A family of metrics on contact structures based on edge ideals*

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February 1, 2008

Abstract

The measurement of the similarity of RNA secondary structures, and in general of contact structures, of a fixed length has several specific applications. For instance, it is used in the analysis of the ensemble of suboptimal secondary structures generated by a given algorithm on a given RNA sequence, and in the comparison of the secondary structures predicted by different algorithms on a given RNA molecule. It is also a useful tool in the quantitative study of sequence-structure maps. A way to measure this similarity is by means of metrics. In this paper we introduce a new class of metrics $d_m$, $m \geq 3$, on the set of all contact structures of a fixed length, based on their representation by means of edge ideals in a polynomial ring. These metrics can be expressed in terms of Hilbert functions of monomial ideals, which allows the use of several public domain computer algebra systems to compute them. We study some abstract properties of these metrics, and we obtain explicit descriptions of them for $m = 3, 4$ on arbitrary contact structures and for $m = 5, 6$ on RNA secondary structures.

Keywords: contact structure, RNA secondary structure, metric, distance, monomial ideal, Hilbert function.

1 Introduction

As it is well known, in the cell and in vitro RNA molecules and proteins fold into three-dimensional structures, which determine their biochemical function. A central problem in molecular biology is the study of these structures, their prediction and comparison. As different levels of precision are suitable for different problems, we can sometimes forget about the detailed description of the three-dimensional structure of a biopolymer and simply focus our attention on what has been called its contact structure: the set of all pairs of monomers (nucleotides in

*This work has been partially supported by the Spanish DGES, grant BFM2000-1113-C02-01.
RNA molecules, amino acids in proteins) that are spatial neighbors in the three-dimensional structure [4]. If we assume the monomers numbered from 1 to \( n \) along the backbone of the polymer, then a contact structure can be understood as an undirected graph without multiple edges or self-loops with set of nodes \( \{1, \ldots, n\} \): its edges are consistently called contacts and its number \( n \) of nodes its length.

The secondary structures of RNA molecules form a special class of contact structures. In them, contacts represent the hydrogen bonds between pairs of bases that held together the three-dimensional structure. A hydrogen bond can only form between bases that are several positions apart in the chain, but we shall not take this restriction into account here and we shall impose that a contact can only exist between non-consecutive bases. A restriction is added to the definition of RNA secondary structure: a base can only pair with at most one base. This restriction is called the unique bonds condition and it is specific of secondary structures.

It is usual to impose a further restriction on RNA secondary structures, by forbidding the existence of (pseudo)knots: a contact between bases at the \( i \)th and \( j \)th positions in the backbone cannot coexist with a contact between bases at the \( k \)th and \( l \)th positions if \( i < k < j < l \). This restriction has its origin in the first dynamic programming methods to predict RNA secondary structures [25, 27, 28], but since real RNA structures can contain knots, which are moreover important structural elements in many RNA molecules, and their existence does not compromise our models, we shall not impose this restriction here.

Contact structures with unique bonds can also be used to represent the basic building blocks of protein structures, like \( \alpha \)-helixes, \( \beta \)-sheets and \( \beta \) and \( \Omega \)-turns (called thus protein secondary structures), which are also held together by means of hydrogen bonds between non-consecutive amino acids.

But, beyond secondary structures, the representation of the neighborhood in three-dimensional structures of RNA molecules and proteins needs contact structures without unique bonds. The full three-dimensional structure of RNA molecules contains contacts that violate the unique bonds condition, like base triplets and guanine platforms [1, 16]. And in the tertiary structure of a protein, represented for instance by means of a self-avoiding walk in a lattice (i.e., a path in \( \mathbb{N}^3 \) that does not visit the same node more than once [14]), one amino acid can be spatial neighbor of several amino acids [5, 7]. But even in this general case, the existence of contacts between pairs of monomers that are next to each other in the backbone is still forbidden in contact structures, because their spatial closeness can be understood as a consequence of their position in the backbone.

As we mentioned, an important problem in molecular biology is the comparison of the three-dimensional structures formed by RNA molecules and proteins, because it is assumed that a preserved three-dimensional structure corresponds to a preserved function. Moreover, the measurement of the similarity of contact structures on biopolymers of a fixed length has an interest in itself. For instance, it can be used in the analysis of the ensemble of suboptimal solutions provided by a given algorithm, like for instance Zuker’s algorithm [26], to the problem of determining the secondary structure of a given RNA molecule; see [27, 17]. It can also be used to compare the output of different prediction algorithms applied to the same RNA molecule or protein, to assess their performance. This similarity measurement lies also at the basis of the study of the mapping that assigns to each RNA molecule or protein the structure it folds into [9, 21] and it can be used in the study of phenotype spaces [10].

The similarity of contact structures can be quantified by means of metrics on the set of all contact structures of a given length. For instance, with the purpose of comparing suboptimal
solutions to the RNA secondary structure prediction problem in order to reduce the number of alternate structures obtained by his algorithm, Zuker introduced from the very beginning its metric $d_Z$ [26, 27] and more recently the mountain metrics [17]. Tree editing distances have also been used in this context [13, 17, 20].

Reidys and Stadler defined in their seminal paper [18] on algebraic models of biopolymer structures three metrics on RNA secondary structures of fixed length $n$, based on their representations as involutions and as permutation subgroups, and on Magarshak’s matrix representation [15], and they discussed their biophysical relevance. These metrics have been recently analyzed from the mathematical point of view [8, 19].

Since their models cannot be used to represent in a one-to-one way contact structures without unique bonds, Reidys and Stadler’s metrics cannot be extended to the set of arbitrary contact structures of a fixed length. In this paper we overcome this drawback, by switching from subgroups of the symmetric group $S_n$ to monomial ideals of a polynomial ring in $n$ variables. More specifically, we represent a contact structure by means of its edge ideal. Edge ideals are a quite popular tool in commutative algebra to represent graphs and to study their properties [23, 24]. By using them, we generalize Reidys and Stadler’s subgroup metric to define a metric through their permutation subgroups model, to define a family of metrics $(d_m)_{m\geq 3}$ on the set of all contact structures of a fixed length. Up to our knowledge, these are the first metrics defined on arbitrary contact structures of a fixed length that are independent of any notion of graph edition. We express these metrics in terms of Hilbert functions, which makes them easily computable using several public domain computer algebra systems like for instance, CoCoA [3] or Macaulay [11]. We also obtain explicit expressions for several of these metrics on contact and RNA secondary structures, which allow to grasp the notion of similarity they measure.

We hope that our metrics will increase the range of sensible metrics available in the applications of the comparison of structures of a fixed length mentioned above: as Moulton, Zuker et al point out, “[…] generally speaking, it is probably safest to try as many metrics as possible” [17, p. 290].

2 Preliminaries

In this section we recall some definitions and facts on contact and RNA secondary structures, and we take the opportunity to fix some notations and conventions that we shall use henceforth, usually without any further notice.

**Contact structures and RNA secondary structures.** From now on, let $[n]$ denote the set $\{1, \ldots, n\}$, for every positive integer $n$. We begin by recalling the definition of contact structure from [18, 22]; contact structures are also called diagrams in [12].

**Definition 1** A contact structure of length $n$ is an undirected graph without multiple edges or self-loops $\Gamma = ([n], Q)$, for some $n \geq 1$, whose arcs $\{i, j\} \in Q$, called contacts, satisfy the following condition:

i) For every $i \in [n]$, $\{i, i + 1\} \notin Q$.

A contact structure has unique bonds when it satisfies the following extra condition:

ii) For every $i \in [n]$, if $\{i, j\}, \{i, k\} \in Q$, then $j = k$.

