Geometric Crossover for Sets, Multisets and Partitions

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Abstract. This paper extends a geometric framework for interpreting crossover and mutation [5] to the case of sets and related representations. We show that a deep geometric duality exists between the set representation and the vector representation. This duality reveals the equivalence of geometric crossovers for these representations.

1 Introduction

Sets, multisets and partitions are natural representations for many important combinatorial optimization problems such as grouping problems, graph coloring and so on. The set representation for evolutionary algorithms was theoretically studied by Radcliffe [10] within his forma analysis framework.

Geometric crossover and geometric mutation are representation-independent search operators that generalize many pre-existing search operators for the major representations used in evolutionary algorithms, such as binary strings [5], real vectors [5], permutations [7], syntactic trees [6] and sequences [8]. They are defined in geometric terms using the notions of line segment and ball. These notions and the corresponding genetic operators are well-defined once a notion of distance in the search space is defined. Defining search operators as functions of the search space is opposite to the standard way [3] in which the search space is seen as a function of the search operators employed. This viewpoint greatly simplifies the relationship between search operators and fitness landscape and has allowed us to give simple *rules-of-thumb* to build crossover operators that are likely to perform well.

In this paper we use the geometric framework [5] to study and design crossover operators for the set representation and related representations such as multi-sets and partitions for the fixed-size and variable-size variants. We also show an illuminating isometric duality between the spaces associated to the set representation and the vector representation that enables us to prove the equivalence of geometric crossovers for these representations.

The paper is organised as follows. In section 2 we present the geometric framework. In section 3, we extend it to sets, multisets and partitions of variable-size. In section 4, we consider the fixed-size case. In section 5, we illustrate the duality between sets and vectors. In section 6, we draw some conclusions.

2 Geometric framework

2.1 Geometric preliminaries

In the following we give necessary preliminary geometric definitions and extend those introduced in [5] and [6]. The following definitions are taken from [2].

The terms *distance* and *metric* denote any real valued function that conforms to the axioms of identity, symmetry and triangular inequality. A simple connected graph is naturally associated to a metric space via its *path metric*: the distance between two nodes in the graph is the length of a shortest path between the nodes.

In a metric space (S, d) a *line segment* (or closed interval) is the set of the form $[x; y] = \{z \in S | d(x, z) + d(z, y) = d(x, y)\}$ where $x, y \in S$ are called extremes of the segment. Metric segment generalises the familiar notion of segment in the Euclidean space to any metric space through distance redefinition. Notice that a metric segment does not coincide with the shortest path connecting its extremes (*geodesic*) as in an Euclidean space. In general, there may be more than one geodesic connecting two extremes; the metric segment is the union of all geodesics.

We assign a structure to the solution set S by endowing it with a notion of distance d. $M = (S, d)$ is therefore a solution *space* and $L = (M, g)$ is the corresponding fitness landscape.

2.2 Geometric crossover definition

The following definitions are *representation-independent* and, therefore, applicable to any representation.

Definition 1. *(Image set) The* image set $Im[OP]$ *of a genetic operator* OP *is the set of all possible offspring produced by* OP *with non-zero probability.*

Definition 2. *(Geometric crossover) A binary operator is a geometric crossover under the metric* d *if all offspring are in the segment between its parents.*

Definition 3. *(Uniform geometric crossover) Uniform geometric crossover* UX *is a geometric crossover where all* z *laying between parents* x *and* y *have the same probability of being the offspring:*

$$f_{UX}(z|x, y) = \frac{\delta(z \in [x; y])}{|[x; y]|}$$

$$Im[UX(x, y)] = \{z \in S | f_{UX}(z|x, y) > 0\} = [x; y].$$

A number of general properties for geometric crossover and mutation have been derived in [5] where we also showed that traditional crossover is geometric under Hamming distance. In previous work we have also studied various crossovers for permutations, revealing that PMX, a well-known crossover for permutations, is geometric under swap distance. Also, we found that Cycle crossover, another traditional crossover for permutations, is geometric under swap distance and under Hamming distance.

