Necessary and Sufficient Conditions for Surrogate Functions of Pareto Frontiers and Their Synthesis Using Gaussian Processes

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Abstract—This paper introduces the necessary and sufficient conditions that surrogate functions must satisfy to properly define frontiers of non-dominated solutions in multi-objective optimization problems. Given that this is the first time that those conditions are elicited, there is no reason to believe that the surrogates already proposed in the literature meet them. As a consequence, dominated solutions can be suggested by already proposed surrogates as valid candidates to represent the Pareto frontier. Conceptually speaking, the new conditions we are introducing work directly on the objective space, thus being agnostic on the evaluation methods. Therefore, real objectives or user-designed objectives’ surrogates are allowed, opening the possibility of linking independent objective surrogates. To illustrate the practical consequences of adopting the proposed conditions, an oversimplified model for the surrogate is shown to be capable of suggesting a valid frontier of non-dominated solutions, though not the exact one from the data provided. On the other hand, when applying Gaussian processes as surrogates endowed with non-dominated soft constraints and with an adjustable degree of flexibility, the necessary and sufficient conditions proposed here are finely managed by the multivariate distribution, guiding to high-quality surrogates capable of suitably synthesizing an approximation to the Pareto frontier in challenging instances of multi-objective optimization.

Index Terms—Gaussian processes; Necessary and sufficient conditions; Non-dominated frontier; Surrogate functions.

I. INTRODUCTION

MULTI-OBJECTIVE optimization (MOO), also called multiple criteria optimization [1], is an extension of the standard single-objective optimization problem, where the objectives may be conflicting with each other [2], [3]. When a conflict exists, we are no more looking for a single optimal solution but for a set of solutions, each one providing a trade-off on the objectives and none being better than the others. This solution set is called the Pareto set and its counterpart in the objective space is denoted the Pareto frontier.

The Pareto frontier is at the core of MOO algorithms, being the foundation of many methods devoted to evaluating the performance and comparing the solutions to each other [4]. However, the frontier is defined by the objectives, which can be expensive to compute [5], [6], [7]. This leads to a variety of surrogate methods that try to approximate the objectives, thus saving computational resources at the cost of possibly reducing accuracy.

Using these surrogates to find good candidates for evaluation and then evaluating with the real objectives can lead to low-quality results, since usually the surrogates are trained or created separately for each objective and do not take into account the innate relationship of the objectives at the frontier [7]. To overcome this limitation, mono-surrogate methods were proposed [8], [9], [10], where one maps directly from the decision space to an evaluation of the solution in comparison to the Pareto frontier. The mapping is constructed using a support vector machine to learn a function where non-dominated solutions provide approximately the same known value and dominated ones provide smaller values. This function then allows the optimization process to grasp inherent relationship between objectives.

Nonetheless, the region indicated as the frontier of non-dominated candidate solutions in these algorithms is a general subspace of the objective space and may violate the definition of a non-dominated frontier. Moreover, these proposed surrogates go from the decision space directly to the evaluation of the frontier, leaving no space for using different methods to approximate each objective, based on prior knowledge.

In this paper, we find the necessary and sufficient conditions that a function must satisfy in order to define a proper frontier of non-dominated candidate solutions, therefore working as a Pareto frontier surrogate. Moreover, the theory is developed based only on the objective space, allowing either correct or approximate objectives to be used, without restricting the format of the objectives’ surrogates. If parametric surrogate objectives are used, their association through the score function can provide feedback on how to adjust their parameters so that the approximation is closer to the real objectives. Furthermore, the theory can also be used to adjust the existing mono-surrogates methods, so that their learnt functions satisfy the conditions required to define a proper Pareto frontier, not simply a generic curve synthesized from a training data set.

Based on the theoretical results, we try to approximate simple but sharp frontiers with very few points using functions as surrogates for the frontier. One of the surrogates is designed to show that, even though it satisfies all theoretical conditions, it does not imply that the expected frontier shape, based on the samples, is the one found by the learning algorithm. The other surrogate is a Gaussian process [11] designed with the theory in mind, which is not restricted to satisfy all conditions and uses them as soft constraints. The proposed Gaussian process correctly finds good approximations, even when the theoretical conditions are slightly violated. This establishes
the gap between the theoretical requirements of surrogates and their capacities to fit the desired Pareto frontier, not an arbitrary one, from its samples, and shows that designing Pareto frontier surrogates with the necessary and sufficient conditions in mind can lead to better approximations.

This paper is organized as follows. Section II introduces the notation and principles of multi-objective optimization used in this paper. Section III shows the conditions that a function must satisfy to define a Pareto frontier, which are then used in Sec. IV to build the two functions to approximate a frontier given some points on it. Finally, Sec. V summarizes the findings and indicates possible further research.

II. MULTI-OBJECTIVE OPTIMIZATION

A multi-objective optimization (MOO) problem is defined by a decision space $\mathcal{X}$ and a set of objective functions $g_i(x): \mathcal{X} \to \mathcal{Y}_i$, $i \in \{1, \ldots, M\}$, where $\mathcal{Y}_i \subseteq \mathbb{R}$ [12]. Since the framework is the same for maximization or minimization, we will consider that minimization is desired in all objectives. For a given point $x$ in the decision space, the point defined by its evaluation using the objectives $y = (g_1(x), \ldots, g_M(x))$ is its counterpart in the objective space $\mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_M$.

Although the objective space usually only makes sense when coupled with the decision space and objectives, which allows for its infeasible region and Pareto frontier to be defined, we will work only with the objective space in this paper, since the results hold for virtually any problem. We will also consider that $\mathcal{Y} = \mathbb{R}^M$, since any restriction on the space for a specific problem is defined by means of the objectives and decision space constraints and are handled transparently.

