

Multi-Objective Mixed-Integer Quadratic Models: A Study on Mathematical Programming and Evolutionary Computation

Ofer M. Shir and Michael Emmerich

Abstract—Within the current literature on multi-objective optimization, there is a scarcity of comparisons between equation-based white-box solvers to evolutionary black-box solvers. It is commonly held that when dealing with linear and quadratic models, equation-based deterministic solvers are generally the preferred choice. The present study aims at challenging this hypothesis, and we show that particularly in box-constrained mixed-integer (MI) problems it is worth employing evolutionary methods when the goal is to achieve a good approximation of a Pareto frontier. To do so, this paper compares a mathematical programming approach with an evolutionary method for set-oriented Pareto front approximation of bi-objective quadratic MI optimization problems. The focus is on convex quadratic under-constrained models wherein the decision variables are either tightly or loosely bounded by box-constraints. Through an empirical assessment of families of quadratic models across varying Hessian forms, variable ranges, and condition numbers, the study compares the performance of the CPLEX-based Diversity Maximization Approach to a state-of-the-art evolutionary multi-objective optimization meta-heuristic with MI mutation and crossover operators. We identify and explain strengths and weaknesses of both approaches when dealing with loosely bounded box-constraints, and prove a theorem regarding the potential undecidability of such multi-objective problems featuring unbounded integer decision variables. The empirical results systematically confirm that black-box and white-box solvers can be competitive, especially in the case of loose box-constraints.

Index Terms—Set-oriented Pareto optimization, MIQP, CPLEX, DMA, SMS-EMOA, population-based meta-heuristics, mathematical programming, non-scalarizing, convex quadratic models, box-constraints, undecidability.

I. INTRODUCTION

Within global optimization, Mixed-Integer (MI) problems [1]–[3] constitute a broad class whose formulations comprise both continuous and discrete decision variables. MI Optimization (MIO) problems are NP-hard already when the objective and constraint functions are linear (MI Linear Programs, MILPs), and finding an optimal solution in practice is often challenging. However, various optimization techniques have been developed to tackle MIO problems, either as White-Box Optimization (WBO) or Black-Box Optimization (BBO). WBO includes Mathematical Programming (MP) algorithms – such as Branch-and-Bound [4], or relaxations to semidefinite programming [5], to name a couple – whereas BBO involves

dedicated meta-heuristics [6]–[8]. These approaches can be applied to a wide range of real-world problems, including design and process optimization, hyperparameters calibration, resource allocation, and network design – see, e.g., [9].

Recently, there is a growing interest in generalizing MIO to multi-objective optimization problems, whose aim is to simultaneously treat a number of conflicting objective functions [10]. *A priori* methods can be contrasted to *a posteriori* methods. In *a priori* approaches a scalarization function has to be defined first, with the target to map the vector of objective function values to a single scalar value, which then undergoes minimization or maximization. Questions related to *a priori* methods, such as weight set decomposition, have been addressed concerning MIO in [11]. In this paper we consider the other approach to locate the Pareto frontier, i.e., by means of *a posteriori* methods. These methods involve computing an approximation of the Pareto optimal solutions, usually in the form of a set of points. The goal is to identify sets of points that can effectively cover and converge to the Pareto frontier. This concept is discussed for MIO problems by Santis [12] and Burachik [13]. The computational problem of unveiling the Pareto frontier of such multi-objective optimization problems [14], [15] can be treated by means of either WBO solvers (often entitled “Multi-Objective Programming” [16]) or BBO meta-heuristics. Notably, when the model complexity does not allow for exact MP-based problem-solving, WBO offers a variety of approximation methods [17]. The common working hypothesis states that problem-specific WBO approaches are superior to general-purpose BBO approaches – when systematic comparisons over specific problems are available. At the same time, the practical relevance of BBO meta-heuristics is rooted in the fact that an explicit problem structure is not a prerequisite for their operation.

Finally, *box-constraints* (also known as bound constraints), refer to limitations placed on the decision variables to fall within specific lower and upper bounds, forming a “box” or an D -dimensional *hyperrectangle* within which the search is allowed to be conducted [18]. Box-constraints reflect typical real-world settings and are very common in both WBO and BBO problem-solving. Their handling within WBO is inherent, subject to the explicit problem formulation. In BBO there are multiple straightforward practices to enforce them, e.g., penalizing a violation, mirroring, or repetitive sampling as long as the new value is outside the box [18], [19]. Recently, a single-objective test-suite dedicated to strict box-constraints was announced [20] and a single-objective MI

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evolution strategy capable of handling explicit constraints was devised [21]. However, we are not aware of any prior work that investigated MI box-constrained multi-objective problems.

Research Question

Our long-term goal is to obtain a systematic empirical and theoretical assessment comparing between WBO algorithms to BBO meta-heuristics on different classes of multi-objective optimization problems. Yet, specifically, we articulate the overarching question of this study as follows:

How do the strengths and weaknesses of Set-Oriented WBO solvers and BBO meta-heuristics compare in treating bi-objective box-constrained MI quadratic models with different shapes of quadratic forms and scenarios of tight or loose bounds?

Our motivation to focus on quadratic MIO problems is driven by the practical observation that real-world MIOs often exhibit non-linearity, and quadratic terms represent a fundamental form of non-linearity. In the realm of continuous non-linear optimization, convex quadratic programming serves as the boundary for efficiently solvable problems. Notably, there exist numerous real-world applications that involve quadratic non-linearities, with one prominent example being the multi-objective portfolio optimization problem formulated by Markowitz [22]. Furthermore, in engineering problems involving binary interactions between process variables, quadratic terms are introduced. An illustrative instance is the utilization of Quadratic Response Surface Models in engineering design. In such cases, some process variables are discretized due to availability constraints and adherence to industrial norms, such as the sizing of equipment or parts. Moreover, discrete variables are introduced in the encoding of process alternatives [23].

In the current study we make a start by empirically exploring the performance of a WBO algorithm versus a BBO meta-heuristic (i.e., a concrete representative per each approach) on the following class of quadratic MIO problems:

- i The discrete variables constitute ordinal integers.
- ii The problems are box-constrained, with various box sizes, where the optimizer does not reside on the boundary.
- iii The quadratic objective functions are convex (in their continuous relaxation).
- iv We study bi-objective optimization problems aiming to compute a sparse point cover of their Pareto frontiers.

Although this problem class might appear simplistic, our study will show that it is already a challenging class for state-of-the-art solvers and these challenges need to be addressed first when departing to more difficult non-linear MIO problems.

Contribution and Paper Organization

The concrete contributions of this paper are the following:

- Identification of a generalized MP weakness in treating unbounded multi-objective quadratic MIO problems by set-oriented approaches: a proof and numerical evidence.
- Empirical analysis of the box-constraints' practical consequences considering this MP weakness (*tightly* versus *loosely* bounded box-constraints).

TABLE I
NOMENCLATURE AND ACRONYMS.

Acronym	Term
BBO	black-box optimization
DMA	Diversity Maximization Approach [32]
EMOA	evolutionary multi-objective algorithm
ES	evolution strategy
LP	linear program
MI(O)	mixed-integer (optimization)
MIES	mixed-integer evolution strategy
MILP	mixed-integer linear program
MIQCQP	mixed-integer quadratically-constrained quadratic program
MIQP	mixed-integer quadratic program
MP	mathematical programming
QP	quadratic program
SMS-EMOA	S-Metric Selection EMOA [33]
WBO	white-box optimization

- Systematic empirical comparison between a single CPLEX-based WBO algorithm to a state-of-the art evolutionary BBO meta-heuristic in Pareto optimization of a class of bi-objective convex quadratic MI problems with box-constraints.
- Assessment of the impact of the Hessian's structure and conditioning on the complexity of solving multi-objective quadratic MIO problems.

The remainder of this paper is organized as follows. Next, Section II begins by stating the targeted problem and providing its mathematical formulation. It then presents the theoretical contribution of this study in the form of a proven theorem on the computational complexity of a certain scenario under our consideration. Section III presents our empirical methodology for the planned systematic comparison, that is, the concrete WBO algorithm and BBO meta-heuristic that we employ. We then describe our experimental planning and setup in Section IV, where we also present preliminary runs and sensitivity analyses. In Section V we describe the systematic comparison of the selected methods on the quadratic models. Finally, we summarize the empirical observations in Section VI, link them to the theoretical results, and conclude this study.

II. PROBLEM STATEMENT AND FORMULATION

Linear optimization problems constitute the foundations of the single-objective constrained optimization domain. Pure Linear Programs (LP) are completely tractable, paving the road to addressing MILPs, which underlie the classical problems of Computer Science [4], [9], [24]. LPs, both pure and MI, have been extensively investigated (see, e.g., [25], [26]), and are likely the most exercised modeling in optimization. Also, they have enjoyed systematic empirical comparisons between WBO and BBO (see, e.g., [27]). At the same time, quadratic models constitute the next-step toward the generalization to nonlinear models. They are well-understood in both WBO and BBO research – with MP having the established Quadratic Programming (QP) branch [28], while evolutionary heuristics enjoying a sheer volume of theoretical results on their behavior over unconstrained quadratic models (see, e.g., [29]–[31]), including single-objective models with MI formulations [3].

