Towards Rigorous Foundations for Metaheuristic Research

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Abstract: Several authors have recently pointed to a crisis within the metaheuristic research field, particularly the proliferation of metaphor-inspired metaheuristics. Common problems identified include using non-standard terminology, poor experimental practices, and, most importantly, the introduction of purportedly new algorithms that are only superficially different from existing ones. In this paper, we argue that although metaphors may be good sources of inspiration and creativity, being the only reason for publication is insufficient. Instead, adopting a formal, mathematically sound representation of metaheuristics is a valuable path to follow. We believe this will lead to more insightful research.

1 INTRODUCTION

The recent past has seen an increase in research that is critical of numerous trends and practices observed in the field of metaheuristics (Aranha et al., 2021; Fister jr et al., 2016; Molina et al., 2020; Sörensen, 2015; Stegherr et al., 2020; Tzanetos & Dounias, 2021). An influential study by (Sörensen, 2015) points out several broad issues, including irresponsible metaphor usage, poor experimental practices, and misconceptions of what a metaheuristic is.

Others have lamented the poor quality and lack of rigor and insights in published works (see https://github.com/fcampelo/EC-Bestiary).
According to (Campelo & Aranha, 2021; Fister Jr et al., 2016; Sörensen, 2015), this has severe consequences for productivity, the credibility of the field, and the capability to stimulate new, valuable insights effectively.

In this paper, we review the issues raised by various researchers, consider proposed solutions, and argue that metaheuristic studies should adopt a mathematically formulated metaheuristic definition where the underlying philosophy is mindful of the issues affecting the metaheuristic field. We also agree with recent sentiments that metaphors are useful to inspire creativity but are insufficient on their own. We then propose a mindful and rigorous core understanding of metaheuristics.

1.1 Metaheuristics

The term 'meta-heuristic' was coined by Glover in (Glover, 1986), where the authors suggested that Tabu Search could be viewed as a metaheuristic "superimposed" on another heuristic. The suggestion is that metaheuristics operate on a higher level than heuristics.

Early definitions of the term metaheuristic were critically analyzed in (Voß, 2001). These definitions generally suggest that a metaheuristic is a higher-level strategy that guides subordinate heuristics, with some auxiliary constituents such as information for the guiding process and intelligent combinations of various exploration and exploitation concepts.

The meta-level is described as dealing with applying control and strategy to a given domain (Ostrowski & Schleis, 2008). In the context of heuristics being the domain, metaheuristics can then be defined as entities that apply control and strategy to heuristics, as depicted in Figure 1. Metaheuristics consists of a base plan, an integrated learning component, and strategic heuristics. The base plan

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and integrated learning component are utilized only in hyper-parameter tuning, while strategic heuristics are required for all metaheuristic activities. The strategic heuristics apply control and strategy to the heuristics.

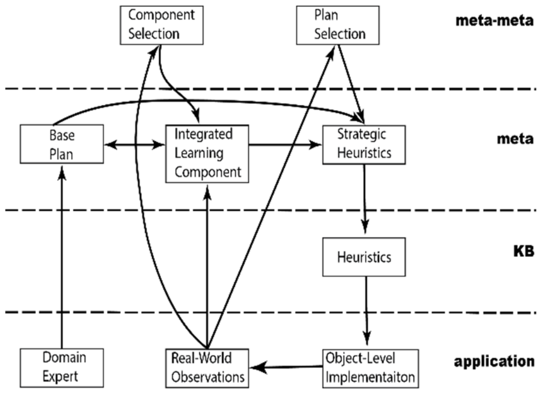

Figure 1: Metarules framework (Ostrowski & Schleis, 2008).

Metaheuristics are described in (Sörensen & Glover, 2013) as frameworks that can be used to derive heuristic optimization algorithms and notes that, in literature, the frameworks and the heuristic optimization algorithms are both referred to as metaheuristics. An elaboration of why the distinction between framework and algorithm is essential when discussing novelty can be found in (Lones, 2020); it can be inferred that, often, a novelty at the algorithm level is hardly a significant feat.

The rest of the paper is structured as follows: a review of several criticisms of the field is given in Section 2. Section 3 briefly reviews potential solutions to these problems discussed in literature. A proposal for instilling rigor in the metaheuristics research space is given in Section 4. This is discussed in Section 5, and Section 6 concludes.

