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Transit sets of k-point crossover operators

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Abstract

k-point crossover operators and their recombination sets are studied from different perspectives. We show that transit functions of k-point crossover generate, for all $k > 1$, the same convexity as the interval function of the underlying graph. This settles in the negative an open problem by Mulder about whether the geodesic convexity of a connected graph G is uniquely determined by its interval function I. The conjecture of Gitchoff and Wagner that for each transit set $R_k(x, y)$ distinct from a hypercube there is a unique pair of parents from which it is generated is settled affirmatively. Along the way we characterize transit functions whose underlying graphs are Hamming graphs, and those with underlying partial cube graphs. For general values of k it is shown that the transit sets of k-point crossover operators are the subsets with maximal Vapnik–Chervonenkis dimension.

Keywords: Genetic algorithms; Recombination; Transit functions; Betweenness; Vapnik–Chervonenkis dimension

1. Introduction

Crossover operators are a crucial component of Genetic Algorithms and related approaches in Evolutionary Computation. Their purpose is to combine the genetic information of two parents to produce one or more

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offspring that are “mixtures” of their parents. In this contribution we will be concerned with the specific setting of crossover operators for strings of fixed length n over an alphabet $\mathcal{A}$ of $a \geq 2$ letters. Given two parental strings $x = (x_1x_2 \dots x_n)$ and $y = (y_1y_2 \dots y_n)$ one may for instance construct recombinant offspring of the form $(x_1x_2 \dots x_i y_{i+1}y_{i+2} \dots y_n)$ and $(y_1y_2 \dots y_i x_{i+1}x_{i+2} \dots x_n)$. The index i serves as a breakpoint at which the two parents recombine. This so-called one-point crossover can be generalized to two or more breakpoints.

Definition 1.1. Given $x, y, z \in \mathcal{A}^n$ we say that z is a k-point crossover offspring of x and y if there are indices $0 = i_0 \leq i_1 \leq i_2 \leq i_k = n$ so that for all ℓ, $1 \leq \ell \leq k$, either $z_j = x_j$ for all $j \in \{i_{\ell-1} + 1, \dots, i_\ell\}$ or $z_j = y_j$ for all $j \in \{i_{\ell-1} + 1, \dots, i_\ell\}$.

Note that this definition states that x and y are broken up into *at most* k intervals that are alternately included into z. This convention simplifies the mathematical treatment considerably and also conforms to the usual practice of including crossovers with fewer than the maximum number of breakpoints. Uniform crossover, where each letter z_i is freely chosen from one of the two parents, is obtained by allowing $k = n - 1$ breakpoints. We note, furthermore, that our definition ensures that the parental strings are also included in the set of possible offspring.

Properties of k-point crossover have been studied extensively in the past. Key algebraic properties are described in [1]. Isomorphisms between the search spaces induced by crossover and mutation with small populations have been analysed by [2]. A formal treatment of multi-point crossover with an emphasis on disruption analysis can be found in [3]. A general review of genetic algorithms from the perspective of stochastic processes on populations can be found in [4]. In this context, crossover operators are represented by stochastic matrices. A similar matrix-based formalism is explored in [5]. Coordinate transformations, more precisely the Walsh transform [6] and its generalizations to non-binary alphabets [7] have played an important role in explaining the functioning of GAs in terms of building blocks and the Schema theorem [8]. As a generalization, an abstract treatment of crossover in terms of equivalence relations has been given by [9].

Gitchoff et al. [10] proposed to consider the function $R : X \times X \to 2^X$ that assigns to each possible pair of parents the set of all possible recombinants. They asked which properties of R could be used to characterize crossover operators in general and explored properties of k-point crossover on strings. In particular, they noted the following four properties:

(T1) $x, y \in R(x, y)$ for all $x, y \in X$,

(T2) $R(x, y) = R(y, x)$ for all $x, y \in X$,

(T3) $R(x, x) = \{x\}$ for all $x \in X$,

(GW4) $z \in R(x, y)$ implies $|R(x, z)| \leq |R(x, y)|$.

Mulder introduced the concept of *transit functions* characterized by the axioms (T1), (T2), and (T3) as a unifying approach to intervals, convexities, and betweenness in graphs and posets in last decade of the 20th century. Available as preprint only but frequently cited for more than a decade, the seminal paper was published only recently [11]. For example, given a connected graph G, its geodetic intervals, i.e., the sets of vertices lying on shortest paths between a pair of prescribed endpoints $x, y \in V(G)$ form a transit function usually denoted by $I_G(x, y)$ [12] and referred as the interval function of a graph G. Unequal crossover, where (T3) is violated, has been rarely explored in the context of evolutionary computation, which the exception of [13]. In this contribution we restrict ourselves exclusively to the simpler case of homologous string recombination. *Thus, from here on we will assume that R satisfies (T1), (T2), and (T3).*

A common interpretation of transit functions is to view $R(x, y)$ as the subset of X lying `between` x and y. Indeed, a transit function is a *betweenness* if it satisfies the two additional axioms

(B1) $z \in R(x, y)$ and $z \neq y$ implies $y \notin R(x, z)$.

(B2) $z \in R(x, y)$ implies $R(x, z) \subseteq R(x, y)$.

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It is natural, therefore, to regard a pair of distinct points x and y without other points between them as *adjacent*. The corresponding graph G_R has X as its vertex set and $\{x, y\} \in E(G_R)$ if and only if $R(x, y) = \{x, y\}$ and $x \neq y$. The graph G_R is known as the *underlying graph* of R.

Moraglio [14] introduced the notion of *geometric crossover operators* relative to a connected reference graph G with vertex set X by requiring – in our notation – that $R(x, y) \subseteq I_G(x, y)$ for all $x, y \in X$. In the setting of [14], the reference graph G was given externally in terms of a metric on X. When studying crossover in its own right it seems natural to consider the transits sets of R in relation to the intervals of G_R itself. Hence we say that R is *MP-geometric* if

(MG) $R(x, y) \subseteq I_{G_R}(x, y)$ for all $x, y \in X$.

Note the condition (MG) is an axiom for transit functions independent of any externally prescribed structure on X. Mulder [11] considered a different notion of "geometric" referring transit functions that satisfy (B2) and the axiom

(B3) $z \in R(x, y)$ and $w \in R(x, z)$ implies $z \in R(w, y)$.

Mulder's version of "geometric" is less pertinent for our purposes because crossover operators usually violate (B2).

Another interpretation of R, which is just as useful in the context of crossover operators, is to regard $R(x, y)$ as the set of offspring reachable from the parents x and y in a single generation. It is natural then to associate with R a function $\widehat{R} : X \times X \to 2^X$ so that $z \in \widehat{R}(x, y)$ if and only if z eventually can be generated from x and y and all their following generations of offspring. Formally, $z \in \widehat{R}(x, y)$ if there is a finite sequence of pairs $\{x_k, y_k\}$ so that $z \in R(x_m, y_m)$, $\{x_k, y_k\} \in R(x_{k-1}, y_{k-1})$ for all $k = 1, \ldots, m$, $x_0 = x$, and $y_0 = y$. By construction, $R(x, y) \subseteq \widehat{R}(x, y)$ for all $x, y \in X$. If R is a transit function, then $\widehat{R}$ is also a transit function.

We say that $R(x, y)$ is *closed* if $R(x, y) = \widehat{R}(x, y)$. Equivalently, a transit set $R(x, y)$ is closed if and only if $R(u, v) \subseteq R(x, y)$ holds for all $u, v \in R(x, y)$, since in this case nothing can be generated from the children of x and y that is not accessible already from x and y itself. In particular, all singletons and all adjacencies, i.e., individual vertices and the edges of G_R, are always closed. A transit function R is called *monotone* if it satisfies

(M) For all $x, y \in X$ and $u, v \in R(x, y)$ implies $R(u, v) \subseteq R(x, y)$,

i.e., if all transit sets are closed. By construction, $\widehat{R}$ satisfies (M) for any transit function R. A simple argument[1] shows that $\widehat{R}(x, y) = \{x, y\}$ if and only if $R(x, y) = \{x, y\}$. Thus R and $\widehat{R}$ have the same underlying graph $G_{\widehat{R}} = G_R$. The sets $\{\widehat{R}(x, y)|x, y \in X\}$, finally, generate a convexity $\mathfrak{C}_R$ consisting of all intersections of the (finitely many) transit sets $\widehat{R}(x, y)$.

