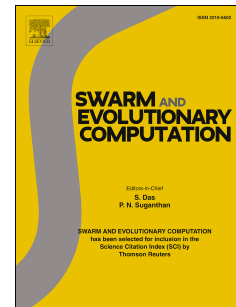


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An Algebraic Framework for Swarm and Evolutionary Algorithms in Combinatorial Optimization

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Abstract

A popular trend in evolutionary computation is to adapt numerical algorithms to combinatorial optimization problems. For instance, this is the case of a variety of Particle Swarm Optimization and Differential Evolution implementations for both binary and permutation-based optimization problems. In this paper, after highlighting the main drawbacks of the approaches in literature, we provide an algebraic framework which allows to derive fully discrete variants of a large class of numerical evolutionary algorithms to tackle many combinatorial problems. The strong mathematical foundations upon which the framework is built allow to redefine numerical evolutionary operators in such a way that their original movements in the continuous space are simulated in the discrete space. Algebraic implementations of Differential Evolution and Particle Swarm Optimization are then proposed. Experiments have been held to compare the algebraic algorithms to the most popular schemes in literature and to the state-of-the-art results for the tackled problems. Experimental results clearly show that algebraic algorithms outperform the competitors and are competitive with the state-of-the-art results.

Keywords: Algebraic Evolutionary Algorithms, Combinatorial search spaces, Algebraic Evolutionary Computation

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1. Introduction

Swarm and evolutionary meta-heuristics are widely applied to solve complex optimization problems where traditional techniques are not able to produce good solutions in a reasonable amount of time. By a slight abuse of terminology, in
 5 this article the term Evolutionary Algorithms (EAs) is used to refer to meta-heuristics based on both evolutionary and swarm intelligence principles.

Depending on the nature of the solution set, it is possible to distinguish between continuous and combinatorial optimization problems and, as a consequence, between numerical and combinatorial EAs. The former work with
 10 solutions represented as real vectors, while the latter tackle problems whose solutions are discrete objects like, for example, bit-strings or permutations.

Though there exist EAs specifically designed to evolve discrete solutions, the wide availability of algorithms for continuous optimization has given rise to a plethora of numerical EAs adapted to solve combinatorial problems. Among
 15 them, see for instance the algorithms described in [1, 2, 3, 4, 5]. One possible motivation for this proliferation is that many nature-inspired algorithms have been historically defined for numerical problems. Therefore, in order to solve a combinatorial problem with a natural principle, it is often easier to adapt an existing numerical algorithm than to design a new combinatorial EA.

20 One of the most used and general technique to adapt a numerical EA to combinatorial problem is to employ decoding procedures which transform numeric vectors into valid discrete solutions for the representation at hand. For instance, the random-key decoder [6] converts a vector in \mathbb{R}^n to a permutation of n integers by sorting the vector indexes according to the corresponding vector
 25 values. Decoder-based schemes have been also proposed to transform numeric vectors into bit-strings [7, 2]. However, this approach has several issues:

- often, the reported good results are only obtained by hybridizing the adapted EA with other techniques (local searches, heuristic functions, restart mechanisms, etc.) and, as far as we know, no study is provided to
 30 understand if the adapted EA alone is effective or not;

- due to obvious cardinality reasons, a single discrete solution can be encoded by a potentially infinite number of numeric vectors, thus introducing large plateaus in the fitness landscape navigated by the underlying algorithm;
- 35 • the intuition of how the EA searches and moves in the continuous space, for which it has been originally designed, is completely lost when the algorithm is integrated with a decoding procedure and its moves are observed in the combinatorial space.

In a previous series of papers [8, 9, 10, 11, 12, 13], we have proposed discrete
 40 evolutionary algorithms, based on algebraic properties of the permutation space, which have reached remarkable results on the permutation flowshop scheduling and the linear ordering problem.

The main contribution of this article is the extension of the approach to a general algebraic framework by which it is possible to derive algebraic variants of
 45 many of the numerical EAs available in literature in order to tackle a large class of combinatorial optimization problems. Conversely from most of the decoder-based schemes, an algebraic algorithm directly evolves a population of discrete solutions by redefining the evolutionary operators of the numerical EA from which it is derived in such a way that the original movements in the continuous
 50 space are simulated in the discrete space.

The proposed method requires that the solution set X forms a finitely generated group. This algebraic structure automatically gives rise to neighborhood relations on X , thus the search space can be seen as a graph of interconnected solutions. For binary and permutation problems, the induced search spaces are
 55 exactly the same spaces widely considered in the fields of local searches and fitness landscape analysis [14, Ch. 5]. In analogy to what happens in \mathbb{R}^n , the algebraic structure also allows to dichotomously interpret discrete solutions both as points and as displacements (i.e., vectors) between points in the space. Hence, it is possible to introduce the operations of addition, subtraction, and
 60 scalar multiplication on X with similar properties as the corresponding vector

operations of \mathbb{R}^n . Therefore, these operations allow to consistently redefine the move equations of most numerical EAs in combinatorial search spaces.

To show the potential of the framework, in this paper we provide Algebraic EAs (AEAs) derived from differential evolution [15] and particle swarm optimization [16]. Abstract definitions, valid for any finitely generated group, are introduced for both AEAs together with their implementations for the search spaces of bit-strings and permutations. Note anyway that the framework is general enough to allow the discretization of other numerical algorithms such as, for instance, the firefly algorithm [17] or the bacterial foraging optimization [18].

Experiments have been held with the aim of comparing the effectiveness of the proposed algorithms with respect to the numerical decoder-based EAs and the state-of-the-art results. NK landscapes [19] have been considered as binary benchmarks, while, for the permutation search space, the experiments have been held on standard instances of the permutation flowshop scheduling [20] and linear ordering problem [21].

In the first set of experiments, both our algorithms and the competitors' have been implemented in their standalone versions. A second set of experiments has been held in order to compare AEAs with the corresponding numerical decoder-based EAs by incorporating additional techniques such as heuristic functions, local search procedures, restart mechanisms, and self-adaptive strategies. Furthermore, the AEAs results have been compared with the best known solutions in literature.

The rest of the paper is organized as follows. Section 2 describes the most used techniques for adapting continuous EAs to discrete problems, and Section 3 provides a critical analysis of the decoder-based approach. Section 4 provides mathematical background concepts used in Section 5, where the algebraic structure and the vector operations of combinatorial search spaces are introduced. The definitions of the algebraic EAs are then provided in Section 6. The experimental analysis is provided in Section 7. Finally, Section 8 concludes the paper by also providing future research directions.

2. Related work

2.1. Differential Evolution and Particle Swarm Optimization

Among the numerical evolutionary algorithms in literature, Differential Evolution and Particle Swarm Optimization are the most studied and effective. Here
 95 we briefly describe them.

The Differential Evolution (DE) algorithm has been originally introduced in [15]. Its key operator is the differential mutation that, in the most used variant rand/1, for every population individuals x_i , generates a mutant y_i according to the following formula

$$y_i \leftarrow x_{r_0} + F \cdot (x_{r_1} - x_{r_2}), \quad (1)$$

where $F \geq 0$ is the scale factor parameter of DE [22], and $x_{r_0}, x_{r_1}, x_{r_2}$ are three randomly chosen population individuals different from each other and with respect to x_i . Then, a crossover operator is applied to y_i and x_i to generate the trial solution z_i that, if fitter than x_i , replaces it in the next generation
 100 population.

The Particle Swarm Optimization (PSO) algorithm has been originally introduced in [16]. PSO iteratively evolves a population of so-called particles. The i -th particle of the population is composed by the current position vector x_i , the velocity vector v_i , the personal best p_i , and the neighborhood best g_i . The communication among the particles is modeled by defining a neighborhood \mathcal{N}_i for every particle i . A variety of neighborhood topologies are possible. One of the most used is the ring topology, where the particles are statically arranged in a ring such that any particle has a neighbor to its left and one to its right. In PSO, at every generation, the velocity and the current position of every particle i are updated according to:

$$v_i \leftarrow [w \cdot v_i] + [(c_1 \cdot r_{1i}) \cdot (p_i - x_i)] + [(c_2 \cdot r_{2i}) \cdot (g_i - x_i)], \quad (2)$$

$$x_i \leftarrow x_i + v_i, \quad (3)$$

where $r_{1i}, r_{2i} \in [0, 1]$ are randomly generated at every step, and $w, c_1, c_2 \geq 0$ are the three PSO parameters called, respectively, inertial, cognitive and social coefficient. Then, the new position x_i updates the personal best p_i if fitter, while g_i is replaced with the fittest vector among the particles in \mathcal{N}_i .

105 2.2. Combinatorial variants of numerical EAs

Although DE and PSO are defined for continuous problems, in the literature there are innumerable attempts to use them in combinatorial optimization. Often, they differ from each other in few details, thus we are here interested in taxonomizing the approaches used for the discretization of a numerical EA.
110 With this regard, two main classes of approaches can be distinguished.

In the first class, the evolutionary algorithms are based on the redefinition of the numerical operators of addition, subtraction, and multiplication. In this way, they can directly use discrete objects with formulae similar to (1), (2), and (3). Most algorithms of this class use ad-hoc definitions of the operators, thus
115 preserving little more than the name of the numerical EAs from which they are derived. For example, the discrete operations used in [23, 24, 25, 26] have just a vague resemblance with the corresponding numerical versions.

