Mathematical Interpretation between Genotype and Phenotype Spaces and Induced Geometric Crossovers

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March 10, 2009

Abstract

In this paper, we present that genotype-phenotype mapping can be theoretically interpreted using the concept of quotient space in mathematics. Quotient space can be considered as mathematically-defined phenotype space in the evolutionary computation theory. The quotient geometric crossover has the effect of reducing the search space actually searched by geometric crossover, and it introduces problem knowledge in the search by using a distance better tailored to the specific solution interpretation. Quotient geometric crossovers are directly applied to the genotype space but they have the effect of the crossovers performed on phenotype space. We give many example applications of the quotient geometric crossover.
Keywords: Geometric crossover, genotype-phenotype mapping, quotient metric space, quotient geometric crossover.

1   Introduction

In evolutionary computation, genotype means solution representation, which is the structure that can be stored in a computer and manipulated. Phenotype means solution itself without any reference to how it is represented. Sometimes it is possible to have a one-to-one mapping between genotypes and phenotypes, so the distinction between genotype and phenotype becomes purely formal. However, in many interesting cases, phenotypes cannot be represented uniquely by genotypes. So the same phenotype is represented by more than one genotype. In such case we say that we have a *redundant representation*. For example, to represent a graph we need to label its nodes and then we can represent it using its adjacency matrix. This representation is

redundant because the same graph can be represented with more than one adjacency matrix by relabeling its nodes.

There are quite a few problems in that it is hard to represent one phenotype by just one genotype using traditional representations. Roughly speaking, redundant representation leads to severe loss of search power in genetic algorithms, in particular, with respect to traditional crossovers [3]. To alleviate the problems caused by redundant representation, a number of methods such as adaptive crossover have been proposed [6, 16, 24, 31]. Among them, a technique called *normalization*[1] is representative. It transforms the genotype of a parent to another genotype to be consistent with the other parent so that the genotype contexts of the parents are as similar as possible in crossover. There have been a number of successful studies using normalization. An extensive survey about normalization is appeared in [4].

We recognized that genotype-phenotype mapping can be theoretically interpreted using the concept of quotient space in mathematics. In this paper, we formally present the general relation between the notion of quotient and genotype-phenotype mapping, and we study the relation between genotype and phenotype spaces and geometric crossovers on them.

For analysis, we adopted the concept of geometric crossover [20] because it is representation-independent and well-defined once a notion of distance in the search space is defined. In this study, we consider only genotype and phenotype spaces that are metric spaces. So the metric for a space is considered as the most important characteristic of its structure. This approach enables to deal with the problem spaces more mathematically.

The remainder of the paper is organized as follows. In Section 2, we preliminarily present some necessary mathematical notions and the geometric framework. In Section 3, the new notion of quotient geometric crossover is introduced in connection with genotype-phenotype mapping. In Section 4, we study several useful examples. In Section 4.1 and 4.2, we show how previous work on groupings [14] and graphs can be recast and understood more simply in terms of quotient geometric crossover. In such problems, quotient geometric crossover has the effect of filtering out inherent redundancy in the solution representation. In Section 4.3, we consider symmetric functions and their problem spaces. The usage of the quotient geometric crossover for circular permutation encodings is discussed in Section 4.4. In Section 4.5, we show how homologous crossover for variable-length sequences [23] can be understood as a quotient geometric crossover. Finally we give our conclusions in Section 5.

2 Preliminaries

2.1 Mathematical Notions

In the following, we give some known mathematical definitions required to present our idea.

Given a set X and an equivalence relation $\sim$ on X, the equivalence class of an element a in X is the subset of all elements in X that are equivalent to a:

$$\bar{a} = \{x \in X : a \sim x\}.$$

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[1]The term of *normalization* is firstly appeared in [11]. However, it is based on the adaptive crossovers proposed in [16, 24].

The set of all equivalence classes in X given an equivalence relation $\sim$ is usually denoted by $X/\sim$ and called the quotient set of X by $\sim$. This operation can be thought (very informally) as the act of "dividing" the input set by the equivalence relation. The quotient set is considered as the set with all the equivalent points identified as a point.

Next, *group* [8] is introduced. A group is an algebraic structure consisting of a set together with an operation that combines any two of its elements to form a third element. To qualify as a group, the set and operation must satisfy a few conditions called group axioms, namely associativity, identity, and invertibility. Formally it is defined as follows:

Definition 1 (Group). *A group $(\mathcal{G}, *)$ is a set $\mathcal{G}$ closed under a binary operation $*$, such that the following axioms are satisfied:*
(i) Associativity: for all $a, b, c \in G$, we have

$$(a * b) * c = a * (b * c).$$

(ii) Identity: there is an element e in G such that for all $x \in G$,

$$e * x = x * e = x.$$

(iii) Invertibility: for each $a \in G$, there is an element a^{-1} in G such that

$$a * a^{-1} = a^{-1} * a = e.$$

In this paper, we will use groups for constructing equivalence relations with *good* properties.

In the following, we view the problem spaces as metric spaces. It is a reasonable assumption because the general solution spaces usually have metrics. For example, binary space has the Hamming distance and real space has Minkowski distances including the Euclidean distance. Formally, the term *metric* - or *distance* - denotes any real-valued function that conforms to the axioms of identity, symmetry, and triangular inequality. Now, we introduce an isometry on a metric space.

Definition 2 (Isometry). *Let (X, d) be a metric space. If $f\colon X \to X$ satisfies the condition*

$$d(f(x), f(y)) = d(x, y)$$

for all $x, y \in X$, then f is called an isometry *of X.*

The set of isometries on X is denoted by $Iso(X)$. $Iso(X)$ forms a group under function composition operator. In our study, an isometry subgroup $\mathcal{G} \subseteq Iso(X)$ will be considered to generate an equivalence relation for quotient metric space.

2.2 Geometric Preliminaries

In this subsection we provide some geometric definitions, which extend those introduced in [18, 19]. The following definitions are taken from [5].

