Geometric Crossovers for Real-code Representation

Yourim Yoon
School of Computer Science & Engineering
Seoul National University
Sillim-dong, Gwanak-gu, Seoul, 151-744, Korea
yryoon@soar.snu.ac.kr

Yong-Hyuk Kim
Department of Mathematical Sciences
Seoul National University
Sillim-dong, Gwanak-gu, Seoul, 151-747, Korea
yhdfly@soar.snu.ac.kr

Alberto Moraglio
Department of Computer Science
University of Essex
Wivenhoe Park, Colchester, CO4 3SQ, UK
amoragn@essex.ac.uk

Byung-Ro Moon
School of Computer Science & Engineering
Seoul National University
Sillim-dong, Gwanak-gu, Seoul, 151-744, Korea
moon@soar.snu.ac.kr

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University of Essex
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ABSTRACT

Geometric crossover is a representation-independent generalization of the class of traditional mask-based crossover for binary strings. It is based on the distance of the search space seen as a metric space. Although real-code representation allows for a very familiar notion of distance, namely the Euclidean distance, there are also other distances suiting it. Also, topological transformations of the real space give rise to further notions of distance. In this paper, we study the geometric crossovers associated with these distances in a formal and very general setting and show that many pre-existing genetic operators for the real-code representation are geometric crossovers. We also propose a novel methodology to remove the inherent bias of pre-existing geometric operators by formally transforming topologies to have the same effect as gluing boundaries.

Keywords

Geometric crossover, real-code representation, crossover bias, glued space

1. INTRODUCTION

Geometric crossover [5] is a representation-independent operator defined over the distance of the search space. Informally, geometric crossover requires the offspring to lie between parents. Despite its simple geometric definition, geometric crossover captures the notion of "real-world" crossover: geometric crossover generalizes many pre-existing search operators for the major representations used in practice, such as binary strings [5], permutations [7], syntactic trees [6] and sequences [9].

The formal definition of geometric crossover enables us to build a representation-independent theory of evolutionary algorithms. It can also be used to guide the design of new specific crossover operators for non-standard representations using distances rooted on the specific representation (e.g., edit distances) as base for geometric crossover [7]. To be effective, specific geometric crossover operators need to be matched to the problem at hand. In order to embed problem knowledge in the crossover operator, this has to be based on a distance that is meaningful for the problem at hand. Previously, Moraglio and Poli [6] have suggested a rule of thumb: the distance chosen should make the resulting fitness landscape "smooth" in some statistical sense, or in other words, closer solutions should tend to have closer fitness.

Geometric crossover encompasses naturally combinatorial and continuous spaces. So far we have focused on the study of geometric crossover for combinatorial spaces and shown that their "geometrization" is not only possible but surprisingly insightful for the analysis and design of search operators. We have left to the intuition the case of continuous space because the definition of geometric crossover seems so natural for this space that no further investigation seems to be required. However this is not true: continuous spaces are as rich in variety as combinatorial spaces. Indeed, beside the traditional Euclidean distance there are many other distances for real vectors, hence there are many different types of geometric crossovers for real vectors with quite different search properties and suitable for different types of continuous problems.

In this paper we start to study the geometric crossovers for continuous spaces. A natural starting point are Minkowski distances that are simple generalizations of the Euclidean distance. Geometric crossovers based on Minkowski distances have an inherent bias toward the center of the space. This bias could be potentially harmful for the search. We then study geometric crossovers for glued versions of these spaces for which the bias disappears. We also show that many pre-existing recombination operators for real-vectors are geometric crossovers.

The reminder of this paper is organized as follows. In Section 2, we review the most frequently used genetic operators for the real-code representation. In Section 3, we introduce the geometric framework. In Section 4, we present geometric crossovers based on p-norms. In Section 5, we introduce the notion of biased crossover and explain why geometric crossovers based on p-norms are biased. In Section 6, we present geometric crossovers based on glued spaces that are unbiased. In Section 7, we show that a number of pre-existing recombination operators for the real-code representation are geometric and the implications of this. In Section 8, we draw conclusions and outline future work.

2. GENETIC OPERATORS FOR REAL-CODE REPRESENTATION

In this section we review the most frequently used recombination operators for the real-code representation. These operators are described into details in [1]. In literature many recombination operators for real-code representation are found. In the following we present a taxonomy of recombination operators that does not consider the specific probability distribution of the offspring but only what offspring can be generated with probability greater than zero given two parents. This taxonomy is important in relation with geometric crossover because the specific class of a recombination operator in this taxonomy is sufficient to tell which kind of geometric crossover it is. This will be shown in Section 7.

There are two main families of recombination operators [11]: discrete recombinations and blend recombinations. Blend recombination can be distinguished into line recombinations and box recombinations. Important variations of the last two recombination operators are the extended-line recombination and the extended-box recombination [10].

The discrete recombination family is the straightforward extension to real vectors of the family of mask-based crossover operators for binary strings including n-point and uniform crossover. The mask is still a binary vector dictating for each position of the offspring vector from which parent the (real) value for that position is taken.

The blend recombination family does not exchange values between parents like discrete recombinations but it averages or blends them. Line recombination returns offspring on the (Euclidean) line segment connecting the two parents. Box recombination returns offspring in the box (hyper-rectangle) whose diagonally opposite corners are the parents. Extended-line recombination picks offspring on an extended segment passing through the parent vectors but extending beyond them and not only in the section between them. Analogously extended-box recombination picks offspring on an extended box whose main diagonal passes through the parents but extends beyond them.

The most common form of mutation for real-code vectors generates an offspring vector by adding a vector M of random variables with expectation zero to the parent vector. There are two types of mutations bounded and unbounded depending on the fact that the range of the random variable is bounded or unbounded. The most frequently used bounded mutations are the creep mutation and the single-variable mutation and for the unbounded case is the Gaussian mutation.

