On the Construction of Pareto-compliant Quality Indicators

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ABSTRACT

The performance comparison of multi-objective evolutionary algorithms (MOEAs) has been a broadly studied research area. For almost two decades, quality indicators (QIs) have been employed to quantitatively compare the Pareto front approximations produced by MOEAs. QIs are set-functions that assign a real value, depending on specific preferences, to such approximation sets. Mainly, QIs aim to measure the capacity of MOEAs to generate nondominated solutions, the diversity of such solutions, and their convergence to the true Pareto front. Regarding convergence QIs, the Pareto-compliance property is crucial to properly assess the performance of MOEAs. However, in specialized literature, the only Pareto-compliant QI is the hypervolume indicator. In this paper, we propose a methodology to construct new Pareto-compliant indicators based on the combination of QIs. Our preliminary experimental results show that our proposed framework to construct Pareto-compliant QIs introduce new preferences over the Pareto front approximations.

CCS CONCEPTS

• **Mathematics of computing → Continuous functions**; • **Theory of computation → Bio-inspired optimization**; • **Computing methodologies → Continuous space search**;

KEYWORDS

Quality Indicators, Pareto Compliance, Multi-Objective Optimization

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1 INTRODUCTION

In the real world, there are several problems that involve the simultaneous optimization of multiple, often conflicting, objective functions [3]. These are the so-called multi-objective optimization problems (MOPs). Mathematically, MOPs are defined as follows:

$$\min_{\vec{x}\in\Omega} \vec{F}(\vec{x}) = (f_1(\vec{x}), f_2(\vec{x}), \ldots, f_m(\vec{x}))^T , \tag{1}$$

where $\vec{x}$ is the vector of decision variables, $\Omega \subseteq \mathbb{R}^n$ is the decision variable space and $\vec{F}(\vec{x})$ is the vector of m (≥ 2) objective functions, where $f_i : \mathbb{R}^n \to \mathbb{R}$, $i = 1, \ldots, m$. Solving an MOP involves finding the set of best possible trade-offs among the objective functions (i.e., solutions in which an objective cannot be improved without worsening another). The set that yields the optimum values is known as the Pareto optimal set and its image in objective space is known as the Pareto optimal front (PF).

To tackle complex MOPs, multi-objective evolutionary algorithms (MOEAs) have arisen as a popular option in recent years. MOEAs are population-based and gradient-free metaheuristics that are based on the principles of the natural evolution of species [3]. The main idea of MOEAs is to drive the population towards PF by selecting the fittest individuals at each generation, typically using as optimality criterion the Pareto dominance relation,[1]. In consequence, an MOEA produces a Pareto front approximation[2] per execution.

Since the early days of MOEAs, their performance comparison has been widely investigated, focusing on determining the quality of the Pareto front approximations. In the early 1990s, researchers analyzed the outcomes of MOEAs based on qualitative comparisons of the convergence and distribution of solutions [6]. However, the need for quantitative comparisons was evident as the dimensionality of the approximation sets increased. In consequence, some isolated efforts were undertaken to numerically assess the performance of MOEAs [4, 11]. It was until 1999 when David van Veldhuizen, in his Ph.D. thesis [12], provided a comprehensive review of most of the quality indicators (QIs) available at that time and also proposed a non-parametric statistical method to analyze the performance of MOEAs on the basis of QIs. As a result, such a thesis can be considered as a cornerstone regarding QIs.

[1]Given $\vec{x}, \vec{y} \in \mathbb{R}^n$ we say that $\vec{x}$ Pareto dominates $\vec{y}$ (denoted as $\vec{x} \prec \vec{y}$) if and only if $f_i(\vec{x}) \leq f_i(\vec{y})$ for $i = 1, \ldots, m$ and $\exists j \in \{1, \ldots, m\}$ such that $f_j(\vec{x}) < f_j(\vec{y})$. In case $f_i(\vec{x}) \leq f_i(\vec{y})$ for all $i = 1, \ldots, m$, $\vec{x}$ is said to weakly Pareto dominate $\vec{y}$ (denoted as $\vec{x} \preceq \vec{y}$).

[2]Let $\mathcal{A}$ be a finite set of m-dimensional objective vectors. $\mathcal{A}$ is called a Pareto front approximation or approximation set if $\forall \vec{u}, \vec{v} \in \mathcal{A}$, $\vec{u} \neq \vec{v}$ it holds that $\vec{u} \npreceq \vec{v}$ and $\vec{v} \npreceq \vec{u}$.