A QP is *standardly* formed [34] to minimize a quadratic objective function whose decision variables are within the unit simplex in \mathbb{R}_+^D (i.e., the vector $\vec{e} \in \mathbb{R}^D$ is of all ones):

$$\text{minimize}_{\vec{x} \in \Delta_D} \vec{x}^T \mathbf{H} \vec{x} \quad \Delta_D := \{\vec{x} \in \mathbb{R}_+^D : \vec{e}^T \vec{x} = 1\}, \quad (1)$$

where \mathbf{H} is a symmetric $D \times D$ real matrix. Notably, the consideration of a non-homogeneous quadratic function is easily achieved by a trivial reformulation [34]. The introduction of integer decision variables renders the problem MI, standardly denoted as MIQP. Importantly, however, pure-QP is already NP-complete [35] – i.e., this standard QP (1) constitutes a hard problem even before introducing the integer decision variables. When such integers are introduced, the resultant MIQP is clearly a harder problem, yet there has been much progress in addressing it in practice [36] (we elaborate further in III-A). Again, one of the important aspects of the MIQP branch is the fact that it constitutes the next-step from the well-established MILP branch (see, e.g., [25]) toward the generalized Mixed-Integer Nonlinear Programming (MINLP) branch [37]. Finally, another degree of complexity is introduced to the model when the formulation encompasses quadratic constraint terms, and it is then called Quadratically-Constrained QP (QCQP) (also known as *all-quadratic programs* [38]; see, e.g., [39] as a single-objective solution approach). Quadratic models, either pure-QP or MIQP, arise in a large variety of problems, ranging from Portfolio optimization (Markowitz's original formulation [40] and its extensions [41]) and resource allocation [42], to population genetics [43] and game theory [44]. When turning to the multi-objective perspective, the nature of the objective function is clearly critical for its treatment by WBO. The multi-objective optimization of quadratic models, which is the focus of this study, has been naturally developed in MP from multi-objective LP, with Benson's method being its renowned baseline [45]. Such extensions yielded approximation methods [17] with the capacity to address nonlinear models [12], [46], [47]. At the same time, exact non-scalarizing MP-based methods exist, and we shall use such a method in our study (see description in Section III-A). Finally, BBO-wise, multi-objective optimization of quadratic models has not received any special attention in meta-heuristics' research, since no presumptions are usually made on the objective functions.

A. Concrete Aims and Assumptions

The current study aims to investigate problem-solving of bi-objective MI quadratic models by means of set-oriented approaches, both WBO and BBO, when subject to box-constraints. To this end, we explicitly consider the following family of MI quadratic objective functions:

$$f_k(\vec{x}) := (\vec{x} - \vec{\xi}_k)^T \cdot \mathcal{H}_k \cdot (\vec{x} - \vec{\xi}_k), \quad (2)$$

where the D -dimensional decision vector \vec{x} is constructed by n_r real-valued decision variables followed by n_z integer decision variables that are defined by the so-called *index set* $I := \{n_r + 1, \dots, n_r + n_z\}$: $\forall i \in I \quad x_i \in \mathbb{Z}$.

Importantly, we hold the following assumptions:

- i the model is unconstrained (that is, removing the requirement in (1) for placement within the unit simplex),

- ii the decision variables' bounds $[\ell, u]$ are not necessarily tight (and may be considered *unbounded* in practice),
- iii the matrices \mathcal{H}_k are positive semidefinite, which render the relaxation obtained by dropping the integrality requirements *convex*.

Overall, we target the Pareto optimization of this family of bi-objective convex quadratic problems with box-constraints (f_k refers to the family defined by (2)):

$$\begin{aligned} &\text{minimize}_{\vec{x}} \quad (f_0(\vec{x}), f_1(\vec{x}))^T \\ &\text{subject to:} \quad \vec{x} \in \mathbb{R}^D \\ &\quad \quad \quad x_i \in \mathbb{Z} \quad \forall i \in I \\ &\quad \quad \quad \ell \leq x_i \leq u \quad \forall i \in \{1, \dots, D\} \end{aligned} \quad (3)$$

with I being the integers' index set, where this vector notation refers to function-wise minimization:

$$f_0(\vec{x}) \mapsto \min, \quad f_1(\vec{x}) \mapsto \min.$$

Notably, the **loosening of boundary constraints** is fundamental (also in terms of computational complexity), as will become clear shortly. In addition we assume non-binary integer ranges, noting that in the case of binary integers linearization of the white-box model is commonly applied (see, e.g., [48]).

B. Complexity of Multi-Objective Unbounded Problems

A striking theorem proved by Jeroslow 50 years ago states that *quadratically-constrained MI unbounded problems are undecidable* [49]. In what follows, we link this result to the framework of multi-objective optimization to obtain a theorem relevant to set-oriented treatment of unbounded quadratic models.

Proposition 1. *Given an unbounded mixed-integer multi-objective optimization problem with quadratic objective functions, treating it with a set-oriented method that seeks to maximize diversity in the objective space necessarily induces unbounded quadratically constrained mixed-integer problems once the set is populated with the first solution.*

Proof. Once the set is populated with the first solution, the model must account for its existence by means of an explicit constraint. Since the objective functions are quadratic, the representation of this solution point within the constraint must take a quadratic form. The unboundness of this model, both in the objective function term, as well as the quadratic constraint, is simply a consequence of the original unboundness property. \square

Theorem 2. *Solving a mixed-integer multi-objective problem with quadratic objective functions by means of a set-oriented method is undecidable.*

Proof. According to Jeroslow's result [49] a quadratically-constrained mixed-integer unbounded problem is undecidable. Given Proposition-1, an unbounded quadratically constrained mixed-integer problem is necessarily induced when treating such multi-objective scenarios by a set-oriented approach, and hence the theorem follows. \square

III. APPROACH AND METHODOLOGY

We would like to conduct a systematic comparison between exact versus approximate multi-objective optimization problem-solvers over instances belonging to the class defined in (3), while exploring the impact of the box-constraints. To this end, we consider a representative per each approach – the Diversity Maximization Approach (DMA) [32], equipped with the CPLEX engine [50], as an exact method, versus the evolutionary-based SMS-EMOA [51]. The DMA is selected among other exact methods for being a set-oriented method with a compact Mathematical Program. Its attractive features will be summarized in the next subsection, and its implementation will be provided in Appendix A. In what follows, we will describe the main principles of the two approaches and then present the experimental planning and setup. Firstly, for the sake of notation definition, let \mathcal{X} denote the set of feasible solutions, $\mathcal{Y} \subset \mathbb{R}^m$ its image in the objective space. If $\vec{x} \in \mathcal{X}$, then $y = f(\vec{x}) \in \mathcal{Y}$, and the i^{th} objective function value is $y^{(i)} = f^{(i)}(\vec{x})$. Finally, we denote the Pareto frontier by \mathcal{Y}_{eff} .

A. WBO: The Diversity Maximization Approach

This subsection describes in detail the operation of the selected WBO algorithm, the so-called DMA. We begin by formally presenting the underlying mathematical definitions and programs in an MP-oriented style. We then offer a high-level overview, which may be helpful for readers who want to understand the basic concepts without getting bogged down in the technical details of the MP formalism.

Given a subset E of \mathcal{Y} and a point $y \in \mathcal{Y}$, we quantify the *diversity measure* of y with respect to this subset ($y_e \in E$):

$$\alpha_E(y) := \max_{y_e \in E} \left(\min_{1 \leq i \leq m} y^{(i)} - y_e^{(i)} \right). \quad (4)$$

Notably, we chose a scaling-free version of this diversity measure,¹ **which lies in the center of this approach**, in order to keep the algorithm as simple as possible and parameter-free. When the set E is unambiguous, we use the notation $\alpha(y)$ instead of $\alpha_E(y)$. Next, we consider E as a partial efficient frontier (evolving set) and state the underlying theorem for the DMA's operation and convergence (lexmin refers to lexicographical minimization of the subsequent list, ordered from the most to the least important, and w_i are positive weights):

Theorem 3. Let $y^* = \text{lexmin}_{y \in \mathcal{Y}} (\alpha(y), \sum_{i=1}^m w_i y^{(i)})$, where $\forall i \ w_i > 0$, and let $E \subseteq \mathcal{Y}_{\text{eff}}$. Then:

- 1) if $\alpha(y^*) < 0$, then $y^* \in \mathcal{Y}_{\text{eff}}$,
- 2) if $\alpha(y^*) = 0$, then $\mathcal{Y}_{\text{eff}} = E$.

See [32] for the full details and the proof.

¹This measure is introduced in the original paper [32] using a positive scaling coefficient Δ_{ie} :

$$\alpha_E(y) := \max_{y_e \in E} \left(\min_{1 \leq i \leq m} \frac{y^{(i)} - y_e^{(i)}}{\Delta_{ie}} \right). \quad (5)$$

Next, we outline the explicit DMA steps (note that the objective functions are implicit in this formulation, and in practice are to appear within the constraints):

Step-0: Solve the following problem with $w_i > 0$ for all i :

$$\begin{aligned} \text{[P0]} \quad & \text{minimize } \sum_{i=1}^m w_i \cdot f^{(i)}(\vec{x}) \\ & \text{subject to: } \vec{x} \in \mathcal{X}, \end{aligned} \quad (6)$$

where \mathcal{X} is deliberately left abstract. Let $y^* = f(\vec{x}^*)$ be the optimal value. Set $E = \{y^*\}$. Choose $\varepsilon > 0$ (say, 10^{-3}).

Step-1: Solve **P1** and let $y^* = f(x^*)$ be the optimal value:

$$\begin{aligned} \text{[P1]} \quad & \text{lexmin}_{y \in \mathcal{Y}} \left(\alpha(y), \sum_{i=1}^m w_i y^{(i)} \right) \\ & \text{subject to:} \\ & \alpha_E(y) := \max_{y_e \in E} \left(\min_{1 \leq i \leq m} y^{(i)} - y_e^{(i)} \right) \\ & \vec{x} \in \mathcal{X}. \end{aligned} \quad (7)$$

Step-2: If $\alpha(y^*) < -\varepsilon$ then $E = E \cup y^*$, go to **Step-1**; else **Terminate**.