One of the most fruitful lines of research in the field of transit functions is the search for axiomatic characterizations of a wide variety of different types of graphs and other discrete structures in terms of their transit functions. It is shown in [15] that a function $I : V \times V \to 2^V$ is the geodesic interval function of a connected graph if and only if I satisfies a set of axioms that are phrased in terms of I only. The axiomatic characterization of $I(u, v)$ was later improved by formulating a nice set of (minimal) axioms [16]. The all-paths function A of a connected graph G (defined as $A(u, v) = \{z \in V(G) : z$ lies on some u, v-path in $G\}$) admits a similar axiomatic characterization [17]. These results immediately raise the question whether other types of transit functions can be characterized in terms of transit axioms only.

Since k-point crossover on strings over a fixed alphabet forms a rather specialized class of recombination operators we ask here whether it can be defined completely in terms of properties of its transit function R_k. Beyond the immediate interest in k-point crossover operators we can hope in this manner to identify generic properties of crossover operators also on more general sets X.

This contribution is organized as follows. In Section 2 we consider transit functions whose underlying graphs G_R are Hamming graphs since, as we show in Section 3, k-point crossover belongs to this class. We then investigate the properties of k-point crossover in more detail from the point of view of transit functions. In Section 4 we switch to a graph-theoretical perspective and derive a complete characterization of k-point crossover on binary alphabets, making use of key properties of partial cubes.

[1] (i) $R(x, y) \subseteq \widehat{R}(x, y)$ by definition, (ii) $R(x, y) = \{x, y\}$ implies $\widehat{R}(x, y) = \{x, y\}$, (iii) if $\widehat{R}(x, y) = \{x, y\}$ but $R(x, y) \neq \{x, y\}$ either (i) or axiom (T1) is violated.

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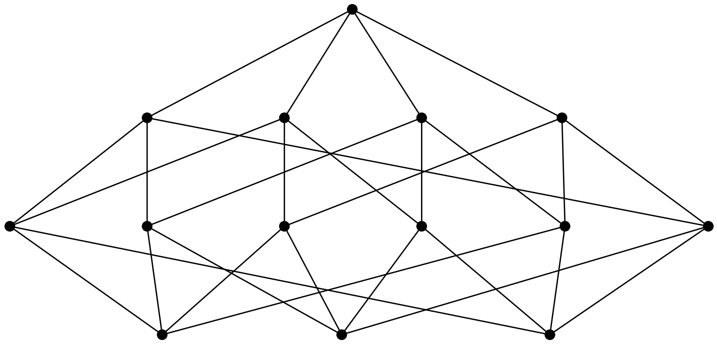

Fig. 1. The last condition of Proposition 2.1, i.e., $|V(G)| = 2^\delta$, is necessary as demonstrated by this example of a $(0, 2)$-graph that is not a hypergraph [12]. It satisfies all but the last requirement from the proposition.

2. Hamming graphs and their geodesic intervals

In most applications, k-point crossover will be applied to binary strings or, less frequently, to strings over a larger, fixed-size alphabet $\mathcal{A}$. In a population genetics context, however, the number of alleles may be different for each locus, hence we consider the most general case here, where each sequence position is taken from a distinct alphabet $\mathcal{A}_i$ with $a_i := |\mathcal{A}_i| \geq 2$ for $1 \leq i \neq n$. The Hamming graph $\prod_i K_{a_i}$ is the Cartesian products of complete graphs K_{a_i} with a_i vertices; we refer to the book [18] for more details on Hamming graphs and product graphs in general. The special case $a_i = 2$ for all i is usually called n-dimensional hypercube K_2^n. The shortest path distance on $\prod_i K_{a_i}$ is the Hamming distance $d(x, y)$, which counts the number of sequence positions at which the strings x and y differ.

Given a transit function R and a point $x \in X$ let $\delta(x) = |\{y \in X \quad | \quad |R(x, y)| = 2\}|$, i.e., $\delta(x) = \delta_R(x)$ is the degree of x in the underlying graph G_R. We write $\delta(R) = \max_{x \in X} \delta(x)$ for the maximal degree of the underlying graph.

The purpose of this section is to characterize transit functions whose underlying graphs are Hamming graphs. Our starting point is the following characterization of hypercubes, which follows from results in [12,19]:

Proposition 2.1. *Suppose G is connected and each pair of distinct adjacent edges lies in exactly one 4-cycle. Then G is isomorphic to n-dimensional hypercube if and only if the minimum degree δ of G is finite and $|V(G)| = 2^\delta$.*

Graphs with the property that any pair of vertices has zero or exactly 2 common neighbours are called $(0, 2)$-graphs [12]. We note that the condition $|V(G)| = 2^\delta$ in Proposition 2.1 is necessary as demonstrated by the example in Fig. 1. Proposition 2.1 can be translated into the language of transit functions as follows:

Corollary 2.2. *Let R be a transit function on a set X with a connected underlying graph. Then the underlying graph G_R is isomorphic to n-dimensional hypercube K_2^n if and only if R satisfies:*

(A1) *For every x, u, v such that $|R(x, u)| = |R(x, v)| = 2$ there exists a unique y such that $|R(y, u)| = |R(y, v)| = 2$,*

(A2) *$\delta(R) = n$ and $|X| = 2^n$.*

Proposition 2.1 was generalized to arbitrary Hamming graphs [20]. For any vertex x in the graph G let $N_i(x)$ denote the number of maximal i-cliques K_i in G that contain the vertex x.

Proposition 2.3 (*[20]*). *Let G be a simple connected graph such that two non-adjacent vertices in G either have exactly 2 common neighbours or none at all, and suppose G has neither $K_4 \setminus e$ nor $K_2 \square K_3 \setminus e$ (Fig. 2) as induced subgraph. Then $N_i(x)$ is independent of x and G is isomorphic to the Hamming graph if and only if $|V(G)| = \prod_{h=1}^{p} h^{N_i(x)}$, where p is the maximum integer such that $N_p(x)$ is nonzero.*

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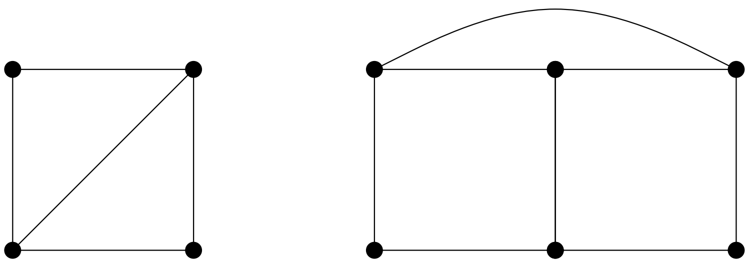

Fig. 2. The forbidden induced subgraphs $K_4 \setminus e$ and $K_2 \Box K_3 \setminus e$ appearing in Proposition 2.3.

These results can again be translated into the language of transit functions:

Corollary 2.4. *Let R be a transit function with a connected underlying graph. Then the underlying graph G_R is isomorphic to Hamming graph K_a^n if and only if R satisfies:*

(A1) *For every x, u, v such that $|R(x,u)| = |R(x,v)| = 2$ there exists unique y such that $|R(y,u)| = |R(y,v)| = 2$,*

(A2') *$\delta(R) = n(a-1)$ and $|X| = a^n$,*

(A3) *There exist no x, y, u, v such that $|R(x,u)| = |R(x,v)| = |R(y,u)| = |R(y,v)| = |R(x,y)| = 2$ and $|R(u,v)| > 2$,*

(A4) *There exist no x, y, u, v, w, z such that $|R(x,u)| = |R(x,v)| = |R(y,u)| = |R(y,v)| = |R(v,w)| = |R(y,z)| = |R(w,z)| = |R(x,w)| = 2$ and $|R(u,v)|, |R(u,w)|, |R(u,z)|, |R(x,y)|, |R(x,z)|, |R(v,z)|, |R(y,w)| > 2$.*

The representation of Hamming graphs as n-fold Cartesian products of complete graphs $H = \prod_{i=1}^{n} K_{a_i}$ implies a "coordinatization", that is, a labelling of the vertices reflects this product structure. The geodesic intervals in Hamming graphs then have very simple description:

$$I_H(x,y) = \left\{ z = (z_1, z_2, \ldots z_n) \middle| z_i \in \{x_i, y_i\} \text{ for } 1 \le i \le n \right\} \tag{1}$$

where $(x_1, x_2, \ldots x_n)$ and $(y_1, y_2, \ldots y_n)$ are the coordinates of the vertices x and y. Thus $G_{I_H(x,y)}$ is a subhypercube of dimension $d(x,y)$ as shown in example in [18]. The intervals of Hamming graphs have several properties that will be useful for our purposes. A graph is called antipodal if for every vertex v there is a unique "antipodal vertex" $\bar{v}$ with maximum distance from v.