In other cases, a more principled method of defining the operators is adopted. For instance, Set-based PSO [27] and DE [28] evolve a set representation of
120 the discrete solutions by employing set-theoretical operators. These schemes have been applied to the traveling salesman problem and the multidimensional knapsack problem. Their main difference with respect to our approach is that they require a new set-based representation of the solutions, while our proposal adopts the classical (binary and permutation) representations. Another impor-
125 tant difference is that [27, 28] require the concept of dimension (which is not required in our proposal) and may introduce constraints among the dimensions of a solution. For this reason, it is difficult to encode, by using the set-based representation, the solutions of a generic permutation-based problem. Indeed, though in [27] a set-based representation for the traveling salesman problem
130 (TSP) is presented, this one relies on the fact that a TSP solution is a collection

of arcs (with constraints), thus it cannot be generalized to other permutation problems such as the ones tackled in the experimental part of this work.

More general methods based on the operators' redefinition which are somehow in line with our algebraic EAs can be found in [29] and [30]. In these works,
 135 the subtraction operation $x - y$ is defined in terms of a sequence of moves which transform y into x . As we will see later, our proposal belongs to this class and its main difference with [29, 30] is that, in our approach, solutions and moves between solutions use the same representation, thus allowing additions, subtractions and scalar multiplications without any restriction. Furthermore, our
 140 approach is general enough to cover different search spaces.

The second class of approaches is based on decoder procedures. Discrete solutions of combinatorial problems are often represented using a proper subset X of the numeric vectors in \mathbb{R}^n , i.e., $X \subset \mathbb{R}^n$. For instance, bit-strings are 0/1 vectors, while a permutation can be represented as a vector of (all different)
 145 ent) integers. However, these vectors are transformed by the move operators to vectors which almost always lie outside the feasible space X . To overcome this issue, continuous-to-discrete decoding schemes have been proposed to transform a numeric vector into a valid solution. Practically, decoder procedures can be devised for any representation and incorporated in any numerical algorithm.
 150 For this reason, we focus on decoder-based schemes on the experimental comparison provided in Section 7. However, though widely used in literature (see for example [7, 2, 31, 5]), this approach has some drawbacks. The most important one is that the intuition of how the underlying numerical EA searches and moves in the continuous space for which it has been originally designed is
 155 totally lost when the same algorithm is integrated with a decoding procedure and its search moves are observed in the combinatorial space. In the following, for the sake of comparison, we briefly describe the most popular combinatorial algorithms based on numerical decoders.

2.3. Binary EAs based on Probabilistic Decoders

160 Binary variants of DE [32] and PSO [7], to which we refer to as BDE and BPSO, aim to optimize an objective function of the form $f : \mathbb{B}^n \rightarrow \mathbb{R}$, where $\mathbb{B} = \{0, 1\}$. They evolve a population of bit-strings by mainly using the move operators of their numerical counterparts. Then, as soon as an unfeasible vector is generated, it is transformed back to a valid binary solution by means of a
 165 probabilistic decoder. Formally, given the non-binary vector $x \in \mathbb{R}^n$, each of its components x_i is converted to 1 or 0 with probability $S(x_i)$ and $1 - S(x_i)$, respectively. The sigmoid function $S(t) = (1 + e^{-t})^{-1}$ is used to monotonically map any real number t to a probability value $S(t) \in [0, 1]$.

In BDE [32], only the differential mutation of equation (1) can generate a
 170 non-binary vector. Hence, the components of a mutant $y \in \mathbb{R}^n$ are converted to bit values according to the probability given by $S\left(\frac{2b(y_i - 0.5)}{1 + 2F}\right)$, where $b > 0$ is a further algorithmic parameter called *bandwidth factor*.

BPSO [7] encodes particle positions as binary strings and velocities as numeric vectors. Hence, a velocity vector $v \in \mathbb{R}^n$ is updated as usual using equa-
 175 tion (2). Then, v is used to generate the update probabilities for its corresponding particle position x , i.e., the i -th bit of x is set to 1 or 0 with probability $S(v_i)$ and $1 - S(v_i)$, respectively.

Applications of BDE and BPSO have been proposed, for instance, in [33, 34, 35, 36]. Finally, there have been proposals to use, in place of the sigmoid
 180 function, other mathematical functions which generate probabilities: a review of them can be found in [1].

2.4. Angle Modulated EAs

The angle modulation technique, first introduced in [37], allows to transform a four-dimensional numeric vector to an n -length binary string, for any
 185 dimensionality n .

Formally, [37] introduces a decoder function $AM : \mathbb{R}^4 \rightarrow \mathbb{B}^n$ which can be used by any numerical algorithm \mathcal{A} to optimize an objective function of the

form $f : \mathbb{B}^n \rightarrow \mathbb{R}$. The only modification to \mathcal{A} is to consider $f(AM(x))$ as the fitness value of a generic individual $x \in \mathbb{R}^4$.

Let $x = (a, b, c, d)$ and its corresponding binary string be $y = AM(x)$, then the i -th bit of y is computed as

$$y(i) = \begin{cases} 1 & \text{if } g(i-1) > 0 \\ 0 & \text{otherwise,} \end{cases} \quad (4)$$

190 where $g(t) = \sin(2\pi \cdot (t-a) \cdot b \cdot \cos(2\pi \cdot (t-a) \cdot c)) + d$ is called *generating function* in [37].

Angle modulated variants of DE and PSO, i.e., AM-DE and AM-PSO, have been introduced in, respectively, [2] and [37], while further applications are proposed in [38, 39].

195 2.5. Random-Key based EAs

The Random-Key (RK) technique has been introduced in [6] to tackle permutation optimization problems.

Formally, [6] introduces a decoding function $RK : \mathbb{R}^n \rightarrow \mathcal{S}_n$ (where \mathcal{S}_n is the set of permutations of $[n] = \{1, \dots, n\}$) which can be used by any numerical
200 algorithm \mathcal{A} to optimize an objective function of the form $f : \mathcal{S}_n \rightarrow \mathbb{R}$. Also in this case, the only modification to \mathcal{A} is to consider $f(RK(x))$ as the fitness value of a generic individual $x \in \mathbb{R}^n$.

RK transforms x to the permutation π such that the sequence $x_{\pi(1)}, \dots, x_{\pi(n)}$ is increasingly ordered. For example, if $x = (0.46, 0.91, 0.33, 0.75, 0.51)$, the de-
205 coded permutation is $\pi = RK(x) = \langle 3, 1, 5, 4, 2 \rangle$. Therefore, RK requires to sort the component indexes of x according to their corresponding values. This can be done in $\Theta(n \log n)$ time.

Also a simple variant of RK has been considered in literature, see for instance [40] and [5]. In this variant, a vector x is decoded to the permutation ρ such that
210 $\rho(i) = r_i$, where r_i is the rank of x_i among the vector components x_1, \dots, x_n sorted in increasing order. It is easy to see that this decoding scheme can be obtained by inverting the result of RK , i.e., $\rho = (RK(x))^{-1}$. Therefore,

we generalize random-key by considering the parametrized decoder RK^k where $k = \pm 1$.

215 Random-key variants of DE and PSO, i.e., RK-DE and RK-PSO, have been used in many works. See for instance [31, 41, 3, 42, 43].

3. Critical analysis of the decoder-based approaches

The decoder-based approaches have two inherent drawbacks: a single discrete solution can be encoded by a potentially infinite number of numeric vectors, and the distance relationships among the discrete objects can be completely
220 upset after the embedding in the continuous space.

The probabilistic decoders described in Section 2.3, though their non-deterministic nature can sometime help to exit search stagnation, introduce a large amount of spatial distortion. Indeed, given a fixed numeric vector, performing multiple
225 decoding steps can result in very different bit-strings. As an extreme example, let consider a BPSO particle with a zero vector as velocity. Since $S(0) = 0.5$, there is equal probability to have a 0 or a 1 for every bit in the decoded bit-string. Hence, the zero vector can be decoded in any one of the 2^n bit-strings with uniform probability, thus completely losing its original “identity”.

230 Regarding the angle modulated approach (see Section 2.4), no explicit proof that equation (4) allows to cover the whole space \mathbb{B}^n for any n is provided in the literature. Moreover, by measuring the distances in the numeric and binary spaces by, respectively, the Euclidean and Hamming distance, we have that distant numeric vectors may correspond to close bit-strings and vice versa. For instance, the Euclidean distance between the vectors $x = (-6.94, 8.24, 0.68, 0.08)$
235 and $y = (-6.89, 8.31, 0.72, 0.11)$ is around 0.1 (a relatively small number with respect to the vector values) but, when $n = 50$, $AM(x)$ differs from $AM(y)$ for 23 bits, i.e., almost half the total number of bits. On the other hand, the vectors $(3.36, -6.6, -2.96, 1.1)$ and $(34.56, 27.14, 10.74, 15.26)$ are very different (their
240 Euclidean distance is around 50), but they encode exactly the same bit-string (again, with $n = 50$).

Similar scenarios happen with the random-key approaches (see Section 2.5). Here we only consider RK^{-1} , though the space distortion induced by RK^{+1} is even more pronounced. For example, the two vectors $x = (0.46, 0.91, 0.33, 0.75, 0.51)$ and $y = (0.4, 0.9, 0.3, 0.7, 0.5)$ correspond to the same permutation, i.e., $RK^{-1}(x) = RK^{-1}(y) = \langle 3, 1, 5, 4, 2 \rangle$. The vectors x and y have a small Euclidean distance, but the same problem can also happens for vector pairs whose distance is arbitrarily large. As an example, let consider the family of vectors $y_\Delta = (0.4, 0.9 + \Delta, 0.3, 0.7, 0.5)$ which encode the same permutation $\langle 3, 1, 5, 4, 2 \rangle$ for every choice of $\Delta \geq 0$. At the same time, given an $\epsilon > 0$, we can find, for every possible permutation $\pi \in \mathcal{S}_n$, a vector $x \in \mathbb{R}^n$ such that its Euclidean distance from the zero vector is ϵ and $RK^{-1}(x) = \pi$.

