# Towards GP-based optimization with finite time horizon

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**Abstract** During the last decade, Kriging-based sequential algorithms like EGO [2] and its variants have become reference optimization methods in computer experiments. Such algorithms rely on the iterative maximization of a sampling criterion, the expected improvement ($EI$), which takes advantage of Kriging conditional distributions to make an explicit trade-off between promizing and uncertain search space points. We have recently worked on a multipoints $EI$ criterion meant to simultaneously choose several points, which is useful for instance in synchronous parallel computation. The research results that we wish to present in this paper concern sequential procedures with a fixed number of iterations. We show that maximizing the 1-point criterion at each iteration ($EI$ algorithm) is suboptimal. In essence, the latter amounts to considering the current iteration as the last one. This work formulates the problem of optimal strategy for finite horizon sequential optimization, provides the solution to this problem in terms of multipoints $EI$, and illustrates the suboptimality of the usual $EI$ algorithm on the basis of a first counter-example.

## 1 Introduction

Gaussian Process (GP) [4] has become a major tool in *metamodeling* for computer experiments. When studying a multivariate numerical simulator with scalar output, $y : \mathbf{x} \in D \subset \mathbb{R}^d \longrightarrow y(\mathbf{x}) \in \mathbb{R}$, GP metamodeling consists of assuming that $y$ is one path of a GP $Y$. The main focus in this paper is on metamodel-based optimization with finite time horizon. In GP-based optimization, it is common to sequentially enrich the current Design of Experiments (DoE) $\mathbf{X} = \{\mathbf{x}^1, \ldots, \mathbf{x}^n\} \in D^n$ ($n \in \mathbb{N}^*$) —denoted by $\mathbf{X} = \mathbf{X}^0$ and $n = n_0$ in the initial state— by maximizing a probabilistic criterion of interest, update the GP model, and iterate. As detailed in [1], the *Expected Improvement* (EI) is now one of the most popular GP-based optimization criteria:

$$EI(\mathbf{x}) = \mathbb{E}\left[(\min(Y(\mathbf{X})) - Y(\mathbf{x}))^+ \,|\, Y(\mathbf{X}) = \mathbf{Y}\right] = \mathbb{E}\left[I(\mathbf{x})|A\right] \tag{1}$$

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where $I(\mathbf{x}) := (\min(Y(\mathbf{X})) - Y(\mathbf{x}))^+$ is the random variable of improvement at $\mathbf{x}$, and $A$ is the event summarizing all available points and corresponding observations. $EI$ is appreciated for providing a trade-off between exploitation of known information and exploration of not already visited zones of the search space. Furthermore, $EI$ is known in closed form (Cf. [2]), which allows very fast evaluations and even analytical calculation of its derivatives. Such a criterion, though regularly updated by taking the new data into account, is most of the time considered at each iteration without structural change. In fact, in $EI$ algorithms like $EGO$, the point $\mathbf{x}^{n+j}$ to be visited at the $j^{\text{th}}$ iteration is set by maximizing a conditional expectation:

**Algorithm 1** EI algorithm with known Kriging parameters and fixed number of iterations $r \in \mathbb{N}^*$

1: **function** EGO($\mathbf{X}$, $\mathbf{Y}$, $r$)
2: **for** $j \leftarrow 1, r$ **do**
3: $A_{j-1} = \left\{Y(\mathbf{x}^1) = y(\mathbf{x}^1), \ldots, Y(\mathbf{x}^{n+j-1}) = y(\mathbf{x}^{n+j-1})\right\}$
4: $\mathbf{x}^{n+j} = \arg\max_{\mathbf{x}\in D} \left\{\mathbb{E}\left[I(\mathbf{x})|A_{j-1}\right]\right\}$
5: **end for**
6: **end function**

*Example 1.* We consider a 1-dimensional test-case where $D = [0,1]$ and the objective fonction is defined by $y_1 : x \in [0,1] \rightarrow y_1(x) = sin(10x+1)/(1+x) + 2\cos(5x)x^4 \in \mathbb{R}$. The initial design of experiments $\mathbf{X}^0$ is a set of $n_0 = 3$ irregularly spaced points, $\{0.1, 0.2, 0.85\}$. Simple Kriging is performed using a Matern covariance kernel ($\nu = \frac{3}{2}$, see [7] for details), with a unit variance and a range of $\frac{\sqrt{3}}{6}$. Fig. 1 illustrates $y_1$ and its actual minimizer, the design of experiments $\mathbf{X}^0$, as well as the associated 1-point $EI$ function and 2-points $EI$ contour lines. Comments are to be found in the caption of fig. 1 and to be resumed in section 3.2.

