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A supermartingale approach to Gaussian process based sequential design of experiments

Julien Bect* François Bachoc† David Ginsbourger‡

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Abstract

Gaussian process (GP) models have become a well-established framework for the adaptive design of costly experiments, and in particular, but not only, of computer experiments. GP-based sequential designs have been proposed for various objectives, such as global optimization (estimating the global maximum or maximizer(s) of a function), reliability analysis (estimating a probability of failure) or the estimation of level sets and excursion sets. In this paper, we tackle the convergence properties of an important class of such sequential design strategies, known as stepwise uncertainty reduction (SUR) strategies. Our approach relies on the key observation that the sequence of residual uncertainty measures, in a SUR strategy, is in general a supermartingale with respect to the filtration generated by the observations. We also provide some general results about GP-based sequential design, which are of independent interest. Our main application is a proof of almost sure convergence for one of the SUR strategies proposed by Bect, Ginsbourger, Li, Picheny and Vazquez (Stat. Comp., 2012). To the best of our knowledge, this is the first convergence proof for a GP-based sequential design algorithm dedicated to the estimation of probabilities of excursion and excursions sets. We also establish, using the same approach, a new proof of almost sure convergence for the expected improvement algorithm, which is the first proof for this algorithm that applies to any continuous GP.

Keywords: Sequential Uncertainty Reduction, Expected Improvement, Convergence.

1 Introduction

Sequential design of experiments is an important and lively field of statistics, where the goal is to allocate experimental resources step by step so as to reduce uncertainties on some quantity, or function, of interest. While the experimental design vocabulary traditionally refers to observations of natural phenomena presenting aleatory uncertainties, the design of computer

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experiments—in which observations are replaced by evaluations of numerical simulators—has become a field of research *per se* (Sacks et al., 1989; Santner et al., 2003), where Gaussian process models are heavily used to define efficient sequential strategies in cases of costly evaluations. The predominance of Gaussian processes in this field is undoubtedly due to their unique combination of modeling flexibility and computational tractability, which makes it possible to compute sampling criteria accounting for the potential effect of adding new experiments.

The expected improvement (EI) is a famous example of such a criterion. Following the foundations laid by Mockus et al. (1978) and the considerable impact of the work of Jones et al. (1998), EI and other Bayesian optimization strategies have spread in a variety of application fields. As an example, they are now commonly used in engineering design (Forrester et al., 2008) and, in the field of machine learning, for the automatic configuration algorithms (see Shahriari et al., 2016, and references therein). Extensions to constrained, multi-objective and/or robust optimization constitute an active field of research (see, e.g., Williams et al., 2000; Emmerich et al., 2006; Picheny, 2014; Binois, 2015; Gramacy et al., 2016; Feliot et al., 2016). In a different context, sequential design strategies based on Gaussian process models have been used to estimate contour lines, probability of failures, profile optima and excursion sets of expensive to evaluate simulators (see, notably, Ranjan et al., 2008; Vazquez and Bect, 2009; Picheny et al., 2010; Bect et al., 2012; Zuluaga et al., 2013; Chevalier et al., 2014; Ginsbourger et al., 2014; Wang et al., 2016).

In the present paper we investigate the convergence properties of a particular class of sequential designs for the Gaussian process model, which are built according to the *step-wise uncertainty reduction* (SUR) paradigm (see Villemonteix et al., 2009; Bect et al., 2012; Chevalier, 2013, and references therein). More precisely, we are interested in the almost sure consistency of these algorithms with respect to the prior distribution, i.e., consistency under the assumption that the function of interest is a sample path of the Gaussian process prior that is used to construct the sequential design. Almost sure consistency has already established for the EI algorithm (Vazquez and Bect, 2010a), a particular case of a SUR strategy, but only under the restrictive assumption that the covariance function satisfies a certain condition—the “No Empty Ball” (NEB) property, recalled in Section 3—which excludes very regular Gaussian processes¹. Moreover, to the authors’ knowledge no proof of almost sure convergence has yet been established for algorithms dedicated to probability of excursion and/or excursion set estimation (referred to as *excursion case* henceforth) such as those of Bect et al. (2012). Here we develop a novel proof scheme, relying notably on a supermartingale approach, that allows addressing the excursion case and also revisiting the convergence of the EI algorithm without the NEB assumption.

Before outlining the paper in more detail, let us briefly introduce its general setting and, in particular, what we mean by SUR strategies. We will focus directly on the case of Gaussian

¹On a related note, Bull (2011) proves an upper-bound for the convergence rate of the expected improvement algorithm under the assumption that the covariance function is Hölder, but his result only holds for functions that belong to the reproducing kernel Hilbert space (RKHS) of the covariance—a condition that, under appropriate assumptions, is almost surely not satisfied by sample paths of the Gaussian process according to Driscoll’s theorem (Lukić and Beder, 2001). Another result in the same vein is provided by Yarotsky (2013b) for the squared exponential covariance in the univariate case, assuming the objective function is analytic in a sufficiently large complex domain around its interval of definition.

processes for clarity, but the SUR principle in itself is much more general, and can be used with other types of models (see, e.g., MacKay, 1992; Cohn et al., 1996; Geman and Jedynak, 1996).

Let ξ be a real-valued Gaussian process defined on some measurable space \mathbb{X} —typically, ξ will be a continuous Gaussian process on a compact metric space, such as $\mathbb{X} = [0, 1]^\ell$ —and assume that evaluations $Y_n = \xi(X_n) + \epsilon_n$ are to be made, sequentially, in order to gather information about some quantity of interest. We will assume the sequence of observation errors $(\epsilon_n)_{n \in \mathbb{N}^*}$ to be independent of the Gaussian process ξ , and composed of independent centered Gaussian variables. The definition of a SUR strategy starts with the choice a “measure of residual uncertainty” for the quantity of interest after n evaluations, which is a functional

$$H_n = \mathcal{H} \left(\mathbb{P}_n^\xi \right) \quad (1)$$

of the conditional distribution \mathbb{P}_n^ξ of ξ given \mathcal{F}_n , where \mathcal{F}_n is the σ -algebra generated by $X_1, Y_1, \dots, X_n, Y_n$. For a given prior distribution \mathbb{P}_0^ξ , assume that this functional \mathcal{H} induces a sequence of measurable functions

$$h_n : (\mathbb{X} \times \mathbb{R})^n \rightarrow \mathbb{R} \quad (2)$$

such that, for all $n \geq 1$,

$$H_n = h_n(X_1, Y_1, \dots, X_n, Y_n); \quad (3)$$

or, equivalently, assume that H_n is an \mathcal{F}_n -measurable random variable. So-called SUR sampling criteria are then defined as