Furthermore, we assume that the optimal solutions describe a set of $M-1$ manifolds on $\mathbb{R}^M$, which correspond to curves in the 2D case and surfaces in the 3D case. Most multi-objective optimization problems have solutions with this property, with noticeable exceptions, such as: i) problems where some of the objectives do not conflict, so that only one of them should be used in the MOO problem with the other conflicting objectives; while the optimality of the ignored objectives is guaranteed because they were redundant; and ii) some problems with less decision variables $D$ than objectives $M$, such as the Viennot function [13].

Since we are dealing with an optimization problem, we must define operators to compare solutions, like the operators $<$ and $\leq$ are used in the mono-objective case. In MOO, this operator is the dominance.

Definition 1 (Dominance). Let $y$ and $y'$ be points in $\mathbb{R}^M$, the objective space. Then $y$ dominates $y'$, denoted $y \preceq y'$, if $y_i \leq y'_i$ for all $i$.

The definition of dominance used in this paper is the same provided in [3], which allows a point to dominate itself. Another common definition is to require that $y_i < y'_i$ for at least one $i$, and both definitions are consistent with the theory developed in this paper.

Definition 2 (Strong Dominance). Let $y$ and $y'$ be points in $\mathbb{R}^M$, the objective space. Then $y$ strongly dominates $y'$, denoted $y < y'$, if $y_i < y'_i$ for all $i$.

The main difference between the dominance operators in Definitions 1 and 2 is that the dominance allows a point to dominate another even when their values on some coordinates are the same. On the other hand, if $y$ is better than $y'$ in all objectives, then $y$ strongly dominates $y'$. Note also that the strong dominance is more restricted than regular dominance, such that $y < y' \Rightarrow y \preceq y'$.

Once defined the comparison operator, we can divide the space $\mathcal{Y}$ in three sets: an estimated Pareto frontier, the set of points strongly dominated by the estimated frontier, and the set of points not strongly dominated by the estimated frontier.

Definition 3 (Estimated Pareto Frontier). A connected set of points $F \subseteq \mathbb{R}^M$ is said to be an estimated Pareto frontier if no point in it exhibits strong dominance over another point also in $F$, that is, $\forall y \in F, \exists y' \in F: y' < y$.

Definition 4 (Estimated Strict Pareto Frontier). A set of points $F^{*} \subseteq \mathbb{R}^M$ is said to be an estimated strict Pareto frontier if no point in it exhibits dominance over another point also in $F^{*}$, that is, $\forall y \in F^{*}, \exists y' \in F^{*}, y' \neq y: y' \preceq y$.

Since the term “Pareto frontier” is frequently used to mean the optimal achievable and feasible solutions to the problem [3], we use the term “estimated” to emphasize that $F$ can be the best connected set capable of estimating the true Pareto frontier at a given stage of the optimization. So the true Pareto frontier will be part of the estimated strict Pareto frontier only when the optimization process converges. The estimated strict Pareto frontier in turn is always part of the estimated Pareto frontier, by definition.

Therefore, the estimated Pareto frontier defined here is a generalization and an approximation of the true Pareto frontier in two ways: i) if the true Pareto frontier is discontinuous, then dominated points are added so that the estimated Pareto frontier $F$ is connected while also guaranteeing that no point in it exhibits strong dominance over any other; and ii) during the underlying algorithm’s execution, the estimated Pareto frontier is simply a set of points that divide the space into dominated and non-dominated solutions.

Consider, for instance, a problem where one of the objectives is given by

$$g_1(x) = \begin{cases} x + 1, & x < 1 \\ x, & \text{otherwise}, \end{cases}$$

and the other is given by $g_2(x) = -x$. Then the true Pareto frontier $F^{*}$ is given by

$$F^{*} = \{(x + 1, -1) \mid x \in \mathbb{R}, x < 1\} \cup \{(x, -x) \mid x \in \mathbb{R}, x \geq 1\},$$

which clearly is not connected. However, if we add the set of points $\tilde{F} = \{(y, -1) \mid y \in [1, 2]\}$ to $F^{*}$, then the resulting connected set $F = F^{*} \cup \tilde{F}$ satisfies Definition 3 despite the fact that every point in $\tilde{F}$ is dominated by $(1, 1) \in F^{*}$, but not strongly dominated by it.

Figure 1 shows the estimated strict Pareto frontier $F^{*}$, which coincides with the true Pareto frontier, and the connected estimated Pareto frontier $F$ for this problem. This makes it clear that, after concluding the optimization, the estimated
Pareto frontier $F$ contains the true Pareto frontier $F^*$, i.e. $F^* \subseteq F$, while providing a connected 1D manifold that splits the whole objective space $\mathbb{R}^2$. Of course, these properties of the estimated Pareto frontier are extensible to $M > 2$ objectives.

With the definition of an estimated Pareto frontier, the objective space is divided into two sets, named dominated and non-dominated sets, also shown in Fig. 1.

**Definition 5** (Dominated Set). The dominated set $D$ for an estimated Pareto frontier $F$ is the set of all points in $\mathbb{R}^M$ where, for each one of them, there is at least one point in $F$ that strongly dominates it, that is, $D = \{y \in \mathbb{R}^M \mid \exists y' \in F: y' \succ y\}$.

**Definition 6** (Non-Dominated Set). The non-dominated set $\overline{D}$ for an estimated Pareto frontier $F$ is the set of all points that are not in $F$ or $D$. This implies that $\overline{D} = \{y \in \mathbb{R}^M \mid \exists y' \in F: y \prec y'\}$.