In a metric space (X, d), a *line segment* (or closed interval) is the set of the form $[x; y]_d = \{z \in X \mid d(x, z) + d(z, y) = d(x, y)\}$, where $x, y \in X$ are called extremes of the segment. Metric

segment generalizes the familiar notions of segment in the Euclidean space to any metric space through distance redefinition. Notice that a metric segment does not coincide to a 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 X by endowing it with a notion of distance d. $M = (X, d)$ is therefore a solution *space* and (M, f) is the corresponding fitness landscape, where f is the fitness function over X.

2.3 Geometric Crossover

Geometric crossover is a representation-independent search operator that generalizes many pre-existing search operators for the major representations used in evolutionary algorithms, such as binary strings [18], real vectors [18, 33], permutations [20], permutations with repetition [17], syntactic trees [19], sequences [23], and sets [21]. It is 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 [10] 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.

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

Definition 3 (Image set). *The* image set $Im[OP]$ *of a genetic operator OP is the set of all possible offspring produced by OP.*

Definition 4 (Geometric crossover). *A binary operator GX is a* geometric crossover *under the metric d if all offspring are in the segment between its parents x and y, i.e.,*

$$Im[GX(x, y)] \subseteq [x; y]_d.$$

A number of general properties for geometric crossover have been derived in [18] where it was also shown that traditional mask-based crossovers are geometric under the Hamming distance. Moraglio and Poli also studied various crossovers for permutations, revealing that PMX (partially matched crossover) [9], a well-known crossover for permutations, is geometric under swap distance. Also, they found that cycle crossover [25], another traditional crossover for permutations, is geometric under swap distance and under the Hamming distance.

Theoretical results of metric spaces can naturally lead to interesting results for geometric crossover. In particular, Moraglio and Poli showed that the notion of *metric transformation* has great potential for geometric crossover in [22]. A metric transformation is an operator that constructs new metric spaces from pre-existing metric spaces: it takes one or more metric spaces as input and outputs a new metric space. The notion of metric transformation becomes extremely interesting when considered together with distances firmly rooted in the syntactic structure of the underlying solution representation (e.g., edit distance). In these cases it gives rise to a simple and *natural interpretation in terms of syntactic transformations*.

Moraglio and Poli extended the geometric framework introducing the notion of product crossover associated with the Cartesian product of metric spaces in [22]. This is a very important tool that allows one to build new geometric crossovers customized to problems with mixed representations by combining pre-existing geometric crossovers in a straightforward way. Using the product geometric crossover, they also showed that traditional crossovers for symbolic vectors and blend crossovers for integer and real vectors are geometric crossover.

3 Quotient Geometric Crossover

3.1 Motivation

Geometric operators are defined as functions of the distance associated to the search space. However, the search space does not come with the problem itself. The problem consists only of a fitness function to optimize, that defines what a solution is and how to evaluate it, but it does not give any structure on the solution set. The act of putting a structure over the solution set is a part of the search algorithm design and it is a designer's choice.

A fitness landscape is the fitness function plus a structure over the solution space. So, for each problem, there is one fitness function but as many fitness landscapes as the number of possible different structures over the solution set. In principle, the designer can choose the structure to assign to the solution set completely independently from the problem at hand. However, because the search operators are defined over such a structure, doing so would make them decoupled from the problem at hand, hence turning the search into something very close to random search.

To avoid such problem, one can exploit problem knowledge in the search. It can be achieved by carefully designing the connectivity structure of the fitness landscape. For example, one can study the objective function of the problem and select a neighborhood structure that couples the distance between solutions and their fitness values. Once it is done, problem knowledge can be exploited by search operators to perform better than random search, even if the search operators are problem-independent (as is the case of geometric operators). Indeed, the fitness landscape is a knowledge interface between the problem at hand and a formal, problem-independent search algorithm.

Under which conditions is a landscape well-searchable by geometric operators? As a rule of thumb, geometric crossover works well on landscapes where the closer pairs of solutions, the more correlated their fitness values. Of course this is no surprise: the importance of landscape smoothness has been advocated in many different contexts and has been confirmed in uncountable empirical studies with many neighborhood search meta-heuristics [27]. We operate according to the following rules-of-thumb:

Rule-of-thumb 1: if we have a good distance for the problem at hand, then we have a good geometric crossover.

Rule-of-thumb 2: a good distance for the problem at hand is a distance that makes the landscape "smooth."
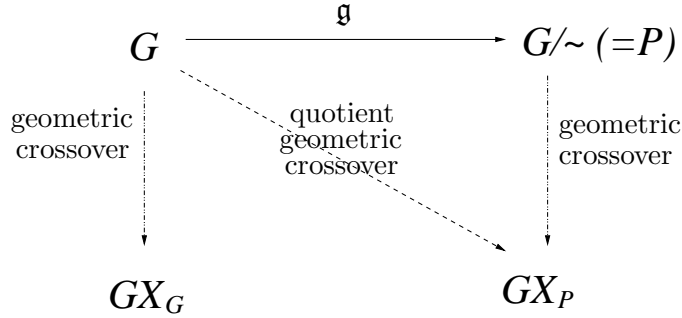
$$G \xrightarrow{\quad \mathfrak{g} \quad} G/\!\sim (=P)$$

geometric crossover   quotient geometric crossover   geometric crossover

$$GX_G \qquad\qquad GX_P$$

Figure 1: Diagram linking genotype, phenotype spaces, and geometric crossovers

3.2 Genotype-Phenotype Mapping

We formally present the general relation between the notion of quotient and genotype-phenotype mapping. Let G and P be genotype space and phenotype one, respectively. Consider a genotype-phenotype mapping $\mathfrak{g}\colon G \to P$ that are not injective (i.e., redundant representation). The mapping $\mathfrak{g}$ induces a natural equivalence relation $\sim$ on the set of genotypes: *genotypes with the same phenotype belong to the same class.* Then the phenotype space P becomes exactly a quotient space $G/\!\sim$ of the genotype space G.