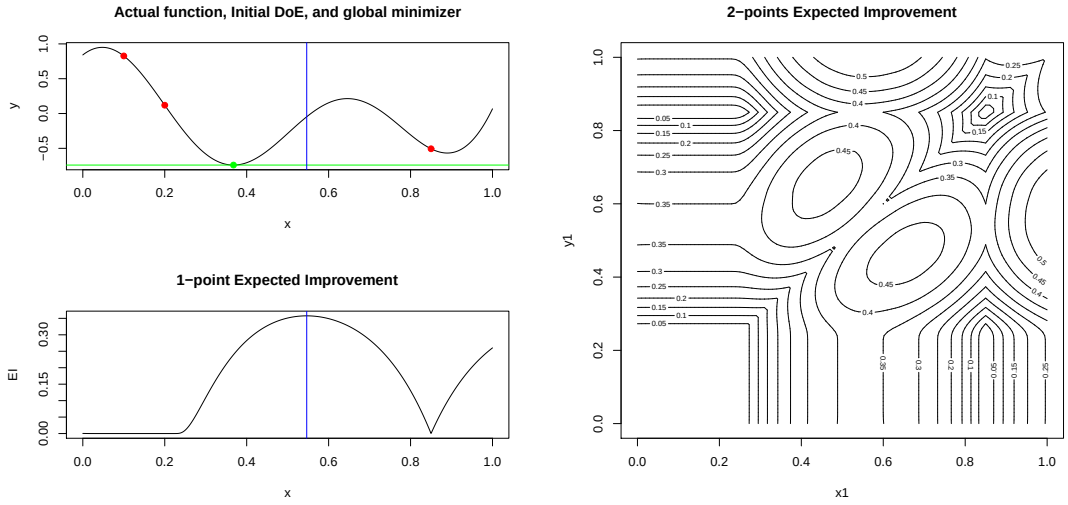


**Fig. 1** $y_1$ (upper left) with its global minimizer (in green) and the design $\mathbf{X}^0$ (in red), 1-point $EI$ and 2-points $EI$ criteria (lower left, and right) corresponding to the Kriging model of example 1. The vertical blue line locates the 1-point $EI$ maximizer, at $\approx 0.55$. The maximum of the 2-points $EI$ is reached with one point as previously, and one point at the boundary point 1.

## 2 What is a strategy and how to measure its performance?

### 2.1 Deterministic strategies with finite horizon

We now propose a definition of sequential deterministic strategies for optimization with finite horizon. Assume that one has a budget of $r$ evaluations after having evaluated $y$ at an arbitrary $n$-points design, $\mathbf{X}$. One step of a sequential strategy essentially consists in looking for the next point where to evaluate $y$, say $\mathbf{x}^{n+1}$. In some sampling procedures like crude Monte Carlo, $\mathbf{x}^{n+1}$ may be determined without taking into account the design $\mathbf{X}$ and the corresponding observations $\mathbf{Y}$. However, in the considered case of adaptive strategies, $\mathbf{x}^{n+1}$ is determined on the basis of the available information. Furthermore, we restrict ourselves here to the case of deterministic strategies, i.e. where $\mathbf{x}^{n+1}$ only depends on the past and doesn't involve any random operator (like mutations in genetic algorithms). So $\mathbf{x}^{n+1}$ is in fact defined as some function of $\mathbf{X}$ and $\mathbf{Y}$:

$$s_1 : (\mathbf{X},\mathbf{Y}) \in (D\times\mathbb{R})^n \longrightarrow \mathbf{x}^{n+1} = s_1(\mathbf{X},\mathbf{Y}) \in D \tag{2}$$

For instance, $s_1(.)$ is defined in Alg. 1 as $\arg\max_{\mathbf{x}\in D}\mathbb{E}[(\min(Y(\mathbf{X})) - Y(\mathbf{x}))^+ | Y(\mathbf{X}) = \mathbf{Y}]$. Back to the notations of the previous section , one can similarly define a fonction $s_j(.) : (D\times\mathbb{R})^{n_0+j-1} \longrightarrow D$ for all $j \in [2,r]$.