$$J_n(x) = \mathbb{E}_{n,x}(H_{n+1}), \quad (4)$$

where $\mathbb{E}_{n,x}$ denotes the conditional expectation with respect to \mathcal{F}_n with $X_{n+1} = x$ (assuming that H_{n+1} is integrable, for any choice of $x \in \mathbb{X}$). The value of the sampling criterion $J_n(x)$ at time n measures the expected residual uncertainty at time $n + 1$ if the next evaluation is made at x . Finally, a (non-randomized) sequential designed is constructed by choosing at each step the point that provides the smallest expected residual uncertainty—or, equivalently, the largest expected uncertainty reduction—, that is,

$$X_{n+1} = \operatorname{argmin}_{x \in \mathbb{X}} J_n(x), \quad (5)$$

assuming for simplicity that the minimum is attained at a single point; more generally, $X_{n+1} \in \operatorname{argmin}_{x \in \mathbb{X}} J_n(x)$. Given a finite measure μ over \mathbb{X} and an excursion threshold $T \in \mathbb{R}$, a typical choice of measure of residual uncertainty in the excursion case (See Bect et al., 2012) is the integrated indicator variance $H_n = \mathcal{H}(\mathbb{P}_n^\xi) = \int_{\mathbb{X}} p_n(1 - p_n) d\mu$ where $p_n(u) = \mathbb{P}_n(\xi(u) \geq T)$ and \mathbb{P}_n denotes the conditional probability with respect to \mathcal{F}_n .

In the optimization case on the other hand, it turns out that the EI criterion is underlaid by the following measure of residual uncertainty (See, e.g., Chevalier, 2013, Section 3.3): $H_n = \mathcal{H}(\mathbb{P}_n^\xi) = \mathbb{E}_n(\max \xi - M_n)$ where $M_n = \max_{i \leq n} \xi(X_i)$ and \mathbb{E}_n refers to the conditional expectation with respect to \mathcal{F}_n .

As developed further in Section 4 it appears in both cases that the associated measures of residual uncertainty are supermartingales. Our approach here is to establish convergence of SUR strategies relying on this property. We prove in particular that a larger class of SUR criteria, built upon quite general loss functions, are supermartingales. Furthermore, we establish convergence results under the requirement that the uncertainty reduction does not vanish too swiftly along the sequence. Then we examine in detail why this requirement is met both in the excursion and Bayesian optimization cases discussed above. An interesting by-product in the excursion case is that the proof also accommodates observation noise.

The paper is structured as follows. In Section 2 we present some preliminary results on Gaussian processes in the sequential design context. These results that mainly concern the limiting behaviour of Gaussian process conditional distributions in the sequential setting, and that might also be of independent interest, prove to be key instruments in the convergence proofs established for the excursion and optimization cases. In Section 3, general considerations about supermartingale properties are exposed, and in particular it is shown that SUR strategies built upon a general risk minimization principle systematically fall into the supermartingale framework. Then a pivotal result is proved, Proposition 3.3, that specifies a technical requirement under which a diversity of limit results can be established for supermartingales such as considered. Section 4 details how the previous results apply in the excursion and Bayesian optimization (EI) cases, establishing the convergence to zero of considered uncertainties and related quantities, both in L^1 and almost sure convergence modes.

2 Preliminary results on Gaussian processes

This section contains results that hold true for any (possibly randomized) sequential design $(X_n)_{n \geq 1}$. We assume that \mathbb{X} is a separable metric space and ξ a Gaussian process with continuous sample paths, defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Consequently, ξ has continuous mean and covariance functions (see, e.g., Lemma 1 in Ibragimov and Rozanov (1978)).

We denote by \mathbb{P}_n the conditional probability with respect to \mathcal{F}_n , and by \mathbb{E}_n (resp. var_n , resp. cov_n) the corresponding conditional expectation (resp. variance, resp. covariance) operator. Similar notations with $n = \infty$ are used to indicate conditioning with respect to the σ -algebra $\mathcal{F}_\infty = \bigvee_{n \geq 1} \mathcal{F}_n$ generated by $\bigcup_{n \geq 1} \mathcal{F}_n$.

Proposition 2.1 (Well-behaved conditional moments). *For each $n \geq 1$, there exist processes $\widehat{\xi}_n$ and k_n , indexed respectively by \mathbb{X} and $\mathbb{X} \times \mathbb{X}$, such that:*

- (i) *for all $x \in \mathbb{X}$, $\widehat{\xi}_n(x)$ is a conditional mean of $\xi(x)$ given \mathcal{F}_n ,*
- (ii) *for all $x, y \in \mathbb{X}$, $k_n(x, y)$ is a conditional covariance of $\xi(x)$ and $\xi(y)$ given \mathcal{F}_n ,*
- (iii) *$\widehat{\xi}_n$ and k_n have continuous sample paths,*
- (iv) *for all $x \in \mathbb{X}$, $\sigma_n^2(x) := k_n(x, x)$ is decreasing (i.e., $\sigma_n^2(x, \omega)$ is decreasing for all $\omega \in \Omega$).*

The processes $\widehat{\xi}_n$ and k_n are the unique processes, up to evanescence, that satisfy (i)–(iii).

Proof. Let $\sum_{i=1}^n \lambda_{i,n}(\cdot; \underline{x}_n) Y_i$ and $k_n^0(\cdot, \cdot; \underline{x}_n)$ denote the conditional mean and covariance functions for a given deterministic n -point design $\underline{x}_n = (x_1, \dots, x_n)$. They are continuous and satisfy the decreasing variance property for any \underline{x}_n . Thus, (i)–(iv) are proved for deterministic designs.

For a general (possibly randomized) sequential design X_1, X_2, \dots , it can be proved recursively that $\hat{\xi}_n = \sum_{i=1}^n \lambda_{i,n}(\cdot; \underline{X}_n) Y_i$ and $k_n = k_n^0(\cdot, \cdot; \underline{X}_n)$ are respectively a conditional mean function and a conditional covariance function of ξ given \mathcal{F}_n , which proves (i) and (ii). The properties of continuity (iii) and decreasing variance (iv) are inherited from the case of deterministic designs, pointwise on Ω . The result is thus proved. \square

Remark 2.2. In other words, we have a well-behaved sequence of continuous conditional moments, which are obtained by plugging, for each $\omega \in \Omega$, the sequence $(X_n(\omega))_{n \geq 1}$ into the expression of the moments for a *deterministic* design $(x_n)_{n \geq 1}$.