The advantage of geometric crossover is that we can formally define a geometric crossover under the distance once a distance is defined. Then what if the quotient space $G/\!\sim$ has a distance d_P induced by the distance d_G of G? If so, the geometric crossover under d_P would be a natural crossover since it reflects the structure of the genotype space G by involving the distance d_G of G.

By applying the formal definition of geometric crossover to the metric spaces (G, d_G) and (P, d_P), we obtain the geometric crossovers GX_G and GX_P, respectively. GX_G searches the space of genotypes and GX_P searches that of phenotypes. Searching the space of phenotypes has a number of advantages: (i) it is smaller than the space of genotypes, hence quicker to search (ii) the phenotypic distance is better tailored to the underlying problem, hence the corresponding geometric crossover works better (iii) the space of phenotypes has different geometric characteristics from the genotypic space. It can be used to remove unwanted bias from geometric crossover.

However, the crossover GX_P cannot be directly implemented because it recombines phenotypes that are objects that cannot be directly represented. So, we propose a notion of quotient geometric crossover to search the space of phenotypes with the crossover GX_P *indirectly* by manipulating the genotypes G. The relationship among G, P, and their geometric crossovers is illustrated through a diagram in Figure 1.

In the next subsection we present more formally the concept of quotient metric space and quotient geometric crossover in relation with genotype-phenotype mapping.

3.3 Quotient Metric Space

Let (X, d) be a metric space and $(\mathcal{G}, \cdot) \subseteq Iso(X)$ be a subgroup of the isometry group, where $\cdot$ means the function composition operator. We introduce a relation $\sim_{\mathcal{G}}$: x and y in X are equivalent if and only if $x = g(y)$ for some $g \in \mathcal{G}$. Then $\sim_{\mathcal{G}}$ is an equivalence relation by the following proposition.

Proposition 1. *Relation $\sim_{\mathcal{G}}$ is an equivalence relation.*

Proof. Assume that x, y, and $z \in X$.
(i) Reflexivity: (Since $\mathcal{G}$ is a group, identity map e is in $\mathcal{G}$.) Since $x = e(x)$, $x \sim_{\mathcal{G}} x$.
(ii) Symmetry: Suppose that $x \sim_G y$, i.e., $x = g(y)$ for some $g \in G$. There exists $g^{-1} \in G$ since G is a group. Then, $y = g^{-1}(x)$. So $y \sim_G x$.
(iii) Transitivity: Suppose that $x \sim_G y$ and $y \sim_G z$. $x = g(y)$ and $y = h(z)$ for some g and $h \in G$. Then $x = g(y) = g(h(z)) = (g \cdot h)(z)$. $g \cdot h$ is in G since G is a group. Hence, $x \sim_{\mathcal{G}} z$. □

For $x \in X$, equivalence class $\bar{x}$ can be written as $\bar{x} = \{g(x) : g \in \mathcal{G}\}$. Now we will give a metric on $X/\sim_G$ (usually denoted by just $X/\mathcal{G}$) induced by the original metric d on X.

Definition 5 (Quotient metric). *Quotient metric $\bar{d}(\bar{x}, \bar{y})$ is defined as $\min\{d(x', y') : x' \in \bar{x}, y' \in \bar{y}\}$.*

It is shown that $\bar{d}$ is actually a metric on $X/\mathcal{G}$ in the following proposition.

Proposition 2. *$(X/G, \bar{d})$ is a metric space, i.e., $\bar{d}$ is a metric in X/G.*

Proof. Assume that x, y, and $z \in X$.
(i) Identity: $0 \leq \bar{d}(\bar{x}, \bar{x}) \leq d(x, x) = 0$.
(ii) Symmetry: There exist $x_1 \in \bar{x}$ and $y_1 \in \bar{y}$ such that $\bar{d}(\bar{x}, \bar{y}) = d(x_1, y_1)$. Then, $\bar{d}(\bar{x}, \bar{y}) = d(x_1, y_1) = d(y_1, x_1) \geq \bar{d}(\bar{y}, \bar{x})$. Similarly, $\bar{d}(\bar{y}, \bar{x}) \geq \bar{d}(\bar{x}, \bar{y})$. Hence, $\bar{d}(\bar{x}, \bar{y}) = d(x_1, y_1)$.
(iii) Triangular inequality: There exist $x_1 \in \bar{x}$ and $y_1 \in \bar{y}$ such that $\bar{d}(\bar{x}, \bar{y}) = d(x_1, y_1)$. Also, There exist $y_2 \in \bar{y}$ and $z_2 \in \bar{z}$ such that $\bar{d}(\bar{y}, \bar{z}) = d(y_2, z_2)$. Since y_1 and y_2 belong to the same equivalence class, there exists $g \in G$ such that $y_1 = g(y_2)$. Then,

$$
\begin{aligned}
& \bar{d}(\bar{x}, \bar{y}) + \bar{d}(\bar{y}, \bar{z}) \\
= {} & d(x_1, y_1) + d(y_2, z_2)) \\
= {} & d(x_1, g(y_2)) + d(y_2, z_2) \\
= {} & d(x_1, g(y_2)) + d(g(y_2), g(z_2)) \quad (\because g \in Iso(X).) \\
\geq {} & d(x_1, g(z_2)) \quad (\because d \text{ is a metric in } X.) \\
\geq {} & \bar{d}(\bar{x}, \bar{z}). \quad (\because z_2 \sim_{\mathcal{G}} g(z_2).)
\end{aligned}
$$

□

The following proposition gives a simpler definition of quotient metric $\bar{d}$.

