Topological Representation of the 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. Moreover, the transit sets of $k$-point crossover on binary strings form topes of uniform oriented matroid of VC-dimension $k + 1$. The Topological Representation Theorem for oriented matroids therefore implies that $k$-point crossover operators can be represented by pseudosphere arrangements. This provides the tools necessary to study the special case $k = 2$ in detail.

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 offsprings 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 $A$ of $a \geq 2$ letters. Given two parental strings $x = (x_1x_2\ldots x_n)$ and $y = (y_1y_2\ldots y_n)$ one may for instance construct recombinant offsprings of the form $(x_1x_2\ldots x_iy_{i+1}y_{i+2}\ldots y_n)$ and $(y_1y_2\ldots y_ix_{i+1}x_{i+2}\ldots x_n)$. 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 Given $x, y, z \in A^n$ we say that $z$ is a $k$-point crossover offspring of $x$ and $y$ if there are indices $0 = i_0 \leq i_1 \leq i_2 \leq \ldots \leq i_k = n$ so that for all $\ell$, $1 \leq \ell \leq k$, either $z_j = x_j$ for all $j \in \{i_{\ell-1} + 1, \ldots, i_{\ell}\}$ or $z_j = y_j$ for all $j \in \{i_{\ell-1} + 1, \ldots, i_{\ell}\}$.

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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 offsprings.

Properties of $k$-point crossover have been studied extensively in the past. [English(1997)] described key algebraic properties and isomorphisms between the search spaces induced by crossover and mutation with small populations have been analyzed by [Culberson(1995)]. A formal treatment of multi-point crossover with an emphasis on disruption analysis can be found in [DeJong and Spears(1992)]. A general review of genetic algorithms from the perspective of stochastic processes on populations can be found in [Schmitt(2001)]. In this context, crossover operators are represented by stochastic matrices. A similar matrix-based formalism is explored in [Stadler et al.(2000)Stadler, Seitz, and Wagner]. Coordinate transformations, more precisely the Walsh transform [Goldberg(1989)] and its generalizations to non-binary alphabets [Field(1995)] have played an important role in explaining the functioning of GAs in terms of building blocks and the Schema theorem [Holland(1975)]. As a generalization, an abstract treatment of crossover in terms of equivalence relations has been given by [Radcliffe(1994)].

[Gitchoff and Wagner(1996)] proposed to consider the function $R : X \times X \rightarrow 2^X$ 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 more than a decade, the seminal paper was published recently [Mulder(2008)]. 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 $I_G(x, y)$ [Mulder(1980)] 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 the work by [Shpak and Wagner(1999)]. 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 $R(x, z) \subseteq R(x, y)$. 

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 and Poli (2004) 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 Moraglio and Poli (2004), 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 transit sets of \( G \) vertices and the edges of \( R \) only if \( R \) satisfies a set of axioms that are phrased in terms of \( R \) itself. Hence we say that \( R \) is *MP-geometric* if

\[
\text{(MG)} \quad R(x, y) \subseteq I_G(x, y) \quad \text{for all} \quad x, y \in X.
\]

Note the condition (MG) is an axiom for transit functions independent of any externally prescribed structure on \( X \). Mulder (2008) considered a different notion of “geometric” referring transit functions that satisfy (B2) and the axiom

\[
\text{(B3)} \quad z \in R(x, y) \quad \text{and} \quad w \in R(x, z) \quad \text{implies} \quad z \in R(w, y).
\]

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 offsprings reachable from the parents \( x \) and \( y \) in a single generation. It is natural then to associate with \( R \) a function \( \hat{R} : X \times X \to 2^X \) so that \( z \in \hat{R}(x, y) \) if and only if \( z \) eventually can be generated from \( x \) and \( y \) and all their following generations of offsprings. Formally, \( z \in \hat{R}(x, y) \) if there is a finite sequence of pairs \( \{x_k, y_k\} \) so that \( z \in \hat{R}(x_{m}, y_m) \), \( \{x_k, y_k\} \in R(x_{k-1}, y_{k-1}) \) for all \( k = 1, \ldots, m \), \( x_0 = x \), and \( y_0 = y \). By construction, \( R(x, y) \subseteq \hat{R}(x, y) \) for all \( x, y \in X \).

If \( R \) is a transit function, then \( \hat{R} \) is also a transit function.

