Proceedings of the ASME 2021 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference IDETC/CIE 2021 August 17-20, 2021, Virtual, Online

IDETC2021-71226

LEVERAGING DESIGN HEURISTICS FOR MULTI-OBJECTIVE METAMATERIAL DESIGN OPTIMIZATION

Roshan Suresh Kumar* Department of Aerospace Engineering Texas A&M University College Station, Texas 77840 roshan94@tamu.edu Srikar Srivatsa Sibley School of Mechanical and Aerospace Engineering Cornell University Ithaca, New York 14850 sms722@cornell.edu

Meredith Silberstein

Sibley School of Mechanical and Aerospace Engineering Cornell University Ithaca, New York 14850 meredith.silberstein@cornell.edu

Daniel Selva

Department of Aerospace Engineering Texas A&M University College Station, Texas 77840 dselva@tamu.edu

ABSTRACT

Design optimization of metamaterials and other complex systems often relies on the use of computationally expensive models. This makes it challenging to use global multi-objective optimization approaches that require many function evaluations. Engineers often have heuristics or rules of thumb with potential to drastically reduce the number of function evaluations needed to achieve good convergence. Recent research has demonstrated that these design heuristics can be used explicitly in design optimization, indeed leading to accelerated convergence. However, these approaches have only been demonstrated on specific problems, the performance of different methods was diverse, and despite all heuristics being "correct", some heuristics were found to perform much better than others for various problems. In this paper, we describe a case study in design heuristics for a simple class of 2D constrained multiobjective optimization problems involving lattice-based metamaterial design. Design heuristics are strategically incorporated into the design search and the heuristics-enabled optimization framework is compared with the standard optimization framework not using the heuristics. Results indicate that leveraging design heuristics for design optimization can help in reaching the optimal designs faster. We also identify some guidelines to help designers choose design heuristics and methods to incorporate them for a given problem at hand.

NOMENCLATURE

- *x* Design variable
- f(x) Objective function
- C_{11} Effective metamaterial stiffness in horizontal direction
- C_{22} Effective metamaterial stiffness in vertical direction
- v_f Volume fraction of complete truss design
- *E* Young's Modulus of constituent material
- *l* Side length of lattice unit
- *d* Diameter of truss member
- *c*_{target} Target stiffness ratio
- $g_{f eas}$ Design feasibility score
- g_{conn} Design connectivity score
- g_{stif} Design stiffness ratio constraint
- g_{pc} Design partial collapsibility score

^{*}Address all correspondence to this author.

g_{np} Design nodal properties score
<i>g</i> orient Design orientation score
<i>g</i> _{inter} Design intersection score
g_{pen} Total penalty function
w_{stif} Penalty weight for stiffness ratio constraint
w _{con} Penalty weight for feasibility and connectivity constraint
PF Pareto Front
<i>d</i> _{PF,pen} Minimum distance to penalized Pareto Front
$d_{PF,true}$ Minimum distance to true Pareto Front
<i>sup</i> Support of association rule
<i>conf</i> Confidence of association rule
<i>lift</i> Lift of association rule

INTRODUCTION

The design of mechanical meta-materials and other complex engineered systems such as spacecraft has traditionally relied on the use of computationally expensive models such as finite element simulations. Moreover, these problems are often nonconvex, constrained, multi-objective, mixed integer optimization problems for which efficient algorithms are not known. Global multiobjective optimization algorithms such as evolutionary algorithms are often used to solve these problems, but in some cases they require many function evaluations to reach the optimal regions of the design space. Several methods have been proposed to reduce the number of function evaluations needed to achieve a certain level of convergence, such as surrogate-assisted methods [1,2], Bayesian optimization [3,4], or using expert knowledge, either biasing the initial population, using hard or soft constraints, or using specialized operators [5,6]. Methods leveraging expert knowledge are particularly interesting, either in isolation or to complement data-driven methods, since: 1) They do not require many expensive function evaluations to tune the models, unlike some data-driven methods. 2) Large databases containing knowledge in the form of design heuristics or lessons learned in a format that facilitates integration into a computational tool (e.g., SysML, knowledge graphs) are becoming more common in organizations [7,8]. Moreover, recent research in design automation has found that incorporating design heuristics explicitly into design optimization has the potential to improve the efficiency of the search for optimal designs [9, 10].

The definition of a design heuristic considered in this paper is taken from Fu et al. [11] and has been derived from an extensive literature survey: A context-driven directive, based on intuition, tacit knowledge, or experiential understanding, which provides design process direction to increase the chance of reaching a satisfactory but not necessarily optimal solution. Extraction of design heuristics can be done using interviews [12], examination of high quality products [13] or through data-driven methods [14, 15]. Heuristics are commonly used in design optimization to overcome computational hurdles [16]. They are essentially rules of thumb, situated in either intuition or domain experience that can be utilized to improve computational efficiency [12, 16] but at the expense of guarantee of optimality and completeness of the solution set [17]. In this paper, we attempt to use such heuristics explicitly to accelerate design optimization. Note that according to this definition, optimal designs do not necessarily need to abide by a heuristic, but searching for heuristic-satisfying designs should lead to satisfactory and optimal designs faster.

For example, in the earth observation satellite system design problem described in [18], wherein the goal is to find satellite constellations maximizing science benefit while minimizing mission cost, examples of the heuristics used include: 1) avoiding satellites in the constellation with payload mass of more than 1500 kg, since that leads to diseconomies of scale and/or insufficient resources on board for all instruments, thus degrading both science and cost; 2) putting synergistic instruments on the same satellites, and separating instrument with negative interactions in different platforms; 3) targeting a satellite size and weight that leads to high packaging efficiency factors given a launch strategy, which leads to launch cost savings without affecting science.

The utility of employing heuristics in the design optimization process is empirically demonstrated in a comparison study in Binder and Paredis [19]. To demonstrate their newly developed Design Decision Framing Method, an algebraic heuristic enabled design method is compared with expert and non-expert variants of a computational optimization based expected utility maximization approach for the design of a pressure vessel. The algebraic design method incorporates a heuristic based inbuilt factor of safety, using it to compute two wall thicknesses and choose the conservative option. It is found that the algebraic heuristic based design method outperforms the non-expert based optimization approach under certain conditions. It is worth mentioning that the algebraic heuristic optimization algorithm is an instance of the incorporation of expert heuristics into the optimization framework.

While the incorporation of design heuristics for design optimization has been demonstrated on specific problems, the utility of this approach has not been systematically demonstrated across a wide range of problems. Here, we seek to extend our understanding of how to utilize heuristics through the example of mechanical metamaterial design. Metamaterials are materials whose properties are determined by geometry of a repeated microstructure, in addition to the intrinsic mechanical properties. The inverse metamaterial design problem has been found to be challenging owing to the potentially large design space. Consequently, design of metamaterials for mechanical properties is a large field, spanning ad hoc knowledge-driven approaches and formal design methodologies [20-22]. Topology Optimization is the most common method for 3D metamaterial design, especially when elastic properties are of interest, thanks to its balance of generality and efficiency [23, 24]. Typically, a finite element based method is used to compute the material properties of the candidate structure filling a certain region of the design space and the numerical optimization approach drives the design search towards the region with the required material properties and density. Many machine learning and system design techniques have also been applied to the metamaterial design problem [25–30]. The particular material design problem in this paper was selected because it has hard constraints that are difficult to satisfy, in addition to two conflicting objectives. This essentially creates a dynamic objective function that focuses first on finding feasible designs, then optimal ones. This aspect was not present in any of the problems previously studied to leverage design heuristics [31–33].