Finally, we have conducted an experiment in order to show the weak correlation between the distances on the continuous and on the permutation space. We have considered the classical distance functions: Euclidean distance for the continuous space, and Kendall's- τ distance for permutations (i.e., the number of pairwise disagreements between two permutations). Given $\sigma > 0$, 10 000 pairs of vectors $x_i, y_i \in \mathbb{R}^{10}$ have been generated such that $d(x_i, y_i) = \sigma$. The Kendall's- τ distance between $RK^{-1}(x)$ and $RK^{-1}(y)$ has been computed as well. Different values of σ in the range $[0.1, 3]$ have been considered. The graph in Figure 1 clearly shows that, though in average both distances have a similar behavior, the variability in terms of Kendall's- τ distance explodes when the Euclidean distance σ increases. Therefore, a large number of nearby vectors correspond to far away permutations and vice versa.

4. Algebraic Background

In many combinatorial optimization problems, the set of discrete solutions X is naturally endowed with a composition operator, i.e., there exists a binary operator \star such that, given two solutions $x, y \in X$, then $x \star y$ is again a solution. Often, X and \star satisfy the group properties [44]. As we will see later, this is the case of the binary and permutation representations that are quite ubiquitous in

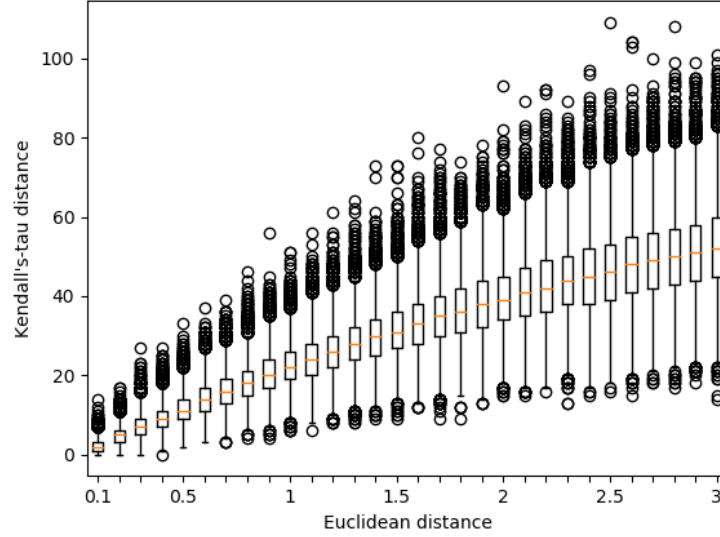


Figure 1: Boxplot chart showing the correlation between Euclidean distance and Kendall's- τ distance.

combinatorial problems: for example in the binary knapsack problem or in the permutation flowshop scheduling problem.

The algebraic structure of the search spaces allows to characterize the geometry of the search space and to describe the search moves. Usually, the search algorithms do not explicitly exploit the algebraic properties of the search spaces. Therefore, the aim of the paper is to show how groups can be used in evolutionary algorithms, while the rest of this section is devoted to introduce the mathematical concepts used later on.

4.1. Groups

A group [44] is an algebraic structure (X, \star) where X is a set and \star is a binary operation on X which fulfills the following properties:

- for all $x, y, z \in X$, $x \star (y \star z) = (x \star y) \star z$ (associativity);
- there exists a unique element $e \in X$ such that, for all $x \in X$, $x \star e =$

$e \star x = x$ (neutral or identity element);

- 285 • for every $x \in X$, there exists a unique element $x^{-1} \in X$ such that $x \star x^{-1} =$
 $x^{-1} \star x = e$ (inverse element).

If \star is commutative, i.e., for all $x, y \in X$, $x \star y = y \star x$, then the group is called Abelian.

A group (X, \star) is finitely generated if there exists a finite subset $H \subseteq X$
 290 such that any $x \in X$ can be written as a composition of elements in H , i.e.,
 $x = h_1 \star h_2 \star \dots \star h_l$ for some $h_1, h_2, \dots, h_l \in H$. H and its elements are called,
 respectively, the generating set and the generators of X , while the sequence
 $\langle h_1, h_2, \dots, h_l \rangle$ is a decomposition of x . Usually, though not strictly necessary,
 H is closed with respect to inversion, i.e., for all $h \in H$ also $h^{-1} \in H$.

295 Generally, every $x \in X$ has many decompositions with possibly different
 lengths. Hence, a useful concept is that of minimal decomposition. A decom-
 position $\langle h_1, h_2, \dots, h_l \rangle$ of a given $x \in X$ is minimal if, for any other decompo-
 sition $\langle h'_1, h'_2, \dots, h'_m \rangle$ of x , we have $l \leq m$. Even minimal decompositions are
 not unique in general, but it is possible to define the weight $|x|$ as the length of
 300 the minimal decompositions of x .

Minimal decompositions allow also to define a partial order on X . Given
 $x, y \in X$, we write $x \sqsubseteq y$ if, for each minimal decomposition s_x of x , there exists
 a minimal decomposition s_y of y such that s_x is a prefix of s_y .

Furthermore, if X is finite, there exists at least one maximal weight element.
 305 For the sake of presentation, here we focus on groups with a unique maximal
 weight element ω such that $x \sqsubseteq \omega$ for all $x \in X$.

4.2. Cayley Graphs

Every group (X, \star) , finitely generated by H , geometrically corresponds to
 the Cayley graph $\mathcal{C}(X, \star, H)$, i.e., the labeled digraph whose vertexes are the
 310 elements of X and there is an arc from x to y labeled by $h \in H$ if and only if
 $y = x \star h$. The graph $\mathcal{C}(X, \star, H)$ is:

- strongly connected, i.e., for all $x, y \in X$ there is a directed path from x to y and from y to x ;
- regular, i.e., every vertex has the same number of incoming and outgoing arcs;
- vertex-transitive, i.e., every vertex has the same set of (incoming and outgoing) arc labels.

These properties guarantee that, for any possible sequence of generators s and for any element $x \in X$, $\mathcal{C}(X, \star, H)$ has exactly one path which starts from the vertex x and whose arcs are labeled according to s . In the Cayley graph, for all $x \in X$, each directed path from the group identity e to x corresponds to a decomposition of x : if the arc labels occurring in the path are $\langle h_1, h_2, \dots, h_l \rangle$, then $x = h_1 \star h_2 \star \dots \star h_l$. As a consequence, shortest paths from e to x correspond to minimal decompositions of x . Hence, if $e \xrightarrow{h_1} x_1 \xrightarrow{h_2} x_2 \xrightarrow{h_3} \dots \xrightarrow{h_l} x_l$ is a shortest path in $\mathcal{C}(X, \star, H)$, then, for any integer $i \in [1, l]$, $\langle h_1, \dots, h_i \rangle$ is a minimal decomposition of x_i , and $|x_i| = i$. Moreover, given $x, y \in X$, $x \sqsubseteq y$ if and only if there exists at least one shortest path from e to y passing by x .

More generally, for all $x, y \in X$, any path from x to y in $\mathcal{C}(X, \star, H)$ has an algebraic interpretation. If the arc labels in the path are $\langle h_1, h_2, \dots, h_l \rangle$, then $x \star (h_1 \star h_2 \star \dots \star h_l) = y$. Hence, $\langle h_1, h_2, \dots, h_l \rangle$ is a decomposition of $x^{-1} \star y$. In particular, shortest paths correspond to minimal decompositions. Starting from this observation, it is possible to define a distance d on the group X generated by H . For all $x, y \in X$, $d(x, y)$ is the length of a shortest path from x to y in $\mathcal{C}(X, \star, H)$ or, equivalently, $d(x, y) = |x^{-1} \star y|$. If H is closed with respect to inversion, the neighborhoods of $\mathcal{C}(X, \star, H)$ are symmetric and d is a metric distance. Finally, the diameter D of a Cayley graph is equal to the maximal weight, i.e., $D = |\omega|$.

4.3. Bit-String Group

The set $\mathbb{B}^n = \{0, 1\}^n$ of the n -length bit-strings forms a group with respect to the bitwise XOR, denoted by \vee . The identity is the “all 0s string” $\mathbf{0}$. Moreover,

\vee is commutative and $x^{-1} = x$, for all $x \in \mathbb{B}^n$.

The most natural and elementary generating set of \mathbb{B}^n is the subset of the n bit-strings with exactly one 1-bit, i.e., the set $U = \{u_i \in \mathbb{B}^n : u_i(i) = 1 \text{ and } u_i(j) = 0 \text{ for } j \neq i\}$, where $u_i(k)$ is the k -th bit of the string u_i . It is
 345 important to note that $x \vee u_i$ corresponds to flipping the i -th bit of x .

The maximal weight element of \mathbb{B}^n with respect to U is the “all 1s string”
 1. Hence, the Cayley graph diameter is n .

Furthermore, the group weight is the Hamming weight, the group distance is the Hamming distance, and the Cayley graph is the binary hypercube.

350 4.4. Permutation Group

The set \mathcal{S}_n of the permutations of $[n] = \{1, 2, \dots, n\}$ forms a group, called the *symmetric group*, with respect to the composition operator \circ . Given $\pi, \rho \in \mathcal{S}_n$, $\pi \circ \rho$ is defined as the permutation $(\pi \circ \rho)(i) = \pi(\rho(i))$ for all the indices $i \in [n]$. \mathcal{S}_n is not Abelian and its identity is the permutation e such that $e(i) = i$ for all
 355 $i \in [n]$.