**Definition 1.** We call *deterministic strategy with horizon r* ($r \in \mathbb{N}^*$) any finite sequence $\mathscr{S} = (s_j)_{j\in[1,r]}$ of measurable functions $s_j(.) : (D\times\mathbb{R})^{n_0+j-1} \longrightarrow D$ ($j \in [1,r]$), and denote by $\mathbb{S}_r$ the space of such $\mathscr{S}$.

In Alg. 1, the $s'_j s$ are implicitely taken as $\arg\max_{\mathbf{x}\in D}\mathbb{E}[I(\mathbf{x})|\mathbf{X}^{j-1}, Y(\mathbf{X}^{j-1})]$ for all $j \in [2,r]$, where $\mathbf{X}^{j-1} = \mathbf{X}^0 \cup \{\mathbf{x}^{n_0+1},\dots,\mathbf{x}^{n_0+j-1}\}$ and $\mathbf{Y}^{j-1} = Y(\mathbf{X}^{j-1})$ denote the augmented design and vector of observations. Hence the only changes in the criteria of such EI algorithm is the updated information. We now consider strategies with a broader generality, where the $s'_j s$ may be subject to structural changes at each iteration.

*After the r function evaluations*, it is possible to evaluate the success of $\mathscr{S} \in \mathbb{S}_r$ by comparing the best response at the initial state, $m_0 := \min(y(\mathbf{X}^0))$ with the best response observed during the additional runs,

$$m_{1:r} := \min(y(\mathbf{x}^{n_0+1}),\dots,y(\mathbf{x}^{n_0+r})). \tag{3}$$

The corresponding performance measure can be written in terms of multipoints improvement [6, 5, 1]:

**Definition 2.** The (*a posteriori*) improvement of $\mathscr{S} \in \mathbb{S}_r$ seen from the initial state is defined as

$$i^0(\mathscr{S}) := (m_0 - m_{1:r})^+ = (m_0 - \min(y(s_1(\mathbf{X}^0,\mathbf{Y}^0)),\dots,y(s_r(\mathbf{X}^{r-1},\mathbf{Y}^{r-1}))))^+ \tag{4}$$

Similarly, the random variable $I^0(\mathscr{S}) = (\min(Y(\mathbf{X}^0)) - \min(Y(\mathbf{x}^{n_0+1}),\dots,Y(\mathbf{x}^{n_0+r})))^+$ denotes the improvement at the points $(\mathbf{x}^{n_0+1},\dots,\mathbf{x}^{n_0+r})$, where $y$ is replaced by the process $Y$. More generally, $i^j(\mathscr{S})$ and $I^j(\mathscr{S})$ $(1 \le j \le r)$ refer to the same objects with $\mathbf{X}^0$ replaced by $\mathbf{X}^j$ in $\min(y(\mathbf{X}^0))$ and $\min(Y(\mathbf{X}^0))$.

Our purpose here is to find strategies that produce the largest possible *a posteriori* improvement in a given number of iterations. In other words, we are looking for the $s_1^*,\dots,s_r^*$ that maximize the improvement of eq. 4. However, evaluating $i(\mathscr{S})$ obviously requires already knowing $\mathbf{X}^r$ and $\mathbf{Y}^r$, i.e. being at the end of the algorithm. So we need a criterion that takes a strategy $\mathscr{S} = (s_j)_{j\in[1,r]}$ as argument while not explicitly depending on the design points and response values to be observed during the algorithm. This is what we will propose in the next subsection with the adaptation of the *Expected Improvement* criterion to *sequential strategies*. Let us first recall a few measurability results and introduce some additional notations.

## 2.2 Expected Improvement of a sequential strategy

### 2.2.1 Measurability with respect to a random variable.

We now consider two arbitrary real random variables $X$ and $Y$ defined over the same probability space $(\Omega, \mathscr{F}, \mathbb{P})$. $\sigma(X)$ denotes the sub-$\sigma$-field of $\mathscr{F}$ generated by $X$. Let us recall that $\sigma(X)$ is the sub-$\sigma$-field $X^{-1}(\mathscr{B}(\mathbb{R}))$ of $\mathscr{F}$ generated by all events of the kind $X^{-1}(B) := \{\omega \in \Omega | X(\omega) \in B\}$, where $B \in \mathscr{B}(\mathbb{R})$.

