# Towards GP-based optimization with finite time horizon

David Ginsbourger and Rodolphe Le Riche

**Abstract** During the last decade, Kriging-based sequential algorithms like EGO [5] 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 article concern sequential procedures with a fixed number of iterations. We show that maximizing the usual $EI$ criterion at each iteration 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 a new multipoints $EI$, and illustrates the suboptimality of maximizing the 1-point $EI$ at each iteration on the basis of a first counter-example.

## 1 Introduction

Gaussian Process (GP) [9] 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 in assuming that $y$ is one path of a GP $Y$. The main focus of 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 [4], the *Expected Improvement* (EI) is now one of the most popular GP-based optimization criteria:

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

David Ginsbourger
CHYN, Université de Neuchâtel, Rue Emile-Argand 11, CP 158 CH-2009 Neuchâtel, Switzerland, e-mail: david.ginsbourger@unine.ch

Rodolphe Le Riche
CNRS (UMR 5146) and Département 3MI, Ecole Nationale Supérieure des Mines, 158 cours Fauriel, Saint-Etienne, France, e-mail: leriche@emse.fr

where $I(\mathbf{x}) := (\min(Y(\mathbf{X})) - Y(\mathbf{x}))^+ = \max(0, \min(Y(\mathbf{X})) - Y(\mathbf{x}))$ 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 unvisited areas of the search space. Furthermore, $EI$ is known in closed form [5], which allows very fast evaluations and even analytical calculation of its derivatives. Such a criterion, though regularly updated by taking new data into account, is typically considered at each iteration without structural change. In fact, in $EI$ algorithms like $EGO$, the point $\mathbf{x}^{n+j}$ visited at the $j^{\text{th}}$ iteration is determined 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 [13] for details), with a unit variance and a range of $\frac{0.3}{\sqrt{3}}$. 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. Further comments can be found in the caption of fig. 1 and in section 3.2.

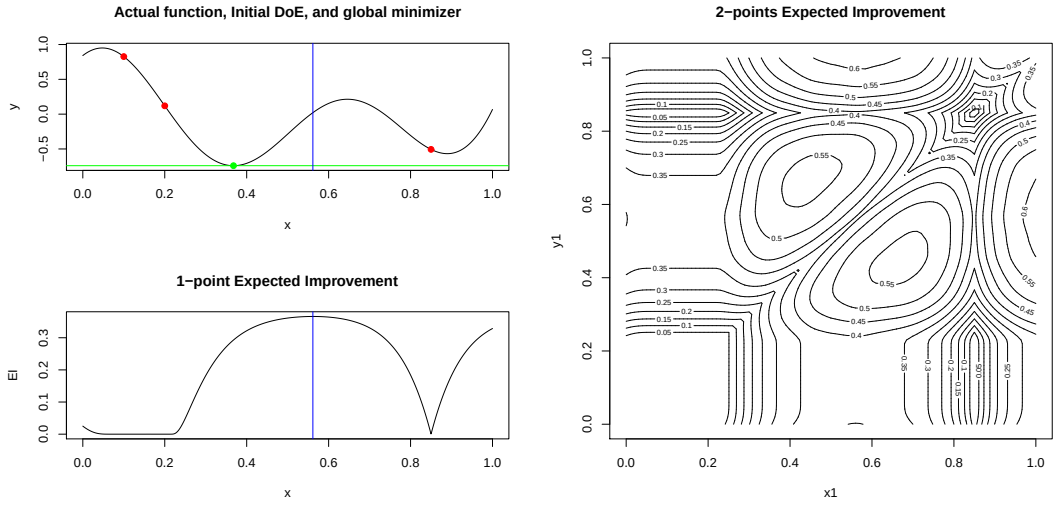


**Fig. 1** $y_1$ (upper left) with its global minimizer (in green) and the design $\mathbf{X}^0$ (in red), 1-point $EI$ and 2-points $EI$ criteria (lower left, and right) corresponding to the Kriging model of example 1. The vertical blue line shows the 1-point $EI$ maximizer, $\mathbf{x} \approx 0.57$. The maximum of the 2-points $EI$ is reached with one point as previously, and one point at the boundary point $\mathbf{x} = 1$.