Note that, from the definition of strong dominance, both $D$ and $\overline{D}$ are open and unbounded sets, with boundaries defined by the estimated Pareto frontier $F$. Furthermore, after convergence of the optimization process, when $F$ contains the true Pareto frontier, $\overline{D}$ is not achievable by the optimization process.

From the partition of the objective space in three sets, one estimated Pareto frontier, one dominated and one non-dominated set, we can define a score function similarly to [8], [9].

**Definition 7** (Score Function). A score function $f(y): \mathbb{R}^M \rightarrow \mathbb{R}$ for a given estimated Pareto frontier $F$ is a function that satisfies

$f(y) = 0, \quad \forall y \in F,$

$f(y) > 0, \quad \forall y \in D,$

$f(y) < 0, \quad \forall y \in \overline{D}.$

Therefore, a score function provides a single value that places its argument in relation to the estimated frontier. Moreover, for a given estimated Pareto frontier $F$, there are many possible choices of score functions $f(y)$ that satisfy the definition and all of them uniquely define $F$ based on their solution set $f(y) = 0$. This allows a score function to work as a surrogate for the estimated Pareto frontier.

III. NECESSARY AND SUFFICIENT CONDITIONS FOR SURROGATE SCORE FUNCTIONS

In this section, we will show how a score function $f(y)$ can induce an estimated Pareto frontier $F$ and the conditions it must satisfy so that the set it defines is indeed an estimated Pareto frontier, that is, no point in it exhibits strong dominance over any other point in it.

The main theory developed is based on the most general notion of a function $f$, but the conditions may be hard to evaluate for a general case. Therefore, we will also provide corollaries that prove the results for functions with additional constraints, like continuous derivatives. Since some of these results depend on Taylor approximations and the first derivative at the required points may be zero, we must define a generalized gradient.

**Definition 8** (Generalized Gradient). Let $h \in C^k$, where $C^k$ is the class of functions where the first $k$ derivatives exist and are continuous, with $k \geq 1$. Let $k^*(h)$ be the first non-zero derivative of $h$ evaluated at 0, that is,

$k^*(h) = \arg \min_{1 \leq i \leq k} \left( \frac{d^i h}{dx^i} \right)_{x=0} \neq 0,$

where $k^*(h)$ is not defined if $h$ is a constant function or no $i$ satisfies the inequality. Then

$\Delta(h) = \begin{cases} 0, & \exists C, \forall x: h(x) = C \\ \frac{1}{k^*(h)!} \frac{d^{k^*(h)} h}{dx^{k^*(h)}} \bigg|_{x=0}, & \text{otherwise} \end{cases}$

is the generalized gradient operator, which is undefined if there is no $i$ that satisfies the inequality.

The generalized gradient can be used in the Taylor approximation as $h(\delta) \approx h(0) + \delta^i \Delta(h)$, where $0 < \delta \ll 1$ and $\delta' = \delta^{k^*(h)}$. Since the result is based on $\delta$ being a small value, the exact power used to compute $\delta'$ is not important for the approximation.

The extensions to continuous functions $f$ rely on the generalized gradient of a single-parameter continuous function $f$, derived from the original $f$, having different signs for opposite directions. However, it does not hold for functions where $k^*(\cdot)$ is even.

1Consider the function $f(x) = x^3$, which has null gradient at $x = 0$, but is strictly increasing.
For example, consider $h(x) = x^2$, which has $k^*(h) = 2$. The Taylor approximation is given by $h(\delta) \approx \delta^2 \Delta(h(x)) = 2\delta^2 = \delta^2 \Delta(h(-x)) \approx h(-\delta)$, which does not give different signs to different directions of $x$. Therefore, the two constraints on $\Delta(f)$ defined in the corollaries that follow can be viewed as a single constraint on $\Delta(f)$ plus the constraint that $k^*(f)$ is odd.

A. Necessary Conditions

The necessary conditions derived are direct applications of the estimated Pareto frontier’s definition and establishes the basic ground on how to define a function $f$ from a given estimated frontier.

**Lemma 1** (General Necessity). Let $F$ be an estimated Pareto frontier. Let $f(y): \mathbb{R}^M \to \mathbb{R}$ be a score function for $F$. Then $f(y + \delta u) > 0$ and $f(y - \delta u) < 0$ for all $y \in F$, $u \in (0, 1]^M$, and $\delta \in \mathbb{R}, \delta > 0$.

**Proof.** Assume there are $y, u$, and $\delta > 0$ such that $f(y + \delta u) \leq 0$. Let $y' = y + \delta u$, so that $y < y'$.

If $f(y') < 0$, then from the definition of a score function there is some $y^* \in F$ such that $y' \prec y^*$. From the transitivity of dominance, we have that $y < y' \prec y^*$, which is a contradiction, since the point $y^*$ in the frontier cannot strongly dominate the point $y$ also in the frontier. Then we must have $f(y') = 0$, which means $y' \in F$ and also creates a contradiction.

Assume that $f(y - \delta u) \geq 0$, and let $y'' = y - \delta u$. Then we can similarly prove that it also creates a contradiction.

Therefore, there are no such $y, u$, and $\delta$ with $f(y + \delta u) \leq 0$ or $f(y - \delta u) \geq 0$.

This result is intuitive, since moving $\delta$ in direction $u$ from $y$ we enter either $D$ or $\mathcal{D}$. If the function has the required derivatives, then the following result holds.

