Product Geometric Crossover

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Abstract. Geometric crossover is a representation-independent definition of crossover based on the distance of the search space interpreted as a metric space. It generalizes the traditional crossover for binary strings and other important recombination operators for the most frequently used representations. Using a distance tailored to the problem at hand, the abstract definition of crossover can be used to design new problem specific crossovers that embed problem knowledge in the search. In this paper, we introduce the important notion of product geometric crossover that allows to build new geometric crossovers combining pre-existing geometric crossovers in a simple way.

Keywords: Theory, Crossover, Representations

1 Introduction

Geometric crossover and geometric mutation are representation-independent search operators that generalize many pre-existing search operators for the major representations used in evolutionary algorithms, such as binary strings [4], real vectors [4], permutations [6], syntactic trees [5] and sequences [7]. They are defined in geometric terms using the notions of line segment and ball. These notions and the corresponding genetic operators are well-defined once a notion of distance in the search space is well-defined. Defining search operators as functions of the search space is opposite to the standard way [3] in which the search space is seen as a function of the search operators employed. This viewpoint greatly simplifies the relationship between search operators and fitness landscape and has allowed us to give simple *rules-of-thumb* to build crossover operators that are likely to perform well.

Theoretical results of metric spaces can naturally lead to interesting results for geometric crossover. In particular, in this paper we focus on the notion of *metric transformation*. 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 underlaying solution representation (e.g. edit distances). In these cases it gives rise to a simple and *natural interpretation in terms of syntactic transformations.*

Metric transformations: there are a number of metric transformations [2] [10]:

- *sub-metric spaces*
- *product spaces*
- *quotient metric space*
- *gluing metric space*
- *combinatorial transformation*
- *non-negative combinations of metric spaces*
- *Hausdorf transformation*
- *Concave transformation*
- *Biotope transform*

Natural syntactic interpretation of a metric transformations: Geometric crossover is well-defined once a metric space is defined. Let us consider the geometric crossover X associated to the original metric space M, and the geometric crossover X' associated to the transformed metric space $M' = mt(M)$ where mt is the metric transformation. The functional relationship among metric spaces and geometric crossovers can be nicely expressed through a commutative diagram (Fig. 1). gx means application of the formal definition of geometric crossover and gt means *induced geometricity-preserving* crossover transformation associated to the metric transformation mt. This diagram becomes remarkably interesting when the metric transformation mt is associated to an induced geometricity-preserving crossover transformation gt that has a simple interpretation in terms of syntactic manipulation. This indeed allows one to get new geometric crossovers starting from recombination operators that are known to be geometric by simple *geometricity-preserving syntax manipulation.*

In this paper we extend the geometric framework introducing the important notion of cartesian product of geometric crossover, that allows to build new geometric crossovers combining preexisting geometric crossovers in a very simple way. The metric transformation considered is a simple product of metric spaces and the corresponding induced crossover transformation is the *product geometric crossover.* This may sound very abstract and impractical. However, it actually is not. Indeed, we put the ideas reported in this paper to the test [8].

The paper is organised as follows. In section 2 we present the geometric framework. In section 3, we extend it with the notion of product geometric crossover. In section 4, we draw conclusions.

2 Geometric framework

2.1 Geometric preliminaries

In the following we give necessary preliminary geometric definitions and extend those introduced in [4] and [5]. The following definitions are taken from [2].

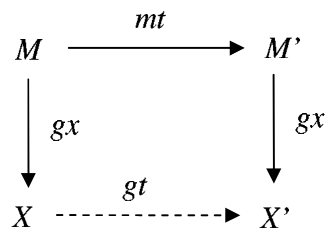

Fig. 1. Commutative diagram linking metric and crossover transformations.

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

In a metric space (S, d) a *line segment* (or closed interval) is the set of the form $[x; y] = \{z \in S | d(x, z) + d(z, y) = d(x, y)\}$ where $x, y \in S$ are called extremes of the segment. Metric segment generalises the familiar 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 S by endowing it with a notion of distance d. $M = (S, d)$ is therefore a solution *space* and $L = (M, g)$ is the corresponding fitness landscape.