2 METAHEURISTICS AND ITS DISCONTENTS

Several authors have recently pointed to problems afflicting metaheuristic research. This section summarizes these issues.

Irresponsible metaphor usage, in the metaheuristic field, is the use of sources of inspiration, e.g., nature, physics, and human behavior, to be the most, if not the only, pivotal aspect to justify the algorithm as a "new" metaheuristic to the field (Aranha et al., 2021; Sörensen, 2015). These works usually include practices that obscure details by using non-standard terminology (terminology specific to the metaphor/inspiration used). Doing so adds to the challenge of positioning the proposed contribution in literature and may give the impression that the research output is novel. Symptoms of this activity are, according to (Aranha et al., 2021; de Armas et al., 2021; Molina et al., 2020; Sörensen, 2015; Tzanetos & Dounias, 2021), a flood of metaheuristics, numerous cases of very similar/overlapping work, lack of novelty, and according to (Molina et al., 2020) instances where inspirational source and algorithm behaviour are disconnected.

Researchers have also pointed to poor experimental practices. Reports such as (Aranha et al., 2021; Sörensen, 2015; Stegherr et al., 2020; Tzanetos & Dounias, 2021) suggest unfair and biased comparisons such as comparing new proposals to older metaheuristics instead of state-of-the-art and tweaking hyperparameters in favor of a metaheuristic to lift its performance above the rest.

Comparative studies are not transparent enough, resulting in difficulties in extending past studies and existing data (Aranha et al., 2021; Sörensen, 2015). A lack of proper motivation for selecting metaheuristics to compare is common (Stegherr et al., 2020). There is also a lack of rigorous data analytics (Sörensen, 2015). Competitive studies produce very little insight and do not answer or aid in answering the how and why (Birattari et al., 2003; Hooker, 1995), yet comparative studies are still widely setup as competitive ones (Campelo & Aranha, 2021; Sörensen, 2015).

The proliferation of metaphor-inspired metaheuristics is also a cause for concern. A GitHub project called the Evolutionary Computational Bestiary lists a vast and ever-growing number of bio-inspired metaheuristics (with only a few exceptional bio-inspired metaheuristics being exempt) (Campelo & Aranha, 2021). The aforementioned project opposes the flood of metaheuristics, especially the creation of new bio-inspired metaheuristics. Articles and other projects that criticize certain metaheuristic research trends are listed, some of which are intended to parody or ridicule the fact that these trends still exist.

The above criticisms have not been universally accepted. One such counter-argument is that metaheuristics are currently being applied in various domains from numerous disciplines and have also been applied to real-world problems (Torres-Jiménez & Pavón, 2014). The view that metaheuristic research is of poor quality may very well be overly pessimistic and aims to make capital out of flaws in research techniques that are merely pragmatic. The pursuit of being theoretically optimal has little benefit to the real world.

Also, the argument goes, there is a long history of using nature to inspire the development of metaheuristic algorithms. Thus, to reject work that uses natural inspiration is to hinder creativity. The researcher pool has a diverse skill set, i.e., not all possess an advanced mathematical background, and researchers have skills/talents which may lie more in creativity than analytics. Therefore, the move to abandon natural inspiration or inspirational sources, in general, can be interpreted as a move to discriminate against researchers that are more creative than analytical.

To refute these arguments, we refer to a study by (Ven & Johnson, 2006) that explores the relationship between scholarly and practical knowledge. It analyses ways in which the discrepancies between these domains have been framed and discusses methods to address this, such as a method of engaged scholarship (proposed by the aforementioned study). From the study, it can be understood that practical and scholarly knowledge have different contexts and objectives. Practical knowledge deals with specific circumstances in certain scenarios, while scholarly knowledge deals with viewing specific circumstances as instances of a more general case to further understand and explain how what is done works. Reaping both benefits can be achieved through methods of communication between both spaces. This entails that the scholarly domain must be robust so that new knowledge can be framed efficiently amongst existing knowledge and communicated effectively to practical domains and other scholarly domains.

Recent studies have shown instances of scholarly work claiming to be novel, but the novelty does not stand up to scrutiny. Comparative studies have been questioned regarding their transparency and choice of experimental practices. The overloading of well-known concepts with non-standard terminology is creating confusion in literature. In summary, the issues highlighted by several publications are indicators that the metaheuristic research space falls extremely short of ideal conditions for a scholarly domain.