**Definition 3.** $Y$ is said $\sigma(X)$-mesurable (or more simply $X$-mesurable) when $\sigma(Y) \subset \sigma(X)$

In essence, saying that $Y$ is $\sigma(X)$-mesurable amounts to saying that knowing the realization $X(\omega)$ specifies enough the state $\omega \in \Omega$ to be able for the observer to deduce $Y(\omega)$. $Y$ can then been seen as a function of $X$:

**Theorem 1.** *(see e.g. [8]) $Y$ is measurable with respect to $\sigma(X)$ if and only if there exists some measurable function $f : (\mathbb{R}, \mathscr{B}(\mathbb{R})) \to (\mathbb{R}, \mathscr{B}(\mathbb{R}))$ such that $Y = f(X)$.*

### 2.2.2 Expected Improvement of a strategy in finite time, and the associated optimality problem

**More notations:** we already know that $(\mathbf{X}^0, \mathbf{Y}^0)$ denotes the initial design and observation vectors, and that the $\mathbf{x}^{n_0+j}$ $(j \in [1,r])$ are the points visited within the considered strategy. Similarly, $\mathbf{X}^{n_0+j}$ and $\mathbf{Y}^{n_0+j}$ denote the initial design and observation vectors respectively augmented by the $\mathbf{x}^{n_0+i}$ and $y(\mathbf{x}^{n_0+i})$ $(1 \leq i \leq j,\ j \in [1,r])$. Note that all these quantities are deterministic from the point of view of an observer having collected information at or after the $j^{th}$ iteration. We now propose additional notations and details for the case where the latter are seen from the past of iteration $j$, and hence inherits from an epistemic random nature:

The $\mathscr{X}^{n_0+j}$'s denote the random variables corresponding to the $\mathbf{x}^{n_0+j}$'s $(j \in [1,r])$, and $\mathbb{X}^{n_0+j} = \mathbf{X}^0 \cup \{\mathscr{X}^{n_0+1}, \ldots, \mathscr{X}^{n_0+j}\}$ the random design corresponding to $\mathbf{X}^{n_0+j}$ with known initial design $\mathbf{X}^{n_0}$. Similarly, $\mathbb{Y}^{n_0+j} = \mathbf{Y}^0 \cup \{Y(\mathscr{X}^{n_0+1}), \ldots, Y(\mathscr{X}^{n_0+j})\}$ denotes the random vector corresponding to $\mathbf{Y}^{n_0+j}$.

In a purely deterministic strategy $\mathscr{S}$ as considered here, $\mathscr{X}^{n_0+1} = s_1(\mathbf{X}^0, \mathbf{Y}^0)$ is in fact non-random. However, $\mathscr{X}^{n_0+2} = s_2(\mathbb{X}^1, \mathbb{Y}^1)$ is random, and is more precisely a $\sigma(Y(\mathbf{X}^{n_0+1}))$- or $\sigma(\mathbb{Y}^1)$-mesurable random variable. More generally, each $\mathscr{X}^{n_0+j}$ is clearly a $\sigma(\mathbb{Y}^{j-1})$-mesurable random variable for the same reason.

Finally, let $A_0 = \{\mathbb{X}^0 = \mathbf{X}^0, Y(\mathbf{X}^0) = \mathbf{Y}^0\}$ denote the information available at the initial state of the strategy, and $A_j = \{\mathbb{X}^j = \mathbf{X}^j, Y(\mathbf{X}^j) = \mathbf{Y}^j\}$ $(1 \leq j \leq r)$ stand for the information available at the $j^{th}$ iteration, i.e. right after the calculation of $\mathscr{X}^{n_0+j}$ and the evaluation of $y$ at this point.