3 Geometric crossover for variable-size sets, multi-sets and partitions

We consider problems where solutions are naturally represented as sets of objects taken from a reference set (universal set). We also consider the simple extension to multi-sets, sets that are allowed to contain repetitions of the same object. A set can be seen also as a bipartition of the universal set (objects in the set and remaining objects in the universal set). A natural extension of the notion of set in this sense is to consider generic multi-partitions of the universal set. We will study this case too.

There is a further aspect of the set representation that has a major impact on the associated geometric crossovers: the search being restricted to fixed-size sets versus the variable-size case. In this section, we study sets, multi-sets and partitions for the easier variable-size case. In section 4, we consider the fixed-size case.

3.1 Distances and crossover for sets

Let U be the universal set and $A, B \subseteq U$. The *symmetric distance* between sets is $d(A,B) = |A \Delta B|$ where $A \Delta B = A \cup B \setminus A \cap B$ is the symmetric difference between sets. The symmetric distance is a metric [2]. When $A = B$, d(A,B)=0; when $A \cap B = \emptyset$, A and B are at maximum distance and $d(A,B) = |A| + |B|$. The *ins/del edit distance* between A and B is the minimum number of elements that need to be deleted or inserted for A to be transformed into B (and *vice versa*).

Theorem 1. *The symmetric distance is the same as the ins/del edit distance.*

Proof. The edit distance corresponds to the symmetric distance because the minimum number of elements that need to be deleted from A are $|A \setminus B|$ and of those that need to be added are $|B \setminus A|$. It is easy to see that $d(A,B) = |A \Delta B| = |A \setminus B| + |B \setminus A|$.

Corollary: since any edit distance is a metric [1], theorem 1 proves also that the symmetric distance is a metric.

Theorem 2. *Given two parent sets A and B any recombination operator OP that returns offspring O such as $A \cap B \subseteq O \subseteq A \cup B$ is geometric crossover under symmetric distance.*

Proof. Proving geometricity under symmetric distance is equivalent to proving geometricity under ins/del edit distance. Any intermediate set C on the minimal ins/del move path to transform A into B is between A and B (in the segment $[A,B]$) under ins/del edit distance (see Fig. 1). Every O such that $A \cap B \subseteq O \subseteq A \cup B$ belongs to such a path because: A can be transformed into B by inserting in A the elements $O \setminus A$, removing from A the elements $A \setminus O$ and then by inserting in B the elements $B \setminus O$, and removing from B the elements $O \setminus B$. So $d(A,O) = |O \setminus A| + |A \setminus O|$ and $d(B,O) = |O \setminus B| + |B \setminus O|$

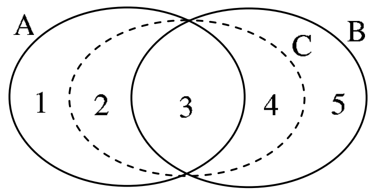

Fig. 1. Venn diagram linking offspring set and parent sets.

Example Let $U = \{a, b, c, d\}$ be the universal set and $A = \{a, b\}$ and $B = \{b, c\}$ two parent sets such that $A, B \subseteq U$. The symmetric distance between A and B is $d_\Delta(A, B) = |A \backslash B| + |B \backslash A| = 1+1 = 2$. Let GX_Δ be a geometric crossover under symmetric distance. Any offspring O of A and B, $O = GX_\Delta(A, B)$, respects the condition $A \cap B \subseteq O \subseteq A \cup B$. So, in our example we have: $\{b\} \subseteq O \subseteq \{a, b, c\}$. These are the sets: $\{b\}, \{a, b\}, \{b, c\}, \{a, b, c\}$. It is easy to verify that every O is in the segment between A and B under d_Δ. For example if we consider $O = \{a, b, c\}$ we have $d_\Delta(A, O) + d_\Delta(O, B) = (0 + 1) + (1 + 0) = 2 = d_\Delta(A, B)$.