**Corollary 1** (Differentiable Necessity). Let $F$ be an estimated Pareto frontier. Let $f(y): \mathbb{R}^M \to \mathbb{R}$ be a score function for $F$. Let $f^+_{y,u}(x) = f(y + xu)$ and $f^-_{y,u}(x) = f(y - xu)$. Let $\Delta(f^+_{y,u})$ and $\Delta(f^-_{y,u})$ be defined for all $y \in F$ and $u \in (0, 1]^M$. Then $\Delta(f^+_{y,u}) > 0$ and $\Delta(f^-_{y,u}) < 0$ for all $y \in F$ and $u \in (0, 1]^M$.

**Proof.** Since $f$ satisfies all conditions from Lemma 1 we have that $f(y + \delta u) > 0$ and $f(y - \delta u) < 0$ for all $y, u$, and $\delta > 0$.

In particular, let $\delta \ll 1$. Approximating using Taylor’s series, we have that $f(y + \delta u) \approx f(y) + \delta' \Delta(f^+_{y,u}) > 0$ and $f(y - \delta u) \approx f(y) + \delta' \Delta(f^-_{y,u}) < 0$, where $\delta'$ is the appropriate power of $\delta$ for the expansion. Since $f(y) = 0$ and $\delta' > 0$, then $\Delta(f^+_{y,u}) > 0$ and $\Delta(f^-_{y,u}) < 0$ must hold.

Although this corollary may appear to provide weaker guarantees on $f$, its proof shows that the inequality constraints on the generalized gradient is equivalent to the direct inequalities on the function defined in the previous lemma.

B. Sufficient Conditions

Once defined how the estimated Pareto frontier relates to a given function, we will show that a function that satisfies the results of the previous lemma and corollary in fact uniquely defines an estimated Pareto frontier $F$.

**Lemma 2** (General Sufficiency). Let $f(y): \mathbb{R}^M \to \mathbb{R}$ be a function. Let $F = \{y \in \mathbb{R}^M \mid f(y) = 0\}$ be a connected set. Let $f(y + \delta u) > 0$ and $f(y - \delta u) < 0$ for all $y \in F$, $u \in (0, 1]^M$, and $\delta \in \mathbb{R}, \delta > 0$. Then $F$ is an estimated Pareto frontier.

**Proof.** For $F$ to be an estimated Pareto frontier, we have to prove that for any $y, y' \in F$, $y \neq y'$ we have $y \not\succ y'$. Assume there are $y$ and $y'$ in $F$ such that $y < y'$. Let $u = y' - y$ and $\delta = 1$. Then we have $f(y + \delta u) = f(y') = 0$, which violates the first inequality on $f(\cdot)$. Alternatively, we have $f(y' - \delta u) = f(y') = 0$, which violates the second inequality.

Therefore, there are no $y$ and $y'$ in $F$ such that $y < y'$, and $F$ is an estimated Pareto frontier.

The restrictions on $f(y \pm \delta u)$ may be hard to verify in general, since they must be valid for all $\delta$. However, if the function has the appropriate derivatives, then it becomes easier to check if it satisfies the requirements.

**Corollary 2** (Differentiable Sufficiency). Let $f(y): \mathbb{R}^M \to \mathbb{R}$ be a function. Let $F = \{y \in \mathbb{R}^M \mid f(y) = 0\}$ be a connected set. Let $f^+_{y,u}(x) = f(y + xu)$ and $f^-_{y,u}(x) = f(y - xu)$. Let $\Delta(f^+_{y,u}) > 0$ and $\Delta(f^-_{y,u}) < 0$ for all $y \in F$ and $u \in (0, 1]^M$. Then $F$ is an estimated Pareto frontier.

**Proof.** To use Lemma 2 we must prove that $f(y + \delta u) > 0$ and $f(y - \delta u) < 0$ for all $y \in F$, $u \in (0, 1]^M$, and $\delta \in \mathbb{R}, \delta > 0$.

Suppose there is some $y, u$, and $\delta$ in the domain such that $f(y + \delta u) = 0$. Moreover, let $\delta$ be the smallest value for which this happens for a given $y$ and $u$. Let $0 < \epsilon < 1$ and $\epsilon < \delta$. Then $f(y + \epsilon u) \approx f(y) + \epsilon' \Delta(f^+_{y,u}) > 0$ and $f((y + \delta u) - \epsilon u) \approx f(y + \delta u) + \epsilon' \Delta(f^-_{y,u}) < 0$, where $\epsilon'$ is the appropriate power of $\epsilon$ for the approximation. However, $f(\cdot)$ cannot go from positive to negative without passing through 0 due to its continuity. Then there must be some $\delta' < \delta$ such that $f(y + \delta' u) = 0$, which contradicts the definition of $\delta$.

Therefore, the first inequality on Lemma 2 holds. We can use a similar method to prove the second inequality, and then use the lemma.

Again, this corollary shows the equivalence between the inequalities on the function and on the generalized gradient.

C. Necessary and Sufficient Conditions

Since the symmetry between Lemmas 1 and 2 is clear, we can build a theorem to merge those two and provide necessary and sufficient conditions for defining an estimated Pareto frontier $F$ from a score function $f(y)$.