By introducing $m \cdot \text{card}\{E\}$ binary decision variables, denoted by $\beta_{i,e}$, **P1** may be linearized and become an MILP (as long as **P0** is an MILP; note that L is a large number):

$$\begin{aligned} \text{[P1*]} \quad & \text{lexmin}_{y \in \mathcal{Y}} \left(\alpha, \sum_{i=1}^m w_i y^{(i)} \right) \\ & \text{subject to:} \\ & \alpha \geq \left(y^{(i)} - y_e^{(i)} \right) + (1 - \beta_{i,e}) \cdot L \\ & \forall i = 1, \dots, m \ \forall y_e \in E \\ & \sum_{i=1}^m \beta_{i,e} = 1 \quad \forall y_e \in E \\ & \beta_{i,e} \in \{0, 1\} \quad \forall i = 1, \dots, m \ \forall y_e \in E \\ & \vec{x} \in \mathcal{X}. \end{aligned} \quad (8)$$

Conceptual Summary and Key Features: The DMA begins by obtaining a single point on the Pareto frontier (solving **P0**) as an aggregated single-objective problem), which is to become the first element in the evolving set. It then iteratively adds individual points to the set, each constituting the non-dominated, farthest point from the existing set with respect to a diversity measure (locating each point by solving **P1*** with a set of constraints that reflects the distances to the existing set elements). In other words, it obtains a new exact non-dominated solution per each iteration. This problem-solving is enabled thanks to the specific diversity measure under consideration and to the fact that maximizing it is possible by solving an MILP. The termination criteria are either information on the attainment of the complete Pareto frontier (available through the diversity measure), or by exhausting a designated number of solution points.

Next, we summarize the DMA's key features:

- Fine distribution of the existing set is guaranteed.
- Optimality gap is provided.
- Solves frontiers of any nature (convex, concave).
- DMA is a MILP if the original problem is a MILP.

The explicit formulation of the DMA by means of a Mathematical Program is provided in Appendix A.

Synopsis, Complexity and Pragmatic Matters: Importantly, within the current context of quadratic models, **the obtained DMA modeling becomes a Mixed-Integer Quadratically-Constrained Quadratic Program (MIQCQP)** (note that the objective functions' formulation is implicit herein). We note a few remarks on this statement:

- 1) Theorem-2 applies to the DMA when treating quadratic objective functions (and thus becoming MIQCQP) and when the decision variables are unbounded. In practice, **the effect of this theorem will become evident as the box-constraints are as loose as $[-10^4, 10^4]$** (see Section IV-B and Figure 1). Yet, despite this theoretical complexity of handling integer quadratically-constrained problems, there has been much practical progress in treating MIQP in general [36] and Quadratically-Constrained problems in particular (e.g., by reformulation to a bilinear programming problem with integer variables [39], or by diverting to Mixed-Integer Second-Order Cone Programming [52] when the model permits).²
- 2) Despite the availability of many linearization and reformulation techniques [54], [55], we cannot apply them herein because a generalized unbounded MIQP cannot be linearized.³ In practice, the hardness of solving the model lies nonetheless within the DMA's MILP.
- 3) The numerical vulnerability of our DMA realization is potentially twofold – the applied linearization to get **[P1*]** and the lack of scaling coefficients, as specified earlier.

B. BBO: SMS-EMOA with MI Operators

To present the considered BBO approach, we first describe the concrete MI mutation and recombination operators, which are adopted from evolutionary single-objective optimization. These operators will then be used in combination with the SMS-EMOA method, a population-based meta-heuristic for multi-objective optimization which uses the hypervolume indicator as a selection criterion. The boundary treatment is as simple as applying truncation at the boundary. Unlike other evolutionary algorithms, SMS-EMOA's selection is based on *rank* rather than the absolute values of the objective function. In that regard, rank-based selection equips it with invariance properties with respect to order-preserving transformations [56], and gives it an advantage in the context of our study. As a steady-state EMOA, it generates and discards a single solution in each generation.

Here, adhering to the nature of the *family of problems* at hand – possessing real-valued, ordinal integer as well as categorical decision variables – we describe in what follows a specific evolutionary heuristic that was selected for the current

task. *Evolution Strategies* (ES) [30] are canonical evolutionary algorithms for global optimization with unique representation as well as specific variation operators. In ES, each individual carries, apart from the vector of decision variables, a vector of *endogenous* strategy parameters, which practically dictates the mutation operation. Both the decision variables, as well as the strategy parameters, evolve and are continuously optimized, according to the so-called *self-adaptation principle* [57]. In MI Evolution Strategies (MIES) [58], unlike the standard ES, the decision variables are categorized to three groups: real-valued variables, integer variables, and possibly categorical variables. Each individual in the population of candidate solutions carries strategy parameters per each category. The defining equations of the mutation operator, which constitutes the primary variation operator in ES, rely on stochastic sampling from the normal and geometric distributions. In this study we are interested only in real-valued and ordinal integer variables, so we do not specify the mutation operator for categorical variables. The MIES's operation is well defined by its self-adaptive mutation operator (Algorithm 1): $\{\vec{x}, \vec{z}\}$ are the real-valued and integer decision variables, respectively, and $\{\vec{s}, \vec{q}\}$ are their strategy parameters, respectively. \mathcal{N} denotes the normal distribution, which plays the dominant role of the real-valued update steps. At the same time, the integer decision variables are mutated by adding a *doubly geometrically* distributed random number, which is denoted by \mathcal{G}_{n_z} and is defined as follows (computed using uniformly distributed random variables $\mathcal{U}(0, 1)$):

$$\begin{aligned} \psi &\leftarrow 1 - (q'_i/n_z) \cdot \left(1 + \sqrt{1 + \left(\frac{q'_i}{n_z}\right)^2}\right)^{-1} \\ g_\ell &\leftarrow \left\lfloor \frac{\log(1-\mathcal{U}(0,1))}{\log(1-\psi)} \right\rfloor \quad \ell = 1, 2 \\ \mathcal{G}_{n_z}(0, q'_i) &:= g_1 - g_2. \end{aligned} \quad (9)$$

The recombination operator of the MIES is the discrete recombination, which randomly chooses a component at a vector position of the child individual from one of the two parents at the same position.

The S-Metric Selection EMOA (SMS-EMOA) [33] is a population-based meta-heuristic for bi-objective optimization that approximates the Pareto frontier using a fixed-size finite number of points. It employs non-dominated sorting to rank the population into layers, which are then ranked by the hypervolume contribution of their points. By using this ranking in a steady-state $(\mu + 1)$ -selection scheme, SMS-EMOA generates a series of populations that semi-monotonically increase the hypervolume indicator, a measure of the quality of Pareto frontier approximation. The choice of mutation and recombination operators should be based on the decision space domain. Note that for many-objective optimization, other methods like DI-MOEA [59], MOEA/D [60], and NSGA-III [61] are more appropriate. Our implementation and parameter settings typically follow [62]. A MI implementation of the SMS-EMOA was also suggested in [63]. The same idea of a MI variation operators can also be employed in the NSGA-II algorithm, which is the most widely used meta-heuristic for solving bi-objective optimization problems. Our preliminary experiments included the NSGA-II (using the implementation

²For pragmatic purposes, convenient implementation interfaces are available – see, e.g., [53].

³Even if the integers $x_i : i \in I$ may be linearized using auxiliary binaries [48], the multiplication of two (loosely bounded) decision variables within \vec{x} cannot be precisely linearized (but could be piecewise approximated upon separation [55]).

```

mutate( $\vec{x}, \vec{s}, n_r, \vec{z}, \vec{q}, n_z$ )
  /* real-valued decision variables */
   $\mathcal{N}_g^{(r)} \leftarrow \mathcal{N}(0, 1), \tau_g^{(r)} \leftarrow \frac{1}{\sqrt{2 \cdot n_r}}, \tau_\ell^{(r)} \leftarrow \frac{1}{\sqrt{2 \cdot \sqrt{n_r}}}$ 
  for  $i = 1, \dots, n_r$  do
     $s'_i \leftarrow$ 
     $\max\left(\varepsilon, s_i \cdot \exp\left\{\tau_g^{(r)} \cdot \mathcal{N}_g^{(r)} + \tau_\ell^{(r)} \cdot \mathcal{N}(0, 1)\right\}\right)$ 

    while true do
      if  $x'_i \leftarrow x_i + \mathcal{N}(0, s'_i) \in [\ell, u]$  then break
    end

  end

  /* integer decision variables */
   $\mathcal{N}_g^{(z)} \leftarrow \mathcal{N}(0, 1), \tau_g^{(z)} \leftarrow \frac{1}{\sqrt{2 \cdot n_z}}, \tau_\ell^{(z)} \leftarrow \frac{1}{\sqrt{2 \cdot \sqrt{n_z}}}$ 
  for  $i = 1, \dots, n_z$  do
     $q'_i \leftarrow$ 
     $\max\left(1, q_i \cdot \exp\left\{\tau_g^{(z)} \cdot \mathcal{N}_g^{(z)} + \tau_\ell^{(z)} \cdot \mathcal{N}(0, 1)\right\}\right)$ 

    while true do
      if  $z'_i \leftarrow z_i + \mathcal{G}_{n_z}(0, q'_i) \in [\ell, u]$  then break
      // see Eq. 9
    end

  end

end
return  $\{\vec{x}', \vec{s}', \vec{z}', \vec{q}'\}$ 

```

Algorithm 1: MIES-based self-adaptive mutation operator utilized by the SMS-EMOA: $\{\vec{x}, \vec{s}\}$ are the real-valued decision variables and strategy parameters, respectively. $\{\vec{z}, \vec{q}\}$ are the integer decision variables and strategy parameters, respectively. \mathcal{N} and \mathcal{G} denote the normal and the geometric distributions, respectively (for the latter see (9)). In our implementation we set $\varepsilon := 10^{-5}$. The box-constraints are enforced using repetitive sampling (the while loops are broken only when the new values are within the box).

of the `pymoo` package [64] and its default settings therein), yet indicated inferior performance on the current testbed.