For the creep (or hyper-box) mutation $M \sim U([-a, a]^n)$ is a vector of uniform random variables where a is a parameter defining the limits of the offspring area. This operator yields offspring within a hyper-box centered in the parent vector.

For the single-variable mutation M is a vector in which all entries are set to zero except for a random entry which is a uniform random variable $\sim U([-a, a])$.

Bounded mutation operators may get stuck in local optima. In contrast, unbounded mutation operators guarantee asymptotic global convergence. The primary unbounded mutation is the Gaussian mutation for which M is a multivariate Gaussian distribution.

3. GEOMETRIC FRAMEWORK

3.1 Geometric Preliminaries

In the following we give necessary preliminary geometric definitions and extend those introduced in [5, 6]. The following definitions are taken from [3].

The terms *distance* and *metric* denote any real valued function that conforms to the axioms of identity, symmetry and triangular inequality.

In a metric space (S, d) a *closed ball* is the set of the form $B_d(x; r) = \{z \in S : d(x, z) \leq r\}$ where r is a positive real number called the radius of the ball. A *line segment* (or closed interval) is the set of the form $[x; y]_d = \{z \in S : d(x, z) + d(z, y) = d(x, y)\}$ where $x, y \in S$ are called extremes of the segment. Metric segment and ball generalize the familiar notions of segment and ball 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 S by endowing it with a notion of distance d. $M = (S, d)$ is therefore a solution *space* and (M, f) is the corresponding fitness landscape, where f is the fitness function over S.

3.2 Definitions of Geometric Operators

The following definitions are *representation-independent* 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.*

DEFINITION 2 (GEOMETRIC MUTATION). *A unary operator GM is a* geometric ε-mutation *operator if $Im[GM(x)] \subseteq B_d(x; \varepsilon)$ where ε is the smallest real value for which this condition holds true.*

DEFINITION 3 (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.,*

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

DEFINITION 4 (UNIFORM GEOMETRIC MUTATION). Uniform geometric ε-mutation UGM *is a geometric ε-mutation* *where all z at most ε away from parent x have the same probability of being the offspring. That is, $UGM(x)$ has the uniform distribution on the ball $B_d(x;\varepsilon)$; the probability density function becomes*

$$f_{UGM}(z|x) = \frac{\delta(z \in B_d(x;\varepsilon))}{\mathrm{vol}(B_d(x;\varepsilon))},$$

where δ is a function which returns 1 *if the argument is true,* 0 *otherwise.*

$$Im[UGM(x)] = \{z \in S : f_{UGM}(z|x) > 0\} = B_d(x;\varepsilon).$$

Definition 5 (Uniform geometric crossover). Uniform geometric crossover *UGX is a geometric crossover where all z laying between parents x and y have the same probability of being the offspring. That is, $UGX(x,y)$ has the uniform distribution on the segment $[x;y]_d$; the probability density function becomes*

$$f_{UGX}(z|x,y) = \frac{\delta(z \in [x;y]_d)}{\mathrm{vol}([x;y]_d)}.$$

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

A number of general properties for geometric crossover and geometric mutation have been derived in [5] where we also showed that traditional crossover is geometric under the Hamming distance.

3.3 Problem versus Fitness Landscape

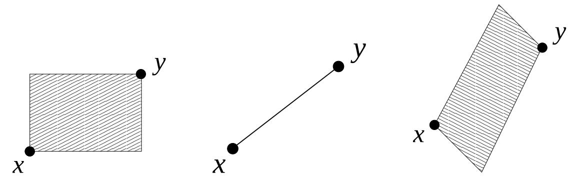
For continuous optimization problems, more than for combinatorial optimization problems, there is the assumption that problem and fitness landscape are completely interchangeable notions. However this is not true: the problem is simply the objective function and it does not come with any a priori notion of distance; the fitness landscape is the objective function plus a notion of distance. The two concepts are normally understood as equivalent because the Euclidean distance is taken for granted.

This assumption however is not always a good one. In fact some problems become easier to solve when the distance chosen for the landscape is more natural for the problem addressed than the Euclidean distance. A more natural distance gives rise to a smoother fitness landscape and the geometric operators associated with it are likely to perform better than those associated with the Euclidean distance. So it is important to study geometric crossovers and geometric mutations for real-code representation based on a number of alternative distances.

4. GEOMETRIC CROSSOVERS BASED ON p-NORMS

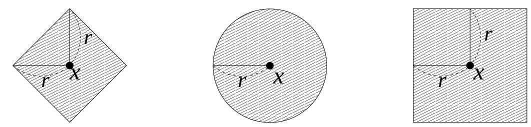
4.1 Metric Segments and Balls Induced by p-norms

Geometric crossover depends on the metric of given space. Although Euclidean distance is ordinarily used for $\mathbb{R}^n$, there exist many other metrics for $\mathbb{R}^n$. We study geometric crossover for real vector space under more general and abstract metric, Minkowski distance.



(A) $[x;y]_{d_1}$ (B) $[x;y]_{d_2}$ (C) $[x;y]_{d_\infty}$

Figure 1: Metric segments induced by p-norms



(A) $B_{d_1}(x;r)$ (B) $B_{d_2}(x;r)$ (C) $B_{d_\infty}(x;r)$

Figure 2: Metric balls induced by p-norms

Given a vector space X, *norm* is a real-valued function on X satisfying the properties of positiveness, positive homogeneity and subadditivity. Considering $\mathbb{R}^n$ as a vector space, we define p-norm on $\mathbb{R}^n$, where p is a natural number.