Lemma 2.5. *Let Q be an induced sub-hypercube of a Hamming graph H. Then for every $x \in Q$ there is a unique vertex $\bar{x} \in Q$ so that $Q = I_H(x, \bar{x})$.*

Proof. This follows from a well known fact that hypercubes are antipodal graphs [12]. □

It is well known that I_H satisfies the monotone axiom (M) and thus also (B2).

Lemma 2.6. *Let Q' and Q'' be two induced sub-hypercubes in a Hamming graph H. Then $Q' \cap Q''$ is again an induced (possibly empty) sub-hypercube of H.*

Proof. For every coordinate i, $Q'_i = \{x_i | x' \in Q\}$ and $Q''_i = \{x_i | x \in Q''\}$ contain at most two different letters from the alphabet $\mathcal{A}_i$. $Q' \cap Q'' = \prod_i (Q'_i \cap Q''_i)$, and hence a hypercube. □

As an immediate consequence we note that I_H satisfies even the stronger property

(MM) For all $u, v, x, y \in X$ holds: if $R(u,v) \cap R(x,y) \neq \emptyset$ then there are $p, q \in X$ so that $R(u,v) \cap R(x,y) = R(p,q)$.

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The disadvantage of the results so far is that we have to require explicitly that G_R is connected. In the light of condition (MG) above it seems natural to require connectedness of G_R for recombination operators in general.

To-date, only sufficient conditions for connectedness of G_R are known. Following ideas outlined in [21], we can show directly that the following property is sufficient:

(CG) For all $a, x, y, z \in X$: If $R(a, x) \subseteq R(a, y)$, then $R(a, x) \subseteq R(a, z) \subseteq R(a, y)$ if and only if $z \in R(x, y)$.

As a technical device we will employ the partial order $\leq_a$ of X defined, for given $a \in X$, by $x \leq_a y$ if and only if $R(a, x) \subseteq R(a, y)$. As usual, we write $x <_a y$ if $x \leq_a y$ and $x \neq y$. For $R = I_G$ we have the equivalence $x \in I_G(a, y)$ if and if only $x \leq_a y$.

Lemma 2.7. *The underlying graph G_R of a transit function R is connected if R satisfies axiom* (CG).

Proof. Let R be a transit function satisfying axiom (CG). Let $a, b \in X$ be two distinct elements, and let $\mathbf{C} = (a = a_0, a_1, \ldots a_t = b)$ be a maximal $\leq_a$-chain between a and b, where the elements are labelled in increasing order $a = a_0 <_a a_1 <_a a_2 <_a \ldots <_a a_t = b$.

We claim that, for any i, $0 \leq i \leq n$, elements a_i and a_{i+1} form an edge in G_R. To see this assume that, on the contrary, there is an element $x \in R(a_i, a_{i+1}) \setminus \{a_i, a_{i+1}\}$ for some i. Then (CG) implies $R(a, a_i) \subseteq R(a, x) \subseteq R(a, a_{i+1})$, i.e., $a_i <_a x <_a x_{i+1}$, contradicting maximality of the chain $\mathbf{C}$. Hence $\mathbf{C}$ consists of consecutive edges whence G_R is a connected graph. □

However, property (CG) is much too strong for our purposes: Setting $x = a$ makes the condition in (CG) trivial, i.e., the axiom reduces to "$R(a, z) \subseteq R(a, y)$ if and only if $z \in R(a, y)$". Since $R(a, z) \subseteq R(a, y)$ implies $z \in R(a, y)$ we are simply left with axiom (B2), i.e., (CG) implies (B2). As we shall see below, however, string crossover in general does not satisfy (B2) and thus (CG) cannot not hold in general. Similarly, we cannot use Lemma 1 of [22], which states that G_R is connected whenever R is a transit function satisfying (B1) and (B2).

Allowing conditions not only on R but also on its closure $\widehat{R}$ we can make use of the fact that $G_R = G_{\widehat{R}}$. Since $\widehat{R}$ satisfies the monotonicity axion (M) by construction, (B2) is also satisfied. Thus R_G is connected if at least one of the following two conditions is satisfied: (i) $\widehat{R}$ satisfies (B1), or (ii) $\widehat{R}$ satisfies

(CG') $x \in \widehat{R}(a, z)$ and $z \in \widehat{R}(a, y)$ if and only if $z \in \widehat{R}(x, y)$

The latter is equivalent to (CG) whenever R satisfies (M). To see this observe that $R(a, x) \subseteq R(a, y)$ implies $x \in R(a, y)$ and by (M) $R(x, y) \subseteq R(a, y)$.

So far, we lack a condition for the connectedness of G_R that can be expressed by first order logic in terms of R alone.

3. Basic properties of k-point crossover

We first show that the underlying graphs of k-point crossover transit functions are Hamming graphs.

Lemma 3.1. $G_{R_k} = \prod_{i=1}^{n} K_{a_i}$ *for all* $1 \leq k \leq n - 1$.

Proof. Since $R_j(x, y) \subseteq R_k(x, y)$ for $j \leq k$ by definition, it suffices to consider R_1. By definition, $R_1(x, y) = \{x, y\}$ if and only if x and y differ in a single coordinate, i.e., for which $d(x, y) = 1$, i.e., x and y are adjacent in $\prod_{i=1}^{n} K_{a_i}$. Obviously, $R_k(x, y) = R_1(x, y)$ in this case. If there are two or more sequence positions that are different between the parents, then the crossover operator can "cut" between them to produce and generate an off-spring different from either parent so that $|R_1(x, y)| > 2$. □

From Lemma 3.1 and Corollary 2.4 we immediately conclude that the k-point crossover transit function R_k satisfies (A1), (A2'), (A3), and (A4).

Lemma 3.2. *Let R_k be the k-point crossover function. Then $\widehat{R_k}(x, y) = I_{G_{R_k}}(x, y)$ for all $x, y \in X$ and all $k \geq 1$.*

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Proof. By construction $z \in \widehat{R_k}(x, y)$ agrees in each position with at least one of the parents, i.e., $z_i \in \{x_i, y_i\}$ for $1 \leq i \leq n$, and thus $\widehat{R_k}(x, y) \subseteq I_{G_R}(x, y)$. Conversely, choose an arbitrary $z \in I_G(x, y)$. Find the first position k in the coordinate representation in which z disagrees with x and form the recombinant $y' \in R_1(x, y)$ that agrees with x for $i < k$ and with y for all $i \geq k$. Then form the $x' \in R_1(x, y') \subseteq \widehat{R_1}(x, y)$ by recombining again after position k. By construction, x' agrees with z at least for all $i \leq k$, i.e., in at least one position more than x. Since $x' \in \widehat{R_1}(x, y)$ we can repeat the argument at most n time to find a sequence $x^{(n)} \in \widehat{R_1}(x, y)$ that agrees with z in all positions. Since $R_1(x, y) \subseteq R_k(x, y)$ for all $k \geq 1$, we conclude that $z \in \widehat{R_k}(x, y)$. □

As an immediate corollary we have:

Corollary 3.3. *k-point crossover is MP-geometric for all $k \geq 1$.*

MP-geometricity is a desirable property for crossover operators in general because it ensures that repeated application eventually produces the entire geodesic interval of the underlying graph structure.