Condition (i) translates the impossibility of a contact between two consecutive monomers, while condition (ii) translates the unique bonds condition in RNA secondary structures men-
tioned in the introduction. We shall call the contact structures with unique bonds RNA secondary structures. As we mentioned in the Introduction, the conventional definition of RNA secondary structure forbids moreover the existence of pseudoknots (pairs of contacts \( \{i,j\} \) and \( \{k,l\} \) such that \( i < k < j < l \)), but we shall not impose this restriction here.

We shall denote from now on a contact \( \{j,k\} \) by \( j \cdot k \) or \( k \cdot j \), without distinction. A node is said to be isolated in a contact structure when it is not involved in any contact.

We shall often represent specific RNA secondary structures without pseudoknots by means of their bracket representation \([13]\), obtained by replacing in the sequence \([n]\) each contact \( i \cdot j \) with \( i < j \) by a “(” in the \( i \)th position and a “)” in the \( j \)th position, and each isolated node by a dot in the corresponding position. For instance,

\[
((((((\ldots))))..((\ldots)))\ldots)
\]

represents the secondary structure

\[
\left( [25], \{1\cdot25, 2\cdot14, 3\cdot13, 4\cdot12, 5\cdot11, 6\cdot10, 17\cdot23, 18\cdot22\} \right).
\]

Knotted RNA secondary structures admit a similar representation, using different types of brackets to represent contacts in order to avoid ambiguities.

Given two contact structures of the same length \( \Gamma_1 = ([n], Q_1) \), \( \Gamma_2 = ([n], Q_2) \), their union is the contact structure

\[
\Gamma_1 \cup \Gamma_2 = ([n], Q_1 \cup Q_2).
\]

From now on, and unless otherwise stated, given any contact structure \( \Gamma \) or \( \Gamma_i \), \( i = 1, 2, \ldots \), we shall always denote its set of contacts by \( Q \) or \( Q_i \), respectively.

Let \( C_n \) and \( S_n \) denote the sets of all contact structures and of all RNA secondary structures of length \( n \), respectively.

**Subgroup metric.** For every \( n \geq 1 \), let \( S_n \) be the symmetric group of permutations of \([n]\). In [18], Reidys and Stadler associated to every RNA secondary structure \( \Gamma \in S_n \) the subgroup \( G(\Gamma) \) of \( S_n \) generated by the set of the transpositions corresponding to the contacts in \( \Gamma \):

\[
G(\Gamma) = \langle \{(i,j) \mid i \cdot j \in Q\} \rangle.
\]

They also proved that the mapping \( \Gamma \mapsto G(\Gamma) \) is an embedding of \( S_n \) into the set \( \text{Sub}(S_n) \) of subgroups of \( S_n \), and they used this representation of RNA secondary structures as permutation subgroups to define the following subgroup metric:

\[
d_{\text{sgr}} : S_n \times S_n \rightarrow \mathbb{R} \quad \Gamma_1, \Gamma_2 \mapsto \ln \left( \frac{|G(\Gamma_1) \cdot G(\Gamma_2)|}{|G(\Gamma_1) \cap G(\Gamma_2)|} \right)
\]

In [19] it was proved that this metric simply measures, up to a scalar factor, the cardinal \(|Q_1 \Delta Q_2|\) of the symmetric difference of the sets of contacts.

Unfortunately, if we extend the mapping \( G \) to the set \( C_n \) of all contact structures of length \( n \), we no longer obtain an embedding into \( \text{Sub}(S_n) \), as the following easy example shows.

**Example 1** Let \( \Gamma_1 = ([5], Q_1) \) and \( \Gamma_2 = ([5], Q_2) \) be contact structures with sets of contacts

\[
Q_1 = \{1\cdot3, 3\cdot5\}, \quad Q_2 = \{1\cdot5, 3\cdot5\}.
\]
see Fig. 1. Then \( G(\Gamma_1) = \langle (1, 3), (3, 5) \rangle \) and \( G(\Gamma_2) = \langle (1, 5), (3, 5) \rangle \) are both equal to

\[
\{ \text{Id}, (1, 3), (1, 5), (3, 5), (1, 3, 5), (1, 5, 3) \}.
\]

Figure 1: The contact structures in Example 1.

This entails in particular that the subgroup metric, when extended to the set \( C_n \), yields only a pseudodistance: it is nonnegative and symmetric and satisfies the triangular inequality, but \( d_{\text{grp}}(\Gamma_1, \Gamma_2) = 0 \) does not imply \( \Gamma_1 = \Gamma_2 \). The scope of the failure of the separability condition is determined by the following result.

**Proposition 2** For every \( \Gamma_1, \Gamma_2 \in C_n \), \( d_{\text{grp}}(\Gamma_1, \Gamma_2) = 0 \) if and only if for every \( i, j \in \Gamma_1 \) there exists a chain of contacts \( k_1 k_2 k_3 \ldots k_{m-2} k_{m-1} k_m \) in \( \Gamma_2 \) with \( m \geq 2 \), \( k_1 = i \) and \( k_m = j \), and vice versa, for every \( i, j \in \Gamma_2 \) there is a similar chain of contacts in \( \Gamma_1 \) going from \( i \) to \( j \).

**Proof.** By [18, Thm. 5], \( d_{\text{grp}}(\Gamma_1, \Gamma_2) = 0 \) if and only if \( G(\Gamma_1) = G(\Gamma_2) \), i.e., if and only if every transposition corresponding to a contact in \( \Gamma_1 \) is a product of transpositions corresponding to contacts in \( \Gamma_2 \), and vice versa, every transposition corresponding to a contact in \( \Gamma_2 \) is a product of transpositions corresponding to contacts in \( \Gamma_1 \), a condition that is equivalent to the one given in the statement.

**Orbits.** Reidys and Stadler also represented an RNA secondary structure \( \Gamma \in S_n \) with set of contacts \( \mathcal{Q} = \{i_1 \cdot j_1, \ldots, i_k \cdot j_k\} \) by the involution

\[
\pi(\Gamma) = \prod_{t=1}^{k} (i_t, j_t) \in S_n.
\]

They also proved that this construction yields and embedding \( \pi : S_n \hookrightarrow S_n \), which they used to induce metrics on \( S_n \) from metrics on \( S_n \) [12, 18].

For every \( \Gamma_1, \Gamma_2 \in S_n \), let \( D(\Gamma_1, \Gamma_2) = \langle \pi(\Gamma_1), \pi(\Gamma_2) \rangle \in \text{Sub}(S_n) \) be the dihedral subgroup of \( S_n \) generated by the involutions associated to them. This subgroup acts on \([n]\). The **orbits** induced by this action can be understood as subsets \( \{i_1, i_2, \ldots, i_m\} \subseteq [n] \), \( m \geq 1 \), such that

\[
i_1 \cdot i_2 \cdot i_3 \cdot \ldots \cdot i_{m-1} \cdot i_m \in Q_1 \cup Q_2
\]

\[1\] Notice that this product is only well-defined if the transpositions appearing in it commute with each other, and thus this definition does not make sense for arbitrary contact structures, at least unless some convention is introduced on the order how these transpositions must be composed; we shall not consider this problem here.
and maximal with this property, i.e., such that any other contact in $Q_1 \cup Q_2$ involving some element of this subset can only be $i_1 \cdot i_m$. Notice that these orbits are exactly the connected components of the graph $\Gamma_1 \cup \Gamma_2$. The unique bonds condition (or, in group-theoretical terms, the fact that $\pi(\Gamma_1)$ and $\pi(\Gamma_2)$ are involutions) implies that if $\{i_1, i_2, \ldots, i_m\}$ is such an orbit, then $i_1 \cdot i_2, i_3 \cdot i_4, \ldots$ belong to one of the sets $Q_1$ or $Q_2$ and $i_2 \cdot i_3, i_4 \cdot i_5, \ldots$ belong to the other one.