According to (Swan et al., 2015), expressing metaheuristics via mathematical formulations facilitates a rigorous definition of the term metaheuristic. Some may criticize and label this decision as systematically marginalizing creative research because mathematical definitions often use cryptic notation that may not be friendly to researchers without an advanced mathematical background and with a different skill set. However, the benefits of using mathematical formulations (more specifically, functional descriptions), as listed and discussed in (Swan et al., 2015), include promoting better communicability, reproducibility, interoperability, facilitating automated metaheuristic assembly, and promoting scientific advancement. Therefore, using mathematical formulations does not marginalize creative research; instead, it guides creativity.

The No Free Lunch theorem (Wolpert & Macready, 1997) being a valid premise in the argument for justifying the existence of a vast number of metaheuristics in the research space, is viewed as unclear in (Lones, 2020). The study also speculates that the argument may have substance as the performance of different optimizers varies when subjected to different problems. However, a discussion is presented in (Camacho-Villalón et al., 2022) that criticizes the aforementioned argument as being based on a misunderstanding of the No Free Lunch theorem for optimization and that the vast number of published metaheuristics based on metaphors are creating confusion in the research space, leading it away from proper scientific goals. Therefore, relying on the No Free Lunch theorem is not advisable to support the creation of a novel metaheuristic.

3 A REVIEW OF POTENTIAL SOLUTIONS

Several authors have not only given critical commentary on the field but have also suggested potential solutions.

The solutions to the metaheuristic research quality issues require adoption by researchers so that their impact, as argued in the respective research publications, may influence the metaheuristic research space. Increasing awareness about issues associated with metaphor-based research is therefore essential to stimulate the adoption of these solutions (Campelo & Aranha, 2021), and it is a recurring theme in many such publications, e.g., (Lones, 2020; Sörensen, 2015; Stegherr et al., 2020; Tzanetos & Dounias, 2021). Projects such as the Evolutionary Computational Bestiary are also ways to raise awareness.

A component-based view of metaheuristics, as a solution to the issues afflicting the metaheuristic research space, is highlighted in (Sörensen, 2015). This view suggests understanding metaheuristics as sets of general concepts, accompanied by the decision to distinguish metaheuristics from the optimization algorithms derived from them. Its widespread adoption may help resolve several of the problems discussed above. The component-based view of metaheuristics deals with conceptualization at the foundational layer, i.e., where definitions, taxonomies, ontologies etc., are crucial.

Applying mathematical formulations to express metaheuristics facilitates a rigorous definition of the term metaheuristic (Swan et al., 2015). Several definitions of the term metaheuristic incorporate tuples. Tuples encapsulate the specifications, main components, and sometimes structures that hold the relationships between the specifications and components.

The study by (Wang, 2010) provides worded definitions for the terms metaheuristic and metaheuristic computing. The study provides a rigorous definition of metaheuristic computing using tuples, in which the elements are concept algebra structures.

A tuple definition for population-based metaheuristics is presented as part of the unified framework for population-based metaheuristics introduced in (Liu et al., 2011).

The work done in (Cruz-Duarte et al., 2020) defines a metaheuristic as a map (expressible in terms of three components: initializer, search operator, and finalizer heuristics) from an arbitrary domain to a feasible domain of an optimization problem.

As part of the proposed design of a software framework to solve combinatorial optimization problems presented in (Peres & Castelli, 2021), a metaheuristic – actually an abstract metaheuristic – is defined as a map from a domain of specifications (encapsulated in a tuple) to a set of possible variations of the metaheuristic.

Swan et al. (Swan et al., 2015) advocate for metaheuristics to be described entirely in terms of functions (which are essentially maps), in which metaheuristics are parameterized by their environment, state, and the environments of the employed components. The environment, in this sense, refers to information required during execution, and the state refers to the solution in chosen representation form. The component heuristics are also parameterized with their environment and state.

The component-based view proposed by (Sörensen, 2015) is meritorious but has drawbacks if not used properly (Achary & Pillay, 2022). Definitions such as those presented by (Cruz-Duarte et al., 2020; Liu et al., 2011) express metaheuristics in terms of components, but as emphasized above, the ambiguity present in the definitions by (Cruz-Duarte et al., 2020) may lead to conflicting understandings. The definition by (Liu et al., 2011) uses biological terminology and thereby promotes the metaphor-based philosophy of metaheuristics. However, metaphor usage, non-standard terminology, and natural inspiration have been criticized in literature, indicating that the perspective used may nullify the long-term advantages of using the component-based view.