Lemma 3.2 also implies a negative answer to one of the questions posed in [11]: "Is the geodesic convexity uniquely determined by the geodesic interval function $I(u, v)$ of a connected graph?". More precisely, Lemma 3.2 shows that the k-point crossover transit function R_k also generates the geodesic convexity and hence that the geodesic convexity is not uniquely determined by the interval function I as the $I_{G_{R_k}}(x, y)$, being the interval in a hypercube, is itself convex.

A trivial consequence of Lemma 3.2, furthermore, is the well known fact that the transit function of uniform crossover R_{n-1} is the interval function on the Hamming graph:

Corollary 3.4. $R_{n-1}(x, y) = \widehat{R_{n-1}}(x, y) = I_{G_R}(x, y)$ *for all* $x, y \in X$.

For small distances, k-point crossover also produces the full geodesic interval in a single step:

Lemma 3.5. $R_k(x, y) = I_{G_R}(x, y)$ *if and only if* $d(x, y) \leq k + 1$.

Proof. If $d(x, y) \leq k+1$ we can place one cross-over cut between any two positions at which x and y differ. In this way we obtain all possible recombinations, i.e., $R_k(x, y)$ is a subhypercube of dimension $k + 1$ in the underlying graph G_R. Conversely if $d(x, y) > k+1$ then there exists a $z \in I_{G_R}(x, y)$ such that z requires more than k cross-over cuts between positions at which x and y, which completes the proof. □

Next, we observe that the transit sets of k-point crossover can be constructed recursively.

Theorem 3.6. $R_k(u, v) = \bigcup_{z \in R_{k-1}(u,v)} [R_1(u, z) \cup R_1(z, v)]$.

Proof. W.l.o.g. we can assume that $u = 0 \ldots 0$ and $v = 1 \ldots 1$. Let $a \in R_k(u, v)$ and without loss of generality we can assume that a ends with 0. Let a_j denote the coordinate, with the last appearance of 1 in a. Let b be an element with $b_i = a_i$ for $1 \leq i \leq j$ and $b_i = 1$ otherwise. It follows that $b \in R_{k-1}(u, v)$ and moreover $a \in R_1(b, v)$. □

A key property in the theory of transit functions is the so-called Pasch axiom

(Pa) For $p, a, b \in X$, $a' \in R(p, a)$ and $b' \in R(p, b)$ implies that $R(a', b) \cap R(b', a) \neq \emptyset$.

Lemma 3.7. *R_1 satisfies the Pasch axiom* (Pa).

Proof. Consider three arbitrary strings a, b, and p. Then $a' \in R_1(a, p)$ is a concatenation of a prefix of a with the corresponding suffix of p, or *vice versa*. Each $b' \in R_1(b, p)$ has an analogous representation, leading to four cases depending on whether p is a prefix or a suffix of a' and b', resp., see Fig. 3. In case 1, $a' \in R_1(b', a)$ if a' has a shorter p-suffix than b'. Otherwise $b' \in R_1(a', b)$. In case 2, a' has a p-prefix up to k and b' has a p-suffix starting at l. If the two parts of p overlap, i.e., $l \leq k$ then $(b_1 \ldots b_l, p_{l+1} \ldots p_k, a_{k+1} \ldots a_n) \in R_1(b, a') \cap R_1(a, b')$. If $k < l$ then a common crossover product is obtained by recombining both b with a' and a with b' at position k. Case 3, a' has a p-suffix and b' has a p-prefix, can be treated analogously. Case 4, in which p matches a prefix of both a' and b' can be treated as in case 1. In summary, thus $R_1(a', b) \cap R_1(a, b') \neq \emptyset$ for any choice of $a' \in R_1(a, p)$ and $b' \in R_1(b, p)$, i.e., R_1 satisfies (Pa). □

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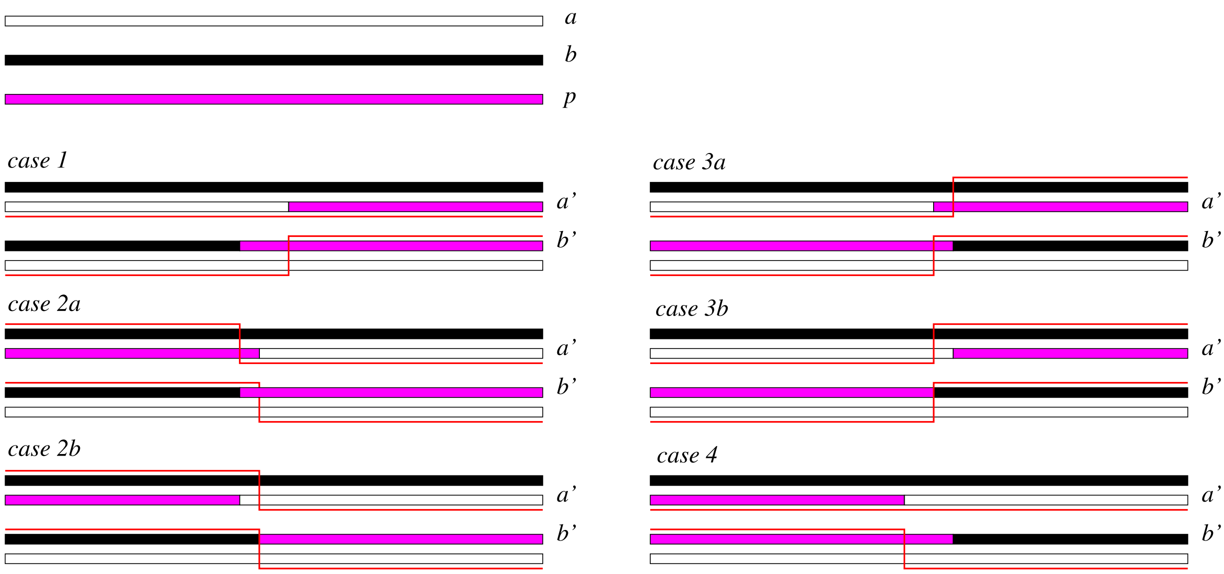

Fig. 3. Sketch of the proof of *Lemma* 3.7. We distinguish 6 cases depending on how a' and b' are constructed in $R_1(a, p)$ and $R_1(b, p)$, respectively. The red lines indicate the explicit construction of an element in $R_1(a, b') \cap R_1(a', b)$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Theorem 3.8. *R_k satisfies axiom* (Pa) *for all* $k \geq 1$.

Proof. For fixed a, b, p let $a' \in R_k(a, p)$ and $b' \in R_k(b, p)$. By Theorem 3.6 we have

$$R_k(a', b) = \bigcup_{z \in R_{k-1}(a',b)} [R_1(a', z) \cup R_1(z, b)] \qquad R_k(a, b') = \bigcup_{y \in R_{k-1}(a,b')} [R_1(b', y) \cup R_1(y, a)]$$

and hence

$$\begin{aligned} & R_k(a', b) \cap R_k(a, b') = \\ & \left(\bigcup_{z \in R_{k-1}(a',b)} [R_1(a', z) \cup R_1(z, b)] \right) \cap \left(\bigcup_{y \in R_{k-1}(a,b')} [R_1(b', y) \cup R_1(y, a)] \right) = \\ & \left(\left(\bigcup_{z \in R_{k-1}(a',b)} [R_1(a', z) \cup R_1(z, b)] \right) \cap \left(\bigcup_{y \in R_{k-1}(a,b')} R_1(b', y) \right) \right) \cup \\ & \left(\left(\bigcup_{z \in R_{k-1}(a',b)} [R_1(a', z) \cup R_1(z, b)] \right) \cap \left(\bigcup_{y \in R_{k-1}(a,b')} R_1(y, a) \right) \right) \\ & \supseteq \bigcup_{\substack{z \in R_{k-1}(a',b) \\ y \in R_k - 1(b',a)}} [R_1(a', z) \cap R_1(y, a)] \end{aligned}$$

Since $z = b \in R_{k-1}(a', b)$ and $y = b' \in R_{k-1}(a, b')$ we conclude $R_k(a', b) \cap R_k(a', b) \supseteq R_1(a', b) \cap R_1(a, b') \neq \emptyset$ by Lemma 3.7. □

The Pasch axiom (Pa) implies in particular (B3), as shown in [23]. Lemma 1 of [16] therefore implies that R_k also satisfies

(C4) $z \in R(x, y)$ implies $R(x, z) \cap R(z, y) = \{z\}$,

which in turn implies (B1).