Such an orbit is cyclic if $m = 2$ and $i_1 \cdot i_2 \in Q_1 \cap Q_2$, or $m \geq 3$ and $i_1 \cdot i_m \in Q_1 \cup Q_2$, and it is linear in all other cases: see Fig. 2. We shall call the cardinal of an orbit its length. The length of a cyclic orbit is always even: if $i_1 \cdot i_2 \in Q_1$ in a cyclic orbit $\{i_1, i_2, \ldots, i_m\}$, then $i_1 \cdot i_m \in Q_2$ and hence $i_{m-1} \cdot i_m \in Q_1$.

![Figure 2: A cyclic orbit of length $m$ (a) and a linear orbit of length $m$ (b).](image)

An orbit is trivial when it is a singleton: it is a linear orbit consisting of a node that it is isolated in both $\Gamma_1$ and $\Gamma_2$. If $\{i_1, i_2, \ldots, i_m\}$ is a non-trivial linear orbit with $i_1 \cdot i_2, i_2 \cdot i_3, \ldots, i_{m-1} \cdot i_m \in Q_1 \cup Q_2$ and $i_1 \cdot i_m \notin Q_1 \cup Q_2$, then $i_1, i_m$ are its end points.

We shall say that a contact $i \cdot j \in Q_1 \cup Q_2$ is involved in an orbit when its vertices $i, j$ belong to this orbit. Every contact in $Q_1 \cup Q_2$ is involved in one and only one orbit, and a contact belongs to $Q_1 \Delta Q_2$ if and only if it is involved in a linear orbit or in a cyclic orbit of length $m > 2$.

Let, for every $k \geq 2$,

$$\Lambda^{(m)}, \: \Lambda \geq k, \: \Theta^{(m)}$$

denote, respectively, the number of linear orbits of length $m$, the number of linear orbits of length $m \geq k$ and the number of cyclic orbits of length $m$ induced by the action of $D(\Gamma_1, \Gamma_2)$ on $[n]$. Since a cyclic orbit of length $m$ involves $m$ contacts, and a linear orbit of length $m$ involves $m - 1$ contacts, we have that

$$|Q_1 \Delta Q_2| = \sum_{m \geq 4} m\Theta^{(m)} + \sum_{m \geq 2} (m - 1)\Lambda^{(m)}.$$

### 3 A family of metrics based on edge ideals

Let $n$ be from now on an integer greater than 2. Let $\mathcal{M}(x_1, \ldots, x_n)$, or simply $\mathcal{M}(\underline{x})$, be the set of all monomials in the variables $x_1, \ldots, x_n$. We shall denote a monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n} \in \mathcal{M}(\underline{x})$ by $x^{\alpha}$ if we let $\underline{\alpha}$ stand for the $n$-tuple $(\alpha_1, \ldots, \alpha_n)$. The total degree of a monomial $x^{\alpha}$ is $\sum_{i=1}^n \alpha_i$. For every $m \geq 0$,
• let $\mathcal{M}(x)^{(m)}$ be the set of all monomials in $\mathcal{M}(x)$ of total degree $m$, and
• let $\mathcal{M}(x)_m$ be the set of all monomials in $\mathcal{M}(x)$ of total degree $\leq m$.

Recall that

$$|\mathcal{M}(x)_m| = \binom{n + m}{n}$$

and

$$|\mathcal{M}(x)^{(m)}| = \binom{n + m - 1}{n - 1}.$$

Let $\mathbb{F}_2$ be the field $\mathbb{Z}/2\mathbb{Z}$ and $\mathbb{F}_2[x_1, \ldots, x_n]$, or simply $\mathbb{F}_2[x]$, the ring of polynomials in the variables $x_1, \ldots, x_n$ with coefficients in $\mathbb{F}_2$. Let $\text{Id}(\mathbb{F}_2[x])$ denote the set of ideals of $\mathbb{F}_2[x]$. For every $I \in \text{Id}(\mathbb{F}_2[x])$ and for every $m \geq 0$,

• let $\mathcal{M}(I) = I \cap \mathcal{M}(x)$ be the set of all monomials that belong to $I$;
• let $\mathcal{M}(I)^{(m)} = I \cap \mathcal{M}(x)^{(m)}$ be the set of all monomials of total degree $m$ that belong to $I$;
• let $\mathcal{M}(I)_m = I \cap \mathcal{M}(x)_m$ be the set of all monomials of total degree $\leq m$ that belong to $I$;
• let $C(I) = \mathcal{M}(x) - \mathcal{M}(I)$ be the set of all monomials that do not belong to $I$; and
• let $C(I)_m = C(I) \cap \mathcal{M}(x)_m$ be the set of all monomials of total degree $\leq m$ that do not belong to $I$.

An ideal $I$ of $\mathbb{F}_2[x]$ is monomial when it is generated by a set of monomials. It should be recalled that, given a monomial ideal $I$ generated by a set of monomials $M$, the monomials in $M(I)$ are exactly those that are divisible by some monomial in $M$ and the polynomials in $I$ are exactly the linear combinations (with coefficients in $\mathbb{F}_2$) of monomials in $M(I)$; in particular, for every two monomial ideals $I$ and $J$ of $\mathbb{F}_2[x]$, $I = J$ if and only if $M(I) = M(J)$.

**Definition 2** For every $\Gamma = ([n], Q) \in C_n$, the edge ideal $I_\Gamma$ of $\Gamma$ is the monomial ideal of $\mathbb{F}_2[x]$ generated by the products of pairs of variables whose indexes form a contact in $\Gamma$:

$$I_\Gamma = \{x_i x_j \mid i \cdot j \in Q\}.$$

**Proposition 3** The mapping $I : C_n \to \text{Id}(\mathbb{F}_2[x])$ that sends every $\Gamma \in C_n$ to its edge ideal, is an embedding.

**Proof.** For every $\Gamma \in C_n$, the monomials in $I_\Gamma$ are exactly those divisible by some $x_i x_j$ with $i \cdot j \in Q$. This implies that

$$M(I_\Gamma)^{(2)} = \{x_i x_j \mid i \cdot j \in Q\},$$

and therefore $\Gamma$ is uniquely determined by $M(I_\Gamma)^{(2)}$. 

\[\blacksquare\]
Given two contact structures $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$, it is clear that

$$I_{\Gamma_1} + I_{\Gamma_2} = \left( \{x_ix_j \mid i \cdot j \in Q_1\} \cup \{x_ix_j \mid i \cdot j \in Q_2\} \right) = I_{\Gamma_1 \cup \Gamma_2}.$$ 

As far as $I_{\Gamma_1} \cap I_{\Gamma_2}$ goes, it is straightforward to prove that it is generated by

$$\{x_ix_j \mid i \cdot j \in Q_1 \cap Q_2\} \cup \{x_ix_jx_k \mid i \cdot j \in Q_1 - Q_2, j \cdot k \in Q_2 - Q_1\} \cup \{x_ix_jx_kx_l \mid i \cdot j \in Q_1 - Q_2, k \cdot l \in Q_2 - Q_1, \{i,j\} \cap \{k,l\} \neq \emptyset\}.$$ 

Using a construction similar to the one introduced by Reidys and Stadler for subgroups, we want to measure the difference between two contact structures $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$ by means of the quotient $(I_{\Gamma_1} + I_{\Gamma_2})/(I_{\Gamma_1} \cap I_{\Gamma_2})$. Notice that this quotient is a singleton if and only if $I_{\Gamma_1} = I_{\Gamma_2}$, i.e., if and only if $\Gamma_1 = \Gamma_2$. Unfortunately, in all other cases this quotient is infinite: if a monomial $x^m$ belongs to, say, $I_{\Gamma_1} - I_{\Gamma_2}$, then all its powers define pairwise different equivalence classes modulo $I_{\Gamma_1} \cap I_{\Gamma_2}$. Thus, to obtain a “finite distance” we move to quotients of $F_2[x]$. 