Mathematically, a unary QI is a function $I : \Psi \rightarrow \mathbb{R}$, where Ψ is the set of all approximation sets of size N. In other words, QIs assign a real value to each approximation set $\mathcal{A}$ related to an MOP [14]. Consequently, QIs impose a total order in Ψ. However, this formal definition does not encompass all the characteristics related to QIs namely, scalability, knowledge-dependence, parameter-dependence, scaling invariance, and performance criteria [8]. Regarding the latter, a QI can measure the number of nondominated solutions, the convergence to PF, the diversity of solutions, or simultaneously the last two aspects. It is worth noting that an important property related to convergence QIs[3] is Pareto compliance[4] that, in summary, ensures that the comparison between the indicator values of two given approximation sets is in accordance with the Pareto dominance relation between both sets. Such property has been extensively studied [14]. Up to date, in the evolutionary multi-objective optimization community, the hypervolume indicator (HV) [13] is the most popular Pareto-compliant QI. HV measures the volume dominated by an approximation set and bounded by an anti-optimal reference set [1]. HV prefers solutions close to the knee of the Pareto front and on its boundary. An important drawback of HV is that its computational cost increases super-polynomially with the number of objective functions. Therefore, other less expensive but weakly Pareto-compliant QIs have been recently proposed, e.g., the $R2$ indicator [2], and the Inverted Generational Distance plus (IGD^+) indicator [7].

Currently, an open research question concerns the possibility to construct new Pareto-compliant QIs having different preferences to those of HV. In this paper, we propose a mathematical methodology to construct Pareto-compliant QIs based on the combination of as many weakly Pareto-compliant QIs as desired with at least one Pareto-compliant QI. To the authors best knowledge, this mathematical framework is the first insight into the combination of QIs in order to produce Pareto-compliant indicators. The advantages of our methodology are threefold: 1) we propose a first methodology to mathematically combine QIs, 2) we extend the number of Pareto-compliant QIs, and 3) it is possible to improve indicators such as $R2$ and IGD^+ by making them Pareto-compliant.

The remainder of this paper is organized as follows. Section 2 presents the mathematical developments to construct Pareto-compliant QIs. Experimental results related to the preferences of the new QIs are shown in Section 3. Finally, Section 4 overviews our preliminary conclusions and some possible research paths.

2 CONSTRUCTING PARETO-COMPLIANT QIS

In the following, we introduce the mathematical framework for the combination of QIs in order to produce Pareto-compliant ones.

Definition 1 (Combination function). *A combination function $C : \mathbb{R}^k \rightarrow \mathbb{R}$ assigns a real value to a vector $\vec{I} = (I_1, I_2, \ldots, I_k)$, where each I_j represents the value of a unary indicator.*

Definition 2 (Combined Indicator). *Given a vector of k indicators $\vec{I} = (I_1, I_2, \ldots, I_k)$ and a combination function C, a combined indicator $\mathcal{I}$ is defined as follows: $\mathcal{I} = C(\vec{I})$.*

[3] For the rest of the paper, we will refer to convergence QIs just as QIs.
[4] Formally defined in the next section.

Clearly, Definitions 1 and 2 describe a combined indicator $\mathcal{I}$ as a general function that transforms a vector of indicator values into a single real value. However, for getting more important theoretical results, we should say something about the properties of each $I_j, j = 1, \ldots, k$ and the combination function. Hansen and Jaszkiewicz [5] defined the case in which the evaluation of two approximation sets by a certain indicator is compatible with the result of a Pareto-based outperformance relation applied to these two sets. Based on this analysis, an indicator could be compliant or weakly compliant with the outperformance relation. In our case, let $\triangleleft$ be the outperformance relation between sets, defined as follows: $\mathcal{A} \triangleleft \mathcal{B}$ means that $\forall \vec{b} \in \mathcal{B}, \exists \vec{a} \in \mathcal{A} \ : \ \vec{a} \preceq \vec{b}$ and $\mathcal{A} \neq \mathcal{B}$. The following two properties formally state both terms. Without loss of generality, let us assume that a greater indicator value corresponds to a higher quality.