$$\|x\|_p = \left\{ \sum_{i=1}^{n} |x_i|^p \right\}^{\frac{1}{p}}.$$

Especially, ∞-norm is defined as follows:

$$\|x\|_\infty = \max_{1 \le i \le n} |x_i| \ .$$

Once the norm $\|\cdot\|$ is defined, we can define a metric on $\mathbb{R}^n$ by $d(x,y) := \|x - y\|$. The metric $d_p(x,y)$ is defined as $\|x - y\|_p$ on $\mathbb{R}^n$. Using these metrics, the metric segment between two points x and y on $\mathbb{R}^n$ under the metric d_p induced by p-norm is defined as follows:

$$[x;y]_{d_p} = \{z \in \mathbb{R}^n : \|x - z\|_p + \|z - y\|_p = \|x - y\|_p\}.$$

Also, the metric r-ball of a point x on $\mathbb{R}^n$ under the metric d_p is the set

$$B_{d_p}(x;r) = \{z \in \mathbb{R}^n : \|x - z\|_p \le r\}.$$

Figure 1 and 2 show an example of metric segments and metric balls on $\mathbb{R}^2$ for the cases that $p = 1, 2$ and ∞ ($[x;y]_{d_2} \subseteq [x;y]_{d_1}$ and $[x;y]_{d_2} \subseteq [x;y]_{d_\infty}$) and a geometric crossover under the metric d_1 is also geometric under the metrics d_2 and d_∞ ($B_{d_1}(x;r) \subseteq B_{d_2}(x;r) \subseteq B_{d_\infty}(x;r)$). We can easily see that a geometric crossover under the metric d_2 is also geometric under the metrics d_1 and d_∞.

Geometric crossover takes offspring that lies in the metric segments. We design new geometric crossovers using the metric segments induced by p-norms by choosing offspring that lie in the segments.

4.2 Implementation of Geometric Crossovers

Although new crossovers are theoretically meaningful, if they cannot be implemented efficiently, they are useless. We consider 1-norm, 2-norm and ∞-norm, and provide methods to implement geometric crossovers induced by the norms.

The metric induced by 2-norm is Euclidean distance. In this case, metric segment is just the line segment that is familiar to us. It is the convex combination of two points. An interesting fact is that this is not unique property of Euclidean space. If only given space has *inner product*, the property that convex combination and metric segment coincide holds by the following theorem.

THEOREM 1. *If H is an inner product space, $[x;y]_{d_H} := \{z \in H : \|x-z\| + \|z-y\| = \|x-y\|\} = \{\lambda x + (1-\lambda)y : 0 \le \lambda \le 1\}$, where $\|x\| := \langle x,x\rangle^{1/2}$.*

PROOF. If $z = \lambda x + (1-\lambda)y$ for some λ such that $0 \le \lambda \le 1$, then,

$$\begin{aligned} & \|x-z\| + \|z-y\| \\ = \; & \|x - \lambda x - (1-\lambda)y\| + \|\lambda x + (1-\lambda)y - y\| \\ = \; & (1-\lambda)\|x-y\| + \lambda\|x-y\| \\ = \; & \|x-y\|. \end{aligned}$$

Hence, $\{\lambda x + (1-\lambda)y : 0 \le \lambda \le 1\} \subset [x;y]_{d_H}$.

Now, to show that $[x;y]_{d_H} \subset \{\lambda x + (1-\lambda)y : 0 \le \lambda \le 1\}$, suppose $\|x-z\| + \|z-y\| = \|x-y\|$.
$\|x-z\|^2 = \|x\|^2 - 2\langle x,z\rangle + \|z\|^2$.
$\|z-y\|^2 = \|z\|^2 - 2\langle z,y\rangle + \|y\|^2$.
$\|x-y\|^2 = \|x\|^2 - 2\langle x,y\rangle + \|y\|^2$.
Let $\lambda = \|z-y\|/\|x-y\|$. Then, $0 \le \lambda \le 1$.

$$\begin{aligned} & z - \lambda x - (1-\lambda)y \\ = \; & z - \frac{\|z-y\|}{\|x-y\|}x - \left(1 - \frac{\|z-y\|}{\|x-y\|}\right)y \\ = \; & \frac{1}{\|x-y\|}\left(\|x-y\|z - \|z-y\|x - \|x-z\|y\right) \\ = \; & \frac{1}{\|x-y\|}\left(\|z-y\|z + \|x-z\|z - \|z-y\|x - \|x-z\|y\right) \\ = \; & \frac{1}{\|x-y\|}\left\{\|z-y\|(z-x) + \|x-z\|(z-y)\right\}. \end{aligned}$$

Using this formula, consider $\|z - \lambda x - (1-\lambda)y\|^2$.

$$\begin{aligned} & \|z - \lambda x - (1-\lambda)y\|^2 \\ = \; & \frac{1}{\|x-y\|^2}\left\| \; \|z-y\|(z-x) + \|x-z\|(z-y) \; \right\|^2 \\ = \; & \frac{1}{\|x-y\|^2}(\|z-y\|^2\|x-z\|^2 \\ & \quad + 2\|z-y\|\|x-y\|\langle z-x, z-y\rangle + \|z-y\|^2\|x-z\|^2) \\ = \; & \frac{\|z-y\|\|x-z\|}{\|x-y\|^2}\left(2\|z-y\|\|x-z\| + 2\langle z-x, z-y\rangle\right) \\ = \; & \frac{\|z-y\|\|x-z\|}{\|x-y\|^2}\{(\|x-z\| + \|z-y\|)^2 \\ & \quad - \|x-z\|^2 - \|z-y\|^2 + 2\langle z-x, z-y\rangle\} \\ = \; & \frac{\|z-y\|\|x-z\|}{\|x-y\|^2}(\|x-y\|^2 - \|x-z\|^2 \\ & \qquad - \|z-y\|^2 + 2\langle z-x, z-y\rangle) \\ = \; & \frac{\|z-y\|\|x-z\|}{\|x-y\|^2}(\|x\|^2 - 2\langle x,y\rangle + \|y\|^2 - \|x\|^2 + 2\langle x,z\rangle \\ & \qquad - \|z\|^2 - \|z\|^2 + 2\langle z,y\rangle - \|y\|^2 \\ & \qquad + 2\|z\|^2 - 2\langle z,y\rangle - 2\langle x,z\rangle + 2\langle x,y\rangle) \\ = \; & 0. \end{aligned}$$

Hence, $z = \lambda x + (1-\lambda)y$. $\square$

```
UGX_2(x, y)
{
    λ ← a random real number in [0, 1];
    for i ← 1 to n
        z_i ← λx_i + (1 − λ)y_i;
    return z = (z_1, z_2, ..., z_n);
}
```

Figure 3: Uniform geometric crossover under d_2

Since Euclidean space has a *dot product*, the next corollary is trivial.