Proposition 2.3. *There exists a continuous process k_∞ on $\mathbb{X} \times \mathbb{X}$ such that*

$$k_\infty(x, y) = \text{cov}_\infty(\xi(x), \xi(y)) \quad \text{for all } x, y \in \mathbb{X}^2, \quad (6)$$

where cov_∞ denotes the conditional variance with respect to \mathcal{F}_∞ , and

$$k_n \rightarrow k_\infty \quad \text{uniformly on the compact subsets of } \mathbb{X} \times \mathbb{X}. \quad (7)$$

Proof. Let $\mu = \sum_{i=1}^p \mu_i \delta_{x_i}$ denote any finitely supported measure on \mathbb{X} , and let

$$\sigma_n^2(\mu) = \sum_{i,j=1}^p \mu_i \mu_j k_n(x_i, x_j) = \sum_{i,j=1}^p \mu_i \mu_j k_n^0(x_i, x_j; \underline{X}_n)$$

denote the conditional variance of $\sum_{i=1}^p \mu_i \xi(x_i)$ given \mathcal{F}_n . Reducing to the case of a deterministic design as above, it is decreasing and therefore converges to a limit $\sigma_\infty^2(\mu)$. Thus,

$$k_n(x, y) = \frac{1}{4} (\sigma_n^2(\delta_x + \delta_y) - \sigma_n^2(\delta_x - \delta_y)) \xrightarrow{n \rightarrow \infty} \frac{1}{4} (\sigma_\infty^2(\delta_x + \delta_y) - \sigma_\infty^2(\delta_x - \delta_y)),$$

which proves convergence to a limit $k_\infty(x, y)$, for all $x, y \in \mathbb{X}$. Moreover, since $\xi(x), \xi(y) \in L^2$, and thus $\xi(x)\xi(y) \in L^1$, it follows from Theorem 7.23 in Kallenberg (2002), that $\text{cov}_n(x, y) \rightarrow \text{cov}_\infty(x, y)$, almost surely and in L^1 , which implies that $k_\infty(x, y)$ is a version of $\text{cov}_\infty(x, y)$.

Let us now prove that k_∞ is continuous. For any $x, y, x', y' \in \mathbb{X}$, we have

$$k_n(x, y) - k_n(x', y') = \text{cov}_n(\xi(x), \xi(y) - \xi(y')) + \text{cov}_n(\xi(x) - \xi(x'), \xi(y')), \quad (8)$$

and thus

$$|k_n(x, y) - k_n(x', y')| \leq \sigma_n(x) \sigma_n(\delta_y - \delta_{y'}) + \sigma_n(y') \sigma_n(\delta_x - \delta_{x'}) \quad (9)$$

$$\leq \sigma_0(x) \sigma_0(\delta_y - \delta_{y'}) + \sigma_0(y') \sigma_0(\delta_x - \delta_{x'}). \quad (10)$$

Letting n go to $+\infty$, we obtain:

$$|k_\infty(x, y) - k_\infty(x', y')| \leq \sigma_0(x) \sigma_0(\delta_y - \delta_{y'}) + \sigma_0(y') \sigma_0(\delta_x - \delta_{x'}). \quad (11)$$

Since the right-hand side goes to zero when $(x', y') \rightarrow (x, y)$ by continuity of σ_0 , the continuity of k_∞ is proved.

Finally, let C denote a compact subset of $\mathbb{X} \times \mathbb{X}$. Consider the sequence of functions $C \rightarrow \mathbb{R}$, $(x, y) \mapsto \sigma_n^2(\delta_x + \delta_y)$. This is a decreasing sequence of continuous functions, which converges pointwise to the continuous function $(x, y) \mapsto \sigma_\infty^2(\delta_x + \delta_y)$. Since C is compact, the convergence is uniform by Dini's first theorem (see, e.g., Theorem 7.13 in Rudin, 1976). The same argument applies to $(x, y) \mapsto \sigma_n^2(\delta_x - \delta_y)$ and therefore to k_n by polarization. \square

Proposition 2.4. *Assume that \mathbb{X} is compact. Then $\mathbb{E}(\sup_{x \in \mathbb{X}} |\xi(x)|) < +\infty$.*

Proof. This is a direct consequence of Theorem 2.9 of Azais and Wschebor (2009), since $\sup_{x \in \mathbb{X}} |\xi(x)| < +\infty$ for a process with continuous sample paths on a compact space. \square

Proposition 2.5. *Assume that \mathbb{X} is compact. Then $\sup_n \left(\sup_{\mathbb{X}} |\widehat{\xi}_n| \right) < \infty$ almost surely.*

Proof. Since ξ has continuous sample paths and \mathbb{X} is compact, the random variable $\xi^* = \sup_{\mathbb{X}} |\xi|$ takes finite values. Furthermore, from Proposition 2.4, $\mathbb{E}(\xi^*) < +\infty$. Hence, from Theorem 7.23 in Kallenberg (2002),

$$\mathbb{E}(\xi^* | \mathcal{F}_n) \xrightarrow[n \rightarrow \infty]{\text{as}, L^1} \mathbb{E}(\xi^* | \mathcal{F}_\infty). \quad (12)$$

The right-hand side of the above display is almost surely finite, as it has a finite expectation by the law of total expectation. Furthermore

$$\sup_{x \in \mathbb{X}} |\widehat{\xi}_n(x)| = \sup_{x \in \mathbb{X}} |\mathbb{E}(\xi(x) | \mathcal{F}_n)| \quad (13)$$

$$\leq \sup_{x \in \mathbb{X}} \mathbb{E}(|\xi(x)| | \mathcal{F}_n) \quad (14)$$

$$\leq \mathbb{E}(\xi^* | \mathcal{F}_n). \quad (15)$$

The sequence $(\mathbb{E}(\xi^* | \mathcal{F}_n))_n$ converges almost surely according to Equation (12), and therefore is almost surely bounded. \square

3 Stepwise uncertainty reduction and supermartingales

An important observation, which is central to the convergence results established in this paper, is that for most of the sequential designs already available in the literature under the ‘‘SUR strategy’’ label, the uncertainty functional \mathcal{H} (see Equation (1)) enjoys the following *supermartingale* property:

Definition 3.1. *The functional \mathcal{H} is said to have the supermartingale property if, for any choice of sequential design X_1, X_2, \dots , the sequence (H_n) is an (\mathcal{F}_n) -supermartingale.*

A direct consequence of this property is that, for any n and $x \in \mathbb{X}$,

$$J_n(x) \leq H_n \quad \text{almost surely.} \quad (16)$$

The key, to understand the origin of this supermartingale property, is to recognize that the final goal of our sequential design is to form a decision D concerning some quantity of interest. This decision can be of various natures: it will be a pointwise estimate of the quantity of interest in the examples of this paper, but it could also be a confidence region or a predictive distribution, for instance². Let \mathbb{D} denote the set of all possible decisions, \mathbb{D}_n the subset of decisions available at time n (possibly depending on $X_1, Y_1, \dots, X_n, Y_n$), and let

$$L : (f, d) \mapsto L(f, d) \in \mathbb{R} \tag{17}$$

denote a loss function, which maps a sample path f and a decision d to a loss value $L(f, d)$. Assume that $L(\xi, \cdot)$ defines a measurable process on \mathbb{D} , such that $L(\xi, d)$ is integrable for all $d \in \mathbb{D}$. Then, a Bayes-optimal decision if we decided to stop after n evaluations would be any decision minimizing the risk (if such a decision exists):

$$D_n^* \in \operatorname{argmin}_{d \in \mathbb{D}_n} \mathbb{E}_n(L(\xi, d)),$$

and the corresponding value of the risk provides a natural measure of uncertainty for the problem at hand:

$$H_n = \mathbb{E}_n(L(\xi, D_n^*)) = \min_{d \in \mathbb{D}_n} \mathbb{E}_n(L(\xi, d)). \tag{18}$$

From this decision-theoretic point of view, the SUR strategy associated to this uncertainty measure (see Equations (4)–(5)) is a one-step look-ahead—sometimes also called myopic, or greedy—sequential decision procedure, associated to the loss function L for the final decision and without observation cost.