**Theorem 1** (General Score Function). Let $f(y): \mathbb{R}^M \to \mathbb{R}$ be a function. Let $F = \{y \in \mathbb{R}^M \mid f(y) = 0\}$ be a connected set. Let $D = \{y \in \mathbb{R}^M \mid \exists y' \in F : y' < y\}$ and $\overline{D} = \mathbb{R}^M \setminus (F \cup D)$. Let $f(y) > 0, \forall y \in D$, and $f(y) < 0, \forall y \in \overline{D}$. Then $F$ is an estimated Pareto frontier if and only if $f(y + \delta u) > 0$ and $f(y - \delta u) < 0$ for all $y \in F$, $u \in (0, 1]^M$, and $\delta \in \mathbb{R}, \delta > 0$. 
Proof. Assume that the constraints on \( f \) are valid. Then, from Lemma 2 we have that \( F \) is an estimated Pareto frontier. Now assume that \( F \) is an estimated Pareto frontier. Then, from Lemma 1 we have that the constraints on \( f \) are valid. \( \blacksquare \)

Instead of requiring knowledge of the sign of \( f(y) \) over the sets, we can use a more strict definition, requiring continuity, to guarantee that the result holds. \( \blacksquare \)

Corollary 3 (Continuous Score Function). Let \( f(y): \mathbb{R}^M \to \mathbb{R} \) be a continuous function where there are points \( v_+ \) and \( v_- \) such that \( f(v_+) > 0, f(v_-) < 0, \) and \( v_- < v_+ \). Let \( F = \{ y \in \mathbb{R}^M \mid f(y) = 0 \} \) be a connected set. Then \( F \) is an estimated Pareto frontier if and only if \( f(y) \) is a strictly increasing function over \( F \) such that \( y < y' \).

Proof. Assume that \( F \) is an estimated Pareto frontier. Assume that there are \( y, y' \in D = \{ y \in \mathbb{R}^M \mid \exists y' \in F : y' < y \} \) such that \( f(y') = 0 \) and \( f(y') < 0 \). From the continuity of \( f \), we have that there is some \( z \in D \) such that \( f(z) = 0 \). However, since \( f(0) = 0 \), it is in \( F \). From the definition of \( D \), there is some \( z' \in F \) such that \( z' < z \), which violates the assumption that \( F \) is an estimated Pareto frontier. Therefore, all points in \( D \) have the same sign over \( F \). The same can be show for \( \overline{D} \).

Since \( v_- < v_+ \), we have that \( v_+ \in D \) and \( v_- \in \overline{D} \). Then \( f \) satisfies all conditions from Theorem 1. \( \blacksquare \)

Again, we can replace the constraints on \( f(y \pm \delta u) \) by the constraint on the generalized gradient.

Corollary 4 (Differentiable Score Function). Let \( f(y): \mathbb{R}^M \to \mathbb{R} \) be a function where there are points \( v_+ \) and \( v_- \) such that \( f(v_+) > 0, f(v_-) < 0, \) and \( v_- < v_+ \). Let \( F = \{ y \in \mathbb{R}^M \mid f(y) = 0 \} \) be a connected set. Let \( f^+_{y,u}(x) = f(y + xu) \) and \( f^-_{y,u}(x) = f(y - xu) \). Let \( \Delta(f^+_{y,u}) \) and \( \Delta(f^-_{y,u}) \) be defined for all \( y \in F \) and \( u \in (0,1)^M \). Then \( F \) is an estimated Pareto frontier if and only if \( \Delta(f^+_{y,u}) > 0 \) and \( \Delta(f^-_{y,u}) < 0 \) for all \( y \in F \) and \( u \in (0,1)^M \).

Proof. We can use Corollary 3 to show that the restrictions on \( f(y \pm \delta u) \) must hold. From Corollaries 1 and 2 we know that the restrictions on \( \Delta(f^+_{y,u}) \) are the same as the restrictions on \( f(y \pm \delta u) \), so this corollary is valid. \( \blacksquare \)

Since Theorem 1 together with the presented lemmas and corollaries, define necessary and sufficient conditions for a score description of an estimated Pareto frontier, the search for approximations for the estimated Pareto frontier using surrogate functions should be constrained to, or at least focused on, the ones that satisfy the results. If not, the resulting manifold obtained from \( f(y) = 0 \) may have any shape, possibly with many dominated and/or strongly dominated points, which could result in reduced performance.

IV. LEARNING SURROGATE FUNCTIONS FROM SAMPLES

After showing what conditions the function \( f \) must satisfy, one could ask how to build such function for a given problem and specially how to learn one from a given set of non-dominated points. This can be a hard question to answer in general, but we can provide an additional lemma that can help in many cases.

Lemma 3 (Strictly Increasing Sufﬁciency). Let \( f(y): \mathbb{R}^M \to \mathbb{R} \) be a strictly increasing function on each coordinate. Let \( F = \{ y \in \mathbb{R}^M \mid f(y) = 0 \} \). Then \( F \) is an estimated Pareto frontier.

Proof. For \( F \) to be an estimated Pareto frontier, we have to prove that for any \( y, y' \in F, y \neq y' \) we have \( y \not< y' \). Assume there are \( y \) and \( y' \) in \( F \) such that \( y < y' \).

Let \( P = (p_0 = y, p_1, \ldots, p_{M-1}, p_M = y') \) be a path between \( y \) and \( y' \) that increments only one coordinate at a time. Since \( f \) is strictly increasing, we have that \( f(p_i) < f(p_{i+1}) \).

Thus \( f(y') < f(y') \), which contradicts the premise that \( f(y) = f(y') = 0 \) because they are both in the frontier.

Therefore, there are no \( y \) and \( y' \) in \( F \) where \( y < y' \) and \( F \) is an estimated Pareto frontier. \( \blacksquare \)

Note that, because \( f \) is strictly increasing, there is no point in \( F \) that even dominates another point in \( F \), which was allowed in Definition 3. This restriction can be relaxed to be only monotonically non-decreasing if one can guarantee that \( f(y) = 0 \) is only a manifold, and not a whole subspace. If \( f(y) = 0 \) is a subspace, then we can find two points in it where one dominates the other, which violates the basic definition of an estimated Pareto frontier. For instance, a function that is monotonically non-decreasing and is constant in at most one dimension at a time does not create a subspace on \( f(y) = 0 \).