IV. EXPERIMENTAL SETUP AND RESULTS

In order to systematically examine the behavior of the set-oriented WBO and BBO approaches, it is necessary to use prescribed test problems and limit the computation time to obtain comparable Pareto frontiers. To this end, we adopt the commonly used quadratic models, namely COCO's Ellipsoidal, Discus and Cigar functions [65].⁴ Explicitly, we consider five Hessian matrices for unconstrained and box-constrained problems: three separable and two non-separable matrices with dimensions $n = n_r = n_z = D/2$:

H-1 DISCUS: $(\mathcal{H}_{\text{disc}})_{11} = c, (\mathcal{H}_{\text{disc}})_{ii} = 1 \quad i = 2, \dots, n;$

H-2 CIGAR: $(\mathcal{H}_{\text{cigar}})_{11} = 1, (\mathcal{H}_{\text{cigar}})_{ii} = c \quad i = 2, \dots, n;$

H-3 ELLIPSE: $(\mathcal{H}_{\text{ellipse}})_{ii} = c^{\frac{i-1}{n-1}};$

H-4 Rotated Ellipse (ROTELLIPSE):

$$\mathcal{H}_{\text{RE}} = \mathcal{R}\mathcal{H}_{\text{ellipse}}\mathcal{R}^{-1}$$

⁴These functions correspond to $\{f_2, f_{10}, f_{11}, f_{12}\}$ at the renowned BBOB suite. The actual rotation of f_{10} is implemented as reported in [31].

where \mathcal{R} is rotation by $\approx \frac{\pi}{4}$ radians in the plane spanned by $(1, 0, 1, 0, \dots)^T$ and $(0, 1, 0, 1, \dots)^T$;

H-5 Hadamard Ellipse (HADELLIPSE):

$$\mathcal{H}_{\text{HE}} = \mathcal{S}\mathcal{H}_{\text{ellipse}}\mathcal{S}^{-1}$$

where the rotation constitutes the normalized Hadamard matrix, $\mathcal{S} := \text{Hadamard}(D)/\sqrt{D}$,

with c denoting a parametric condition number. We set two points about which the quadratic models are centered:

$$\vec{\xi}_0 := (+7, -7, +7, -7, \dots, +7, -7)^T$$

$$\vec{\xi}_1 := (-4, +4, -4, +4, \dots, -4, +4)^T.$$

For the separable cases (1-3) we construct the $D \times D$ -dimensional Hessian matrix as a concatenation of two $n \times n$ -dimensional matrices, in order to introduce the conditioning effect to both types of variables:

$$\mathbf{H} := \begin{pmatrix} \mathcal{H} & \mathbf{0} \\ \mathbf{0} & \mathcal{H} \end{pmatrix}.$$

After the $D \times D$ -dimensional Hessian matrix is set, the two objective functions are calculated *de facto* as follows:

$$\begin{aligned} f_0 &= \frac{1}{c} \cdot \left[\left(\vec{x} - \vec{\xi}_0 \right)^T \mathbf{H} \left(\vec{x} - \vec{\xi}_0 \right) \right] \\ f_1 &= \frac{1}{c} \cdot \left[\left(\vec{x} - \vec{\xi}_1 \right)^T \mathbf{H} \left(\vec{x} - \vec{\xi}_1 \right) \right]. \end{aligned} \quad (10)$$

Figure 11 depicts contour maps of the objective function values per a variety of 2D landscapes. Next, after laying out the setup in Section IV-A, we will describe the following experimental studies:

- Section IV-B will present a sensitivity analysis on the choice of bounds, where we will increasingly loosen the box-constraints and assess their impact on the behavior of the methods. They will reveal a major problem of the WBO solver to handle loosely bounded models. The sensitivity analysis will not constitute a comprehensive benchmark, but will unveil valuable insights. We will also analyze the parameter settings of the SMS-EMOA and the extent to which it can adapt step-sizes.
- Section V will present a benchmark on a wider set of problems with a focus on the tight bounds of $[-10, 10]$. Evidently, the selected WBO and BBO approaches can be considered to perform competitively when subject to such box-constraints, and we will reveal how exactly they compare over a variety of problems and for a range of conditioning levels of the Hessian matrix.

A. Experimental Planning and Numerical Setup

The experimental results in what follows show approximations of 2D Pareto frontiers with 15 points. Our rationale for selecting 15 points for the approximation was based on several considerations. First and foremost, the nature of the two-dimensional Pareto frontiers in our study exhibits a relatively simple shape, which we suppose is related to the convex nature of the continuous relaxations. This simplicity allows

us to capture the essential characteristics of the frontier with a relatively small number of points. We have carefully assessed the quality indicators, specifically the hypervolume, for this approximation. The results consistently demonstrate that the 15-point approximation captures the essential features of the frontier, yielding high-quality results. To check the validity of our claims, we conducted additional experiments with 30 points to explore the potential benefits of a larger set. However, the outcomes of these experiments showed only insignificant changes in the quality indicators, particularly the hypervolume. Evidently, the resultant 30-point sets possess only a negligible addition of 1%-2% per the hypervolume indicator value with respect to the 15-point sets (see Supplementary Materials for the numerical comparisons). Importantly, the resultant 30-point sets never introduced “breaking” points nor modified the ranking of the two approaches under consideration. It is worth noting that the computational effort for the 30-point sets is approximately doubled with respect to the 15-point sets. The insignificant improvement with the increased set cardinality does not justify the additional computational resources and the space needed to obtain these results.

Preliminary runs indicated that the DMA required long computation times for obtaining an exact solution to problem [P1*]. At the same time, the SMS-EMOA exhibited convergence per a single run after 10^7 function evaluations. Therefore, we set a pragmatic time limit for solving each problem instance: $12\frac{1}{2}$ computation hours (see below details concerning the specifications of machines), which break down to a single DMA run with a time limit of 50min per each solution point (`cplex.tilim` = 3000 times 15 points), or to 10 SMS runs each with a budget of 10^7 function evaluations. It may be argued that the DMA benefits from a CPU advantage over the SMS-EMOA, which requires repetitions due to its stochasticity. **Importantly, we will focus in Section V on experimenting in depth the 64-dimensional use-case (i.e., $n = 32$, $D = 64$).** Preliminary runs reflected equivalent algorithmic behavior on various dimensions (e.g., $D \in \{32, 64, 128\}$), and yet, this particular dimension is selected for being an interesting tradeoff between high dimensionality to known scalability issues of ESs [66]. Also, per the HADELLIPSE definition, we set the baseline ellipse therein to $(\mathcal{H}_{\text{ellipse}})_{ii} = 1 + \frac{(c-1)(i-1)}{n-1}$. Next, we provide the technical specifications of our numerical simulations.⁵

a) WBO Setup: The DMA was implemented in IBM ILOG CPLEX Optimization Studio 12.8 in OPL and its associated scripting language (javascript-based). All the experiments were run using the Python API (for sequential execution) and executed on Windows Intel(R) Xeon(R) CPU E5-1620 v4 @ 3.50GHz with 16 processing units. The relative MIP optimality gap was set to 10^{-3} (`cplex.epgap` = 0.001), and the `polish` procedure [67] was enabled after reaching an integer solution. Otherwise, the CPLEX engine was employed in its default settings, which in this convex MIQCQP case translate into a Branch & Cut scheme that relies on a QP solver [50].

b) BBO Setup: The SMS-EMOA was implemented in Mathwork's MATLAB 2016a. All runs, using a population of 15 individuals, were deployed on Linux Intel(R) Xeon(R) CPU E5-2670 v3 @ 2.30GHz with 48 processing units.

B. Sensitivity analyses: boundaries and parameters' settings

The DMA fails to converge under the scenario of totally loose bounds ($[-10^6, 10^6]$). In order to investigate this failure, we conducted additional runs where we gradually set them loose. We designed a series of DMA runs along which we increased the bounding box size of each decision variable, i.e., $\forall i \ x_i \in B$

$$B := \{[-10, 10], [-50, 50], [-200, 200], [-1000, 1000], [-5000, 5000], [-10^4, 10^4], [-10^5, 10^5], [-10^6, 10^6]\}. \quad (11)$$

We experimented the entire set of problems and conditioning levels, yet choose to *qualitatively* report herein on the results without quantitative analysis. To illustrate the trend of the current experiment, we present representative outcomes when loosening the bounds of the DMA program on two 64-dimensional problem instances – Figure 1[LEFT] depicts Pareto frontiers obtained by the DMA for the separable ELLIPSE problem ($\mathcal{H}_{\text{ellipse}}$) with a conditioning level of $c = 10000$, and Figure 1[RIGHT] depicts the equivalent outcome for the non-separable ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 1000$ (the figures also contain zoom-in insets). Evidently, the DMA obtains solid Pareto frontiers up until the bounding box of $[-5000, 5000]$, where the quality of the frontier starts to deteriorate. It is fair to state that the DMA begins to diverge as of the bounding box of $[-10^4, 10^4]$ when subject to the current time limit. Importantly, we carried out additional experiments with extended time-limits (a single DMA run was limited up to 48 hours, that is, `cplex.tilim` = 11500 times 15 points). The DMA behavior under the loose boundaries' scenario was observed to be consistent throughout these experiments. **We consider this behavior as a clear indication for the effect of Theorem-2 - that is, the MP problem becomes harder as the box-constraints' bounds are set loose.**

We recorded the MIES' step-sizes per each decision variable, $\{\vec{s}, \vec{q}\}$, to better understand the behavior on the different scales of search-spaces. Figure 2 depicts step-sizes of randomly-selected decision variables during a successful SMS-EMOA run on the 64-dimensional ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 1000$. It encompasses the real-valued step-size s_i (LEFT) as well as the discrete step-size q_i (RIGHT), accounting for the two boundaries scenarios - tight within $[-10, 10]$ (TOP) and loose $[-10^6, 10^6]$ (BOTTOM - mind should be given to the log-scaled y-axes). The data is down-sampled to values recorded once every 50000 iterations. Importantly, the plots that we chose to show well represent the other problem instances at the various conditioning levels. A few observations are evident from this figure – firstly, there is no step-size convergence in the tight scenario, that is, the median values in the end of the run resemble its beginning. This behavior is expected in multi-objective optimization,

⁵The source code is available at <https://github.com/ofersh/moMIQP>.