Proposition 3. *If we let $\tilde{d}(\bar{x}, \bar{y}) := \min\{d(x, y') : y' \in \bar{y}\}$, $\tilde{d}(\bar{x}, \bar{y}) = \bar{d}(\bar{x}, \bar{y})$.*

Proof. Let $\bar{x}, \bar{y} \in X/G$. It is clear that $\tilde{d}(\bar{x}, \bar{y}) \geq \bar{d}(\bar{x}, \bar{y})$ by the definition. Now we will show that $\tilde{d}(\bar{x}, \bar{y}) \leq \bar{d}(\bar{x}, \bar{y})$. Suppose that $\bar{d}(\bar{x}, \bar{y}) = d(x_1, y_1)$. Since x and x_1 belong to the same equivalence class, there exists $g \in G$ such that $x = g(x_1)$. Since g is an isometry, $d(x_1, y_1) = d(g(x_1), g(y_1)) = d(x, g(y_1))$. $g(y_1) \sim_G y_1 \sim_G y$. So $\tilde{d}(\bar{x}, \bar{y}) \leq d(x_1, y_1) = \bar{d}(\bar{x}, \bar{y})$. $\qquad\square$

This metric space $(X/\mathcal{G}, \bar{d})$ is called *quotient metric space*. Quotient space conceptually corresponds to the phenotype space. The line segment and the geometric crossover in the quotient metric space are defined in the same way as in other metric spaces. However, since in general cases solutions are represented only in the genotype space, we need to define line segments and crossovers on (X, d), not on $(X/\mathcal{G}, \bar{d})$, to practically apply the concept.

In a metric space (X, d), a *quotient line segment* is the set of the form $[x;y]_{\bar{d}} = \{z \in X \mid \bar{d}(\bar{x}, \bar{z}) + \bar{d}(\bar{z}, \bar{y}) = \bar{d}(\bar{x}, \bar{y}), \bar{z} \in X/G\}$, where $\bar{x}, \bar{y} \in X/G$.

Proposition 4. *If $\bar{d}(\bar{x}, \bar{y}) = d(x, y^*)$, $[x;y^*]_d \subseteq [x;y]_{\bar{d}}$.*

Proof. Let $z \in [x;y^*]_d$. Then, $\bar{d}(\bar{x}, \bar{z}) + \bar{d}(\bar{z}, \bar{y}) \leq d(x, z) + d(z, y^*) = d(x, y^*) = \bar{d}(\bar{x}, \bar{y})$. Since $\bar{d}(\bar{x}, \bar{z}) + \bar{d}(\bar{z}, \bar{y}) \geq \bar{d}(\bar{x}, \bar{y})$ by the property of triangular property, $\bar{d}(\bar{x}, \bar{z}) + \bar{d}(\bar{z}, \bar{y}) = \bar{d}(\bar{x}, \bar{y})$. So, $z \in [x;y]_{\bar{d}}$. $\qquad\square$

Now we can define the *quotient geometric crossover*.

Definition 6 (Quotient geometric crossover). *A binary operator GX_q is a quotient geometric crossover under the metric d and the equivalence relation $\sim_G$ if all offspring are in the quotient line segment between its parents x and y, i.e., $GX_q(x, y) \subseteq [x;y]_{\bar{d}}$.*

In the following we define the *induced quotient crossover*, which is a kind of quotient geometric crossovers. This crossover is defined using the original geometric crossover under the original distance d. This crossover is not only concrete but also easily implemented while the quotient geometric crossover is conceptual.

Definition 7 (Induced quotient crossover). *First, find y^* in the equivalence class $\bar{y}$ of the second parent y such that $\bar{d}(\bar{x}, \bar{y}) = d(x, y^*)$. Then, do the geometric crossover on X using the first parent x and the normalized second parent y^*.*

Corollary 1. *Induced quotient crossover is a quotient geometric crossover.*

Proof. Let $y^* \in \bar{y}$ be a normalized second parent i.e., $\bar{d}(\bar{x}, \bar{y}) = d(x, y^*)$. Then, $[x;y^*]_d \subseteq [x;y]_{\bar{d}}$ by Proposition 4. This satisfies the definition of quotient geometric crossover. $\qquad\square$

Induced quotient crossover can be a bridge between the original geometric crossover and the quotient geometric crossover. We can redraw Figure 1 including the induced quotient crossover. It is shown in Figure 2.

In the next section, we consider a number of equivalence classes for the quotient operation and its related induced genotypic crossover transformation.
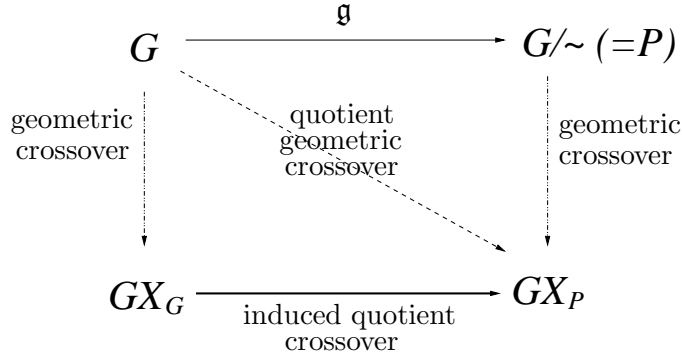
Figure 2: Diagram linking genotype, phenotype spaces, and crossovers including induced quotient crossover

4 Examples

In this section, we introduce examples of quotient geometric crossovers. In some examples (groupings in Subsection 4.1 and sequences in Subsection 4.5), previously proposed crossovers are reinterpreted as quotient geometric crossovers. In other examples, we introduce new crossovers consistent with genotype-phenotype mapping of given problems using the concept of quotient geometric crossover.

4.1 Groupings

Grouping problems [7] are commonly concerned with partitioning given item set into mutually disjoint subsets. Examples belonging to this class of problems are multiway graph partitioning, graph coloring, bin packing, and so on. Grouping representation is also used to solve the joint replenishment problem, which is a well-known problem appeared in the field of industrial engineering [26]. In this class of problems, the normalization decreased the problem difficulty and led to notable improvement in performance.