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Furthermore, $\widehat{R}$ also satisfies (M) and therefore in particular (B2). As an immediate consequence we conclude that $\widehat{R_k}$ is geometric in the sense of Nebeský. Note that this is not true for R_k itself since (B2) is violated for all $k < n-1$ for all pairs of vertices with distance $d(x, \bar{x}) = n$. Lemma 1 of [22], furthermore, implies that $G_{\widehat{R_k}} = G_{R_k}$ is connected since $\widehat{R_k}$ is a transit function satisfying (B1) and (B2).

The requirement that G is connected in Corollaries 2.2 and 2.4 can therefore be replaced also by requiring that $\widehat{R}$ satisfies (Pa).

The main result of [24], see also [16], states that a geometric transit function R equals the interval function of its underlying graph, $R = I_{G_R}$, if and only if R satisfies in addition the two axioms

(S1) $|R(x, y)| = |R(z, w)| = 2$, $x \in R(y, w)$, and $y, w \in R(x, z)$, implies $z \in R(y, w)$.

(S2) $|R(x, y)| = |R(y, w)| = 2$, $y \in R(x, y)$, $w \notin R(x, z)$, $z \notin R(y, w)$ implies $y \in R(x, w)$.

Again we need (S1) and (S2) to hold for $\widehat{R}$ rather than R itself.

Lemma 3.9. *The 1-point crossover operator R_1 satisfies the* (S1) *axiom.*

Proof. Let R_1 be 1-point crossover operator. Since $|R(u, x)| = |R(v, y)| = 2$, it follows that u and x as well as v and y differ in only a single coordinate. Writing $u = (u_1, u_2, \ldots, u_i, u_{i+1}, \ldots, u_n)$ and assuming $u \in R(x, y)$ we must have either

(1) $u = (u_1, u_2, \ldots, u_i, u_{i+1}, \ldots, u_n) = (x_1, x_2, \ldots, x_i, y_{i+1}, \ldots, y_n)$, or

(2) $u = (u_1, u_2, \ldots, u_i, u_{i+1}, \ldots, u_n) = (y_1, y_2, \ldots, y_i, x_{i+1}, \ldots, x_n)$.

W.l.o.g., suppose u is of the form (1), therefore $u_1, u_2, \ldots, u_i = x_1, x_2, \ldots, x_i$ and $u_{i+1}, \ldots, u_n = y_{i+1}, \ldots, y_n$. Let $x \in R(u, v)$. Since u is of the form (1), we have $u_1, u_2, \ldots, u_i = x_1, x_2, \ldots, x_i$ and $x_{i+1}, \ldots, x_n = v_{i+1}, \ldots, v_n$. Let $y \in R(u, v)$. since u is of the form (1), we have $y_1, y_2, \ldots, y_i = v_1, v_2, \ldots, v_i$ and $y_{i+1}, \ldots, y_n = u_{i+1}, \ldots, u_n$. Hence $v = (v_1, v_2, \ldots, v_i, v_{i+1}, \ldots, v_n)$ can be written as $v = (y_1, y_2, \ldots, y_i, x_{i+1}, \ldots, x_n)$, which implies $v \in R(x, y)$. Thus the axiom (S1) follows. □

Lemma 3.10. *The 1-point crossover operator R_1 satisfies axiom* (S2).

Proof. From $|R(u, x)| = |R(v, y)| = 2$, it follows that u and x differ in only one coordinate, say i, and v and y differ in a single coordinate, say j. W.l.o.g., let $i \le j$. Since $v \notin R(x, y)$, y and v differ only in position j, we conclude that

(*) $x_j, \ldots, x_n \neq v_j, \ldots, v_n$.

From $x \in R(u, v)$ and (*) we obtain $x_1, \ldots, x_{j-1} = v_1, \ldots, v_{j-1} = y_1, \ldots, y_{i-1}$. Hence $x_j, \ldots, x_n = u_j, \ldots, u_n$. Therefore $x = (x_1, \ldots, x_{j-1}, x_j, \ldots, x_n) = (y_1, \ldots, y_{j-1}, u_j, \ldots, u_n)$. This implies $x \in R(u, y)$ and axiom (S2) follows. □

As shown in [16], the axiom

(MO) $R(x, y) \cap R(y, z) \cap R(z, x) \neq \emptyset$

implies both (S1) and (S2).

On hypercubes, i.e., assuming an alphabet with just two letters, uniform crossover $R = \widehat{R_k}$ satisfies $|R(x, y) \cap R(y, z) \cap R(z, x)| = 1$. The unique *median* $m = R(x, y) \cap R(y, z) \cap R(z, x)$ is defined coordinate-wise by majority voting of $x_i, y_i, z_i \in \{0, 1\}$, see [12]. On hypercubes, $\widehat{R_k}$ thus satisfy (MO). This argument fails, however, for general Hamming graphs. The reason is that axiom (MO) fails for each position at which the three sequences x, y, z are pairwise distinct: $\{0, 1\} \cap \{1, 2\} \cap \{2, 0\} = \emptyset$.

For $z \in R_k(x, y)$ let I denote the set of indices $0 = i_0 \le i_1 \le i_2 \le i_k = n$ from Definition 1.1 such that z is a k-point crossover offspring of x and y. If z is an offspring such that x is placed before y in the definition we denote this by $z = x \times_I y$ and $z = y \times_I x$ otherwise.

Lemma 3.11. *Let $d(a, b) > k+1$. If $s = a \times_I b$, $t = a \times_I b$ and $|I| = k$, then $s \times_j t \notin R_k(a, b)$ and $t \times_j s \notin R_k(a, b)$ holds for all $j \notin I$.*

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Proof. Since $j \notin I$ it follows that $s \times_j t = (a \times_I b) \times_j (b \times_I a)$ and $t \times_j s = (b \times_I a) \times_j (a \times_I b)$, we have $s \times_j t, t \times_j j \in R_{k+1}(a, b) \setminus R_k(a, b)$. □

Gitchoff et al. [10] conjectured that for each transit set $R_k(x, y)$ there is a unique pair of parents from which it is generated unless $R_k(x, y)$ is a hypercube. We settle this conjecture affirmatively:

Theorem 3.12. *If $d(u, v), d(x, y) > k + 1$ then $R_k(u, v) = R_k(x, y)$ if and only if $\{u, v\} = \{x, y\}$.*

Proof. The implication from right to left is trivial. For other direction we use Lemma 3.11. Assume, for contradiction, that $R_k(u, v) = R_k(x, y)$ and $\{u, v\} \neq \{x, y\}$. Then $x, y \in R_k(u, v)$ and $u, v \in R_k(x, y)$. From $R_k(u, v) = R_k(x, y)$ it follows also that $\widehat{R_k}(u, v) = \widehat{R_k}(x, y)$, which in turn implies $d(u, v) = d(x, y)$. Therefore, there exists a set of indices I, $|I| = k$, such that $x = u \times_I v$ and $y = v \times_I u$. From $d(x, y) > k+1$ and Lemma 3.11 we conclude that there exists $j \notin I$ such that $x \times_j y \notin R_k(u, v)$. Hence $R_k(u, v) \neq R_k(x, y)$. This contradiction completes the proof of the theorem. □

For the special case $k = 1$, Theorem 3.12 for $k = 1$ implies the following statement.

(H3) For every $x, y, u, v \in X$, $u \neq v$, $x \neq y$, $|R(x, y)| > 4$, $R(u, v) \subseteq R(x, y)$ implies that either $R(u, v) = \{u, v\}$ or $\{u, v\} = \{x, y\}$.

For $x, y \in X$ with $d(x, y) = t \geq 3$, the transit set $R_1(x, y)$ induces a cycle of size $2t$, and hence the only other transit sets that are included in $R_1(x, y)$ are singletons and edges.

4. Graph theoretical approach for k-point crossover operators

Transit sets $R(x, y)$ inherit a natural graph structure as an induced subgraph of the underlying graph G_R. In the case of crossover operators and their corresponding transit sets $R_k(x, y)$, the distance in the underlying graph plays a crucial role in their characterization.