**Definition 4.** The Expected Improvement of a strategy $\mathscr{S} = (s_j)_{j \in [1,r]}$ seen from its initial state is given by

$$\begin{aligned} EI^0(\mathscr{S}) :&= \mathbb{E}\left[(\min(Y(\mathbf{X}^0)) - \min(Y(s_1(\mathbf{X}^0, \mathbf{Y}^0)), Y(s_2(\mathbb{X}^1, \mathbb{Y}^1)), \ldots, Y(s_r(\mathbb{X}^{r-1}, \mathbb{Y}^{r-1}))))^+ | A_0\right] \\ &= \mathbb{E}\left[I^0(s_1(\mathbf{X}^0, \mathbf{Y}^0), s_2(\mathbb{X}^1, \mathbb{Y}^1), \ldots, s_r(\mathbb{X}^{r-1}, \mathbb{Y}^{r-1})) | A_0\right], \end{aligned} \tag{5}$$

**Definition 5.** We denote by $\mathscr{P}_r$ the problem: find $\mathscr{S}_r^* = (s_j^*)_{j \in [1,r]}$ maximizing $EI^0$.

# 3 Towards deriving the optimal strategy in finite time

## 3.1 Main results

We restrict ourselves here to the case where $D$ is a compact subset of $\mathbb{R}^d$, and assume for convenience that each considered $\mathbb{E}[I^j(\mathbf{x},\ldots)|A_j]$ $(0 \leq j \leq r)$ possesses one unique global maximizer over $D$. This working hypothesis grossly means that the possible symmetries have been taken into account, and that there is enough expected improvement in the vicinity of the current DoE not to be damned to explore $D$ far away from the observation points, where the predictions are all close to each other (in the case of $1^{st}$ order stationarity). Let us first write a trivial property of strategies with horizon 1 which will nevertheless be crucial in the sequel:

**Lemma 1.** *The solution of $\mathscr{P}_1$ is given by $s_1^*(\mathbf{X}^0,\mathbf{Y}^0) = \arg\max_{\mathbf{x}\in D}\mathbb{E}[I^0(\mathbf{x})|A_0]$.*

*Proof.* Directly follows from the definition of $\mathscr{P}_1$.

**Lemma 2.** $\forall (a,b,c)\in\mathbb{R}^3,\ (a-min(b,c))^+ = (a-b)^+ + (min(a,b)-c)^+$.

*Proof.* If $a = min(a,b,c)$, then both left and right terms are 0. If $b = min(a,b,c)$, both terms equal $(a-b)$ since $min(b,c) = b$ and $(min(a,b)-c)^+ = 0$. Finally, if $c = min(a,b,c)$, the left term equals $(a-c)$ and the right one equals $0+(a-c)$ if $b \geq a$ and $(a-b)+(b-c) = (a-c)$ else. □

**Theorem 2.** *In $\mathscr{P}_r$, choosing $\mathbf{x}^{n_0+r}$ after $r-1$ iterations amounts to maximizing $\mathbb{E}[I^{r-1}(.)|A_{r-1}]$*

*Proof.* After $r-1$ iterations, $\{\mathbf{X}^{r-1},\mathbf{Y}^{r-1}\}$ is known, and the maximization of $EI$ over $\mathbb{S}_r$ reduces to a simpler problem over $\mathbb{S}_1$. Noting $M_0 = \min(Y(\mathbf{X}^0))$ and $M_{1:r-1} = \min(Y(\mathbf{x}^{n_0+1}),\ldots,Y(\mathbf{x}^{n_0+r-1}))$, we have:

$$\begin{aligned}\mathbf{x}^{n_0+r} &= \arg\max_{\mathbf{x}\in D}\mathbb{E}[(M_0-\min(Y(\mathbf{x}^{n_0+1}),\ldots,Y(\mathbf{x}^{n_0+r-1}),Y(\mathbf{x})))^+|A_{r-1}]\\ &= \arg\max_{\mathbf{x}\in D}\mathbb{E}[(M_0-\min(M_{1:r-1},Y(\mathbf{x})))^+|A_{r-1}]\end{aligned} \tag{6}$$

We then use lemma 2 with $a = \min(Y(\mathbf{X}^0))$, $b = M_{1:r-1}$, $c = Y(\mathbf{x})$ and get:

$$\begin{aligned}\mathbb{E}[(M_0-\min(M_{1:r-1},Y(\mathbf{x})))^+|A_{r-1}] &= \mathbb{E}[(M_0-M_{1:r-1})^+ + (\min(Y(\mathbf{X}^0),M_{1:r-1})-Y(\mathbf{x}))^+|A_{r-1}]\\ &= (M_0-M_{1:r-1})^+ + \mathbb{E}[I^{r-1}(\mathbf{x})|A_{r-1}]\end{aligned} \tag{7}$$