For every $n \geq 1$ and $m \geq 3$, let us consider the quotient ring

$$R_{n,m} = F_2[x_1, \ldots, x_n]/(M(x)^{(m)}),$$

and let $\pi_m : F_2[x_1, \ldots, x_n] \to R_{n,m}$ be the corresponding quotient ring homomorphism. For every $I \in \text{Id}(F_2[x_1, \ldots, x_n])$, let $\pi_m(I)$ be the image of $I$ in $R_{n,m}$.

**Proposition 4** For every $m \geq 3$, the mapping $d'_m : \mathcal{C}_n \times \mathcal{C}_n \to \mathbb{R}$ defined by

$$d'_m(\Gamma_1, \Gamma_2) = \log_2 \left| \frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} \right|$$

is a metric on $\mathcal{C}_n$.

**Proof.** When we perform the quotient $R_{n,m} = F_2[x]/(M(x)^{(m)})$, all monomials with total degree greater or equal than $m$ are cancelled. Then, each element in $R_{n,m}$ has a unique representative that is a linear combination with coefficients in $F_2$ of monomials of total degree at most $m - 1$. Since $F_2$ is a finite field, this implies that $R_{n,m}$ is finite, and in particular it is a finite commutative group with the sum of quotient classes of polynomials as operation. Let $\text{Sub}(R_{n,m})$ denote its set of subgroups.

On the other hand, since $m \geq 3$, the quotient homomorphism $\pi_m$ does not identify any monomial of total degree 2 with any other monomial. Thus, $\pi_m(I_{\Gamma_1}) = \pi_m(I_{\Gamma_2})$ implies $M(I_{\Gamma_1})^{(2)} = M(I_{\Gamma_2})^{(2)}$ and hence, as we saw in Proposition 3, $\Gamma_1 = \Gamma_2$. In other words, the mapping $\pi_m \circ I : \mathcal{C}_n \to \text{Sub}(R_{n,m})$ sending every $\Gamma \in \mathcal{C}_n$ to $\pi_m(I_{\Gamma})$, is an embedding.

Then, since by [18, Thm. 5] the mapping

$$\Psi(I, J) = \log_2 \left| \frac{I + J}{I \cap J} \right|, \quad I, J \in \text{Sub}(R_{n,m})$$

is a metric on $\text{Sub}(R_{n,m})$, the mapping

$$d'_m(\Gamma_1, \Gamma_2) = \Psi(\pi_m(I_{\Gamma_1}), \pi_m(I_{\Gamma_2})), \quad \Gamma_1, \Gamma_2 \in \mathcal{C}_n$$

is a metric on $\mathcal{C}_n$, as we claimed. 

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We have used $\log_2$ instead of $\ln$ in the definition of $d'_m$ in order to avoid unnecessary scalar factors: cf. [19, Prop. 4].

These metrics $d'_m$ have a simple description in terms of symmetric differences of sets of monomials.

**Proposition 5** For every $m \geq 3$ and for every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,

$$d'_m(\Gamma_1, \Gamma_2) = |M(\Gamma_1)_{m-1} \Delta M(\Gamma_2)_{m-1}|.$$  

**Proof.** Notice that, for every $I \in \text{Id}(\mathbb{F}_2[x])$,

$$\pi_m(I) = \pi_m(I + \langle M(x)^{(m)} \rangle).$$

Then, for every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,

$$\frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} = \frac{\pi_m(I_{\Gamma_1} + \langle M(x)^{(m)} \rangle) + \pi_m(I_{\Gamma_2} + \langle M(x)^{(m)} \rangle)}{\pi_m(I_{\Gamma_1} + \langle M(x)^{(m)} \rangle) \cap \pi_m(I_{\Gamma_2} + \langle M(x)^{(m)} \rangle)}$$

$$= \frac{(I_{\Gamma_1} + \langle M(x)^{(m)} \rangle) \cap (I_{\Gamma_2} + \langle M(x)^{(m)} \rangle)}{I_{\Gamma_1} + I_{\Gamma_2} + \langle M(x)^{(m)} \rangle}$$

where the equality

$$(I_{\Gamma_1} + \langle M(x)^{(m)} \rangle) \cap (I_{\Gamma_2} + \langle M(x)^{(m)} \rangle) = (I_{\Gamma_1} \cap I_{\Gamma_2}) + \langle M(x)^{(m)} \rangle$$

used in the last step holds because $I_{\Gamma_1}, I_{\Gamma_2}$ and $\langle M(x)^{(m)} \rangle$ are monomial ideals.

To simplify the notations, set

$$J = I_{\Gamma_1} + I_{\Gamma_2} + \langle M(x)^{(m)} \rangle,$$

$$K = (I_{\Gamma_1} \cap I_{\Gamma_2}) + \langle M(x)^{(m)} \rangle,$$

so that

$$\frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} \approx \frac{J}{K}.$$  

These ideals $J$ and $K$ are also monomial and

$$M(J) = M(I_{\Gamma_1})_{m-1} \cup M(I_{\Gamma_2})_{m-1} \cup \bigcup_{r>m-1} M(x)^{(r)},$$

$$M(K) = (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1}) \cup \bigcup_{r>m-1} M(x)^{(r)}.$$

A polynomial belongs to $J$ (resp. $K$) if and only if it is a linear combination, with coefficients in $\mathbb{F}_2$, of elements of $M(J)$ (resp. $M(K)$). This implies that every quotient class in $J/K$ has a unique representative of the form $\sum_{x \in M_0} x^a$ for some finite subset $M_0$ of $M(J) - M(K)$ (the zero class corresponds to $M_0 = \emptyset$). Since

$$M(J) - M(K) = (M(I_{\Gamma_1})_{m-1} \cup M(I_{\Gamma_2})_{m-1}) - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1})$$

$$= M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1}$$
is a finite set, this implies that
\[ \left| \frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} \right| = \frac{J}{K} = 2^{M(I_{\Gamma_1})_{m-1} - M(I_{\Gamma_2})_{m-1}}, \]
as we claimed.

Proposition 5 allows us to express the metrics \( d'_m \) in terms of Hilbert functions. For every monomial ideal \( I \) of \( \mathbb{F}_2[q] \) and for every \( m \geq 0 \), let \( H_I : \mathbb{N} \rightarrow \mathbb{N} \) be the mapping defined by
\[ H_I(m) = |C(I)_m|, \quad m \in \mathbb{N}; \]
i.e., \( H_I(m) \) is the number of monomials of total degree \( \leq m \) that do not belong to \( I \). This mapping is called the (affine) Hilbert function of \( I \). It can be computed explicitly from a given finite set of generators of \( I \) [2]; actually, several freely available computer algebra systems like, for instance, CoCoA [3] or Macaulay [11], compute Hilbert functions.

For every contact structure \( \Gamma \in \mathcal{C}_n \), let \( H_\Gamma \) denote the Hilbert function of its edge ideal.