Recall that n-dimensional hypercubes are antipodal graphs, i.e., for any vertex v there is a unique antipodal vertex $\overline{v}$ with $d(v, \overline{v}) = \text{diam}(G) = n$, where diam$(G)$ denotes the diameter of graph G. The vertex $\overline{v}$ is obtained from v by reversing all coordinates.

Theorem 4.1. *$R_k(x, y)$ induces an antipodal graph such that $\overline{x} = y$, $\overline{y} = x$, and for each $u \in R_k(x, y)$ of the form $u = x \times_I y$ we have $\overline{u} = y \times_I x$.*

Proof. The definition of R_k immediately implies that x and y are at the maximal distance from each other and every other $v \in R_k(x, y)$, $v = x \times_I y$, has a unique vertex at maximal distance in $R_k(x, y)$, that is $\overline{v} = y \times_I x$. □

Note that here v and $\overline{v}$ are antipodal in a subgraph $R_k(x, y)$ and will not be antipodal in the underlying graph G_R, unless $d(v, \overline{v}) = \text{diam}(G_R)$. This is not the only property inherited from hypercubes. We say that H is an *isometric subgraph* of a graph G if for every pair of vertices $u, v \in V(H)$ the distance from G is preserved, i.e., if $d_H(u, v) = d_G(u, v)$. Isometric subgraphs of hypercubes are known as *partial cubes* [18,25]. It is shown in [10] (1) that $R_1(x, y)$ induces C_{2t}, a cycle of length $2t$, where $t = d(x, y)$, and (2) that $d_{C_{2t}}(u, v) = d_{G_{R_1}}(u, v)$ holds for every pair $u, v \in R_1(x, y)$. In other words $R_1(x, y)$ is a partial cube. Theorem 3.6 implies that this result holds in general:

Corollary 4.2. *The k-point crossover operator R_k induces a partial cube.*

In particular, therefore, R_k always induces a connected subgraph of G_R.

In the remainder of this section we consider only the binary case.

Definition 4.1. Let R be a transit function R on a set X. Then we set $uv \parallel xy$ if and only if $v, x \in R(u, y)$ and $u, y \in R(v, x)$.

The binary relation $\parallel$ was introduced in [26] in the context of a characterization of so called X-nets, a structure from phylogenetic combinatorics that is intimately connected with partial cubes. Indeed, $\parallel$ can be used to characterize partial cubes [26]:

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Proposition 4.3. *Let G be a graph and $R = I_G$, then G is a partial cube if and only if the relation $\|$ is an equivalence relation on the set of its edges.*

By the definition, the relation $\|$ is reflexive and symmetric. Therefore it suffices to require that $\|$ is a transitive relation. Proposition 4.3 thus can be translated into the language of transit functions:

Theorem 4.4. *Let R be a transit function on a set X. Then the underlying graph G_R is partial cube if and only if R satisfies:*

(AX) *for all $a, b, c, d, e, f \in X$, with $|R(a, b)| = |R(c, d)| = |R(e, f)| = 2$ and $ab \| cd$ and $cd \| ef$ it follows that $ab \| ef$.*

It is worth noting that the axiom (AX) can be also described purely in a transit sets notation as follows:

(AX') for all $a, b, c, d, e, f \in X$, with $|R(a, b)| = |R(c, d)| = |R(e, f)| = 2$ and $b, c \in R(a, d)$, $a, d \in R(b, c)$, $d, e \in R(c, f)$ and $c, f \in R(d, e)$ it follows that $b, e \in R(a, f)$ and $a, f \in R(b, e)$.

For a partial cube G, the equivalence classes of the relation $\|$ are called *cuts* and we denote the set of all cuts by $\mathcal{C} = \{C_1, C_2, \ldots, C_n\}$, where n is the dimension of the smallest hypercube into which G embeds isometrically. Cuts form a minimal edge partition of the edge set in a partial cube with the property that removal of all edges from a given cut results in a disconnected graph with exactly two connected components. These are called *splits* [25,27].

Cuts of the partial cubes correspond to the coordinates in the corresponding isometric embedding into the hypercube and they induce a binary labelling of the strings: for a cut C_i vertices from one part of the split induced by C_i are labelled “0” in coordinate i, and vertices from the other part of the split are labelled “1” in coordinate i. For any pair of parallel edges xy, uv in a partial cube the notation can be chosen such that $d(u, x) = d(v, y) = d(u, y) - 1 = d(v, x) - 1$. The distance between any two vertices in a partial cube therefore can be computed as the Hamming distance between the corresponding binary labellings, which in turn corresponds to the number of cuts that separate the two vertices. In other words, any shortest path between two vertices in a partial cube is determined by the cuts it traverses. Moreover, any shortest path traverses each cut at most once. We refer to [18,25] for the details; there, the cuts are called Θ-classes.

Let us denote the cuts appearing in the partial cube $R_1(x, y)$ by $C(x, y)$. We have $|C(x, y)| = d(x, y)$. For any pair of vertices x, y in a hypercube with $d(x, y) = t$ we have $t!$ possible ways to choose a shortest path between them, because each of the $t!$ possible orders in which the corresponding cuts that are traversed results in a distinct path. Therefore there are also $t!$ ways to choose an isometric cycle through x and y. The definition of the 1-point crossover operator, on the other hand, identifies a unique isometric cycle between $x, y \in V(G_R)$.

The binary labelling of vertices in a partial cube naturally induces a lexicographic ordering of vertices. Similarly, by taking first the labelling of the minimal vertex and concatenating it with the labelling of the remaining vertex, we can also lexicographically order the edges of a partial cube (Fig. 5). The idea can further be generalized to a lexicographic ordering of all paths and cuts of a partial cube. The following result shows the 1-point crossover is intimately related to this lexicographic order.

Theorem 4.5. *Let $x, y \in X = \{0, 1\}^n$. Then $R_1(x, y)$ consist of all vertices appearing on lexicographically minimal and maximal paths between x and y.*

Proof. The statement follows immediately from the definition of the 1-point crossover operator. □

Problem 4.1. Is it true that $R_k(x, y)$ consist of all vertices appearing on $\frac{k!}{2}$ pairs of first and last lexicographically minimal and maximal paths between x and y?

For $x, y \in X\{0, 1\}^n$ and any shortest path between them, there is exactly one path along which the cuts appear in the reverse order. Consider any $u \in R_1(x, y) \setminus \{x, y\}$. There is exactly one shortest path between u and x in $R_1(x, y)$. For $k > 1$ and $d(x, y) = t$ both x and y have exactly t neighbours in $R_k(x, y)$. Moreover as shown above, see Fig. 4, for $u \in R_k(x, y)$, it may be the case that $R_k(x, u) = \widehat{R_k}(x, u) \subseteq R_k(x, y)$. Hence the lexicograpic order of cuts does not uniquely determine a shortest path in $R_k(u, x)$. The structure of $R_k(u, v)$ hence is much richer and calls for more “dimensions”.

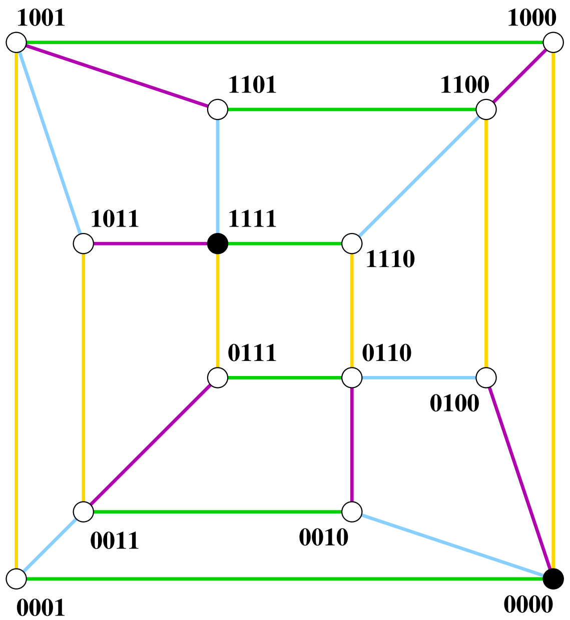

Fig. 4. $R_2(0000, 1111)$ together with coloured cuts. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Problem 4.2. Compute the size of cuts for R_k, i.e., the number of edges belonging to the common cut.