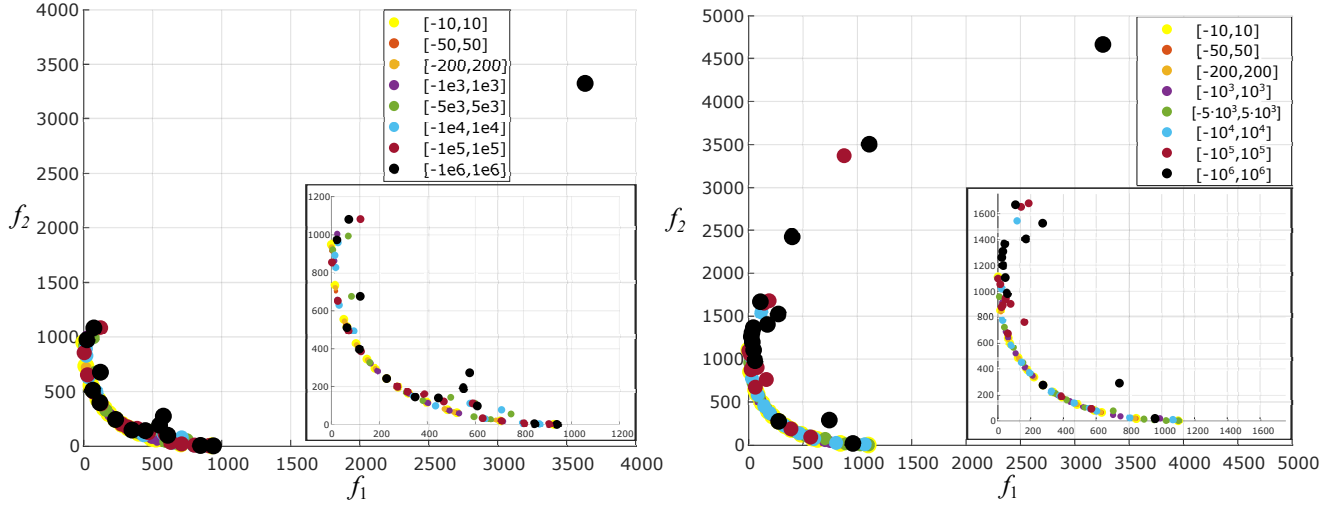


Fig. 1. Pareto frontiers obtained by the DMA on 8 problem-instances subject to loosening the box-constraints' bounds: [LEFT] the separable 64-dimensional ELLIPSE problem ($\mathcal{H}_{\text{ellipse}}$) with a conditioning level of $c = 10000$, and [RIGHT] the non-separable 64-dimensional ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 1000$. The increasing bounds of the box-constraints per the 8 problem-instances, whose attained frontiers are depicted in different colors, are indicated in the legends. Insets: zoom-in of the same datasets. The observed divergence on both landscapes is indicative of the practical effect of Theorem-2 — WBO problem-solving of such quadratic landscapes, when using the DMA, becomes harder as the decision variables' bounds are set loose.

since the self-adaptation principle is well defined for single-objective optimization, and moreover, a new offspring is injected into the (small) population in every generation with default step-size values. Secondly, the step-size values in the loose scenario exhibit dramatic large values, whose standard deviations gradually shrink upon convergence. We identify this pattern as the indication for the MIES' capability to handle the enormous bounding box of $[-10^6, 10^6]$ per each decision variable, relying on step-size adaptation.

To further investigate the SMS-EMOA's behavior, we conducted additional experiments where the recombination operator was suspended in the scenario of loose boundaries (the variation was restricted then to mutation only). Figure 3 depicts the summary of this investigation on selected 64-dimensional problem instances – separable at the TOP ((a) presents the CIGAR problem ($\mathcal{H}_{\text{cigar}}$) with a conditioning level of $c = 100$, and (b) presents the ELLIPSE problem ($\mathcal{H}_{\text{ellipse}}$) with a conditioning level of $c = 1000$), and non-separable at the BOTTOM ((c) presents the ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 100$, and (d) presents the HADELLIPSE problem (\mathcal{H}_{HE}) with a conditioning level of $c = 10$). For reference, the outputs of the DMA as well as the default SMS-EMOA are also presented (altogether five approximate frontiers, where each frontier of the SMS-EMOA constitutes the non-dominated solutions of the union of results). The outcome of the modified meta-heuristic (“NoRecomb”), depicted by black stars, is evidently inferior in its coverage, but competitive in its accuracy when compared to the default SMS-EMOA. Figure 3(d) should be inspected with care, keeping in mind that the default SMS-EMOA was challenged on the Hadamard landscape in the first place, regardless of the examined scenarios. In other words, the mutation operator is responsible for the MIES' ability to handle the loosely bounded decision variables (via self-adaptation), and to enable a focused search in a tight regime.

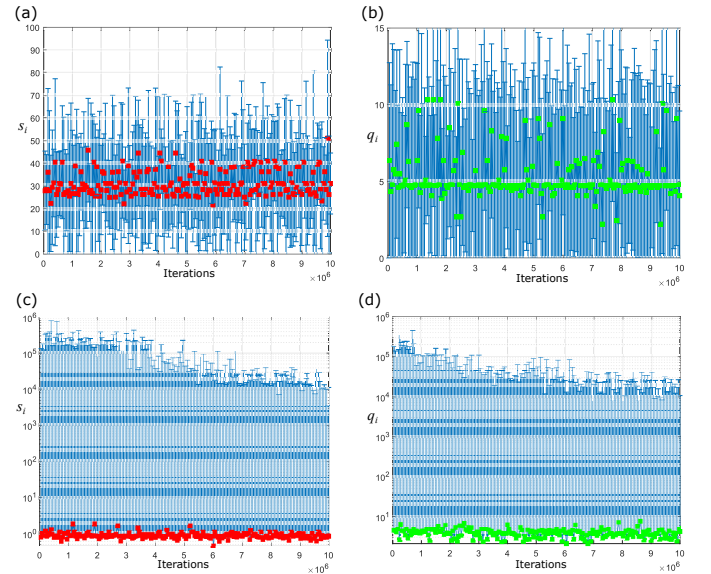


Fig. 2. Recorded step-sizes of a successful SMS-EMOA run on the 64-dimensional ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 1000$ – per randomly selected decision variables, subject to tight boundaries [TOP: (a)+(b)] and loose boundaries [BOTTOM: (c)+(d)]. The data is down-sampled to values recorded once every 50000 iterations. The populations' median values are depicted by points, while the error-bars represent the standard deviation within the population: (a) the real-valued step-size s_i subject to a bounding box of $[-10, 10]$; (b) the discrete step-size q_i subject to a bounding box of $[-10, 10]$; (c) the real-valued step-size s_i subject to a bounding box of $[-10^6, 10^6]$, with a log-scaled y-axis; (d) the discrete step-size q_i subject to a bounding box of $[-10^6, 10^6]$, with a log-scaled y-axis.

At the same time, lacking the recombination operator hampers the ability of the SMS-EMOA to explore tradeoff areas and results in deteriorated coverage of the approximate frontier.

V. BENCHMARK ON QUADRATIC TEST PROBLEMS

In the next study, we compare the performance of DMA and SMS-EMOA on five commonly used test problems: DISCUS

