ABSTRACT

Black-box and preference-based optimization algorithms are global optimization procedures that aim to find the global solutions of an optimization problem using, respectively, the least amount of function evaluations or sample comparisons as possible. In the black-box case, the analytical expression of the objective function is unknown and it can only be evaluated through a (costly) computer simulation or an experiment. In the preference-based case, the objective function is still unknown but it corresponds to the subjective criterion of an individual. So, it is not possible to quantify such criterion in a reliable and consistent way. Therefore, preference-based optimization algorithms seek global solutions using only comparisons between couples of different samples, for which a human decision-maker indicates which of the two is preferred. Quite often, the black-box and preference-based frameworks are covered separately and are handled using different techniques. In this paper, we show that black-box and preference-based optimization problems are closely related and can be solved using the same family of approaches, namely surrogate-based methods. Moreover, we propose the generalized Metric Response Surface (gMRS) algorithm, an optimization scheme that is a generalization of the popular MSRS framework. Finally, we provide a convergence proof for the proposed optimization method.

Keywords  Global optimization, Black-box optimization, Preference-based optimization, Bayesian optimization.

1 Introduction

In many applications there is the need to find the “optimal” value for a decision variable, i.e. the one that maximizes a measure of performance, minimizes some cost or best satisfies a human decision-maker’s criterion. For instance, in the context of control systems, we might be interested in tuning the parameters of a controller to achieve some desired performance. However, in some cases, it might be impossible to objectively quantify the “goodness” of a certain decision variable. For instance, an evaluation of a controller performance might depend on a human operator, that expresses a judgement through visual inspection (or other sensory evaluations) of the behavior achieved by the system under control. These optimization problems can be stated as: find the global solution of an optimization problem whose objective function can either be: (i) completely known (i.e. its analytical expression is available), (ii) unknown but measurable or (iii) unknown and not objectively quantifiable. Further complications arise if the evaluation of the objective function is expensive, i.e. a non-negligible amount of resources needs to be spent to assess the “goodness” of a
decision variable (for instance, its measure might require running a time-expensive computer simulation or performing experiments on a real system). Depending on (i) the knowledge available on the objective function, as well as (ii) how easy it is to acquire information on it, different optimization frameworks should be employed, see Figure 1.

Whenever the objective function is known or is quite cheap to evaluate, it is best to employ global optimization techniques, that can either be derivative-based [26] or derivative-free [31]. In the first case, it is possible to combine a derivative-based local search algorithm with a multi-start method [24] to reach the global solution. Instead, derivative-free techniques are quite useful whenever the objective function is not differentiable or if the derivative information is unreliable (e.g. if it is obtained by finite differentiation of noisy measures). Some popular derivative-free algorithms are DIvide a hyper-RECTangle (DIRECT) [21], Particle Swarm Optimization (PSWARM) [35] and evolutionary algorithms [18].

The main drawback of the aforementioned techniques is the often excessive number of function evaluations required to find the global solution. This could be quite prohibitive when the objective function is unknown and expensive to measure. When that is the case, a better suited class of algorithms are black-box optimization techniques [11], which aim to both minimize the number of function evaluations and obtain the global optimizer. A family of procedures within such framework is called surrogate-based (or surface response) methods. These algorithms aim to both approximate the unknown objective function, using a so-called surrogate model, and explore the domain of the decision variable sufficiently enough to converge to the global solution. In practice, such methods iteratively propose new samples to be evaluated by properly trading-off exploitation (local search) and exploration (global search). This is done by defining a suitable acquisition function and the next candidate sample is obtained by minimizing or maximizing it. Some good and extensive surveys on the topic are [36] [20]. The most popular surface response methods either approximate the black-box function using Gaussian Processes, giving rise to Bayesian Optimization [6], or through Radial Basis Functions, see for example the algorithm proposed by Gutmann [Gutmann-RBF] [16]. Constrained Optimization using Response Surfaces (CORS) [29], Metric Stochastic Response Surface Method (MSRS) [30] and the more recent GLobal minimum using Inverse distance weighting and Surrogate radial basis functions (GLIS) [2].

When the objective function can only be evaluated subjectively, or rather it describes a human decision-maker’s criterion that cannot be expressed analytically, a possible way to solve the optimization problem consists of iteratively asking the user to compare couples of different samples, expressing preferences between them. All the information that concerns the tastes of an individual is encapsulated in a preference relation, which describes the outcomes of the comparisons. There exist many fundamental results in utility theory that, under some hypotheses, allow us to represent the preference relation with a (latent) utility function [27], i.e. a function that assigns an abstract degree of “goodness” to all possible values of the decision variable. In this case, the best sample for a human decision-maker is the one that has the highest utility. To find the maximizer of the utility function, it is possible to use (active) preference-based optimization algorithms (sometimes referred to as active preference learning) [2], which also aim to minimize the number of pairwise comparisons. Surface response methods for preference-based optimization build a surrogate model for the latent utility function using the preferences expressed by the individual. Similarly to the black-box case, a suitable acquisition function needs to be defined in order to find the next candidate sample to evaluate. Most preference-based

[2] We want to make a clear distinction between preference learning and preference-based optimization. The former aims to approximate the latent utility function [14] with a predictive model, as commonly done in machine learning. Instead, the latter aims to find the global optimizer of an optimization problem using only the information brought by the preferences. In practice, many preference-based optimization methods still use a predictive model, yet its prediction accuracy is not the main concern.
optimization algorithms are extensions of Bayesian Optimization, see for example [7, 15, 4]. Quite recently, the authors of [2] proposed an extension of GLIS in the preference-based framework, called GLISp [3], that is based on a radial basis function surrogate.

Global, black-box and preference-based optimization are often treated separately in the literature. Moreover, a unified view for the resolution of these optimization problems has not yet been proposed. In this paper, we show how black-box and preference-based frameworks can be seen as particular cases of global optimization, since they all aim to find the global solution of an optimization problem. At the same time, preference-based optimization can be interpreted as an instance of black-box optimization, where the objective function is both unknown (black-box) and cannot be measured explicitly. Considering preference-based optimization as a specific case of black-box optimization can ease the definition of new algorithms for the former framework. Moreover, results and techniques applied for black-box procedures can be carried over to preference-based ones. The main contributions of this work are:

1. Provide a thorough comparison of black-box and preference-based optimization, highlighting key similarities and differences, and show that, from an utility theory perspective, they both aim to solve the same optimization problem;
2. Propose a general surrogate-based optimization scheme that can be applied to both black-box and preference-based frameworks;
3. Provide a proof of convergence for such surrogate-based scheme. Notably, it is possible to prove the convergence in the preference-based case by leveraging results from the global optimization literature and the utility theory framework.

The paper is organized as follows. Section 2 introduces and compares the black-box and preference-based optimization problems. Section 3 describes two popular surrogate models, based on Radial Basis Functions and Gaussian Processes. Section 4 proposes an acquisition function suited for both black-box and preference-based optimization, while Section 5 provides a general surrogate-based optimization scheme, based on the proposed acquisition function. Its convergence is proven both in the black-box and preference-based frameworks. An example of the proposed optimization scheme is shown in Section 6. Finally, Section 7 is devoted to concluding remarks.

2 Problems formulation

In this Section we are going to compare the black-box and preference-based optimization frameworks, showing how they both solve the same optimization problem using different information on the objective function.