COROLLARY 1. $[x;y]_{d_2} = \{\lambda x + (1-\lambda)y : 0 \le \lambda \le 1\}$.

PROOF. For $x, y \in \mathbb{R}^n$, define $\langle x,y\rangle$ as the dot product $\sum_{i=1}^n x_i y_i$. Then, $\langle \; , \; \rangle$ is the inner product and $\|x\|_2^2 = \langle x,x\rangle$ [4]. $\square$

Geometric crossover chooses offspring in the segments between parents. We can design uniform geometric crossover UGX_2 to choose a random vector in the segments between parents as offspring. If we use the metric d_2, the segment is the convex combination of parents by Corollary 1. We implement UGX_2 by choosing a random real value λ between 0 and 1 and computing $\lambda x + (1-\lambda)y$. Figure 3 shows the algorithm of UGX_2. Traditional arithmetic crossover [2] is a geometric crossover under d_2. In arithmetic crossover, the value of λ is fixed to 1/2; it chooses only *midpoints* between parents. However, it is not uniform geometric crossover under d_2. A restricted version of line recombination proposed by Mühlenbein and Schlierkamp-Voosen [11] is the uniform geometric crossover under d_2.

The metric d_1 induced by 1-norm is Manhattan distance. To implement geometric crossover under the Manhattan distance, we can get hints from Figure 1. In $\mathbb{R}^2$, the segment between two points is a rectangle bounded by the coordinate value of each point. Theorem 2 shows that this property holds for general cases.

THEOREM 2. $[x;y]_{d_1} = \{(z_1, z_2, \ldots, z_n) : \min(x_i, y_i) \le z_i \le \max(x_i, y_i), \; \forall i = 1, 2, \ldots, n\}$.

PROOF. Suppose that $\min(x_i, y_i) \le z_i \le \max(x_i, y_i)$ for each $i = 1, 2, \ldots, n$. Then, $\sum_{i=1}^n |x_i - z_i| + \sum_{i=1}^n |z_i - y_i| = \sum_{i=1}^n (|x_i - z_i| + |z_i - y_i|)$. For each i, if $x_i \ge y_i$, $y_i \le z_i \le x_i$, and hence $|x_i - z_i| + |z_i - y_i| = x_i - y_i = |x_i - y_i|$. If $x_i < y_i$, $x_i \le z_i \le y_i$, and hence $|x_i - z_i| + |z_i - y_i| = -x_i + y_i = |x_i - y_i|$. Hence, $\sum_{i=1}^n |x_i - z_i| + \sum_{i=1}^n |z_i - y_i| = \sum_{i=1}^n |x_i - y_i|$. This implies that $z \in [x;y]_{d_1}$.

Now, suppose that $\sum_{i=1}^n |x_i - z_i| + \sum_{i=1}^n |z_i - y_i| = \sum_{i=1}^n |x_i - y_i|$. Assume that $\min(x_i, y_i) \le z_i \le \max(x_i, y_i)$ does not hold for all i. That is, there exists k such that $z_k > \max(x_k, y_k)$ or $z_k < \min(x_k, y_k)$.

If $z_k > \max(x_k, y_k)$, $\sum_{i=1}^n |x_i - y_i| = \sum_{i=1}^n |x_i - z_i| + \sum_{i=1}^n |z_i - y_i| = \sum_{i \ne k}(|x_i - z_i| + |z_i - y_i|) + |x_k - z_k| + |z_k - y_k| \ge \sum_{i \ne k}(|x_i - z_i| + |z_i - y_i|) + 2z_k - x_k - y_k$. If $x_k \ge y_k$, $z_k \le x_k$. This contradicts the assumption that $z_k > \max(x_k, y_k)$. If $x_k < y_k$, $z_k \le y_k$. This is also a contradiction.

In the case that $z_k < \min(x_k, y_k)$, we can also obtain a contradiction in a similar way. So, we showed that $\sum_{i=1}^n |x_i - z_i| + \sum_{i=1}^n |z_i - y_i| = \sum_{i=1}^n |x_i - y_i|$ for all i. $\square$

```
UGX_1(x, y)
{
    for i ← 1 to n
        z_i ← a random real number in [min(x_i, y_i), max(x_i, y_i)];
    return z = (z_1, z_2, ..., z_n);
}
```

Figure 4: Uniform geometric crossover under d_1

Since the segment under d_1 is a region bounded by coordinate value of each point, we design uniform geometric crossover UGX_1 by choosing a random real number between two coordinate values for each coordinate. Figure 4 shows this algorithm. Traditional n-point/uniform crossovers (discrete recombinations) are geometric under d_1 since it chooses extreme points of the segment under d_1 as offspring. However, they are not uniform geometric crossover under d_1. A restricted version of intermediate recombination (box recombination) proposed by Mühlenbein and Schlierkamp-Voosen [11] is the uniform geometric crossover under d_1.

In Figure 1, $[x; y]_{d_\infty}$ is the parallelogram of which sides have the slope ± 1. For higher dimensional cases, we can also guess that the shape of the segment is something of which surfaces (hyperplanes) have the slope ± 1. Theorem 3 represents $[x; y]_{d_\infty}$ formally.