Since $(M_0-M_{1:r-1})^+$ doesn't depend on $\mathbf{x}$, maximizing the left term or $\mathbb{E}[I^{r-1}(\mathbf{x})|A_{r-1}]$ are equivalent. □

**Theorem 3.** *The solution $\mathscr{S}^* = (s_1^*,\ldots,s_r^*)$ of $\mathscr{P}_r$ is given by the following recursion:*

$$\begin{cases}\mathbf{x}^{n_0+r} = s_r^*(\mathbf{X}^{r-1},\mathbf{Y}^{r-1}) = \arg\max_{\mathbf{x}\in D}\mathbb{E}[I^{r-1}(\mathbf{x})|A_{r-1}]\\ \mathbf{x}^{n_0+r-1} = s_{r-1}^*(\mathbf{X}^{r-2},\mathbf{Y}^{r-2}) = \arg\max_{\mathbf{x}\in D}\mathbb{E}[I^{r-2}(\mathbf{x},s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x})))|A_{r-2}]\\ \ldots\\ \mathbf{x}^{n_0+1} = s_1^*(\mathbf{X}^0,\mathbf{Y}^0) = \arg\max_{\mathbf{x}\in D}\mathbb{E}[I^0(\mathbf{x},s_1^*(\mathbb{X}^1(\mathbf{x}),\mathbb{Y}^1(\mathbf{x})),\ldots,s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x})))|A_0]\end{cases}$$

*Proof.* The first equality directly follows from theorem 2. Now, the point $\mathbf{x}^{n_0+r-1}$ is obtained after observation of $\mathbf{X}^{r-1}, \mathbf{Y}^{r-1}$ by maximizing the overall criterion

$$\begin{aligned}&\mathbb{E}\left[(M_0 - \min(Y(\mathscr{X}^{n_0+1}),\ldots,Y(\mathscr{X}^{n_0+r-2}),Y(\mathbf{x}),Y(\mathscr{X}^{n_0+r}))^+|A_{r-2}\right]\\ =&\mathbb{E}\left[(m_0 - \min(y(\mathbf{x}^{n_0+1}),\ldots,y(\mathbf{x}^{n_0+r-2}),Y(\mathbf{x}),Y(s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x}))))^+|A_{r-2}\right]\end{aligned}$$

where the equality is due to the facts that $\mathscr{X}^{n_0+j}$ and $Y(\mathscr{X}^{n_0+j})$ $(1 \leq j \leq r-2)$ are known conditional on $A_{r-2}$, and $\mathscr{X}^{n_0+r} = s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x}))$ by the last result. Applying again lemma 2 with $a = m_0$, $b = m_{1:r-2}$, $c = \min\left(Y(\mathbf{x}),Y(s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x})))\right)$ leads to maximizing $\mathbb{E}[I^{r-2}(\mathbf{x},s_r^*(\mathbb{X}^{r-1}(\mathbf{x}),\mathbb{Y}^{r-1}(\mathbf{x})))|A_{r-2}]$. The remaining points are similarly determined by backward induction.

### 3.2 Example: decomposing the $EI$ of a two-iterations strategy

We consider for convenience a family of elementary 2-iterations strategies $\mathscr{S}(\mathbf{a})$ $(\mathbf{a} \in D)$ defined as follows:

$$\mathscr{S}(\mathbf{a}) = \text{"choose } \mathbf{a} \text{ at the first iteration, and then maximize the 1-point } EI\text{"} \tag{8}$$

Our purpose is to show that in some cases, there exists a better strategy than sequentially maximizing the 1-point $EI$ like in Alg. 1. Let us develop $EI(\mathscr{S}(\mathbf{a}))$ for some fixed $\mathbf{a} \in D$. The second point is given by

$$\mathscr{X}^{n_0+2} = s_2^*(\mathbb{X}^1,\mathbb{Y}^1) = \arg\max_{\mathbf{x}\in D} \mathbb{E}\left[\left(\min(\mathbb{Y}^1) - Y(\mathbf{x})\right)^+ |A_0, Y(\mathbf{a})\right] \tag{9}$$