Most normalization studies for grouping problems were focused on the k-way partitioning problem. In the problem, the k-ary representation, in which k subsets are represented by the integers from 0 to $k-1$, has been generally used. In this case, one phenotype (a k-way partition) is represented by $k!$ different genotypes. In the problem, a normalization method was used in [11]. Other studies for the k-way partitioning problem used the same technique [3, 12]. In the sense that normalization pursues the minimization of genotype inconsistency among chromosomes, in [13], Kim and Moon proposed an optimal, efficient normalization method for grouping problems and a distance measure, the *labeling-independent distance*, that eliminates such dependency completely.

Now we reinterpret the previous work in terms of quotient space. Let $a, b \in X = \{1, 2, \ldots, k\}^n$ be k-ary encodings (fixed-length vectors on a k-ary alphabet) and Σ_k be a set of all permutations of length k. For each $\sigma \in \Sigma_k$, we can view σ as a function on X by defining $\sigma(a)$ be a permuted encoding of a by a permutation σ. For example, in the case that $a = (1, 2, 3, 3, 2, 4, 1, 4)$ is a 4-ary encoding and $\sigma = \left(\begin{smallmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 3 & 1 \end{smallmatrix}\right) \in \Sigma_4$, $\sigma(a) = (2, 4, 3, 3, 4, 1, 2, 1)$.

$$X = \{1, 2, 3\}^4$$

$$x = (1, 2, 3, 1), y = (2, 1, 2, 3) \in X$$

Σ_k	$\bar{y}$	$H(x, \sigma(y))$
$\sigma_1 = (1, 2, 3)$	$\sigma_1(y) = (2, 1, 2, 3)$	$H(x, \sigma_1(y)) = 4$
$\sigma_2 = (1, 3, 2)$	$\sigma_2(y) = (3, 1, 3, 2)$	$H(x, \sigma_2(y)) = 3$
$\sigma_3 = (2, 1, 3)$	$\sigma_3(y) = (1, 2, 1, 3)$	$H(x, \sigma_3(y)) = 2$
$\sigma_4 = (2, 3, 1)$	$\sigma_4(y) = (3, 2, 3, 1)$	$H(x, \sigma_4(y)) = 1$
$\sigma_5 = (3, 1, 2)$	$\sigma_5(y) = (1, 3, 1, 2)$	$H(x, \sigma_5(y)) = 3$
$\sigma_6 = (3, 2, 1)$	$\sigma_6(y) = (2, 3, 2, 1)$	$H(x, \sigma_6(y)) = 3$

$$y^* = \sigma_4(y) = (3, 2, 3, 1)$$

$$\bar{d}(\bar{x}, \bar{y}) = 1$$

Figure 3: An example of grouping

It is well known that permutations form a group. Hence, Σ_k is a group. Moreover, when we use the Hamming distance H on X, it is easy to check that each $\sigma \in \Sigma_k$ is an isometry. So $\sim_{\Sigma_k}$ becomes an equivalence relation and the quotient metric in Definition 5 is well defined by Proposition 2. The quotient metric was introduced as labeling-independent distance in [13]. In the context of this study, it is rewritten as follows:

$$\bar{d}(\bar{a}, \bar{b}) := \min_{\sigma \in \Sigma_k} H(a, \sigma(b)).$$

An example case is shown in Figure 3.

The definition of labeling-independent crossover presented in [14] is in the following.

Definition 8 (Labeling-independent crossover)**.** *Normalize the second parent to the first under the Hamming distance. Then, do the normal crossover using the first parent and the normalized second parent.*

This crossover is exactly the induced quotient crossover. For the process of normalization, it is possible to enumerate all $k!$ permutations and find an optimal one among them. However, for a large k, such a procedure is intractable. Fortunately, it can be done in $O(k^3)$ time using the *Hungarian method* proposed by Kuhn [15].

In summary, we have the following.

Example	Groupings
Genotype space X	$\{1, 2, \ldots, k\}^n$
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	Σ_k: a set of all permutations of length k
Metric d on X	Hamming distance H
Original geometric crossover	traditional crossover for vectors
Induced quotient crossover	Labeling-independent crossover in [14]

From understanding normalization for grouping problems in terms of quotient geometric crossover, we can understand the benefit of normalization in terms of landscape analysis. We have already done this in our previous work [17].

4.2 Graphs

In this subsection, we consider any problem naturally defined over a graph in which the fitness of the solution does not depend on the labels on the nodes but only on the structural relationship, i.e., edge between nodes.

Formally, let $A \in \mathfrak{M}_n$ be the adjacency matrix of a labeled graph using labels of n nodes and let $\mathcal{P}_n$ be a set of all $n \times n$ permutation matrices[2]. Then, for each permutation matrix $P \in \mathcal{P}_n$, the matrix PAP^T means the labeled graph obtained by relabeling A according to the permutation represented by P. The fitness $f : \mathfrak{M}_n \to \mathbb{R}$ satisfies that for every $A \in \mathfrak{M}_n$ and every permutation matrix P, $f(A) = f(PAP^T)$.

Let $(\mathfrak{M}_n, H)$ be a metric space on the labeled graphs under the Hamming distance H. Notice that this metric is labeling-dependent. In particular, $H(A, PAP^T)$ may not be zero although A and PAP^T represent the same structure. If A is equal to PBP^T for some permutation matrix P, we define A and B to be in relation $\sim_{\mathcal{P}_n}$, i.e., $A \sim_{\mathcal{P}_n} B$. Since a set of permutation matrices $\mathcal{P}_n$ forms a group, the relation $\sim_{\mathcal{P}_n}$ is an equivalence relation by Proposition 1.