THEOREM 3. *Let k be the one of the indices such that $\|x-y\|_\infty = |x_k - y_k|$. If $x_k \geq y_k$, $[x; y]_{d_\infty} = \{(z_1, z_2, \ldots, z_n) : \min(x_k, y_k) \leq z_k \leq \max(x_k, y_k)$ and for each i, $|x_i - z_i| \leq |x_k - z_k|$ and $|z_i - y_i| \leq |z_k - y_k|\}$.*

PROOF. Let $z \in [x; y]_{d_\infty}$. Then, $\|x - z\|_\infty + \|z - y\|_\infty = \|x - y\|_\infty$. There exist s and t satisfying $\|x - z\|_\infty = |x_s - z_s|$ and $\|z - y\|_\infty = |z_t - y_t|$, i.e., $|x_s - z_s| \geq |x_i - z_i|$ and $|z_t - y_t| \geq |z_i - y_i|$ for all i.

The above formula can be rewritten as $|x_s - z_s| + |z_t - y_t| = |x_k - y_k|$. Then, $|z_t - y_t| = |x_k - y_k| - |x_s - z_s| \geq |z_k - y_k|$. So, $|x_s - z_s| \leq |x_k - y_k| - |z_k - y_k| \leq |(x_k - y_k) - (z_k - y_k)| = |x_k - z_k|$. This implies $|x_s - z_s| = |x_k - z_k|$. Similarly, $|z_t - y_t| = |z_k - y_k|$.

$|x_s - z_s| + |z_t - y_t| = |x_k - z_k| + |z_k - y_k| = |x_k - y_k|$, i.e., $z_k \in [x_k; y_k]_{d_1}$ in $\mathbb{R}$. Hence, $\min(x_k, y_k) \leq z_k \leq \max(x_k, y_k)$ by Theorem 2. Moreover, for all i, $|x_i - z_i| \leq |x_s - z_s| \leq |x_k - z_k|$ and $|z_i - y_i| \leq |z_t - y_t| \leq |z_k - y_k|$.

Now, assume that z satisfies $\min(x_k, y_k) \leq z_k \leq \max(x_k, y_k)$ and for each i, $|x_i - z_i| \leq |x_k - z_k|$ and $|z_i - y_i| \leq |z_k - y_k|$ hold. Then, $\|x - z\|_\infty = |x_k - z_k|$ and $\|z - y\|_\infty = |z_k - y_k|$. If $x_k \geq y_k$, $\|x - z\|_\infty + \|z - y\|_\infty = |x_k - z_k| + |z_k - y_k| = x_k - z_k + z_k - y_k = x_k - y_k = \|x - y\|_\infty$. If $y_k > x_k$, $\|x - z\|_\infty + \|z - y\|_\infty = |x_k - z_k| + |z_k - y_k| = z_k - x_k + y_k - z_k = y_k - x_k = \|x - y\|_\infty$. So, $z \in [x; y]_{d_\infty}$. $\square$

By Theorem 3, the implementation of UGX_∞ has become possible though we cannot imagine its shape in the concrete.

The algorithm for UGX_∞ is given in Figure 5. We first choose the index k such that $\|x - y\|_\infty = |x_k - y_k|$, i.e., $|x_k - y_k| \geq |x_i - y_i|$ for every i. And then, we choose the value of z_k between x_k and y_k. Using this value of z_k, for each coordinate, we choose z_i satisfying $|x_i - z_i| \leq |x_k - z_k|$ and $|z_i - y_i| \leq |z_k - y_k|$. This is done by calculating the minimum and maximum values that z_i can be and choosing a random real number between them.

```
UGX_∞(x, y)
{
    k ← argmax_{1≤i≤n} |x_i − y_i|;
    z_k ← a random real number in [min(x_k, y_k), max(x_k, y_k)];
    for i ← 1 to n
        z_i ← a random real number in
                [max(x_i − |x_k − z_k|, y_i − |z_k − y_k|),
                    min(x_i + |x_k − z_k|, y_i + |z_k − y_k|)];
    return z = (z_1, z_2, ..., z_n);
}
```

Figure 5: Uniform geometric crossover under d_∞

5. CROSSOVER BIAS

Let us introduce the notion of *bias* of an operator. Let OP be a search operator $z = OP(p_1, p_2, \ldots, p_n)$ where p_is are the parents in S and $z \in S$ is the offspring. We say that a search operator is *unbiased* if we choose parents independently and uniformly in the solution set S we obtain offspring uniformly at random in the solution set S. In formulas: OP is unbiased if $p_i \sim U(S)$ and independent implies $z = OP(p_1, p_2, \ldots, p_n) \sim U(S)$. Biasedness is the inherent preference of a search operator for specific areas of the search space and it is an important search property of a search operator: an evolutionary algorithm using that operator, without selection, is attracted to the areas the search operator prefers. Arguably, also when selection is present, the operator bias acts as a background force that makes the search more keen to go toward the areas preferred by the search operator. This is not necessarily bad if the bias is toward the optimum or an area with high-quality solutions. However, it is bad if the bias is toward an area of poor-quality solutions. When the location of good solutions of a problem is not known, it would be better to leave selection to guide the search on the basis of the fitness values only. In fact the operator bias could be potentially deleterious for performances because it interferes with selection.

Interestingly, uniform geometric crossover is unbiased on the Hamming space but the very same operator is biased toward the center on the Euclidean space. This is easy to verify by picking random parents in the two spaces and generating offspring in the respective segments. One way to compensate for such a bias in Euclidean and Manhattan spaces is using extended-line and extended-box recombinations. Another way to compensate for the bias relies on understanding the origin of this bias.