The following result establishes the supermartingale property of the sequence (H_n) defined by Equation (18), under mild technical assumptions. The reader is referred to Molchanov (2006) for definitions and background results on random closed sets.

Proposition 3.2. *Let ξ be a measurable process and let X_1, X_2, \dots be a given, possibly randomized, sequential design. Assume that*

- (i) \mathbb{D} is a Polish space and \mathbb{D}_n an \mathcal{F}_n -measurable random closed subset of \mathbb{D} ,
- (ii) $\mathbb{D}_n \subset \mathbb{D}_{n+1}$ for all n , and
- (iii) there exists an \mathcal{F}_n -measurable version \bar{L}_n of $d \mapsto \mathbb{E}_n(L(\xi, d))$ that is bounded from below and has lower semi-continuous (LSC) sample paths.

Then the sequence (H_n) , with $H_n = \inf_{d \in \mathbb{D}_n} \bar{L}_n(d)$, is an (\mathcal{F}_n) -supermartingale.

Proof. Let us first prove that H_n is a real-valued \mathcal{F}_n -measurable random variable. It is clearly real-valued because of the boundedness assumption on \bar{L}_n . Then, since \mathbb{D} is Polish, the \mathcal{F}_n -measurable random closed set \mathbb{D}_n admits by Theorem 2.3 in Molchanov (2006) a Castaing representation: $\mathbb{D}_n = \operatorname{cl}\{U_{n,k}, k \in \mathbb{N}\}$, where cl denotes the closure in \mathbb{D} and $(U_{n,k})$ is a

²The example of a predictive distribution is relevant to the use of Shannon's entropy as a measure of uncertainty (see, e.g., Villemonteix et al., 2009)

sequence of \mathbb{D} -valued random variables. Let $\mathbb{D}_{n,0} = \{U_{n,k}, k \in \mathbb{N}\}$. Using the LSC property of \bar{L}_n , we conclude that $\inf_{\mathbb{D}_n} \bar{L}_n = \inf_{\mathbb{D}_{n,0}} \bar{L}_n = \inf_{k \in \mathbb{N}} \bar{L}_n(U_{n,k})$ is \mathcal{F}_n -measurable.

Let $\varepsilon > 0$. The set $F_{n,\varepsilon} = \mathbb{D}_n \cap \{\bar{L}_n \leq H_n + \varepsilon\}$ is a \mathcal{F}_n -measurable random closed set, which is not empty since $H_n = \inf_{\mathbb{D}_n} \bar{L}_n$. By the fundamental selection theorem in Polish spaces (see Molchanov, 2006, Theorem 2.13), there exists an \mathcal{F}_n -measurable selection $D_{n,\varepsilon}$ in $F_{n,\varepsilon}$ (i.e., a \mathbb{D} -valued \mathcal{F}_n -measurable random variable such that $D_{n,\varepsilon} \in F_{n,\varepsilon}$ almost surely). Then we have

$$H_{n+1} = \inf_{\mathbb{D}_{n+1}} \bar{L}_{n+1} \leq \bar{L}_{n+1}(D_{n,\varepsilon})$$

almost surely, since $D_{n,\varepsilon} \in F_{n,\varepsilon} \subset \mathbb{D}_n \subset \mathbb{D}_{n+1}$ almost surely, and therefore

$$\mathbb{E}_n(H_{n+1}) \leq \mathbb{E}_n(\bar{L}_{n+1}(D_{n,\varepsilon})) = \bar{L}_n(D_{n,\varepsilon}) = H_n + \varepsilon. \quad (19)$$

We conclude that (H_n) is an \mathcal{F}_n -supermartingale, since Equation (19) holds almost surely for any $\varepsilon > 0$. \square

The following result states an important consequence of the supermartingale property, which is central to our general approach for the convergence of SUR strategies.

Proposition 3.3. *Let ξ be a measurable process. Let a SUR strategy for ξ be given in terms of a sequence (h_n) of measurable functions, as in Equations (2)–(4). Assume that, at each step of the construction of the design,*

(i) $x \mapsto \mathbb{E}_{n,x}(H_{n+1})$ admits a version J_n that is \mathcal{F}_n -measurable and has LSC sample paths.

Then there actually exists an \mathcal{F}_n -measurable random variable X_{n+1} , not necessarily unique, that satisfies Equation (5). Assume further that

(ii) *The sequence (H_n) is an (\mathcal{F}_n) -supermartingale, bounded in L^1 .*

Then $H_n - \min_{x \in \mathbb{X}} J_n(x) \rightarrow 0$ almost surely.

Proof. Since J_n is \mathcal{F}_n -measurable and has LSC sample paths, $\operatorname{argmin} J_n$ is a non-empty \mathcal{F}_n -measurable random closed subset of \mathbb{X} . It is non-empty since \mathbb{X} is compact (LCS functions attain their minimum on compact sets) and therefore, by the fundamental selection theorem (see Molchanov, 2006, Theorem 2.13), there exists an \mathcal{F}_n -measurable selection X_{n+1} in $\operatorname{argmin} J_n$. In other words, there exists an \mathcal{F}_n -measurable random variable X_{n+1} that satisfies Equation (5).

Let us now prove that $H_n - \min_{x \in \mathbb{X}} J_n(x) \rightarrow 0$. Since X_{n+1} is \mathcal{F}_n -measurable, we have:

$$\begin{aligned} J_n(X_{n+1}) &= \mathbb{E}_n(h_{n+1}(X_1, Y_1, \dots, x, \xi(x) + \epsilon_{n+1}))|_{x=X_{n+1}} \\ &= \mathbb{E}_n(h_{n+1}(X_1, Y_1, \dots, X_{n+1}, Y_{n+1})) = \mathbb{E}_n(H_{n+1}). \end{aligned} \quad (20)$$

Set $\Delta_{n+1} = H_n - H_{n+1}$ and $\bar{\Delta}_{n+1} = \mathbb{E}_n(\Delta_{n+1}) = H_n - \mathbb{E}_n(H_{n+1})$. The random variables $\bar{\Delta}_n$ are positive in as much as (H_n) is a supermartingale and, using Equation (20) and (5), we have

$$\bar{\Delta}_{n+1} = H_n - \mathbb{E}_n(H_{n+1}) = H_n - J_n(X_{n+1}) = H_n - \min_{x \in \mathbb{X}} J_n.$$