Different generating sets are possible in \mathcal{S}_n (see [9, 45, 46]). One of the most elementary is the subset of the $n - 1$ simple transpositions, i.e., the set $ST = \{\sigma_i \in \mathcal{S}_n : 1 \leq i < n\}$, where σ_i is defined as: $\sigma_i(i) = i + 1$, $\sigma_i(i + 1) = i$, and $\sigma_i(j) = j$ for $j \in [n] \setminus \{i, i + 1\}$. Since the inverse of a simple transposition
 360 is itself, ST is closed with respect to inversion. The maximal weight element of \mathcal{S}_n , with respect to ST , is the permutation r such that $r(i) = n + 1 - i$ for all $i \in [n]$. Its weight, thus the Cayley graph diameter, is $\binom{n}{2}$.

For all $\pi \in \mathcal{S}_n$, the composition $\pi \circ \sigma_i$ corresponds to swap the adjacent items at positions i and $i + 1$ in π . The weight $|\pi|$ is equivalent to the number of
 365 inversions in π , i.e., the pairs of indexes $i, j \in [n]$ such that $i < j$ and $\pi(i) > \pi(j)$. Finally, the distance $d(\pi, \rho)$ between $\pi, \rho \in \mathcal{S}_n$ is known as bubble-sort distance and counts the minimum number of adjacent swaps required to transform π in ρ (or vice versa) [45].

5. Algebra of Combinatorial Search Spaces

370 In all the combinatorial optimization problems, the search space is usually described by the set X of discrete solutions and the set O of operators, such that any $o \in O$ can be applied to any solution $x \in X$ to obtain a (neighbor) solution $o(x) \in X$. Therefore, the neighborhood of any $x \in X$ is $\mathcal{N}(x) = \{y \in X : \exists o \in O \text{ s.t. } y = o(x)\}$. Usually, O contains the most elementary variations of
 375 the solution representation adopted, e.g., bit-flips for binary strings or adjacent swaps for permutations.

It is important to note that, in many cases, the search space (X, O) has an algebraic structure: it can be represented by a finitely generated group. This happens when there exist:

- 380 1. a binary operation \star satisfying the group properties on X ,
2. a finite subset $H \subseteq X$ that generates the group (X, \star) , and
3. a one-to-one correspondence which associates to every $o \in O$ a generator $h \in H$ such that $o(x) = x \star h$.

This algebraic structure gives rise to a Cayley graph that geometrically represents the search space and the same neighborhood relations induced by O . For
 385 instance, the previously described \mathbb{B}^n and \mathcal{S}_n are search spaces representable by finitely generated groups. Moreover, though not studied in this paper, also other search spaces satisfy the properties (1–3) like, for instance, the space of integer vectors.

390 In the rest of this section we show how, in a combinatorial search space represented by a group (X, \star) finitely generated by H , it is possible to naturally introduce the operations of addition \oplus , subtraction \ominus , and scalar multiplication \odot in a meaningful way and with similar properties as the analogous operations of the Euclidean vector space. This, in turn, will allow to consistently redefine the
 395 move equations of numerical EAs (like differential evolution or particle swarm optimization) for combinatorial search spaces.

The key observation is the dichotomous interpretation of an element of X . From Section 4, any element $x \in X$ can be decomposed and seen as a sequence

of generators, hence x corresponds to a sequence of arc labels in several paths of
 400 $\mathcal{C}(X, \star, H)$. This observation is crucial, because the elements of X can be seen
 both as *points*, i.e., vertices in the Cayley graph, and as *vectors*¹, i.e., sequences
 of generators in shortest paths of the Cayley graph.

5.1. Abstract Addition and Subtraction

The addition $z = x \oplus y$ is defined as the application of the vector $y \in X$
 to the point $x \in X$. The result z is computed by choosing a decomposition
 $\langle h_1, h_2, \dots, h_l \rangle$ of y and by finding the end point of the path which starts from
 x and whose arc labels are $\langle h_1, h_2, \dots, h_l \rangle$, i.e., $z = x \star (h_1 \star h_2 \star \dots \star h_l)$.
 By noting that $h_1 \star h_2 \star \dots \star h_l = y$, the addition \oplus is independent from the
 generating set and is defined as

$$x \oplus y := x \star y. \quad (5)$$

Continuing the analogy with the Euclidean space, the difference between two
 points is a vector. Given $x, y \in X$, the difference $y \ominus x$ produces the sequence of
 labels $\langle h_1, h_2, \dots, h_l \rangle$ in a path from x to y . Since $h_1 \star h_2 \star \dots \star h_l = x^{-1} \star y$, we
 can replace the sequence of labels with its product, thus making the difference
 independent from the generating set. Therefore, \ominus is uniquely defined as

$$y \ominus x := x^{-1} \star y. \quad (6)$$

Both \oplus and \ominus , like their numerical counterparts, are consistent with each
 405 other: $x \oplus (y \ominus x) = y$ for all $x, y \in X$.

5.2. Abstract Scalar Multiplication

Again, as in the Euclidean space, it is possible to multiply a vector by a
 non-negative scalar in order to stretch its length.

Given $a \geq 0$ and $x \in X$, we denote their multiplication with $a \odot x$ and we
 410 first identify the conditions that $a \odot x$ has to verify in order to simulate, as much
 as possible, the scalar multiplication of vector spaces:

¹Here, with “vector” we intend “free vector”, i.e., a vector without point of application.

(C1) $|a \odot x| = \lceil a \cdot |x| \rceil$;

(C2) if $a \in [0, 1]$, $a \odot x \sqsubseteq x$;

(C3) if $a \geq 1$, $x \sqsubseteq a \odot x$.

415 Clearly, the scalar multiplication of \mathbb{R}^n satisfies a slight variant of (C1) where the Euclidean norm replaces the group weight and the ceiling is omitted. Besides, similarly to scaled vectors in \mathbb{R}^n , (C2) and (C3) intuitively encode the idea that $a \odot x$ is the element x scaled down or up, respectively.

It is important to note that, fixed a and x , there may be more than one
420 element of X satisfying (C1–C3). This is a clear consequence of the non-uniqueness of minimal decompositions. Therefore, different strategies can be devised to compute $F \odot x$. Nevertheless, since our aim is to apply the operation in evolutionary algorithms, we denote with $a \odot x$ a randomly selected element satisfying (C1–C3).

425 Note also that the diameter D induces an upper bound on the possible values for the scalar a . For any $x \in X$, let $\bar{a}_x = \frac{D}{|x|}$, if $a > \bar{a}_x$, (C1) would imply $|a \odot x| > D$, which is impossible. Therefore, we define

$$a \odot x := \bar{a}_x \odot x, \quad \text{when } a > \bar{a}_x. \quad (7)$$

For the sake of clarity, we separately define the operation $a \odot x$ for the two cases $a \in [0, 1]$ and $a > 1$.

430 Both cases employ an abstract procedure which returns a randomly selected minimal decomposition of the element in input.

When $a \in [0, 1]$, let $l = |x|$ and consider a random shortest path from e to x such as $e \xrightarrow{h_1} \dots \xrightarrow{h_k} x_k \dots \xrightarrow{h_l} x_l$, where $x_l = x$. For the Cayley graph properties, (C1) and (C2) are satisfied by setting $a \odot x = x_k$, with $k = \lceil a \cdot l \rceil$.

435 Moreover, when $a = 1$, $a \odot x = x$ and this satisfies both (C2) and (C3).

When $a > 1$, let $l = |x|$ and consider a random shortest path from e to ω passing by x such as $e \xrightarrow{h_1} \dots \xrightarrow{h_l} x_l \xrightarrow{h_{l+1}} \dots \xrightarrow{h_k} x_k \xrightarrow{h_{k+1}} \dots \xrightarrow{h_D} \omega$, where $x_l = x$. For the Cayley graph properties, (C1) and (C3) are satisfied by setting $a \odot x = x_k$, with $k = \lceil a \cdot l \rceil$.

440 Anyway, it is possible to make the computation more efficient by exploiting
 that $a \odot x = (h_1 \star \dots \star h_l) \star (h_{l+1} \star \dots \star h_k) = x \star (h_{l+1} \star \dots \star h_k)$, thus only the
 sub-path from x to ω , which forms a minimal decomposition of $\omega \ominus x = x^{-1} \star \omega$,
 needs to be known. Since $|x| + |x^{-1} \star \omega| = D$, thus $|x| = D - |x^{-1} \star \omega|$, then
 $a \odot x$ can be computed by taking a minimal decomposition of $x^{-1} \star \omega$, truncating
 445 it after $\lceil a \cdot |x| \rceil - |x|$ generators, and right-composing the truncated sequence
 with x .

These two abstract methods are valid for any finitely generated group. Their
 implementations mainly require a concrete randomized decomposition algorithm
 for the group at hand.

450 5.3. Vector Operations for Bit-Strings

The bit-string representation can be used in a very large number of problems
 such as, for example, NK landscape optimization, binary knapsack problems,
 number partitioning, any subset selection problem, etc. As described in Section
 4.3, for the search space of bit-strings \mathbb{B}^n , we consider the bitwise XOR operator
 455 \vee and the generating set U representing the bit-flip moves.

Thanks to properties of this group, \oplus and \ominus coincide and are defined as

$$x \oplus y = x \ominus y := x \vee y. \quad (8)$$

These operations are both commutative, and the time complexity to compute
 them is $\Theta(n)$.

The operation \odot is implemented by considering that the search space di-
 ameter is n and the maximal weight bit-string is the “all 1s string” $\mathbf{1}$. The
 460 randomized decomposition algorithm is RandBits, presented in Algorithm 1.