3.2 Distances and crossover for multi-sets

A multi-set (sometimes also called a bag) differs from a set in that each member has a *multiplicity*, which is a natural number indicating how many times it occurs in the multi-set. A multi-set can be formally defined as a pair (A, m) where A is some set and $m : A \to \mathbb{N}$ is a function from A to the set of natural numbers $\mathbb{N}$. The set A is called the underlying set of elements. The *size* of the multi-set (A, m) is the sum of all multiplicities for each element of A: $|(A, m)| = \sum_{a \in A} m(a)$. A *submultiset* (B, n) of a multiset (A, m) is a subset $B \subseteq A$ and a function $n : B \to \mathbb{N}$ such that $\forall b \in B : n(b) \leq m(b)$. The usual operations of union and intersection for sets can easily be generalized to multisets. Suppose (A, m) and (B, n) are multisets. The *union* can be defined as $(A \cup B, f)$ where $f(x) = \max\{m(x), n(x)\}$. The *intersection* can be defined as $(A \cap B, f)$ where $f(x) = \min\{m(x), n(x)\}$.

Hence we can define the *symmetric difference* between multisets as $(A \Delta B, f)$ where $f(x) = \max\{m(x), n(x)\} - \min\{m(x), n(x)\} = |m(x) - n(x)|$. The *symmetric distance* for multisets becomes $d((A, m), (B, n)) = |(A, m) \Delta (B, n)| = \sum_{x \in A \Delta B} |m(x) - n(x)|$. The symmetric distance between multisets can be seen as a simple generalization of the *ins/del edit distance* for sets in which the edit move becomes the insertion or deletion of a *single occurrence* of an element.

The geometricity theorem for sets under symmetric distance can be extended to the case of multisets. Given two parent multisets (A, m) and (B, n) any recombination operator OP that returns offspring (O, f) such as $(A, m) \cap (B, n) \subseteq (O, f) \subseteq (A, m) \cup (B, n)$ is geometric crossover under symmetric distance.

Example Let $U = \{a, b, c, d\}$ be the universal set, $A = \{a, b\}$ and $B = \{b, c\}$ be two sets such as $A, B \subseteq U$. Let us consider the parent multiset $M_A = \{a, a, b\} =$

(A, m) where $m(a) = 2$ and $m(b) = 1$ and the parent multiset $M_B = \{b, b, c, c\} = (B, n)$ where $n(b) = 2$ and $n(c) = 2$. Their sizes are $|M_A| = 3$ and $|M_B| = 4$. Their union is $M_A \cup M_B = (A, m) \cup (B, n) = (A \cup B, f)$ where $f = max(m, n)$. In our example we have $M_A \cup M_B = \{a, a, b, b, c, c\}$. Their intersection is $M_A \cap M_B = (A, m) \cap (B, n) = (A \cap B, f)$ where $f = min(m, n)$. In our example we have $M_A \cap M_B = \{b\}$. Their symmetric difference is $M_A \Delta M_B = (A \Delta B, f)$ where $f = max(m, n) - min(m, n)$. In our example we have $M_A \Delta M_B = \{a, a, b, c, c\}$. The symmetric distance between M_A and M_B is, therefore, $d_\Delta(M_A, M_B) = |M_A \Delta M_B| = 5$. Let GX_Δ be a geometric crossover under symmetric distance for multisets. Any offspring M_O of M_A and M_B, $M_O = GX_\Delta(M_A, M_B)$, respects the condition $M_A \cap M_B \subseteq M_O \subseteq M_A \cup M_B$. So, in our example we have: $\{b\} \subseteq M_O \subseteq \{a, a, b, b, c, c\}$. Thus, any multiset $M_O = (O, f)$ such as $0 \leq f(a) \leq 2, 1 \leq f(b) \leq 2, 0 \leq f(c) \leq 2$ is a possible offspring of M_A and M_B.

3.3 Distances and crossover for partitions

In this paper we restrict our focus on partitioning problems with labeled partitions and a fixed number of partitions. In this section we consider the case where the same partition may have different size in different solutions. In section 4 we will consider the case in which all solutions are required to have the same size for the same partition.

A partition of a set X is a division of X into non-overlapping subsets that cover all of X. When the set X is partitioned into n subsets we say that they form a n-partition of X. A n-partition generalizes the notion of set A seen as partitioning the universal set U in two subsets A and $\overline{A}$ (bipartition).

The symmetric distance between two n-partitions $\mathcal{A} = \{A_1, \ldots, A_n\}$ and $\mathcal{B} = \{B_1, \ldots, B_n\}$ of a set X is a simple generalization of the symmetric distance for sets: $d(\mathcal{A}, \mathcal{B}) = \sum |A_i \Delta B_i|$.