Nonetheless, this lemma can be used as a guide on how to build a function for the general case. We will build two models that try to approximate the true Pareto frontier from a few of its samples: a guaranteed strictly increasing function, based on the hyperbolic tangent, and an approximated monotonically increasing function, based on Gaussian processes.

Both functions will try to find suitable score functions from samples of the Pareto frontiers, as this is usually the available information that the optimizing algorithm provides. The two test frontiers are given by \( P_1 = [(0,1), (\epsilon, \epsilon), (1,0)] \), which is a convex frontier, and \( P_2 = [(0,1), (1-\epsilon, 1-\epsilon), (1,0)] \), which is a concave frontier, both with \( \epsilon = 10^{-3} \). Note that the points were purposely selected to test the ability to model very sharp frontiers.

A. Strictly Increasing Function

The hyperbolic tangent

\[
\tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1}
\]

is a strictly increasing function of its argument. Thus we can build a strictly increasing function on \( y \) as:

\[
f(y) = a \tanh(b^T y + c) , \quad a, b_i > 0,
\]

whose solution set is given by the plane \( b^T y + c = 0 \).

Since \( f(y) \) is differentiable, we would expect to be able to learn its parameters, and an appropriate estimated Pareto frontier, by reducing the error between the evaluation of points and their target values. A common approach to this problem is to use the gradient descent with squared error.

Since \( f(y) \) must be zero for all points in the frontier, we must define additional points to avoid the trivial solution \( a \to \)
0. Following the definition of $f$ in Corollary 3, we provide $v_- = (-0.5, -0.5)$ and $v_+ = (1.5, 1.5)$ such that their target values are $-1$ and $1$, respectively.

Figure 2 shows the learned function. The set $f(y) = 0$, which is given by the line $b^T y + c = 0$, is indeed a valid estimated Pareto frontier, as expected from the lemma. However, it is very distant from the expected curved shape, which makes it clear that this kind of surrogate is not able to fit the data the way we expected. In this particular case, the surrogate function does not have enough flexibility to learn the desired Pareto frontier.

This example shows that, although the theory is valid, its use to learn an estimated Pareto frontier from a set of points depends on appropriate choices for $f(y)$, which should be able to learn the underlying true shape. Therefore, blindly following the theory developed in this paper and using any function that satisfies the requirements to define an estimated Pareto frontier from its samples, when expecting that the existence of the function means that it will be a good approximate for the desired frontier, is misleading and one must be careful.

B. Gaussian Process As a Function Approximation Problem

Since we have shown that the model should have enough flexibility to fit the given data, an appropriate choice for a surrogate function is a Gaussian process, which always has enough capacity to fit the data. Before describing how a Gaussian process is used to approximate the Pareto frontier, we provide the reader with an overview of how they work. For a more detailed description, we refer the reader to [11].

A Gaussian process (GP) is a generalization of the multivariate normal distribution to infinite dimensions and can be used to approximate a regression problem. A GP defines a probability distribution over functions, such that the outputs are jointly normally distributed.

To better understand this concept, consider two infinite vectors $x, y \in \mathbb{R}^\infty$. Then a function $f: \mathbb{R} \rightarrow \mathbb{R}$ can be described by associating the vector indexes, such that $f(x_i) = y_i$. The GP relies on the fact that the relationship between $x$ and $y$ can be written as:

$$y \sim \mathcal{N}(\mu(x), K(x)),$$

which states that all dimensions of $y$ are distributed according to a multivariate normal distribution with mean $\mu(x)$ and covariance $K(x)$. Moreover, the mean for a given dimension is given by $\mathbb{E}[y_i] = \mu(x_i)$ and the covariance is given by $\text{Cov}(y_i, y_j) = k(x_i, x_j)$, where $k(\cdot, \cdot)$ is a positive semi-definite kernel function.

Although continuous functions, and thus Gaussian processes, are defined for an infinite number of points, which caused the vectors $x$ and $y$ to have infinite dimensions, only a finite number of observations are actually made in practice. Let $N$ be such number of observations. Then, by the marginalization property of the multivariate normal distribution, we only have to consider $N$ observed dimensions of $x$ and $y$. Furthermore, the finite-dimension version of $y$ still is normally distributed according to Eq. (1) when considering only the observed dimensions.

Usual choices for the mean and covariance functions are the null mean, such that $\mu(x) = 0$, and the squared exponential kernel, defined by:

$$k(x, x') = \eta^2 \exp \left( -\frac{1}{2} \frac{(x - x')^2}{\rho^2} \right),$$

where $\eta, \rho > 0$ and $\rho$ is the scale parameter, which defines a representative scale for the smoothness of the function.

Figure 3a shows the prior distribution over functions using the squared exponential kernel with $\eta = 1$ and $\rho = 0.5$ and the zero mean. This highlights the fact that the GP defines a distribution over functions, not a unique function. Three sample functions from this GP are also shown in the same figure. Note that the functions are not shown as continuous, which would require an infinite number of points, but as finite approximations.

To use the GP to make predictions, the observed values of $x$ are split into a training set $X$, whose output $Y$ is known,
and a test set $X_*$, whose output $Y_*$ we want to predict. Since all observations are jointly normally distributed, we have that the posterior distribution is given by:

$$Y_*|X_*, X, Y \sim \mathcal{N}(\mu_*, \Sigma_*)$$  \hfill (2a)

$$\mu_* = K(X_*, X)K(X, X)^{-1}Y$$  \hfill (2b)

$$\Sigma_* = K(X_*, X_*) - K(X_*, X)K(X, X)^{-1}K(X, X_*)$$  \hfill (2c)

where $K(\cdot, \cdot)$ are matrices built by computing the kernel function for each combination of the arguments values.