The degree sequence of the graphs induced by 1-point crossover and uniform crossover operators are monotone. In the first case all values are equal to 2, and in the second case they equal the length of the string n.

Problem 4.3. Let $d(a, b) = t > k + 1 > 2$. Determine degree sequences of the graphs induced by $R_k(a, b)$.

Lemma 4.6. *Let $a, b \in X = \{0, 1\}^n$ and $k > 1$. Then the maximum and the minimum degree of a graph induced by $R_k(a, b)$ equal n and $k + 1$, respectively.*

Proof. Clearly the graph induced by $R_2(a, b)$ includes all neighbours of x and y in $\{0, 1\}^n$, hence the maximum degree of a graph induced by $R_2(a, b)$, and consequently of graphs induced by $R_k(a, b)$, for $k > 2$, is n. W.l.o.g., let $a = 0 \dots 0$ and $b = 1 \dots 1$. Then $R_k(a, b)$ consist of all binary strings with less than $k+1$ blocks of consecutive 0's or 1's. Hence the minimum degree in a graph induced by $R_k(a, b)$ is attained by vertex corresponding to a binary string consisting of exactly k different blocks of consecutive 0's or 1's, and they have exactly $k + 1$ neighbours in a graph induced by $R_k(a, b)$. □

A solution of Problem 4.3 could help solve

Problem 4.4. Does R_k induce a k-connected graph?

For an axiomatic characterization of R_1 in terms of transit functions axioms it is easy to translate graph theoretic properties related to the fact that $R_1(x, y)$ induces an isometric cycle in $\{0, 1\}^n$ in the language of transit functions. In addition, however, it would also be necessary to express a consistent ordering of the cuts that appear in the isometric cycles in terms of transit function. While this appears possible, it seems to be cumbersome and does not promise additional insights into the structure of the transit sets. Hence we do not pursue this issue further.

5. Combinatorial properties of recombination sets

Since the monotonicity axiom (M) fails for k-point crossover with $k < n - 1$, an alternative axiom was proposed in [10]:

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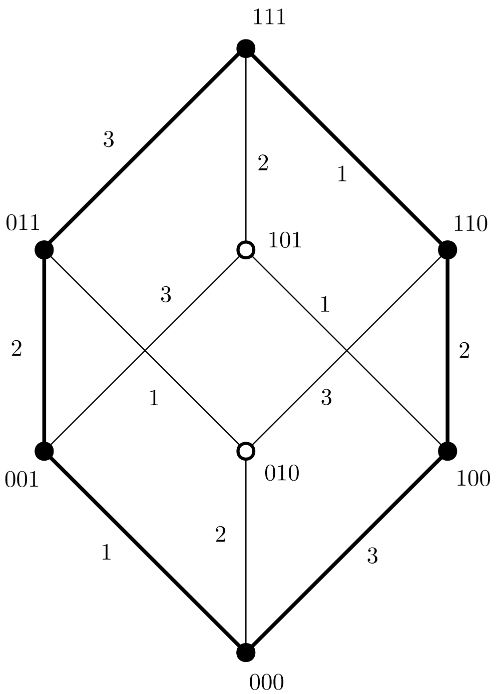

Fig. 5. $R_1(000, 111)$ in K_2^3 is represented with black vertices and fat edges. Lexicographic ordering of the vertices of K_2^3: starting at 000 bottom-up and then in each level from left to right; labelling of the edges corresponds to the induced lexicographic ordering of cuts.

(GW3) For all $x, y \in X$ and all $u, v \in R(x, y)$ holds $|R(u, v)| \leq |R(x, y)|$.

stipulating monotonicity in size. This is proper relaxation of (M), which obviously (M) implies (GW3). In order to derive explicit expressions for $|R_k(x, y)|$ we note that, for given vertices x and y, the hypercube can be relabelled in such a way that x becomes the all-zero string and y is a 01-string with 1's at exactly the positions where x and y differ. Thus the size of the recombination sets $|R_k(x, y)| =: r_k(t)$ depends only on the order k of the recombination operator and the Hamming distance $t := d(x, y)$. In the following we write

$$\Phi_h(n) := \sum_{i=0}^{h} \binom{n}{i}. \tag{2}$$

In order to compute $r_k(t)$, we have to distinguish the case of small and large Hamming distances.

Theorem 5.1. *Let $1 \leq k < t$. Then*

$$r_k(t) = \begin{cases} 2^t & \text{if} \quad t \leq k \\ 2\,\Phi_k(t-1) & \text{if} \quad t > k \end{cases} \tag{3}$$

Proof. Consider two strings x and y. From [10] we know that $|R_1(x, y)| = 2t$. For all children of x and y that are obtained by i-point crossover, $1 \leq i \leq k$ with exactly i cuts, we have i possibilities for choosing the cuts along $t-1$ positions. This amounts to a total of $\binom{t-1}{i}$ possibilities in 2 different choices for the ordering of parents. If $t \leq k$ cuts may be placed simultaneously between any two positions in which x and y differ, i.e., i takes values from 0 to $t-1$. Thus $r_k(t) = 2\sum_{i=0}^{t-1}\binom{t-1}{i} = 2\,\Phi_{t-1}(t-1) = 2 \cdot 2^{t-1} = 2^t$. For $t > k$ the number of possible cuts is limited by k and hence $r_k(t) = 2\,\Phi_k(t-1)$. □

Parts of this result were already observed by [10]. In particular, $r_1(t) = 2t$ for $t > 1$, $r_2(t) = t^2 - t + 2$ for $t > 2$, $r_k(k+1) = 2^{k+1}$, and $r_k(k+2) = 2^{k+1} - 2$.

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The latter equation shows that $R_{k-1}(x, y)$ for $d(x, y) = k + 1$ misses exactly two points compared to $R_k(x, y)$, i.e., $R_k(x, y) \setminus R_{k-1}(x, y) = \{a, b\}$. Thus we can conclude immediately that $a = x \times_I y$, $b = y \times_I x$ with $|I| = k$. Since every $x, y, x \neq y$, has a unique a, b with the above property, we obtain another simpler proof of Theorem 3.12.

From $r_k(t) = 2^t$ for $t \leq k + 1$ and the fact that $\widehat{R_k}(x, y)$ is a hypercube K_2^t of dimension t for $d(x, y) = t$ we immediately conclude that $R_k(x, y)$ is also a hypercube for $t \leq k + 1$.

Let G be partial cube and let H be a graph obtained by contracting some of the cuts of G, i.e. by forgetting some of the coordinates in binary labelling of vertices. If H is isomorphic to some hypercube, then we say that H is a *cube minor* of G.

Lemma 5.2. *Consider $R_k(x, y)$ as an induced subgraph of the boolean hypercube K_2^n, and suppose $d(x, y) \geq k+1$. Then the largest cube minors of $R_k(x, y)$ are isomorphic to K_2^{k+1}.*

Proof. This is an immediate consequence of Lemma 3.5 and Theorem 3.6. □

The Vapnik–Chervonenkis dimension (or VC-dimension) measures the complexity of set systems. Originally introduced in learning theory [28], it has found numerous applications e.g. in statistics, combinatorics and computational geometry, see [29]. Consider a base set X and family $\mathcal{H} \subseteq 2^X$. A set $C \subseteq X$ is *shattered by* $\mathcal{H}$ if $\{Y \cap C | Y \in \mathcal{H}\} = 2^C$. The VC-dimension of $\mathcal{H}$ is the largest integer d_{VC} such that there is a set C of cardinality d_{VC} that is shattered by $\mathcal{H}$. For $\mathcal{H} = \emptyset$, $d_{VC} = -1$ by definition.

Clearly, X is shattered by $\mathcal{H} = 2^X$, hence the VC-dimension of the Boolean hypercube $\{0, 1\}^d$ is d. Now consider an even cycle C_{2t} of length $2t$, isometrically embedded into t dimensional hypercube. It is not hard to check that the VC-dimension of C_{2t} is 2 for any $t \geq 2$. More generally, the VC-dimension of a partial cube G, with d cuts, equals the dimension of the largest cube-minor in G, because this is the largest cardinality of a set of coordinates that can be shattered by the set of all d of cuts of G.

