} The above discussion assumes an orthonormal basis for \(P\) with respect to \(\tau\). This is needed, in particular, to define the sampling measures in \eqref{eq:3.6}. In practice, such a basis may not be given in advance, but it can be readily computed via QR decomposition. This is, in fact, the reason for defining \(\tau\) as a measure supported on a finite grid as opposed to the whole of \(\Omega\). We now describe the construction of such a basis and how to sample from the corresponding measures \eqref{eq:3.6}.

Since \(\tau\) is a measure defined over \(Z\) we can write
\[ d\tau(y) = \sum_{i=1}^K \tau_i \delta(y - z_i), \]
where \(\tau_i = \mathbb{P}(y = z_i)\) for \(y \sim \tau\). Now let \(\{\psi_i\}_{i=1}^N\) be a nonorthogonal basis for \(P\),
\[ B = \{\sqrt{\tau_i}\psi_j(z_i)\}_{i,j=1}^{K,N} \in \mathbb{C}^{K \times N}, \]
and suppose that $B$ has QR decomposition $B = QR$, where $Q \in \mathbb{C}^{K \times N}$ and $R \in \mathbb{C}^{N \times N}$. Write $Q = \{q_j\}_{j=1}^{K,N}$. Then it follows straightforwardly that

$$\phi_i(y) = \sum_{j=1}^{i} (R^{-\top})_{ij} \psi_j(y), \quad i = 1, \ldots, N.$$  

Thus, the orthonormal basis functions $\phi_i$ are easily computed from the $\psi_j$’s. Moreover, if $M = kN$ and $(j-1)k < i \leq jk$, then the measure $\mu_i$ defined in (3.6) is given by

$$d\mu_i(y) = |\phi_j(y)|^2 d\tau(y) = \sum_{k=1}^{K} \tau_k |\phi_j(z_k)|^2 \delta(y - z_k) dy = \sum_{k=1}^{K} |q_{kj}|^2 \delta(y - z_k) dy.$$  

Hence, $\mu_i$ is the discrete measure with $y \sim \mu_i$ if $P(y = z_k) = |q_{kj}|^2$ for $k = 1, \ldots, K$. Therefore, sampling from $\mu_i$ is equivalent to drawing an integer $l$ randomly from the set $\{1, \ldots, K\}$ according to the distribution $\{|q_{kj}|^2\}_{k=1}^{K}$ and then setting $y = z_l$.

### 3.2 ASUD

We now return to the main problem considered in this paper – namely, where $\Omega$ is unknown – and introduce the ASUD method. ASUD is an instance of GDAS in which we use the ideas from ASGD to construct the sampling measures. To this end, we make the following assumption:

**Assumption 3.3.** There are sequences of sampling ratios $0 = k_0 < k_1 \leq k_2 \leq \ldots$ and integers $0 = N_0 < N_1 \leq N_2 \leq N_3 \leq \ldots$ such that $M_l = k_l N_l$ for $l = 0, 1, 2, \ldots$. Furthermore, there is a sequence of nested, finite-dimensional subspaces $P_1 \subseteq P_2 \subseteq P_3 \subseteq \ldots \subseteq L^2(D, \tau)$ of dimensions $\dim(P_l) = N_l$ and functions $\psi_1, \psi_2, \ldots$ such that $P_l = \text{span}\{\psi_i\}_{i=1}^{N_l}$ for $l = 1, 2, \ldots$. These subspaces may either be defined beforehand or generated adaptively during GDAS.

The basic idea behind the second part of this assumption is that the $P_l$ are subspaces in which we expect $f$ to be well approximated, i.e. the best approximation error decreases rapidly in $l$. In this paper, we consider the case where the subspaces are defined a priori beforehand. However, it is also possible to generate them adaptively, typically in a greedy manner (see, e.g., [11, 22, 24]).

With Assumption 3.3 in hand, we now describe how ASUD constructs the sampling measures $\mu_1, \mu_2, \ldots$. Consider the first step $l = 1$ of GDAS, in which we first need to define the measures $\mu_1, \ldots, \mu_{M_1}$. We do this via the same approach as ASGD. For convenience, we now also write $\Omega_0 = D$ for the first estimate of the domain $\Omega$, $Z_0 = Z$ for the first estimate of the discrete domain $\Omega \cap Z$ and $\tau_0 = \tau$. Let $P_1$ be the first subspace. We construct an orthonormal basis $\{\phi_j^{(1)}\}_{j=1}^{N_1}$ for $P_1$ over $Z_0$, so that

$$P_1 = \text{span}\{\phi_j^{(1)}, \ldots, \phi_{N_1}^{(1)}\} \subseteq L^2(Z_0, \tau_0) \equiv L^2(D, \tau).$$

Then we define the measures exactly as in ASGD, i.e.

$$d\mu_i(y) = |\phi_j^{(1)}(y)|^2 d\tau_0(y), \quad y \in D, \quad (j-1)k_1 < i \leq jk_1, \quad j = 1, \ldots, N_1.$$  

Notice that condition (3.5) holds for these measures. Specifically, we have

$$\frac{1}{M_1} \sum_{i=1}^{M_1} d\mu_i(y) = K(P_1, L^2(Z_0, \tau_0))(y) d\tau_0(y), \quad y \in D.$$
Hence, these sampling measures are suitable (in the sense of (3.2)) for approximation over the initial domain estimate $\Omega_0$.

Now consider step $l = 2$ of GDAS. We have a new grid $Z_1$ (computed in stage (d) of step $l = 1$) and a new subspace $P_2$. To apply the ASGD methodology, we first restrict $\tau$ to $Z_1$. This gives the discrete probability measure

$$d\tau_1(y) = \frac{\mathbb{I}_{Z_1}(y)}{\int_{Z_1} d\tau(y)} d\tau(y), \quad y \in D.$$  