**Corollary 6** For every \( \Gamma_1, \Gamma_2 \in \mathcal{C}_n \) and for every \( m \geq 3 \),
\[ d'_m(\Gamma_1, \Gamma_2) = H_{\Gamma_1}(m - 1) + H_{\Gamma_2}(m - 1) - 2H_{\Gamma_1 \cup \Gamma_2}(m - 1). \]

**Proof.** We have that
\begin{align*}
M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1} & = (M(I_{\Gamma_1})_{m-1} - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1})) \cup (M(I_{\Gamma_2})_{m-1} - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1})) \\
& = (M(I_{\Gamma_1} + I_{\Gamma_2})_{m-1} - M(I_{\Gamma_2})_{m-1} \cup (M(I_{\Gamma_1} + I_{\Gamma_2})_{m-1} - M(I_{\Gamma_1})_{m-1}) \\
& = (C(I_{\Gamma_2})_{m-1} - C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1}) \cup (C(I_{\Gamma_1})_{m-1} - C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1})
\end{align*}
and thus, this union being disjoint,
\begin{align*}
|M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1}| & = (|C(I_{\Gamma_2})_{m-1}| - |C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1}|) + (|C(I_{\Gamma_1})_{m-1}| - |C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1}|) \\
& = (H_{\Gamma_2}(m - 1) - H_{\Gamma_1 \cup \Gamma_2}(m - 1)) + (H_{\Gamma_1}(m - 1) - H_{\Gamma_1 \cup \Gamma_2}(m - 1)),
\end{align*}
as we claimed.

To close this section, we want to point out that the metrics \( d'_m \) grow with \( n \) and \( m \), and thus it is convenient to normalize them in order to avoid unnecessarily high figures. More specifically, let \( \Gamma_0 = ([n], 0) \) be the empty RNA secondary structure of length \( n \) and let \( \Gamma_1 \) be an RNA secondary structure of length \( n \) with only one contact, say \( i \cdot j \) with \( i < j \). Then \( I_{\Gamma_0} = \{0\}, I_{\Gamma_1} = I_{\Gamma_0} + I_{\Gamma_1} = \langle x_i x_j \rangle \), and therefore, for every \( m \geq 3 \),
\[ d'_m(\Gamma_0, \Gamma_1) = H_{\Gamma_0}(m - 1) - H_{\Gamma_1}(m - 1), \]
where
\begin{align*}
H_{\Gamma_0}(m - 1) & = |\mathcal{M}(\emptyset)_{m-1}| = \binom{n+m-1}{n} \\
H_{\Gamma_1}(m - 1) & = |\mathcal{M}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)_{m-1}| \\
& \quad + |\mathcal{M}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n)_{m-1}| \\
& \quad - |\mathcal{M}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n)_{m-1}| \\
& = 2\binom{n+m-2}{n-2} - \binom{n+m-3}{n-2},
\end{align*}
and
and hence
\[d'_m(\Gamma_0, \Gamma_1) = \binom{n + m - 1}{n} - 2\binom{n + m - 2}{n - 1} + \binom{n + m - 3}{n - 2} = \binom{n + m - 3}{n}.\]

If we take 1 as the “natural” value for the distance between \(\Gamma_0\) and \(\Gamma_1\), then instead of using the metrics \(d'_m\) on \(\mathcal{C}_n\), we must divide them by \(\binom{n + m - 3}{n}\).

**Definition 3** For every \(m \geq 3\), the edge ideal \(m\)th metric on \(\mathcal{C}_n\) is
\[d_m(\Gamma_1, \Gamma_2) = \frac{1}{\binom{n + m - 3}{n}}d'_m(\Gamma_1, \Gamma_2), \quad \Gamma_1, \Gamma_2 \in \mathcal{C}_n.\]

So, for instance, on \(\mathcal{C}_n\)
\[d_3 = d'_3, \quad d_4 = \frac{1}{n + 1}d'_4, \quad d_5 = \frac{1}{\binom{3}{2}}d'_5, \quad \text{and so on.}\]

Even after this modification, the metric \(d_m\) is sensitive to \(n\), in the sense that if we add to two contact structures of a given length \(n\) an isolated point, making them contact structures of length \(n + 1\), then their distance \(d_m\) (for \(m \geq 4\); see Proposition 7 below) may grow. For instance, let \(\Gamma_0\) be again the empty RNA secondary structure of length \(n \geq 6\) and let now \(\Gamma_1 = ([n], \{1, 3, 4, 6\})\). Then
\[d_m(\Gamma_0, \Gamma_1) = \frac{1}{\binom{n + m - 3}{n}}(H_{\Gamma_0}(m - 1) - H_{\Gamma_1}(m - 1)).\]

We have seen above that \(H_{\Gamma_0}(m - 1) = \binom{n + m - 1}{n}\), and we shall see in Proposition 14 below that (with the convention that \(\binom{i}{n} = 0\) if \(i < n\))
\[H_{\Gamma_1}(m - 1) = \binom{n + m - 1}{n} - 2\binom{n + m - 3}{n} + \binom{n + m - 5}{n}.
\]

Therefore,
\[d_m(\Gamma_0, \Gamma_1) = \frac{1}{\binom{n + m - 3}{n}}(2\binom{n + m - 5}{n} - \binom{n + m - 3}{n}) = 2 - \binom{m - 3}{n} - \binom{n + m - 5}{n} = 2 - \binom{m - 3}{n} - \binom{n + m - 5}{n},\]
which increases with \(n\) if \(m \geq 5\).

Since we are only interested in comparing contact structures of the same length, this sensitivity of the edge ideal metrics to the length \(n\) is not a major drawback.

### 4 Some computations

In this section we shall compute explicitly some edge ideal \(m\)th metrics on \(\mathcal{C}_n\) and \(\mathcal{S}_n\), for low values of \(m\). We begin with \(m = 3\).

**Proposition 7** For every \(\Gamma_1, \Gamma_2 \in \mathcal{C}_n\),
\[d_3(\Gamma_1, \Gamma_2) = |Q_1 \Delta Q_2|.
\]

**Proof.** Notice that \(M(I_{\Gamma})_1 = \emptyset\) for every \(\Gamma \in \mathcal{C}_n\). Therefore
\[M(I_{\Gamma_1})_2 \Delta M(I_{\Gamma_2})_2 = M(I_{\Gamma_1})_2(2) \Delta M(I_{\Gamma_2})_2(2) = \{x_i \cdot x_j \mid i, j \in (Q_1 - Q_2) \cup (Q_2 - Q_1)\}\]
and hence \(|M(I_{\Gamma_1})_2 \Delta M(I_{\Gamma_2})_2| = |Q_1 \Delta Q_2|\). \(\blacksquare\)
Actually, it is not difficult to prove that, for every \( \Gamma \in S_n \), the mapping \( G(\Gamma) \rightarrow \pi_3(I_\Gamma) \) sending every permutation \( \sigma = (i_1, j_1) \cdots (i_t, j_t) \in G(\Gamma) \), with \( i_1, j_1, \ldots, i_t, j_t \in Q \), to the equivalence class of the polynomial \( x_{i_1} x_{j_1} + \cdots + x_{i_t} x_{j_t} \in I_\Gamma \) modulo \( \langle M(\mathbb{Z}) \rangle \), is an isomorphism of groups, considering \( \pi_3(I_\Gamma) \) as a subgroup of \( R_{n, 3} \). This is not true for arbitrary contact structures, because in this case \( G(\Gamma) \) need not be commutative, while \( \pi_3(I_\Gamma) \) is always so. Therefore, the embedding \( \pi_3 \circ I : C_n \hookrightarrow Sub(R_{n, 3}) \) generalizes the embedding \( G : S_n \hookrightarrow Sub(S_n) \), and hence the metric \( d_3 \) generalizes (up to a scalar factor) the subgroup metric \( d_{sgr} \) at a level deeper than their raw value.

The edge ideal \( m \)th metrics for \( m > 3 \) have a much more involved expression. In their computation we shall use the following lemma; notice that the edge ideals of contact structures are radical monomial proper (i.e., \( \neq \mathbb{F}_2[\mathbb{F}] \)) ideals.