Two main challenges exist in leveraging expert knowledge in design optimization: selecting heuristics and selecting methods to leverage those heuristics. Hitomi and Selva [5] noted that even though by definition all design heuristics are "good" (in the sense that they capture a directive which when applied to the specific context described in the heuristic should improve the quality of the design), not all heuristics actually have a positive impact when used in a specific problem. For example, in [5], some of the heuristics used were naturally satisfied by most designs in the design space due to the specifics of the problem formulation, rendering that heuristic not useful for the problem. Another reason why good heuristics may not be useful for a particular problem is that the heuristic could be aligned with some of the objectives but actually conflict with a more important objective or hard constraint. Even if the best possible set of heuristics were chosen for a given problem, there are still questions about the best methods to leverage those heuristics. Design heuristics have been used in different ways to accelerate optimization, including as repair search operators, as soft or hard constraints, or as biased prior probability distributions to generate initial populations [34,35]. For example, biasing an initial population is a very soft method of incorporating heuristics. As demonstrated in [5], different methods may lead to widely different performance, and there is little guidance about when to use different methods.

In this paper, we describe a case study in design heuristics for a simple class of 2D constrained multiobjective optimization problems involving design of lattice-based metamaterials for targeted mechanical properties. In addition to comparing the heuristics enabled optimization framework to a standard optimization framework (based on the popular ϵ -MOEA algorithm [36]), guidelines on how to leverage design heuristics for design optimization, identified during the course of the case study, are presented.

The paper is structured as follows: First the case study is presented, followed by a detailed discussion on the different methods of representation of design heuristics and the methods to incorporate them into the design optimization process, recommendations on heuristic metrics, results from the case study, and finally recommendations for future utilization of heuristics.



FIGURE 1: An example design in the 2D 3x3 square node grid design space is shown in (1a) with an example truss design is illustrated with the nodes in red and the members in black. The same lattice is shown in a 3x3 repeated form in (1b).

CASE STUDY PROBLEM FORMULATION

The constant radius truss design problem considers a 2D 3x3 node grid shown in Fig. 1a. This 2D node grid represents a single repeat unit cell of the metamaterial and is the design space to explore. The design decisions are binary variables that represent the presence or absence of truss members within the 3x3 node grid. Allowing for all possible connections between pairs of nodes, there are 36 possible truss members. However, to account for repetition of lattice units in the two orthogonal directions, the design decisions corresponding to members on opposite edges must be the same. For this problem, the decisions for the left and bottom edge members are determined by the optimization algorithm and replicated for the right and top edge members respectively– thus making the design vector to be optimized 30 elements long. All model evaluation was performed with custom MATLAB scripts as described conceptually below.

The full stiffness matrix for each design is evaluated by modeling the lattice as a truss - each linear elastic member can only deform axially and connects to other members only at the nodes, which are modeled as pin joints. The stiffness values of individual members are combined based on shared member endpoints to form the global stiffness matrix. The effective material stiffness tensor is then calculated by applying a series of controlled displacements to the boundary of the lattice, calculating force, and normalizing by area to obtain stress components. In this paper, we are focused on the normal horizontal and vertical moduli, C_{11} and C_{22} respectively, which are components of this stiffness tensor. The volume fraction of the design is found by dividing the sum of the volumes of all members by a volume of the same side length and thickness of the unit cell. Based on convergence of the moduli, all values were calculated using 3x3 repeats of the 3x3 node grid as depicted in Fig. 1b. The radius of each member and side length of the lattice unit are fixed at 250 μm and 10 mm respectively. The constituent material is assumed to be SIL (elastic modulus of 1.8162 MPa).

An unrestricted design space of all possible connectivity between nodes contains many designs that are not realizable as metamaterials. First, nodes cannot be connected to exactly 1 member, as this member will then not actually connect with the rest of the material. Second, no members can cross or overlap since they would then occupy the same physical space. These hard requirements are enforced as the connectivity function (g_{conn}) and feasibility function ($g_{f eas}$), respectively. To facilitate the optimization, constraint functions are defined for each constraint that span from 0 to 1, with 1 representing no violations and 0.1 subtracted for each violation.

The selected multiobjective combinatorial design optimization problem is formalized in Eqn. 1. The goal is to maximize vertical stiffness while minimizing volume fraction of the repeated lattice configuration, subject to constraints on design feasibility, design connectivity and an additional constraint representing a target stiffness ratio.

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) = \begin{bmatrix} -C_{22} & v_f \end{bmatrix}^T$$
s.t.
$$1 - g_{f eas}(\mathbf{x}) = 0$$

$$1 - g_{conn}(\mathbf{x}) = 0$$

$$g_{stif} = 0$$
(1)

Here, $g_{stif} = \left| \frac{C_{22}}{C_{11}} - c_{target} \right|$, and we will present results only for $c_{target} = 1$. The feasibility and connectivity constraints are enforced using the interior penalty method [37] with a base 10 logarithm. The log_{10} function gives a zero value for completely feasible and fully connected designs and a greater negative value the further a design is from full feasibility and connectivity. The lowest feasibility and/or connectivity score a design can achieve is 1.1×10^{-16} (as a result of MATLAB's precision limitations), so the largest penalty that can be levied on a design for complete infeasibility or non-connectivity is near 16. The constraint penalty terms are appended to the objectives with their corresponding weights and the multi-objective optimization algorithm optimizes the two penalized objectives, shown in Eqn. 2. The penalty term $g_{pen}(\mathbf{x})$ is defined in Eqn. 3.

$$f_{pen}(\mathbf{x}) = \begin{bmatrix} -\frac{C_{22}}{v_F^E} \\ \frac{v_F^E}{0.96} \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} g_{pen}(\mathbf{x})$$
(2)
$$g_{pen}(\mathbf{x}) = w_{con} \left(\frac{\frac{\log_{10}(g_{feas})}{16} + \frac{\log_{10}(g_{conn})}{16}}{2} \right) + w_{stif} \frac{g_{stif}}{10}$$
(3)

In order to interpret the weights w_{con} and w_{stif} solely in terms of assigning relative priority for the optimization algorithm, the objectives and the penalty terms are normalized to the best extent possible to have a value between 0 and 1. g_{stif} is normalized by 10 based on observations from multiple runs. v_f is normalized by 0.96 which is the volume fraction of the truss design with all possible member connections (i.e. the highest possible volume fraction ignoring feasibility limits). For the purpose of this pa-



FIGURE 2: Illustration of the different heuristic representations and their corresponding handling methods.

per, both w_{con} and w_{stif} are taken as 10 to emphasize constraint satisfaction over objective minimization, since both the feasibility and stiffness ratio constraints are rather hard to satisfy, as is shown later.

Four design heuristics are considered for this problem based on expert knowledge of the authors for good design of mechanical metamaterials. Importantly, they were not all developed for this particular problem, but may be related to some of the objectives and constraints. They are:

- Partial Collapsibility: This design heuristic embodies the resistance of the truss design to collapse due to shear loading. It dictates that each half of the unit cell, both vertically and horizontally, must contain at least one diagonal member.
- 2. Nodal Properties: This design heuristic directs designs to be physically stable. It dictates that each node have at least three connections unless completely unused, to prevent snap-through instability in joints under loading. This heuristic also caps the number of unused nodes per design to 1. As a result its main goal is to aid in the satisfaction of the connectivity constraint.
- 3. **Orientation**: This design heuristic directs designs to achieve a certain target average orientation of its members, computed from the target stiffness ratio. Thus the heuristic is aimed at satisfying the stiffness ratio constraint.
- 4. **Intersection**: This design heuristic has been developed to reduce the number of intersections between the members of the truss design. It is therefore associated with the feasibility constraint.

INCORPORATION OF HEURISTICS INTO OPTIMIZA-TION FRAMEWORK

Figure 2 shows the different means of representation of design heuristics and the handling methods that utilize the appropriate representations of the heuristics to incorporate them into the design optimization framework. It must be stressed that any heuristic can be formulated into any of the illustrated representations. These representations capture the underlying directives of the heuristics in a manner suitable for their incorporation into the design search. It is worth mentioning that although the design heuristic representations were developed with evolutionary algorithms in mind - a popular method to solve metamaterial design problems - they can trivially be extended for use in other optimization techniques. What follows applies to any global multiobjective optimization strategy that uses random generation of an initial set of solutions and performs some kind of hill climbing by iteratively applying one or more moves or operators.