The posterior distribution for the previous GP, after four observations marked as black dots, is shown in Fig. 3b. Note that the uncertainty around the observed points is reduced due to the observation themselves, and the mean function passes over the points, as expected. Again, three functions are sampled from the posterior, and all agree on the value the function must assume over the observations.

In order to avoid some numerical issues and to consider noisy observations, we can assume that the covariance has a noisy term. Assuming that $y_i = f(x_i) + \epsilon_i$, where $\epsilon_i$ is normally distributed with zero mean and variance $\sigma^2$, then the covariance of the observations is given by $\text{Cov}(y_i, y_j) = k(x_i, x_j) + \sigma^2 \delta_{ij}$. The noiseless value $l_i = f(x_i)$ can then be estimated by:

$$L_*|X_*, X, Y \sim \mathcal{N}(\mu_*, \Sigma_*)$$

$$\mu_* = K(X_*, X)\Omega Y$$

$$\Sigma_* = K(X_*, X_*) - K(X_*, X)\Omega K(X, X_*)$$

$$\Omega = \left[K(X, X) + \sigma^2 I\right]^{-1},$$

which is similar to Eq. (2), except for the added term in $\Omega$ corresponding to the noise.

\section{C. Gaussian Processes with Monotonicity Soft Constraint as Surrogates}

Just like in the previous section, we consider the null mean function and the squared exponential kernel. However, since now we are mapping from the objective space $\mathbb{R}^M$ to a value in $\mathbb{R}$, according to Definition 7 the input values are the objectives $y$ and the outputs the scores $z$.

Since $y$ is multi-dimensional, we use a modified kernel, defined by:

$$k(y, y') = \eta^2 \exp \left(-\frac{1}{2} \sum_{i=1}^{M} \frac{(y_i - y'_i)^2}{\rho_i^2}\right),$$

where $\eta, \rho_i > 0$ and $\rho_i$ are the scale parameters, which defines characteristic length-scales for each objective. This allows automatic relevance determination [11], which ponders the distance measure in each objective automatically.

Let $Y \in \mathbb{R}^{N \times M}$ be a set of $N$ input points and $Z \in \mathbb{R}^N$ their desired targets for training. We define the latent variable $L$ between the two, such that

$$L|X \sim \mathcal{N}(0, K(Y, Y)),$$

where $K(Y, Y)_{i, j} = k(y_i, y_j)$. The latent variable then produces the observed values $Z$ through

$$Z|L \sim \mathcal{N}(L, \sigma^2 I),$$

where $I$ is the identity matrix.

This model is the same as the one described in Sec. 1V-B. However, only the mean prediction will be used in this paper to describe the estimated Pareto frontier. Moreover, we will show how changing the allowed noise level $\sigma$ affects the Pareto frontier approximation.

Besides the observations of $f(y)$ at the desired points, the GP framework also accepts observations of its derivative, since differentiation is a linear operator [15], [16], that is, the
The derivative of a GP is also a Gaussian process. However, since we do not know the desired value of the gradient, only that it should be positive, from Corollary 4 and Lemma 5 forcing an arbitrary value may lead to reduced performance.

Another option is to introduce a probability distribution over the gradient in order to favor positive values, introducing monotonicity information [17]. This new distribution can be viewed as adding constraints to the Gaussian process, making it feasible to include the monotonicity information to the existing framework.

Ideally, the probability distribution over the gradient is the step function, which provides a probability of zero if the gradient is negative and the same probability for all positive gradients. However, the step function defines a hard threshold and does not allow small errors, which can cause some problems for the optimization. Therefore, a smooth function that approximates the step is used to define a soft constraint over the gradient.

Let \( m_{d_i}^{(i)} \) be the indication that the \( i \)-th sample is monotonic in the direction \( d_i \). Then the following probability distribution can be used to approximate the step function:

\[
p \left( m_{d_i}^{(i)} \big| \frac{\partial f^{(i)}}{\partial y_{d_i}} \right) = \Phi \left( \frac{\partial f^{(i)}}{\partial y_{d_i}} \nu \right)
\]

\[
\Phi(\nu) = \int_{-\infty}^{\nu} \mathcal{N}(t|0, 1) \, dt,
\]

where we assume the probit function \( \Phi(\cdot) \) as the derivative probability. The parameter \( \nu \) allows us to define how strict the distribution should be, with \( \nu \to 0 \) approximating the step function or a hard constraint. In this paper, following the suggestion of [17], we use \( \nu = 10^{-6} \).

Since this probability is not normal, it has to be approximated by a normal distribution to be used in the GP framework. We used the expectation propagation algorithm [18], with the update equations described in [17].

Besides this monotonicity constraint, we also would like that the errors between the provided values for the points \( z \) and their latent values \( l \) are small, so that the estimated shape of the Pareto frontier is closer to the true one. This can be achieved by placing a prior inverse-gamma distribution over \( \sigma^2 \), whose density is given by:

\[
p(x; \alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} \exp \left( -\frac{\beta}{x} \right),
\]

where \( \Gamma(\cdot) \) is the gamma function. As \( \beta \to \infty \), this prior is ignored, while \( \beta \to 0 \) indicates that there is no noise. In the results shown, we fix \( \alpha = 3 \) and vary \( \beta \).

We define \( f(y) \) as the final expected value \( E[l^*|y^*, Z, Y, \theta] \), and the parameters \( \theta \) are optimized to maximize the full likelihood, including gradient probability and \( \sigma^2 \) prior, of the training data \( Y \) and \( Z \). We also add the monotonicity constraint on all training data for all directions, but it should be noted that we can also add only monotonicity constraint at a point without defining its desired value. This allows us to find points that have \( f(y) = 0 \) but negative gradient and add the constraint on them, which in turn could improve the estimation.