Notice that $Z_1$ is nonempty by construction and $\tau$ is supported on $Z$. Hence the denominator is nonvanishing, and therefore $\tau_1$ is well defined. We now orthogonalize $P_2$ with respect to this measure, and write

$$P_2 = \text{span}\{\phi^{(2)}_1, \ldots, \phi^{(2)}_{N_2}\} \subset L^2(Z_1, \tau_1),$$

where $\{\phi^{(2)}_i\}$ is an orthonormal basis for $P_2$, when considered as a subspace of $L^2(Z_1, \tau_1)$. Using this, we then define the new measures $\mu_{M_1+1}, \ldots, \mu_{M_2}$ by

$$d\mu_i(y) = |\phi^{(2)}_j(y)|^2 d\tau_1(y), \quad y \in D, \; j = 1, \ldots, N_2,$$

where $i$ satisfies

$$(j-1)(k_2 - k_1) + M_1 < i \leq j(k_2 - k_1) + M_1, \quad j = 1, \ldots, N_1,$$

$$(j-1)k_2 < i \leq jk_2, \quad j = N_1 + 1, \ldots, N_2.$$  

Step $l \geq 2$ of GDAS proceeds in a similar manner. We have a new grid $Z_{l-1}$ (computed in stage (d) of the previous step) and a new subspace $P_l$. We restrict $\tau$ to $Z_{l-1}$, giving a discrete probability measure

$$d\tau_{l-1}(y) = \frac{\mathbb{I}_{Z_{l-1}}(y)}{\int_{Z_{l-1}} d\tau(y)} d\tau(y), \quad y \in D,$$  

which is once again well defined. We now orthogonalize $P_l$ with respect to the measure $\tau_{l-1}$, and write

$$P_l = \text{span}\{\phi^{(l)}_1, \ldots, \phi^{(l)}_{N_l}\} \subset L^2(Z_{l-1}, \tau_{l-1}),$$

where $\{\phi^{(l)}_i\}_{i=1}^{N_l}$ is the corresponding orthonormal basis for $P_l$, when considered as a subspace of $L^2(Z_{l-1}, \tau_{l-1})$. Then we define the new measures $\mu_{M_{l-1}+1}, \ldots, \mu_{M_l}$ as

$$d\mu_i(y) = |\phi^{(l)}_j(y)|^2 d\tau_{l-1}(y), \quad y \in D, \; j = 1, \ldots, N_l,$$

where $i$ satisfies

$$(j-1)(k_l - k_{l-1}) + M_{l-1} < i \leq j(k_l - k_{l-1}) + M_{l-1}, \quad j = 1, \ldots, N_{l-1},$$

$$(j-1)k_l < i \leq jk_l, \quad j = N_{l-1} + 1, \ldots, N_l.$$  

**Remark 3.4** As with ASGD, in ASUD we use the orthonormal basis $\{\phi^{(l)}_i\}_{i=1}^{N_l}$ for $P_l$ to construct the sampling measures. We once more compute this basis using QR decomposition. To do this, we first write the measure $\tau_{l-1}$ as

$$d\tau_{l-1}(y) = \sum_{i=1}^{K_{l-1}} \tau_i^{(l-1)} \delta(y - z_i^{(l-1)}),$$
where \( z_i^{(l-1)} \) is the \( i \)th point in the grid \( Z_{l-1} = \{ z_i^{(l-1)} \}_{i=1}^{K_l-1} \) and \( \tau_i^{(l-1)} = \mathbb{P}(y = z_i^{(l-1)}) \) for \( y \sim \tau_{l-1} \).

Now, let \( \{ \psi_1, \ldots, \psi_{N_l} \} \) be a nonorthogonal basis for \( P_l \) and

\[
B_l = \left\{ \sqrt{\tau_i^{(l-1)}} \psi_j(z_i^{(l-1)}) \right\}_{i,j=1}^{K_l-1, N_l} \in \mathbb{C}^{K_l-1 \times N_l}.
\]

Let \( B_l \) have a QR decomposition \( B_l = Q_l R_l \), where \( Q_l \in \mathbb{C}^{K_l-1 \times N_l} \) and \( R_l \in \mathbb{C}^{N_l \times N_l} \), and write

\[
Q_l = \{ q_j^{(l)} \}_{j=1}^{N_l} \in \mathbb{C}^{K_l-1 \times N_l}.
\]

Then, as before,

\[
\phi_i^{(l)}(y) = \sum_{j=1}^{i} (R_l^{-\top})_{ij} \psi_j(y), \quad i = 1, \ldots, N_l,
\]

is an orthonormal basis for \( P_l \) in \( L^2(Z_{l-1}, \tau_{l-1}) \). Therefore, for \( j = 1, \ldots, N_l \) and \( i \) satisfying (3.8), we can write the sampling measure \( \mu_i \) as

\[
d\mu_i(y) = |\phi_j^{(l)}(y)|^2 \ d\tau(y) = \sum_{k=1}^{K_l-1} \tau_k^{(l-1)} |\phi_j^{(l)}(z_k^{(l-1)})|^2 \delta(y - z_k^{(l-1)}) \ dy
\]

\[
= \sum_{k=1}^{K_l-1} |q_{kj}^{(l)}|^2 \delta(y - z_k^{(l-1)}) \ dy.
\]

Hence \( \mu_i \) is the discrete probability measure with \( y \sim \mu_i \) if \( \mathbb{P}(y = z_k^{(l-1)}) = |q_{kj}^{(l)}|^2 \) for \( k = 1, \ldots, K_l-1 \). Sampling from \( \mu_i \) is equivalent to drawing an integer \( t \) randomly from \( \{1, \ldots, K_l-1\} \) based on distribution \( \{ |q_{ij}^{(l-1)}|^2 \}_{j=1}^{K_l-1} \) and then setting \( y = z_t^{(l-1)} \).

With this remark in hand, we have now fully described the ASUD for GDAS. The resulting procedure is summarized in Method 2.
Method 2. GDAS with Adaptive Sampling for Unknown Domains (ASUD)

**Inputs:** Finite grid $Z$, probability measure $\tau$ over $Z$, subspace dimensions $0 = N_0 < N_1 < N_2 < \cdots$ and sampling ratios $1 \leq k_1 \leq k_2 \leq \cdots$ such that $M_l = k_l N_l$ for all $l$, function $Q$ as in [2,1].

**Initialize:** Set $K_0 = |Z|$, $Z_0 = \{z_i^{(0)}\}_{i=1}^{K_0} = Z$, $I_0 = \{1, \ldots, K_0\}$, $F_0 = 0$, $S_1 = R_1 = \emptyset$.

For $l = 1, 2, \ldots$ do

**Stage (a)**

(i) Unless already defined, construct an approximation space $P_l = \text{span}\{\psi_j\}_{j=1}^{N_l} \subset L^2(D, \tau)$ of dimension $N_l$ and set $M_l = k_l N_l$.

(ii) Construct the matrix $B_l = \{\sqrt{\tau_{i,j}} \psi_j(z^{(l-1)}_i)\}_{i,j=1}^{K_{l-1}, N_l}$.

(iii) Compute the QR decomposition $B_l = Q_l R_l$ and write $Q_l = \{q_{ij}^{(l)}\}_{i,j=1}^{K_{l-1}, N_l}$.