The equivalence class $\bar{A}$ is represented as follows:

$$\bar{A} := \{PA : P \in \mathcal{P}_n\}.$$

It corresponds to an *unlabeled graph* and the quotient space $\mathfrak{M}_n/\mathcal{P}_n$ can be understood as *unlabeled-graph space*. $\mathfrak{M}_n/\mathcal{P}_n$ is a quotient metric space by Proposition 2. So we obtain induced quotient metric on $\mathfrak{M}_n/\mathcal{P}_n$. It can be written as follows:

$$\bar{d}(\bar{A}, \bar{B}) = \min_{P \in \mathcal{P}_n} H(A, PB).$$

An example for graphs is shown in Figure 4.

Now we design induced quotient crossover. In this example, the process of finding the normalized second parent y^* can be understood as graph matching in terms of graphs which are not adjacency matrices.
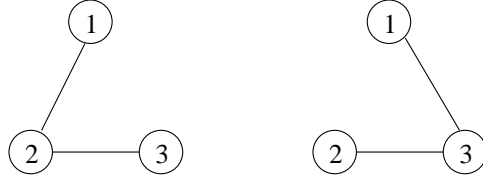
Definition 9 (Induced quotient crossover for graphs)**.** *Do the graph matching of the second parent B to the first A under the Hamming distance H, i.e.,*

$$B^* := \underset{B' \in \bar{B}}{\operatorname{argmin}} H(A, B').$$

---

[2] Permutation matrix is a $(0, 1)$-matrix with exactly one 1 in every row and column.

$$X = \mathfrak{M}_3$$

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, B = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \in X$$

$\mathcal{P}_3$		$\bar{B}$		$H(A, PBP^T)$
$P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$		$P_1 B P_1^T = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$		$H(A, P_1 B P_1^T) = 4$
$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$		$P_2 B P_2^T = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$		$H(A, P_2 B P_2^T) = 0$
$P_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$		$P_3 B P_3^T = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$		$H(A, P_3 B P_3^T) = 4$
$P_4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$		$P_4 B P_4^T = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$		$H(A, P_4 B P_4^T) = 0$
$P_5 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$		$P_5 B P_5^T = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$		$H(A, P_5 B P_5^T) = 4$
$P_6 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$		$P_6 B P_6^T = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$		$H(A, P_6 B P_6^T) = 4$

$$B^* = P_2 B P_2^T \text{ or } P_4 B P_4^T$$

$$\bar{d}(\bar{A}, \bar{B}) = 0$$

Figure 4: An example of graph

Then, do the normal crossover using the first parent A and the graph-matched second parent B^*.

The induced quotient crossover is defined over unlabeled graphs $\mathfrak{M}_n/\mathcal{P}_n$. This space is much smaller than labeled graphs $\mathfrak{M}_n$. More precisely, $|\mathfrak{M}_n/\mathcal{P}_n| = |\mathfrak{M}_n|/n!$. This means that the more the labels are, the smaller the unlabeled-graph space is when compared with the labeled-graph space. Smaller space means better performance, given the same amount of evaluations.

Now we tell how to guide the implementation using graph matching for specific geometric crossovers. To implement the geometric crossover over unlabeled graphs, we need to use labeled graphs. The labeling results are necessary to represent and handle the solution, even if in fact it is only an auxiliary function and can be considered as not being part of the problem to solve. Graph matching before crossover allows to implement the geometric crossover on the unlabeled-graph space. We use the corresponding geometric crossover over the auxiliary space of the labeled graph after graph matching.

Example	Graphs
Genotype space X	$\mathfrak{M}_n$ (the set of all $n \times n$ adjacency matrices)
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	$\mathcal{P}_n$: a set of all $n \times n$ permutation matrices
Metric d on X	Hamming distance H
Original geometric crossover	traditional crossover on adjacency matrices seen as length-n^2 vectors
Induced quotient crossover	graph matching before traditional crossover (newly introduced in this study)

By applying the quotient geometric crossover on graphs, we can design a crossover better tailored to graphs. The notion of graph matching before crossover arises directly from the definition of quotient geometric crossover. Graphs are very important because they are ubiquitous. In future work we will test this crossover on some applications. Graphs and groupings can be seen as particular cases of labeled structures in which the fitness of a solution depends only on the structure and not on the specific labeling. In future work we will also study the class of labeled structures in combination with quotient geometric crossover.

4.3   Symmetric Functions

A symmetric function on n variables $x_1, x_2, \ldots, x_n$ is a function that is unchanged by any permutation of its variables. That is , if $f(x_1, x_2, \ldots, x_n) = f(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(n)})$ for any permutation σ, the function f is called symmetric function. In this subsection, we consider problems of which fitness function is symmetric. Some evolutionary studies have been made on such problems [28, 32]. More properties about specific symmetric functions are introduced in [2, 30].

Solutions for symmetric functions are typically represented as n-dimensional vectors, i.e., length-n strings. Let X be the solution space (or domain) of given symmetric function and Σ_n be a set of all permutations of length n. Similarly to the example of grouping in Section 4.1, $\sigma \in \Sigma_n$ can be understood as a function. For example, in the case that $x = (x_1, x_2, x_3, x_4)$ and

$$X = \mathbb{R}^3$$

$$x = (1, 4, 5), y = (3, 0, 6) \in X$$

Σ_3	$\bar{y}$	$H(x, \sigma(y))$
$\sigma_1 = (1, 2, 3)$	$\sigma_1(y) = (3, 0, 6)$	$E(x, \sigma_1(y)) = \sqrt{21}$
$\sigma_2 = (1, 3, 2)$	$\sigma_2(y) = (3, 6, 0)$	$E(x, \sigma_2(y)) = \sqrt{33}$
$\sigma_3 = (2, 1, 3)$	$\sigma_3(y) = (0, 3, 6)$	$E(x, \sigma_3(y)) = \sqrt{3}$
$\sigma_4 = (2, 3, 1)$	$\sigma_4(y) = (0, 6, 3)$	$E(x, \sigma_4(y)) = 3$
$\sigma_5 = (3, 1, 2)$	$\sigma_5(y) = (6, 3, 0)$	$E(x, \sigma_5(y)) = \sqrt{51}$
$\sigma_6 = (3, 2, 1)$	$\sigma_6(y) = (6, 0, 3)$	$E(x, \sigma_6(y)) = 3\sqrt{5}$

$$y^* = \sigma_3(y) = (0, 3, 6)$$

$$\bar{d}(\bar{x}, \bar{y}) = \sqrt{3}$$

Figure 5: An example of symmetric function under the Euclidean distance

$\sigma = \left(\begin{smallmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 3 & 1 \end{smallmatrix} \right) \in \Sigma_4$, $g_\sigma(x) = (x_2, x_4, x_3, x_1)$. As mentioned in Section 4.1, Σ_n is a group and each σ is an isometry.