RandBits produces a random minimal decomposition of x by returning a ran-
 dom permutation of the generators corresponding to the 1-bits of x . RandBits
 and \odot can be computed in time $\Theta(n)$.

For the sake of clarity, we provide an illustrative example. Let consider the
 465 two bit-strings of $n = 5$ bits $x = (10101)$ and $y = (01100)$. We compute the
 difference $z = x \ominus y = x \vee y = (11001)$ which, as expected, has a 1-bit in the

Algorithm 1 Randomized decomposition algorithms for bit-strings

```

1: function RANDBITS( $x$ )
2:    $s \leftarrow \langle \rangle$  ▷  $s$  is a sequence of generators
3:   for  $i \leftarrow 1$  to  $n$  do
4:     if  $x(i) = 1$  then ▷  $x(i)$  is the  $i$ -th bit of  $x$ 
5:        $s \leftarrow \text{Concatenate}(\langle u_i \rangle, s)$  ▷  $u_i$  is a generator
6:    $s \leftarrow \text{Shuffle}(s)$  ▷ Uniform random shuffle of  $s$ 
7:   return  $s$  ▷  $s$  is now a min. decomposition of  $x$ 
8: end function

```

positions where x and y differ. Adding z to y , as expected, we get back to x , i.e., $y \oplus z = y \vee z = (10101) = x$. Now, let $a = 0.66$ and let analyze the scalar multiplication $a \odot z$. First, a (random) minimal decomposition of z is obtained as follows: $\text{RandBits}(z) = \langle u_5, u_1, u_2 \rangle$, where the u_i are the generator bit-strings with exactly one 1-bit (see Section 4.3). From the decomposition it is easy to see that $|z| = 3$, thus the computation of $0.66 \odot z$ simply requires to compose the first $\lceil 0.66 \cdot 3 \rceil = 2$ generators of z , i.e., $0.66 \odot z = u_5 \vee u_1 = (00001) \vee (10000) = (10001)$. The case $a > 1$ is slightly different. Let analyze the computation of $1.33 \odot z$. First, we need the maximum-weight bit-string $\mathbf{1} = (11111)$ (see Section 4.3) and a (random) minimal decomposition of the difference $\mathbf{1} \ominus z = (00110)$, i.e., $\text{RandBits}(\mathbf{1} \ominus z) = \langle u_4, u_3 \rangle$. Exploiting the equivalences $D = n = 5$ and $|z| + |\mathbf{1} \ominus z| = D$, we compute, as expected, $|z| = 3$. Therefore, $1.33 \odot z$ simply requires to compose z with the first $\lceil 1.33 \cdot 3 \rceil - 3 = 1$ generator of $\mathbf{1} \ominus z$, i.e., $1.33 \odot z = z \vee u_4 = (11011)$.

5.4. Vector Operations for Permutations

The permutation representation can be used in many problems such as, for example, the linear ordering problem, the permutation flowshop scheduling, the quadratic assignment problem, etc. As described in Section 4.4, for the permutation space \mathcal{S}_n , we consider the composition operator \circ and the generating set ST representing the adjacent swap moves.

The operations \oplus and \ominus are defined as:

$$x \oplus y := x \circ y, \quad (9)$$

$$y \ominus x := x^{-1} \circ y. \quad (10)$$

Both are non-commutative and can be computed in time $\Theta(n)$.

The operation \odot is implemented by considering that the search space diameter is $\binom{n}{2}$ and the maximal weight permutation is the reversed identity r . The randomized decomposition algorithm is RandBS, presented in Algorithm 2.

RandBS iteratively sorts x in increasing order (hence obtaining e) by iteratively choosing a random adjacent swap moves from the set of adjacent inversions A . Then, A is efficiently updated by considering that the adjacent swap σ_i can only affect three adjacent inversions $(i-1, i), (i, i+1), (i+1, i+2)$. As also highlighted in [8], RandBS and \odot are computed in time $\Theta(n^2)$.

Algorithm 2 Randomized decomposition algorithms for permutations

```

1: function RANDBS( $x$ )
2:    $s \leftarrow \langle \rangle$   $\triangleright s$  is a sequence of generators
3:    $A \leftarrow \{\sigma_i \in ST : i < i+1 \text{ and } x(i) > x(i+1)\}$ 
4:   while  $A \neq \emptyset$  do  $\triangleright A \neq \emptyset \iff x \neq e$ 
5:      $\sigma \leftarrow$  select an element from  $A$  uniformly at random
6:      $x \leftarrow x \circ \sigma$   $\triangleright \sigma$  is a generator
7:      $s \leftarrow \text{Concatenate}(\langle \sigma \rangle, s)$ 
8:      $A \leftarrow \text{Update}(A, \sigma)$   $\triangleright \Theta(1)$  complexity
9:   return  $s$   $\triangleright s$  is now a min. decomposition of  $x$ 
10: end function

```

For the sake of clarity, we provide an illustrative example. Let consider the two permutations of $n = 5$ items $x = \langle 12534 \rangle$ and $y = \langle 41532 \rangle$. In order to compute the difference $x \ominus y$, we need the inverse of y , i.e., $y^{-1} = \langle 25413 \rangle$. Then, $z = x \ominus y = y^{-1} \circ x = \langle 25341 \rangle$. Adding z to the right of y , as expected, we obtain again x , i.e., $y \oplus z = y \circ z = \langle 12534 \rangle = x$. Now, let $a = 0.33$ and let analyze the computation of $a \odot z$. First, a (random) minimal decomposition of z

is obtained as follows: $RandBS(z) = \langle \sigma_1, \sigma_2, \sigma_4, \sigma_3, \sigma_4, \sigma_2 \rangle$, where the σ_i are the generators defined as in Section 4.4. From the decomposition it is easy to see that $|z| = 6$, thus the computation of $0.33 \odot z$ simply requires to compose the first
505 $\lceil 0.33 \cdot 6 \rceil = 2$ generators of z , i.e., $0.33 \odot z = \sigma_1 \circ \sigma_2 = \langle 21345 \rangle \circ \langle 13245 \rangle = \langle 23145 \rangle$.
The case $a > 1$ is slightly different. Let analyze the computation of $1.5 \odot z$. First, we need the maximum-weight permutation $r = \langle 54321 \rangle$ (see Section 4.4) and a (random) minimal decomposition of the difference $r \ominus z = \langle 24315 \rangle$, i.e., $RandBS(r \ominus z) = \langle \sigma_1, \sigma_2, \sigma_3, \sigma_2 \rangle$. Exploiting the equivalences $D = \binom{5}{2} = 10$ and
510 $|z| + |r \ominus z| = D$, we compute, as expected, $|z| = 6$. Therefore, $1.5 \odot z$ simply requires to compose z with the first $\lceil 1.5 \cdot 6 \rceil - 6 = 3$ generators of $r \ominus z$, i.e., $1.5 \odot z = z \circ \sigma_1 \circ \sigma_2 \circ \sigma_3 = \langle 53421 \rangle$.

5.5. Algebraic Properties

It is easy to prove that the operations \oplus, \ominus, \odot satisfy the following properties:

- 515 (i) \oplus is associative;
- (ii) \oplus is commutative, if \star is commutative;
- (iii) e is the neutral element for \oplus ;
- (iv) $x \oplus x^{-1} = x^{-1} \oplus x = e$ for each $x \in X$;
- (v) $1 \odot x = x$ for each $x \in X$;
- 520 (vi) $a \odot (b \odot x) = (ab) \odot x$ for each $x \in X$ and $a, b \geq 0$;
- (vii) $0 \odot x = e$ for each $x \in X$;
- (viii) $x \oplus (y \ominus x) = y$ for each $x, y \in X$.

The properties (i–viii) make X similar to a vector space over \mathbb{R} . Besides property (ii), the two vector space's properties that do not hold in general are
525 the distributivity laws of \odot with respect to \oplus and to $+$.

6. Algebraic Evolutionary Algorithms

In this section we describe an algebraic method to adapt an evolutionary algorithm \mathcal{A} , originally designed for continuous optimization, to solve a combinatorial optimization problem \mathcal{P} . The adaptation is possible under the following

530 two conditions: 1) the search space X of \mathcal{P} is representable by a finitely generated group, and 2) the evolutionary operators of \mathcal{A} are linear combinations of population individuals.

When both conditions are met, the original evolutionary operators, expressed with the usual numerical vector operations, can be rewritten using \oplus , \ominus , and
 535 \odot . The adapted algorithms, called *algebraic*, directly navigate the combinatorial search space by means of the operations defined on the underlying group. Therefore, algebraic evolutionary algorithms (AEAs) simulate the search moves of their numerical counterparts in the combinatorial search space at hand.

AEAs can be defined for the most popular and effective numerical evolutionary algorithms in literature. Here, we consider the most used ones: Differential
 540 Evolution (DE) [15] and Particle Swarm Optimization (PSO) [16]. Anyway, the same technique can be applied also to other evolutionary algorithms like, for instance, Firefly Algorithm [17], Bacterial Foraging Optimization Algorithm [18], and Artificial Bee Colony [47], and simple univariate Evolution Strategies [48].

545 In the following we introduce the abstract forms of the algebraic variants of DE and PSO, namely, ADE and APSO. By replacing the abstract \oplus , \ominus , \odot with their bit-string or permutation implementations, we have AEAs for, respectively, binary or permutation problems. The precedences among the algebraic operations are assumed to be as in their numerical counterparts.