Moreover, for any n , we have $\sum_{k=0}^{n-1} \Delta_k = H_0 - H_n$, and therefore

$$\mathbb{E} \left(\sum_{k=0}^{n-1} \bar{\Delta}_k \right) = \mathbb{E} \left(\sum_{k=0}^{n-1} \Delta_k \right) = \mathbb{E} (H_0 - H_n) \leq 2 \sup_k \mathbb{E} (|H_k|) < +\infty$$

since (H_n) is bounded in L^1 . It follows that $\mathbb{E} (\sum_{k=0}^{\infty} \bar{\Delta}_k) < +\infty$, and therefore $\bar{\Delta}_{n+1} = H_n - \min_{x \in \mathbb{X}} J_n(x) \rightarrow 0$ almost surely. \square

Remark 3.4. By Doob's supermartingale convergence theorem (see, e.g., Kallenberg, 2002, Theorem 7.18), there exists under Condition ii) of Proposition 3.3 a random variable H_∞ such that $H_n \rightarrow H_\infty$ almost surely, and therefore $\min_{x \in \mathbb{X}} J_n(x) \rightarrow H_\infty$ as well.

Propositions 3.2 and 3.3 can be used to study the convergence of various SUR strategies as follows:

- A. Show that (H_n) is an (\mathcal{F}_n) -supermartingale using Proposition 3.2 (i.e. exhibit a decision space \mathbb{D} , a loss function L , etc.) and check that it is bounded in L^1 .
- B. Find an event $B \in \mathcal{F}$ such that $H_n \rightarrow H^* := \min_P \mathcal{H}(P)$ on B and

$$\limsup_{n \rightarrow \infty} \left(H_n - \min_{x \in \mathbb{X}} J_n(x) \right) \text{ on } \Omega \setminus B. \quad (21)$$

- C. Deduce from Proposition 3.3 that Equation (21) defines a negligible event, and thus $H_n \rightarrow H^*$ almost surely.

Two examples will be worked out in detail in the following section.

Remark 3.5. Proposition 3.3 will, typically, be applied to events B where $\sup \sigma_\infty^2 = 0$ (see Section 4), in which case it follows that the sequence of design points X_1, X_2, \dots is almost surely dense in \mathbb{X} for processes that are not “too regular”, in the sense of the following definition:

Definition 3.6 (Vazquez and Bect, 2010a). *A Gaussian process ξ (or, equivalently, its covariance function k) is said to have the no-empty-ball (NEB) property if, for all sequences $(x_n)_{n \geq 1}$ in \mathbb{X} and all $y \in \mathbb{X}$, the following assertions are equivalent:*

- (i) y is an adherent point of the set $\{x_n, n \geq 1\}$;
- (ii) $\sigma_n^2(y) \rightarrow 0$ if ξ is observed at $X_n = x_n, n \geq 1$.

Gaussian processes with a Matérn covariance functions are examples of processes with the NEB property. Gaussian processes with a squared exponential covariance function, on the other hand, do not have the NEB property (Vazquez and Bect, 2010b). The NEB property was a key ingredient in the proof by Vazquez and Bect (2010a) of the convergence of the expected improvement algorithm, which is revisited in Section 4.2 without assuming the NEB property.

4 Applications in probability of excursion estimation and in Bayesian optimization

We assume in this section that \mathbb{X} is a compact metric space and ξ a Gaussian process with continuous sample paths.

4.1 Convergence of a SUR strategy for probability of excursion estimation

Let $T \in \mathbb{R}$ be a given threshold and let μ be a given finite measure over \mathbb{X} . We consider here the following measure of uncertainty (See, e.g., Bect et al. (2012), where it is denoted by $J_{4,n}^{\text{SUR}}$) for the excursion set $\Gamma = \{\xi \geq T\}$:

$$H_n = \mathbb{E}_n \left(\left\| \mathbb{1}_\Gamma - \mathbb{1}_{\widehat{\Gamma}_n} \right\|_{L^2(\mu)}^2 \right) = \int_{\mathbb{X}} \text{var}_n (\mathbb{1}_{\xi(u) \geq T}) d\mu(u) = \int_{\mathbb{X}} p_n (1 - p_n) d\mu, \quad (22)$$

where $\widehat{\Gamma}_n = \{\widehat{\xi}_n \geq T\}$ and $p_n(u) = \mathbb{P}_n(\xi(u) \geq T)$. The corresponding SUR sampling criterion is given by

$$J_n(x) = \mathbb{E}_{n,x}(H_{n+1}) = \int_{\mathbb{X}} \mathbb{E}_{n,x}(p_{n+1}(u)(1 - p_{n+1}(u))) d\mu(u). \quad (23)$$

We now prove that Proposition 3.3 applies to the just-presented SUR criterion. For clarity of exposition, we assume that the variances of the $(\epsilon_n)_{n \in \mathbb{N}}$ are constant. This condition can be relaxed.

Proposition 4.1. *Assume that for all $n \in \mathbb{N}$, $\text{var}(\epsilon_n) = \tau^2 < \infty$. Then the conditions i) and ii) of Proposition 3.3 hold. As a consequence, $\sigma_\infty^2 \equiv 0$.*

Proof. For checking i), it is useful to note that $p_n(u)(1 - p_n(u)) = \text{var}_n(\mathbb{1}_{\xi(u) \geq T})$. From there,

$$J_n(x) = \int_{\mathbb{X}} \mathbb{E}_n (\text{var}_n(\mathbb{1}_{\xi(u) \geq T} | \xi(x) + \epsilon_{n+1})) d\mu(u) \leq \int_{\mathbb{X}} \text{var}_n(\mathbb{1}_{\xi(u) \geq T}) d\mu(u) = H_n \quad (24)$$

by applying the law of total variance to the integrand, and it appears that (H_n) is indeed an (\mathcal{F}_n) -super martingale. It is bounded in L^1 since $\text{var}_n(\mathbb{1}_{\xi(u) \geq T}) \leq \frac{1}{4}$ and μ is a finite measure. Regarding ii), let us remark first that for any $x \in \mathbb{X}$

$$\begin{aligned} J_n(x) - H_n &= \int_{\mathbb{X}} \mathbb{E}_n (\text{var}_n(\mathbb{1}_{\xi(u) \geq T} | \xi(x) + \epsilon_{n+1})) d\mu(u) - \int_{\mathbb{X}} \text{var}_n(\mathbb{1}_{\xi(u) \geq T}) d\mu(u) \\ &= - \int_{\mathbb{X}} \text{var}_n(\mathbb{E}_n (\mathbb{1}_{\xi(u) \geq T} | \xi(x) + \epsilon_{n+1})) d\mu(u) = - \int_{\mathbb{X}} \text{var}_n(p_{n+1}(u; x)) d\mu(u). \end{aligned} \quad (25)$$

We then need to establish that with probability one $\exists x^* \in \mathbb{X}$, $\sigma_\infty^2(x^*) > 0$ implies that $\limsup_{n \rightarrow \infty} \int_{\mathbb{X}} \text{var}_n(p_{n+1}(u; x^*)) d\mu(u) > 0$. Before proving it let us recall an inequality which will be used below.