If X is a real space, we can use the Euclidean distance E. In that case, induced quotient metric on $X/\mathcal{G}$ is defined as follows:

$$\bar{d}(\bar{x}, \bar{y}) := \min_{\sigma \in \Sigma_n} E(x, \sigma(y))$$

Figure 5 will be helpful to understand the quotient metric space for this case.

Induced quotient crossover can also be defined as in Definition 7. Because it uses permutation, it can be performed in $O(n^3)$ time by the Hungarian method similarly to groupings.

Summary for this Euclidean case is as follows:

Example	Symmetric functions on real space
Genotype space X	$\mathbb{R}^n$
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	Σ_n: a set of all permutations of length n
Metric d on X	Euclidean distance E
Original geometric crossover	traditional crossover on real vectors
Induced quotient crossover	rearranging before traditional crossover (newly proposed in this study)

On the other hand, if X is a discrete space as in binary or k-ary encoding, we can use the Hamming distance. Then, induced quotient metric on $X/\mathcal{G}$ is defined as follows:

$$\bar{d}(\bar{x}, \bar{y}) := \min_{\sigma \in \Sigma_n} H(x, \sigma(y))$$

Induced quotient crossover for this case can also be performed in $O(n^3)$ time by the Hungarian method. In sum, we have:

Example	Symmetric functions on discrete space
Genotype space X	$\{0,1\}^n$
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	Σ_n: a set of all permutations of length n
Metric d on X	Hamming distance H
Original geometric crossover	traditional crossover on binary or k-ary vectors
Induced quotient crossover	rearranging before traditional crossover (newly proposed in this study)

4.4 Circular Permutations

Here we consider the case that solutions of a problem are represented as circular permutations such as traveling salesman problem (TSP). Gluing head and tail of the permutation obtains a circular permutation. Circular permutations cannot be represented directly. They are typically represented with simple permutations. Then each circular permutation is represented by more than one permutation. For example, permutations $(1,2,3)$, $(2,3,1)$, and $(3,1,2)$ represent the same phenotype, i.e., circular permutation. In such problem, the genotype space is a set of permutations and the phenotype space is a set of circular permutations. We can consider this problem in view of genotype-phenotype mapping using the concept of quotient space.

Let Σ_n be a set of all permutations with length n. A function $s_k : \Sigma_n \to \Sigma_n$ is defined by k-step circular shift operation to right. For example, $s_2(1,2,3) = (2,3,1)$. A set of all shift operations $S_n = \{s_k : k = 0, 1, 2, \ldots, n-1\}$ is a group. And it is easy to check that each s_k is an isometry on Σ_n. If Σ_n has a metric, Σ_n/S has an induced quotient metric by Proposition 2.

Now we consider various distances for permutation encoding. The most typical distance is the Hamming distance H. Under the Hamming distance, it is known that cycle crossover is geometric [19]. In this case, quotient metric is defined as follows:

$$\bar{d}(\bar{x}, \bar{y}) := \min_{s \in S_n} H(x, s(y)).$$

An example case is shown in Figure 6.

Then we can define induced quotient crossover.

Definition 10 (Position-independent cycle crossover)**.** *Normalize the second parent to the first under the Hamming distance H. Then, do the cycle crossover using the first parent and the normalized second parent.*

Normalizing the second parent takes $O(n)$ time because the equivalence class of the second parent has exactly n elements by shift operations.

Cycle crossover is also geometric under the swap distance. The induced quotient crossover can be defined in a similar way using the swap distance instead of the Hamming distance. Summary for the case of applying the cycle crossover is as follows:

$$X = \Sigma_6$$

$$x = (2, 4, 5, 1, 6, 3), y = (4, 6, 1, 5, 3, 2) \in X$$

S_6	$\bar{y}$	$H(x, s(y))$
s_0	$s_0(y) = (4, 6, 1, 5, 3, 2)$	$H(x, s_0(y)) = 6$
s_1	$s_1(y) = (2, 4, 6, 1, 5, 3)$	$H(x, s_1(y)) = 2$
s_2	$s_2(y) = (3, 2, 4, 6, 1, 5)$	$H(x, s_2(y)) = 6$
s_3	$s_3(y) = (5, 3, 2, 4, 6, 1)$	$H(x, s_3(y)) = 5$
s_4	$s_4(y) = (1, 5, 3, 2, 4, 6)$	$H(x, s_4(y)) = 6$
s_5	$s_5(y) = (6, 1, 5, 3, 2, 4)$	$H(x, s_5(y)) = 5$

$$y^* = s_1(y) = (2, 4, 6, 1, 5, 3)$$

$$\bar{d}(\bar{x}, \bar{y}) = 2$$

Figure 6: An Example of circular permutation under the Hamming distance

Example	circular permutations
Genotype space X	Σ_n
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	S_n: a set of all shift operations
Metric d on X	Hamming distance H (or swap distance)
Original geometric crossover	cycle crossover
Induced quotient crossover	rearranging before cycle crossover (newly proposed in this study)

On the other hand, we can use another well-known distance for Σ_n - *reversal distance*. Its neighborhood structure is the one based on the 2-opt move. The reversal move selects any two points along the permutation then reverses the subsequence between these points. This move induces a graphic distance between circular permutations: the minimum number of reversals to transform one circular permutation into the other. The geometric crossover associated with this distance belongs to the family of sorting crossovers [19]: it picks offspring on the minimum sorting trajectory between parent circular permutations sorted by reversals.