The edit distance between two n-partitions is a natural generalization of the ins/del edit distance for sets. We define the edit distance between two n-partitions as the minimum number of edit moves to transform one partition into the other where the edit move considered is moving one element from one subset to another. This edit move transforms a partition of X into another partition of X for which the conditions of full coverage of X and mutual exclusivity of subsets are respected. This edit distance is a generalization of the ins/del edit distance for sets in that when one considers a set A as a bipartition of the universal set U into A and $\overline{A}$, inserting or deleting one element from A implies respectively deleting or inserting the same element in $\overline{A}$. So, this is equivalent of moving one element from A to $\overline{A}$. The symmetric distance between partitions does not equal their ins/del edit distance (although these distances are related).

Example Let $X = \{a, b, c, d\}$ be the universal set (the set to be partitioned), and be $\mathcal{A} = (\{a, b\}, \{c, d\})$ and $\mathcal{B} = (\{b, c, d\}, \{a\})$ two ordered (or labeled) bipartitions of X. Since we consider ordered partitions, $(\{a, b\}, \{c, d\}) \neq (\{c, d\}, \{a, b\})$. The edit distance between $\mathcal{A}$ and $\mathcal{B}$ is the minimum number of elements that need to be transferred from one subset to another to transform $\mathcal{A}$ into $\mathcal{B}$ (or viceversa). In our case, in order to transform $\mathcal{A}$ into $\mathcal{B}$, we need to transfer c and d from the second subset to the first subset and transfer a from the first subset to the second for a total of 3 edit moves. So the edit distance $ed(\mathcal{A}, \mathcal{B}) = 3$. The geometric crossover under edit distance requires the offspring partition $\mathcal{O} = (O_1, \ldots, O_n)$ to satisfy $\forall i : A_i \cap B_i \subseteq O_i \subseteq A_i \cup B_i$. Notice that the sets O_i needs to form a partition of X hence need to be chosen so as to be non-overlapping and covering X completely (so their choices cannot be made independently). In our example we have $\{b\} \subseteq O_1 \subseteq \{a, b, c, d\}$ and $\emptyset \subseteq O_2 \subseteq \{a, c, d\}$. Considered independently, O_1 can be any subset of X including b (8 possible subsets) and O_2 can be any subset of $\{a, c, d\}$ (8 possible subsets). However since O_1 and O_2 need to form a partition of X, we have only 8 choices (and not 8^2) which are $\mathcal{O} = (O_1, \overline{O}_1)$ where $\{b\} \subseteq O_1 \subseteq \{a, b, c, d\}$.

4 Geometric crossover for fixed-size sets, multi-sets and partitions

Substitution edit distance Let U be the universal set and $\mathcal{X}_n$ the set of all subsets of U of size n, $\mathcal{X}_n = \{A : A \subseteq U, |A| = n\}$, and let $A, B \in \mathcal{X}_n$.

The *edit distance between sets under element substitution move* between A and B is the minimum number of elements of A that need to be substituted with an element in $U \setminus A$ to be transformed into B (or vice versa). Since this distance is an edit distance it is a metric.

For any two sets of the same size, their ins/del edit distance is twice their substitution edit distance because every substitution is equivalent to one deletion and one insertion operation and there are no shorter ways to transform one set into another of the same size using deletions and insertions. The substitution edit distance is well-defined only for sets of the same size because sets of different size cannot be transformed into each other by substitutions only.

Geometric crossover under substitution edit distance Given two parent sets $A, B \in \mathcal{X}_n$ any recombination operator OP that returns offspring $O \in \mathcal{X}_n$ such that $A \cap B \subseteq O \subseteq A \cup B$ is geometric crossover under substitution edit distance. So, this geometric crossover is a geometric crossover under ins/del edit distance restricted to sets of size n.
Proof: if we restrict the image set of a geometric crossover from X to $S \subseteq X$ we obtain a new geometric crossover that for any two parents $a, b \in S$ returns offspring in $[a, b] \cap S$. So, restricting the geometric crossover associated to ins/del edit distance from the set 2^U to the set $\mathcal{X}_n \subseteq 2^U$, we obtain a new geometric crossover based on the ins/del distance that returns offspring of the same size of the parents.