2.1 Black-box optimization

The aim of black-box optimization is to solve the following global optimization problem:

\[
x^* = \arg \min_x f(x) \quad \text{s.t.} \quad x \in \Omega,
\]

where \( x = [x^{(1)} \ldots x^{(n)}]^T \in \mathbb{R}^n \) is the decision variable, \( f : \mathbb{R}^n \to \mathbb{R} \) is a black-box cost function (unknown and expensive to evaluate) and \( \Omega \subset \mathbb{R}^n \) is the constraint set which, in its most general formulation, is given by

\[
\Omega = \left\{ x : l \leq x \leq u, \begin{array}{l} A_{ineq} \cdot x \leq b_{ineq}, \\
A_{eq} \cdot x = b_{eq}, \\
g_{ineq}(x) \leq 0_{p_{ineq}}, \\
g_{eq}(x) = 0_{p_{eq}} \end{array} \right\}
\]

In (2), \( l, u \in \mathbb{R}^n, A_{ineq} \in \mathbb{R}^{q_{ineq} \times n}, b_{ineq} \in \mathbb{R}^{q_{ineq}}, A_{eq} \in \mathbb{R}^{q_{eq} \times n}, b_{eq} \in \mathbb{R}^{q_{eq}}, g_{ineq} : \mathbb{R}^n \to \mathbb{R}^{p_{ineq}} \) and \( g_{eq} : \mathbb{R}^n \to \mathbb{R}^{p_{eq}} \). Notation-wise, \( 0_{p_{ineq}} \) represents the \( p_{ineq} \) zero column vector (and similarly for \( 0_{p_{eq}} \)). We suppose that: (i) all of these constraints are completely known and (ii) Problem (1) is, at least, bound constrained. If \( \Omega \) is compact and \( f(x) \) is continuous, then Problem (1) admits a solution according to the Extreme Value Theorem (1).

Surrogate-based methods solve Problem (1) starting from a set \( \mathcal{X} \) of \( N \) distinct samples of the decision variable, defined as:

\[
\mathcal{X} = \{ x_i : i = 1, \ldots, N, x_i \in \Omega, x_i \neq x_j, \forall i \neq j \},
\]
as well as the corresponding values assumed by the cost function at those samples. In practice, the measure of \( f(x) \) could be affected by noise, which is assumed to be a zero-mean Gaussian white noise with variance \( \sigma_n^2 \). We define the set of measures as:

\[
\mathcal{Y} = \left\{ y_i : y_i = f(x_i) + \eta_i, x_i \in \mathcal{X}, \eta_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma_n^2) \right\}.
\]  

(4)

The cardinality of sets \( \mathcal{X} \) and \( \mathcal{Y} \) is \( |\mathcal{X}| = |\mathcal{Y}| = N \).

### 2.2 Preference-based optimization

In the preference-based framework, there is no function \( f(x) \) to be measured explicitly. Instead, a human decision-maker expresses his/her preferences between couples of samples. A fundamental question to ask is:

*Can an arbitrary criterion of an individual be “translated” into a mathematical function \( f(x) \) such that solving Problem [1] leads to finding his/her most preferred value for the decision variable?*

To answer such question, we will now give a brief overview of some important results in utility theory [27], which allow us to formalize the preference-based optimization framework. Consider the constraint set \( \Omega \) in [2], we define a generic binary relation \( R \) on \( \Omega \) as a subset \( R \subseteq \Omega \times \Omega \). Notation-wise, given two samples \( x_i, x_j \in \Omega \), we denote the ordered pairs for which the binary relation holds, \( (x_i, x_j) \in R \), as \( x_i \succ R x_j \) [27].

A preference relation, \( \succ \subseteq \Omega \times \Omega \), is a preorder (a specific case of binary relation) which is commonly used to describe the tastes of an individual. In this context, \( x_i \succ x_j \) implies that a human decision-maker with preference relation \( \succ \) deems sample \( x_i \) at least as good as \( x_j \). The fact that the preference relation is a preorder encompasses the rationality of the individual, since the following holds:

1. Reflexivity, i.e. \( x_i \succ x_i, \forall x_i \in \Omega \) (any alternative is as good as itself),
2. Transitivity, i.e. \( \forall x_i, x_j, x_k \in \Omega \), if \( x_i \succ x_j \) and \( x_j \succ x_k \) hold, then \( x_i \succ x_k \) (consistency of the preferences expressed by the individual).

The preference relation \( \succ \) is usually “split” into two transitive binary relations:

- The strict preference relation \( \succ \) on \( \Omega \), i.e. \( x_i \succ x_j \) if and only if \( x_i \succ x_j \) but not \( x_j \succ x_i \) (\( x_i \) is “better than” \( x_j \)), and
- The indifference relation \( \sim \) on \( \Omega \), i.e. \( x_i \sim x_j \) if and only if \( x_i \succ x_j \) and \( x_j \succ x_i \) (\( x_i \) is “as good as” \( x_j \)).

Another common assumption on \( \succ \) is that it is a complete binary relation, i.e. either \( x_i \succ x_j \) or \( x_j \succ x_i \) hold \( \forall x_i, x_j \in \Omega \). Completeness of \( \succ \) implies that the human decision-maker is never uncertain, that is he/she is always able to express a preference between any couple of samples. One last relevant property for \( \succ \) is continuity. Here, we avoid a formal definition of the continuity of a binary relation [27] but, intuitively, if \( \succ \) is continuous and \( x_i \succ x_j \), then an alternative \( x_k \) which is “very close” to \( x_j \) should also be deemed strictly worse than \( x_i \).

Having defined the preference relation \( \succ \), the goal of preference-based optimization is to find the \( \succ \)-maximum of \( \Omega \), i.e. the sample \( x^* \in \Omega \) such that \( x^* \succ x, \forall x \in \Omega \) (the most preferred by the individual). Concerning the existence of \( x^* \), we can state the following Proposition, which can be seen as a generalization of the Extreme Value Theorem [1] for preference relations.

**Proposition 1** (Existence of a \( \succ \)-maximum of \( \Omega \) [27]). A \( \succ \)-maximum of \( \Omega \) is guaranteed to exist if \( \Omega \) is a compact subset of a metric space (in our case \( \Omega \subset \mathbb{R}^n \)) and \( \succ \) is a continuous and complete preference relation on \( \Omega \).

Proposition 1 allows us to prove the convergence of the proposed optimization scheme (Section 5) in the preference-based case. One of the most important results in utility theory is the following Theorem.

**Theorem 1** (Debreu’s Utility Representation Theorem for \( \mathbb{R}^n \) [10]). Let \( \Omega \) be any nonempty subset of \( \mathbb{R}^n \) and \( \succ \) be a complete preference relation on \( \Omega \). If \( \succ \) is continuous, then it can be represented by a continuous utility function \( u_\succ : \Omega \to \mathbb{R} \) such that, \( \forall x_i, x_j \in \Omega \):

\[
x_i \succ x_j \text{ if and only if } u_\succ(x_i) \geq u_\succ(x_j).
\]

Moreover, we have that:

\[
\begin{align*}
x_i &> x_j \text{ if and only if } u_\succ(x_i) > u_\succ(x_j), \\
x_i &\sim x_j \text{ if and only if } u_\succ(x_i) = u_\succ(x_j).
\end{align*}
\]
Using Theorem 1, we can build an optimization problem to find the \( \succeq \)-maximum of \( \Omega \) as
\[
\mathbf{x}^* = \arg \max \ u_\succeq (\mathbf{x}) \tag{5}
\]
subject to \( \mathbf{x} \in \Omega \),

which is equivalent to Problem (1) by setting \( f(\mathbf{x}) = -u_\succeq (\mathbf{x}) \). To avoid confusion, we refer to \( f(\mathbf{x}) \) in the preference-based framework as the scoring function and, similarly to the black-box case, its analytical formulation is unknown.

**Remark 1.** Formally, \( f(\mathbf{x}) \) in the black-box framework and \( u_\succeq (\mathbf{x}) \) in the preference-based one have different domains (\( \mathbb{R}^n \) and \( \Omega \) respectively). However, assuming that \( u_\succeq (\mathbf{x}) \) is continuous and \( \Omega \) is a compact subset of \( \mathbb{R}^n \) (which are either results or assumptions of Proposition 1 and Theorem 1), then there exists a continuous extensions of \( u_\succeq (\mathbf{x}) \) with domain \( \mathbb{R}^n \) (Tietze Extension Theorem [22]).