So, what is the origin of the different bias of geometric crossover for the Hamming space and for the Euclidean space? The answer relies on the notion of *isotropy* of the underlaying metric space. Informally, a metric space is *isotropic* if all its points are equivalent: every point has the same properties in terms of distance. The Euclidean space, more precisely a bounded hyper-rectangular subspace of the Euclidean space, is not isotropic because the existence of the boundaries introduces an asymmetry on the types of points: the space has boundaries and has a center, hence each point is different from each other depending on how far from the boundaries and the center it is. Each point has a special status, hence the space is not isotropic. Conversely, in the Hamming space, each point is the center and at the same time is a boundary point, so each point has the same sta-

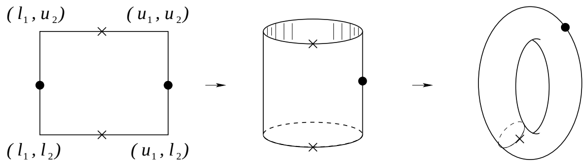


Figure 6: Glued space on $\mathbb{R}^2$. This can be considered as a quotient space.

tus and the Hamming space is therefore isotropic. Let us consider now a new metric space obtained by gluing the opposite extremities of the Euclidean hyper-rectangle; in the case of a simple two-dimensional rectangle the space we obtain is the surface of a torus. Notice that the metric associated with this space is not the Euclidean metric anymore, because points that were at opposite sides of the rectangle are close to each other in the new space. The new space is isotropic because the boundaries, that are the origin of the inhomogeneity of types of points in the Euclidean space, are not there anymore. The uniform geometric crossover based on this new space is unbiased because there cannot be bias toward the center given that every point is the center of the new space as in the case of the Hamming space. *It is therefore the isotropy of the space that causes the bias of the search operator to cease being.* In the next section we present geometric crossovers for glued spaces in a formal setting.

6. GEOMETRIC CROSSOVERS IN GLUED SPACE

In general, solution space of real-coded problems has the range. Let the solution space X be $\{x \in \mathbb{R}^n : l_i \leq x_i < u_i \text{ for each } i\}$ where $l = (l_1, l_2, \ldots, l_n)$ is a lower bound and $u = (u_1, u_2, \ldots, u_n)$ is an upper bound. If we apply geometric crossover on this bounded domain, offspring have bias toward the center of the space. One method to eliminate this bias is gluing the boundaries by identifying u_i to l_i for each i. Figure 6 shows this glued space for $\mathbb{R}^2$ case.

Formally, the glued space is considered as a quotient space. To make a quotient space which gives an effect equivalent to gluing, equivalence relation on $\mathbb{R}^n$ is defined as follows:

Definition 6. *$x \sim y$ if and only if for each $i = 1, 2, \ldots, n$, there exists $a_i \in \mathbb{Z}$ such that $x_i - y_i = a_i(u_i - l_i)$.*

Theorem 4. *The relation $\sim$ is an equivalence relation.*

Proof. Assume that x, y and $z \in \mathbb{R}^n$.
(i) *Reflexive*: $x_i - x_i = 0(u_i - l_i)$ for each $i = 1, 2, \ldots, n$. Since $0 \in \mathbb{Z}$, $x \sim x$.
(ii) *Symmetric*: If $x \sim y$, for each $i = 1, 2, \ldots, n$, there exists $a_i \in \mathbb{Z}$ such that $x_i - y_i = a_i(u_i - l_i)$. Then, $y_i - x_i = -(x_i - y_i) = -a_i|u_i - l_i|$ and $-a_i \in \mathbb{Z}$. Hence, $y \sim x$.
(iii) *Transitive*: If $x \sim y$ and $y \sim z$, for each $i = 1, 2, \ldots, n$, there exists $a_i \in \mathbb{Z}$ such that $x_i - y_i = a_i(u_i - l_i)$ and $b_i \in \mathbb{Z}$ such that $y_i - z_i = b_i(u_i - l_i)$. $x_i - z_i = (x_i - y_i) + (y_i - z_i) = a_i(u_i - l_i) + b_i(u_i - l_i) = (a_i + b_i)(u_i - l_i)$. $a_i + b_i \in \mathbb{Z}$ since a_i and $b_i \in \mathbb{Z}$. So, $x \sim z$. $\square$

Let $\langle x \rangle$ be the equivalence class of $x \in \mathbb{R}^n$. In Figure 7, points indicated by bullets are in the same equivalent class on $\mathbb{R}^2$.

X can be considered as a quotient set $\mathbb{R}^n / \sim$ by considering $x \in X$ as $\bar{x} \in \mathbb{R}^n / \sim$. However, this gives another

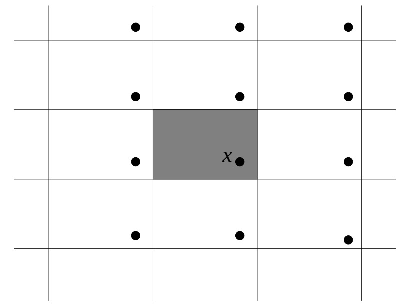


Figure 7: Equivalent class of x on $\mathbb{R}^2$. The shadowed rectangle represents given bounded real space X. Each rectangle has the same size as X.

topology to the same set. We need to define a distance tailored to this new topology. We define a new distance on $\mathbb{R}^n / \sim$ using the distance on $\mathbb{R}^n$. Let $x, y \in X$.