Property 1 (Pareto compliance). *Given two approximation sets $\mathcal{A}$ and $\mathcal{B}$, a unary indicator I is $\triangleleft$-compliant (Pareto compliant) if $\mathcal{A} \triangleleft \mathcal{B} \Rightarrow I(\mathcal{A}) > I(\mathcal{B})$.*

Property 2 (Weakly Pareto compliance). *Given two approximation sets $\mathcal{A}$ and $\mathcal{B}$, a unary indicator I is weakly $\triangleleft$-compliant (weakly Pareto compliant) if $\mathcal{A} \triangleleft \mathcal{B} \Rightarrow I(\mathcal{A}) \geq I(\mathcal{B})$.*

Based on the above definitions, we construct a special vector of indicators that is necessary for the refinement of the combined indicator model.

Definition 3 (Compliant Indicator Vector). *The vector of indicator values $\vec{I} = (I_1, I_2, \ldots, I_k) \in Q$ is called a compliant indicator vector (CIV) if $\forall j = 1, \ldots, k$, I_j is weakly Pareto compliant and there exists at least an index $t \in \{1, \ldots, k\}$ such that I_t is Pareto compliant. $Q \subseteq \mathbb{R}^k$ is called the quality space.*

Theorem 1 (Construction of Pareto-compliant combined indicators). *Let $I_1, \ldots, I_k$ be unary indicators that form a compliant indicator vector $\vec{I}$. A combined indicator $\mathcal{I}(\vec{I})$ is $\triangleleft$-compliant if it has the order-preserving property:*

$$\forall \vec{u}, \vec{v} \in \mathbb{R}^k, \vec{u} \succ \vec{v} \Rightarrow \mathcal{I}(\vec{u}) > \mathcal{I}(\vec{v}).$$

Proof. Consider two approximation sets $\mathcal{A}$ and $\mathcal{B}$ such that $\mathcal{A} \triangleleft \mathcal{B}$ and let $\vec{I}^{\mathcal{A}} = \vec{I}(\mathcal{A})$ and $\vec{I}^{\mathcal{B}} = \vec{I}(\mathcal{B})$, where $\vec{I}$ is a CIV. Then, $\mathcal{A} \triangleleft \mathcal{B} \Rightarrow \vec{I}^{\mathcal{A}} \succ \vec{I}^{\mathcal{B}}$ because the Pareto-compliant indicators get better and the weakly Pareto-compliant ones get better or stay equal. Moreover, by definition $\vec{I}^{\mathcal{A}} \succ \vec{I}^{\mathcal{B}} \Rightarrow \mathcal{I}(\vec{I}^{\mathcal{A}}) > \mathcal{I}(\vec{I}^{\mathcal{B}})$. Hence, by transitivity of $\Rightarrow$, it holds $\mathcal{A} \triangleleft \mathcal{B} \Rightarrow \mathcal{I}(\vec{I}^{\mathcal{A}}) > \mathcal{I}(\vec{I}^{\mathcal{B}})$, i.e., $\mathcal{I}$ is Pareto-compliant. □

Theorem 1 provides a sufficient condition for constructing Pareto-compliant combined indicators on the basis of compliant indicator vectors. In other words, a combined indicator preserves the Pareto-compliant property because of the use of order-preserving combination functions.

Remark 1. *The condition of Theorem 1 is suffcient but not necessary. For instance, given $\vec{I} = (I_1, I_2, \ldots, I_k)$ where I_1 is Pareto-compliant and the $I_j, j = 2, \ldots, k$ are not Pareto-compliant, the combined indicator $\mathcal{I}(\vec{I}) = I_1$ is also Pareto-compliant. Hence, there is a large number of possibilities to construct combined indicators.*

There exist many combination functions that have the property of Theorem 1. However, in this paper, we focus on certain utility functions $u : \mathbb{R}^k \to \mathbb{R}$ that hold the desired property [10]. A utility function (UI) is a model of the Decision Maker preferences that assigns to each k-dimensional vector a utility value. Thus, a combination function C can be defined in terms of these functions. Generally, UIs employ a convex weight vector $\vec{w} \in \mathbb{R}^k$ (i.e., a vector that holds $\sum_{i=1}^{k} w_i = 1, w_i \geq 0$). However, for our purposes, we only consider $w_i > 0, i = 1, \ldots, k$ such that all indicator values are considered in the combined indicator. Based on the above, a Pareto-compliant utility indicator (PCUI) is defined as follows:

Definition 4 (Utility indicator). *Given a utility function $u : \mathbb{R}^k \to \mathbb{R}$, an indicator vector $\vec{I} \in \mathbb{R}^k$ that assesses an approximation set $\mathcal{A}$ and a weight vector $\vec{w} \in \mathbb{R}^k$ such that $w_i > 0, i = 1, \ldots, k$, we denote a utility indicator as $u_{\vec{w}}(\vec{I}(\mathcal{A}))$. If u is also order-preserving as required in Theorem 1, $u_{\vec{w}}(\vec{I}(\mathcal{A}))$ is denoted as a Pareto-compliant utility indicator.*

There is a large number of utility functions in the specialized literature [10]. However, we focused our attention on one of the simplest UIs, i.e., the Weighted Sum function (WS). Before using WS to produce PCUIs as claimed in Def. 4, we have to prove that WS is an order-preserving function.

Definition 5. *The weighted sum (WS) is defined by the following formula:*

$$WS_{\vec{w}}(\vec{x}) = \sum_{i=1}^{k} w_i x_i, \tag{2}$$

where $\vec{x}, \vec{w} \in \mathbb{R}^k$ and $w_i \geq 0, i = 1, \ldots, k$.

Lemma 2. *Given two CIVs $\vec{x}, \vec{y} \in \mathbb{R}^k$ and a weight vector $\vec{w} \in \mathbb{R}^k, w_i > 0, i = 1, \ldots, k$, then if $\vec{x} \succ \vec{y} \Rightarrow WS_{\vec{w}}(\vec{x}) > WS_{\vec{w}}(\vec{y})$.*

Proof. Let's prove this lemma by induction. Let us consider, without loss of generality, that the first component of both CIVs is related to a Pareto-compliant indicator and the rest of components are related to weakly Pareto-compliant indicators, i.e., $x_1 > y_1 \wedge x_i \geq y_i, i = 2, \ldots, k$.

Base case:

For $k = 2$, we have $x_1 > y_1 \wedge x_2 \geq y_2$. Then $w_1 x_1 + w_2 x_2 > w_1 y_1 + w_2 y_2$.

Inductive hypothesis:

Given $\vec{x}, \vec{y} \in \mathbb{R}^k$, then $\sum_{i=1}^{k} w_i x_i > \sum_{i=1}^{k} w_i y_i$.

Inductive step:

We want to prove that $\sum_{i=1}^{k} w_i x_i + w_{k+1} x_{k+1} > \sum_{i=1}^{k} w_i y_i + w_{k+1} y_{k+1}$. Without loss of generality, let us assume that the $(k+1)$ components are related to a weakly Pareto-compliant indicator, then $x_{k+1} \geq y_{k+1}$ and for every $w_{k+1} > 0$ it follows that $w_{k+1} x_{k+1} \geq w_{k+1} y_{k+1}$. From the above statement and the inductive hypothesis, we have the following:

$$\sum_{i=1}^{k} w_i x_i + w_{k+1} x_{k+1} > \sum_{i=1}^{k} w_i y_i + w_{k+1} y_{k+1}$$

$$\mathrm{WS}_{\vec{w}}(\vec{x}) > \mathrm{WS}_{\vec{w}}(\vec{y})$$

Hence, $\vec{x} \succ \vec{y} \Rightarrow \mathrm{WS}_{\vec{w}}(\vec{x}) > \mathrm{WS}_{\vec{w}}(\vec{y})$. □

3 EXPERIMENTAL RESULTS

The aim of the experimentation is to investigate the preferences of two PCUIs, i.e., $\mathrm{WS}_{\vec{w}}(\mathrm{HV}, \mathrm{R2})$ and $\mathrm{WS}_{\vec{w}}(\mathrm{HV}, \mathrm{IGD}^+)$ that in the following will be denoted as WS(HV, R2) and WS(HV, IGD$^+$). In both cases, we set $\vec{w} = (0.1, 0.9)$, where the greater component is related to the weakly Pareto-compliant indicator. These two PCUIs represent the Pareto-compliant versions of the $R2$ and IGD$^+$ indicators. The study of preferences is based on correlation analysis, using the Kendall rank correlation coefficient τ which is a rank-based nonlinear correlation coefficient measure [9]. Hence, we investigate the correlation of preferences between HV, $R2$, IGD$^+$, WS(HV, R2) and WS(HV, IGD$^+$) to analyze how they rank the set of all approximation sets. For this purpose, the adopted QIs ranked different Pareto front approximations (related to the Lamé superspheres problems having convex, linear and concave Pareto front shapes) produced by the algorithms SMS-EMOA, NSGA-III, MOEA/D, MOMBI2, NSGA-II, SPEA2, MOVAP, Δ_p-MaOEA, and IGD$^+$-MaOEA. All these MOEAs are adopted in order to have a sample of the set of all approximation sets for such MOPs. The way each QI ranked the MOEAs is analyzed using the Kendall's τ correlation test using a significance value of 0.05.