**return** The discrete distributions $\{|q_{ij}^{(l)}|^2\}_{i=1}^{K_{l-1}}$ for $j = 1, \ldots, N_l$.

**Stage (b)**

if $l > 1$ do

for $t = 1, \ldots, N_{l-1}$ do

for $s = 1, \ldots, k_{l-1} - k_{l-2}$ do

Draw an integer $v$ randomly and independently from $I_{l-1}$ according to the discrete distribution $\{|q_{it}^{(l-1)}|^2\}_{i=1}^{K_{l-1}}$. If $Q(f(z_v)) = 0$ then add $z_v$ to $R_l$. Repeat until $Q(f(z_v)) = 1$ and then add $z_v$ to $S_l$.

end for

end for

for $t = N_{l-1} + 1, \ldots, N_l$ do

for $s = 1, \ldots, k_l$ do

Draw an integer $v$ randomly and independently from $I_{l-1}$ according to $\{|q_{it}^{(l-1)}|^2\}_{i=1}^{K_{l-1}}$. If $Q(f(z_v)) = 0$ then add $z_v$ to $R_l$. Repeat until $Q(f(z_v)) = 1$ and then add $z_v$ to $S_l$.

end for

end for

**return** Sample points $S_l = \{y_t\}_{t=1}^{M_l}$ and rejected points $R_l = \{u_{ij}\}_{ij=1}^{T_l}$, total number of function evaluations $F_l = F_{l-1} + G_l$, where $G_l$ is the number of evaluations of $f$ used in this stage, and $T_l = F_l - M_l$.

**Stage (c)** Compute an approximation $\tilde{f}_l$ to $f$ from the data $\{f(y_t)\}_{t=1}^{M_l}$.

**Stage (d)** Compute $Z_l = \{z \in Z : Q(\tilde{f}_l(z)) = 1\} \cup S_l \setminus R_l$. Define a new set of indices $I_l = \{j_1, \ldots, j_{K_l}\}$ so that $Z_l = \{z_{j_i}\}_{i=1}^{K_l} = \{z_i^{(l)}\}_{i=1}^{K_l}$, where $K_l = |Z_l|$.

Update $S_{l+1} = S_l$ and $R_{l+1} = R_l$.

end for

**Output:** The sequences of function approximations $\{\tilde{f}_l\}_{l \geq 1}$ and domain approximations $\{Z_l\}_{l \geq 1}$.
4 Approximation methods for $\tilde{f}$

Note that ASUD allows for arbitrary methods of approximation in stage (c). We now discuss the two approaches for doing this that we consider later in our numerical experiments. Both approaches assume that the subspaces $P_l$ are defined \textit{a priori} as a sequence of nested finite-dimensional subspaces $P_1 \subseteq P_2 \subseteq \ldots \subseteq L^2(D, \tau)$. Note that other approaches are possible within our framework, including those that adaptively generate the $P_l$. See §3 for some further discussion on this point.

4.1 (Weighted) least-squares approximation

Let $N_l = \dim(P_l)$ and suppose that $M_l \geq N_l$. Let $y_1, \ldots, y_{M_l}$ be the sample points generated up to and including stage (b) of step $l$ of ASUD. Let $\tau_l, \mu_l$ and $Z_{l-1}$ be as in §3.2 and let

$$w_l = (K(P_l, L^2(Z_{l-1}, \tau_{l-1})))^{-1},$$

where $K(P_l, L^2(Z_{l-1}, \tau_{l-1}))$ is the reciprocal Christoffel function of $P_l$ as a subspace of $L^2(Z_{l-1}, \tau_{l-1})$ (see (3.4)). Then, similar to in Remark 3.1 we define the (weighted) least-squares approximation of $f$ as

$$\tilde{f}_l = \arg\min_{p \in P_l} \left\{ \frac{1}{M_l} \sum_{i=1}^{M_l} w_l(y_i) |f(y_i) - p(y_i)|^2 \right\}. \quad (4.1)$$

Write $\tilde{f}_l = \sum_{i=1}^{N_l} c^{(l)}_i \phi^{(l)}_i$ in terms of the orthonormal basis $\{\phi^{(l)}_j\}_{j=1}^{N_l}$ for the subspace $P_l \subseteq L^2(Z_{l-1}, \tau_{l-1})$. Then the coefficients $c^{(l)}_i$ of $\tilde{f}_l$ are a solution of the algebraic least-squares problem

$$c^{(l)} = (c^{(l)}_i)_{i=1}^{N_l} \in \arg\min_{x \in \mathbb{C}^{N_l}} \frac{1}{2} \left\| A^{(l)} x - b^{(l)} \right\|_2^2, \quad (4.2)$$

where

$$A^{(l)} = \left\{ \sqrt{\frac{w_l(y_i)}{M_l}} \phi^{(l)}_j(y_i) \right\}_{i=1,j=1}^{M_l,N_l} \in \mathbb{C}^{M_l \times N_l}, \quad b^{(l)} = \left\{ \sqrt{\frac{w_l(y_i)}{M_l}} f(y_i) \right\}_{i=1}^{M_l} \in \mathbb{C}^{M_l}.$$

Now, as in stage (a)(iii) of ASUD (Method 2), let $Q_l$ be the matrix arising from the QR factorization of $B_l$, with entries $\{q^{(l)}_{i,j}\}_{i,j=1}^{K_{l-1},N_l}$. Since the points $y_1, \ldots, y_{M_l}$ belong to $Z_{l-1}$, we can write $y_i = z^{(l)}_{j_i}$, where $j_i \in \{1, \ldots, K_{l-1}\}$ for $i = 1, \ldots, M_l$. Hence, we can rewrite $A^{(l)}$ and $b^{(l)}$ as

$$A^{(l)} = \left\{ \frac{q^{(l)}_{i,j}}{\sqrt{\frac{M_l}{N_l} \sum_{t=1}^{N_l} |q^{(l)}_{j,t}|^2}} \right\}_{i,j=1}^{M_l,N_l}, \quad b^{(l)} = \left\{ \frac{f(y_i)}{\sqrt{\frac{M_l K_{l-1}}{N_l} \sum_{t=1}^{N_l} |q^{(l)}_{j,t}|^2}} \right\}_{i=1}^{M_l},$$

in terms of the matrix $Q_l$. In particular, $A^{(l)}$ consists of rows of $Q_l$ corresponding to the indices $j_1, \ldots, j_{M_l}$, scaled by values $\sqrt{w_l(y_i)/M_l}$.