We say that \( R(x, y) \) is *closed* if \( R(x, y) = \hat{R}(x, y) \). 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

\[
\text{(M)} \quad \text{For all} \quad x, y \in X \quad \text{and} \quad u, v \in R(x, y) \quad \text{implies} \quad R(u, v) \subseteq R(x, y),
\]

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

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. Nebeský (2001) showed 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. Later, Mulder and Nebeský (2009) improved the axiomatic characterization of \( I(u, v) \) by formulating a nice set of (minimal) axioms. The all-paths function \( A \) of a connected graph \( G \) (defined as \( A(u, v) = \{z \in V(G) : z \text{ lies on some } u, v \text{-path in } G\} \) admits a similar axiomatic characterization Changat et al. (2001). Changat, Klavžar, and Mulder. These results

\[\text{(i)} \quad R(x, y) \subseteq \hat{R}(x, y) \quad \text{by definition,} \quad \text{(ii)} \quad R(x, y) = \{x, y\} \quad \text{implies} \quad \hat{R}(x, y) = \{x, y\}, \quad \text{and} \quad \text{(iii)} \quad \text{if } \hat{R}(x, y) = \{x, y\} \quad \text{but} \quad R(x, y) \neq \{x, y\} \quad \text{either (i) or axiom (T1) is violated.}\]
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 specialised 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 organised 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. In order to generalize these results we consider topological aspects of $k$-point crossover in section 6 and explore its relationship with oriented matroids. We conclude our presentation with several open questions.

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 $A_i$ with $a_i := |A_i| \geq 2$ 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 by [Hammack et al. (2011)]Hammack, Imrich, and Klavžar 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 $K_n^2$. 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 string $x$ and $y$ differ.

Given a transit function $R$ and a point $x \in X$ let $\delta(x) = |\{y \in X \mid |R(x, y)| = 2\}|$, 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 by [Mulder(1980)] and [Laborde and Rao Hebbare(1982)].

Proposition 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 $\delta$ 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 [Mulder(1980)]. We note that the condition $|V(G)| = 2^\delta$ in Proposition 1 is necessary as demonstrated by the example in Fig. 1.

Proposition 1 can be translated into the language of transit functions as follows:

Corollary 1 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 $K_n^2$ if and only if $R$ satisfies:

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

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Figure 1. The last condition of Proposition 1, i.e., $|V(G)| = 2^δ$, is necessary as demonstrated by this example of a $(0,2)$-graph that is not a hypergraph [Mulder(1980)]. It satisfies all but the last requirement from the proposition.

(A2) $δ(R) = n$ and $|X| = 2^n$.

Later, [Mollard(1991)] generalized Proposition 1 to arbitrary Hamming graphs. 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 ([Mollard(1991)]) Let $G$ be a simple connected graph such that two non-adjacent vertices in $G$ either have exactly 2 common neighbors or none at all, and suppose $G$ has neither $K_4 \backslash e$ nor $K_2 \square K_3 \backslash e$ (Figure 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.

Figure 2. The forbidden induced subgraphs $K_4 \backslash e$ and $K_2 \square K_3 \backslash e$ appearing in Proposition 2.

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

Corollary 2 Let $R$ be a transit function with a connected underlying graph. Then the underlying graph $G_R$ is isomorphic to Hamming graph $K_n^a$ 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') $δ(R) = n(a - 1)$ 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 $|R(u, v)|, |R(u, w)|, |R(u, z)|, |R(v, u)|, |R(x, u)|, |R(v, z)| > 2.$
The representation of Hamming graphs as $n$-fold Cartesian products of complete graphs $H = \prod_{i=1}^{n} K_{2}$, implies a “coordinatization”, that is, a labeling of the vertices the reflects this product structure. The geodesic intervals in Hamming graphs then have very simple description:

\[ I_H(x, y) = \{ z = (z_1, z_2, \ldots, z_n) | z_i \in \{x_i, y_i\} \text{ for } 1 \leq i \leq n \} \]

(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 the book by [Hammack et al. (2011)].

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 1** 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 [Mulder (1980)]. □ It is well known that $I_H$ satisfies the monotone axiom (M) and thus also (B2).

**Lemma 2** 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 $Q''_i = \{x_i | x \in Q''\}$ contains at most two different letters from the alphabet $A_i$. $Q' \cap Q'' = \bigcap_i (Q'_i \cap Q''_i)$, 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 $R(u, v) \cap R(x, y) = \emptyset$ then there are $p, q \in X$ so that $R(u, v) \cap R(x, y) = R(p, q)$.

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 by [van de Vel (1983)], 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 only if $x <_a y$.

**Lemma 3** 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 $C = (a = a_0, a_1, \ldots, a_t = b)$ be a maximal $\leq_a$-chain between $a$ and $b$, where the elements are labeled 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., $a_i <_a x <_a a_{i+1}$.
contradicting maximality of the chain $C$. Hence $C$ 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 hold in general. Similarly, we cannot use Lemma 1 of Changat, Mathew, and Mulder, 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 $\hat{R}$ we can make use of the fact that $G_R = G_{\hat{R}}$. Since $\hat{R}$ satisfies the monotonicity axiom (M) by construction, (B2) is also satisfied. Thus $R_G$ is connected if at least one of the following two conditions is satisfied: (i) $\hat{R}$ satisfies (B1), or (ii) $\hat{R}$ satisfies

\[(CG') \quad x \in \hat{R}(a, z) \mbox{ and } z \in \hat{R}(a, y) \mbox{ if and only if } z \in \hat{R}(x, y)\]

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) $R(x, y) \subseteq R(x, y)$.