**Lemma 8** Let \( I \) be a radical monomial proper ideal of \( \mathbb{F}_2[\mathbb{F}] \) and, for every \( k \geq 1 \), let \( SF_k(I) \) be the number of square free monomials of total degree \( k \) belonging to \( M(I) \). Then, for every \( m \geq 0 \),

\[
H_I(m) = \binom{n+m}{n} - \sum_{k=1}^{m} \binom{m}{k} SF_k(I).
\]

**Proof.** If \( I \) is a radical monomial ideal, then a monomial of the form \( x_{i_1}^{\alpha_1} \cdots x_{i_k}^{\alpha_k} \), with \( i_1, \ldots, i_k \) pairwise different and each \( \alpha_i \geq 1 \), belongs to \( M(I) \) if and only if the corresponding square free monomial \( x_{i_1} \cdots x_{i_k} \) belongs to \( M(I) \). Therefore, each one of the \( SF_k(I) \) square free monomials \( x_{i_1} \cdots x_{i_k} \) of total degree \( k \geq 1 \) in \( M(I) \) adds as many monomials \( x_{i_1}^{\alpha_1} \cdots x_{i_k}^{\alpha_k} \) to \( M(I)_m \) as vectors \( (\alpha_1, \ldots, \alpha_k) \in (\mathbb{N} - \{0\})^k \) such that \( \sum_{i=1}^{k} \alpha_i \leq m \) there exist, and the number of the latter is \( \binom{k+m-k}{k} = \binom{m}{k} \). Since all monomials in \( M(I)_m \) added in this way are pairwise different and \( 1 \notin I \) by assumption, this proves that

\[
|M(I)_m| = \sum_{k=1}^{m} \binom{m}{k} SF_k(I),
\]

and hence

\[
|C(I)_m| = |M(\mathbb{Z})_m| - |M(I)_m| = \binom{n+m}{n} - \sum_{k=1}^{m} \binom{m}{k} SF_k(I),
\]

as we claimed. \( \square \)

Notice that if \( \Gamma \in C_n \), then \( SF_1(I_{\Gamma}) = 0 \) and \( SF_2(I_{\Gamma}) = |Q| \).

Let us compute now \( d_4 \) on \( C_n \). For every contact structure \( \Gamma \in C_n \), let

\[
A(\Gamma) = \left\{ \{i,j,k\} \subseteq Q \mid j \neq k \right\}, \\
T(\Gamma) = \left\{ \{i,j,k\} \subseteq [n] \mid i \cdot j \cdot k, i-k \in Q \right\}.
\]

In other words, \( A(\Gamma) \) and \( T(\Gamma) \) are respectively the numbers of indices and triangles in \( \Gamma \). Notice that each triangle contains three different indices and therefore \( 3T(\Gamma) \leq A(\Gamma) \).

**Proposition 9** For every \( \Gamma_1, \Gamma_2 \in C_n \),

\[
d_4(\Gamma_1, \Gamma_2) = |Q_1 A Q_2| - \frac{1}{n+1} \left( 2A(\Gamma_1 \cup \Gamma_2) - A(\Gamma_1) - A(\Gamma_2) + 2T(\Gamma_1 \cup \Gamma_2) - T(\Gamma_1) - T(\Gamma_2) \right)
\]

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Proof. For every $\Gamma = ([n], Q) \in \mathcal{C}_n$ we have that

$$H_\Gamma(3) = \binom{n+3}{n} - 3SF_1(\Gamma) - 3SF_2(\Gamma) - SF_3(\Gamma),$$

where $SF_1(\Gamma) = 0$ and $SF_2(\Gamma) = |Q|$. It remains to compute $SF_3(\Gamma)$:

1. For every $i \cdot j \in Q$, there are $(n-2)$ square free monomials $x_i x_j x_k$ in $M(\Gamma)$: this makes $(n-2)|Q|$ such monomials.

2. Now, if $i \cdot j \cdot k \in Q$ form an angle, the monomial $x_i x_j x_k$ was counted twice in (1): therefore, to count these monomials only once, we must subtract $A(\Gamma)$.

3. Finally, if the nodes $i, j, k$ form a triangle in $\Gamma$, then the monomial $x_i x_j x_k$ was counted three times in (1) and it was subtracted three times in (2): therefore, to retrieve these monomials, we must add $T(\Gamma)$ again.

Therefore

$$SF_3(\Gamma) = (n-2)|Q| - A(\Gamma) + T(\Gamma)$$

and

$$H_\Gamma(3) = \binom{n+3}{n} - (n+1)|Q| + A(\Gamma) - T(\Gamma).$$

We have then

$$d'_4(\Gamma_1, \Gamma_2) = H_{\Gamma_1}(3) + H_{\Gamma_2}(3) - 2H_{\Gamma_1 \cup \Gamma_2}(3)$$

$$= \binom{n+3}{n} - (n+1)|Q_1| + A(\Gamma_1) - T(\Gamma_1) + \binom{n+3}{n} - (n+1)|Q_2| + A(\Gamma_2) - T(\Gamma_2)$$

$$- 2\left(\binom{n+3}{n} - (n+1)|Q_1 \cup Q_2| + A(\Gamma_1 \cup \Gamma_2) - T(\Gamma_1 \cup \Gamma_2)\right)$$

$$= (n+1)|Q_1 \Delta Q_2| - (2A(\Gamma_1 \cup \Gamma_2) - A(\Gamma_1) - A(\Gamma_2) + 2T(\Gamma_1 \cup \Gamma_2) - T(\Gamma_1) - T(\Gamma_2));$$

in the last equality we have used that $2|Q_1 \cup Q_2| - |Q_1| - |Q_2| = |Q_1 \Delta Q_2|$.

Dividing by $n+1$ this last expression for $d'_4(\Gamma_1, \Gamma_2)$, we obtain the expression for $d_4(\Gamma_1, \Gamma_2)$ given in the statement. 

A simple computation shows that, for every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,

$$2A(\Gamma_1 \cup \Gamma_2) - A(\Gamma_1) - A(\Gamma_2)$$

$$= \left| \left\{ i \cdot j \cdot k \mid i \neq k, \ (i \cdot j, j \cdot k \in Q_s) \text{ and } (i \cdot j \text{ or } j \cdot k \notin Q_t), \text{ for some } \{s, t\} = \{1, 2\} \right\} \right|$$

$$+ 2 \left| \left\{ i \cdot j \cdot k \mid i \cdot j \in Q_1 - Q_2, j \cdot k \in Q_2 - Q_1 \right\} \right|$$

$$2T(\Gamma_1 \cup \Gamma_2) - T(\Gamma_1) - T(\Gamma_2)$$

$$= \left| \left\{ i \cdot j \cdot k \mid (i \cdot j, j \cdot k \in Q_s) \text{ and } (i \cdot j \cdot k \text{ or } i \cdot k \notin Q_t), \text{ for some } \{s, t\} = \{1, 2\} \right\} \right|$$

$$+ 2 \left| \left\{ i \cdot j \cdot k \mid i \cdot j \cdot k \in Q_s, \text{ and } i \cdot k \in Q_t - Q_s, \text{ for some } \{s, t\} = \{1, 2\} \right\} \right|$$

Example 10 Let $\Gamma_0 = ([9], \{1, 3, 4, 6\})$, and consider the following “modifications” of it:

$$\Gamma_1 = ([9], \{1, 3, 4, 6, 7, 9\}), \quad \Gamma_2 = ([9], \{1, 3, 4, 6, 6, 9\}), \quad \Gamma_3 = ([9], \{1, 3, 4, 6, 1, 6\})$$

$$\Gamma_4 = ([9], \{1, 3, 4, 7\}), \quad \Gamma_5 = ([9], \{1, 3, 3, 6\}), \quad \Gamma_6 = ([9], \{1, 3, 3, 5\}), \quad \Gamma_7 = ([9], \{1, 3, 5, 7\})$$

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The contact structures $\Gamma_1$, $\Gamma_2$ and $\Gamma_3$ are obtained by adding a contact to $\Gamma_0$ in three different ways, $\Gamma_4$ and $\Gamma_5$ are obtained by shifting the contact 4-6 in two different ways, and $\Gamma_6$ and $\Gamma_7$ are obtained by displacing this contact in two more ways. Notice that $\Gamma_0, \Gamma_1, \Gamma_4$ and $\Gamma_7$ are RNA secondary structures, but not the others.