Instead of considering the preference relation explicitly (or the utility theory framework), most preference-based optimization algorithms define an (unknown) preference function \( \pi : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \{-1, 0, 1\} \) which describes the output of the comparison between two samples. Here, we consider \( \pi(\mathbf{x}_i, \mathbf{x}_j) \) as defined in (3):
\[
\pi(\mathbf{x}_i, \mathbf{x}_j) = \begin{cases} 
-1 & \text{if } f(\mathbf{x}_i) < f(\mathbf{x}_j) \iff \mathbf{x}_i \succ \mathbf{x}_j \\
0 & \text{if } f(\mathbf{x}_i) = f(\mathbf{x}_j) \iff \mathbf{x}_i \sim \mathbf{x}_j . \\
1 & \text{if } f(\mathbf{x}_i) > f(\mathbf{x}_j) \iff \mathbf{x}_j \succ \mathbf{x}_i
\end{cases} \tag{6}
\]

The preference function (6) is obtained from the utility representation of the binary relation \( \succeq \) (see Theorem 1) and from the fact that \( f(\mathbf{x}) = -u_\succeq (\mathbf{x}) \). Reflexivity and transitivity of the preorder \( \succeq \) are highlighted by the following properties of \( \pi(\mathbf{x}_i, \mathbf{x}_j) \):

1. \( \pi(\mathbf{x}_i, \mathbf{x}_i) = 0, \ \forall \mathbf{x}_i \in \mathbb{R}^n \),
2. \( \pi(\mathbf{x}_i, \mathbf{x}_j) = \pi(\mathbf{x}_j, \mathbf{x}_k) = b \Rightarrow \pi(\mathbf{x}_i, \mathbf{x}_k) = b, \ \forall \mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k \in \mathbb{R}^n \).

In the context of preference-based optimization, surrogate-based methods aim to find the \( \succeq \)-maximum of \( \Omega \) (by solving Problem (5) which is equivalent to Problem (1)) starting from a set of samples \( \mathcal{X} \) as defined in (3), and a set of \( M \) preferences expressed by the human decision-maker
\[
\mathcal{B} = \{ b_h : h = 1, \ldots, M, b_h \in \{-1, 0, 1\} \} . \tag{7}
\]

\( b_h \) in (7) is the \( h \)-th preference obtained by comparing a certain couple of samples, as highlighted by the following mapping set:
\[
\mathcal{S} = \left\{ (\ell(h), \kappa(h)) : h = 1, \ldots, M, \ell(h), \kappa(h) \in \mathbb{N}, \right. \\
\quad \quad \quad \quad \quad \quad \left. b_h = \pi(\mathbf{x}_{\ell(h)}, \mathbf{x}_{\kappa(h)}) , \right. \\
\quad \quad \quad \quad \quad \quad \left. b_h \in \mathcal{B}, \mathbf{x}_{\ell(h)}, \mathbf{x}_{\kappa(h)} \in \mathcal{X} \right\} , \tag{8}
\]
where \( \ell : \mathbb{N} \rightarrow \mathbb{N} \) and \( \kappa : \mathbb{N} \rightarrow \mathbb{N} \) are two mapping functions that associate the indexes of the samples, contained inside \( \mathcal{X} \), to their respective preferences in \( \mathcal{B} \). This time, the cardinalities are \( |\mathcal{X}| = N \) and \( |\mathcal{B}| = |\mathcal{S}| = M \). Also note that \( 1 \leq M \leq \binom{N}{2} \).

Table 1 summarizes the formulations of the black-box and preference-based optimization problems.

### 3 Surrogate models

In the context of surrogate-based methods, a *surrogate model* \( \hat{f} : \mathbb{R}^n \rightarrow \mathbb{R} \) is an approximation of the black-box cost function or the scoring function \( f(\mathbf{x}) \) that is (usually) inexpensive to evaluate. Its objective is to drive the optimization algorithm towards candidate samples that are minimizers of \( f(\mathbf{x}) \). The most commonly used surrogate models are based either on Radial Basis Functions (RBFs) or Gaussian Processes (GPs). In this Section, we show how both models can be used to approximate either the black-box cost function or the scoring function.

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\[ \text{There exist different formulations of the preference function. For example, the authors of [15] define } \pi(\mathbf{x}_i, \mathbf{x}_j) \text{ as the probability of } \mathbf{x}_i \text{ being preferred over } \mathbf{x}_j. \]
Set of samples
Information on Preference mapping:

\[ x^* = \arg \min_{x \in \Omega} f(x) \]

\[ \pi \]

\[ x^* = \arg \min_{x \in \Omega} f(x) \]

\[ \mathcal{X} \]

\[ \text{Expressed preferences: } \mathcal{B} \]

\[ \text{Preference mapping: } \mathcal{S} \]

Table 1: Summary of the information used to solve black-box and preference-based optimization problems.

### 3.1 Surrogates based on Radial Basis Functions

In this case, the surrogate model is defined by a \textit{radial basis function expansion} \cite{12} as

\[
\hat{f}(x) = \sum_{i=1}^{N} \beta^{(i)} \cdot \varphi(\epsilon \cdot \|x - x_i\|_2)
= \phi(x)^\top \beta,
\]

where \( \varphi : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R} \) is a properly chosen \textit{radial function} \cite{13}, \( \phi(x) \in \mathbb{R}^N \) is the radial basis function vector,

\[ \phi(x) = [\varphi(\epsilon \cdot \|x - x_1\|_2) \ldots \varphi(\epsilon \cdot \|x - x_N\|_2)]^\top, \]

\[ \epsilon \in \mathbb{R}_{\geq 0} \]

is the so-called \textit{shape parameter} (which needs to be tuned) and \( \beta = [\beta^{(1)} \ldots \beta^{(N)}]^\top \in \mathbb{R}^N \) is a vector of weights that has to be computed from data at hand.

#### 3.1.1 Black-box optimization

In the context of black-box optimization, especially if the measures of \( f(x) \) in \( \mathcal{Y} \) are noiseless, it is desirable to have a surrogate model that interpolates the given points. That is because, as the number of samples increases, \( \hat{f}(x) \) gets sufficiently expressive to capture where the global minimizer of \( f(x) \) is located \cite{20}. To do so, we enforce the \textit{interpolation conditions} and calculate \( \beta \) in (9) by solving the following linear system:

\[
\Phi \cdot \beta = y,
\]

where \( \Phi \in \mathbb{R}^{N \times N} \) is a symmetric matrix whose \((i,j)\)-th element is \( \Phi^{(i,j)} = \varphi(\epsilon \cdot \|x_i - x_j\|_2) \) and \( y \in \mathbb{R}^N \) is a vector which contains the entries of set \( \mathcal{Y} \), i.e. \( y = [y_1 \ldots y_N]^\top \).

The matrix \( \Phi \) might be singular depending on the choice of the radial function and on the points contained in \( \mathcal{X} \) \cite{16}. Moreover, the shape parameter \( \epsilon \) as well as the number and the distribution of the samples \( x_i \in \mathcal{X} \) affect the condition number of \( \Phi \) \cite{12,32}. In \cite{2}, the authors propose to solve the linear system in (10) using a low-rank approximation of \( \Phi \). Alternatively, a polynomial function of a certain degree can be added to the surrogate model \cite{9}, ensuring the existence of a unique interpolant \cite{16}.