Let $c^{(l)}$ be a solution of the algebraic least-squares problem. In order to perform stage (d) of ASUD, we need to evaluate the corresponding function $\tilde{f}_l$ over the grid $Z_0$. This can be done straightforwardly using the matrix $R_l$ arising from the QR factorization of $B_l$, as well as the matrix

$$C_l = \left\{ \psi_j(z^{(0)}_i) \right\}_{i,j=1}^{K_0,N_l}.$$
Specifically, the vector
\[ \tilde{f}_l = C_l(R_l)^{-1} c^{(l)}, \]
contains the values of \( \tilde{f}_l \) over \( Z_0 \). Indeed, the action of \( (R_l)^{-1} \) on \( c^{(l)} \) yields the coefficients of \( \tilde{f}_l \) in the nonorthogonal basis \( \{ \psi_i \}_{i=1}^{N_l} \) for \( P_l \), and the subsequent action of \( C_l \) evaluates an expansion in this basis (given its coefficients) on the grid \( Z_0 \). Indeed, consider \( z_l^{(0)} \in Z_0 \) and (3.9). Then
\[
\tilde{f}_l(z_l^{(0)}) = \sum_{i=1}^{N_l} c_l^{(l)}(0) \phi_l^{(l)}(z_l^{(0)}) = \sum_{i=1}^{N_l} \sum_{j=1}^{M_l} (R_l)_{ij}^{-\top} \psi_j(z_l^{(0)}) = \sum_{i=1}^{N_l} \sum_{j=1}^{M_l} (C_l)_{ij}(R_l)_{ij}^{-\top},
\]
which is precisely \( (C_l(R_l)^{-1} c^{(l)})_l \), as required. Note that computing \( \tilde{f}_l \) is not only necessary for stage (d) of ASUD, it also allows us to represent \( \tilde{f}_l \) over the domain approximation \( Z_l \) and, in simulations, the true (discrete) domain \( \Omega \cap Z \). Hence, instead of the function \( \tilde{f}_l \), we consider the vector \( \hat{f}_l \) as the output of the weighted least-squares approximation. This approximation is summarized below:

**Inputs:** \( C_l, \) QR decomposition \( Q_l R_l \) of \( B_l \), and indices \( i_1, \ldots, i_{M_l} \).

(i) Define \( A^{(l)} \in \mathbb{C}^{M_l \times N_l} \) and \( b^{(l)} \in \mathbb{C}^{M_l} \) as
\[
A^{(l)} = \left\{ \frac{q_{j,k}^{(l)}}{\sqrt{M_l \sum_{i=1}^{N_l} |q_{ji,t}^{(l)}|^2}} \right\}_{i,j=1}^{M_l,N_l} \quad \text{and} \quad b^{(l)} = \left\{ \frac{f(y_i)}{\sqrt{M_l \sum_{i=1}^{N_l} |q_{ji,t}^{(l)}|^2}} \right\}_{i=1}^{M_l}.
\]

(ii) Compute \( c^{(l)} = \arg\min_{x \in \mathbb{C}^{N_l}} \| A^{(l)} x - b^{(l)} \|_2 \) and \( \hat{f}_l = C_l(R_l)^{-1} c^{(l)} \).

**Return** Approximation \( \hat{f}_l \) to \( f \).

### 4.2 Augmented (weighted) least-squares approximation

A limitation of the approximation described previously is that it makes no use of the rejected points \( R_l \). There are a number of ways that one might strive to incorporate these points into an approximation scheme. We now describe a modification of the previous procedure that can lead to significantly better domain learning for certain functions.

As before, we consider a sequence of nested finite-dimensional subspaces \( P_1 \subseteq P_2 \subseteq \ldots \subseteq L^2(D, \tau) \) with \( N_l = \dim(P_l) \). We now make several modifications to Method 2. First, we modify stage (b) to only reject a point \( z_u \) if \( f(z_u) = +\infty \). In other words, we accept points both inside \( \Omega \) and outside \( \Omega \). Then, in Stage (d) we modify the domain update as follows:

\[
Z_l = \left\{ z \in Z : Q(\tilde{f}_l(z)) = 1 \right\} \cup \left\{ y_i : Q(f(y_i)) = 1, \ i = 1, \ldots, M_l \right\}
\]
\[
\setminus \left\{ y_i : Q(f(y_i)) = 0, \ i = 1, \ldots, M_l \right\} = \cup \left\{ u_i \right\}_{i=1}^{T_l}.
\]

In other word, our domain estimate includes all points in \( Z \) for which \( Q(\tilde{f}_l(z)) = 1 \) and all the sample points \( y_i \) which belong to \( \Omega \), and excludes those sample points that do not belong to \( \Omega \) and any rejected points \( u_i \) (i.e. those for which \( f = +\infty \)).
Given these modifications, we define the resulting approximation exactly as before, via weighted least squares. Since it uses points both inside and outside of \( \Omega \), we term this procedure augmented (weighted) least-squares approximation.

5 Numerical experiments

In this section, we present numerical experiments demonstrating the performance of ASUD with both unaugmented and augmented weighted least-squares approximation.

5.1 Experimental setup

In this section, we describe our experimental setup. Throughout, we consider the domain \( D = [-1, 1]^d \). We let \( Z_0 = Z \) be a uniform grid of size \( K = 30000 \), drawn uniformly and randomly from \( D \), and let \( \tau \) be the uniform measure over \( Z \). Throughout, we consider the approximation of smooth functions using polynomials. To do so, we choose

\[
P_l = \mathcal{P}_{\Lambda_{n_l}} = \text{span} \{ y \mapsto y^n : n \in \Lambda_{n_l} \},
\]

where \( \Lambda_{n_l} \) is the hyperbolic cross index set of index \( n \):

\[
\Lambda_{n_l} = \left\{ n = (n_1, \ldots, n_d) \in \mathbb{N}_0^d : \prod_{k=1}^d (n_k + 1) \leq n + 1 \right\}.
\]

The initial basis \( \{ \psi_1, \ldots, \psi_{N_l} \} \) for \( P_l \) is constructed by taking the restrictions to \( Z_{l-1} \) of the orthonormal Legendre polynomials on \([-1, 1]^d\) with indices in \( \Lambda \). We also define sampling rates \( 0 = M_0 < M_1 < \ldots < M_r = M_{\text{max}} \) as \( M_l = k_l N_l \), where \( N_l = \dim(P_l) \), \( 1 \leq N_1 < \ldots < N_r = N_{\text{max}} \leq 1000 \) and \( k_l \) is the closest integer to \( \log(N_l) \).