Definition 7. *Let $x, y \in X$. If d is a distance for $\mathbb{R}^n$,*

$$d_q(x, y) := \min_{x' \in \langle x \rangle, y' \in \langle y \rangle} d(x', y').$$

Theorem 5. *If the distance d is induced by a norm, d_q is a metric for X.*

Proof. Assume that x, y and $z \in X$.
(i) *Identity*: $0 \leq d_q(x, x) \leq d(x, x) \leq 0$.
(ii) *Symmetry*: $d_q(x, y) = d(x', y')$ for some $x' \in \langle x \rangle$ and $y' \in \langle y \rangle$. Then, $d_q(x, y) = d(x', y') = d(y', x') \geq d_q(y, x)$. Similarly, $d_q(y, x) \geq d_q(x, y)$.
(iii) *Triangular inequality*: $d_q(x, y) + d_q(y, z) = d(x', y') + d(y'', z'')$ for some $x' \in \langle x \rangle$, $y', y'' \in \langle y \rangle$, and $z'' \in \langle z \rangle$. Since d is induced by a norm, $d(y'', z'') = d(y'' - y'' + y', z'' - y'' + y') = d(y', z'' - y'' + y')$. Since $y'_i - y''_i = k_i|u_i - l_i|$ for each i, $z'' - y'' + y' \in \langle z \rangle$. Hence,

$$\begin{aligned} d_q(x, y) + d_q(y, z) &= d(x', y') + d(y'', z'') \\ &= d(x', y') + d(y', z'' - y'' + y') \\ &\geq d(x', z'' - y'' + y') \\ &\geq d_q(x, y). \end{aligned}$$

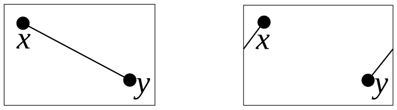
$\square$

It is impossible to calculate $d_q(x, y)$ considering all points in equivalence class since the number of the points is infinite. Fortunately, there is a practical way to calculate it.

Let $x, y \in X$. For each i, let $T_i(y) = \{y_i, y_i + (u_i - l_i), y_i - (u_i - l_i)\}$ and $M_i(y) = \operatorname{argmin}_{m \in T_i(y)}\{|x_i - m|\}$. $M_i(y)$ is the set because the number of maximizers can be more than one. Let $M(y) = \{(y'_1, y'_2, \ldots, y'_n) \in \mathbb{Z}^n : y'_i \in M_i(y) \text{ for each } i\}$.

Theorem 6. *Let x and $y \in X$. If a metric d is induced by p-norm and $y^* \in M(y)$, $d(x', y') \geq d(x, y^*)$ for all $x' \in \langle x \rangle$ and $y' \in \langle y \rangle$, i.e., d_q is well-defined and $d_q(x, y) = d(x, y^*)$. Moreover, $M(y) = \{y' \in \langle y \rangle : d_q(x, y) = d(x, y')\}$.*

Proof. $d(x', y') = (\sum_{i=1}^{n} |x'_i - y'_i|^p)^{1/p}$.
For each i, $|x'_i - y'_i| = |x'_i - y'_i + x_i - x_i + y_i - y_i| = |(x_i - y_i) + (x'_i - x_i) + (y_i - y'_i)|$. Since $x \sim x'$ and $y \sim y'$, $(x'_i - x_i) + (y_i - y'_i) = k_i(u_i - l_i)$ for some $k_i \in \mathbb{Z}$. Then, $|x'_i - y'_i| = |(x_i - y_i) + k_i(u_i - l_i)|$.



(A) $[x;y]_{d_2}$ (B) $[x;y]_{d_q}$

Figure 8: Line segments on Euclidean space and glued space

If $k_i \geq 2$, $|(x_i - y_i) + k_i(u_i - l_i)|$ is positive since $x_i - y_i$ cannot be greater than $u_i - l_i$. So, $|x'_i - y'_i| = |(x_i - y_i) + k_i(u_i - l_i)| > |(x_i - y_i) + (u_i - l_i)| = |x_i - \{y_i + (u_i - l_i)\}| \geq |x_i - y^*_i|$. Similarly, in the case that $k_i \leq -2$, $|(x_i - y_i) + k_i(u_i - l_i)|$ is negative. Hence, $|x'_i - y'_i| = |(x_i - y_i) + k_i(u_i - l_i)| > |(x_i - y_i) - (u_i - l_i)| = |x_i - \{y_i - (u_i - l_i)\}| \geq |x_i - y^*_i|$. Finally, if $k_i = 0, 1, -1$, $|x'_i - y'_i| = |(x_i - y_i) + k_i(u_i - l_i)| \geq |x_i - y^*_i|$ by the definition of $M(y)$.

So, $d(x', y') = \{\sum_{i=1}^n |x'_i - y'_i|^p\}^{1/p} \geq \{\sum_{i=1}^n |x_i - y^*_i|^p\}^{1/p} = d(x, y^*)$.

Now, we will show that $M(y) = \{y' \in \langle y \rangle : d_q(x, y) = d(x, y')\}$. Suppose that $y' \in \langle y \rangle$ satisfies $d_q(x, y) = d(x, y')$ but $y' \notin M(y)$. Then, there exists a nonempty index set $J = \{j : |x_j - y'_j| \neq |x_j - y^*_j|\}$. For each $j \in J$, $|x_j - y'_j| = |x_j - y_j - k_j(u_j - l_j)|$. If $k_j \geq 2$ or $k_j \leq -2$, $|x_j - y'_j| > |x_j - y^*_j|$ by the same way as the above. If $k_j = 0, 1, -1$, $|x_j - y'_j| \geq |x_j - y^*_j|$. By the assumption, $|x_j - y'_j| \neq |x_j - y^*_j|$ and hence $|x_j - y'_j| > |x_j - y^*_j|$. Therefore, $d(x, y') = (\sum_{i=1}^n |x_i - y'_i|^p)^{1/p} > d(x, y^*)$ and it is contradiction. □

According to Theorem 6, to calculate $d_q(x, y)$, we need only to find y^* by choosing minimizer among three elements from $T_i(y)$ for each coordinate and get Euclidean distance between x and y^*. Now, the segment between x and y on quotient space is induced by the segment between x and y^* on $\mathbb{R}^n$.