#### 3.1.2 Preference-based optimization

In the context of preference-based optimization, a surrogate model \( \hat{f}(x) \) can be used to define the \textit{surrogate preference function} \( \hat{\pi} : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \{-1, 0, 1\} \). Differently from \( \pi(x_i, x_j) \) in \cite{6}, we consider a tolerance \( \sigma \in \mathbb{R}_{> 0} \) to avoid using strict inequalities and equalities and define \( \hat{\pi}(x_i, x_j) \) as \cite{3}:

\[
\hat{\pi}(x_i, x_j) = \begin{cases} -1 & \text{if } |\hat{f}(x_i) - \hat{f}(x_j)| \leq -\sigma \\ 0 & \text{if } |\hat{f}(x_i) - \hat{f}(x_j)| \leq \sigma \\ 1 & \text{if } |\hat{f}(x_i) - \hat{f}(x_j)| \geq \sigma \end{cases} \tag{11}
\]

Instead of enforcing the interpolation conditions, \textit{we are interested in a surrogate preference function that correctly describes the preferences expressed in } \( \mathcal{B} \) \textit{and} \( \mathcal{S} \). This, in turn, translates into constraints on the surrogate model \( \hat{f}(x) \),
which can be used to find $\beta$ in (9). In order to do so, the authors of [3] define the following optimization problem:

$$\arg \min_{x, \beta} \frac{\lambda}{2} \cdot \beta^\top \cdot \beta + g^\top \cdot \varepsilon$$

s.t. $\hat{f}(\mathbf{x}_i) - \hat{f}(\mathbf{x}_j) \leq -\sigma + \varepsilon(h)$ \hspace{1cm} $\forall h : b_h = -1$

$|\hat{f}(\mathbf{x}_i) - \hat{f}(\mathbf{x}_j)| \leq \sigma + \varepsilon(h)$ \hspace{1cm} $\forall h : b_h = 0$

$\hat{f}(\mathbf{x}_i) - \hat{f}(\mathbf{x}_j) \geq \sigma - \varepsilon(h)$ \hspace{1cm} $\forall h : b_h = 1$

$\varepsilon \geq 0_M$

$h = 1, \ldots, M$,

where $\varepsilon = [\varepsilon^{(1)} \ldots \varepsilon^{(M)}] ^\top \in \mathbb{R}^M$ is a vector of slack variables (one for each preference), $g = [g^{(1)} \ldots g^{(M)}] ^\top \in \mathbb{R}^M$ is a vector of weights and $\lambda \in \mathbb{R}_{\geq 0}$ plays the role of a regularization parameter.

Problem (12) ensures that, at least approximately, $\hat{f}(\mathbf{x})$ is a suitable representation of the unknown preference relation $\succeq$ which generated the data (see Theorem 1). The slacks $\varepsilon$ are added because the surrogate model might not be complex enough to describe the given preferences, or in case some of them are expressed inconsistently by the individual. In practice, Problem (12) can be employed for any choice of $\hat{f}(\mathbf{x})$ which depends upon some parameters vector $\beta$. If the surrogate model is linear in $\beta$ (such as the one in (9)), then Problem (12) is a convex Quadratic Program (QP) for $\lambda > 0$ or a Linear Program (LP) for $\lambda = 0$ [3].

3.2 Surrogates based on Gaussian Processes

In this case, we impose a Gaussian Process (GP) [38] prior distribution on the unknown cost function as

$$f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}_i, \mathbf{x}_j)).$$

(13)

The mean of the GP is assumed to be the zero function and $k(\mathbf{x}_i, \mathbf{x}_j)$ is a suitable kernel (or covariance function) which possibly depends on some hyperparameters. Under the assumption in (13), the probability associated to the latent values $f = [f(\mathbf{x}_1) \ldots f(\mathbf{x}_N)] ^\top \in \mathbb{R}^N$ assumed by $f(\mathbf{x})$ at the sampled points in $\mathcal{X}$ is

$$p(f) = \mathcal{N}(0_N, K),$$

(14)

where $K \in \mathbb{R}^{N \times N}$ is a symmetric matrix whose $(i, j)$-th entry is $K_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$ and $\mathcal{N}(\mu_N, \Sigma_N)$ is a Gaussian distribution with mean $\mu_N$ and covariance $\Sigma_N$.

Based on the specific optimization framework, a suitable likelihood which describes the dataset at hand, i.e. either $\mathcal{Y}$ or $\mathcal{B}$ and $\mathcal{S}$, needs to be defined. Here, we will denote the likelihood as $p(D|f, \mathcal{X})$, where $D$ indicates a generic dataset, containing either the function measures or the preferences. Once $p(D|f, \mathcal{X})$ has been defined, it is possible to marginalize it with respect to $\mathbf{f}$ to obtain the marginal likelihood $p(D|\mathcal{X})$. The latter is often used to recalibrate the hyperparameters of the kernel [38]. Finally, using Bayes’ Theorem [3], we can calculate the posterior distribution $p(f|D, \mathcal{X})$ and, more importantly, the predictive distribution $p(f|D, \mathcal{X}, \tilde{x})$, whose mean can be used as the surrogate model $\tilde{f}(\mathbf{x})$.

3.2.1 Black-box optimization

In the black-box framework, given that $y_i = f(\mathbf{x}_i) + \eta_i$ as reported in (4) and $\eta_i$ is a realization of a Gaussian white noise, the likelihood is

$$p(D|f, \mathcal{X}) = \mathcal{N}(f, \sigma^2 \cdot I_{N \times N}),$$

(15)

where $I_{N \times N}$ is the $N \times N$ identity matrix. Using the properties of Gaussian distributions [38], it is possible to compute the expression of the predictive distribution in closed form as

$$p(f|D, \mathcal{X}, \tilde{x}) = \mathcal{N}(\mu_f, \Sigma_f),$$

(16a)

$$\mu_f = k(\tilde{x})^\top \cdot [K + \sigma^2 \cdot I_{N \times N}]^{-1} \cdot y,$$

(16b)

$$\Sigma_f = k(\tilde{x}, \tilde{x}) - k(\tilde{x})^\top \cdot [K + \sigma^2 \cdot I_{N \times N}]^{-1} \cdot k(\tilde{x}),$$

(16c)

Footnote: The radial functions $\varphi \cdot \|x_i - x_j\|_2$ used in (9) are suitable kernels.
where $k(\bar{x}) = [k(x_1, \bar{x}) \ldots k(x_N, \bar{x})]^{\top} \in \mathbb{R}^N$ is the kernel vector. The surrogate model is the expected value of the predictive distribution in (16a), which can be written as

$$\hat{f}(x) = k(x)^{\top} \cdot \beta$$

(17)

Notice that (17) is quite similar to (9), but this time $\beta = [K + \sigma_n^2 \cdot I_{N \times N}]^{-1} \cdot y$.

In practice, $\sigma_n^2$ is unknown and needs to be estimated from data. If data is assumed to be noiseless ($\sigma_n^2 = 0$) then, provided that $K$ is nonsingular, $\hat{f}(x)$ in (17) interpolates the samples in $\mathcal{X}$ and $\mathcal{Y}$.

### 3.2.2 Preference-based optimization

Gaussian Processes have also been employed in the context of preference learning and preference-based optimization. A widely used likelihood is proposed in [9], where the authors only consider the strict preference relation $\succ$ instead of $\succeq$ (the indifference relation $\sim$ is not handled explicitly). Under this assumption, it is possible to define the mapping functions $\ell(h), \kappa(h)$ in (8) so that

$$x_{\ell(h)} \succ x_{\kappa(h)}, \quad \forall h = 1, \ldots, M,$$

making the set $B$ in (7) redundant. Additionally, the scoring function $f(x)$ is assumed to be affected by a Gaussian white noise $\eta_{\ell(h)} \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma_n^2)$, i.e.

$$y_{\ell(h)} = f(x_{\ell(h)}) + \eta_{\ell(h)},$$

and similarly for those values indexed by $\kappa(h)$. Then, $x_{\ell(h)} \succ x_{\kappa(h)}$ whenever $y_{\ell(h)} < y_{\kappa(h)}$. The noise is used to capture possible inconsistencies in the preferences expressed by the individual (similarly to the role of the slacks in Problem (13)). The likelihood proposed in (9) reads as

$$p(D|f, \mathcal{X}) = \prod_{h=1}^{M} p\left(y_{\ell(h)} < y_{\kappa(h)} | f_{\ell(h)}, f_{\kappa(h)}, x_{\ell(h)}, x_{\kappa(h)}\right)$$

$$= \prod_{h=1}^{M} \Phi_{\mathcal{N}}\left(\frac{f_{\kappa(h)} - f_{\ell(h)}}{\sqrt{2 \cdot \sigma_n^2}}\right),$$

(18)

where $\Phi_{\mathcal{N}}(\cdot)$ is the standard cumulative normal distribution. In this case, it is not possible to obtain the posterior distribution in closed form. Instead, the authors of [9] resort to its Laplace Approximation [5], which requires solving an additional optimization problem to find the Maximum A Posteriori (MAP) estimate of the latent function values, $f_{MAP} \in \mathbb{R}^n$. In particular,

$$p(f|D, \mathcal{X}) \approx \mathcal{N}\left(f_{MAP}, [K^{-1} + \Lambda_{MAP}]^{-1}\right),$$

where $\Lambda_{MAP} \in \mathbb{R}^{N \times N}$ is the Hessian of the negative log likelihood $-\ln p(D|f, \mathcal{X})$ evaluated at $f_{MAP}$. Finally, the predictive distribution can be obtained using the Laplace Approximation of the posterior distribution:

$$p\left(\hat{f}|D, \mathcal{X}, \bar{x}\right) = \mathcal{N}\left(\mu_{\hat{f}}, \Sigma_{\hat{f}}\right),$$

(19a)

$$\mu_{\hat{f}} = k(\bar{x})^{\top} \cdot K^{-1} \cdot f_{MAP},$$

(19b)

$$\Sigma_{\hat{f}} = k(\bar{x}, \bar{x}) - k(\bar{x})^{\top} \cdot [K + \Lambda_{MAP}^{-1}]^{-1} \cdot k(\bar{x}).$$

(19c)

The surrogate model is the expected value of the predictive distribution, which can be written as in (17) with $\beta = K^{-1} \cdot f_{MAP}$.