We consider the following test functions:

\[
f_1(y) = \left( \frac{10}{7} - \frac{1}{y_1^2 + y_2^2} \right) \exp\left( -\sum_{i=1}^d y_i / 2d \right),
\]

\[
f_2(y) = \log\left( 8 \sum_{i=1}^d y_i^2 \right) - 2 \left( \sum_{i=1}^d y_i^2 \right),
\]

\[
f_3(y) = \left( 1 - \frac{(d - 2)}{100} (d^2 - 10d + 29) \right) \log\left( \frac{16}{d} \sum_{i=1}^d y_i^2 \right) - \frac{4}{d} \left( \sum_{i=1}^d y_i^2 \right),
\]

\[
f_4(y) = \prod_{i=1}^d \frac{d/4}{d/4 + (y_i + (-1)^{i+1}/(i + 1))^2}.
\]

We define the corresponding domain \( \Omega = \Omega_i \) for the function \( f_i \) as

\[
\Omega_i = \{ z \in D : 0 \leq f_i(y) < \infty \}, \quad i = 1, 2, 3, \quad \Omega_4 = \{ z \in D : 0.18 \leq f_4(z) \leq 0.72 \}.
\]

Examples of these domains in \( d = 2 \) dimensions are shown in Fig. 2. Note that \( f_2 = f_3 \) when \( d = 2 \). All four functions are smooth (analytic) within their respective domains. Notice, however, that \( f_2 \) and \( f_3 \) have singularities at \( y = 0 \in D \) and \( f_1 \) has a singularity at any \( y \in D \) for which \( y_1 = y_2 = 0 \). The reason for considering functions with singularities at certain points is that it
allows us to model cases where the ‘black box’ evaluating $f$ returns an exit flag (NaN, Inf), which we think of as $+\infty$.

To measure the error between $f$ and its approximation $\tilde{f}$, we consider the relative approximation error

$$E_l(f) = \frac{\|f - \tilde{f}\|_{L^2(\Omega, \bar{\tau})}}{\|f\|_{L^2(\Omega, \bar{\tau})}}, \quad d\bar{\tau}(y) := \frac{\mathbb{I}_\Omega(y)}{\int_{\Omega} d\tau(y)} d\tau(y),$$

(5.1)

where $\bar{\tau}$ is the restriction of $\tau$ to $\Omega$. In order to measure the approximation of the true domain, we define the mismatch volume between $\Omega$ and $Z_l$ as

$$V_l(f) = \frac{|(Z_\Omega \setminus Z_{l-1}) \cup (Z_{l-1} \setminus Z_\Omega)|}{|Z_\Omega|},$$

(5.2)

where $Z_\Omega = \Omega \cap Z$ is the discrete representation of $\Omega$. As we mentioned in Section 2.3, we also compute the rejection rate as

$$R_l(f) = \frac{F_l - M_l}{F_l},$$

(5.3)

where $F_l$ is the number of function evaluations of ASUD at the $l$th step. Since our methods involve random sampling, we perform multiple trials and then average the corresponding quantities $E_l(f)$, $V_l(f)$ and $R_l(f)$. Throughout, we present the mean values of these quantities averaged over 50 trials.

We consider ASUD with either the least-squares approximation of Section 4.1, which we term ASUD-LS, or the augmented least-squares approximation of Section 4.2, which we term ASUD-ALS. We also compare these schemes against two other methods. The first is the ASGD method of [4], which was discussed earlier in Section 3.1. We term this ASGD-LS. Note that this method assumes the domain $\Omega$ is known. Thus, it provides a benchmark against which to compare the performance of ASUD. Since the number of function evaluations $F_l = M_l$ in this case, we do not report the rejection rate $R_l(f)$ for this method. At the other end of the spectrum, we also consider (unweighted) least-squares with Monte Carlo sampling, which we term MC-LS. As discussed in Section 1, this method is often used in practice. Yet it can be wasteful, since it does not adapt the sampling to a domain estimate. Later, we will see that this method often has a high rejection rate.

### 5.2 Experimental results

In Fig. 3, we show results for the function $f = f_1$. We see a clear benefit of ASUD-LS over MC-LS in lower dimensions with respect number of function evaluations needed to obtain a certain accuracy.
In fact, the ASUD-LS approximation error is quite close to that of ASGD-LS, despite it assuming no a priori knowledge of the domain. As shown in the right column of this figure, the rejection rate $R_l(f)$ for MC-LS is around 40%, since $\text{Vol}(\Omega)/\text{Vol}(D) \approx 0.6$ in all dimensions. Conversely, the rejection rate is decreasing for ASUD-LS, and close to zero in dimensions $d = 2, 3, 5$ for large enough $l$. Even in higher dimensions, however, the rejection rate is significantly smaller than for MC-LS. This translates to it needing fewer function evaluations to achieve a certain error. Indeed, when $d = 15$ we achieve the minimum error using roughly $2 \times 10^3$ function evaluations versus $3 \times 10^3$ function evaluations for MC-LS.

It is notable that ASUD-ALS gives a significantly worse approximation than the other methods. We discuss the reasons for this later. In particular, the mismatch volume $V_l(f)$ for this method is never below 20%, while the other methods can achieve close to zero domain learning errors in the lower-dimensional cases. On the other hand, when $d = 15$ ASUD-LS achieves a similar domain learning error for large enough numbers of function evaluation, despite yielding a much worse approximation error.

In Fig. 4 we show experiments for $f = f_2$. Both ASUD-LS and ASUD-ALS can generally be seen to have decreasing error as we increase the number of functions evaluations used in computing their respective approximations, while this is not the case for MC-LS. This latter effect is indicative of a general property of Monte Carlo sampling with least-squares approximation: namely, it can be unstable and nonconvergent when the sampling rate is log-linear in the dimension of the polynomial subspace (note that in this case, $M_l \approx N_l \log(N_l)$, where $N_l = \dim(P_l)$). See [3, Sec. 5.4.4] and [21] for further discussion. Markedly, the errors of ASGD-LS and ASUD-LS follow a similar trend, with the latter requiring slightly more function evaluations due to lack of domain knowledge of $\Omega_2$ and the nonzero rejection rate (as shown in the right column of Fig. 4). Overall, ASUD-LS performs better than MC-LS when approximating the function, while both methods perform similarly when learning the domain. The mismatch volume is approximately 10% for these methods in $d = 2$ and $d = 3$ dimensions. Notice also that for ASUD-ALS, the mismatch volume decreases faster than ASUD-LS and MC-LS in all dimensions studied. It is important to mention that this domain has decreasing volume relation to $D$ as the dimension increases. Consequently, the rejection rate for MC-LS increases with dimension as can be seen in the third column of Fig. 4. On the other hand, the rejection rate for ASUD-LS is asymptotically decreasing in $l$ in all dimensions.