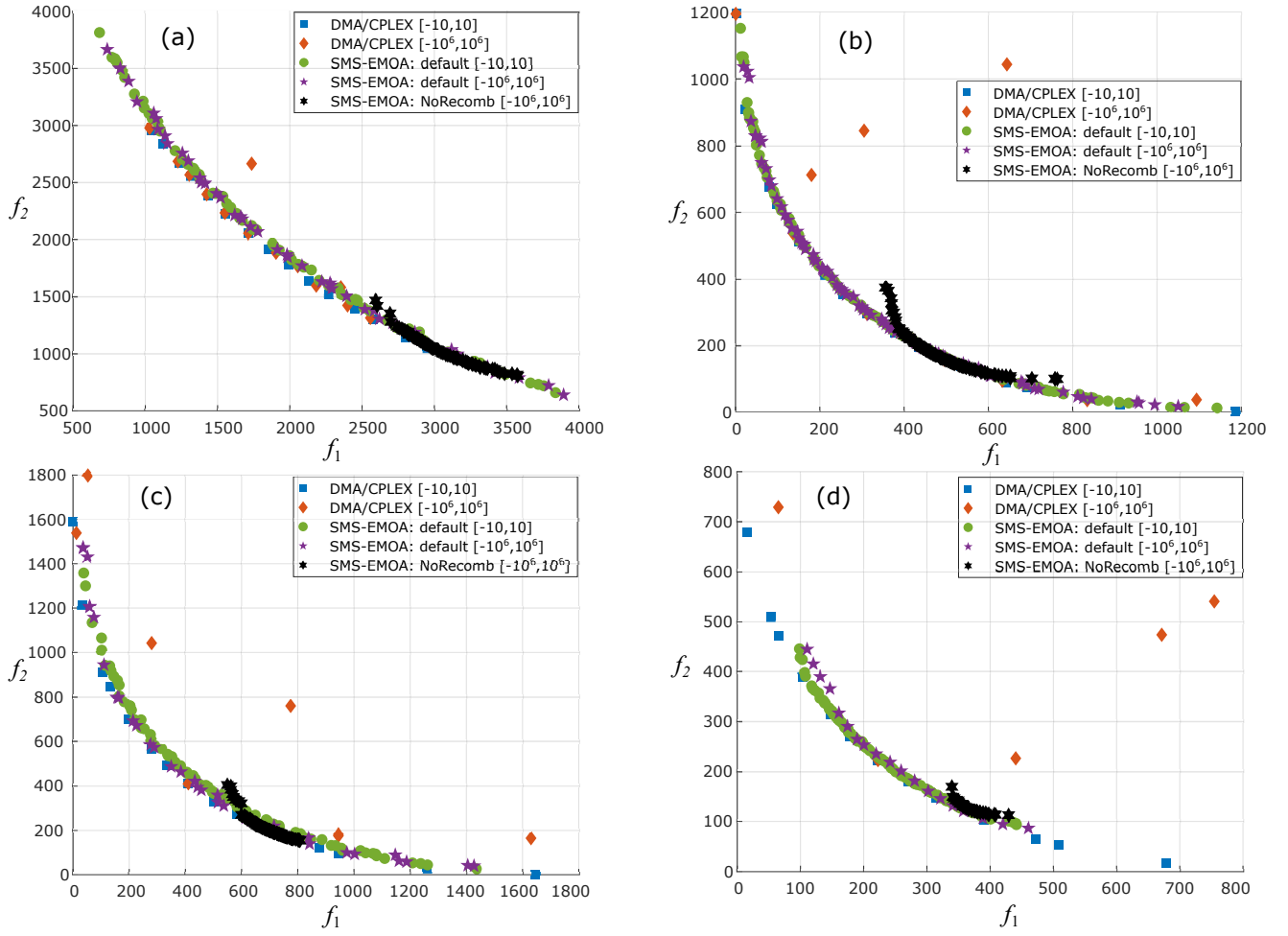


Fig. 3. Investigating the suspension of the MIES recombination operator on the SMS-EMOA performing over 64-dimensional problem instances (clockwise starting at top-left): (a) presents the CIGAR problem ($\mathcal{H}_{\text{cigar}}$) with a conditioning level of $c = 100$; (b) presents the ELLIPSE problem ($\mathcal{H}_{\text{ellipse}}$) with a conditioning level of $c = 1000$; (c) presents the ROTELLIPSE problem (\mathcal{H}_{RE}) with a conditioning level of $c = 100$, and (d) presents the HADELLIPSE problem (\mathcal{H}_{HE}) with a conditioning level of $c = 10$. For reference, the outputs of the DMA as well as the default SMS-EMOA are also presented (altogether five approximate frontiers, where the frontier of the SMS-EMOA constitutes an aggregation of its runs).

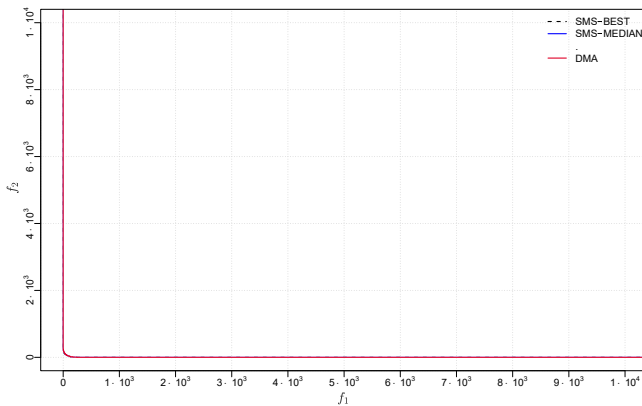


Fig. 4. Median attainment curves of the stochastic SMS-EMOA (median and best over 10 runs) versus the deterministic DMA (single run) for the DISCUS problem with $c = 10^5$. Evidently, the curves collide in this case, and hence indicate equivalent performance on this problem instance (see also Fig. 9).

($\mathcal{H}_{\text{disc}}$; Figure 4), CIGAR ($\mathcal{H}_{\text{cigar}}$; Figure 5), ELLIPSE ($\mathcal{H}_{\text{ellipse}}$; Figure 6), ROTELLIPSE (\mathcal{H}_{RE} ; Figure 7), and HADELLIPSE (\mathcal{H}_{HE} ; Figure 8). Each test problem is evaluated over six differ-

ent conditioning levels, ranging from $c = 10$ to $c = 1000000$, at dimension $D = 64$. We focus on the tight box-constraints (the bounded scenario of $[-10, 10]$), although we conducted experiments for the loose scenario as well and will mention it occasionally. We use median attainment curves to compare the algorithms, which provide a visual representation of the trade-off between the objectives. The median attainment curve shows the boundary of the region that is attained in at least half of total number of the runs, when considering multiple runs of the stochastic meta-heuristic.⁶ For the stochastic SMS-EMOA the curves summarize the median and the best over 10 runs, whereas we use a single run to produce the attainment curve of the deterministic DMA.⁷ Due to space limitations we present herein only a subset of the calculated attainment curves; The remaining curves, which consistently support the reported trends, are placed in the Supplementary Material Section. Furthermore, to enhance the robustness of our findings, we employed the hypervolume indicator as a suitable scalar

⁶We use the R package implementing empirical attainment surfaces [68].

⁷The raw datasets are available at <https://github.com/ofersh/moMIQP/tree/main/datasets>.

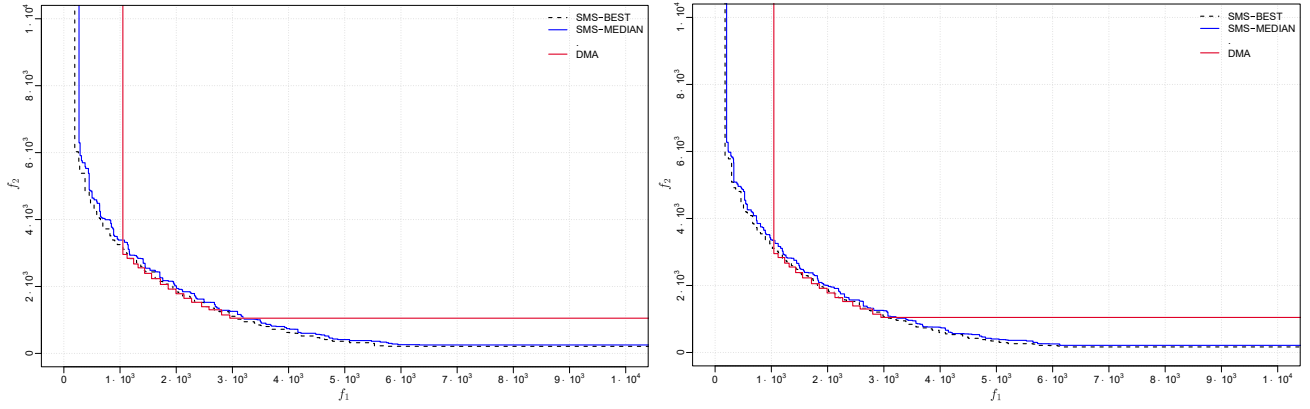


Fig. 5. Median attainment curves of the stochastic SMS-EMOA (median and best over 10 runs) versus the deterministic DMA (single run) for the CIGAR problem: $c = 10$ [LEFT] and $c = 10^6$ [RIGHT]. The DMA underperforms on these problem instances (see also Fig. 9).

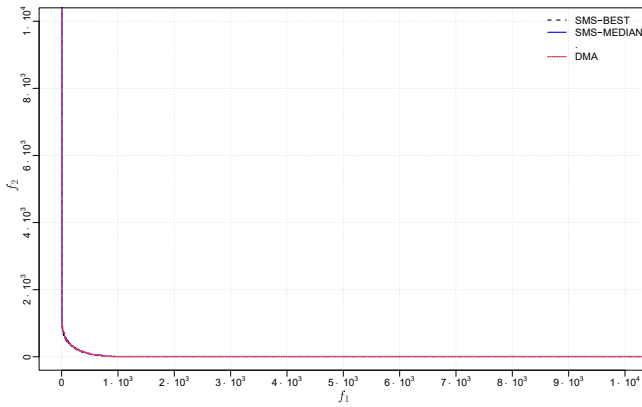


Fig. 6. Median attainment curves of the stochastic SMS-EMOA (median and best over 10 runs) versus the deterministic DMA (single run) for the ELLIPSE problem with $c = 10^4$. The curves collide and thus indicate equivalent performance (see also Fig. 9).

measure for pairwise performance comparisons. We illustrate the hypervolume calculations using statistical box-plots, which display the normalized indicator of the SMS-EMOA divided by the hypervolume indicator achieved by the DMA. In this context, a value of 1.0 represents equivalent performance, while values exceeding 1.0 indicate superior performance. It is important to note that the reference point was determined by considering the worst objective function values obtained from the dataset of the merged Pareto front approximations of all algorithms. These box-plots are organized based on the 5 Hessian types and encompass the 6 conditioning levels, resulting in a total of 30 box-plots. Figure 9 showcases the box-plots for the tight (bounded) scenario. The equivalent plot for the loose (unbounded) scenario, which suffers from occasional divergence of the DMA (see Section IV-B and the link therein to Theorem-2), was placed in the Supplementary Material Section. The hypervolume statistics confirm the overall trends observed in the empirical attainment curves and adds further validation to our claims.