Theorem 7. *If d is induced by p-norm, the line segment $[x;y]_{d_q}$ is the set*

$$\bigcup_{y' \in M(y)} \{z \in X : z \sim z' \text{ for some } z' \in [x;y^*]_d\}.$$

Proof. Let $y^* \in M(y)$ and $z \sim z'$ for some $z' \in [x;y^*]_d$. Then, $d_q(x, z) + d_q(z, y) \leq d(x, z') + d(z', y^*) = d(x, y^*) = d_q(x, y^*)$. Since $d_q(x, z) + d_q(z, y) \geq d_q(z, y)$ by triangular property, $d_q(x, z) + d_q(z, y) = d_q(z, y)$. So, $z \in [x;y]_{d_q}$.

Now, let $z \in [x;y]_{d_q}$. There exist z' such that $d_q(x, z) = d(x, z')$ and y' such that $d_q(z, y) = d(z, y')$ in $\mathbb{R}^n$ by Theorem 6. Let $y^* := y' - z + z'$. Then, $y^* \sim y' \sim y$ and $d_q(x, y) = d_q(x, z) + d_q(z, y) = d(x, z') + d(z, y') = d(x, z') + d(z', y' - z + z') = d(x, z') + d(z', y^*) \geq d(x, y^*)$ since d is a metric. By the definition of d_q, $d_q(x, y) \leq d(x, y^*)$ is true and hence $d_q(x, y) = d(x, y^*)$. This implies $y^* \in M(y)$ and $d(x, z') + d(z', y^*) = d(x, y^*)$. □

In Figure 8, (A) shows the segment on Euclidean space and (B) shows the segment on glued space (quotient space). In quotient space, segments may cross the boundaries.

7. GEOMETRICITY OF PRE-EXISTING CROSSOVERS

In this section we consider pre-existing operators for the real-code representation and tell whether they are geometric operators and if so for what distances. Knowing that a recombination operator is geometric is important because there is a growing body of theory that applies to geometric crossovers. Also, knowing the distance for which an operator is geometric allows us to tell a priori by a simple landscape analysis if the operator is going to perform well or not. Although this practice is a standard for mutation, the geometric framework extends this to crossover. Alternatively, the knowledge of a natural distance for a given problem immediately tells us what geometric crossover to use because, as a rule of thumb, the geometric crossover associated with this distance is likely to perform well.

It is immediate to see that line recombination and box recombination are geometric crossovers under Euclidean and Manhattan distance respectively because offspring are in the segments between parents under these two distances.

Discrete recombination is geometric under Manhattan distance because it can be seen as a special case of box recombination in which offspring are at the corners of the hyper-box identified by the parents. It is easy to verify that discrete recombination is also geometric under Hamming distance extended to real vectors. This distance is simply the number of positions in the two vectors containing different real values.

Are extended-line recombination and extended-box recombination geometric? Let us consider the case of extended-line recombination. Obviously this recombination is not a geometric crossover under the Euclidean distance, because of the possibility of generating offspring outside the Euclidean segment between parents. However this does not exclude that the extended line recombination may be geometric under some other notion of distance. That indeed would make it a geometric crossover. So, wouldn't it be possible to do some topological transformation of the underlying real space, a gluing for example, and find a space endowed with a distance for which segments are extended segment in the Euclidean space? Even if this seems to be a promising way of approaching the problem, this leads nowhere. Previously Moraglio and Poli [8] have shown axiomatically that there is no distance such as the extended-line crossover is geometric, hence there is no topological transformation of the space that does the trick. So extended-line crossover is not a geometric crossover. The extended-box recombination can be proven non-geometric analogously.

The results for real vectors extend immediately to integer vectors. Since integer vectors can be understood as a subsets of real vectors, cardinal and ordinal recombinations between integer vectors can be seen as special cases of respectively discrete and box recombinations, so they are geometric crossovers under Hamming and Manhattan distances, respectively.

Let us now turn to mutation operators. Creep mutation is the uniform geometric a-mutation under d_∞. Single-variable mutation is a geometric a-mutation under any Minkowski distance. Gaussian mutation is a geometric δ-mutation under any Minkowski distance, where δ is the semi-diameter of the search space.

8. CONCLUSIONS AND FUTURE WORK

In this paper we have applied the geometric framework to the real-vector representation. We have made the following contributions.

- Although the definition of geometric crossover is fairly intuitive for the case of Euclidean metric, there are other distances suiting real vectors. We have studied formally and in a very general settings geometric crossovers for the family of Minkowski metrics and given efficient algorithms to implement them.

- We have seen that geometric crossover specified for the Minkowski metrics is a bias operator: it produces offspring toward the center of the space with higher probability from uniformly distributed parents. We have explained that the origin of this bias has to be found in the fact that these spaces are non-isotropic: all points are not fully-symmetric in relation with the distance.

- Minkowski spaces can be made isotropic by gluing their opposite sides together and considering the distances associated with these glued spaces. We have then studied formally and in full generality the unbiased geometric crossovers associated with these new spaces.

- We have also shown that a number of pre-existing recombination operators for real vectors are geometric crossovers under some Minkowski distances. This is important because it allows us to apply to them a growing body of theoretical results for the class of geometric crossover.

In future work we want to implement the new crossovers presented in this paper and test them on problems for which we expect them to perform well from the study of their fitness landscapes.

There are other interesting metrics associated with real spaces of potential use for specific applications. For example, we could consider vectors as polar coordinates instead of Cartesian coordinates and define metrics and geometric crossovers suited to them. These crossovers are likely to perform well on problems that are naturally expressed in terms of polar coordinates such as problems naturally defined on a sphere, for example, finding locations of antennas to maximize the signal coverage on the surface of the earth respecting some constraints.

In future work we will explore more metrics for the real-code representation and associated geometric operators in conjunction with specific problems because this is a powerful and straightforward way of embedding problem knowledge in the search that has been completely neglected in the specific case of continuous optimization for which the Euclidean distance has been always implicitly chosen.

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