Lemma 2 then enables us once again to provide an interesting decomposition of the expected improvement:

$$\begin{aligned}EI(\mathscr{S}(\mathbf{a})) &= \mathbb{E}\left[\left(\min(\mathbf{Y}^0) - \min(Y(\mathbf{a}),Y(\mathscr{X}^{n_0+2}))\right)^+ |A_0\right]\\ &= \underbrace{\mathbb{E}\left[\left(\min(\mathbf{Y}^0) - Y(\mathbf{a})\right)^+ |A_0\right]}_{EI^0_{0:1}(\mathbf{a}) := EI(\mathbf{a})} + \underbrace{\mathbb{E}\left[\left(\min(\mathbb{Y}^1) - Y(\mathscr{X}^{n_0+2})\right)^+ |A_0\right]}_{EI^0_{1:2}(\mathbf{a})}\end{aligned} \tag{10}$$

The latter hence appears as the sum of the 1-point $EI$ at point $\mathbf{a}$ —denoted here by $EI^0_{0:1}(\mathbf{a})$, i.e. "the expected improvement between iteration 0 and 1, seen from the initial state"— and the expected value of the future expected improvement at $\mathscr{X}^{n_0+2}$ —similarly denoted by $EI^0_{1:2}(\mathbf{a})$. Since $EI(\mathbf{a})$ is analytically known, calculating $EI(\mathscr{S}(\mathbf{a}))$ amounts to computing the second term of this sum. Now, seen from the initial state (before evaluating $y$ at $\mathbf{a}$), $Y(\mathbf{a})$ is a random variable. Under usual assumptions of centered GP with known covariance kernel, the law of $Y(\mathbf{a})$ conditional on $A_0$ is well known and sends back to the results:

$$Y(\mathbf{a})|A_0 \sim \mathscr{N}\left(m_0(\mathbf{a}), s_0^2(\mathbf{a})\right), \tag{11}$$

where the Simple Kriging equations [4] write $\begin{cases} m_0(\mathbf{a}) := \mathbf{k}_0^T(\mathbf{a})\mathbf{K}_0^{-1}\mathbf{Y}^0 \\ s_0^2(\mathbf{a}) := k(\mathbf{a},\mathbf{a}) - \mathbf{k}_0(\mathbf{a})^T\mathbf{K}_0^{-1}\mathbf{k}_0(\mathbf{a}) \end{cases}$

Using the law of total expectation (See [8] for details) and conditional simulations based on eq. 11 will finally allow us to compute the term $EI^0_{1:2}(\mathbf{a})$ by Monte-Carlo in the next subsection.

### *3.3 Numerical application*

Back to the framework of *example* 1, $EI^0(\mathscr{S}(\mathbf{a}))$ is computed for the boundary point $\mathbf{a}=1$ and compared to the $EI$ value obtained with two iterations of Alg. 1 (i.e. maximizing twice the regular $EI$). As detailed in Alg. 3.3, the computation of $EI^0_{1:2}(\mathbf{a})$ is based on the following:

$$EI^0_{1:2}(\mathbf{a}) \approx \frac{1}{m}\sum_{i=1}^{m} \mathbb{E}\left[\left(\min(\mathbb{Y}^1(\mathbf{a})) - Y(\mathscr{X}^{n_0+2}(\mathbf{a}))\right)^+ \middle| A_0, Y(\mathbf{a}) = y_a^i\right] \tag{12}$$

where the $y_a^i \sim \mathscr{N}(m_0(\mathbf{a}), s_0^2(\mathbf{a}))$ are independently drawn ($1 \leq i \leq m$). Figure 2 sums up the results obtained by running Alg. 3.3 with $m=100$, with both $\mathbf{a}=1$ and $\mathbf{a}$ fixed to the maximizer of the 1-point $EI$.

**Algorithm 2** Computation of $EI(\mathscr{S}(\mathbf{a}))$ by Monte-Carlo

**function** $\widehat{EI}(\mathbf{X}, \mathbf{Y}, \mathbf{a}, m)$
  $EI_1^0 = \mathbb{E}\left[I^0(\mathbf{a})|A_0\right]$
  $\mathbf{X}^1 = \mathbf{X}^0 \cup \{\mathbf{a}\}$
  **for** $j \leftarrow 1, m$ **do**
    $y_{sim} \sim \mathscr{N}\left(m_0(\mathbf{a}), s_0^2(\mathbf{a})\right)$
    $\mathbf{Y}^1 = \mathbf{Y}^0 \cup \{y_{sim}\}$
    $\mathbf{x}_{sim}^{n_0+2} = \arg\max_{\mathbf{x}\in D}\left\{\mathbb{E}\left[I^1(\mathbf{x})|A_1\right]\right\}$
    $v_j = \mathbb{E}\left[I^1(\mathbf{x}_{sim}^{n_0+2})\middle|A_1\right]$
  **end for**
  **return** $\widehat{EI^0_{1:2}} = EI_1^0 + \frac{1}{m}\sum_{j=1}^m v_j$
**end function**