Here are the main observations concerning the tight scenario:

- 1) For the DISCUS and ELLIPSE problems, both DMA and SMS-EMOA achieved equally good approximations based on the median attainment curves and the hypervolume statistics – this holds across all conditioning levels.
- 2) The SMS-EMOA obtained better approximations for the CIGAR problem compared to the DMA. This outperformance is statistically significant across all conditioning levels. In particular, the DMA failed to reach the outer flanks of the CIGAR problem's Pareto frontier.
- 3) For the ROTELLIPSE problem, the relative performance of the DMA and SMS-EMOA is dependent upon the condition number. Interestingly, while SMS-EMOA underperforms across the moderate condition numbers ($c = \{10, 100, 1000\}$), the trend is flipped at higher condition numbers. Specifically, the SMS-EMOA outperforms the DMA on the high condition numbers of $c = \{10^5, 10^6\}$.
- 4) For the HADELLIPSE problem, the DMA consistently outperforms the SMS-EMOA, regardless of the condition number, with statistical significance. This result can be attributed to the narrow cone of dominating solutions, which makes it difficult for isotropic mutation, as generated by the MIES, to find improvements towards the Pareto frontier. In contrast, DMA can exploit the explicit quadratic form of the problem to place points with precision in the dominating cone, leading to better results.
- 5) For both ROTELLIPSE and HADELLIPSE, our objective was to assess the proximity of the solution to the true Pareto frontier. To achieve this, we constructed a lower bound envelope for the Pareto frontier by solving the continuous relaxation of the MIQP problem using DMA/CPLEX with a larger set of 30 points. The obtained results reveal a noticeable disparity between the bounds derived from the continuous relaxation and the outcomes obtained through MIQP. Upon assuming the accuracy of the continuous relaxation solution, we deduce that for a value of $c = 10$, the discrepancy in integrality is negligible. Consequently, we believe that SMS-EMOA possesses the capability to achieve optimality in solving the problem. However, the integrality gap fails to account for the observation that DMA yields a sparse approximation of the Pareto frontier. This discrepancy is attributed to DMA's inherent inability to bridge the gaps present in the approximation of the Pareto frontier.
- 6) The overall results, across separable and non-separable

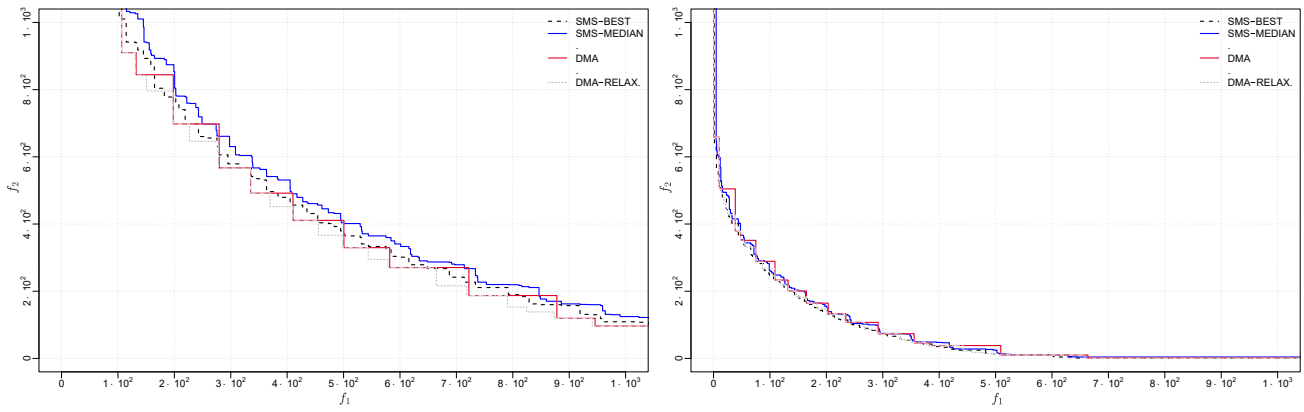


Fig. 7. Median attainment curves of the stochastic SMS-EMOA (median and best over 10 runs) versus the deterministic DMA (single run) for the ROTELLIPSE problem: $c = 100$ [LEFT] and $c = 10^5$ [RIGHT]. The SMS-EMOA underperforms on the low-conditioning instances, but, surprisingly, outperforms the DMA on the ill-conditioning instances (see also Fig. 9).

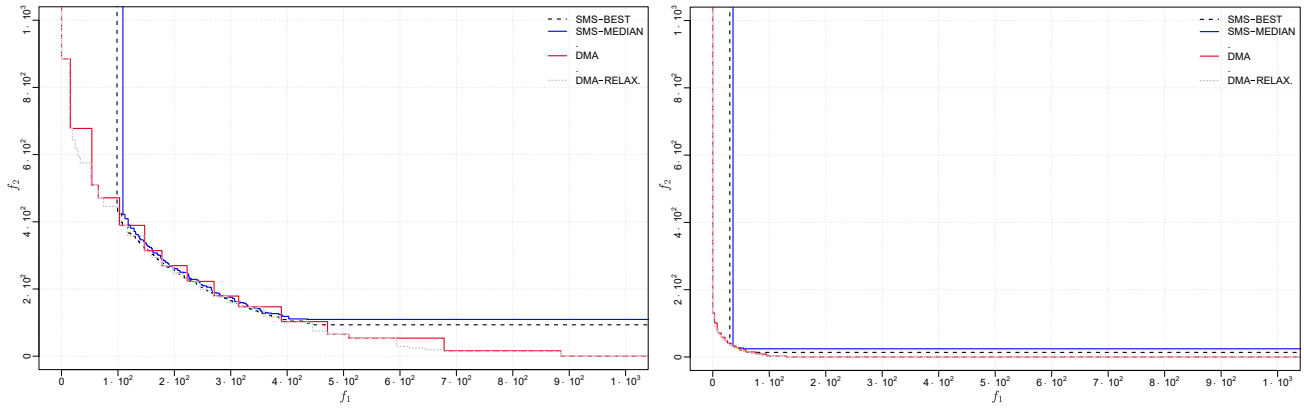


Fig. 8. Median attainment curves of the stochastic SMS-EMOA (median and best over 10 runs) versus the deterministic DMA (single run) for the HADELLIPSE problem: $c = 10$ [LEFT] and $c = 1000$ [RIGHT]. The SMS-EMOA underperforms on this problem instance across all conditioning levels (see also Fig. 9).

problems, demonstrate that the type of interaction is usually more significant in the problem difficulty than the condition number. Furthermore, we observe that problems with interaction between real variables and high conditioning are the most challenging for meta-heuristic algorithms.

The aforementioned findings are grounded in empirical observations, which demand elucidation. Rather than embarking on a formal analysis, we will present two graphical explanations to depict the impact of the condition number and non-separability on the inherent complexity of the problem.

The illustration of an elliptic contour, as it might manifest in either the context of ROTELLIPSE or HADELLIPSE, is presented in Figure 10 (Left). The point $(-2, 2)$ can only be enhanced by transitioning to $(-1, -1)$, which unfortunately does not align with an adjacent point on the integer lattice (especially in the consideration of a Hamming neighborhood). This instance serves to exemplify that non-separable quadratic integer programming can induce **multimodal landscapes**, even in scenarios without constraints. As a result, stochastic hill-climbing strategies like the MIES and the isotropic mutation based SMS-EMOA can become trapped in such landscapes. It is worth noting that this particular issue does not arise when the principal axes of the ellipses are parallel

to the coordinate axes, constituting a separable problem.

In Figure 10 (Right), the contours of two elliptic quadratic functions across a continuous domain are depicted. The solid yellow region represents the domain where points superior to x are situated. This region is extremely narrow, making it challenging to position points within it to approach the efficient set (and the Pareto frontier). Narrow elliptical contours manifest when there is a substantial variance in eigenvalues, indicating a high condition number in the Hessian matrix.

VI. DISCUSSION AND SUMMARY

The proven proposition (Theorem-2) on the potential undecidability of set-oriented approaches when treating unbounded multi-objective MIQP constitutes a WBO weakness. In some sense, this weakness is not surprising, since MP is known to operate well under constraints (e.g., the broad relevance of interior-point methods). Indeed, this weakness becomes an opportunity for BBO methods to prove themselves effective. Our empirical study focused on the strengths and limitations of a CPLEX-based WBO algorithm (the DMA) versus an evolutionary BBO meta-heuristic (the MIES-based SMS-EMOA). We looked at three main factors of problem complexity: the tightness of the box-constraints, the interaction between decision variables (separability), and the conditioning of the

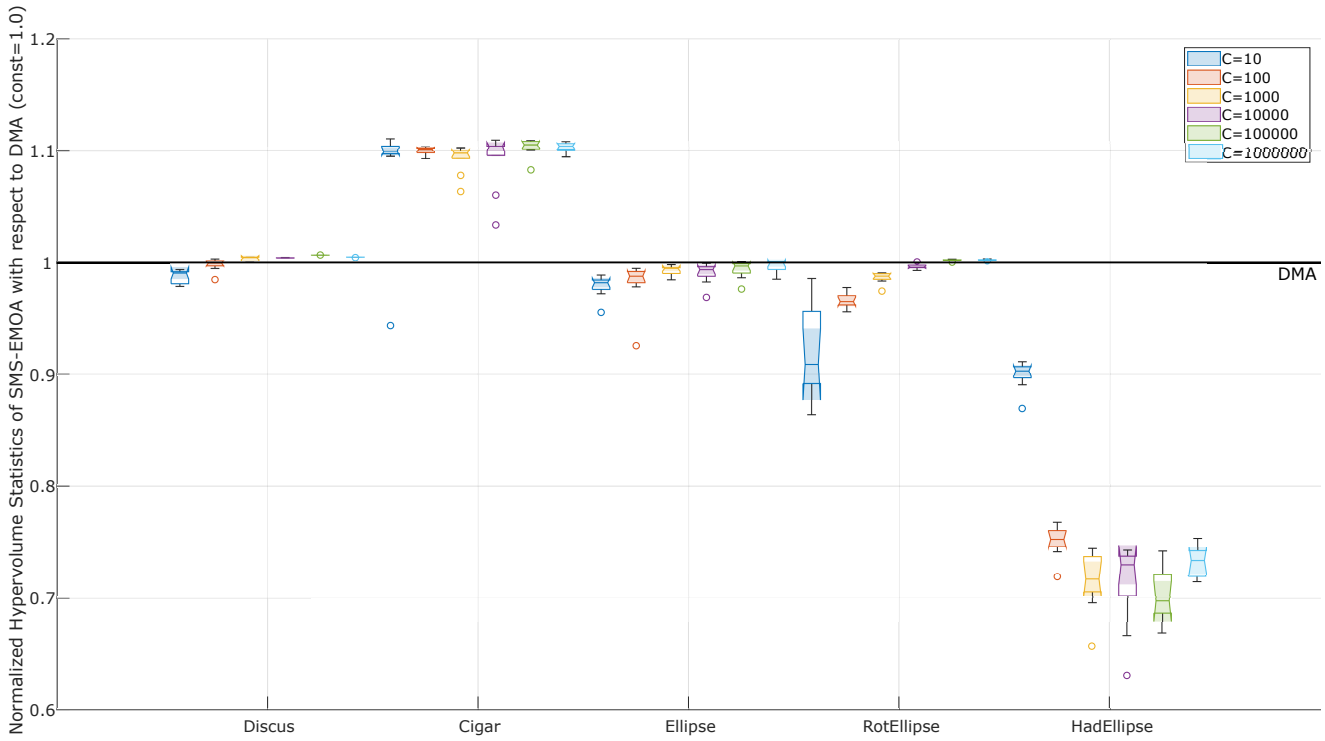


Fig. 9. Statistical box-plots of the hypervolume indicator obtained by the stochastic SMS-EMOA when normalized with respect to the deterministic DMA on the **tight** (bounded) use-cases. The flat function of the constant 1.0 value represents the DMA reference. The box-plots are group-organized according to the 5 Hessian types (see x-axis' ticks) and group-colored according to the 6 conditioning levels (see legend) – with 30 box-plots altogether.