Figure 1 shows the correlation results using heatmaps. Concerning the correlation between the PCUIs, the preferences of both PCUIs for all convex and linear MOPs are independent for all the objective space dimensions. For concave MOPs, both PCUIs are positively correlated in all cases for 2 objective functions. However, they become independent as the objective dimensionality increases. Such results mean that the preferences of both PCUI are overall different. Regarding the correlation between PCUIs and their base indicators, the following can be claimed: WS(HV, R2) is regularly correlated in a positive way with both HV and $R2$ for 2 and 3 objective functions. However, for 4 objectives, WS(HV, R2) is strongly correlated with $R2$ and its preferences are independent to those of HV in all cases. Hence, WS(HV, R2) shows a switching behavior of preferences between the ones of HV and those of $R2$. This behavior could be an insight of compensation of weaknesses of one QI with the strengths of the other. To validate this hypothesis, WS(HV, R2) could be integrated into the selection mechanism of an MOEA. WS(HV, IGD$^+$) acts in a similar way to WS(HV, R2) with the exception that it presents cases where its preferences are simultaneously independent to both baseline QIs. Additionally, for highly concave MOPs in 4 objectives, WS(HV, IGD$^+$) is correlated to both baseline QIs unlike WS(HV, R2) that is always correlated with $R2$ and independent to HV.

4 CONCLUSIONS AND FUTURE WORK

In this paper, we introduced a mathematical framework for the combination of quality indicators. We proposed to combine several weakly Pareto-compliant QIs with at least one Pareto-compliant indicator, using an order-preserving function, for example, the Weighted Sum function, to generate a new Pareto-compliant QI. The main consequences of our mathematical development are threefold: 1) to provide the first guideline to combine QIs, 2) to increase the number of Pareto-compliant QIs, and 3) to improve weakly

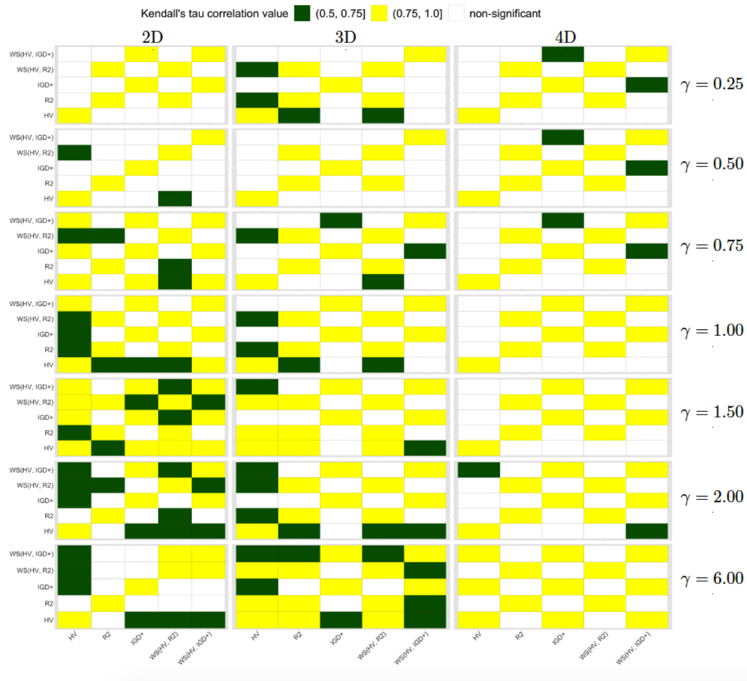

Figure 1: Heatmaps corresponding to the correlation of preferences.

Pareto-compliant indicators, such as $R2$ and IGD$^+$, by making them Pareto-compliant. In the experimental results, we showed a preference analysis of the Pareto-compliant versions of the indicators $R2$ and IGD$^+$ constructed by our methodology. As part of our future work, an in-depth study of the preferences of the PCUIs is necessary to understand their properties. Additionally, we want to study the effect of other order-preserving utility functions for the combination.

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