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 4** $G_{R_k} = \prod_{i=1}^n K_{a_i}$ 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 4 and Corollary 2 we immediately conclude that the $k$-point crossover transit function $\hat{R}_k$ satisfies (A1), (A2'), (A3), and (A4).

**Lemma 5** Let $R_k$ be the $k$-point crossover function. Then $\hat{R}_k(x, y) = I_{G_{R_k}}(x, y)$ for all $x, y \in X$ and all $k \geq 1$.

**Proof** By construction $z \in \hat{R}_k(x, y)$ 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 $\hat{R}_k(x, y) \subseteq I_{G_{R_k}}(x, y)$. Conversely, choose an arbitrary $z \in I_{G_k}(x, y)$. 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 $x' \in R_1(x, y') \subseteq R_1(x, y)$ by recombinating 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 $x' \in \hat{R}_1(x, y)$ we can repeat the argument at most $n$ time to find a sequence $x^{(n)} \in \hat{R}_1(x, y)$ 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 $z \in \hat{R}_k(x, y)$.

As an immediate corollary we have:

**Corollary 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 5 also implies a negative answer to one of the questions posed by [Mulder, 2008]: “Is the geodesic convexity uniquely determined by the geodesic interval function \( I(u, v) \) of a connected graph?” More precisely, Lemma 5 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 \( I_{G_n}(x, y) \), being the interval in a hypercube, is itself convex.

A trivial consequence of Lemma 5, 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 4** \( R_{n-1}(x, y) = \overline{R_{n-1}}(x, y) = I_{G_n}(x, y) \) for all \( x, y \in X \).

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

**Lemma 6** \( R_k(x, y) = I_{G_n}(x, y) \) if and only if \( d(x, y) \leq k + 1 \).

**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 \( a_i \) 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 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. [22]. 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 \( (b_1 \ldots b_1, p_{l+1} \ldots p_k, a_{k+1} \ldots a_n) \in R_1(b, a') \cap R_1(a, b') \). 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).

**Theorem 2** \( R_k \) satisfies axiom (Pa) for all \( k \geq 1 \).
Figure 3. Sketch of the proof of Lemma 7. We distinguish 6 cases depending on how $a'$ and $b'$ are constructed in $R_1(a,b)$ and $R_1(a',b')$, respectively. The red lines indicate the explicit construction of an element in $R_1(a,b') \cap R_1(a',b)$.

Proof For fixed $a, b, p$ let $a' \in R_k(a,p)$ and $b' \in R_k(b,p)$. By Theorem 1 we have

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

and hence

$$R_k(a',b) \cap R_k(a,b') =$$

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

$$\left( \bigcup_{z \in R_{k-1}(a',b)} [R_1(a',z) \cup R_1(z,b)] \right) \cap \left( \bigcup_{y \in R_{k-1}(a,b')} R_1(b',y) \right) \cup$$

$$\left( \bigcup_{z \in R_{k-1}(a',b)} [R_1(a',z) \cup R_1(z,b)] \right) \cap \left( \bigcup_{y \in R_{k-1}(a,b')} R_1(y,a) \right) \supseteq \bigcup_{z \in R_{k-1}(a',b') \cap R_1(y,a)} [R_1(a',z) \cap R_1(y,a)]$$

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 7.

The Pasch axiom (Pa) implies in particular (B3), as shown by van de Vel (1993). Lemma 1 of Mulder and Nebeský (2009) 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).

Furthermore, $\hat{R}$ also satisfies (M) and therefore in particular (B2). As an immediate consequence we conclude that $\hat{R}_k$ 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 $d(x,\hat{x}) = n$. Lemma 1 of Changat et al. (2010) Changat, Mathew, and Mulder.
furthermore, implies that $G_{\hat{R}} = G_R$ is connected since $\hat{R}$ is a transit function
satisfying (B1) and (B2).

The requirement that $G$ is connected in Corollary \ref{cor:1} and \ref{cor:2} can therefore be replaced
also by requiring that $\hat{R}$ satisfies (Pa).