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

**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 consists in looking for the next point where to evaluate $y$, say $\mathbf{x}^{n+1}$. In some sampling procedures like crude Monte Carlo, $\mathbf{x}^{n+1}$ is 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 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 defined as a 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 $\arg\max_{\mathbf{x}\in D}\mathbb{E}[I(\mathbf{x})|A_0]$. 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 $\mathbf{X}^{j-1} = \mathbf{X}^0 \cup \{\mathbf{x}^{n_0+1},\ldots,\mathbf{x}^{n_0+j-1}\}$ 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 consider here more general strategies, 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, $m_0 := \min(y(\mathbf{X}^0))$ to the best response observed during the additional runs,

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

The corresponding performance measure can be written in terms of multipoints improvement [12, 11, 4]:

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

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

Similarly, the random variable $I^0(\mathscr{S}) = (\min(Y(\mathbf{X}^0)) - \min(Y(\mathbf{x}^{n_0+1}),\ldots,Y(\mathbf{x}^{n_0+r})))^+$ denotes the improvement at the points $(\mathbf{x}^{n_0+1},\ldots,\mathbf{x}^{n_0+r})$, where $y$ is replaced by the process $Y$. More generally,

$$i^j(\mathscr{S}) := \big(m_j - m_{(j+1):r}\big)^+ = \big(\min(y(\mathbf{X}^j)) - \min(y(s_{j+1}(\mathbf{X}^j,\mathbf{Y}^j)),\ldots,y(s_r(\mathbf{X}^{r-1},\mathbf{Y}^{r-1})))\big)^+ \tag{5}$$

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 $\min(Y(\mathbf{X}^0))$, and stand for the cumulative improvement obtained between the $j^{\text{th}}$ step and the end of strategy $\mathscr{S}$.

Our purpose 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 $s_1^*,\ldots,s_r^*$ that maximize the improvement of eq. (4). However, evaluating $i^0(\mathscr{S})$ obviously requires already knowing $(\mathbf{X}^r,\mathbf{Y}^r)$, 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*.

**EI of a finite time sequential strategy**

*Additional notations:* we already know that $(\mathbf{X}^0, \mathbf{Y}^0)$ denotes the initial design and observation vectors, and that the $\mathbf{x}^{n_0+j}$'s $(j \in [1,r])$ 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 $\mathbf{x}^{n_0+i}$'s and $y(\mathbf{x}^{n_0+i})$'s $(1 \leq i \leq j,\ j \in [1,r])$. 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 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:

$\mathscr{X}^{n_0+j}$ denotes the random variable corresponding to $\mathbf{x}^{n_0+j}$ , 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 $\mathbf{X}^{n_0}$ (in all cases, $j \in [1,r]$). 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 $\mathbf{Y}^{n_0+j}$. Note that in a purely deterministic strategy $\mathscr{S}$ as considered here, $\mathscr{X}^{n_0+1} = s_1(\mathbf{X}^0, \mathbf{Y}^0)$ is 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 3.** The Expected Improvement of a strategy $\mathscr{S} = (s_j)_{j\in[1,r]}$ seen from its initial state is given by

$$EI^0(\mathscr{S}) := \mathbb{E}\left[(\min(Y(\mathbf{X}^0)) - \min(Y(s_1(\mathbf{X}^0, \mathbf{Y}^0)), Y(s_2(\mathbb{X}^1, \mathbb{Y}^1)), \ldots, Y(s_r(\mathbb{X}^{r-1}, \mathbb{Y}^{r-1}))))^+ | A_0\right] \qquad (6)$$