Soft Constraint Form

The soft constraint form of design heuristics quantifies the degree of satisfaction of that heuristic by an input design by means of a function $g: X \to \mathbb{R}$, where $x \in X$ represents a design from the design space and g(x) represents the degree of satis faction of heuristic g by design x. This function can then be incorporated into the problem formulation as a soft constraint. Note that from the very definition of a heuristic, it is not guaranteed to lead to optimal solutions, and it is only applicable to a certain context. Therefore, a heuristic should not be implemented as a hard constraint. The soft constraint forms of the partial collapsibility and nodal properties heuristics award a value of 1 to designs that fully satisfy the heuristic directive and 0.1 is subtracted for each subsequent violation. The orientation soft constraint form calculates a design's orientation as the average orientation of all individual members relative to the horizontal axis, then assigns a score based on the deviation of the design's orientation from the target orientation. This function assigns a continuous score spanning from 0 to 1 (properly oriented). The intersection soft constraint form, used solely for the computation of heuristic alignment metrics introduced below, is identical to the feasibility constraint.

The soft constraint form can be handled using two types of methods: penalty and stochastic. Penalty methods are generic constraint handling methods. As the name suggests, designs are penalized for violations of the design heuristic directives. Examples of methods belonging to this class of constraint handling methodologies include coevolutionary [38], metric [39] and the interior [37] penalty methods. The choice of the penalization method and the inherent weights is left to the designer and can vary based on the severity of the penalty for heuristic violation. For example, for heuristics that are harder to satisfy the dominance operator can be modified so designs are compared based on constraint satisfaction first, with Pareto dominance in objective space being used to break ties. Normalization of the objectives and constraint penalty functions facilitates the interpretation of the penalty weights.

Stochastic constraint enforcement is a class of heuristic handling methodologies that are softer than penalty methods. Two examples of stochastic constraint enforcement methods are Disjunctive Normal Form (DNF) and Adaptive Constraint Handling (ACH) [5]. ACH applies a constraint in a probabilistic manner based on the fraction of solutions in the current archive (approximate Pareto set with one point per epsilon-box in objective space [36]) that violates the constraint. The cumulative constraint violations of two designs are compared to find the dominating design, with Pareto objective dominance being used in case of ties. In this case, the probabilistic application of the heuristic violation penalties to a design ensures diversity in the archive in terms of heuristic satisfaction, which in turn leads to a balance between design space exploration and design heuristic exploitation. An example of soft constraint enforcement is Michalski [40] which classifies designs as acceptable if they satisfy at least one of the knowledge-dependent constraints.

Operator Form

The operator form encodes the prescriptive action or directive represented by the heuristic to improve a design's optimality in the form of a move in design space, i.e. a function that takes a design as an input and returns a design as an output $O: X \to X$. This form is consistent with the representation of heuristics considered in Filingim et. al. [12] where heuristics are considered to prescribe an action towards improving a design. The operator form acts upon a design to produce a new design that adheres to the directives of the heuristic to a greater extent. The partial collapsibility operator form aims to add a diagonal member otherwise absent at random to an input design to improve satisfaction of the heuristic. The nodal properties operator form adds a connection at random to any violating node in order to improve satisfaction of the Nodal Properties directive. The orientation operator form adds either a horizontal or vertical member at random to the input design based on whether the design orientation is higher or lower than the target orientation. The intersection operator form removes an intersecting or overlapping truss member from the design at random. Heuristic-based operators (called knowledge-directed operator in [41]) should be used in conjunction with other knowledge-independent operators so as not to limit the design search. The random aspect of the operator is important for maintaining exploration. The operator form can be handled either using a fixed operator selection strategy that continuously applies the same set of knowledgedirected operators throughout the design search, or by Adaptive Operator Selection (AOS). AOS [42] uses a multi-arm bandit approach for selecting operators to improve the design search. A pool of knowledge-independent (e.g. crossover and mutation) and knowledge-directed operators is maintained, with operators being selected based on their relative cumulative performance. AOS will be used to encode operators in the presented case study. Offspring-parent domination is used as the credit assignment strategy with 1 credit being awarded for the offspring dominating the parent, 0.5 credits for both the offspring and the parent being non-dominated and 0 credits for the parent dominating the offspring. Probability matching is used as the operator selection strategy with α and p_{min} values of 0.6 and 0.03 respectively. In order to reduce reliance on the knowledge-dependent operators in the later stages of the optimization, p_{min} (the minimum probability of selection for an operator) is reduced by 0.01 every 500 function evaluations until a value of 0 is reached to encourage design space exploration by the selection of poorly performing operators. Since the assumption in this work is that heuristics are only useful in the beginning of the design search, it is assumed that the knowledge dependent operators will perform poorly compared to knowledge-independent operators at the later stages of the optimization run.

Biased Prior Distribution Form

The biased prior distribution form encodes the heuristic in the form of a probability distribution that produces a set of designs that statistically tend to satisfy the directives of the heuristic. In population-based algorithms, the biased set of designs can be used as the initial population, with the expectation that the initial presence of some aspects of 'good designs' will accelerate convergence [35]. Again, the stochastic satisfaction aspect is particularly important as it allows for further design space exploration rather than limiting the design search strictly to the heuristic-adhering region of the design space. The partial collapsibility biased initialization strategy assigns a probability of 0.75 for the presence of a diagonal member in a design as opposed to 0.5 for the presence of straight members. For nodal properties, the biased initialization strategy involves increasing the probability of the presence of members so as to statistically reach more number of members in each truss design of the initial population. The population is divided into 4 clusters, the designs in each cluster are biased to statistically contain 15, 18, 20 and 22 members respectively (not counting the repeated members). The initial population biasing strategy for the orientation heuristic involves acceptance of randomly generated designs only if their orientation is in the margin of 10° from the target orientation. The intersection biased initialization strategy involves dividing the population into 4 clusters, with each cluster statistically biased to contain 6, 9, 12 and 15 members respectively with the motivation that designs with fewer members have a lower probability of having intersecting or overlapping members. The methods to implement biased initialization are essentially methods that sample from a given prior probability distribution. For standard random variables, sampling functions are available in most scientific computing software packages. The inverse sampling method can be used if the cumulative distribution function is known. The soft constraint form of the heuristic g(x) can also be used in a rejection sampling scheme.

IDENTIFICATION OF PROMISING HEURISTICS

As mentioned in the introduction, not all "correct" heuristics are actually useful for a given problem at hand. Some of the methods presented above are more forgiving than others when poor heuristics are incorporated (e.g., AOS) but in general, incorporating poor heuristics will hurt performance. This section provides some specific metrics and tests, as identified by the authors, for designers to apply when down-selecting heuristics to incorporate into their optimization problem.

The following types of metrics are recommended to assess how promising a heuristic is:

- 1. Ease or degree of full satisfaction of the heuristic and the quantity it is targeting (Pareto dominance in the true objectives space or specific constraints).
- 2. Alignment with Pareto dominance (e.g., distance to Pareto front) in the true objective space or alignment with one or more constraints. Alignment with Pareto dominance can be a) in the complete range of the true objective space or b) in a portion of the true objective space (e.g., low stiffness/low volume fraction). More succinctly, alignment with Pareto dominance in the *penalized* objective space takes into account both the true objectives and the constraints with the relevant weights as defined in the problem formulation.

In general, these metrics can be evaluated on a set of randomly generated designs. If, like in the problem at hand, the constraints are too hard to be satisfied in a small random sample, a population generated by a preliminary search process can be used instead. The degree of full satisfaction of a heuristic or constraint can be computed using the fraction of randomly generated designs that fully satisfy it. Intuitively, heuristics strongly aligned with more important or harder to satisfy objectives and constraints will help the most. The ease of satisfaction of the heuristic itself will also inform the heuristic handling method. Of note, this metric evaluation step is not strictly necessary for all heuristic are useful for the problem at hand and which are not. However, the performance of AOS degrades when the number of operators in the pool is very large.