In Fig. 5 we show experiments for $f = f_3$. In two dimensions this function coincides with the function $f_2$. In higher dimensions, however, the volume of $\Omega_3$ relative to $D$ remains roughly constant, unlike in the case of $f_2$. Correspondingly, the rejection rate for MC-LS is roughly constant, and approximately 30%. In each of the dimensions, ASUD-LS outperforms MC-LS for approximating the target function. As in the experiments in Fig. 4 with $f = f_2$, the domain-learning performance is similar for the three methods, i.e. generally decreasing with increasing number of evaluations. However, ASUD-ALS decreases faster than both ASUD-LS and MC-LS.

Finally, in Fig. 6 we show experiments for $f = f_4$. It is notable that ASUD-ALS performs similarly to ASUD-LS and ASGD-LS in terms of approximating the function in this case, and achieves better domain learning. We discuss the reasons behind this further in the next section.

6 Theoretical discussion

6.1 Accuracy and stability of weighted least squares

Consider a domain $\Omega$ with a probability measure $\tau_{\Omega}$ and a weight function $w$ that is positive and finite almost everywhere on $\text{supp}(\tau_{\Omega})$. Let $y_1, \ldots, y_M$ be $M$ sample points and consider the
Figure 3: Approximation of the function $f = f_1$ and domain $\Omega = \Omega_1$ in $d = 2, 3, 5, 10, 15$ dimensions (top to bottom). Left: the relative error $E_l(f)$ versus the number of function evaluations $F_l$. Middle: the mismatch volume $V_l(f)$ versus $F_l$. Right: the rejection rate $R_l(f)$ versus $M_l$.

weighted least-squares approximation

$$\hat{f} \in \arg\min_{p \in P} \left\{ \frac{1}{M} \sum_{i=1}^{M} w(y_i) |f(y_i) + e_i - p(y_i)|^2 \right\},$$

(6.1)
of a function $f \in L^2(\Omega, \tau_\Omega)$ in a subspace $P \subseteq L^2(\Omega, \tau_\Omega)$ with $\dim(P) = N \leq M$. Here, the values $e_i$ represent noise. Then the accuracy and stability (to noise) of this approximation are both controlled by the following discrete stability constant

$$\alpha = \inf \left\{ \|p\|_{\text{disc}} : p \in P, \|p\|_{L^2(\Omega, \tau_\Omega)} = 1 \right\},$$

where $\|g\|_{\text{disc}} = \sqrt{M^{-1} \sum_{i=1}^M w(y_i) |g(y_i)|^2}$. Specifically, if $\alpha > 0$ then the approximation is unique and it satisfies

$$\|f - \tilde{f}\|_{L^2(\Omega, \tau_\Omega)} \leq \|f - p\|_{L^2(\Omega, \tau_\Omega)} + \alpha^{-1} \|f - p\|_{\text{disc}} + \alpha^{-1} \|e\|, \quad \forall p \in P,$$

Figure 4: Approximation of the function $f = f_2$ and domain $\Omega = \Omega_2$ in $d = 2, 3, 4, 5$, dimensions (top to bottom). Left: the relative error $E_i(f)$ versus the number of function evaluations $F_i$. Middle: the mismatch volume $V_i(f)$ versus $F_i$. Right: the rejection rate $R_i(f)$ versus $M_i$. 

$$\frac{20}{3}$$
Figure 5: Approximation of the function $f = f_3$ and domain $\Omega = \Omega_3$ in $d = 2, 3, 4, 5$, dimensions (top to bottom). Left: the relative error $E_l(f)$ versus the number of function evaluations $F_l$. Middle: the mismatch volume $V_l(f)$ versus $F_l$. Right: the rejection rate $R_l(f)$ versus $M_l$.

where $\|e\| = \sqrt{\frac{1}{M} \sum_{i=1}^{M} w(y_i)|e_i|^2}$ (see, e.g., [3, Chpt. 5]). Thus, accuracy and stability of the approximation follow whenever $1/\alpha$ is not too large. Note that

$$\|p\|_{\text{disc}} \geq \alpha \|p\|_{L^2(\Omega, \tau_\Omega)}.$$ 

Thus, when $1/\alpha$ is not too large, this states that the discrete norm over the sample points can be estimated from below by the underlying norm $\|\cdot\|_{L^2(\Omega, \tau_\Omega)}$ in which accuracy and stability of the approximation are estimated.

The discrete constant can be computed whenever the domain $\Omega$ is known. In that case, we compute an orthonormal basis $\{\phi_1, \ldots, \phi_N\} \subseteq L^2(\Omega, \tau_\Omega)$ of $P \subseteq L^2(\Omega, \tau_\Omega)$ (if $\tau_\Omega$ is a finitely-supported measure, as it is in this paper, then we do this via QR decomposition, as described
Figure 6: Approximation of the function $f = f_4$ and domain $\Omega = \Omega_4$ in $d = 2, 3, 5, 10, 15$, dimensions (top to bottom). Left: the relative error $E_l(f)$ versus the number of function evaluations $F_l$. Middle: the mismatch volume $V_l(f)$ versus $F_l$. Right: the rejection rate $R_l(f)$ versus $M_l$.

previously) and then use this to construct the matrix

$$B = \left( \sqrt{w(y_i) \phi_j(y_i)} \right)_{i,j=1}^{M,N}.$$
The constant $\alpha$ is then precisely $\sigma_{\text{min}}(B)$.

In Fig. 7 we compute this constant for several different examples. As we see, in all cases MC-LS leads to a large constant that increases exponentially with the number of iterations (recall the earlier discussion). All three adaptive methods lead to much smaller constants, and therefore better stability. ASUD-LS and ASGD-LS have similar constants, neither of which grow with the iteration number, and remain less than 10 in magnitude. ASUD-ALS has a slightly large constant that can grow as large as roughly $10^2$ is size in these examples.

This figure also shows the corresponding approximation errors. As we expect, the corresponding MC-LS approximation error is also larger than the ASUD-LS error, since the former has a much larger constant. It is notable that the ASUD-ALS error can be large, even though the constant $1/\alpha$ is small. The reason for this can be traced to the error bound (6.2). For the MC-LS and ASUD-LS approximations, the term $\|f - p\|_{\text{disc}}$ is a discrete error over the sample points $y_i$. Since in these methods the sample points are drawn from $\Omega$, this error is expected to be small whenever $f$ is well approximated over $\Omega$ by a function from $P$. However, in ASUD-ALS, the sample points are not restricted to belong to $\Omega$. They can, in theory, come from anywhere in $D$. Hence, the term $\|f - p\|_{\text{disc}}$ may be much larger in this case, since the functions considered are less smooth (in fact, in some cases, singular) over $D \setminus \Omega$. This results stand in contrast to those for function $f_2$, which has a quadratic singularity at $y = 0$ and for which ASUD-ALS performs the worst, see Fig 3.