550 6.1. Algebraic Differential Evolution

In the Algebraic DE (ADE), previously introduced in [8] for permutation problems, the differential mutation is defined as

$$y_i \leftarrow x_{r_0} \oplus F \odot (x_{r_1} \ominus x_{r_2}), \quad (11)$$

which is the algebraic version of equation (1). The recombination between y_i and x_i is performed using one of the discrete crossover operators available in literature (both for bit-strings and permutations). Then, the same one-to-one selection of numerical DE decides which solution enters the next-generation
 555 population.

Finally, it is worth to note that, though we are limiting our attention to rand/1, all the known differential mutation variants (rand/2, best/1, current-to-best/1, etc.) [49] can be replaced with their algebraic counterparts.

6.2. Algebraic Particle Swarm Optimization

In the Algebraic PSO (APSO), preliminary proposed in [10, 50] for permutation problems, the velocity and position update rules of the i -th particle are defined as:

$$v_i \leftarrow [w \odot v_i] \oplus [(c_1 \cdot r_{1i}) \odot (p_i \ominus x_i)] \oplus [(c_2 \cdot r_{2i}) \odot (g_i \ominus x_i)], \quad (12)$$

$$x_i \leftarrow x_i \oplus v_i, \quad (13)$$

560 which are the algebraic versions of, respectively, equations (2) and (3). The personal and social best p_i and g_i are then updated as in the numerical PSO.

Replacing the velocity v_i in equation (13) with the right side of equation (12), we have that, differently from ADE, the solution x_i is updated by adding three terms to it. Though x_i can be reasonably interpreted as a point in the
 565 space, the three terms composing v_i have natural interpretations as vectors. This generates an ambiguity when \oplus is not commutative (for instance, in the permutations space). Hence, in these cases, the three terms of equation (12) are randomly arranged in one of the $3! = 6$ possible orders.

6.3. Search Characteristics of the AEAs

570 Thanks to the properties of the algebraic framework from which ADE and APSO are derived, their search moves are geometrically similar with respect to the movements performed by their numerical counterparts. Anyway, the discrete nature of the combinatorial spaces inevitably introduces some differences with the numerical algorithms.

575 The main one is the lack of continuity. Indeed, since discrete spaces are finite (or at most countable) an individual cannot get infinitesimally closer to a given solution. Another way of looking at the same issue is that the discrete

spaces are graphs (Cayley graphs in our cases), hence the distance between two solutions is integer-valued. The practical consequence in AEAs, but also
580 in other combinatorial algorithms, is that loss of population diversity is more drastic than in continuous space.

Another difference with numerical algorithms is that when the underlying group is not Abelian, the \oplus operation is not commutative. This issue has been considered in APSO for the permutations space (see Section 6.2).

585 Furthermore, in the case of bit-strings, both \oplus and \ominus are actually the bit-wise XOR operator, hence $x \oplus x = x \ominus x = e$ for all $x \in \mathbb{B}^n$. This implies that, when the population reaches consensus on a bit (i.e., when all individuals have their i -th bit set to the same value), it is impossible to flip that bit in the future generations by using movement equations that only consider linear
590 combinations of population individuals and multiplication by scalars not larger than 1. Anyway, note that this aspect is counter-balanced by the fact that the binary underlying group is Abelian. Indeed, when the composition is commutative, the number of possible minimal decompositions of a generic group element is intuitively large. Just look at RandBits of Algorithm 1 and observe
595 that any possible permutation of the 1-bits of the input string corresponds to a minimal decomposition sequence. This implies that there are intuitively many ways of truncating a decomposition sequence, that in turn likely slows down the convergence to population consensus on a bit.

7. Experimental Analysis

600 The proposed algebraic EAs (AEAs) have been experimentally analyzed on both binary and permutation problems. The benchmarks and the experimental setup adopted are described in, respectively, Sections 7.1 and 7.2. Algorithm parameters are tuned as reported in Section 7.3, while different experimental scenarios have been considered. A first set of experiments is described in Section
605 7.4, where standalone versions of the AEAs are compared with the standalone decoder-based numerical EAs described in Sections 2.3, 2.4, and 2.5. Then,

Section 7.5 describes a second set of experiments designed to compare enhanced versions of both classes of algorithms. Lastly, in Section 7.6, the best AEAs results are compared to the state-of-the-art results in literature for the tackled
 610 problems.

7.1. Benchmarks

Benchmark problems and instances have been selected for both the binary and permutation cases. Due to their generality, NK Landscapes (NKL) [19] have been considered as binary benchmarks, while, for permutation problems, the
 615 experiments have been held on the Permutation Flowshop Scheduling Problem (PFSP) with the total flowtime as objective function [20] and on the Linear Ordering Problem (LOP) [21].

An NKL instance of n bits and epistasis K is provided as n tabulated sub-functions $f_i : \mathbb{B}^{K+1} \rightarrow \mathbb{R}$, with $i \in \{1, \dots, n\}$, each one defined on $K + 1$ bits of
 620 an n -length bit-string including its i -th bit. The objective is to maximize the sum of the sub-function values.

A PFSP instance consists of n jobs, m machines, and a processing time $p_{i,j}$ for every job $i \in \{1, \dots, n\}$ in every machine $j \in \{1, \dots, m\}$. Given a permutation of jobs $\pi \in \mathcal{S}_n$, the completion time of job $\pi(i)$ in machine j
 625 is recursively computed as $c_{\pi(i),j} = p_{\pi(i),j} + \max\{c_{\pi(i-1),j}, c_{\pi(i),j-1}\}$ by also considering the terminal cases $c_{i,0} = c_{0,j} = 0$. The total flowtime objective requires to minimize $f(\pi) = \sum_{i=1}^n c_{\pi(i),m}$.

A LOP instance is provided as an $n \times n$ matrix H and the objective is to find a permutation $\pi \in \mathcal{S}_n$ which maximizes $f(\pi) = \sum_{i=1}^n \sum_{j=i+1}^n H_{\pi(i),\pi(j)}$.

630 Sixty instances for each one of the three problems have been selected from widely adopted benchmark suites as follows.

- NKL instances come from the combinatorial black-box optimization contest organized at GECCO 2015², where they have been randomly generated using different dimensionalities and epistasis values.

²<http://web.mst.edu/~tauritzd/CBBOC/GECCO2015>.

- PFSP instances are taken from the Taillard benchmark suite³ and, as explained in [51], they are the most difficult instances (basing on few algorithms chosen by the author) among a randomly generated set of instances.
- LOP instances are from the benchmark sets LOLIB, SGB and MB⁴: LOLIB is a real-world dataset of input-output tables used in economics, while SGB and MB are randomly generated instances with different dimensionalities and levels of sparsity.

Finally, note that the subset of $60 \times 3 = 180$ instances used in our work has been selected from these datasets by uniformly covering their inner characteristics. For the sake of space, the names of the selected instances are provided as supplementary material on the web [52].

7.2. Setup of the experiments

ADE and APSO have, each one, two implementations: for the binary and permutation space, thus we have a total of four algebraic algorithms. Both in the standalone and enhanced comparison scenarios (see Sections 7.4 and 7.5), ADE and APSO have been compared with the decoder-based numerical EAs described in Sections 2.3, 2.4 and 2.5. Therefore, six binary algorithms have been compared on the NKL instances, while four algorithms for permutation problems have been analyzed on PFSP and LOP instances. We use the same acronyms defined in Section 2 and, for the sake of presentation, we report them in Table 1.

All the PSO-based schemes adopt the ring topology. With regards to the DE-based algorithms, the standard binomial crossover of classical DE is used without any modification on the binary problems, while the OBX crossover [9] is adopted for the permutation problems. Indeed, OBX can be regarded as a simple feasible variant of the binomial crossover for the permutation representation.

³<http://mistic.heig-vd.ch/taillard>.

⁴<http://www.opticom.es/lolib>.

Table 1: Acronyms of the algorithms compared in the experimentation

Search space	Problems	Algorithms Acronyms	Algorithms Descriptions
Binary	NKL	ADE	Algebraic DE for the binary space
		APSO	Algebraic PSO for the binary space
		BDE [32]	Binary DE (see Section 2.3)
		BPSO [7]	Binary PSO (see Section 2.3)
		AM-DE [2]	Angle Modulated DE (see Section 2.4)
		AM-PSO [37]	Angle Modulated PSO (see Section 2.4)
Permutation	PFSP	ADE	Algebraic DE for the permutation space
	LOP	APSO	Algebraic PSO for the permutation space
		RK-DE [31]	Random-key DE (see Section 2.5)
		RK-PSO [3]	Random-key PSO (see Section 2.5)

For every instance, all the algorithms have been executed 20 times using, as termination criteria, both a given budget of fitness evaluations and of computational time. The final fitness values produced by the executions of every algorithm have been aggregated for each instance using the Average Relative Percentage Deviation (ARPD) measure, which is computed according to

$$\text{ARPD}_{\text{Inst}}^{\text{Alg}} = \frac{1}{20} \sum_{i=1}^{20} \frac{|\text{Alg}_{\text{Inst}}^{(i)} - \text{Best}_{\text{Inst}}|}{\text{Best}_{\text{Inst}}} \times 100, \quad (14)$$

where $\text{Alg}_{\text{Inst}}^{(i)}$ is the final fitness value produced by the algorithm Alg in its i -th run on the instance Inst, while $\text{Best}_{\text{Inst}}$ is the best result obtained on the given instance by any algorithm in any run of the considered experiment. The ARPDs have to be minimized both for maximization and minimization problems. Statistical analyses have been conducted by means of the well known Wilcoxon signed-rank test [53].

Finally, a state-of-the-art comparison has been carried out by comparing the best objective values obtained by the algebraic algorithms with the best known solutions so far of every benchmark instance (see Section 7.6).