Theorem 4.2. (See Cacoullos (1982); Klaassen (1985)) Let $Z \sim \mathcal{N}(\mu, \sigma^2)$ and g, g' be real valued functions on \mathbb{R} such that g is an indefinite integral of g' and $\text{var}(g(Z)) < +\infty$. Then,

$$\sigma^2 \mathbb{E}(g'(Z))^2 \leq \text{var}(g(Z)) \leq \sigma^2 \mathbb{E}(g'(Z)^2). \quad (26)$$

Coming back to the proof of Proposition 4.1, we finally want to prove that almost surely $\text{var}_n(p_{n+1}(u; x^*)) \geq \delta > 0$ for n large enough and u in a suitable neighbourhood of x^* . Let Φ and ϕ be the cdf and pdf of the standard normal distribution. First note that, with the convention that $\Phi(0/0) = 1$, we have for $u, x \in \mathbb{X}$

$$p_{n+1}(u; x) = \Phi \left(\frac{\mathbb{E}_n(\xi(u)|\xi(x) + \epsilon_{n+1}) - T}{\sqrt{\text{var}_n(\xi(u)|\xi(x) + \epsilon_{n+1})}} \right) = g_n(\xi(x) + \epsilon_{n+1}; u, x), \quad (27)$$

where $g_n(\cdot; u, x) : t \in \mathbb{R} \rightarrow g_n(t; u, x) = \Phi(a_n(u; x) + b_n(u; x)t)$ with $\lambda_{n+1}(u; x) = \frac{k_n(x, u)}{\sigma_n^2(x) + \tau^2}$, $a_n(u; x) = \frac{\hat{\xi}_n(u) - \lambda_{n+1}(u; x)\hat{\xi}_n(x) - T}{\sqrt{\sigma_n^2(u) - (\sigma_n^2(x) + \tau^2)\lambda_{n+1}(u; x)^2}}$ and $b_n(u; x) = \frac{\lambda_{n+1}(u; x)}{\sqrt{\sigma_n^2(u) - (\sigma_n^2(x) + \tau^2)\lambda_{n+1}(u; x)^2}}$. Using Equation (26),

$$\text{var}_n(p_{n+1}(u; x)) \geq (\sigma_n^2(x) + \tau^2)b_n^2(u; x) \mathbb{E}_n(\phi(a_n(u; x) + b_n(u; x)[\xi(x) + \epsilon_{n+1}]))^2. \quad (28)$$

We now state and prove a technical lemma enabling to write more explicitly the above mean value.

Lemma 4.3. Let $N \sim \mathcal{N}(0, 1)$. Then, for all $\alpha, \beta \in \mathbb{R}$,

$$\mathbb{E}(\phi(\alpha + \beta N)) = \frac{1}{\sqrt{2\pi}\sqrt{\beta^2 + 1}} \exp\left(-\frac{1}{2} \frac{\alpha^2}{\beta^2 + 1}\right). \quad (29)$$

Proof. Using that $\phi(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$, we get

$$\begin{aligned} \mathbb{E}(\phi(\alpha + \beta N)) &= \int_{\mathbb{R}} \phi(\alpha + \beta u)\phi(u)du = \frac{1}{2\pi} \int_{\mathbb{R}} \exp\left(-\frac{1}{2}((\alpha + \beta u)^2 + u^2)\right) du \\ &= \frac{1}{2\pi} \int_{\mathbb{R}} \exp\left(-\frac{1}{2}\left((\beta^2 + 1)\left(u + \frac{\alpha\beta}{\beta^2 + 1}\right)^2 + \alpha^2\left(1 - \frac{\beta^2}{\beta^2 + 1}\right)\right)\right) du. \end{aligned}$$

One concludes by noting that $\int_{\mathbb{R}} \exp\left(-\frac{1}{2}\left((\beta^2 + 1)\left(u + \frac{\alpha\beta}{\beta^2 + 1}\right)^2\right)\right) du = \frac{\sqrt{2\pi}}{\sqrt{\beta^2 + 1}}$. \square

Coming back to the proof of Proposition 4.1 and applying Lemma 4.3 with $\alpha \leftarrow a_n(u; x) +$

$b_n(u; x)\widehat{\xi}_n(x), \beta \leftarrow b_n(u; x)\sqrt{\sigma_n^2(x) + \tau^2}$ we get:

$$\begin{aligned}
\text{var}_n(p_{n+1}(u; x)) &\geq \frac{[\sigma_n^2(x) + \tau^2]b_n^2(u; x)}{2\pi(b_n^2(u; x)[\sigma_n^2(x) + \tau^2] + 1)} \exp\left(-\frac{(a_n(u; x) + b_n(u; x)\widehat{\xi}_n(x))^2}{b_n^2(u; x)[\sigma_n^2(x) + \tau^2] + 1}\right) \\
&= \frac{[\sigma_n^2(x) + \tau^2]}{2\pi([\sigma_n^2(x) + \tau^2] + b_n^{-2}(u; x))} \exp\left(-\frac{(T - \widehat{\xi}_n(u))^2}{\sigma_n^2(u)}\right) \\
&\geq \frac{k_n^2(x, u)}{2\pi[\sigma_n^2(x) + \tau^2]\sigma_n^2(u)} \exp\left(-\frac{\left[|T| + \limsup_{n \rightarrow +\infty} \sup_{v \in \mathbb{X}} (|\widehat{\xi}_n(v)|)\right]^2}{\sigma_n^2(u)}\right).
\end{aligned} \tag{30}$$

From Equation (30), taking $x = x^*$, noting that $\sigma_\infty^2(x^*) > 0$ and applying Proposition 2.3, we have that, almost surely, there exists $N \in \mathbb{N}$, $\alpha, \epsilon > 0$ so that for $\|u - x^*\| \leq \alpha$, for $n \geq N_1$,

$$\frac{k_n^2(x, u)}{2\pi[\sigma_n^2(x) + \tau^2]\sigma_n^2(u)} \geq \epsilon$$

and $\sigma_n^2(u) \geq \epsilon$. Also from Proposition 2.5, almost surely, there exists $C < \infty$, so that for $n \geq N_2$,

$$\left[|T| + \limsup_{n \rightarrow +\infty} \sup_{v \in \mathbb{X}} (|\widehat{\xi}_n(v)|)\right]^2 \leq C.$$

Thus, almost surely, for $n \geq N$ and $\|u - x^*\| \leq \alpha$,

$$\text{var}_n(p_{n+1}(u; x)) \geq \epsilon \exp\left(-\frac{C}{\epsilon}\right).$$

Hence, almost surely for $n \geq N$,

$$\int_{\mathbb{X}} \text{var}_n(p_{n+1}(u; x^*)) d\mu(u) \geq \int_{\mathbb{X}} \mathbb{1}_{\|u - x^*\| \leq \alpha} \epsilon \exp\left(-\frac{C}{\epsilon}\right) d\mu(u).$$

This finishes the proof of ii). \square

In the next corollary, we show that Proposition 4.1 implies that the uncertainty on the set $\{t \in \mathbb{X}; \xi(t) \geq T\}$, as measured by H_n , goes to zero.