### 4 Handling exploration and exploitation

As previously mentioned, surrogate-based methods iteratively propose new samples to try with the aim of solving Problem (1), while also minimizing the number of costly evaluations/comparisons. Suppose that, at iteration $k$, we have at our disposal the set of samples $\mathcal{X}$, $|\mathcal{X}| = N$, and either set $\mathcal{Y}$ or sets $B$ and $S$. We denote the best sample found so far by the procedure (i.e. the one that either achieved the lowest function value or that is preferred by the user) as

$$x_{\text{best}}(N) \in \mathbb{R}^n, x_{\text{best}}(N) \in \mathcal{X}, |\mathcal{X}| = N,$$

such that

$$x_{\text{best}}(N) = \arg \min_{x_i \in \mathcal{X}} y_i, y_i \in \mathcal{Y}$$

or

$$x_{\text{best}}(N) \succeq x_i, \forall x_i \in \mathcal{X}.$$
The new candidate sample,

\[ x_{N+1} \in \mathbb{R}^n, x_{N+1} \notin X, \]

is obtained by solving an additional optimization problem:

\[
x_{N+1} = \arg \min_x a(x) \quad \text{s.t.} \quad x \in \Omega, \tag{20}
\]

where \( a : \mathbb{R}^n \to \mathbb{R} \) is a properly defined acquisition function which trades off exploration and exploitation. Once \( x_{N+1} \) has been computed:

- In the black-box optimization case, we measure the black-box function at the new sample, obtaining \( y_{N+1} = f(x_{N+1}) + \eta_{N+1} \).
- In the preference-based framework, we let the user express a preference between the best sample found so far and the new one, obtaining \( b_{M+1} = \pi(x_{N+1}, s_{\text{best}}(N)) \).

In both cases, \( x_{N+1} \) is added to the set \( X \) and, similarly, \( Y, B, S \) are also updated with either \( y_{N+1} \) or \( b_{M+1} \). The process is iterated until a certain condition is met. Usually, a budget, or rather a maximum number of samples to evaluate \( N_{\text{max}} \), is set and the procedure is stopped once it is reached.

In this work, \( a(x) \) is defined starting from a surrogate model and an exploration function \( z : \mathbb{R}^n \to \mathbb{R} \) which leads the optimization procedure towards regions of \( \Omega \) where few samples have been tried and/or where the surrogate model is most uncertain. We assume that both \( f(x) \) and \( z(x) \) are continuous functions. The acquisition function that we adopt here is an explicit trade-off between these two functions:

\[
a(x) = \delta \cdot \frac{\hat{f}(x) - \hat{f}_{\min}(X_{\text{aug}})}{\Delta F(X_{\text{aug}})} + (1 - \delta) \cdot \frac{z(x) - z_{\min}(X_{\text{aug}})}{\Delta Z(X_{\text{aug}})}, \tag{21}
\]

where:

- \( \delta \in [0, 1] \) is a parameter which defines the exploration-exploitation trade-off.
- \( \hat{f}(x) \) and \( z(x) \) have been rescaled using min-max normalization \(^{17}\) in order to make them assume the same range \([0, 1]\) (or, at least, make them comparable). In particular, given any function \( h : \mathbb{R}^n \to \mathbb{R} \) and a set of samples \( X_{\text{aug}} \), we define

\[
\hat{h}_{\min}(X_{\text{aug}}) = \min_{x \in X_{\text{aug}}} h(x), \tag{22a}
\]

\[
\hat{h}_{\max}(X_{\text{aug}}) = \max_{x \in X_{\text{aug}}} h(x), \tag{22b}
\]

\[
\Delta H(X_{\text{aug}}) = \hat{h}_{\max}(X_{\text{aug}}) - \hat{h}_{\min}(X_{\text{aug}}). \tag{22c}
\]

Note that, to avoid dividing by zero in \((21)\), \( \Delta H(X_{\text{aug}}) \) can be set to \( \hat{h}_{\max}(X_{\text{aug}}) \) or 1 whenever \( \hat{h}_{\min}(X_{\text{aug}}) = \hat{h}_{\max}(X_{\text{aug}}) \neq 0 \) or \( \hat{h}_{\min}(X_{\text{aug}}) = \hat{h}_{\max}(X_{\text{aug}}) = 0 \) respectively.

- \( X_{\text{aug}} = \{x_{\text{aug}} : i = 1, \ldots, N_{\text{aug}}, x_{\text{aug}} \in \Omega\} \) is the so-called augmented sample set, which needs to be defined so that

\[
\hat{f}_{\min}(X_{\text{aug}}) \approx \min_{x \in \Omega} \hat{f}(x), \tag{23a}
\]

\[
\hat{f}_{\max}(X_{\text{aug}}) \approx \max_{x \in \Omega} \hat{f}(x), \tag{23b}
\]

\[
z_{\min}(X_{\text{aug}}) = \min_{x \in \Omega} z(x), \tag{23c}
\]

\[
z_{\max}(X_{\text{aug}}) = \max_{x \in \Omega} z(x). \tag{23d}
\]

In practice, this means that \( X_{\text{aug}} \) needs to be sufficiently expressive to allow for a proper comparison between the surrogate model and the exploration function in \((21)\). There are different ways to obtain the augmented sample set. The most accurate (and expensive) one would be to solve four additional optimization problems to find the minimizers and maximizers of \( \hat{f}(x) \) and \( z(x) \). Alternatively, as it has been done for MSRS \(^{30}\), the augmented sample set can be obtained by randomly sampling \( \Omega \). If a-priori knowledge on the stationary points of \( \hat{f}(x) \) and/or \( z(x) \) is available, then it can be used to build \( X_{\text{aug}} \), see for example \((28)\). Finally, a possible choice is \( X_{\text{aug}} = X \), however it is not recommended because, as we will see in Section 4.1, \( z(x) \) is usually maximal at the sampled points. Therefore, \( X \) is not expressive enough to rescale the exploration function.
As a final note, \( a(x) \) in (21) is often a multimodal function. Therefore, global optimization procedures need to be employed to solve Problem (20). However, compared to the black-box cost function or the interaction with the individual, \( a(x) \) is cheap to evaluate and therefore we are not particularly concerned with its number of function evaluations.

**Remark 2.** The acquisition function (21) can be seen as a generalized version of the one proposed in \( \text{MSRS} [30] \), where the function \( z(x) \) is fixed a-priori. Instead, the proposed \( a(x) \) in (21) can use any (proper) \( z(x) \). Moreover, (21) will be employed in the proposed general optimization scheme for both black-box and preference-based problems.

### 4.1 Exploration functions

In Section 3, we showed different models that can be used as surrogates for the acquisition function (21). Here, we define possible exploration functions \( z(x) \) that are suited for (21).