The highest expected improvement —and especially the median value— obtained with $\mathbf{a}=1$ supports the belief that maximizing $EI$ at each iteration is not (always) the best thing to do in a sequential strategy with fixed horizon. In this particular example, this phenomenon seems due to the good delayed payoff associated with sampling at $\mathbf{a}=1$. Indeed, evaluating $y$ there at the first iteration leaves room to explore the most interesting zone with a little bit more information at iteration 2 than what we initially had. In the straightforward strategy however, one greedily visits the main bump of the 1-points $EI$ at the first iteration and then almost systematically sample $y$ at the boundary point during the second shot (See fig. 2, upper left).

## 4 Conclusion and perspectives

The results presented in this paper extend the field of pertinence of the *multipoints expected improvement* to the framework of optimization strategies with finite time horizon. Thanks to an adequate modeling of the future points and associated observations in terms of random variables, the latter criterion is used to derive the sequence of decisions to be made during the optimal algorithm for any fixed horizon. It is in particular illustrated on the basis of a dedicated example that the classical $EI$ algorithm is suboptimal, and that the strategic value of a point can be decomposed as sum of its 1-point expected improvement plus a more delayed criterion of interest, which can be estimated by Monte-Carlo using conditional simulations.

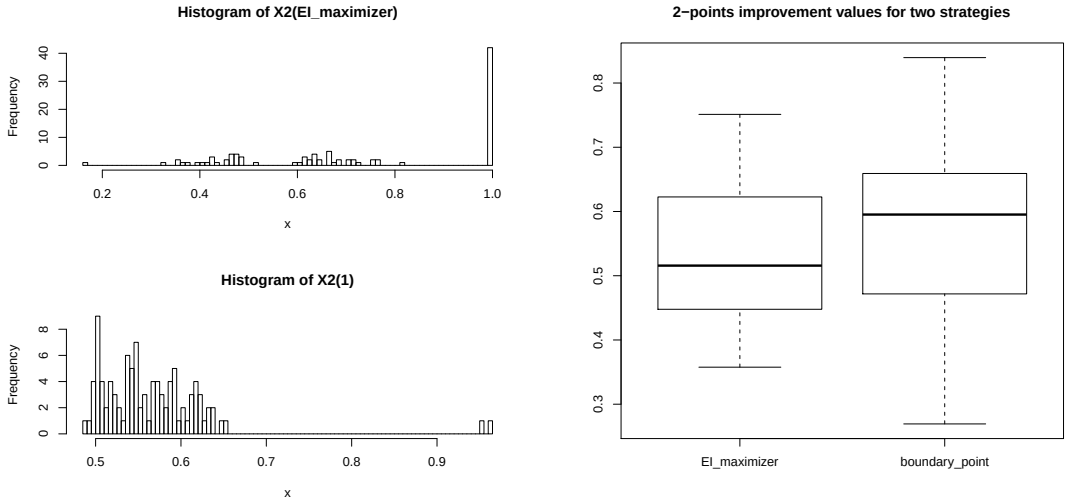


**Fig. 2** The left graphics represents the two populations of $\mathscr{X}^{n_0+2}$ points (100 each) corresponding to both strategies, and the right one compares the samples of improvement values obtained in both cases.

Perspectives include a detailed study and improvements of the latter Monte-Carlo method. Dimension reduction techniques and well-suited heuristics may be required to afford the computation of reasonable estimates for the $EI$ of a strategy with horizon $r \geq 3$. Furthermore, both large-scale practical examples and deeper connections with existing works in the field of sequential strategies, but also in control theory, are currently considered. In particular, the close (but not similarly proven nor illustred) results given in the piece of work [3] very recently discovered by the authors motivate revisting this book two decades later with both the scientific approach in fashion and the increased computation capacity for testing and implementing ideas.

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