Theorem 5.3. *The VC-dimension of $R_k(x, y)$ equals $k + 1$ whenever $d(x, y) > k$. Otherwise the VC-dimension of $R_k(x, y)$ equals $d(x, y)$.*

Proof. If $d(x, y) \leq k$ then $R_k(x, y)$ induces graph isomorphic to d-dimensional hypercube, where $d = d(x, y)$. Let $d = d(x, y)$. If $d > k$ then we need to contract $d - k - 1$ cuts (ignore the corresponding coordinates) to obtain a cube minor of dimension $k + 1$. □

6. Concluding remarks

Crossover operators are a key ingredient in the construction of algorithms in Evolutionary and Genetic Programming. Their purpose is to construct offspring that are a "mixture" of the two parental genotypes, an idea that is captured well by the concept of transit functions. In this contribution we have investigated in detail the transit sets of homologous crossover operators for strings of fixed length and their combinatorial, graph theoretic, and topological properties. As shown by [10] 1-point crossover operators correspond to circles, that is, rather simple 2-dimensional objects. For $k > 1$ we have shown that k-point crossover operators are of more complex nature and correspond to higher dimensional objects, which is appropriately measured by the VC-dimension. The connection of k-point crossover on binary strings with oriented matroids and pseudosphere arrangements will be explored in a forthcoming contribution.

The results presented here suggest to consider transit sets of recombination operators for state spaces other than strings. Natural candidates are many crossover operators for permutation problems. A subset of these was compared e.g. in [30,31] but very little is known about the algebraic, combinatorial, and topological properties. Interestingly, the 1-point crossover operator R_1 satisfies all axioms except (B2) of the axioms characterizing the interval function of an arbitrary connected graph. Nevertheless, there are striking differences even though both functions induce the same convexity as noted in Lemma 3.2.

Finally, recombination operators influence in a critical manner the way how genetic information is passed down through the generalizations in diploid populations. The corresponding nonassociative algebraic structures so far have been studied mostly as generalizations of Mendel's laws [32,33], see also [34,35]. We suspect that a better understanding of the structure of recombination operators will also be of interest in this context.

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References

[1] T.M. English, Some geometric and algebraic results on crossover, in: Evolutionary Programming VI, in: Lect. Notes Comp. Sci., vol. 1213, Springer Verlag, Heidelberg, 1997, pp. 285–295.
[2] J.C. Culberson, Mutation-crossover isomorphisms and the construction of discriminating functions, Evol. Comp. 2 (1995) 279–311.
[3] K. DeJong, W.M. Spears, A formal analysis of the role of multi-point crossover in genetic algorithms, Ann. Math. Artif. Intell. 5 (1992) 1–26.
[4] L.M. Schmitt, Theory of genetic algorithms, Theoret. Comput. Sci. 259 (2001) 1–61.
[5] P.F. Stadler, R. Seitz, G.P. Wagner, Evolvability of complex characters: population dependent Fourier decomposition of fitness landscapes over recombination spaces, Bull. Math. Biol. 62 (2000) 399–428.
[6] D. Goldberg, Genetic algorithms and Walsh functions: a gentle introduction, Complex Syst. 3 (1989) 129–152.
[7] P. Field, Nonbinary transforms for genetic algorithm problems, Complex Syst. 9 (1995) 11–28.
[8] J. Holland, Adaptation in Natural and Artificial Systems, MIT Press, Cambridge, MA, 1975.
[9] N.J. Radcliffe, The algebra of genetic algorithms, Ann. Math. Artif. Intell. 10 (1994) 339–384.
[10] P. Gitchoff, G.P. Wagner, Recombination induced hypergraphs: a new approach to mutation-recombination isomorphism, Complexity 2 (1996) 47–43.
[11] H.M. Mulder, Transit functions on graphs (and posets), in: M. Changat, S. Klavžar, H.M. Mulder, A. Vijayakumar (Eds.), Convexity in Discrete Structures, in: RMS Lecture Notes Series, 2008, pp. 117–130.
[12] H.M. Mulder, The Interval Function of a Graph, in: Math. Centre Tracts, vol. 132, Math. Centre, Amsterdam, NL, 1980.
[13] M. Shpak, G.P. Wagner, Asymmetry of configuration space induced by unequal crossover: implications for a mathematical theory of evolutionary innovation, Artif. Life 6 (1999) 25–43.
[14] A. Moraglio, R. Poli, Topological interpretation of crossover, in: K. Deb, R. Poli, W. Banzhaf, H.G. Beyer, E. Burke, P. Darwen, D. Dasgupta, D. Floreano, J. Foster, M. Harman, O. Holland, P.L. Lanzi, L. Spector, A. Tettamanzi (Eds.), Genetic and Evolutionary Computation – GECCO 2004, in: Lect. Notes Comp. Sci., vol. 3102, 2004, pp. 1377–1388.
[15] L. Nebeský, The interval function of a connected graph and a characterization of geodetic graphs, Math. Bohem. 126 (2001) 247–254.
[16] H.M. Mulder, L. Nebeský, Axiomatic characterization of the interval function of a graph, European J. Combin. 30 (5) (2009) 1172–1185.
[17] M. Changat, S. Klavžar, H.M. Mulder, The all-paths transit function of a graph, Czechoslovak Math. J. 51 (2) (2001) 439–448.
[18] R. Hammack, W. Imrich, S. Klavžar, Handbook of Product Graphs, second ed., CRC Press, Boca Raton, FL, 2011.
[19] J.M. Laborde, S.P. Rao Hebbare, Another characterization of hypercubes, Discrete Math. 39 (2) (1982) 161–166.
[20] M. Mollard, Two characterizations of generalized hypercube, Discrete Math. 93 (1) (1991) 63–74.
[21] M. van de Vel, Matching binary convexities, Topol. Appl. 16 (1983) 207–235.
[22] M. Changat, J. Mathew, H.M. Mulder, The induced path function, monotonicity and betweenness, Discrete Appl. Math. 156 (2010) 426–433.
[23] M. van de Vel, Theory of Convex Structures, vol. 50, North Holland, Amsterdam, 1993.
[24] L. Nebeský, A characterization of the interval function of a connected graph, Czechoslovak Math. J. 44 (1994) 173–178.
[25] S. Ovchinnikov, Graphs and Cubes, Springer, New York, NY, 2011.
[26] A.W.M. Dress, The category of X-nets, in: J. Feng, J. Jost, M. Qian (Eds.), Networks: From Biology to Theory, Springer, London, UK, 2007, pp. 3–22.
[27] A.W.M. Dress, K.T. Huber, J. Koolen, V. Moulton, A. Spillner, Basic Phylogenetic Combinatorics, Cambridge University Press, Cambridge, UK, 2012.
[28] V. Vapnik, A. Chervonenkis, On the uniform convergence of relative frequencies of events to their probabilities, Theory Probab. Appl. 16 (1971) 264–280.
[29] V. Vovk, H. Papadopoulos, A. Gammerman (Eds.), Measures of Complexity: Festschrift for Alexey Chervonenkis, Springer, Heidelberg, 2015.
[30] K. Puljić, R. Manger, Comparison of eight evolutionary crossover operators for the vehicle routing problem, Math. Commun. 18 (2013) 359–375.
[31] A. Bala, A.K. Sharma, A comparative study of modified crossover operators, in: H. Saini, S.P. Ghrera, V.K. Sehgal (Eds.), Third International Conference on Image Information Processing, ICIIP, IEEE, Piscataway, NJ, 2015, pp. 281–284.
[32] S. Bernstein, Demonstration mathématique de la loi d’hérédité de Mendel, C. R. Acad. Sci. Paris 177 (1923) 528–531.
[33] I.M.H. Etherington, Genetic algebras, Proc. Roy. Soc. Edinburgh 59 (1939) 242–258.
[34] A. Wörz-Busekros, Algebras in Genetics, vol. 36, Springer-Verlag, New York, 1980.
[35] Y.I. Lyubich, Mathematical Structures in Population Genetics, Springer-Verlag, New York, 1992.