670 7.3. Tuning of the parameters

Due to the different characteristics of the search spaces navigated by the algebraic and decoder-based algorithms, in order to perform a fair comparison, the parameters of the algorithms have been separately tuned using SMAC [54], i.e., a popular tool for automatic algorithm configuration based on statistical and machine learning techniques. To avoid the over-tuning phenomenon [55], SMAC calibrations have been run using a separate set of instances with respect to those used for algorithm comparisons. The list of the 30 selected calibration instances for each problem class is provided as supplementary material on the web [52]. Every SMAC calibration has been set to run for 72 hours of computational time, while every algorithm execution terminates after $100n^2$ fitness evaluations have been performed. The ranges of the parameters in input to SMAC are as follows: $N \in \{20, 60, 100\}$; $F, CR \in [0, 1]$ for DE schemes; $w \in [0, 1]$ and $c_1, c_2 \in [0, 2]$ for PSO schemes; $b \in [20, 100]$ for BDE; $k \in \{-1, 1\}$ for the random-key schemes. The tuned parameter settings resulting from the SMAC executions are provided in Table 2.

As expected, the different morphologies of the search landscapes are reflected on the noticeable differences among the calibrated parameter values.

7.4. Standalone Algorithms Comparison

The aim of this section is to verify if our proposals are competitive with respect to the decoder-based variants of DE and PSO. Therefore, in this set of experiments all the algorithms have been implemented in their basic versions as depicted by Sections 2 and 6.

The algorithms comparison has been performed by using the calibrated settings of Table 2 and considering two termination criteria: $100n^2$ fitness evaluations (as in calibration), and $50n^2$ milliseconds of computational time. The second criterion is motivated by the inherently different computational complexities of the algebraic and decoder-based algorithms.

The results of the executions are presented in aggregated form in Tables 3, 4, and 5, respectively, for NKL, PFSP, and LOP instances. For each algorithm

Table 2: Calibrated settings obtained with SMAC

Problem	Algorithm	Parameter Settings
NKL	ADE	$N = 100, F = 0.22, CR = 0.22$
	BDE [32]	$N = 100, F = 0.78, CR = 0.65, b = 98.77$
	AM-DE [2]	$N = 60, F = 0.12, CR = 0.32$
	APSO	$N = 100, w = 0.04, c_1 = 0.58, c_2 = 1.7$
	BPSO [7]	$N = 20, w = 0.79, c_1 = 1.64, c_2 = 1.33$
	AM-PSO [37]	$N = 20, w = 0.73, c_1 = 1.77, c_2 = 1.44$
PFSP	ADE	$N = 100, F = 0.13, CR = 0.65$
	RK-DE [31]	$N = 100, F = 0.4, CR = 0.95, k = 1$
	APSO	$N = 20, w = 4 \cdot 10^{-5}, c_1 = 1.4, c_2 = 1.05$
	RK-PSO [3]	$N = 100, w = 0.8, c_1 = 1.78, c_2 = 1.76, k = -1$
LOP	ADE	$N = 100, F = 0.05, CR = 0.42$
	RK-DE [31]	$N = 60, F = 0.9, CR = 0.95, k = 1$
	APSO	$N = 60, w = 0.003, c_1 = 1.74, c_2 = 1.09$
	RK-PSO [3]	$N = 100, w = 0.8, c_1 = 1.73, c_2 = 1.64, k = -1$

and for both termination criteria, any of such tables provides four performance measures: 1) the overall ARPD, 2) the non-parametric average rank (of the algorithm's ARPDs), 3) the intra-class success rate defined as the number of instances where the algorithm obtained the best ARPD compared to the same-class competitors⁵, and 4) the p-value of the Wilcoxon test with respect to the best performing competitor in the same algorithmic class.

The results clearly show that the algebraic algorithms outperform the decoder-based approaches with very high statistical evidence in every problem and considering both termination criteria. In general, the algebraic DE is the best scheme in every problem. Indeed, ADE obtained 1 as average rank both for PFSP and LOP experiments, meaning that ADE has obtained the best ARPD

⁵This is not the standard definition of success rate, i.e., the frequency with which the best known solution has been obtained in n trials. Note anyway that, since our intra-class success rate consider the ARPD values, it takes implicitly into account also the multiple trials performed by the algorithm.

Table 3: Experimental results of standalone algorithms on NKL

Termination Criterion	Performance Measure	ADE	BDE [32]	AM-DE [2]	APSO	BPSO [7]	AM-PSO [37]
Evaluations	Overall ARPD	0.29	12.32	12.83	0.79	6.85	12.31
	Avg Rank	1.25	4.59	5.88	1.84	2.91	4.53
	Success Rate	60/60	0/60	0/60	56/60	4/60	0/60
	p-value	best	$< 10^{-10}$	$< 10^{-10}$	best	$< 10^{-10}$	$< 10^{-10}$
Time	Overall ARPD	0.25	12.40	12.90	0.43	6.93	12.39
	Avg Rank	1.39	4.58	5.88	1.62	2.99	4.54
	Success Rate	60/60	0/60	0/60	60/60	0/60	0/60
	p-value	best	$< 10^{-10}$	$< 10^{-10}$	best	$< 10^{-10}$	$< 10^{-10}$

Table 4: Experimental results of standalone algorithms on PFSP

Termination Criterion	Performance Measure	ADE	RK-DE [31]	APSO	RK-PSO [3]
Evaluations	Overall ARPD	0.62	13.72	5.78	6.58
	Avg Rank	1.00	4.00	2.10	2.90
	Success Rate	60/60	0/60	54/60	6/60
	p-value	best	$< 10^{-10}$	best	$< 10^{-8}$
Time	Overall ARPD	0.38	11.72	4.59	4.83
	Avg Rank	1.00	4.00	2.31	2.69
	Success Rate	60/60	0/60	42/60	18/60
	p-value	best	$< 10^{-10}$	best	0.006

Table 5: Experimental results of standalone algorithms on LOP

Termination Condition	Performance Measure	ADE	RK-DE [31]	APSO	RK-PSO [3]
Evaluations	Overall ARPD	0.14	19.40	3.52	4.11
	Avg Rank	1.00	4.00	2.17	2.83
	Success Rate	60/60	0/60	50/60	10/60
	p-value	best	$< 10^{-10}$	best	$< 10^{-9}$
Time	Overall ARPD	0.08	16.93	2.95	3.12
	Avg Rank	1.00	4.00	2.28	2.72
	Success Rate	60/60	0/60	42/60	18/60
	p-value	best	$< 10^{-10}$	best	$< 10^{-3}$

on every single PFSP and LOP instance. Moreover, in the binary NKL instances, though ADE is anyway the best algorithm in average, APSO reached quite comparable results.

In order to analyze the convergence behaviors, Figure 2 presents the convergence graphs obtained by the median execution of every algorithm in three benchmark instances, one per problem. The data provided are typical data which have been observed also in other executions and benchmark instances. The graphs show behavior of the objective value – of the best solution in the population – with respect to the number of evaluations performed so far. Since the PFSP is the only minimization problem, for the sake of homogeneity, we present the opposite objective values.

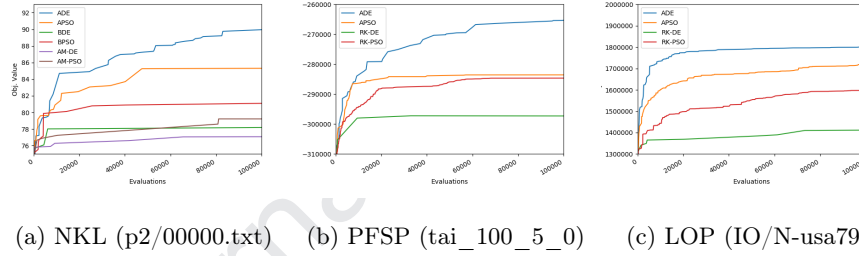


Figure 2: Convergence graphs in three selected instances of the algorithms ADE, APSO, BDE [32], BPSO [7], AM-DE [2], AM-PSO [37], RK-DE [31], RK-PSO [3].

The most interesting observation which follows from these graphs is that, in general, most of the decoder-based schemes seem to converge earlier than algebraic algorithms. One only exception looks to be RK-PSO, in particular in the LOP benchmark. This premature convergence looks to be a plausible explanation of the different performances among the schemes.

Finally, we refer the interested reader to the supplementary material [52] for the full details of the experimental results.

7.5. Enhanced Algorithms Comparison

In order to provide a more complete analysis, additional experiments have been held with the aim of comparing enhanced versions of the AEAs and

decoder-based schemes. The algorithms from both classes have been equipped with four additional components commonly employed in literature to improve the performance of an evolutionary algorithm: a heuristic initialization, a restart
 735 mechanism, a local search procedure, and a self-adaptive strategy for the algorithms' parameters.

The heuristic initialization works by generating one initial solution by means of a heuristic procedure purposely defined for the problem at hand, while the remaining $N - 1$ individuals are randomly generated. For PFSP and LOP, we
 740 have adopted very popular and effective constructive procedures: respectively, the Liu-Reeves [56] and best-insertion [57] heuristics. For NK landscapes, as far as we know, there is no heuristic available in literature, thus we have designed a simple procedure: randomly generate $n(K + 1)$ bit-strings and select the best one. Though being very simple, we have experimentally observed that it
 745 guarantees a good starting point for the algorithms.

Restarts are triggered when the best population solution has not been improved during the last T generations. After some preliminary experiments, T has been set to 1000. In the DE-based schemes, as done for example in [8], the restart randomizes all the solutions except the best one, while in the PSO-
 750 based schemes we have adopted the restart strategy described in [58], i.e., all the personal best solutions are randomized except for the global best particle that randomizes its velocity.