2.2 Geometric crossover definition

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

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

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

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

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

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

A number of general properties for geometric crossover and mutation have been derived in [4] where we also showed that traditional crossover is geometric under Hamming distance. In previous work we have also studied various crossovers for permutations, revealing that PMX, a well-known crossover for permutations, is geometric under swap distance. Also, we found that Cycle crossover, another traditional crossover for permutations, is geometric under swap distance and under Hamming distance.

2.3 Formal evolutionary algorithm and problem knowledge

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 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 could 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.

In order to avoid this one can exploit problem knowledge in the search. This 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 this 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 crossover and mutation). 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 mutation and geometric crossover work 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 context and has been confirmed in uncountable empirical studies with many neighborhood search meta-heuristics [9]. We operate according to the following rule-of-thumbs:

Rule-of-thumb 1: if we have a good distance for the problem at hand than we have good geometric mutation and good geometric crossover

Rule-of-thumb 2: a good distance for the problem at hand is a distance that makes the landscape "smooth"

3 Product geometric crossover

We first introduce the general notion of geometricity-preserving transformations. Then we consider a specific geometricity-preserving transformation associated with the product metric. We introduce product metrics for vector spaces, that are metric preserving transformations, and stress how they can be seen as natural generalization of simple metrics for vector spaces. We then introduce the notion of interval space that naturally bridges the metric and representation aspects of geometric crossover, and recall a few results form interval spaces theory. We use these results to prove our main result of this paper on the product of geometric crossovers. We then give a number of examples of applications. Finally we discuss how to further generalize this theorem to a general structural composition of geometric crossovers.

3.1 Geometricity-preserving transformations

In previous work we have proven that a number of important pre-existing recombination operators for the most frequently used representations are geometric crossovers. We have also applied the abstract definition of geometric crossover to distances firmly rooted in a specific solution representation and designed brand-new crossovers. An appealing way to build new geometric crossovers is starting from recombination operators that are known to be geometric and derive new geometric crossovers by *geometricity-preserving transformations/combinations* that when applied to geometric crossovers, return geometric crossovers.

We study those metric-preserving transformations which induced geometricity-preserving transformations have a simple and natural interpretation on the solution representation.

3.2 N-dimensional real spaces and product metric spaces

Metric spaces on $\mathbb{R}^2$. Let $S = \mathbb{R}^2$, and $x = (x', x'')$, $y = (y', y'')$. The following are metric spaces on S:

$d_1(x, y) = |x' - y'| + |x'' - y''|$ (Manhattan space)

$d_2(x, y) = \sqrt{|x' - y'|^2 + |x'' - y''|^2}$ (Euclidean space)

$d_\infty(x, y) = Max\{|x' - y'| + |x'' - y''|\}$ (Chessboard space)

These may be proved to be metrics [10]. These definitions may be extended to n-dimensional real spaces.

Product metric spaces. Given two metric spaces $M' = (S', d')$ and $M'' = (S'', d'')$, we may define several metrics on $S' \times S''$. For example, if $x = (x', x'')$ and $y = (y', y'')$ are in $S' \times S''$, let

$d_1(x, y) = d'(x', y') + d''(x'', y'')$ (Manhattan product)

$d_2(x, y) = \sqrt{d'(x', y')^2 + d''(x'', y'')^2}$ (Euclidean product)

$d_\infty(x, y) = Max\{d'(x', y') + d''(x'', y'')\}$ (Chessboard product)

These may be proved to be metrics [10]. These definitions may be extended to the product of any finite number of metric spaces.

It is interesting to notice that product spaces can be considered as generalization of n-dimensional real spaces, where the absolute value metric at each dimension is replaced by a generic metric. This is important because the generalization involves two different types of objects: a *simple metric* for a structured space and a structural *metric transformation* of generic metric spaces. More on this in the section 4.

3.3 Product interval spaces

Metric spaces can be associated to geometric interval spaces. The latter are a more natural setting for geometric crossover than the former. We review the notion of interval space and present results that draw a parallel between metric spaces and interval spaces. Then we use them to prove specific results for geometric crossover.