Many metrics can be used to ascertain the alignment of the heuristics with the constraints and Pareto dominance of the true or penalized objectives. The Pearson's Correlation Coefficient [43] and the Spearman's Correlation Coefficient [44] measure the degree of linearity and monotonicity respectively between the independent and dependent variable. In case of insignificant results for the previous two correlation coefficients, various interestingness measures from association rule mining theory can be leveraged. Measures such as support [45], confidence [46] and lift [47] can be used to compute the interestingness of association rules of the form {low/high heuristic} \rightarrow {low/ $d_{PF,true}$, low/high objective} {low/high heuristic} \rightarrow {low/high constraint value} {low/high heuristic} \rightarrow {low/high $d_{PF,pen}$ }

The support, confidence and lift measures for an association rule $A \rightarrow B$ can be computed using the equations below, taken from [48].

$$sup(A \to B) = P(A \cup B)$$
 (4)

$$conf(A \to B) = P(B|A) = \frac{sup(A \cup B)}{sup(A)}$$
 (5)

$$lift(A \to B) = \frac{conf(A \to B)}{sup(B)}$$
(6)

In situations where linear or monotonic alignment cannot be ascertained, the association rule mining based interestingness measures provide valuable information regarding how to leverage the heuristics for optimal design search.

RESULTS AND DISCUSSION Identification of promising heuristics

The metrics described in the Section titled "Identification of promising heuristics", were computed for each of the four heuristics. The heuristics were assessed using 10 trials with 400 designs each. 100 of these designs were randomly generated unique designs and 300 designs were from the final population of 3ϵ -MOEA runs optimizing the problem represented by Eqn. 1. This approach provides a mix of designs that have both high and low constraint satisfaction for an unbiased calculation of the metrics. Specifically, the feasibility constraint is very hard to satisfy and randomly generated designs tend to have very low feasibility scores. It is worth noting that the utilization of ϵ -MOEA generated designs for metrics computation in general is not necessary if enough randomly generated designs can fully satisfy the constraints.

The first metric is ease of satisfaction. Table 1 shows the fraction of the designs that show complete satisfaction of the different constraints and heuristics as well as the mean score of the heuristics and constraints (values of the soft constraint form for the heuristics and the constraint functions) across all designs in all trials. It can be seen that feasibility is indeed very hard to satisfy given the low mean fraction of fully satisfying designs and high standard deviation of the score. It must be mentioned that there is no variation in the mean fraction of fully satisfying designs for feasibility across the trials since the main source of variability in the feasibility scores came from the ϵ -MOEA runs and the random designs all generated zero feasibility score designs. The intersection heuristic shows the same behaviour as feasibility as the feasibility function is used to compute the metrics for the intersection heuristic. In contrast, the connectivity mean fraction of fully satisfying designs and mean scores are extremely high with negligible standard deviation. This indicates the rather

Parameter	$\frac{ g(\mathbf{x})=1 }{ \cup }$	$\frac{\sum(g(\boldsymbol{x}))}{ \cup }$		
PF	0.0175 ± 0.0000	-		
g_{feas}	0.36 ± 0.0000	0.6222 ± 0.3906		
8conn	0.9797 ± 0.0084	0.9977 ± 0.0162		
<i>Sstif</i>	0.045 ± 0.0000	0.0982 ± 0.2376		
8 pc	0.8882 ± 0.0026	0.9845 ± 0.0468		
8np	0.975 ± 0.0104	0.9973 ± 0.0176		
<i>8</i> orient	0.0042 ± 0.0026	0.9784 ± 0.0249		
<i>Sinter</i>	0.36 ± 0.00	0.6222 ± 0.3906		

TABLE 1: Fraction of fully satisfying designs and mean scores for the Pareto front designs, the 3 constraints, and the 4 heuristics across the 10 trials (mean $\pm 1\sigma$).

high ease of satisfaction of the connectivity constraint and thus it may not require further improvement through the incorporation of a heuristic. The stiffness ratio constraint is difficult to satisfy, which is evidenced through the small mean fraction of fully satisfying designs. In addition it can take a wide range of values, which results in a standard deviation greater than the mean value. Partial collapsibility and nodal properties heuristics are reasonably easy to satisfy given the high mean scores and corresponding low standard deviations. The orientation mean fraction of fully satisfying designs and mean score suggests that there are very few designs that fully satisfy it but a high number of designs come very close to it. The small value of fraction of designs in the Pareto front signifies the fact that this constrained multiobjective problem is not easy to solve.

The second metric is alignment of the heuristics with Pareto dominance in the true objective space or with one or more constraints. This is computed either using the Pearson or Spearman correlation coefficients or the interestingness measures (mainly confidence and lift). For computation of the lift, the objectives, constraints, heuristics and distances to the true and penalized Pareto front are thresholded into high or low values. The 75th percentile of combined data for all 10 trials was used as the thresholding limit for C_{22} , $g_{f eas}$, g_{conn} , g_{pc} , g_{np} , g_{orient} and g_{inter} . The 25th percentile was used for v_f and g_{stif} . $d_{PF,pen}$ and $d_{PF,true}$ were thresholded using the 60th and 70th percentile values respectively. Heuristics are assessed based on their associations with desirable consequents containing the constraint or objectives they target. For example, since we want g_{stif} to go to zero, the orientation heuristic would be considered promising if the association rule - high $g_{orient} \rightarrow \log g_{stif}$ was found to be significant. Similarly, high $g_{np} \rightarrow$ high g_{conn} and high $g_{inters} \rightarrow$ high $g_{f eas}$ would imply that both nodal properties and intersection are promising heuristics.

Table 2 presents the statistics for the Pearson and Spearman correlation coefficients as computed for significant combinations of heuristics and either minimum distance to true Pareto front or constraints across the 10 trials. The Pareto fronts are computed for each trial using normalized objectives. The minimum distances to the Pareto front are computed in the normalized objective space. The lower part of Table 2 presents the correlation coefficients for the heuristics with the minimum distance to the penalized Pareto front, combining the true objectives and the constraints. Just like for the distance to true Pareto front, the penalized Pareto front is computed in the normalized penalized objectives space in order to prevent the influence of any penalized objective on the minimum distance calculation. Correlation with the distance to penalized Pareto front provides an aggregate perspective of the heuristics' ability to both reach optimal designs and satisfy constraints. Concerning the association rule mining, the complete set of interestingness measures computed for all relevant association rules is provided in Appendix A. Some examples of rules that were found to have high degree of association as inferred by their lift values are: low $g_{pc} \rightarrow \log g_{stif}$ (lift = 3.85 \pm 0.09), high $g_{orient} \rightarrow \text{low } d_{PF,pen}$ (lift = 1.77 \pm 0.56), high $g_{orient} \rightarrow \log g_{stif}$ (lift = 3.89 ± 0.05), high $g_{inter} \rightarrow high$ $g_{f\,eas}$ (lift = 2.77 ± 0) and low $g_{np} \rightarrow \log g_{conn}$ (lift = 9.21 ± 5.57).