## 3 Towards deriving the optimal strategy in finite time

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). Under these working assumptions, we denote by $\mathscr{P}_r$ the problem: find $\mathscr{S}_r^* = (s_j^*)_{j\in[1,r]}$ maximizing $EI^0$. Let us first write a trivial property of strategies with horizon 1 which will nevertheless be useful 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 1.** *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:

$$\begin{aligned}\mathbf{x}^{n_0+r} &= \arg\max_{\mathbf{x}\in D}\mathbb{E}[(M_0-\min(Y(\mathbf{x}^{n_0+1}),\ldots,Y(\mathbf{x}^{n_0+r-1}),Y(\mathbf{x})))^+|A_{r-1}]\\ &= \arg\max_{\mathbf{x}\in D}\mathbb{E}[(M_0-\min(M_{1:(r-1)},Y(\mathbf{x})))^+|A_{r-1}]\end{aligned} \tag{7}$$

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

$$\begin{aligned}\mathbb{E}[(M_0-\min(M_{1:(r-1)},Y(\mathbf{x})))^+|A_{r-1}] &= \mathbb{E}[(M_0-M_{1:(r-1)})^+ + (\min(Y(\mathbf{X}^0),M_{1:(r-1)})-Y(\mathbf{x}))^+|A_{r-1}]\\ &= (m_0-m_{1:(r-1)})^+ + \mathbb{E}[I^{r-1}(\mathbf{x})|A_{r-1}]\end{aligned} \tag{8}$$

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. □

**Corollary 1.** *The solution $\mathscr{S}^*=(s_1^*,\ldots,s_r^*)$ of $\mathscr{P}_r$ is given by the following recursion:*

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

*Proof.* The first equality directly follows from theorem (1). 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 $Y(\mathscr{X}^{n_0+j})$ $(1\le j\le r-2)$ 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 Dynamic Programming (see theorem 5.2 of [1] for a more general result, and chapter 1 of [3] for the underlying basics).

**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:

$$\mathscr{S}(\mathbf{a}) = \text{"choose } \mathbf{a} \text{ at the first iteration, and then maximize the 1-point } EI\text{"} \tag{9}$$

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

$$\mathscr{X}^{n_0+2} = s_2^*(\mathbb{X}^1, \mathbb{Y}^1) = \arg\max_{\mathbf{x}\in D} \mathbb{E}\left[\left(\min(\mathbb{Y}^1) - Y(\mathbf{x})\right)^+ | A_0, Y(\mathbf{a})\right] \tag{10}$$

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

$$\begin{aligned} EI^0(\mathscr{S}(\mathbf{a})) &= \mathbb{E}\left[\left(\min(\mathbf{Y}^0) - \min(Y(\mathbf{a}), Y(\mathscr{X}^{n_0+2}))\right)^+ | A_0\right] \\ &= \underbrace{\mathbb{E}\left[\left(\min(\mathbf{Y}^0) - Y(\mathbf{a})\right)^+ | A_0\right]}_{EI^0_{0:1}(\mathbf{a}) := EI(\mathbf{a})} + \underbrace{\mathbb{E}\left[\left(\min(\mathbb{Y}^1) - Y(\mathscr{X}^{n_0+2})\right)^+ | A_0\right]}_{EI^0_{1:2}(\mathbf{a})} \end{aligned} \tag{11}$$

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 kernel, the law of $Y(\mathbf{a})$ conditional on $A_0$ is well known [9] and sends back to the results of Simple Kriging:

$$Y(\mathbf{a})|A_0 \sim \mathscr{N}\left(m_0(\mathbf{a}), s_0^2(\mathbf{a})\right), \text{ where } \begin{cases} m_0(\mathbf{a}) := \mathbf{k}_0^T(\mathbf{a})\mathbf{K}_0^{-1}\mathbf{Y}^0 \\ s_0^2(\mathbf{a}) := k(\mathbf{a},\mathbf{a}) - \mathbf{k}_0(\mathbf{a})^T\mathbf{K}_0^{-1}\mathbf{k}_0(\mathbf{a}) \end{cases} \tag{12}$$

Using the law of total expectation (See [14] for details) and conditional simulations based on eq. (12) will finally allow us to compute the term $EI^0_{1:2}(\mathbf{a})$ by Monte-Carlo in the forthcoming numerical application.