The framework proposed in (Peres & Castelli, 2021) resolves this ambiguity by providing mathematically formulated definitions of conceptual-level and concrete-level metaheuristics. Both are formulated as maps. The former maps from a tuple of abstract specifications to a set of concrete heuristic optimization algorithms, and the concrete heuristic optimization algorithms map from their concrete specifications to an optimal solution.

4 A PROPOSED SOLUTION

4.1 Towards a Rigorous Foundation for Metaheuristic Research

Conducting meaningful metaheuristic research for both the long and short term requires metaheuristic research to adopt strong foundations and a rigorous core.

The study by (Campelo & Aranha, 2021) summarizes some promising alternative approaches to conducting research in metaheuristics rather than relying on metaphor-based techniques. They propose understanding metaheuristics as frameworks of semi-independent modules that influence one or more intrinsic algorithmic structures. This is similar to the proposal made in (Sörensen, 2015) to see metaheuristics as frameworks and not concrete heuristic optimization algorithms. Defining metaheuristics as functions is advocated in (Swan et al., 2015), which also suggested a specific template for expressing these functions. Describing metaphor-based metaheuristics using standard terminology that effectively describes similarities and differences between metaheuristics is motivated in (Lones, 2020). Comparing metaheuristics with structure-wise similarity metrics, which facilitates determining special-case and general-case relationships between metaheuristics, is made possible by the work in (de Armas et al., 2021). Using existing taxonomies from literature rigorously is facilitated by work done in (Achary & Pillay, 2022).

Each of the above contributions has little overlap and a strict scope. Using these contributions together may be effective for establishing strong foundations for metaheuristic research and stimulating good quality, insightful research.

A rigorous foundation for metaheuristic research that makes use of the contributions, advice, and guidelines of existing literature is proposed below.

A philosophy of metaheuristics that is mindful of the issues affecting the field is provided by (Sörensen & Glover, 2013) and further explained in (Sörensen, 2015). In this view, metaheuristics are problem-independent frameworks that provide a set of guidelines to create heuristic optimization algorithms and are not the heuristic optimization algorithms themselves.

Mathematical definitions are known to be rigorous, and there are also added benefits to expressing metaheuristics as functions (Swan et al., 2015). Metaheuristics could be formulated as:

$$M: S \rightarrow A \tag{1}$$

Where M is an arbitrary metaheuristic and S is a set of tuples of specifications. The metaheuristic M has an influence on the tuple format, and a tuple of the set S must contain at least one heuristic operator. A is the set of heuristic optimization algorithms, each of which the rules of M can construct using a certain element of S. A proof-of-concept for the formulation in (1) can be found in Section 4.2.

The format and values of the tuples in the set S may be determined using the works of (Lones, 2020) and (Achary & Pillay, 2022). The novelty and influence of metaheuristics can be determined by applying the work of (de Armas et al., 2021) to metaheuristics defined in terms of (1).

This map formulation (1) aligns with the component-based view, as it guides the researcher to elucidate which components are variable in the specification tuple, thus providing scope for experiments in future research.

The restriction that an element of S must contain at least one heuristic operator enforces the component-based view and avoids scenarios where hyper-parameter values are the only elements of a specification tuple.

This map is very abstract and does not have many restrictions on how one may specialize it with details. Its intended use is to be a rigorous underlying conceptualization of what a metaheuristic is when proposing a concrete formulated definition for future research; this underlying conceptualization enforces alignment with the component-based view and considers the insights, advice, suggestions, and guidelines from existing literature on the problems within the metaheuristic field.

4.2 Proof of Concept

The Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Bat Algorithm (BAT), and Differential Evolution (DE) metaheuristics are used to illustrate how the formulation in (1) could be used; a description of each of the aforementioned metaheuristics can be found in (Yang, 2020).

4.2.1 Genetic Algorithm

1. Substitute GA in place of M.
2. An element of S would then contain the initializer, crossover operator, mutation operator, selector, and terminating condition.
3. An element of A will be a resulting concrete Genetic Algorithm.

4.2.2 Particle Swarm Optimization

1. Substitute PSO in place of M.
2. An element of S would then contain the initializer, location update, velocity update, and terminating condition.
3. An element of A will be a resulting concrete Particle Swarm Optimization algorithm.