Results from both the correlation and association rule mining tests show that the partial collapsibility exhibits significant negative correlations with distance to the true Pareto front and feasibility (high Pearson and Spearman correlations between g_{pc} and $d_{PF,true}$, low $g_{pc} \rightarrow \{ \text{low } d_{PF,true}, \text{low } v_f \}$ (lift = 4.27 ± 1.13) and low $g_{pc} \rightarrow \text{high } g_f eas$ (lift = 2.67 ± 0.06)), which implies that contradicting the directive of partial collapsibility leads to promising designs. Nodal properties shows significant correlations with connectivity (low $g_{np} \rightarrow \log g_{conn}$ (lift = 9.21 \pm 5.57)) and stiffness ratio constraint (low $g_{np} \rightarrow$ high g_{stif} (lift = 1.33 ± 0)) but no corresponding significant correlations for high g_{np} thus implying it may not be a promising heuristic. Orientation and intersection on the other hand display very favourable correlations that indicate that they can be help find optimal designs quickly. Orientation has positive correlation with feasibility and negative correlation with stiffness ratio constraint (i.e. positive correlation with reaching target stiffness ratio). The latter is consistent with the main goal of developing the orientation heuristic while the former is a nice bonus. The intersection heuristic not only improves stiffness ratio constraint satisfaction but also moves the design search towards the true Pareto front as designs improve their levels of intersection satisfaction (high $g_{inter} \rightarrow \{ \text{low } d_{PF,true}, \text{low } v_f \}$ (lift = 2.45 ± 0.52)). The full positive correlation of intersection with feasibility is obvious given that the feasibility function is used to compute the metrics for the intersection heuristic. The alignment metrics with the penalized objectives confirm all these results.

Corr. Pairs	Pearson Coeff.	Spearman Coeff.		
ginter, gf eas	1 ± 0	1 ± 0		
gorient, gstif	-0.7214 ± 0.035	-0.6402 ± 0.0342		
gorient, gf eas	0.6640 ± 0.0368	0.7577 ± 0.0369		
ginter, gstif	-0.5934 ± 0.0725	-0.6519 ± 0.0084		
$g_{pc}, d_{PF,true}$	0.4277 ± 0.0191	0.4461 ± 0.0107		
$g_{inter}, d_{PF,pen}$	-0.92 ± 0.0019	-0.975 ± 0.000		
$g_{orient}, d_{PF,pen}$	-0.631 ± 0.041	-0.839 ± 0.0335		
$g_{np}, d_{PF,pen}$	-0.272 ± 0.0548	-0.212 ± 0.0409		
$g_{pc}, d_{PF,pen}$	0.187 ± 0.0049	0.4365 ± 0.0128		

TABLE 2: Alignment metrics between heuristics and aspects of the problem formulation (min. distance to true Pareto front, penalized Pareto front and constraints) (mean $\pm 1\sigma$).

In summary, the study identifies the orientation and intersection heuristics as the most promising candidates for incorporation into the optimization framework, since they are strongly aligned with the problem's objectives and important and hard to satisfy constraints.

Efficacy of the heuristics to accelerate convergence

The constrained multiobjective optimization problem formalized in Eq. 1 is solved using the ϵ -MOEA algorithm with different cases incorporating different heuristics/combinations of heuristics. The value of ϵ is chosen to be 0.01 on both directions of the normalized objective space. Single-point crossover with a crossover probability of 1 and bit-flip mutation with a mutation probability of $\frac{1}{30}$ are employed as the knowledge-independent operators. The population size is set to 100 and the maximum number of function evaluations for termination of the optimization routine is set to 3,000.

Four cases are considered:

- 1. Case 1: No heuristics incorporated
- 2. Case 2: Orientation heuristic incorporated as repair operator using AOS and Intersection heuristic incorporated as repair operator using AOS and as biased prior distribution
- Case 3: Orientation heuristic incorporated as repair operator using AOS
- 4. Case 4: Partial Collapsibility and Nodal Properties repair operators incorporated using AOS

Case 2 considers the two heuristics identified as promising in the previous section. The combination of low mean fraction of fully satisfying designs and high mean score of the orientation heuristic in the studies conducted in the "Identification of



FIGURE 3: Combined feasible pareto fronts from the 30 runs of the four cases at different NFE values in true objective space is shown. The utopia point is located towards the bottom right.

promising heuristics" subsection warrants the use of a representation and handling methodology that is reasonably firm in enforcing heuristic satisfaction. Hence for this problem, the orientation heuristic is represented using its repair operator form and handled with AOS. The intersection heuristic, owing to the difficulty in fully satisfying the feasibility constraint as seen from the metrics study, is represented using both its repair operator (handled using AOS) and its biased prior probability distribution forms. Case 3 is considered in order to emphasize and illustrate the value of incorporating the intersection heuristic as opposed to just the orientation. The intersection repair operator (which removes an intersecting member at random) and the biased prior distribution (which consists of designs with statistically lower number of members that have a lower probability of having intersections or overlaps) improve feasibility, the hardest constraint to satisfy. This is demonstrated in the results shown. Case 4 is considered to demonstrate that the heuristics identified as not promising in the previous study indeed do not perform well. Both partial collapsibility and nodal properties do have reasonably high mean fractions of fully satisfying designs and mean scores, as seen in Table 1. Selective application of their repair operators at appropriate times in the optimization run through AOS is therefore the best way to leverage the heuristics.

Figure 3 shows the feasible designs in the combined Pareto fronts from the 30 runs of each case over the true objectives space at different points in the search (NFE=250, 500, 1500 and 3000).



FIGURE 4: The plot of the hypervolume values over the penalized objectives space as a function of NFE for the four cases is shown. The solid lines represent the median values while the dashed lines represent the inter quartile range.

It shows that Case 2 is the first to reach feasible designs by 500 function evaluations. This clearly demonstrates the utility of the intersection heuristic.

Figure 4 shows the hypervolume values plotted as a function of number of function evaluations (NFE) in the penalized objectives space. It can be seen that Case 2, which incorporates both orientation and intersection heuristics, performs the best and is close to convergence at 3000 NFE. However Case 1, that does not incorporate heuristics, has not yet converged at 3000 NFE. It is worth mentioning that in global optimization, any non-flawed algorithm will eventually reach the true pareto front. So for large NFE, Cases 1,3 and 4 would eventually catch up with Case 2.

Since the main goal of incorporating heuristics into optimization is to reduce the NFE needed to achieve convergence, Fig. 5 shows the fraction of the 30 runs for each case that attain convergence (defined as HV ≥ 0.75) at different values of NFE. It is clearly seen that the incorporation of both orientation and intersection not only allows for reaching convergence faster but also keeping that advantage to reach further optimal designs in the later stages of the optimization run. In contrast, Case 3 is able to reach more optimal designs in the early stages of the design search but it eventually loses out to the ϵ -MOEA algorithm since it does not have a strategy to improve the feasibility of designs. Case 4, which incorporates partial collapsibility and nodal properties, never overcomes the other cases owing to the fact that maximizing partial collapsibility hurts the design search towards the penalized Pareto front as concluded from the positive Spearman coefficient of g_{pc} and $d_{PF,pen}$. This validates the fact that both partial collapsibility and nodal properties are not promising heuristics for this problem.



FIGURE 5: The fraction of the 30 runs that achieve the threshold hypervolume value of 0.75 is plotted as a function of NFE for the four cases.

CONCLUSIONS

This paper shows the potential of methods that explicitly use design heuristics in optimization to help find optimal or at least satisfying designs faster, using the case study of 2D lattice-based mechanical metamaterials. Figure 5 suggests that Cases 2 and 3 succeeded in this objective. However, the point of getting to better designs faster is to enable evolutionary algorithms to get to even more optimal designs towards the end of the optimization run. In this respect, Cases 3 and 4 failed since they could not improve upon the ϵ -MOEA result towards the end of the optimization run.

Further, the main motivation behind the introduction of the metrics of ease of satisfaction and alignment is to identify the heuristics that can help with a given problem at hand. Designers can come up with many heuristics that may seem useful for a class of problems, but their usefulness for a given problem instance is hard to predict due to couplings between the heuristics and the objectives and constraints. For example, the partial collapsibility heuristic was meant to improve shear stability on maximization, a goal that is not directly related to any of the objectives or constraints in the problem considered. The metrics study thus found that using the partial collapsibility heuristic would be detrimental to the design search and thus partial collapsibility was deemed not promising for this problem. A more subtle example of misalignment between heuristics and problem formulations is the nodal properties heuristic that was specifically developed to improve design member connectivity. This is one of the constraints of the problem and hence a prime candidate to be investigated using the metrics study. However, the metrics study concluded that nodal properties did not have any significant correlations with either minimum distance to the Pareto front or any of the constraints, not even connectivity which it was created to improve. The main cause for this low impact is the easy satisfaction of the nodal properties heuristic and its relatively low variation across the design space. The metrics study found that the orientation and intersection heuristics would not only improve the constraints they were developed to improve but also direct the search towards more optimal regions.