The main result of \cite{Nebesky1994}, see also \cite{MulderNebesky2009}, states that a
geometric transit function $R$ equals the interval function of its underlying graph,
$R = I_{G_n}$, if and only if $R$ satisfies in addition the two axioms

\begin{align}
\text{(S1)} & \quad |R(x, y)| = |R(z, w)| = 2, \ x \in R(y, w), \text{ and } y, w \in R(x, z), \text{ implies } z \in R(y, w). \\
\text{(S2)} & \quad |R(x, y)| = |R(y, w)| = 2, \ y \in R(x, y), \ w \notin R(x, z), \ z \notin R(y, w) \text{ implies } y \in R(x, w).
\end{align}

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

**Lemma 8** 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 $u$

\[ u = (u_1, u_2, \ldots, u_i, v_{i+1}, \ldots, v_n) \] 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. \hfill $\Box$

**Lemma 9** 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 $i \leq j$. Since $v \notin R(x, y)$, $y$ and $v$ differ only in position $j$, we conclude that

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

From $x \in R(u, v)$ and (*) we obtain $x_1, \ldots, x_{j-1} = v_1, \ldots, v_{j-1} = y_1, \ldots, y_{j-1}$. 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. \hfill $\Box$

As shown in \cite{MulderNebesky2009}, the axiom

\text{(MO)} \quad 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
$R = \hat{R}_k$ satisfies $|R(x, y) \cap R(y, z) \cap R(z, x)| = 1$. The unique median
$m = \hat{R}(x, y) \cap R(y, z) \cap R(z, x)$ is defined coordinate-wise by majority voting of
\[ x_i, y_i, z_i \in \{0, 1\}, \] see \cite{Mulder1980}. On hypercubes, $\hat{R}_k$ 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 \( 0 = i_0 \leq i_1 \leq i_2 \leq i_k = n \) from definition \(^\text{[1]}\) 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 10** Let \( d(a,b) > k + 1 \). If \( s = a \times_I b \), \( t = a \times_I b \) and \( |I| = k \), then 
\[
\{a, b\} \not\subseteq R_k(a, b) \text{ and } t \times_j s \not\subseteq R_k(a, b) \text{ holds for all } j \not\in I.
\]

**Proof** Since \( j \not\in I \) 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 \( s \times_j t, t \times_j j \in R_{k+1}(a, b) \setminus R_k(a, b). \)

\text{[Gitchhoff and Wagner(1996)]} 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** If \( d(u,v), d(x,y) > k + 1 \) then \( R_k(u,v) = R_k(x,y) \) if and only if \( \{u,v\} \subseteq \{x,y\} \).

**Proof** The implication from right to left is trivial. For other direction we use Lemma \(^\text{[10]}\). Assume, for contradiction, that \( R_k(u,v) = R_k(x,y) \) and \( \{u,v\} \not\subseteq \{x,y\} \). 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 \( R_k(u,v) = R_k(x,y) \), 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 \(^\text{[10]}\) we conclude that there exist \( j \not\in I \) such that \( x \times_j y \not\subseteq R_k(u,v) \). Hence \( R_k(u,v) \not\subseteq R_k(x,y) \). This contradiction completes the proof of the theorem. \(\square\)

For the special case \( k = 1 \), Theorem \(^\text{[8]}\) 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 \( R_t(x,y) \) induces a cycle of size \( 2t \), an hence the only other transit sets that are included in \( R_t(x,y) \) 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 \( \text{diam}(G) \) denotes the diameter of graph \( G \). The vertex \( \overline{v} \) is obtained from \( v \) by reversing all coordinates.

**Theorem 4** \( R_k(x,y) \) induces an antipodal graph such that \( \overline{y} = y, \overline{x} = x \), 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 $\pi = y \times I x$.

Note that here $v$ and $\pi$ are antipodal in a subgraph $R_k(x, y)$ and will not be
antipodal in the underlying graph $G_R$, unless $d(v, \pi) = \text{diam}(G_R)$. 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

\text{[Hammack et al.(2011), Hammack, Imrich, and Klavzar, Ovchinnikov(2011)]}. Gitchoff and Wagner(1996) showed (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
implies that this result holds in general:

Corollary 5 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 2 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 by [Dress(2007)] in the context of a
characterisation of so called $X$-nets, a structure from phylogenetic combinatorics that is
intimately connected with partial cubes. Indeed, [Dress(2007)] showed that $\parallel$ can be
used to characterize partial cubes:

Proposition 3 ([Dress(2007)]) Let $G$ be a graph and $R = I_G$, then $G$ is a partial
cube if and only if the relation $\parallel$ is an equivalence relation on the set of its edges.

By the definition, the relation $\parallel$ is reflexive and symmetric. Therefore it suffices to
require that $\parallel$ is a transitive relation. Proposition 3 thus can be translated into the
language of transit functions:

Theorem 5 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 $ab \parallel cd \parallel ef$ it follows that $ab \parallel ef$.