The aim of \( z(x) \) is to drive the optimization procedure towards regions of \( \Omega \) where few samples are present. To do so, the exploration function must use the information available at the current iteration, i.e. \( \mathcal{X} \) and, possibly but not necessarily, either the measures of the cost function \( \gamma \) or the preferences in \( \mathcal{B} \) and \( \mathcal{S} \). We provide the following Definition to highlight which functions \( z(x) \) are suitable to be used as an exploration function for (21).

**Definition 1 (Proper exploration function).** Suppose that \( \Omega \) is a compact subset of \( \mathbb{R}^n \). Then, a function \( z : \mathbb{R}^n \to \mathbb{R} \) is a proper exploration function if it is continuous and the solution of Problem (20) with \( \delta = 0 \), or equivalently

\[
x_{N+1} = \arg \min_x z(x)
\]

s.t. \( x \in \Omega \),

is not already present in \( \mathcal{X} \), i.e. \( x_{N+1} \notin \mathcal{X} \).

Compactness of \( \Omega \) and continuity of \( z(x) \) ensure that Problem (24) has at least one solution. If instead it has multiple solutions, then at least one of them must not be in \( \mathcal{X} \).

An exploration function could also depend on the choice of the surrogate model. For instance, if \( \hat{f}(x) \) is obtained by imposing a GP prior on \( f(x) \), then we can use the negative standard deviation of the predictive distribution as exploration function, namely

\[
z(x) = - \sqrt{k(x,x) - k(x)^\top \cdot \left[ K + \sigma_n^2 \cdot I_{N \times N} \right]^{-1} \cdot k(x)}
\]

in the black-box case (16a) and

\[
z(x) = - \sqrt{k(x,x) - k(x)^\top \cdot \left[ K + \Lambda_{MAP}^{-1} \right]^{-1} \cdot k(x)}
\]

in the preference-based one (19a).

The functions \( z(x) \) in (25) and in (26) are continuous if the chosen kernel function \( k(\cdot, x) \) is continuous. Moreover, the variance of the predictive distribution is minimal at the sampled values in \( \mathcal{X} \) [38], while it assumes higher values where the surrogate model is most uncertain. Therefore, \( z(x) \) in (25) and in (26) are proper exploration functions.

Alternative exploration functions that are not related to the surrogate model \( \hat{f}(x) \) exist. For example, the authors of GLIS [2] proposed the Inverse Distance Weighting (IDW) distance function:

\[
z(x) = \begin{cases} 
0 & \text{if } x \in \mathcal{X} \\
- \frac{\pi}{2} \cdot \arctan \left( \frac{1}{\sum_{i \neq x} w_i(x)} \right) & \text{otherwise }
\end{cases}
\]

(27)

where \( w_i : \mathbb{R}^n \setminus \{ x_i \} \to \mathbb{R}_{>0} \), \( w_i(x) = \frac{1}{\| x - x_i \|_2} \), is the IDW function [33]. In [2], the authors also prove that \( z(x) \) is differentiable everywhere on \( \mathbb{R}^n \) and hence it is continuous. Another exploration function is the one used in MSRS [30]:

\[
z(x) = - \min_{x_i \in \mathcal{X}} \| x - x_i \|_2,
\]

(28)

which is continuous since it is the composition of continuous functions. Both \( z(x) \) in (27) and in (28) are zero only at \( x_i \in \mathcal{X} \) and assume negative values \( \forall x \notin \mathcal{X} \). Thus, they are proper exploration functions.
4.2 Relationship to other surrogate-based algorithms

Often, acquisition functions based on explicit trade-offs between a surrogate model and an exploration function exhibit the following structure:

\[ a(x) = \hat{f}(x) + \alpha \cdot z(x), \]  

where \( \alpha \in \mathbb{R} \) is a suitable coefficient that can be varied in between iterations of the optimization procedure. The proposed acquisition function (21) belongs to this rationale. It is possible to prove that, for \( \delta \neq 0 \), (21) has the same minimizer as:

\[ a(x) = \hat{f}(x) + \frac{1 - \delta}{\delta} \cdot \frac{\Delta \hat{F}(X_{\text{aug}})}{\Delta Z(X_{\text{aug}})} \cdot z(x). \]  

(30)

For some specific choices of \( \hat{f}(x) \) and \( z(x) \), the proposed acquisition functions \( a(x) \) in (21) or (30) can be seen as a generalization of the acquisition functions used by some other popular surrogate-based methods, like

1. **MSRS** [30] is a black-box optimization algorithm which uses the same acquisition function (21), does not make any assumption on the surrogate model \( \hat{f}(x) \), and adopts the exploration function (28). Moreover, the points in \( X_{\text{aug}} \) are generated randomly and, instead of explicitly solving Problem (20), the new candidate sample is selected as

\[ x_{N+1} = \arg \min_{x \in X_{\text{aug}}} a(x). \]

2. In the context of Bayesian Optimization, a popular acquisition function is the so called **Lower Confidence Bound** (often referred to as GP-LCB) [6], which can be obtained by using the acquisition function (29) with \( \hat{f}(x) \) defined as in Section 3.2 and \( z(x) \) as (25) or (26), depending on the optimization framework. In practice, \( \alpha \) in (29) for GP-LCB [6] is often kept constant throughout the whole optimization procedure.

3. In the preference-based framework, algorithm **GLISp** [3] uses a RBF surrogate model (9) and \( z(x) \) as in (27). Its acquisition function is defined as

\[ a(x) = \frac{\hat{f}(x)}{\Delta \hat{F}(X)} + \alpha \cdot z(x), \]

which has the same minimizer as the one in (30) for \( X_{\text{aug}} = X \) and a proper choice of \( \delta \).

4.3 Choosing the trade-off parameter

Many black-box optimization algorithms explicitly vary the exploration-exploitation trade-off in between the iterations of the procedure. Just to cite a few:

- **Gutmann-RBF** [16] uses an acquisition function that is a measure of “bumpiness” of the RBF surrogate, which depends upon a target value \( t \) to aim for. The values of \( t \) are cycled between two extrema to alternate between local and global search.

- The authors of **MSRS** [30], which uses the acquisition function (21) with \( z(x) \) as in (28), propose to cycle between different values of \( \delta \) as to prioritize exploration or exploitation more.

- In algorithm **SO-SA** [37], which is a revisitation of **MSRS** [30], the weight \( \delta \) is chosen in a random fashion at each iteration. Moreover, the authors adopt a greedy strategy, i.e. the trade-off is kept unaltered until it fails to find a significantly better solution.

- In the context of Bayesian optimization, a popular way to find the next candidate sample is to maximize the **Probability of Improvement**, which is defined as

\[ p\left(f(x) \leq \hat{f}_{\text{min}}(X) - \xi \right) = \Phi_N \left( \frac{\hat{f}_{\text{min}}(X) - \xi - \hat{f}(x)}{-z(x)} \right), \]

where \( \hat{f}(x) \) and \( -z(x) \) are the mean and the standard deviation of the predictive distribution (see Section 5.2), while \( \xi \in \mathbb{R}_{\geq 0} \) is a trade-off parameter that needs to be tuned. In [23], \( \xi \) is initialized to a high value so that the algorithm prioritizes exploration in the early iterations and gets progressively smaller to give more importance to the surrogate later on.
In this work, we use the greedy δ-cycling strategy, which we proposed in [28] and we now briefly review. We define a set of \( N_{\text{cycle}} \geq 1 \) weights to cycle:

\[
\Delta_{\text{cycle}} = \{ \delta_0, \ldots, \delta_{N_{\text{cycle}}-1} \}.
\]

The set \( \Delta_{\text{cycle}} \) should contain values that are well spread within the \([0, 1]\) range as to properly alternate between local and global search. Then, as long as \( x_{\text{best}}(N) \) varies from an iteration to the other (i.e. there has been some improvement), hyperparameter \( \delta \) in \([21]\) is kept unchanged. Viceversa, whenever the algorithm produces an \( x_{N+1} \) that is not better than the best sample found so far \( x_{\text{best}}(N) \), the weight is cycled following the order proposed in \( \Delta_{\text{cycle}} \). More formally, suppose that, at iteration \( k \), we have at our disposal \(|\mathcal{X}| = N\) samples and denote the trade-off parameter \( \delta \) in \([21]\) as \( \delta(k) \) to highlight the iteration number. Furthermore, assume \( \delta(k) = \delta_j \in \Delta_{\text{cycle}} \), which has been used to find the new candidate sample \( x_{N+1} \) at iteration \( k \) by solving Problem \([20]\). Then, at iteration \( k+1 \), we select \( \delta(k+1) \in \Delta_{\text{cycle}} \) as:

\[
\delta(k+1) = \begin{cases} 
\delta_j & \text{if } x_{\text{best}}(N+1) = x_{N+1} \\
\delta_{(j+1) \mod N_{\text{cycle}}} & \text{if } x_{\text{best}}(N+1) = x_{\text{best}}(N) 
\end{cases}
\]

The convergence of the optimization scheme that we propose in the next Section is strictly related to the choice of the cycling set \([31]\).