In the course of conducting the case study, we identified certain guidelines that help to identify promising heuristics that can be leveraged to improve our constrained optimization framework. They are shown below.

- Heuristics that are likely to improve search performance are those that are aligned with Pareto dominance in the penalized objective space, which takes into account both objectives and constraints with their respective weights as provided in the problem formulation. This means that heuristics must be aligned either with Pareto dominance in the true objective space or with any of the constraints.
- 2. Heuristics may be aligned with Pareto dominance only in a certain region of the objective space (e.g., low stiffness/low volume fraction). This is consistent with the definition of design heuristics as context-specific. In such cases, the heuristics can be selectively leveraged based on the current state of the design search (e.g., density of solutions in a given region).
- 3. Heuristics are useful only in the beginning of the design search. Heuristics are supposed to be directives that lead to satisfactory but not necessarily optimal designs faster. Overenforcement of heuristics will eventually lead to a reduction of exploration and result in premature convergence. To alleviate this issue, heuristics must be eventually "shut off" and more exploratory strategies must be favored in the later stages of the search.

The case study presented here not only shows the usefulness of the proposed metrics to predict how promising the design heuristics are for a given problem, but also the potential of heuristic-handling mechanisms (and in particular AOS) to significantly accelerate convergence in highly-constrained multiobjective design problems without impeding exploration and steady-state performance.

In future work, the guidelines proposed in this paper will be tested as hypotheses on a wide range of design optimization problems and formalized into a framework including a design heuristics taxonomy based on the metrics discussed.

ACKNOWLEDGMENT

This work is supported and funded by the National Science Foundation under CMMI Nos. 1825444 and 1825521.

REFERENCES

- Dong, H., Song, B., Wang, P., and Dong, Z., 2018. "Hybrid surrogate-based optimization using space reduction (HSOSR) for expensive black-box functions". *Applied Soft Computing Journal*, *64*, pp. 641–655.
- [2] Dong, H., Song, B., Wang, P., and Dong, Z., 2018. "Surrogate-based optimization with clustering-based space exploration for expensive multimodal problems". *Structural and Multidisciplinary Optimization*, 57(4), pp. 1553– 1577.
- [3] Snoek, J., Hugo Larochell, and Adams, R. P. "Practical Bayesian Optimization of Machine Learnign Algorithms".
- [4] Shahriari, B., Swersky, K., Wang, Z., Adams, R. P., and De Freitas, N., 2016. "Taking the human out of the loop: A review of Bayesian optimization". *Proceedings of the IEEE*, **104**(1), pp. 148–175.
- [5] Hitomi, N., and Selva, D., 2018. "Incorporating expert knowledge into evolutionary algorithms with operators and constraints to design satellite systems". *Applied Soft Computing Journal*, 66, pp. 330–345.
- [6] Shrivastava, P., and O'Mahony, M., 2007. "Design of Feeder Route Network Using Combined Genetic Algorithm and Specialized Repair Heuristic". *Journal of Public Transportation*, 10(2), pp. 109–133.
- [7] Ji, S., Pan, S., Cambria, E., Marttinen, P., and Yu, P. S., 2020. "A survey on knowledge graphs: Representation, acquisition and applications". *arXiv*, 14(8), pp. 1–27.
- [8] Friedenthal, S., Moore, A., and Steiner, R., 2014. A Prractical Guide to SysML: The Systems Modelling Language. Morgan Kaufmann.
- [9] Li, C., Gupta, S., Rana, S., Nguyen, V., Robles-kelly, A., and Venkatesh, S., 2020. "Incorporating Expert Prior Knowledge into Experimental Design via Posterior Sampling". arXiv.
- [10] Chattha, M. A., Siddiqui, S. A., Malik, M. I., van Elst, L., Dengel, A., and Ahmed, S., 2019. "KINN: Incorporating expert knowledge in neural networks". *arXiv*, **2**.
- [11] Fu, K. K., Yang, M. C., and Wood, K. L., 2016. "Design principles: Literature review, analysis, and future directions". *Journal of Mechanical Design, Transactions of the ASME*, **138**(10), pp. 1–13.
- [12] Fillingim, K. B., Nwaeri, R. O., Borja, F., Fu, K., and Paredis, C. J. J., 2020. "Design Heuristics: Extraction and Classification Methods With Jet Propulsion Laboratory's Architecture Team". *Journal of Mechanical Design*, 142(8), pp. 1–13.
- [13] Yilmaz, S., Seifert, C., Daly, S. R., and Gonzalez, R., 2016.
 "Design Heuristics in Innovative Products". *Journal of Mechanical Design, Transactions of the ASME,* 138(7), pp. 1–12.
- [14] Puentes, L., Cagan, J., and McComb, C., 2021. "Data-Driven Heuristic Induction from Human Design Behavior".

Journal of Computing and Information Science in Engineering, **21**(2).

- [15] Mehta, P., Malviya, M., McComb, C., Manogharan, G., and Berdanier, C. G. P., 2020. "Mining Design Heuristics for Additive Manufacturing Via Eye-Tracking Methods and Hidden Markov Modeling". *Journal of Mechanical Design*, *142*(12).
- [16] Lee, B., Fillingim, K. B., Binder, W. R., Fu, K., and Paredis, C. J. J., 2017. "Design Heuristics: A Conceptual Framework and Preliminary Method for Extraction". In International Design Engineering Technical Conferences and Computers and Information in Engineering Conference.
- [17] Moore, R. A., Romero, D. A., and Paredis, C. J., 2014.
 "Value-based global optimization". *Journal of Mechanical Design, Transactions of the ASME,* 136(4), pp. 1–14.
- [18] Hitomi, N., and Selva, D., 2016. "A hyperheuristic approach to leveraging domain knowledge in multi-objective evolutionary algorithms". *Proceedings of the ASME Design Engineering Technical Conference*, 2B-2016.
- [19] Binder, W. R., and Paredis, C. J. J., 2017. "Optimization under uncertainty versus algebraic heuristics: A research method for comparing computational design methods". In ASME 2017 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference.
- [20] Surjadi, J. U., Gao, L., Du, H., Li, X., Xiong, X., Fang, N. X., and Lu, Y., 2019. "Mechanical Metamaterials and Their Engineering Applications". *Advanced Engineering Materials*, 21(3), pp. 1–37.
- [21] Bertoldi, K., Vitelli, V., Christensen, J., and Van Hecke, M. "Flexible Mexhanical Metamaterials". *Nature Reviews Materials*, 2(11), pp. 1–11.
- [22] Yu, X., Zhou, J., Liang, H., Jiang, Z., and Wu, L., 2018. "Mechanical metamaterials associated with stiffness, rigidity and compressibility: A brief review". *Progress in Materials Science*, 94, pp. 114–173.
- [23] Vogiatzis, P., Chen, S., Wang, X., Li, T., and Wang, L., 2017. "Topology optimization of multi-material negative Poisson's ratio metamaterials using a reconciled level set method". *CAD Computer Aided Design*, *83*, pp. 15–32.
- [24] Andreassen, E., Lazarov, B. S., and Sigmund, O., 2014.
 "Design of manufacturable 3D extremal elastic microstructure". *Mechanics of Materials*, *69*(1), pp. 1–10.
- [25] White, D. A., Arrighi, W. J., Kudo, J., and Watts, S. E., 2019. "Multiscale topology optimization using neural network surrogate models". *Computer Methods in Applied Mechanics and Engineering*, 346, pp. 1118–1135.
- [26] Sharpe, C., Seepersad, C. C., Watts, S., and Tortorelli, D., 2018. "Design of mechanical metamaterials via constrained Bayesian optimization". *Proceedings of the ASME Design Engineering Technical Conference, 2A-2018*, pp. 1–11.
- [27] Wang, J., Callanan, J., Ogunbodede, O., and Rai, R.,

2020. "Hierarchical combinatorial design and optimization of non-periodic metamaterial structures". *Additive Manufacturing*, p. 101632.