### 6.2 Can accuracy and stability be numerically verified?

As noted, the constant $\alpha$ can only be computed when the domain $\Omega$ is known. In this case, accuracy and stability of the approximation can numerically verified a priori. Unfortunately, this cannot be done when the domain is unknown, as it is in this paper. At a general step of ASUD-LS we compute a weighted least-squares approximation using an orthonormal basis $\{\phi_1, \ldots, \phi_N\} \subseteq L^2(\Omega', \tau')$, where $\Omega'$ an estimate for the true domain $\Omega$ and $\tau'$ is the normalized restriction of the measure $\tau$ on $D$ to $\Omega'$. If $y_1, \ldots, y_M$ are the sample points, then we form the least-squares matrix

$$A = \left(\sqrt{w(y_i)\phi_j(y_i)}\right)_{i,j=1}^{M,N}.$$ 

It is clearly possible to compute the constant $\beta = \sigma_{\text{min}}(A)$. Unfortunately, this may not describe the stability and accuracy of the approximation in the $L^2(\Omega, \tau_{\Omega})$-norm. Indeed, this constant is precisely

$$\beta = \inf \left\{ \|p\|_{\text{disc}} : p \in P, \|p\|_{L^2(\Omega', \tau')} = 1 \right\}.$$ 

Recall that the discrete norm $\|p\|_{\text{disc}}$ is an approximation to the continuous norm $\|p\|_{L^2(\Omega, \tau_{\Omega})}$ over $\Omega$. Thus, $\beta$ will only serve as a useful surrogate for the true stability constant $\alpha$ when $\Omega'$ approximates the domain $\Omega$ sufficiently well. To see this, let $p \in P$. Then

$$\|p\|_{\text{disc}} \geq \beta\|p\|_{L^2(\Omega', \tau')}.$$ 

Suppose that $\Omega \subseteq \Omega'$, i.e. the true domain is a subset of the estimated domain. Then, if $c_{\Omega} = \int_{\Omega} d\tau(y)$ and $c_{\Omega'} = \int_{\Omega'} d\tau(y)$, we obtain the bound

$$\alpha \geq \sqrt{c_{\Omega}/c_{\Omega'}} \beta \geq \sqrt{c_{\Omega}} \beta,$$
Figure 7: Approximation of the functions $f = f_1, f_2, f_4$ and domains $\Omega = \Omega_1, \Omega_2, \Omega_4$ (left to right) in $d = 2$ dimensions. First row: the relative error $E_l(f)$ versus the number of function evaluations $F_l$. Second row: the mismatch volume $V_l(f)$ versus $F_l$. Third row: the rejection rate $R_l(f)$ versus $M_l$. Fourth row: the constant $1/\alpha$ versus $l$. Fifth row: the constant $1/\beta$ versus $l$.

where in the second step we use that fact that $c_{\Omega'} \leq 1$, since $\Omega' \subseteq D$. Hence, in this case, we expect $\beta$ to provide a reasonable surrogate for $\alpha$. Unfortunately, if $\Omega \not\subseteq \Omega'$ then this is not the case.
Indeed, in general we have
\[ \alpha \geq \beta \gamma, \quad \gamma := \inf \left\{ \| p \|_{L^2(\Omega', \tau')} : p \in P, \| p \|_{L^2(\Omega, \tau_\Omega)} = 1 \right\}. \]
The latter term can easily be large unless \( \Omega' \) is a very good estimate of \( \Omega \). For simplicity, consider the case \( \Omega' \subseteq \Omega \). Then \( 1/\gamma \) determines how large an element \( p \in P \) can grow on the larger domain \( \Omega \) in relation to its size over \( \Omega' \). In the case of polynomial subspaces, this is essentially a type of Remez inequality. Such inequalities are known to grow exponentially in the polynomial degree with a rate depending on the relative volumes of the two domains (see, e.g., \([32, 14]\)).

In Fig. 7 we also show the constant \( 1/\beta \) for the various approximations. For MC-LS it grows large, much like the constant \( 1/\alpha \), since the approximation is unstable. For ASUD-LS the constant can also grow large, depending on the problem and the domain estimate. Indeed, comparing it with the domain mismatch volume, we see that the size of the behaviour of this constant closely tracks with when the domain estimate gets worse. On the other hand, \( 1/\beta \) remains small for the ASUD-ALS approximation. This is indicative of the fact that this scheme performs an approximation over the whole estimated domain. However, as we have seen, this scheme often leads to worse approximation errors for precisely this reason.

The main conclusion of this section is that computing the constant \( \beta \) is of limited value for ASUD-LS, since \( 1/\beta \) being large does not necessarily imply a poor approximation (to either the function or the domain) and \( 1/\beta \) being small need not imply a good approximation (to either the function or the domain).

7 Conclusions

In this paper, we introduced a new method, ASUD, for function approximation and domain learning over unknown domains of interest. This method combines previous work on weighted least-squares approximation on general domains (ASGD) with a domain estimation procedure. As shown in our numerical experiments, this procedure can lead to significant advantages over standard Monte Carlo sampling (MC-LS), even in higher dimensions.

There are several avenues for further investigations. A first one is to enhance the sampling efficiency further. In recent work \([15]\), a boosting procedure for weighted least-squares approximations has been introduced. This procedure uses resampling and a greedy strategy to selectively remove sample points. Incorporating this into ASUD has the potential to further enhance its performance. Another topic for future research involves changing the approximation scheme. In this work we have used (weighted) least squares based on a fixed sequence of subspaces \( P_1 \subseteq P_2 \subseteq \cdots \). An interesting extension is the case where the subspaces are also generated adaptively, via, for instance, greedy adaptive methods \([11, 22, 24]\). A related approach involves using compressed sensing via (weighted) \( \ell^1 \)-minimization (see, e.g., \([2, 3]\)). See \([5]\) for recent work on polynomial approximation via compressed sensing on irregular domains. Finally, there is also increasing interest in using deep learning for high-dimensional approximation tasks arising in UQ (see, e.g., \([11, 6]\) and references therein). An interesting open problem is to combine the adaptive sampling procedure developed in this paper with a suitable deep neural network training strategy.

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References

[1] B. Adcock, S. Brugiapaglia, N. Dexter, and S. Moraga. Deep neural networks are effective at learning high-dimensional Hilbert-valued functions from limited data. In J. Bruna, J. S. Hesthaven, and L. Zdeborová, editors, *Proceedings of The Second Annual Conference on Mathematical and Scientific Machine Learning*, volume 145 of *Proc. Mach. Learn. Res. (PMLR)*, pages 1–36. PMLR, 2021.