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
\begin{itemize}
  \item $b, c \in R(a, d)$, $a, d \in R(b, c)$, $d, e \in R(c, f)$ and $c, f \in R(d, e)$ it follows that $b, e \in R(a, f)$ and $a, f \in R(b, e)$.
\end{itemize}

For a partial cube $G$, the equivalence classes of the relation $\parallel$ 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 [Dress et al.(2012), Dress, Huber, Koolen, Moulton,
and Spillner(2011)].

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 labeled “0” in coordinate $i$, and vertices from the other part of the split are labeled “1” in coordinate $i$. For a 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 labelings, which in turn correspond 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 [Hammack et al. (2011)Hammack, Imrich, and Klavžar; Ovchinnikov (2011)] 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. 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 6** 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 1** Is it true that $R_k(x, y)$ consist of all vertices appearing on $\begin{pmatrix} k \\ 2 \end{pmatrix}$ 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 $u \in R_1(x, y) \setminus \{x, y\}$.

---

**Figure 4.** $R_2(0000, 1111)$ together with colored cuts.
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 example 4, for \( u \in R_k(x, y) \), it may be the case that \( R_k(x, u) = \hat{R}_k(x, u) \subseteq R_k(x, y) \). Hence the lexicographic 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”. We explore this structure in more details in the sections 6 below.

**Problem 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 3** Let \( d(a, b) = t > k + 1 > 2 \). Determine degree sequences of the graphs induced by \( R_k(a, b) \).

We will solve this problem completely for the special case of 2-point crossover operators in Section 6.

**Lemma 11** Let \( a, b \in X = \{0, 1\}^n \) and \( k > 1 \). Then the maximum and 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 \( a = 0 \ldots 0 \) and \( b = 1 \ldots 1 \). 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 \( 3 \) could help solve

**Problem 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 \( k < n - 1 \), [Gitchoff and Wagner(1996)] proposed the axiom

\[
(GW3) \text{ For all } x, y \in X \text{ and all } u, v \in R(x, y) \text{ holds } |R(u, v)| \leq |R(x, y)|.
\]

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 relabeled 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

\[
\Phi_h(n) := \sum_{i=0}^{h} \binom{n}{i}.
\]  

(2)

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

**Theorem 7** Let \( 1 \leq k < t \). Then

\[
r_k(t) = \begin{cases} 2^t & \text{if } t \leq k \\ 2\Phi_k(t-1) & \text{if } t > k \end{cases}
\]  

(3)

**Proof** Consider two strings \( x \) and \( y \). From [Gitchoff and Wagner(1996)] 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 a total of \( \binom{t}{i} \) 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

\[
r_k(t) = 2 \sum_{i=0}^{t-1} \binom{t}{i} = 2\Phi_{t-1}(t-1) = 2 \cdot 2^{t-1} = 2^t.
\]

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 [Gitchoff and Wagner(1996)]. 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 \( r_k(k + 2) = 2^{k+1} - 2 \).

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 the Theorem \( 3 \).
From \( r_k(t) = 2^t \) for \( t \leq k + 1 \) and the fact that \( \widetilde{R}_k(x, y) \) is a hypercube \( K_2^d \) 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 12** 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 6 and Theorem 1.

The Vapnik-Chervonenkis dimension (or VC-dimension) measures the complexity of set systems. Originally introduced in learning theory by Vapnik and Chervonenkis [1971], it has found numerous applications e.g. in statistics, combinatorics and computational geometry, see monograph edited by Vovk et al. [2015] Vovk, Papadopoulos, and Gammerman. 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 8** 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 Topological representation of the \( k \)-point crossover operators

Oriented matroids [Björner et al. (1999)] Björner, Las Vergnas, Sturmfels, White, and Ziegler are an axiomatic combinatorial abstraction of geometric and topological structures such as vector configurations, (pseudo)hyperplane arrangements, convex polytopes, point configurations in the Euclidean space, directed graphs, linear programs, etc. They reflect properties such as linear dependencies, facial relationship, convexity, duality, and have bearing on solutions of associated optimization problems. Beyond their connection with many areas of mathematics, the theory of oriented matroids has in recent years found applications in diverse areas of science and technology, including metabolic network analysis [Gagneur and Klamt (2004)] Müller et al. Müller, Regensburger, and Steuer, Reimers (2014), electronic circuits [Chaiken (1996)] geographic information science [Stell and Webster (2007)], and quantum gravity [Brumemann and Rideout (2010)].

In order to explore the relationships of \( k \)-point crossover operators and oriented matroids it will be convenient to change the coordinates of the vertices of the hypercube.
For the remainder of this section we write \( + \) instead of 1 and \( - \) instead of 0 to conform with the traditional notation in this field. Among several equivalent axiomatizations of oriented matroids, the face or covector axioms best captures the geometric flavour and thus is the most convenient one for our purposes.