**Algorithm 2** Computation of $EI^0(\mathscr{S}(\mathbf{a}))$ by Monte-Carlo

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

**Numerical application.** Back to *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. (2), the computation of $EI^0_{1:2}(\mathbf{a})$ is based on the following:

$$EI^0_{1:2}(\mathbf{a}) \approx \frac{1}{m}\sum_{i=1}^m \mathbb{E}\left[\left(\min(\mathbb{Y}^1(\mathbf{a})) - Y(\mathscr{X}^{n_0+2}(\mathbf{a}))\right)^+ | A_0, Y(\mathbf{a}) = y_a^i\right] \tag{13}$$

where the $y_a^i$ ($1 \le i \le m$) are independently drawn following $\mathscr{N}(m_0(\mathbf{a}), s_0^2(\mathbf{a}))$. Figure 2 sums up the results obtained by running Alg. (2) with $m = 1000$, with both $\mathbf{a} = 1$ and $\mathbf{a}$ fixed to the maximizer of the 1-point $EI$.

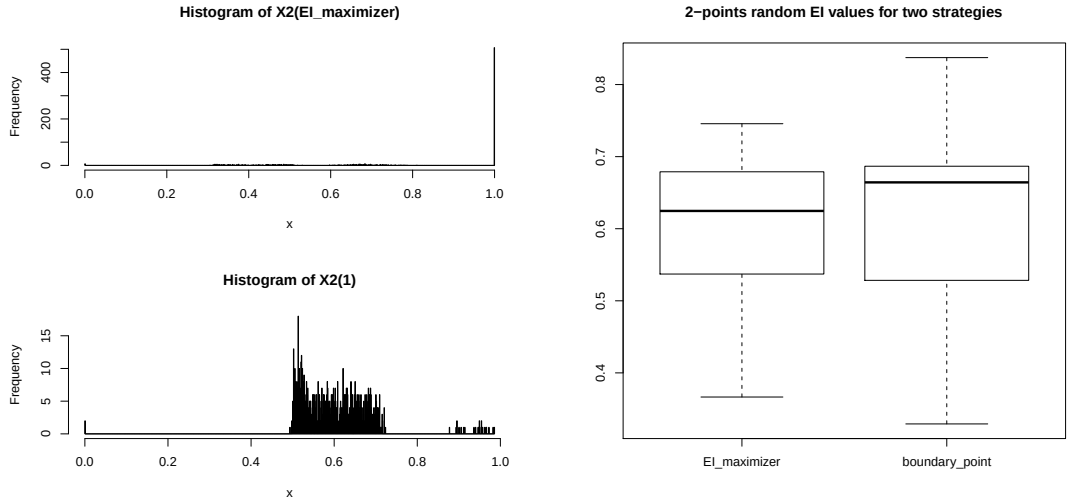


**Fig. 2** The left graphics represents the two populations of $\mathscr{X}^{n_0+2}$ points (1000 each) corresponding to both strategies, and the right one compares the samples of improvement values, $i^0(\mathscr{S})$ (from eq. (4)), obtained in both cases.

We compared the estimates $\widehat{EI^0}$ obtained for the two strategies by means of a Welch t-test —using the *t.test* function of the *stats* R package [8]. With respective estimates of 0.6061772 and 0.6132014 for the means, the second corresponding to $\mathbf{a} = 1$, the t-test with alternative hypothesis "the true difference in means is less than 0" returned a p-value of 0.05611 (with $t = -1.5891$ and $df = 1847.001$).

The slightly higher expected improvement hence 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, the 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 samples $y$ at the boundary point $\mathbf{x} = 1$ during the second shot (See fig. (2), upper left).