As suggested in [59], in every generation, local search is applied to every solution with probability $1/N$. Hence, in average, one solution per generation
 755 undergoes local search. Additionally, in order to refine the search as much as possible, we apply the local search also to the best solution after every restart and at the end of the evolution. A complete best-improvement local search procedure has been employed. The bit-flip neighborhood has been used in NKL instances, while for PFSP and LOP, the commonly used neighborhood based
 760 on item's insertion moves has been considered [45].

In order to automatically calibrate the parameters during the evolution we have used two popular self-adaptive mechanisms: the jDE scheme for the DE-

based algorithms [60], and the self-adaptive PSO scheme introduced in [61]. Both schemes extend each population individual with a personal copy of the parameters which are evolved similarly to the genotype solution. Therefore, no parameter setting is required except for the population size N and the random-key parameter k that have been set as in Table 2.

The enhanced algorithms are denoted as: ADE^+ , $APSO^+$, BDE^+ , $BPSO^+$, $AM-DE^+$, $AM-PSO^+$, $RK-DE^+$, and $RK-PSO^+$. Note also that, both in the heuristic initialization and after any application of the local search, the random-key and the angle modulated schemes require to encode the obtained discrete solution to a numerical vector. For random-key schemes, this is done by normalizing the permutation to a numerical vector such that any dimension is within the allowed numerical bounds. However, as far as we know, there is no known method to invert the AM decoder of equation (4), therefore, $AM-DE^+$ and $AM-PSO^+$ actually do not use heuristic initialization and adopt a Baldwinian local search, i.e., the (hopefully) improved solution is recorded but does not enter the population. Moreover, $BPSO^+$ has been further improved by setting $v_{\max} = \ln(n - 1)$, as suggested in [62].

Experiments have been held using the set of selected instances, every algorithm has been executed 20 times per instance, and each execution terminates after 10 consecutive restarts without improvement of the best solution or after 10 minutes of computational time. The aggregated experimental results are presented in Tables 6, 7, and 8 for, respectively, the NKL, PFSP and LOP benchmarks. The same layout described in Section 7.4 is used.

Table 6: Experimental results of enhanced algorithms on NKL

Performance Measure	ADE^+	BDE^+ [32]	$AM-DE^+$ [2]	$APSO^+$	$BPSO^+$ [7]	$AM-PSO^+$ [37]
Overall ARPD	0.16	12.85	13.68	0.25	1.29	4.15
Avg Rank	1.32	6.00	4.00	1.78	5.00	2.90
Success Rate	60/60	0/60	0/60	60/60	3/60	0/60
p-value	best	$< 10^{-10}$	$< 10^{-10}$	best	$< 10^{-10}$	$< 10^{-10}$

Table 7: Experimental results of enhanced algorithms on PFSP

Performance Measure	ADE ⁺	RK-DE ⁺ [31]	APSO ⁺	RK-PSO ⁺ [3]
Overall ARPD	0.42	1.06	0.59	0.92
Avg Rank	1.48	3.13	2.45	2.93
Success Rate	49/60	11/60	41/60	19/60
p-value	best	$< 10^{-7}$	best	$< 10^{-5}$

Table 8: Experimental results of enhanced algorithms on LOP

Performance Measure	ADE ⁺	RK-DE ⁺ [31]	APSO ⁺	RK-PSO ⁺ [3]
Overall ARPD	0.01	0.29	0.20	0.24
Avg Rank	1.22	3.10	2.58	3.10
Success Rate	57/60	4/60	41/60	20/60
p-value	best	$< 10^{-9}$	best	0.018

The results clearly show that the AEAs outperform the decoder-based approaches in every problem also when both classes of algorithms are enhanced with additional algorithmic components. Indeed, as in the previous experiments, the reported p-values largely indicate that all the comparisons have very high significance, thus definitely validating our proposals with respect to the decoder-based competitors.

In general, all algorithms, apart few exceptions (BDE⁺, AM-DE⁺, AM-PSO⁺ in NKL instances), decrease their overall ARPDs with respect to the experiments of Section 7.4. This is a consequence of the additional algorithmic components which tend to reduce performance differences among multiple runs of the same algorithms. In a few instances, the decoder-based approaches have been able to reach the ARPDs of the algebraic algorithms. This is shown by the non-zero success rates obtained by BPSO⁺ in the NKL instances, and by RK-DE⁺ and RK-PSO⁺ in both the PFSP and LOP instances. However, also the AEAs have consistently improved their overall ARPDs: the best one is 0.01%

(ADE⁺ in the LOP problem), while the worst one is only 0.59% (APSO⁺ in the PFSP problem). Finally, it is worth to note that, as in the previous set of experiments, ADE⁺ is clearly the best algorithm, though APSO⁺ reaches a quite comparable average rank on NKL instances.

805 Finally, we refer the interested reader to the supplementary material [52] for the full details of the experimental results.

7.6. Comparison with State-of-the-art Results

Though the algebraic algorithms clearly outperform the decoder-based approaches, the previous experiments say nothing about the general performances 810 of AEAs with respect to pure combinatorial algorithms. Therefore, in this section we compare the AEAs performances with respect to the state-of-the-art results on the tackled problems.

The analysis has been conducted by comparing, on every instance, the best objective function values obtained by both ADE⁺ and APSO⁺ with respect to 815 the best known solutions available in literature. In particular, these latter have been obtained from: the CBBOC website for NKL (see footnote 2), the LOLIB website for LOP (see footnote 4), and from [8, Table III] for PFSP. With this regard, it is important to stress out that the best known solutions have been obtained by a variety of different algorithms, often purposely designed for the 820 problem at hand. We think that this comparison is much more explanatory and comprehensive than comparing the AEAs with a bunch of chosen algorithms.

Both for ADE⁺ and APSO⁺, the analysis is summarized by the indices provided in Table 9 where, aggregated over the instances of every problem, it is reported: the average, maximum and minimum percentage improvement with 825 respect to the best known solution (BKS) together with the number of BKSs that have been matched or improved by our proposals.

In the NK landscapes, all the best known solutions have been improved (46 cases), or at least reached (14 cases), by both ADE⁺ and APSO⁺. Though these instances have been only investigated during the CBBOC competition, the 830 results are anyway interesting since they clearly show that algebraic algorithms

Table 9: Comparison with state-of-the-art results

Performance Measure	NKL Instances		PFSP Instances		LOP Instances	
	ADE ⁺	APSO ⁺	ADE ⁺	APSO ⁺	ADE ⁺	APSO ⁺
Avg Improvement	+2.06%	+2.05%	−0.60%	−0.93%	−0.0005%	−0.02%
Max Improvement	+10.96%	+10.85%	0.00%	0.00%	0.00%	0.00%
Min Improvement	0.00%	0.00%	−2.54%	−2.85%	−0.03%	−0.19%
BKs reached	60/60	60/60	20/60	20/60	58/60	31/60
BKs improved	46/60	46/60	0/60	0/60	0/60	0/60

are competitive on binary problems.

In the selected LOP instances, it is worth to note that the best known solutions have been proven to be optimal [21]. Hence, Table 9 shows that ADE⁺ has been able to reach the optimum in almost the totality of the instances while
835 its average deviation from the optimum, though negative, is almost negligible. Moreover, the worst deviation obtained by APSO⁺ is only 0.19%.

For PFSP, though both of our proposals have matched the state-of-the-art results in the 20 smaller instances, the average deviations from the best known solutions are slightly larger than in LOP, but they are anyway not greater
840 than 1%.

In conclusion, this analysis shows that the algebraic framework here proposed is quite general and effective also from a practical point of view.

8. Conclusion and Future Work

The main contribution of this work is the general algebraic framework by
845 which it is possible to adapt a large class of numerical evolutionary algorithms to tackle an important class of combinatorial optimization problems.

The framework has been abstractly described by means of the algebraic properties of finitely generated groups, while concrete implementations are provided for binary and permutation search spaces. Discrete vector operations have
850 been proposed in such a way that their geometric interpretations are consistent

throughout the different spaces and with respect to their numerical counterparts.

The algebraic variants of two popular algorithms have been proposed: Algebraic Differential Evolution (ADE) and Algebraic Particle Swarm Optimization (APSO).
855

These algorithms have been implemented and compared with six algorithms in literature which use the decoder-based schemes, i.e., classical numerical algorithms endowed with decoding procedures that convert continuous individuals to discrete solutions. To the best of our knowledge, this is the only technique in
860 literature that guarantees a level of applicability comparable to our framework.

Experiments have been held both on binary and permutation problems by considering two scenarios: standalone and enhanced implementations of the algorithms. The experimental results show that the algebraic algorithms clearly outperform the competitors in both scenarios. Importantly, a further comparison
865 with state-of-the-art results in literature shows that our proposals are also competitive with pure combinatorial algorithms. These empirical results, together with the strong mathematical foundations over which our proposal is built, allow us to suggest our framework in the design of new algorithms for combinatorial optimization problems.

A future research of direction is to apply the proposed framework to other
870 search spaces such as, for instance, the space of integer vectors. Moreover, since the Cartesian product of search spaces representable as groups form itself a group (the so-called product group), we are also planning to expand the applications of the framework to more complex search spaces that are usually tackled
875 by means of co-evolutionary algorithms. Another research direction is to propose algebraic variants for other numerical algorithms like, for example, Firefly Algorithm or Bacterial Foraging Optimization scheme. Finally, it is interesting to study the potentialities of the framework in order to provide a new perspective in the theoretical analysis of combinatorial meta-heuristics. Preliminary
880 investigations in some of these directions are presented in [63, 64].

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