Corollary 4.4. *We have that $H_n \rightarrow_{n \rightarrow \infty} 0$ almost surely and in L^1 .*

Proof. Let us first show the convergence in L^1 . Consider a fixed $u \in \mathbb{X}$. Then $p_n(u) = \mathbb{E}(\mathbb{1}_{\xi(u) \geq T} | \mathcal{F}_n) \rightarrow_{a.s.} \mathbb{E}(\mathbb{1}_{\xi(u) \geq T} | \mathcal{F}_\infty)$ from Theorem 7.23 in Kallenberg (2002).

Now, from Equation (12), $\mathbb{E}(\xi(u) | \mathcal{F}_n) \rightarrow_{a.s.} \mathbb{E}(\xi(u) | \mathcal{F}_\infty)$. By Proposition 4.1 and the fact that $\sigma_n(u) \rightarrow_{n \rightarrow \infty} 0$, $\mathbb{E}(\xi(u) | \mathcal{F}_n) \rightarrow_{a.s.} \xi(u)$. Hence, there exists a \mathcal{F}_∞ -measurable random variable $\tilde{\xi}(u)$ so that $\xi(u) = \tilde{\xi}(u)$ a.s. It follows that, a.s., $\mathbb{E}(\mathbb{1}_{\xi(u) \geq T} | \mathcal{F}_\infty) = \mathbb{E}(\mathbb{1}_{\tilde{\xi}(u) \geq T} | \mathcal{F}_\infty) = \mathbb{1}_{\tilde{\xi}(u) \geq T} = \mathbb{1}_{\xi(u) \geq T}$ and therefore $p_n(u) \rightarrow_{n \rightarrow \infty} \mathbb{1}_{\xi(u) \geq T}$ almost surely.

In addition, by dominated convergence $\mathbb{E}(p_n(u)(1-p_n(u)) \rightarrow_{n \rightarrow \infty} \mathbb{E}(\mathbf{1}_{\xi(u) \geq T}(1-\mathbf{1}_{\xi(u) \geq T})) = 0$. By dominated convergence again and by Fubini's theorem we obtain that $\mathbb{E}(H_n) \rightarrow_{n \rightarrow \infty} 0$.

Let us finally address the almost sure convergence of H_n . By *i*) in Proposition 3.3 and Theorem 7.23 in Kallenberg (2002), H_n converges almost surely to a random variable, which is thus equal to 0 almost surely. \square

4.2 Convergence of the expected improvement algorithm, revisited

As a second example we consider the noiseless case where $\epsilon_i = 0$ for all $i \in \mathbb{N}$. We revisit the case of expected improvement criterion (Mockus et al., 1978; Jones et al., 1998) for the estimation of $\max \xi$, which is usually written as:

$$\text{EI}_n(x) = \mathbb{E}_n(\max(0, \xi(x) - M_n)), \quad (31)$$

where $M_n = \max_{i \leq n} \xi(X_i)$. This criterion can be interpreted as the expected uncertainty reduction for the estimator M_n with L^1 uncertainty measure

$$H_n = \mathbb{E}_n(|\max \xi - M_n|) = \mathbb{E}_n(\max \xi) - M_n. \quad (32)$$

In other words, for all $x \in \mathbb{X}$,

$$\text{EI}_n(x) = H_n - J_n(x), \quad (33)$$

where J_n is defined by Equation (4). Thus, although it is not usually introduced as such, Equation (31) is an example of a SUR criterion. Vazquez and Bect (2010a, Theorem 6) proved that the sequence of points generated by the associated SUR strategy is almost surely dense in \mathbb{X} , and therefore that $M_n \rightarrow \max \xi$ almost surely, if the covariance function has the NEB property (see Section 3). We provide here an alternative proof of the same result, which uses the supermartingale approach of Section 3. In addition, we also provide a direct proof of the fact that $M_n \rightarrow \max \xi$ almost surely, which does not assume the NEB property and therefore holds for very regular covariance functions as well (such as the squared exponential one).

Theorem 4.5. *The conditions *i*) and *ii*) of Proposition 3.3 hold for the expected improvement criterion with*

$$B = B_1 \cup B_2, \quad B_1 = \left\{ \sup \sigma_\infty^2 > 0 \right\}, \quad B_2 = \left\{ \limsup_{n \rightarrow \infty} \left(\max \widehat{\xi}_n - M_n \right) > 0 \right\}. \quad (34)$$

As a consequence, the following convergences hold almost surely and in L^1 :

(a) σ_n^2 converges uniformly to $\sigma_\infty^2 \equiv 0$,

(b) $\max \widehat{\xi}_n - M_n \xrightarrow[n \rightarrow \infty]{} 0$,

(c) $H_n \xrightarrow[n \rightarrow \infty]{} 0$, and

(d) $M_n \xrightarrow[n \rightarrow \infty]{} \max \xi$.

Proof. Condition i) is easily verified: H_n is clearly non-negative and dominated by $2 \sup |\xi|$, which is integrable by Proposition 2.4. Moreover, the supermartingale property follows from the general argument given in Section 3—explicitly:

$$\begin{aligned} \mathbb{E}_n(H_{n+1}) &= \mathbb{E}_n(\mathbb{E}_{n+1}(\max \xi) - M_{n+1}) = \mathbb{E}_n(\max \xi) - \mathbb{E}_n(M_{n+1}) \\ &\geq \mathbb{E}_n(\max \xi) - M_n = H_n, \end{aligned}$$

since (M_n) is increasing.

Let us now establish Condition ii). Recall from Section 3 in Vazquez and Bect (2010a) that the expected improvement is a continuous and non-negative function γ of $z_n(x) := \widehat{\xi}_n(x) - M_n$ and $\sigma_n^2(x)$, with the following properties:

- $\gamma(z, s^2) > 0$ if $s^2 > 0$,
- $\gamma(z, s^2) \geq z > 0$ if $z > 0$.