- [28] Bostanabad, R., Chan, Y. C., Wang, L., Zhu, P., and Chen, W., 2019. "Globally approximate Gaussian processes for big data with application to data-driven metamaterials design". *Journal of Mechanical Design, Transactions of the ASME*, 141(11), pp. 1–11.
- [29] Wang, L., Chan, Y. C., Ahmed, F., Liu, Z., Zhu, P., and Chen, W., 2020. "Deep generative modeling for mechanistic-based learning and design of metamaterial systems". *Computer Methods in Applied Mechanics and Engineering*, 372, pp. 1–41.
- [30] Chan, Y.-c., Ahmed, F., Wang, L., and Chen, W., 2020. "METASET: Exploring Shape and Property Spaces for Data-Driven Metamaterials Design". pp. 1–27.
- [31] Bonissone, P. P., Subbu, R., Eklund, N., and Kiehl, T. R., 2006. "Evolutionary algorithms + domain knowledge = real-world evolutionary computation". *IEEE Transactions on Evolutionary Computation*, 10(3), pp. 256–280.
- [32] Chabuk, T., Reggia, J., Lohn, J., and Linden, D., 2012. "Causally-guided evolutionary optimization and its application to antenna array design". *Integrated Computer-Aided Engineering*, **19**(2), pp. 111–124.
- [33] Mahbub, M. S., Wagner, M., and Crema, L., 2016. "Incorporating domain knowledge into the optimization of energy systems". *Applied Soft Computing*, 47, pp. 483–493.
- [34] Kazimipour, B., Li, X., and Qin, A. K., 2014. "A review of population initialization techniques for evolutionary algorithms". *Proceedings of the 2014 IEEE Congress on Evolutionary Computation, CEC 2014*, pp. 2585–2592.
- [35] Surry, P. D., and Radcliffe, N. J., 1996. "Inoculation to initialise evolutionary search". *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, 1143, pp. 269–285.
- [36] Deb, K., Mohan, M., and Mishra, S., 2005. "Evaluating the ϵ -domination based multi-objective evolutionary algorithm for a quick computation of Pareto-optimal solutions". *Evolutionary Computation*, **13**(4), pp. 501–525.
- [37] Coello, C., and Carlos, A., 1999. "A survey of constraint handling techniques used with evolutionary algorithms". *Lania-RI-99-04, Laboratorio Nacional de ...*, pp. 1–33.
- [38] Coello Coello, C. A., 2000. "Use of a self-adaptive penalty approach for engineering optimization problems". *Computers in Industry*, **41**(2), pp. 113–127.
- [39] Hoffmeister, F., and Sprave, J., 1996. "Problem-Independent Handling of Constraints by Use of Metric Penalty Functions". *Proceedings of the Fifth Annual Conference on Evolutionary Programming*, pp. 289–294.
- [40] Michalski, R. S., 2000. "Learnable evolution model: evolutionary processes guided by machine learning". *Machine*

Learning, 38(1), pp. 9-40.

- [41] Hitomi, N., Bang, H., and Selva, D., 2018. "Adaptive knowledge-driven optimization for architecting a distributed satellite system". *Journal of Aerospace Information Systems*, 15(8), pp. 485–500.
- [42] Fialho, A., 2010. "Adaptive Operator Selection for Optimization". PhD thesis, Universite Paris Sud-Paris XI.
- [43] Lee Rodgers, J., and Alan Nice Wander, W., 1988. "Thirteen ways to look at the correlation coefficient". *American Statistician*, 42(1), pp. 59–66.
- [44] Zar, J. H., 2005. "Spearman Rank Correlation". Encyclopedia of Biostatistics.
- [45] Agrawal, R., Imielinski, T., and Swami, A., 1993. "Mining Association Rules between Sets of Items in Large Databases". In Proceedings of the 1993 ACM SIGMOD international conference on Management of data - SIGMOD '93, pp. 207–216.
- [46] Hahsler, M., Grün, B., and Hornik, K., 2005. "Arules -A computational environment for mining association rules and frequent item sets". *Journal of Statistical Software*, 14.
- [47] Brin, S., Motwani, R., and Silverstein, C., 1997. "Beyond Market Baskets: Generalizing Association Rules to Correlations". In Proceedings of the 1997 ACM SIGMOD international conference on Management of data - SIGMOD '97.
- [48] Prajapati, D. J., Garg, S., and Chauhan, N., 2017. "Interesting association rule mining with consistent and inconsistent rule detection from big sales data in distributed environment". *Future Computing and Informatics Journal*, 2(1), pp. 19–30.

Appendix A: Interestingness Measures of Significant Association Rules

The interestingness measures from association rule mining are used to determine the statistical alignment between heuristics and minimum distance to the Pareto front (penalized or true objective space) and the constraints. The full results are shown in this section.

Table 3 presents the support values of the antecedent, consequent and their intersection as well as the confidence value of the forward rule, confidence of the reverse rule and the lift values for significant association rules with either partial collapsibility or nodal properties in the antecedent. It can be seen from the interestingness measures that pursuing maximization of partial collapsibility would lead the design search away from the true Pareto front and that it hurts feasibility satisfaction. The rule low $gpc \rightarrow \log g_{stif}$ does not have a counterpart for high g_{pc} implying that maximizing partial collapsibility will hurt stiffness ratio constraint satisfaction. The interestingness metrics for association rules with nodal properties in the antecedent are all for low g_{np} with no counterpart with high g_{np} as antecedent. This may be the reason the correlation coefficients between nodal properties and the distance to true Pareto front and constraints were found to be insignificant and are not included in Tab. 2.

Table 4 shows the support values of the antecedent, consequent and their intersection as well as the confidence value of the forward rule, confidence of the reverse rule and the lift values for significant association rules with either orientation or intersection in the antecedent. In this case, the correlation coefficients in Tab. 2 are in complete agreement regarding the inference that both orientation and intersection have significant correlations with both feasibility and stiffness ratio constraint. In addition, the association rule mining interestingness measures have an ability to determine the alignment of heuristics within specific regions in the Pareto front. For example, the significance of the rule high $g_{inter} \rightarrow \{ \text{low } d_{PF,true}, \text{ low } v_f \}$ implies that maximizing the satisfaction of the intersection heuristic leads the design search towards the low v_f region of the true Pareto front.

Table 5 presents the antecedent, consequent and intersection support values as well as the forward rule and reverse rule confidence and lift values for the significant heuristics associations with being close to the true or penalized Pareto front as the consequent. This provides an overall picture of the alignment of heuristics to being close to the true or penalized Pareto front. As mentioned in the "Identification of Promising Heuristics" section, the metrics can be used to find associations with either the full Pareto front or the part of the Pareto front. The previous analysis computes alignment with specific regions in the true Pareto front but this analysis computes alignment of the heuristic with being close to the complete true Pareto front. The interestingness measures indicate that maximizing partial collapsibility satisfaction would hurt the search for optimal designs whereas maximizing orientation and intersection would aid in the search for optimal designs. This makes sense, since the intersection heuristic is aimed at improving feasibility satisfaction and orientation is aimed at improving stiffness ratio constraint satisfaction which drives the design search towards the optimal region of the penalized objective space. This mirrors the inference from the correlation coefficients of the heuristics with $d_{PF,pen}$ shown in Tab. 2.