Interval space and Geometric interval space. Let X be a set and let $I : X \times X \to 2^X$ be a function with the following properties:

- *Extensive Law*: $a, b \in I(a, b)$
- *Symmetry Law*: $I(a, b) = I(b, a)$

Then I is called an *interval operator on* X, and $I(a, b)$ is the *interval between* a *and* b. The resulting pair (X, I) is called an *interval space.*
An interval operator I on a set X is *geometric* provided the following hold.

- *Idempotent Law*: $\forall b \in X : I(b, b) = \{b\}$
- *Monotone Law*: if $a, b, c \in X$ and $c \in I(a, b)$, then $I(a, c) \subseteq I(a, b)$
- *Inversion Law*: if $a, b \in X$ and $c, d \in I(a, b)$, then $c \in I(a, d)$ implies $d \in I(c, b)$

A set with a geometric interval operator is called a *geometric interval space.*

Interval space associated to a metric space. The geodesic operator $[\bullet, \bullet]_d$ that associates extremes of a metric segment to all the points that constitute it is a geometric interval operator [1].

Product segment. Let us define the product segment as $[a, b]_{d \times d'} = \{(x_1, x_2) | x_1 \in [a_1, b_1]_d, x_2 \in [a_2, b_2]_{d'}\}$ where $a = (a_1, a_2), b = (b_1, b_2)$
Product segment theorem: The product segment corresponds to the segment of the Manhattan product space: $[(a_1, a_2), (b_1, b_2)]_{d \times d'} = [(a_1, a_2), (b_1, b_2)]_\rho$ where $\rho((a_1, a_2), (b_1, b_2)) = d(a_1, b_1) + d'(a_2, b_2)$ [1]
This result may be extended to the product segment of any finite number of metric spaces.

Interval spaces connect very naturally with the notion of geometric crossover. There is a wealth of results for geometric interval spaces that can easily be transferred to geometric crossover.

3.4 Product geometric crossover

A *product geometric crossover* of the geometric crossovers X_i based on the metric spaces (S_i, d_i) is a recombination operator defined over the cartesian product set $\prod_i S_i$ that applies the geometric crossover X_i to the projection S_i. From the results in the previous section we have the following

Theorem 1. *Any cartesian product of geometric crossovers is a geometric crossover under the distance given by the sum of the distances of the compounding crossovers*

Proof. This follows immediately from the definition of geometric crossover and the product segment theorem.

The geometric crossovers in each projection of the product geometric crossover do not need to be independent for the product crossover to be geometric. This is because casting any form of dependency between geometric crossovers in different projections results in a reduction of the pool of offspring allowed to be created by the product geometric crossover. From the definition of geometric crossover, such a restriction does not affect its geometricity.

The theorem above is useful because it allows to build new geometric crossovers combining crossovers that are known to be geometric. In particular, this applies to crossovers for mixed representations. Examples of application of product geometric crossovers:

- Multi-crossover: same representation same crossover n times
- Hybrid crossover: same representation different crossover for each projection
- Hybrid representation crossover: different representation for each projection (and different crossover)
- Dependent crossover: different projections represent a single entity and they are mutually constrained (This occurs very often in real-world problems. e.g. for neural networks one projection could be a variable-size graph representing the structural part, a second projection could be a variable-length sequence of real representing the weights. Clearly recombination of the first projection imposes constraints on the recombination of the second projection to obtain a feasible offspring)

3.5 Simplification and generalization of geometricity of traditional crossover

Definition (Discrete metric space). Let A be any non-empty set and define d by

$$d(x, y) = \begin{cases} 1, x \neq y \\ 0, x = y \end{cases}$$

This is a metric and is called the *discrete metric* of A. The discrete metric space is the path metric of the fully-connected graph with nodes A. The interval operator associated with the discrete metric space is: $\forall a, b \in A : [a, b] = \{a, b\}$ (all segments are edges).

We call the geometric crossover associated to the discrete metric, the *discrete metric geometric crossover* DM-GX. Clearly, the only possible offspring of DM-GX are the parents.
Definition (Hamming metric space). Let us consider the set A which elements are vectors of length n over some alphabet A of size $|A|$. The Hamming distance between two vectors is the number of coordinates where they differ. The Hamming space is denoted by $H(n, |A|)$.
Discrete metrics and Hamming space are linked as follows: the product metric of n discrete metric spaces of the alphabet A is the Hamming space $H(n, |A|)$.