This restricted crossover is also geometric crossover under substitution edit distance because given $A, B \in \mathcal{X}_n$, $O \in [A, B]$ under ins/del edit distance iff $O \in [A, B]$ under substitution edit distance because ins/del edit distance is twice of substitution edit distance and proportional metrics have the same metric intervals.

Example Let $U = \{a, b, c, d\}$ be the universal set and $A = \{a, b\}$ and $B = \{b, c\}$ two parent sets such as $A, B \subseteq U$. The substitution edit distance between A and B is $d_{sub}(A, B) = 1$: A can be transformed into B by substituting a single element in A, the element b with c. Their ins/del edit distance, which equals their symmetric distance, is $d_{\Delta}(A, B) = 2 \cdot d_{sub}(A, B) = 2$.

Any offspring O of A and B by geometric crossover under ins/del edit distance GX_{Δ}, $O = GX_{\Delta}(A, B)$, respects the condition $A \cap B \subseteq O \subseteq A \cup B$. These are the sets: $\{b\}, \{a, b\}, \{b, c\}, \{a, b, c\}$. The offspring obtained by geometric crossover under substitution edit distance are those that have the same parent size, size 2 in this case: $\{a, b\}, \{b, c\}$. They are in the segment between parents A and B under substitution edit distance (in this case the only offspring are the parents themselves).

5 Geometric duality of sets and vectors

In this section we show that the same metric spaces considered in section 3 and 4, arising from the set and related representations, arise from the vector representation and permutations with repetitions. In other words, set spaces and vector spaces are isometric. This enables us to show that the geometric crossovers considered in section 3 and 4 for sets, multi-sets and partitions all have equivalent dual geometric crossovers based on vectors in the variable-size case and on permutations with repetitions in the fixed-size case (see Table 1).

5.1 Dual equivalence of geometric crossovers for sets and vectors

Geometric crossovers based on isometric spaces are equivalent. The space of sets endowed with the symmetric distance is isometric to the space of vectors endowed with Hamming distance. Hence, symmetric crossover for sets is equivalent to the traditional crossover for vectors. In the following, we prove the duality and illustrate it with an example.

Definition 4. *(Indicator function) The indicator function of a subset A of a set U is a function $I_A : U \to \{0, 1\}$ defined as* $I_A(x) = \begin{cases} 1 \text{ } if \text{ } x \in A, \\ 0 \text{ } if \text{ } x \notin A. \end{cases}$

Definition 5. *(Isometry) Let X and Y be metric spaces with metrics d_X and d_Y. A map $f : X \to Y$ is called* distance preserving *if for any $x, y \in X$ one has $d_Y(f(x), f(y)) = d_X(x, y)$. A distance preserving map is automatically injective. A* global isometry *is a bijective distance preserving map. Two metric spaces X and Y are called* isometric *if there is a global isometry from X to Y.*

Let U be the universal set, d_Δ the symmetric distance between sets and $M = (2^U, d_\Delta)$ the metric space based on the set of all subsets of U together with the symmetric distance.

Let I_A be the indicator function of $A \subseteq U$ where $U = \{x_1, \cdots, x_n\}$ and V_A be the vector $(I_A(x_1), \cdots, I_A(x_n))$. The map $V : A \to V_A$ mapping a set A and its indicator values vector V_A is bijective.

Let $M' = (\{0,1\}^n, d_H)$ be the metric space of the binary vectors of size n endowed with the Hamming distance d_H.

Theorem 3. *The metric spaces* $M = (2^U, d_\Delta)$ *and* $M' = (\{0,1\}^n, d_H)$ *are isometric.*

Proof. It is sufficient to prove that the the map $V : A \to V_A$ is a distance preserving map. It is immediate to see that for any $A, B \subseteq U$ we have $d_\Delta(A, B) = d_H(V_A, V_B)$. To transform A into B with the minimum number of ins/del operations, the elements that need to be inserted into A are those x_i for which $V_A(i) = 0$ and $V_B(i) = 1$ and the elements that need to be deleted from A are those x_j for which $V_A(j) = 1$ and $V_B(j) = 0$. These are the only positions in which V_A and V_B differ. Since V is bijective, the opposite implication, $V_A, V_B \in \{0,1\}^n : d_\Delta(V^{-1}(V_A), V^{-1}(V_B)) = d_H(V_A, V_B)$, is also true. This completes the proof.