The interestingness measures for various association rules linking heuristics with distance to Pareto front in the penalized and true objective spaces and constraints provide the same amount of information, if not more, when compared to the correlation tests. This study can thus be used as a substitute for the correlation tests to ascertain alignment of heuristics with Pareto dominance in the true or penalized objective spaces and constraints.

Association Rule $\{A\} \rightarrow \{B\}$	sup(A)	sup(B)	$sup(A \cap B)$	$conf \\ (\{A\} \to \{B\})$	$conf \\ (\{B\} \to \{A\})$	lift
$lowg_{pc} \rightarrow \\ \{lowd_{PF,true}, lowC_{22}\}$	0.11 ± 0.003	0.55 ± 0.01	0.11 ± 0.001	0.97 ± 0.02	0.20 ± 0.04	1.82 ± 0.36
$lowg_{pc} \rightarrow \\ \{lowd_{PF,true}, lowv_f\}$	0.11 ± 0.003	0.24 ± 0.08	0.11 ± 0	0.96 ± 0.02	0.48 ± 0.13	4.27 ± 1.13
$lowg_{pc} \rightarrow highg_{feas}$	0.11 ± 0.003	0.36 ± 0	0.11 ± 0	0.96 ± 0.02	0.29 ± 0	2.67 ± 0.06
$\log_{pc} \rightarrow \log_{stif}$	0.11 ± 0.003	0.25 ± 0	0.11 ± 0	0.96 ± 0.02	0.43 ± 0	3.85 ± 0.09
$lowg_{np} \rightarrow \\ \{lowd_{PF,true}, highC_{22}\}$	0.03 ± 0.01	0.14 ± 0.05	0.01 ± 0.004	0.46 ± 0.20	0.08 ± 0.03	3.27 ± 0.94
$lowg_{np} \rightarrow lowg_{feas}$	0.03 ± 0.01	0.64 ± 0.00	0.03 ± 0.01	1 ± 0	0.04 ± 0.02	1.56 ± 0
$lowg_{np} \rightarrow lowg_{conn}$	0.03 ± 0.01	0.02 ± 0.01	0.004 ± 0.003	0.19 ± 0.13	0.21 ± 0.11	9.21 ± 5.57
$low g_{np} \rightarrow high g_{stif}$	0.03 ± 0.01	0.75 ± 0	0.03 ± 0.01	1 ± 0	0.03 ± 0.01	1.33 ± 0

TABLE 3: Interestingness measures for significant association rules with partial collapsibility or nodal properties as antecedent (mean $\pm 1\sigma$).

Association Rule				conf	conf	
$\{A\} \to \{B\}$	sup(A)	sup(B)	$sup(A \cap B)$	$(\{A\} \to \{B\})$	$(\{B\} \to \{A\})$	lift
$ \begin{array}{c} \text{low}g_{orient} \rightarrow \\ \{\text{low}d_{PF,true},\text{high}v_f\} \end{array} $	0.74 ± 0.003	0.44 ± 0.07	0.39 ± 0.07	0.53 ± 0.09	0.88 ± 0.04	1.18 ± 0.05
$lowg_{orient} \rightarrow lowg_{feas}$	0.74 ± 0.003	0.64 ± 0	0.63 ± 0.003	0.85 ± 0.000	0.99 ± 0.005	1.33 ± 0.001
$lowg_{orient} \rightarrow lowg_{conn}$	0.74 ± 0.003	0.02 ± 0.008	0.02 ± 0.008	0.03 ± 0.01	0.98 ± 0.04	1.32 ± 0.06
$lowg_{orient} \rightarrow highg_{stif}$	0.74 ± 0.003	0.75 ± 0	0.74 ± 0.003	1 ± 0	0.99 ± 0.004	1.33 ± 0
$\begin{array}{l} \text{high} g_{orient} \rightarrow \\ \{\text{low} d_{PF,true}, \text{low} C_{22}\} \end{array}$	0.26 ± 0.003	0.55 ± 0.09	0.22 ± 0.04	0.87 ± 0.17	0.41 ± 0.06	1.59 ± 0.26
$\begin{array}{l} \operatorname{highg}_{orient} \rightarrow \\ \left\{ \operatorname{low} d_{PF,true}, \operatorname{low} v_{f} \right\} \end{array}$	0.26 ± 0.003	0.24 ± 0.08	0.20 ± 0.02	0.79 ± 0.06	0.88 ± 0.19	3.43 ± 0.71
$highg_{orient} \rightarrow highg_{f eas}$	0.26 ± 0.003	0.36 ± 0	0.25 ± 0	0.97 ± 0.01	0.69 ± 0	2.7 ± 0.04
$highg_{orient} \rightarrow lowg_{stif}$	0.26 ± 0.003	0.25 ± 0	0.25 ± 0	0.97 ± 0.01	1 ± 0	3.89 ± 0.05
$lowg_{inter} \rightarrow \\ \{lowd_{PF,true}, highv_f \}$	0.64 ± 0	0.44 ± 0.07	0.39 ± 0.07	0.62 ± 0.11	0.89 ± 0.04	1.39 ± 0.06
$lowg_{inter} \rightarrow lowg_{feas}$	0.64 ± 0	0.64 ± 0	0.64 ± 0	1 ± 0	1 ± 0	1.56 ± 0
$low g_{inter} \rightarrow low g_{conn}$	0.64 ± 0	0.02 ± 0.008	0.02 ± 0.008	0.03 ± 0.01	1 ± 0	1.56 ± 0
$low g_{inter} \rightarrow high g_{stif}$	0.64 ± 0	0.75 ± 0	0.64 ± 0	1 ± 0	0.85 ± 0	1.33 ± 0
$\begin{array}{c} \text{high}g_{inter} \rightarrow \\ \{\text{low}d_{PF,true}, \text{low}v_f\} \end{array}$	0.36 ± 0	0.24 ± 0.08	0.20 ± 0.02	0.56 ± 0.04	0.88 ± 0.19	2.45 ± 0.52
$highg_{inter} \rightarrow highg_{feas}$	0.36 ± 0	0.36 ± 0	0.36 ± 0	1 ± 0	1 ± 0	2.78 ± 0
$highg_{inter} \rightarrow lowg_{stif}$	0.36 ± 0	0.25 ± 0	0.25 ± 0	0.69 ± 0	1 ± 0	2.78 ± 0

TABLE 4: Interestingness measures for different association rules with orientation or intersection as antecedent (mean $\pm 1\sigma$).

Association Rule $\{A\} \rightarrow \{B\}$	sup(A)	sup(B)	$sup(A \cap B)$	$conf \\ (\{A\} \to \{B\})$	$conf \\ (\{B\} \to \{A\})$	lift
$\log_{pc} \rightarrow \log d_{PF,true}$	0.11 ± 0.003	0.69 ± 0.09	0.11 ± 0.002	0.99 ± 0.01	0.16 ± 0.02	1.47 ± 0.21
$highg_{orient} \rightarrow lowd_{PF,true}$	0.26 ± 0.003	0.69 ± 0.09	0.25 ± 0.002	0.99 ± 0.01	0.38 ± 0.05	1.46 ± 0.20
$\log_{pc} \rightarrow \log d_{PF,pen}$	0.11 ± 0.003	0.6 ± 0.17	0.11 ± 0	0.96 ± 0.02	0.19 ± 0.06	1.75 ± 0.55
high $g_{orient} \rightarrow \text{low} d_{PF,pen}$	0.26 ± 0.003	0.6 ± 0.17	0.25 ± 0	0.97 ± 0.01	0.45 ± 0.15	1.77 ± 0.57
high $g_{inter} \rightarrow \text{low} d_{PF,pen}$	0.36 ± 0	0.6 ± 0.17	0.36 ± 0	1 ± 0	0.66 ± 0.21	1.82 ± 0.59

TABLE 5: Interestingness measures for significant association rules with the heuristics as antecedent and being close to the true or penanlized Pareto front as the consequent (mean $\pm 1\sigma$).