Theorem 2. *Any traditional mask-based crossover for discrete vectors taking values on the alphabet A is geometric under Hamming distance.*

Proof. This follows from the fact that any traditional mask-based crossover is the product crossover of n DM-GX, one for each projection.

When the alphabet A is a set of integer, beside the discrete metric we can consider also the absolute value of their difference (ABD) for each projection as a metric to be used as base of the product crossover. It is easy to see that the geometric crossover associated to ABD produces integers within the interval having the parents integers as extremes. The product geometric crossover is in this case a blending-type crossover (in contrast with the discrete metric that gives rise to a discrete recombination-type crossover).

4 Future investigations

Structural composition of geometric crossovers: the previous result could be generalized in a very interesting way, extending the geometric framework to complex representations. In the following we discuss this.

Basic representations such as vectors, permutations, sequences, trees, graphs and sets, to mention only the most common, all can be seen as structures containing generic objects. These objects do not need to be necessarily numbers or atomic symbols from a given alphabet. Such objects can well be structures themselves, so we can consider derived structures obtained by structural composition, such for example sets of trees. The composition can be repeated recursively with different types of representations so obtaining a wealth of derived representations, potentially suited to any problem conceivable.

Given geometric crossovers X_A and X_B for the structure A and B associated to the metric spaces M_A and M_B, what is the derived geometric crossover for the derived structure $A \circ B$? What is the derived metric space associated to the derived geometric crossover and the derived structure?

With the product geometric crossover, we have seen that when the structure is a vector, the structural composition with any other representations is connected to a natural derived geometric crossover consisting of a simple geometric crossover for each position in the vector, and associated to a derived metric that is simply the sum of the metric for each position.

In the case of vectors, we have a number of possible structural compositions (a number of metric product operators) but only one notion of metric product that has a natural interpretation on the representation, making it the only one actually useful. In the case of other structures, there could be more than one (or even none) possible structural composition that has a natural interpretation on the representation. Furthermore, in the case of structures other than vectors, we do not have standard metric transformations such as the metric product that naturally suit them. So, where can we start our generalization from?

There seems to be a way suggested by the case of vectors: we have seen that simple metrics on the vector space (structured objects) can be easily generalized to a structural metric transformations of generic metric spaces retaining the overall structure of the original object (vector of metric spaces). We could do the same to generalize metrics for other type of structures to structural metric transformations. The starting point is noticing that distances for structured representations are naturally expressed as some aggregating function of marginal contributions due to the difference in the structural subcomponents. The way of measuring the difference between two components is normally a very simple notion of metric, discrete metric for difference between symbols, or just absolute value for numeric components. In the case of vectors, the aggregating function is a simple sum, and the distance between components is the absolute value. So, the way to pass from metric distance to metric transformation is to replace the simple component-metric with generic metrics, exactly how it was done for the case of vectors.

This seems to be a general and very promising starting point to extend simple metrics on any type of structured object to structural metric transformations naturally associated with its shape. In future work, we will explore these metric transformations and study their induced geometricity-preserving transformations to reveal the effect on the representation of the derived geometric crossovers.

Other metric transformations: Most of the metric transformations listed in the introduction have corresponding syntactic crossover transformations, that can be used for other purposes than actually constructing new geometric crossovers. Indeed, we are currently using some of these transformations to attack the following important open issue regarding geometric crossover. Given a geometric crossover, there is in general more than one distance for which the crossover is geometric (for example cycle crossover is geometric under Hamming distance and swap distance). The question is: is there a distance that can be said to be the best distance to consider for a specific geometric crossover? If so, what is this distance? The answer relies heavily on the notion of metric transformation.

5 Conclusions

In this paper we have extended the geometric framework introducing the notion of cartesian product crossover. This is a very general result that allows to build new geometric crossovers customized to problems with mixed representations by combining pre-existing geometric crossovers in a straightforward way. We have presented this notion in the more general setting of metric transformations and discussed promising future investigations. Using the product geometric crossover theorem, we have also shown that traditional crossovers for symbolic vectors and blending crossovers for integer and real vectors are geometric crossover by looking at them as product crossovers.

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