Let \( E \) be a finite set. A signed vector \( X \) on \( E \) is a vector \( (X_e : e \in E) \) with coordinates \( X_e \in \{+,-,0\} \). The support of a sign vector \( X \) is the set \( \mathcal{X} = \{ e \in E | X_e \neq 0 \} \). The composition \( X \circ Y \) of two signed vectors \( X \) and \( Y \) is the signed vector on \( E \) defined by \( (X \circ Y)_e = X_e \) if \( X_e \neq 0 \), and \( (X \circ Y)_e = Y_e \) otherwise, and their difference set is \( D(X,Y) = \{ e \in E | X_e = -Y_e \} \). We denote by \( \leq \) the product (partial) ordering on \( \{-,0,+\}^E \) relative to the standard ordering \( - < 0 < + \) of signs.

An oriented matroid \( M \) is ordered pair \( (E,\mathcal{F}) \) of a finite set \( E \) and a set of covectors \( \mathcal{F} \subseteq \{+,-,0\}^E \) satisfying the following (face or covector) axioms:

\( (F0) \) \( 0 = (0,0,\ldots,0) \in \mathcal{F} \).

\( (F1) \) If \( X \in \mathcal{F} \), then \( -X \in \mathcal{F} \).

\( (F2) \) If \( X,Y \in \mathcal{F} \), then \( X \circ Y \in \mathcal{F} \).

\( (F3) \) If \( X,Y \in \mathcal{F} \) and \( e \in D(X,Y) \), then there exists \( Z \in \mathcal{F} \) such that \( Z_e = 0 \) and \( Z_f = (X \circ Y)_f \) for all \( f \in E \setminus D(X,Y) \).

A simple example for an oriented matroid are the sign vectors of a vector subspace. More precisely, consider a subspace \( V \subseteq \mathbb{R}^E \), define, for every \( v \in V \), its sign vector \( s(v) \) coordinate-wise by \( s_v(e) = \text{sgn}(v_e) \) for all \( e \in E \), and denote by \( \mathcal{F} \) the set of all sign vectors of \( V \). Then \( M = (E,\mathcal{F}) \) satisfies the axioms \((F0)-(F3)\). Oriented matroids obtained from a vector space in this manner are called representable or linear.

The set \( \mathcal{C} \subseteq \mathcal{F} \) of non-zero covectors that are minimal with respect to the partial order \( \leq \) are called cocircuits or vertices of \( M \). The set of cocircuits determines the oriented matroid: \( X \) is a covector if and only if its composition with any tope is again a tope, i.e.,

\[ \mathcal{F} = \{ X \in \{+,-,0\}^E | \forall T \in \mathcal{T} : X \circ T \in \mathcal{T} \}. \]

where \( \mathcal{T} \subseteq \{0\} \setminus \{0\} \) is the set of topes of \( M \). The big face lattice \( \mathcal{F} \) is a lattice obtained by adding the unique maximal element \( \hat{1} \) to the partial order \( \leq \) on \( \mathcal{F} \). The rank of a covector \( X \) is defined as its height in \( \mathcal{F} \) and rank of oriented matroid is the maximal rank of its covectors.

As an example consider \( R_2(x,y) \) with \( d(x,y) = 5 \). It can be verified that the elements of \( R_2(\ldots,\ldots) \) are exactly the topes of the oriented matroid corresponding to the Rhombododecahedron in Fig. [5] Its big face lattice is shown in Figure [7].

This observation can be generalized with the help of the following

**Proposition 4 (Gärtner and Welzl(1994))** \( T \subseteq \{+,--\}^X \) of VC-dimension \( d \) is the set of topes of a uniform oriented matroid \( M \) on \( X \) if and only if \( T = -T \) and \( |T| = 2d - 1(|X| - 1) \).

By Proposition [8] and Theorems [7] and [4] this immediately implies

**Theorem 9** For \( x,y \in \{+,--\}^X \), with \( d(x,y) = |X| = n \) the elements of \( R_k(x,y) \) form the set of topes of a uniform oriented matroid \( M \) on \( X \) with VC-dimension \( k + 1 \) and corank \( n - k - 1 \).
One of the cornerstones of the theory of oriented matroids is the Topological Representation Theorem, which connects oriented matroids with pseudosphere arrangements, see Appendix A for detailed definitions. Together with Theorem 9, it immediately implies the following topological characterization of the recombination sets of $k$-point crossover:

**Theorem 10** For $x, y \in \{+, -\}^X$, with $d(x, y) = |X| = n$, the recombination set $R_k(x, y)$ can be topologically represented by a pseudosphere arrangement of dimension $k$, where the minimal elements in the big face lattice correspond to the intersections of exactly $k$ pseudospheres, and there are $2\binom{n}{k-1}$ such intersections.