We have that

$$d_3(\Gamma_0, \Gamma_1) = d_3(\Gamma_0, \Gamma_2) = d_3(\Gamma_0, \Gamma_3) = 1,$$
$$d_3(\Gamma_0, \Gamma_4) = d_3(\Gamma_0, \Gamma_5) = d_3(\Gamma_0, \Gamma_6) = d_3(\Gamma_0, \Gamma_7) = 2,$$

while

$$d_4(\Gamma_0, \Gamma_1) = 1, \quad d_4(\Gamma_0, \Gamma_2) = 0.9, \quad d_4(\Gamma_0, \Gamma_3) = 0.8,$$
$$d_4(\Gamma_0, \Gamma_4) = 1.8, \quad d_4(\Gamma_0, \Gamma_5) = 1.7, \quad d_4(\Gamma_0, \Gamma_6) = 1.9, \quad d_4(\Gamma_0, \Gamma_7) = 2.$$

The expression for $d_4$ on RNA secondary structures is much simpler. Recall that, for every $\Gamma_1, \Gamma_2 \in S_n$, $A_{\geq 2}$ stands for the number of linear orbits of length $\geq 2$, i.e., of non-trivial linear orbits induced by the action of $D(\Gamma_1, \Gamma_2)$ on $[n]$.

**Proposition 11** For every $\Gamma_1, \Gamma_2 \in S_n$,

$$d_4(\Gamma_1, \Gamma_2) = |Q_1 \Delta Q_2| - \frac{2}{n+1} A(\Gamma_1 \cup \Gamma_2)$$

$$= |Q_1 \Delta Q_2| - \frac{2}{n+1} (|Q_1 \Delta Q_2| - A_{\geq 2}).$$

**Proof.** Notice that the unique bonds condition implies in this case that

$$A(\Gamma_1) = A(\Gamma_2) = T(\Gamma_1) = T(\Gamma_2) = T(\Gamma_1 \cup \Gamma_2) = 0,$$

from which the first equality follows. It remains to prove that if $\Gamma_1, \Gamma_2 \in SE$, then

$$A(\Gamma_1 \cup \Gamma_2) = |Q_1 \Delta Q_2| - A_{\geq 2}.$$

To prove it, notice that if $\{i, j, k\}$ forms an angle in $\Gamma_1 \cup \Gamma_2$, then, again by the unique bonds condition, one these contacts must belong to $Q_1 - Q_2$ and the other one to $Q_2 - Q_1$, and the nodes $i, j, k$ belong to the same orbit of length at least 3. Now, each cyclic orbit of length $m > 2$ contains $m$ such pairs of contacts, while any linear orbit of length $m \geq 2$ contains $m - 2$ such pairs. Then

$$A(\Gamma_1 \cup \Gamma_2) = \sum_{m \geq 4} m \Theta(m) + \sum_{m \geq 2} (m - 2) \Lambda(m)$$

$$= \sum_{m \geq 4} m \Theta(m) + \sum_{m \geq 2} (m - 1) \Lambda(m) - \sum_{m \geq 2} \Lambda(m) = |Q_1 \Delta Q_2| - A_{\geq 2},$$

as we wanted to prove. $\blacksquare$

Therefore, on $S_n$, the metric $d_4$ increases with the cardinal of $Q_1 \Delta Q_2$, but decreases with the number of pairs of contacts in $Q_1 \Delta Q_2$ that share a node. Notice moreover that

$$0 \leq |Q_1 \Delta Q_2| - A_{\geq 2} \leq |Q_1 \Delta Q_2|;$$

the lower bound is achieved when all non-trivial orbits are linear of length 2 (i.e., when $\Gamma_1 \cup \Gamma_2$ is again an RNA secondary structure), and the upper bound when all non-trivial orbits are cyclic (i.e., when $\Gamma_1$ and $\Gamma_2$ have exactly the same isolated nodes).
Example 12 According to [22, §5.3.2], most RNA AU-sequences of length 16 do not fold at all, i.e., they form the empty RNA secondary structure $\Gamma_0 = ([16], \emptyset)$. But some of these sequences (about a 3% of them) do fold, forming one of the following three RNA secondary structures without pseudoknots:

$\Gamma_1 : (((((...)))))) \quad \Gamma_2 : (((((...)))))) \quad \Gamma_3 : (((((...))))))$

Recall that these are the bracket representations of

$\Gamma_1 = ([16], \{2\cdot16, 3\cdot15, 4\cdot14, 5\cdot13, 6\cdot12, 7\cdot11\})$

$\Gamma_2 = ([16], \{1\cdot15, 2\cdot14, 3\cdot13, 4\cdot12, 5\cdot11, 6\cdot10\})$

$\Gamma_3 = ([16], \{1\cdot16, 2\cdot15, 3\cdot14, 4\cdot13, 5\cdot12, 6\cdot11\})$

They have pairwise disjoint sets of contacts, and hence

$d_3(\Gamma_1, \Gamma_2) = d_3(\Gamma_1, \Gamma_3) = d_3(\Gamma_2, \Gamma_3) = 12.$

But

$d_4(\Gamma_1, \Gamma_2) = \frac{184}{17}, \quad d_4(\Gamma_1, \Gamma_3) = d_4(\Gamma_2, \Gamma_3) = \frac{182}{17},$

which shows that, under $d_4$, $\Gamma_1$ and $\Gamma_2$ are closer to $\Gamma_3$ than to each other.

Example 13 Let us consider a hairpin with an interior loop $\Gamma_0 \in S_{21}$ with bracket representation

$((.(((...))))(....))$

One possible rearrangement of this secondary structure splits the hairpin into a multibranched loop by means of two shift moves, yielding a multibranched structure:

$\Gamma_0 : ((.(((...))))(....)) \implies \Gamma_1 : ((.(((...))(...)).)) \implies \Gamma_2 : ((.(((...))(...)...())))$

Another possible rearrangement through shift moves widens the final loop of the hairpin by moving a one-nucleotide bulge:

$\Gamma_0 : ((.(((...))))(....)) \implies \Gamma_1' : (((.((...)))*)((...))) \implies \Gamma_2' : (((.((...)))*)((...)))$

Now notice that

$d_3(\Gamma_0, \Gamma_1) = d_3(\Gamma_0, \Gamma_1') = 2, \quad d_3(\Gamma_0, \Gamma_2) = d_3(\Gamma_0, \Gamma_2') = 4.$

But, although

$d_4(\Gamma_0, \Gamma_1) = d_4(\Gamma_0, \Gamma_1') = \frac{21}{17},$

it turns out that

$d_4(\Gamma_0, \Gamma_2) = \frac{42}{11}, \quad d_4(\Gamma_0, \Gamma_2') = \frac{41}{11}.$

Therefore, under $d_4$, $\Gamma_2'$ is closer to $\Gamma_0$ than $\Gamma_2.$
As \( m \) grows, the description of \( d_m \) on \( C_n \) gets more and more involved or, if we want it to remain simple, more and more uninformative. The same happens on \( S_n \), but at a lower pace. Therefore, from now on, we shall only consider edge metrics on RNA secondary structures.