Assume that the event $A := \{\sup_n \max_{\mathbb{X}} |\widehat{\xi}_n| < +\infty\}$, which has probability one by Proposition 2.5, is realized. If B_1 holds, i.e., if $\sigma_\infty^2(x^*) > 0$ for some $x^* \in \mathbb{X}$, then the first argument of γ , $z_n(x^*)$, is bounded as $n \rightarrow +\infty$ (since $\sup_n \max_{\mathbb{X}} |\widehat{\xi}_n| < +\infty$) and the second argument, $\sigma_n^2(x^*)$, is bounded away from zero since $n \mapsto \sigma_n^2(x^*)$ is decreasing (by Proposition 2.1); therefore, $\text{EI}_n(x^*) = \gamma(z_n(x^*), \sigma_n^2(x^*))$ is bounded away from zero³. If B_2 holds, i.e., if $\limsup_{n \rightarrow \infty} (\max \widehat{\xi}_n - M_n) > 0$, then there exists $\varepsilon > 0$ and a sequence x_n^* such that $z_n(x_n^*) = \widehat{\xi}_n(x_n^*) - M_n \geq \varepsilon > 0$ on a subsequence, which also proves that $\limsup_{n \rightarrow \infty} \text{EI}_n(x_n^*) > 0$. In both cases, we have proved that $\limsup_{n \rightarrow \infty} (H_n - \min J_n) > 0$ since $\max \text{EI}_n = H_n - \min J_n$ according to Equation (33). Condition ii) is thus established.

We have proved so far that Conditions i) and ii) in Proposition 3.3 hold with B given by Equation (34). Therefore

$$\overline{B} = \left\{ \sup \sigma_\infty^2 = 0 \right\} \cap \left\{ \limsup_{n \rightarrow \infty} \left(\max \widehat{\xi}_n - M_n \right) \leq 0 \right\}$$

holds with probability one. It follows readily from Proposition 2.3 that σ_n^2 converges uniformly to 0, almost surely⁴. Moreover, observe that

$$\max \widehat{\xi}_n \geq \max_{i \leq n} \widehat{\xi}_n(X_i) = \max_{i \leq n} \xi(X_i) = M_n,$$

which implies that b) is satisfied on \overline{B} , and thus holds almost surely.

Let us now prove that $\mathbb{E}_\infty(\max \xi) \stackrel{\text{a.s.}}{=} \max \xi$. For any $x \in \mathbb{X}$, we have by the martingale convergence theorem (see, e.g., Theorem 7.23 in Kallenberg (2002)) that

$$\widehat{\xi}_n(x) \xrightarrow[n \rightarrow \infty]{} \mathbb{E}_\infty(\xi(x))$$

and $\mathbb{E}_\infty(\xi(x)) \stackrel{\text{a.s.}}{=} \xi(x)$, since $\sigma_\infty^2(x) = \text{var}_\infty(\xi(x)) = 0$ almost surely. Let $\{x_i, i \in \mathbb{N}\}$ be a countable dense subset of \mathbb{X} . Then, using the continuity of the sample paths of ξ , it holds with probability one that

$$\max \xi = \max_i \xi(x_i) = \max_i \mathbb{E}_\infty(\xi(x_i)) = \max_i \lim_{n \rightarrow \infty} \widehat{\xi}_n(x_i). \quad (35)$$

³Observe that this proves that $\liminf_{n \rightarrow \infty} \text{EI}_n(x^*) > 0$, which is stronger than what we actually need.

⁴which is enough to obtain Theorem 6 of Vazquez and Bect (2010a)

It follows that $E_\infty(\max \xi) \stackrel{\text{a.s.}}{=} \max \xi$, since the right-hand side of Equation (35) is \mathcal{F}_∞ -measurable, and

$$\max \xi = \max_i \lim_{n \rightarrow \infty} \widehat{\xi}_n(x_i) \leq \liminf_{n \rightarrow \infty} \max \widehat{\xi}_n. \quad (36)$$

Moreover, using again the martingale convergence theorem, we have $E_n(\max \xi) \rightarrow E_\infty(\max \xi)$ almost surely, and thus

$$\max \widehat{\xi}_n = \max_{x \in \mathbb{X}} E_n(\xi(x)) \leq E_n(\max \xi) \rightarrow E_\infty(\max \xi) = \max \xi \quad (37)$$

almost surely. Combining Equations (36) and (37) with b) yields d) in the almost sure sense. Finally, $H_n = E_n(\max \xi) - M_n \rightarrow 0$ also holds almost surely, as a consequence of d) and the fact that $E_n(\max \xi) \rightarrow E_\infty(\max \xi) = \max \xi$ almost surely.

We conclude the proof by observing that all four convergence results (a–d) also hold in the L^1 -sense by the dominated convergence theorem. \square

5 Discussion

We have established convergences for a class of Stepwise Uncertainty Reduction (SUR) strategies relying on a supermartingale approach. Under mild technical conditions, results apply in particular to SUR strategies derived from risk minimization, to which the expected improvement algorithm and a probability of excursion estimation SUR strategy from Bect et al. (2012) belong, that is, correspond to adequate loss functions. This is of practical relevance as, while SUR strategies dedicated to probability of excursion estimation are in use in applications, to the best of our knowledge this is the first convergence proof for one of them. Furthermore results provably hold in the case of noisy observations. Here for brevity the noise is assumed centred Gaussian with constant variance; however generalizations can easily be obtained, for instance in the case of variances evolving along the sequence provided that their limsup remains finite. Besides this, convergence results proved here for the expected improvement algorithm usefully complement those of Vazquez and Bect (2010a), notably as they do not require the No-Empty-Ball assumptions and hence allow for very smooth covariance functions such as the squared-exponential one, for which the convergence of EI algorithms was tackled in Yarotsky (2013a) and Yarotsky (2013b). Let us also remark that in both optimization and excursion cases, the presented convergence results directly extend to batch-sequential settings, that is if several points are sought at each iteration (See, e.g., Chevalier et al., 2014).

Following consistency results, a natural but non-trivial extension of this work would be to establish convergence rates of SUR strategies, for which the results of Bull (2011) on the expected improvement algorithm and variants thereof could be used as a starting point, together with detailed investigations on existing convergence rate results for supermartingales. Further perspectives also include extensions to the case of estimated hyperparameters or the full Bayesian one, investigating when sequentiality of the design actually helps regarding the considered goals, and also what is gained in parallelization speed-ups and/or lost in terms of uncertainty reduction per evaluation when appealing to batch-sequential settings. Beyond the current framework where the objective function is assumed to be a realization of the Gaussian

Process underlying the sequential design, another question of interest is to characterize the set of functions on which given strategies would converge or conversely present failure modes.

On a different note and coming back to the present settings, our results ought to be generalized to other SUR strategies for which the supermartingale property holds. These include in particular Knowledge Gradient strategies presented in (Frazier et al., 2009) and related works, Bayesian optimization algorithms based on the conditional entropy of the minimizer (Villemonteix et al., 2009; Hernández-Lobato et al., 2014), and also strategies relying on further criteria of Bect et al. (2012) such as the one based on the variance of the excursion volume.

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