4.2.3 Bat Algorithm

1. Substitute BAT in place of M.
2. An element of S would then contain the initializer, position update, velocity update, local search technique, and terminating condition.
3. An element of A will be a resulting concrete Bat Algorithm.

4.2.4 Differential Evolution

1. Substitute DE in place of M.
2. An element of S would then contain the initializer, crossover operator, mutation operator, and terminating condition.
3. An element of A will be a resulting concrete Differential Evolution algorithm.

5 DISCUSSION

The definition of metaheuristics adopted by a researcher will significantly influence their metaheuristic research.

A contributing factor to the proliferation of novel metaheuristics is arguably the ambiguity of whether metaheuristics are frameworks, concrete heuristic optimization algorithms, or both. The study in (Sörensen, 2015) remarks that it is unfortunate that the term "metaheuristic" is used for both general, problem-independent, algorithmic frameworks and concrete heuristic optimization algorithms derived from these frameworks and further expresses that metaheuristics are not algorithms, but they are each a set of ideas, concepts, and operators from which heuristic optimization algorithms can be derived.

The definitions presented in (Cruz-Duarte et al., 2020; Liu et al., 2011; Voß, 2001; Wang, 2010) fail to resolve this ambiguity. Difficulty in determining the novelty of new proposals may result from this ambiguity since a heuristic optimization algorithm could be related to a few or many concepts, ideas, or operators of a framework, garnished with a metaphor and non-standard terminology, then published as a novel metaheuristic.

Comparative studies of metaheuristics have received criticism in the literature (Aranha et al., 2021; Sörensen, 2015). A flaw that has been highlighted is that the implementations of metaheuristics, whose selections are poorly motivated (Stegherr et al., 2020), are compared, and the results could be misunderstood as representative of the framework.

Using metaphors and natural sources of inspiration has led to the creation of well-known, influential, and disruptive contributions such as Particle Swarm Optimization, Genetic Algorithm, Simulated Annealing, and Ant Colony Optimization, as indicated in (Camacho-Villalón et al., 2022). However, the incorporation of natural inspiration in research must outweigh the cost.

Research into the trends of metaphor and inspirational source usage (Aranha et al., 2021; Campelo & Aranha, 2021; Fister jr et al., 2016; Sörensen, 2015; Tzanetos & Dounias, 2021) has shown that metaphors and non-standard terminology introduce challenges when trying to frame metaheuristics amongst existing literature. It facilitates work similar to existing literature to be published as novel work. Non-standard terminology confuses readers and clouds the relevance and the link of the phenomenon described by the terms to the metaheuristic.

A flood of metaheuristics has been linked to metaphor and inspiration source usage. Research by (Molina et al., 2020) showed that there are many more inspiration sources than algorithmic behaviors. Hence, it can be said that inspiration source usage is a heuristic, in the general sense, for creativity, similar to the exploration of ideas. However, there is too much exploration and not enough rigor. Since metaphor/inspiration usage enhances creativity, it is insufficient on its own; this analogy is similar to those used in (Fister jr et al., 2016; Lones, 2020) with the similar computational optimization terminology

Although various publications argue that new novel metaheuristics are not needed at this point in the field's timeline, if a metaheuristic is to be published, it should be accompanied by a formulation of the metaheuristic in the format of (1). M represents the abstract pseudocode, ideas, and concepts that make up the metaheuristic. The format of elements of S will convey which components are variable, i.e., different concrete components can be substituted in their respective placeholders, which is then passed to M to create a concrete optimization algorithm of the set denoted by A in the formulation.

6 CONCLUSION

In this study, it is argued that metaheuristics studies should adopt a mathematically formulated metaheuristic definition where the underlying philosophy is mindful of the issues affecting the metaheuristic field; in other words, adopt definitions that sustain good quality research. Mathematical formulated definitions are rigorous and leave less room for vagueness that can lead to convenient interpretations. Ambiguities in adopted or proposed definitions can potentially allow choosing a definition/perspective/interpretation of the shelf that suits a requirement for publication, leading to low-quality research. The underlying philosophy of the mathematically formulated definition must be mindful of issues affecting metaheuristic research to prevent the definition from having the potential to stimulate problematic trends.

This work takes the stance that inspiration source usage is a good heuristic for creativity but is not needed right now; it has the capacity to become saturated, which is detrimental to the field. Intensifying research on existing work would be a better practice at present.

Increasing theoretical insight, better analytical techniques, and solid foundations should be a top priority of metaheuristic research.

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