5 General optimization scheme and convergence

Algorithm [1] describes a general procedure that can be used to solve Problem \([1]\), either in the black-box or preference-based framework. We will refer to the proposed scheme as generalized Metric Response Surface (gMRS for short) since it can be seen as an extension of the MSRS \([30]\) procedure. Differently from MSRS \([30]\), gMRS can handle both optimization frameworks and different exploration functions.

As with any surrogate-based method, gMRS starts from an initial set of samples \( \mathcal{X} \) that needs to be generated using a suitable space-filling experimental design \([36]\), for example Latin Hypercube Designs (LHDs) \([25]\). Then, the samples in \( \mathcal{X} \) are evaluated either by measuring the value of the black-box cost function \( f(x) \) or by asking the individual to compare them. In any case, the initial best sample \( x_{\text{best}}(N) \) is obtained, either as the one that achieved the lowest \( y_1 \in \mathcal{Y} \) or by properly guiding the comparisons, using the transitive property of the preference relation \( \succ\) (see Section 2).

Iteratively, until the budget \( N_{\text{max}} \) is exhausted, the surrogate model \( \hat{f}(x) \) is built (or updated) and, together with a proper exploration function \( z(x) \), used to find a new candidate sample \( x_{N+1} \) by solving Problem \([20]\). The sample \( x_{N+1} \), suggested by the algorithm, replaces the best sample found so far, \( x_{\text{best}}(N) \), either if

\[
y_{N+1} = y_{\text{best}}(N),
\]

where \( y_{\text{best}}(N) \) is the measure of the black-box cost function at \( x_{\text{best}}(N) \), or if

\[
x_{N+1} \succ x_{\text{best}}(N).
\]

After that, the information brought by \( x_{N+1} \) is added to the respective sets \( \mathcal{X}, \mathcal{Y}, \mathcal{B} \) and \( \mathcal{S} \).

Note that \( \hat{f}(x) \) possibly contains some hyperparameters that might need to be recalibrated. In the case of RBF surrogates, this can be done by employing cross-validation (see [32, 8] for black-box optimization and [33] for the preference-based case). Instead, for GP surrogates, we can maximize the marginal likelihood (see [38] and [9] for black-box and preference-based optimization respectively). Recalibration might not be performed at every iteration but only at certain ones.

**Remark 3.** Further algorithmic details, such as the possibility of rescaling the decision variable \( x \) (see for example \([22]\)) or handling the case when \( x_{N+1} \) returned by Problem \([20]\) has already been tried, i.e. \( x_{N+1} \in \mathcal{X} \) (this could happen if \( \delta = 1 \), are not covered in Algorithm [1] but can easily be included.

5.1 Convergence of gMRS

It is possible to guarantee the convergence of any global optimization algorithm to the global minimizer of Problem \([1]\) by proving the following Theorem.

**Theorem 2** (Convergence of a global optimization algorithm \([34]\)). Consider the global optimization problem in \([1]\). Let \( \Omega \subset \mathbb{R}^n \) be a compact set and \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) be a continuous function. Then, an algorithm converges to the global minimum of every continuous function on \( \Omega \) if and only if its sequence of iterates,

\[
\langle x_i \rangle_{i \geq 1} = \langle x_1, x_2, \ldots \rangle,
\]

is everywhere dense in \( \Omega \).
Algorithm 1 gMRS optimization scheme

Input:
(i) Constraint set \( \Omega \) in (2),
(ii) Initial number of samples \( N \) (must be greater than 2 in the preference-based case),
(iii) Budget \( N_{\text{max}} > N \),
(iv) Surrogate model \( \hat{f} (x) \) (Section 3) with, possibly, its hyperparameters,
(v) Proper exploration function \( z (x) \) (Section 4.1),
(vi) Exploration-exploitation trade-off cycle \( \Delta_{\text{cycle}} \) (Section 4.3).

Output:
(i) Best sample obtained by the procedure \( x_{\text{best}} (N_{\text{max}}) \).

1: Select a set of starting points \( X, |X| = N \), using a suitable experimental design [36]
2: Evaluate the samples in \( X \), obtaining some information on the cost function \( f (x) \) (either set \( Y \) in (4) or sets \( B \) and \( S \) in (7) and (8)), and get the initial best sample \( x_{\text{best}} (N) \)
3: for \( k = 1, 2, \ldots, N_{\text{max}} - |X| \) do
4: (Optional) Recalibrate the hyperparameters of the surrogate model \( \hat{f} (x) \)
5: Build or update surrogate model \( \hat{f} (x) \) from \( X \) and the information on \( f (x) \) at hand
6: Build the augmented sample set \( X_{\text{aug}} \)
7: Select \( \delta \) for the current iteration from \( \Delta_{\text{cycle}} \) (Section 4.3)
8: Solve Problem (20) to obtain the new candidate sample \( x_{N+1} \)
9: Either measure the value of the cost function for \( x_{N+1} \) or let the human decision-maker express a preference between \( x_{N+1} \) and \( x_{\text{best}} (N) \)
10: if \( x_{N+1} \) achieved a better result than \( x_{\text{best}} (N) \) then
11: Set \( x_{\text{best}} (N + 1) = x_{N+1} \)
12: else
13: Set \( x_{\text{best}} (N + 1) = x_{\text{best}} (N) \) (no improvement)
14: Update the set of samples \( X \) and either the collection of measures \( Y \) or the user-expressed preferences \( B \) and \( S \).
15: Set \( N = N + 1 \)

Concerning Algorithm 1, we can generalize the convergence result obtained for GLISp-r in [28] to gMRS, as claimed by the following Theorem.

Theorem 3 (Convergence of gMRS). Let \( \Omega \subset \mathbb{R}^n \) be a compact set and either:

- \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) be a continuous function (black-box case) or,
- \( \succeq \) be a continuous and complete preference relation (preference-based case).

If \( z (x) \) is a proper exploration function, as defined in Definition 1 and there \( \exists \delta_j \in \Delta_{\text{cycle}} \) such that \( \delta_j = 0 \), then, for \( N_{\text{max}} \rightarrow \infty \), gMRS converges to the global minimizer of Problem (1) for any set of initial points \( X, |X| = N \), as well as any continuous surrogate model \( \hat{f} (x) \).

Proof. In the black-box framework, continuity of \( f (x) \) and compactness of \( \Omega \) ensure that there exists a global minimizer for Problem (1) (Extreme Value Theorem [1]) and are required for Theorem 2. Similarly, continuity and completeness of \( \succeq \) guarantee that there exists a \( \succeq \)-maximum of \( \Omega \) for Proposition 1. Moreover, from Theorem 1
there exists a continuous scoring function \( f(x) \) that represents \( \succeq \) and such that solving Problem (1) leads to find the \( \succeq \)-maximum of \( \Omega \). In turn, this makes it possible to apply Theorem 2 also in the preference-based framework.

Consider the sequence of iterates \( \langle x_i \rangle_{i \geq 1} \) produced by Algorithm 1. We define

- \( X_\infty \) as the set containing all the elements of \( \langle x_i \rangle_{i \geq 1} \),
- The subsequence of \( \langle x_i \rangle_{i \geq 1} \) containing only its first \( k \) entries as \( \langle x_i \rangle_{i=1}^k = \langle x_1, \ldots, x_k \rangle \),
- \( X_k \) as the collection of the points in \( \langle x_i \rangle_{i=1}^k \).