Definition 11 (Position-independent sorting-by-reversals crossover). *Normalize the second parent to the first under the graphic distance. Then, do the crossover based on sorting by reversals for permutation using the first parent and the normalized second parent.*

Example	circular permutations
Genotype space X	Σ_n
Isometry group $\mathcal{G}$ inducing phenotype space $X/\mathcal{G}$	S_n: a set of all shift operations
Metric d on X	reversal distance
Original geometric crossover	sorting-by-reversals crossover for permutations [19]
Induced quotient crossover	sorting-by-reversals crossover for circular permutation [19]

There is a problem in implementing the geometric crossover under the reversal distance. Sorting linear or circular permutations by reversals is NP-hard [1, 29]. So, the geometric crossover under the reversal distance cannot be implemented efficiently. Nevertheless, this example of quotient geometric crossover illustrates how to obtain a geometric crossover for a transformed representation (circular permutation) starting from a geometric crossover for the original representation (permutation). So in this case quotient geometric crossover is used as a tool to build a new crossover for a derivative representation from a known geometric crossover for the original representation. From [19], we know that the sorting-by-reversals crossover for permutations is an excellent crossover for TSP. In future work we want to test the sorting-by-reversals crossover for circular permutations. Since they are a direct representation, we expect it to perform even better.

4.5 Sequences

An application in this subsection is not exactly fitted to a quotient framework by the isometry subgroup like applications introduced earlier. However, we present this application because it follows the quotient approach except that the equivalence relation is not from an isometry subgroup.

We recast alignment before recombination in variable-length sequences as a consequence of quotient geometric crossover. Consider the case that we use *stretched* sequences as genotypes of sequences. Stretched sequences mean sequences created by interleaving '-' anywhere and in any number in the sequences. We can define a relation $\sim$ on stretched sequences: *each stretched sequence belongs to the class of its unstretched version*. Then, we can easily check that the relation $\sim$ is an equivalence relation.

In [23], Moraglio et al. have applied geometric crossover to variable-length sequences. The distance for variable-length sequences they used there is the *edit distance LD*[3]: the minimum number of insertion, deletion, and replacement of single character to transform one sequence into the other. The geometric crossover associated with this distance is proposed in [23]. It is called *homologous geometric crossover*: two sequences are aligned optimally before recombination. Alignment here means allowing parent sequences to be stretched to match better with each other. Two parent stretched sequences are aligned by interleaving or removing '-' to create two stretched sequences of the same length that have minimal Hamming distance. For example, if we want to recombine `agcacaca` and `acacacta`, we need to align them optimally first: `agcacac-a`

---

[3]The notation LD comes from *Levenshtein distance* that is another name of edit distance.

and `a-cacacta`. Notice that the Hamming distance between the aligned sequences is less than the Hamming distance between the non-aligned sequences. After the optimal alignment, one does the normal crossover and produce a new *stretched* sequence. The offspring is obtained by removing '-', so by unstretching the sequence.

From [23], we can easily check that edit distance for sequences is a metric and hence the phenotype space - the space of variable-length sequences - is a quotient metric space. In fact, the edit distance corresponds to a quotient metric and the homologous geometric crossover corresponds to induced quotient crossover. Suppose that we deal with only genotypes, i.e., stretched sequences. We leave offspring produced by homologous crossover just stretched - not removing '-'. Then the offspring exactly lies on quotient line segment. So the crossover is a quotient geometric crossover in terms of stretched sequences. In sum, we have:

Example	sequences
Genotype space X	stretched sequences
Equivalence relation $\sim$ inducing phenotype space $X/\sim$	stretched sequences with the same unstretched sequence
Metric d on X	edit distance
Original geometric crossover	traditional crossover on stretched sequences
Induced quotient crossover	homologous crossover [23]

Phenotypes are variable-length sequences that are directly representable. So in this case the quotient geometric crossover is not used to search a non-directly representable space (phenotypes) through an auxiliary directly representable space (genotypes). The benefit of applying the quotient geometric crossover on variable-length sequences is that the homologous crossover over sequences GX_P is naturally understood as a transformation of the geometric crossover GX_G over stretched sequences G rather than a crossover acting directly on sequences P. This is because the notion of optimal alignment is inherently defined on stretched sequences and not on simple sequences. In [23], Moraglio et al. have tested the homologous crossover on the protein motif discovery problem. In future work we want to study how the optimal alignment transformation affects the fitness landscape associated with geometric crossover with and without alignment.

5   Concluding Remarks

In this paper we have mathematically analyzed genotype and phenotype spaces by introducing the notion of quotient space. Phenotype space can be regarded as quotient space by a genotype-phenotype mapping. Geometric crossovers has the advantage in that they can also be formally defined once a distance is defined. Owing to this advantage we can connect a solution space - as a metric space - and crossovers. Moreover, geometric crossover based on the appropriate distance of a space reflects properties of given space. We introduced quotient metric on phenotype space. Since the quotient metric is a part of the phenotype space structure, the geometric crossover by the metric reflects the properties of phenotype space more effectively than the original geometric crossover.

As shown in application examples, quotient geometric crossover is not only theoretically significant but also has a practical effect of making search more effective by reducing the search

space or removing the inherent bias. In the example of grouping, we newly reinterpreted geometric crossover [17] that was previously proposed by the authors to be theoretically complete. In the examples of graphs, symmetric functions, and circular permutations, we induced new crossovers better tailored to phenotype space using the proposed methodology. In the example of sequence, we successfully analyzed previous study [23] in view of our quotient theory though it is slightly escaped from the framework we presented.

In future work, we will test the proposed induced quotient crossovers in solving the problems using genetic algorithms. Also, more examples and applications for each example case are left for future study.

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