The significance of this result is that it provides a representation of crossover operators in terms of topological objects. In order to illustrate the usefulness of Theorem 10, we now turn to a full characterization of the transit graphs of 2-point crossover operators. The smallest non-trivial examples are the graphs $R_2(----, ++++)$ in Fig. 6 and $R_2(------, +++++)$ in Fig. 8.

**Theorem 11** $R_2(a, b)$ with $d(a, b) = t > 3$ induces antipodal planar quadrangulation, that is, a partial cube of diameter $t$ with $t^2 - t + 2$ vertices, $2t^2 - 2t$ edges, $t^2 - t$ quadrangles, and all cuts of size $2t - 2$.

**Proof** Let $|V|$, $|E|$, $|Q|$ and $|C|$ denote number of vertices, edges, 4-faces, and edges in a cut, respectively. From the definition of crossover operator, we can arbitrarily permute coordinates, hence it follows that each cut has the same number of edges, this justifies that we study $|C|$. From Theorem 9 it follows that vertices of $R_2(a, b)$ form the set of topes of uniform oriented matroid of rank 3 and corank $t - 3$. As shown by Fukuda and Handa(1993) and in the book by Björner *et al.*(1999)Björner, Las Vergnas, Sturmfels, White, and Ziegler, rank 3 oriented matroids can be represented by pseudocircle arrangement on $S^2$. The corresponding tope graph is therefore planar. Hence $R_2(a, b)$ induces in particular a planar antipodal partial cube.
Figure 8. The transit graph $R_2(----,++++)$.

Figure 9. Topological representation of rhombododecahedron (l.h.s.) in terms of its pseudocircle arrangement (doted curves) and the corresponding hyperplane arrangement (r.h.s.).

Corank $t - 3$ implies that each intersection of pseudocurves is the intersection of exactly two of them. Hence all faces of the dual – the tope graph – are 4-cycles, therefore $R_2(a,b)$ induces planar quadrangulation. Moreover, each intersection of two pseudocircles corresponds to cocircuit. In uniform oriented matroid of corank $t - 3$ there are exactly $2\binom{t}{2}$ cocircuits, which correspond to the 4-cycles in the dual graph.

Quadrangulations are maximal planar bipartite graphs – no edge can be added so that graph remains planar and bipartite. Using Euler formula for planar graphs [Nishizeki and Chiba(1988)], we obtain $|E| = 2|V| - 4$. Theorem 7 furthermore, implies $|E| = 2t^2 - 2t$ and thus $|C| = |E|/t = 2t - 2$.

As an example, Fig. 9 shows the pseudocircle arrangement of transit graph $R_2(----,++++)$ of Fig. 6 and its equivalent hyperplane arrangement.

In order to get a better intuition on the structure of the graphs induced by 2-point crossover operators, we finally derive their degree sequence.

**Theorem 12** Let $d(a,b) = t > 3$. The degree sequence of a graph induced by $R_2(a,b)$ equals $(t, t, 4, \ldots, 4, 3, \ldots, 3)$, where there are $t^2 - 3t$ vertices of degree 4 and $2t$ vertices of degree 3.
Proof W.l.o.g., let $a = 0 \ldots 0$ and $b = 1 \ldots 1$. For any vertex $c = x \ldots xyx \ldots x$, $x, y \in \{0, 1\}$ we have that $c \in R_2(a, b)$, hence $\deg(a) = \deg(b) = t$. Let $c \in R_2(a, b) \setminus \{a, b\}$. Then we have two cases:

**Case 1.** $c = xx \ldots xxyy \ldots yy$ and $\{x, y\} = \{0, 1\}$. Then $c$ has at most four neighbours in $R_2(a, b)$: $c_1 = yx \ldots xxyy \ldots yy$, $c_2 = xx \ldots xxyy \ldots yx$, $c_3 = xx \ldots xxyy \ldots yy$ and $c_4 = xx \ldots xxyy \ldots yy$. Since $t > 3$ it follows $c$ also has at least three neighbours in $R_2(a, b)$.

**Case 2.** $c = x \ldots xxxy \ldots yyxx \ldots x$ and $\{x, y\} = \{0, 1\}$. Then $c$ has at most four neighbours in $R_2(a, b)$: $c_1 = xx \ldots xxyy \ldots yyxx \ldots x$, $c_2 = x \ldots xxxy \ldots yyxx \ldots x$, $c_3 = x \ldots xxxy \ldots yyxx \ldots x$ and $c_4 = x \ldots xxxy \ldots yyxx \ldots x$. Since $t > 3$ it follows $c$ also has at least three neighbours in $R_2(a, b)$.