In practice, the first \( N \) entries of \( \langle x_i \rangle_{i \geq 1} \) constitute the initial set of samples \( X \) (obtained by an experimental design), i.e. \( X_N = X \), while the remaining ones are obtained by solving Problem (20), which always admits a solution since both \( f(x) \) and \( z(x) \) are assumed to be continuous. Any sample \( x_i \) obtained either by the experimental design or by solving Problem (20) is such that \( x_i \in \Omega \), therefore \( X_\infty \subseteq \Omega \).

Suppose now that \( \Delta_{cycle} = \{0\} \), then, at each iteration, the new candidate sample \( x_{k+1} \) \((k > N)\) is found by solving Problem (24) (pure exploration) using \( k \) samples (contained in \( X_k \)). Since \( z(x) \) is a proper exploration function, \( x_{k+1} \notin X_{k} \), which implies that, given any \( x \in \Omega \), \( x \in X_k \) for \( k \to \infty \). In other words, any point \( x \in \Omega \) will eventually be sampled by Problem (24), provided that \( z(x) \) is proper. Thus, we can define a sequence
\[
\langle \tilde{x}_i \rangle_{i \geq 1} = \langle \tilde{x}_1, \tilde{x}_2, \ldots \rangle
\]
in \( X_\infty \) as the concatenation of a sequence \( \langle x_i \rangle_{i=1}^k \) for \( k \) such that \( x_k = x \) and a constant sequence of \( x \), i.e.
\[
\langle \tilde{x}_i \rangle_{i \geq 1} = \langle x_1, \ldots, x_{k-1}, x, x, \ldots \rangle.
\]

By construction, \( \langle \tilde{x}_i \rangle_{i \geq 1} \) is such that
\[
\lim_{i \to \infty} \tilde{x}_i = x. \tag{32}
\]

We have proven that:

- \( X_\infty \subseteq \Omega \),
- Given any \( x \in \Omega \), there exists a sequence \( \langle \tilde{x}_i \rangle_{i \geq 1} \) in \( X_\infty \) which satisfies (32).

Thus, we can conclude that \( X_\infty \) is dense in \( \Omega \) and, consequently, so is the corresponding sequence of iterates \( \langle x_i \rangle_{i \geq 1} \). Finally, by Theorem 3, \( gRMS \) converges to the global minimizer of Problem (1). We can reach the same conclusion for any \( \Delta_{cycle} \) that includes a zero entry. \( \square \)

**Remark 4.** Combining the utility theory framework [27] with preference-based optimization allows us to extend Theorem 2 as to cover the convergence to the \( \succeq \)-maximum of \( \Omega \). In this case, we must ensure that the preference relation admits a continuous representation (Theorem 7) and we need to guarantee that a \( \succeq \)-maximum of \( \Omega \) exists (Proposition 1). Under these assumptions, we are able to prove the convergence of \( gRMS \) in the preference-based case. Instead, other preference-based algorithms often neglect a formal proof of convergence.

**Remark 5.** Theorem 3 guarantees the convergence of \( gRMS \) but does not give any indication on its rate. In practice, it depends on a multitude of factors, such as the choice of the surrogate model, exploration function and cycling set. Setting \( \Delta_{cycle} = \{0\} \) basically results in performing exhaustive search [1], which is quite inefficient but is guaranteed to converge to the minimizer of Problem (1) under the assumptions of Theorem 3. We suggest to use a \( \Delta_{cycle} \) in (31) that contains values which are well spread within the \([0, 1] \) range, including a zero entry to guarantee the convergence.

### 6 Illustrative example

Suppose that we want to solve the following global optimization problem:
\[
x^* = \arg \min_x f(x)
\]
\[
\text{s.t. } [-1, -1]^T \leq x \leq [2, 1]^T
\]
where the cost function \( f(x) \) is the Adjiman function in [19], i.e.
\[
f(x) = \cos(x^{(1)}) \cdot \sin(x^{(2)}) - \frac{x^{(1)}}{(x^{(2)})^2 + 1}
\]
We show the performances of two algorithms that follow the gRMS paradigm (Algorithm 1), in the black-box and preference-based frameworks respectively. For this example, we assume that, in the black-box case, we are able to measure \( f(x) \) without noise \((\sigma^2_f = 0)\). We approximate \( f(x) \) using surrogate model \((9)\) with \( \beta \) computed as in GLIS \([2]\). Viceversa, in the preference-based framework, we use the preference function in \((6)\) to compare different samples. We still use \( \hat{f}(x) \) in \((2)\) but find \( \beta \) by solving Problem \((12)\), as it is done for GLISp \([3]\). In both cases, we use \( z(x) \) in \((27)\) and define the augmented sample set \( X_{aug} \) using some information on the stationary points of the chosen exploration function, as proposed in \((28)\). Moreover, we adopt the same cycling set \( \Delta_{cycle} = \{0.95, 0.7, 0.35, 0\} \) for black-box and preference-based optimization.

We compare the previously described instances of gRMS to GLIS \([2]\) and GLISp \([3]\) since they both use the same surrogate models and exploration function \([2]\) but employ different acquisition functions. For this reason, we refer to them as GLIS-r and GLISp-r, where the r stands for the same hyperparameters for the surrogates of GLIS \([2]\) and GLIS-r, as well as GLISp \([3]\) and GLISp-r (see \([28]\) for a more formal definition of this algorithm), and set them to the values proposed in their respective papers. The remaining hyperparameters for GLIS \([2]\) and GLISp \([3]\) are selected as suggested by the authors. We remark that, in the original methods, no cycling is performed for their respective exploration-exploitation trade-off parameters. We perform \( N_{MC} = 100 \) Monte Carlo simulations starting from different sets of samples and with budget \( N_{max} = 70 \). Moreover, in the black-box framework we start from 4 samples while in the preference-based one we begin from 8 samples and 7 preferences. The initial sample set \( X \) is generated using a Latin Hypercube Design \([25]\). Figure 2 depicts the results of the Monte Carlo simulations. In the black-box framework, GLIS \([2]\) and GLIS-r exhibit similar performances (same convergence speed). Instead, in the preference-based case, median-wise GLISp \([3]\) finds the global minimizer slightly faster compared to GLISp-r but can get stuck on a local minima (as highlighted by its worst-case performances), see \([28]\) for a more in-depth look. Viceversa, cycling \( \delta \) in \((21)\) as proposed in Section 4.3 leads GLISp-r to converge to \( x^* \) on all Monte Carlo simulations.

![Figure 2: Performance comparison between the different algorithms in the black-box and preference-based frameworks. The thick colored lines denote the median value, the shadowed areas remark the best and worst case instances, the dashed black line is the global minimum \( f(x^*) \) and the black vertical line divides the initial sampling phase and the one based on the minimization of the acquisition function.](image)

7 Conclusions

In this paper, we have thoroughly analyzed and compared the black-box and the preference-based optimization frameworks. Using utility theory, we have shown that, if \( \succeq \) associated to the individual’s criterion is a continuous and complete preference relation, then both black-box and preference-based algorithms aim to solve the same problem, that is Problem \((1)\). The only difference is the information available of the latent \( f(x) \). We focused our attention on surrogate-based methods, which approximate \( f(x) \) using only the data at hand. Then, we proposed a general acquisition function \( a(x) \) in \((21)\), which is an explicit trade-off between the surrogate model \( \hat{f}(x) \) and a proper exploration function \( z(x) \), and shown how it relates to the ones used by other popular surface response methods. After that, we formalized gRMS (Algorithm 1), a general optimization scheme that can be used both in the black-box and preference-based frameworks. Its convergence is guaranteed provided that the chosen exploration function is a proper one and \( \Delta_{cycle} \) includes at least a zero entry.

\[5\text{Formally, GLIS} \([2]\) uses an additional exploration function \( s(x) \), called the IDW variance function, and thus its acquisition function is defined as a weighted sum between \( \hat{f}(x) \), \( z(x) \) and \( s(x) \).]
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