Similarly to the hyperbolic tangent proposition, using only the points defined by \( P_1 \) and \( P_2 \) leads to a solution where \( f(y) \) is almost 0 everywhere. To avoid this problem, we add a point \((1, 1)\), with target value 1, to \( P_1 \) and a point \((0, 0)\), with target value \(-1\), to \( P_2 \).

Figure 5 shows the resulting curves for different values of \( \beta \). The first thing we notice is that, although \( \beta \to \infty \) does not place any restriction on \( \sigma \), which allows the observed points in the frontier to be far from their latent values that actually define the frontier, the resulting curve is at least more similar to the expected one than the frontier defined by the hyperbolic tangent, shown in Fig. 2.

As we reduce the value of \( \beta \), the observed variance \( \sigma^2 \) is required to be smaller and the frontier shape gets better and better. Ideally, with \( \beta = 0 \), the latent points would be the same as the observed points, but this causes numeric problems due to the monotonicity information and can make it harder to satisfy the monotonicity constraint, due to the smoothness of the GP.
Figure 5: Contours for the $f(y)$ learned using Gaussian process with derivative constraint. The black dots are the frontier points provided.
When we reduce the value to $\beta = 0.01$ and beyond, the resulting frontier is not valid anymore, with noticeable points with negative derivative. However, the largest difference in the concave problem is between points $(0.82, 1.055)$ and $(0.2, 0.985)$, with a total reduction in $y_2$ of just 0.07, and a similar result is obtained for the convex case. Therefore, this approximation is still close to the correct frontier and could be used to evaluate proposed solutions because it was built with the theoretical developments of this paper in mind and tries to approximate them, which most likely provides better frontier estimates than methods that use traditional regression solutions, such as [8], [9], [10], where the manifold $f(y) = 0$ can have any shape.

To evaluate the effect of using the gradient constraint, Fig. 4 shows a similar GP but without any information on the gradients. Although the expected Pareto frontier is correctly identified, there are also many points that do not belong to the frontier and where $f(y) = 0$. Since the unconstrained GP had better frontier estimates for the extreme points than the constrained GP, as all points between them and the knee satisfy the conditions, it appears that not every point benefits from the gradient constraint.

Even though both GP models failed to satisfy the theoretical conditions, we consider that the GP with derivative restriction performed better, both because there are some parameter sets that are able to satisfy the frontier conditions and because it does not violate the restrictions as much. Moreover, if the variance, which is not shown but is higher for points far from the inputs provided, is taken into account, then the violations of the GP with derivatives occur in a region with higher uncertainty than the violations of the pure GP.

Therefore, despite the minor violations of the GP with derivative constraints, this approximation is still close to the correct frontier and could be used to evaluate the proposed solutions.

V. Conclusion

In this paper, we have introduced the necessary and sufficient conditions that functions must satisfy so that their solution space describes an estimated Pareto frontier. These conditions follow from the definition of an estimated Pareto frontier and are extended for differentiable functions, which allows easier verification of the conditions.

Based on these conditions, two function families were tested with very sharp true Pareto frontier. The first one satisfies all the conditions and indeed defines a linear estimated Pareto frontier, but fails to learn the desired frontier shape. This shows that just using a function that fits the theory does not mean that the resulting approximation is close to what would be expected, which happens if the model does not have enough flexibility.

The second descriptor was a Gaussian process, where the theoretical conditions were inserted as soft probabilistic constraints, and a regularization term was added to avoid large deviations from the points and their latent values. The mean latent value is used as surrogate for the Pareto frontier, and some values of the regularization constant allows a correct frontier estimate to be found.

However, when the regularization becomes too strong, the surrogate violates the constraints that define a valid estimated Pareto frontier on some points, but this occurs far from the given inputs and the deviation is small. This suggests that, even under these conditions, the proposed function could be used to provide insight on the shape of the true Pareto frontier, and possibly provide more realistic estimates than other methods that do not take the restrictions into consideration during their design.

We highlight that, although Gaussian processes were used together with the theory on this paper to approximate the Pareto frontier, the theory is general and does not depend on the specific choice of the function descriptor. Therefore, other models that are able to deal with the constraints imposed by the theory, in either a soft or hard way, should be able to learn the desired shape of the Pareto frontier too. Nonetheless, we are not aware of any other method to create the score function in which the constraints are as easy to include as in the Gaussian process. Additionally, a Gaussian process provides robustness to changing the number of points used in the estimation.

Further investigations involve studying the behavior of the Gaussian process to approximate the Pareto frontier with real benchmarks and using some multi-objective optimization algorithm, such as NSGA-II [19], to provide the points. Since the objectives tend to be smoother than in the example frontier provided [20], we expect the estimated Pareto frontier described by a Gaussian process to fit the true Pareto frontier even better in these problems. If this is the case, we will investigate the possibility of integrating the frontier surrogate with other surrogate models for the objectives, so that all of them are learned directly and the number of function evaluations could be reduced.

Another interesting front is to evaluate when the derivative constraints on the points provided is beneficial, since in some points it avoids incorrect association of other points with the frontier, like around the knee in the unconstrained Gaussian process shown in this paper, and in others it may make the estimated shape not satisfy the constraints, like the points in the constrained Gaussian process also shown in this paper. This could not only provide better fit, but may also increase the fitting speed, since less constraints needs to be evaluate, which reduces the size of the Gaussian process and the number of expectation propagation steps required. Therefore an iterative algorithm that adds the constraints as needed should be pursued.

Acknowledgment

The authors would like to thank CNPq for the financial support.

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