[2] B. Adcock, S. Brugiapaglia, and C. G. Webster. Compressed sensing approaches for polynomial approximation of high-dimensional functions. In H. Boche, G. Caire, R. Calderbank, M. Márs, G. Kutyniok, and R. Mathar, editors, *Compressed Sensing and its Applications: Second International MATHEON Conference 2015*, Appl. Numer. Harmon. Anal., pages 93–124. Birkhäuser, Cham, Switzerland, 2017.

[3] B. Adcock, S. Brugiapaglia, and C. G. Webster. *Sparse Polynomial Approximation of High-Dimensional Functions*. Comput. Sci. Eng. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2021.

[4] B. Adcock and J. M. Cardenas. Near-optimal sampling strategies for multivariate function approximation on general domains. *SIAM J. Math. Data Sci.*, 2(3):607–630, 2019.

[5] B. Adcock, J. M. Cardenas, N. Dexter, and S. Moraga. Towards optimal sampling for learning sparse approximations in high dimensions. In A. Nikgibali, P. Pardalos, A. Raigorodskii, and M. T. Rassias, editors, *High Dimensional Optimization and Probability*. Springer (to appear), 2022.

[6] B. Adcock and N. Dexter. The gap between theory and practice in function approximation with deep neural networks. *SIAM J. Math. Data Sci.*, 3(2):624–655, 2021.

[7] B. Adcock and D. Huybrechs. Approximating smooth, multivariate functions on irregular domains. *Forum Math. Sigma*, 8:e26, 2020.

[8] B. Arras, M. Bachmayr, and A. Cohen. Sequential sampling for optimal weighted least squares approximations in hierarchical spaces. *SIAM J. Math. Data Sci.*, 1(1):189–207, 2019.

[9] C. Audet, G. Caporossi, and S. Jacquet. Binary, unrelaxable and hidden constraints in blackbox optimization. *Oper. Res. Lett.*, 48(4):467–471, 2020.

[10] A. Cohen and G. Migliorati. Optimal weighted least-squares methods. *SMAI Journal of Computational Mathematics*, 3:181–203, 2017.

[11] A. Cohen and G. Migliorati. Multivariate approximation in downward closed polynomial spaces. In J. Dick, F. Y. Kuo, and H. Woźniakowski, editors, *Contemporary Computational Mathematics – A Celebration of the 80th Birthday of Ian Sloan*, pages 233–282. Springer, Cham, Switzerland, 2018.

[12] M. Dolbeault and A. Cohen. Optimal sampling and Christoffel functions on general domains. *arXiv:2010.11040*, 2020.

[13] O. G. Ernst, A. Mugler, H.-J. Starkloff, and E. Ullmann. On the convergence of generalized polynomial chaos expansions. *ESAIM. Math. Model. Numer. Anal.*, 46(2):317–339, Mar. 2012.

[14] M. I. Ganzburg. Polynomial inequalities on measurable sets and their applications. *Constr. Approx.*, 17:275–306, 2001.

[15] C. Haberstich, A. Nouy, and G. Perrin. Boosted optimal weighted least-squares. *arXiv:1912.07075*, 2019.

[16] J. Hampton and A. Doostan. Coherence motivated sampling and convergence analysis of least squares polynomial chaos regression. *Comput. Methods Appl. Mech. Engng.*, 290:73–97, 2015.

[17] J. D. Jakeman, F. Franzelin, A. Narayan, M. Eldred, and D. Pflüger. Polynomial chaos expansions for dependent random variables. *Comput. Methods Appl. Mech. Engng.*, 351:643–666, 2019.

[18] V. K. Ky, C. D’Ambriosso, Y. Hamadi, and L. Liberti. Surrogate-based methods for black-box optimization. *International Transactions in Operational Research*, 24(3):393–424, 2016.

[19] O. Le Maître and O. M. Knio. *Spectral Methods for Uncertainty Quantification: With Applications to Computational Fluid Dynamics*. Sci. Comput. Springer, Dordrecht, Netherlands, 2010.
[20] H. Lee, R. Gramacy, C. Linkletter, and G. Gray. Optimization subject to hidden constraints via statistical emulation. *Pacific Journal of Optimization*, 7(4):467–478, 2011.

[21] G. Migliorati. *Polynomial approximation by means of the random discrete $L^2$ projection and application to inverse problems for PDEs with stochastic data*. PhD thesis, Politecnico di Milano, 2013.

[22] G. Migliorati. Adaptive polynomial approximation by means of random discrete least squares. In A. Abdulle, S. Deparis, D. Kressner, F. Nobile, and M. Picasso, editors, *Numerical Mathematics and Advanced Applications – ENUMATH 2013*, pages 547–554, Cham, Switzerland, 2015. Springer.

[23] G. Migliorati. Adaptive approximation by optimal weighted least squares methods. *arXiv:1807.00402*, 2018.

[24] G. Migliorati. Adaptive approximation by optimal weighted least squares methods. *SIAM J. Numer. Anal.*, 57(5):2217–2245, 2019.

[25] G. Migliorati. Multivariate approximation of functions on irregular domains by weighted least-squares methods. *arXiv:1907.12304*, 2019.

[26] J. Müller and M. Day. Surrogate optimization of computationally expensive black-box problems with hidden constraints. *INFORMS J Comput.*, 31(4):689–702, 2018.

[27] P. Nevai. Géza Freud, orthogonal polynomials and Christoffel functions. A case study. *J. Approx. Theory*, 48(1):3–167, 1986.

[28] K. Sargsyan, C. Safta, H. N. Najm, B. J. Debusschere, D. Ricciuto, and P. Thornton. Dimensionality reduction for complex models via Bayesian compressive sensing. *Int. J. Uncertain. Quan.*, 4(1):63–93, 2014.

[29] R. C. Smith. *Uncertainty Quantification Theory, Implementation, and Applications*. SIAM, 2013.

[30] C. Soize and R. Ghanem. Physical systems with random uncertainties: chaos representations with arbitrary probability measure. *SIAM J. Sci. Comput.*, 26(2):395–410, Jan. 2004.

[31] T. J. Sullivan. *Introduction to Uncertainty Quantification*, volume 63. Springer, Texts Appl. Math., Cham, Switzerland edition, 2015.

[32] V. Temlyakov and S. Tikhonov. Remez-type inequalities for the hyperbolic cross polynomials. *Constr. Approx.*, 46(3):593–615, 2017.