**Computational cost of finite horizon strategies.** As seen in the previous application, computing the expected improvement of a strategy is already an issue: $m^2$ simulations needed for a 2-step strategy (only $m$ with the trick of using the analytical EI at the last step), $m$ EI maximizations, not to mention the $m$ Kriging model updates and other auxiliary computation costs. Similarly, a naive extension of this computation scheme to strategies with horizon $r \geq 3$ would cost to the order of $m^r$ operations, hence exponentially increasing with the number of steps. This is one instance of Bellman's famous *curse of dimensionality* [2]. Now, deriving the optimal strategy is even worse: not only is the computation time exponentially increasing in $m$, but it is also exponentially increasing in the time needed to optimize one-point criteria. Concretely, considering for pedagogical purposes an exhaustive maximization of the $EI$'s and $EI(\mathscr{S}(\mathbf{a}))$'s over a $p$-points grid, finding the optimal strategy (without analytical formula for the last EI) costs $p \times m \times (p-1) \times m$ improvement computations, which becomes $A_p^r m^r$ in the case of a general horizon $1 \leq r \leq p-1$. It is then clear that finding the optimal strategy by such a direct method is limited to an horizon of 2 or 3, and only makes sense in the case of very costly objective functions, for which the optimal strategy is likely to bring a

higher improvement than would do the same computation time invested in some additional evaluations of $y$. However, 2- or 3-steps optimal strategies might remain attractive in the following potential applications:

- Sequential evaluations of $y$ with consecutive blocs of 2-steps optimal strategies
- Sequential-parallel evaluations of $y$ with consecutive blocs of $q \in 2\mathbb{N}$ points, each bloc of two $q$-points designs being optimal in the sense of a 2-steps strategy (the second designs maximizing the $q$-EI of [4]).

## 4 Conclusion and perspectives

The results presented in this paper extend the *multipoints expected improvement* to optimization strategies with finite time horizons. Thanks to an adequate modeling of the future points and associated observations in terms of random variables, the latter criterion is proposed and analyzed to derive the sequence of decisions to be made by the optimal fixed horizon algorithm, obtained by dynamic programming. It is in particular illustrated on the basis of a dedicated example that the classical $EI$ algorithm is suboptimal. To this end, the strategic value of a point is decomposed as the sum of its one-point expected improvement plus a delayed payoff, which can be estimated by Monte-Carlo based on gaussian process conditional simulations.

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 and approximate dynamic programming [7], are currently considered. In particular, the close (but not similarly proven nor illustred) results given in [6] very recently discovered by the authors, motivate revisting this book two decades later with the contemporary scientific approach and the increased computation capacity.

**Aknowledgements:** This work was funded by the *Optimisation Multi-Disciplinaire* (OMD) project of the French Research Agency (ANR). The authors would like to thank Julien Bect (Ecole Supérieure d'Electricité) for providing them with the neighbouring results published by Jonas Mockus [6].

## References

1. A. Auger and O. Teytaud. Continuous lunches are free plus the design of optimal optimization algorithms. *Algorithmica*.
2. R. Bellman. *Dynamic Programming*. Princeton University Press, Princeton, 1957.
3. D.P. Bertsekas. *Dynamic Programming and Optimal Control, Vol. 1*. Athena Scientific, Belmont, MA, 2007.
4. D. Ginsbourger, R. Le Riche, and L. Carraro. *Computational Intelligence in Expensive Optimization Problems*, chapter "Kriging is well-suited to parallelize optimization". Studies in Evolutionary Learning and Optimization. Springer-Verlag.
5. D.R. Jones, M. Schonlau, and W.J. Welch. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13:455–492, 1998.
6. J. Mockus. *Bayesian Approach to Global Optimization*. Kluwer academic publishers, 1988.
7. W.B. Powell. *Approximate Dynamic Programming. Solving the Curses of Dimensionality*. Wiley, 2007.
8. R Development Core Team. R: A language and environment for statistical computing, 2006.
9. C.E. Rasmussen and K.I. Williams. *Gaussian Processes for Machine Learning*. M.I.T. Press, 2006.
10. B.D. Ripley. *Stochastic Simulation*. John Wiley and Sons, New York, 1987.
11. T.J. Santner, B.J. Williams, and W.J. Notz. *The Design and Analysis of Computer Experiments*. Springer, 2003.
12. M. Schonlau. *Computer Experiments and Global Optimization*. PhD thesis, University of Waterloo, 1997.
13. M.L. Stein. *Interpolation of Spatial Data, Some Theory for Kriging*. Springer, 1999.
14. D. Williams. *Probability with Martingales*. Cambridge University Press, 1991.