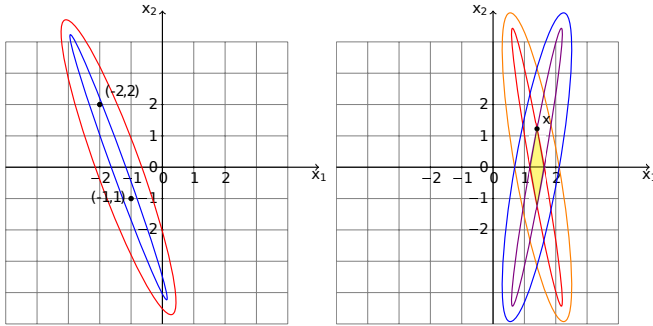


Fig. 10. LHS: Plot of an elliptic contour as it might occur for the problems ROTELLIPSE or HADELLIPSE. The point $(-2, 2)$ can only be improved by a move to $(-1, -1)$ which is not a neighboring point on the integer lattice. RHS: Contours of two elliptic quadratic functions over a continuous domain. The opaque yellow area is the region where points dominating x reside.

Hessian matrix of the objective functions. These difficulties were represented in a set of five selected test problems, which were scalable in terms of bound-tightness and conditioning.

An empirical observation indicated that the HADELLIPSE (\mathcal{H}_{HE}) constituted a challenging landscape for the SMS-EMOA, which practically failed to obtain a fair coverage of the Pareto frontier. Additional runs using the reference BBO meta-heuristic, the NSGA2, concluded with a similar outcome. We argue that the explanation for this difficulty is rooted in this landscape's nature. Firstly, it is well-known that the Pareto frontier is mapped onto the line connecting the two ellipsoids' basins of attraction (see, e.g., [69]). Secondly, as an illustration, we depict in Figure 11 contour maps of the ob-

jective function values per multiple 2D landscapes. Evidently, the Hadamard rotation keeps the two basins aligned, whereas it induces major barriers along their connecting line (Figure 11 BOTTOM). At the same time, the “conventional” rotation keeps the two basins close without dramatic barriers. Notably, the CIGAR landscape also introduces barriers on the connector, which grow as the conditioning increases, but possesses the separability property that enables effective attainment of the frontier by the SMS-EMOA. Counter-intuitively to some extent, the DMA failed to cover the Pareto frontier of this separable CIGAR across all condition numbers. Altogether, the DMA and the SMS-EMOA performed similarly on the DISCUS, ELLIPSE and ROTELLIPSE problems, and finally, the DMA underperformed on the CIGAR problem while the SMS-EMOA underperformed on the HADELLIPSE problem.

Evidently, it is not a clear cut decision whether to employ a WBO algorithm or a BBO meta-heuristic – in our study, the relative performance of the selected representatives largely depended on the characteristics of the quadratic form and the box constraints. Notably, the conditioning is not the main factor in determining the complexity, but it must be viewed in concert with the interaction between variables as dictated by the structure of the Hessian matrix. Moreover, our study shows that the isotropic mutation of integer variables might be an inferior strategy in case of rotated Hessian matrices, and mechanisms such as the covariance matrix adaptation [70] might have to be adopted to make BBO meta-heuristics competitive on high-conditioned non-separable MI problems. On the side of WBO algorithms, the observed problem with loosely bounded decision variables should be regarded as an

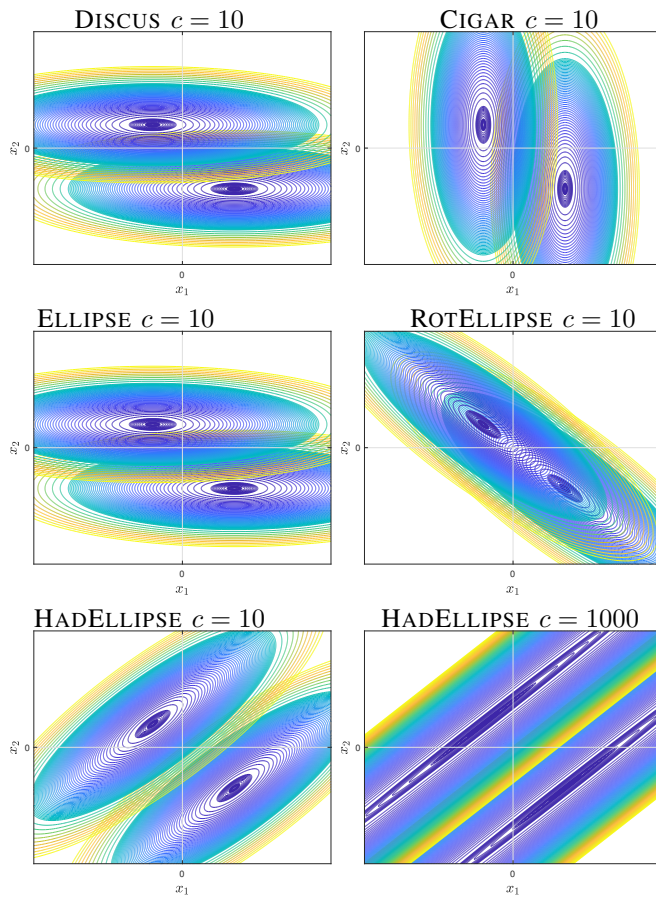


Fig. 11. Contour plots of function values of various 2D problem instances. TOP: DISCUS (Left) and CIGAR (Right), both with conditioning level of $c = 10$; MIDDLE: separable ELLIPSE (Left) and ROTELLIPSE (Right), both with conditioning level of $c = 10$; BOTTOM: two HADELLIPSE instances at conditioning of $c = 10$ (Left) and $c = 1000$ (Right).

incentive for further research, but the DMA's underperformance on certain problems also deserves attention. Finally, it is worth noting that the ability to leverage explicit expressions of equations can provide an advantage to white-box solvers compared to their model-agnostic counterparts. Currently, there are few deterministic set-oriented white-box methods available for mixed-integer non-linear Pareto optimization. One promising new direction is the concept of hypervolume scalarization, as discussed in [71], which could be extended from discrete to mixed-integer domains. This approach follows a mechanism similar to DMA but, instead of determining new points solely based on a diversity metric, it aims to maximize the increment in the hypervolume indicator. Evaluating the potential of these new white-box solvers, in addition to further enhancements of black-box solvers as discussed in this paper, will be of significant interest.

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APPENDIX

A. DMA'S MATHEMATICAL PROGRAM IN OPL

We provide the explicit DMA program per MIQP. CPLEX solves this model per each Pareto point, that is, it receives the evolving efficient set `eObjs` as input:

```

// Excluded: predefined parameters/constants
dvar float x[d in 1..N] in -10..10;
dvar int z[d in 1..N] in -10..10; // <== int
dvar float obj[r in 1..NumObj];
dvar float alpha;
dvar boolean Beta[1..MaxPoints][1..NumObj]
int BigN=2000; // <==== LARGE INTEGER
tuple eObj {
    int id;
    float obj[1..NumObj];
}
float H[1..2*N][1..2*N]=...; //The Hessian
{eObj} eObjs = ...; // evolving efficient set
//THE MODEL:
dexpr float y[i in 1..2*N] = (i in
    1..N)?x[i]:z[i-N];
minimize walpha*alpha + sum(m in
    1..NumObj) (w[m]*obj[m]);
subject to {
    obj[1]==(sum(d1,d2 in 1..2*N)
        H[d1][d2]*(y[d1]-c1[d1])*(y[d2]-c1[d2]))/C;
    obj[2]==(sum(d1,d2 in 1..2*N)
        H[d1][d2]*(y[d1]-c2[d1])*(y[d2]-c2[d2]))/C;
    forall(i in (card(eObjs)+1)..MaxPoints, r in
        1..NumObj) Beta[i][r] == 0;
    forall( e in eObjs, i in 1..NumObj )
        alpha>=obj[m]-e.obj[i] +
        (1-Beta[e.id][i])*BigN;
    forall( e in eObjs ) sum(i in 1..NumObj)
        Beta[e.id][i] == 1;
}

```



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Michael Emmerich is a researcher in the field of Multiobjective Optimization. He holds the position of a university researcher at the Multiobjective Optimization Group of the University of Jyväskylä, and is a guest researcher and former Associate Professor at Leiden University. Besides working for universities, Michael is employed as a Lead AI Scientist at the Nordic AI company Silo.ai. Dr. Emmerich currently lives in Jyväskylä, Finland and was born in Coesfeld, Germany, where he conducted his chemical engineering and informatics studies,

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