Let $x_3$ and $x_4$ denote the number of vertices of degree 3 and 4 respectively. By the handshaking lemma $2|E| = \sum_{v \in V(G)} \deg(v)$. Therefore, it follows from arguments above and Theorem 11 that

$$4t^2 - 4t = 2t + \sum_{v \in V(G) \setminus \{a, b\}} \deg(v)$$

$$4t^2 - 6t = 3x_3 + 4x_4$$

Theorem 11 also implies $t^2 - t = x_3 + x_4$. Solving this system of linear equations yields $x_3 = 2t$ and $x_4 = t^2 - 3t$. \qed

7 Concluding remarks

Crossover operators are a key ingredient in the construction of algorithms in Evolutionary and Genetic Programming. Their purpose is to construct offsprings 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 [Gitchoff and Wagner (1996)] 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. For the case of binary alphabets, we explored the close connection with oriented matroids and found that the elements of transit sets form the topes. Furthermore, there is an equivalent characterization in terms of pseudosphere arrangements. Since string recombination operators effectively only distinguishes whether a sequences position is equal or different between the two parents, the results on the graph-theoretical structures of the transit rests directly carry over to arbitrary Hamming graphs.

Linear oriented matroids are exactly those that can be represented by sphere arrangements, i.e., every member of such arrangement is $(d - 1)$-dimensional sphere in $S^d$, which is in turn equivalent to the representation of oriented matroid by a central hyperplane arrangement, e.g. their tope graphs are zonotopes. This suggest the following open

**Problem 5** Are uniform oriented matroids corresponding to the $k$-point crossover operators realizable? In the case of positive answer, find equations describing the hyperplanes in the corresponding hyperplane arrangement.

The results presented here also 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. by [Puljic and
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 5.

Finally, recombination operators influence in a critical manner they 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 [Bernstein(1923), Etherington(1939)], see also the books by [Wörz-Busekros(1980)] and [Lyubich(1992)]. We suspect that a better understanding of the structure of recombination operators will also be of interest in this context.

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Appendix A: Pseudosphere Arrangements

Consider the $d$-dimensional sphere $S^d$ in $\mathbb{R}^{d+1}$ and the corresponding $(d+1)$-dimensional ball $B^{d+1} = \{(x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} \mid x_1^2 + \ldots + x_{d+1}^2 \leq 1\}$, whose boundary surface is $S^d$.

A pseudosphere $S \subset S^d$ is a tame embedded $(d-1)$-dimensional sphere. Its complement in $B^d$ consist of exactly two regions, hence $S$ can be oriented, by labelling one region by $S_e^+$ and the other by $S_e^-$. A pseudosphere arrangement $S = \{S_e \mid e \in E\}$ in the Euclidean space $\mathbb{R}^d$ is a collection of $(d-1)$-dimensional pseudospheres on the $d$-dimensional unit sphere $S^d$, where the intersection of any number of spheres is again a sphere and the intersection of an arbitrary collection of closed sides is either a sphere or a ball, i.e., for all $R \subset E$ holds

(i) $S_R = S^d \cap \cap_{i \in R} S_i$ is empty or homeomorphic to a sphere.

(ii) If $e \in E$ and $S_R \not\subset S_e$ then $S_R \cap S_e$ is a pseudosphere in $S_R$, $S_R \cap S_e^+ \neq \emptyset$ and $S_R \cap S_e^- \neq \emptyset$.

For a pseudosphere arrangement $S$, the position vector $\sigma(x)$ of a point $x \in S^d$ is defined as

$$\sigma(x)_e = \begin{cases} +, & \text{for } x \in S_e^+ \\ 0, & \text{for } x \in S_e^- \\ -, & \text{for } x \in S_e^- \end{cases}$$

The set of all position vectors of $S$ is denoted by $\sigma(S)$.

A famous theorem due to [Folkman and Lawrence(1978)] establishes an correspondence between oriented matroids and pseudosphere arrangement.

Topological Representation Theorem. Let $M = (E, F)$ be an oriented matroid of rank $d$. Then there exists a pseudosphere arrangement $S$ in $S^d$ such that $\sigma(S) = F$.

Conversely, if $S$ is a pseudosphere arrangement in $S^d$, then $(E, \sigma(S))$ is an oriented matroid of rank $d$.

A simple alternative proof was given by [Bokowski et al.(2005)].
A pseudosphere arrangement naturally induces a cell complex on $S^d$, whose partial order of faces corresponds precisely to the partial order $\leq$ on covectors of the corresponding oriented matroid. This fact serves as motivation for concept of covectors in the theory of oriented matroids.