Example Let $A = \{a, b\}$ and $B = \{b, c, d\}$. Their offspring O obtained by geometric crossover under symmetric distance are $\{b\} \subseteq O \subseteq \{a, b, c, d\}$. Dually, for the set A the vector of the values of the indicator function is $V_A = (1, 1, 0, 0)$ and for B is $V_B = (0, 1, 1, 1)$. The set of their offspring under traditional crossover is the schema $(*, 1, *, *)$. For the duality, these offspring vectors correspond to the offspring sets above via their indicator functions as it is easy to verify.

5.2 Interesting uses of the duality

Thanks to these results we can use the two representations interchangeably. In particular, we can use the most convenient representation, knowing that the search done in one space is equivalent to the search in the other. For example, it is more convenient to work with partitions of both variable structure or fixed structure in their dual spaces based on permutations with repetitions because the constraints of mutual exclusion, full covering and structure preserving are much easier to deal with in operators defined on this space. We have exploited this property in previous work on the graph partitioning problem [4]. On the other hand, it may be more convenient to work with sets of small size (small compared to the size of the universal set) rather than on their dual vectors of fixed size (all the same size of the universal set).

6 Conclusions

We have considered three related representations – sets, multisets and partitions – in their variable size and fixed size variants.

For the variable size case we have considered the ins/del edit distance, that for sets corresponds to the symmetric distance, and its extensions to the case of multi-sets and partitions, for which it becomes the move edit distance.

We have shown that the geometric crossovers associated to the ins/del edit distance for sets is a crossover that requires offspring to be supersets of the intersection of the two parent sets and subsets of their union. The geometric crossovers associated to the ins/del distance for multisets and partitions are simple extensions of the inter/union crossover for sets.

For the fixed size case we have considered the substitution edit distance, that is equivalent to the ins/del edit distance when restricted to set of fixed size. Therefore, geometric crossover under substitution edit distance is a restricted version of the inter/union crossover where all offspring are required to have fixed size. The geometric crossover associated to multisets and partitions for the fixed size case are analogous to the restricted inter/union crossover for sets.

We have proved a duality between geometric crossover for sets, multisets and partitions on the one hand, and binary strings, integer vectors, and permutations with repetitions on the other. Interestingly, this allows the interchangeable use of representations and operators, being equivalent in terms of search, but exploiting their differences in terms of expressing constraints.

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Table 1. Crossovers dual equivalence

	PRIMAL	DUAL
Representation:	Sets - variable size	Binary vectors
Map:	Indication function	
Distance:	Ins/del edit distance	Hamming distance
Crossover:	Inter/union crossover	Traditional crossover
Representation:	Sets - fixed size	Binary permutations with repetitions
Map:	Indication function	
Distance:	Substitution edit distance	Permutation swap edit distance
Crossover:	Inter/union crossover restricted to fixed size	Sorting crossover by swap
Representation:	Multisets - variable size	Integer vectors
Map:	Multiplicity function	
Distance:	Ins/del edit distance	Absolute value distance
Crossover:	Inter/union crossover	Integer blending crossover
Representation:	Multisets - fixed size	Integer distributions
Map:	Multiplicity function	
Distance:	Substitution edit distance	Absolute value distance
Crossover:	Inter/union crossover restricted to fixed size	Integer blending crossover restricted to constant sum
Representation:	Partitions - variable structure	Multary vectors
Map:	Partition label function	
Distance:	Partition move edit distance	Hamming distance
Crossover:	Partitionwise inter/union crossover restricted to mutual exclusion restricted to complete covering	Traditional crossover
Representation:	Partitions - fixed structure	Permutations with repetitions
Map:	Partition label function	
Distance:	Partition swap edit distance	Permutation swap edit distance
Crossover:	Partitionwise inter/union crossover restricted to mutual exclusion restricted to complete covering restricted to same structure	Sorting crossover by swaps
Representation:	n-partitions of set size n	Permutations
Map:	Partition label function	
Distance:	Partition swap edit distance	Permutation swap edit distance
Crossover:	Partitionwise inter/union crossover restricted to mutual exclusion restricted to complete covering restricted to single element subsets	Sorting crossover by swaps, PMX, Cycle crossover