We have a closed formula for the Hilbert function of the edge ideal of an RNA secondary structure, given by the following result, which we consider interesting in itself. In it we use the convention that \( \binom{0}{0} = 1 \) and \( \binom{0}{j} = 0 \) if \( j > 0 \).

**Proposition 14** For every \( \Gamma = ([n], Q) \in S_n \) and for every \( m \geq 0 \),
\[
H_\Gamma(m) = \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j \binom{|Q|}{j} \binom{n + m - 2j}{n}.
\]

*Proof.* To begin with, notice that the Hilbert function \( H_\Gamma \) only depends on \( |Q| \) because, for every two RNA secondary structures \( \Gamma_1, \Gamma_2 \) with the same number of contacts, their edge ideals are the same up to a permutation of the variables and thus \( |C(I_{\Gamma_1})_m| = |C(I_{\Gamma_2})_m| \) for every \( m \geq 0 \). For every \( k \geq 0 \), let \( H_k \) denote the Hilbert function of the edge ideal of any \( \Gamma \in S_n \) with \( |Q| = k \).

Now, notice that if \( \Gamma = ([n], Q) \in S_n \) with \( Q = \{i_1, j_1, \ldots, i_k, j_k\} \), then no monomial \( x_{i_1}x_{j_1}, \ldots, x_{i_k}x_{j_k} \), for \( t = 1, \ldots, k \), is a zero divisor modulo the ideal \( (x_{i_1}x_{j_1}, \ldots, x_{i_{t-1}}x_{j_{t-1}}) \). This implies, by [6, §9.4, Cor. 5] (or, rather, its proof) that
\[
H_{k+1}(m) = H_k(m) - H_k(m-2), \quad \text{for every } k \geq 0, \ m \geq 2,
\]
and hence
\[
H_{k+1}(m) = H_0(m) - \sum_{i=0}^{k} H_i(m-2), \quad \text{for every } k \geq 0, \ m \geq 2;
\]
we shall use this recursion to prove the expression in the statement by induction on \( m \).

To begin with, we know that
\[
H_0(m) = |M(\mathcal{M})_m| = \binom{n + m}{n}, \quad \text{for every } m \geq 0,
\]
which clearly satisfies the expression in the statement (with \( |Q| = 0 \)). Moreover,
\[
H_k(0) = 1, \quad H_k(1) = n + 1, \quad \text{for every } k \geq 0,
\]
because, for every \( \Gamma \in S_n \),
\[
C(I_{\Gamma})_0 = \{1\}, \ C(I_{\Gamma})_1 = \{1, x_1, \ldots, x_n\}.
\]
These values for \( H_k(0) \) and \( H_k(1) \) clearly satisfy the expression given in the statement. Now, as induction hypothesis, assume that
\[
H_k(m_0) = \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{k}{j} \binom{n + m_0 - 2j}{n} \quad \text{for every } k \geq 0.
\]
Then, for every $k \geq 0$,

$$H_{k+1}(m_0 + 2) = H_0(m_0 + 2) - \sum_{i=0}^{k} H_i(m_0)$$

$$= \binom{n+m_0+2}{n} - \sum_{i=0}^{k} \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{j}{i} \binom{n+m_0-2j}{n}$$

$$= \binom{n+m_0+2}{n} + \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{n+m_0-2j}{n} \binom{k+1}{j+1}$$

$$= \binom{n+m_0+2}{n} + \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{n+m_0-2j}{n} \binom{k+1}{j+1}$$

$$= \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{k+1}{j+1} \binom{n+m_0+2-2j}{n},$$

where the second equality uses the induction hypothesis and the fourth equality uses that

$$\sum_{i=0}^{k} \binom{j}{i} = \binom{k+1}{j+1}. \quad \blacksquare$$

Thus, for instance, for every $\Gamma = ([n], Q) \in S_n$,

$$H_{I_1}(2) = \binom{n+2}{3} - |Q|$$

$$H_{I_1}(3) = \binom{n+3}{4} - (n+1)|Q|$$

$$H_{I_1}(4) = \binom{n+4}{5} - \binom{n+2}{2}|Q| + \binom{|Q|}{2}$$

$$H_{I_1}(5) = \binom{n+5}{6} - \binom{n+3}{2}|Q| + (n+1)\binom{|Q|}{2}$$

$$H_{I_1}(6) = \binom{n+6}{7} - \binom{n+4}{2}|Q| + \binom{n+2}{2}\binom{|Q|}{2} - \binom{|Q|}{3}$$

Unfortunately, we do not have a similar explicit expression for the Hilbert function of arbitrary contact structures, including unions of RNA secondary structures, and then we still use Lemma 8 to compute the Hilbert functions of the latter.

To close this paper, we shall provide explicit descriptions of $d_5$ and $d_6$ on the set $S_n$, just to grasp what they measure. Their proofs are simple, but long and technically involved, and we delay them until the Appendix at the end of this paper.

**Proposition 15** For every $\Gamma_1, \Gamma_2 \in S_n$,

$$d_5(\Gamma_1, \Gamma_2) = |Q_1 \Delta Q_2|$$

$$- \frac{1}{12} \left(2(n-1)(|Q_1 \Delta Q_2| - \Lambda_{\geq 2}) + 2(|Q_1 \cup Q_2|) - (|Q_1|) - (|Q_2|) + 2(\Lambda_{\geq 3} + \Theta(4))\right)$$

**Example 16** Consider the RNA secondary structures of length 15

$$\Gamma_1 : (.),(.),(.),(.), \quad \Gamma_2 : (.),(.),(.),(.),(.) \quad \Gamma_3 : (.),(.),(.),(.)$$

Then

$$d_3(\Gamma_1, \Gamma_2) = d_3(\Gamma_1, \Gamma_3) = 7$$

and

$$d_4(\Gamma_1, \Gamma_2) = d_4(\Gamma_1, \Gamma_3) = \frac{25}{4},$$

but

$$d_5(\Gamma_1, \Gamma_2) = 5 + \frac{71}{136}, \quad d_5(\Gamma_1, \Gamma_3) = 5 + \frac{69}{136}.$$

Thus, under $d_5$, $\Gamma_3$ is closer to $\Gamma_1$ than to $\Gamma_2$. 

17
It is interesting to observe that, contrary to what happens with $d_3$ and $d_4$, the term $2(|Q_1 ∪ Q_2|) - (|Q_1|) - (|Q_2|)$ makes the value of $d_5(Γ_1, Γ_2)$ depend not only on the cardinal and structure of the set $Q_1 Δ Q_2$, but also on $|Q_1 ∩ Q_2|$. For instance, it is not difficult to check that if $Γ_1, Γ_2, Γ'_1, Γ'_2 ∈ S_n$ are such that $Q_1 - Q_2 = Q'_1 - Q'_2$ and $Q_2 - Q_1 = Q'_2 - Q'_1$, then

$$d_5(Γ_1, Γ_2) < d_5(Γ'_1, Γ'_2) ⇔ |Q_1 ∩ Q_2| > |Q'_1 ∩ Q'_2|;$$

i.e., the greater the set of contacts they share is, the closer they are.

**Example 17** Consider again the hairpin with an interior loop $Γ_0$ and its rearrangement $Γ_1$ given in Example 13

$$Γ_0 : (((((...))))(....)), \quad Γ_1 : (((((...))(...)....)).$$

Let now $Γ'_0$ and $Γ'_1$ be the RNA secondary structures of the same length 21 obtained by removing from $Γ_0$ and $Γ_1$ their outer stacked pair of contacts:

$$Γ'_0 : ...(((...))))(....), \quad Γ'_1 : ...((...))((...)....).$$

Since $Q_1 Δ Q_2 = Q'_1 Δ Q'_2 = \{4\cdot14, 14\cdot18\}$, we have that

$$d_3(Γ_0, Γ_1) = d_3(Γ'_0, Γ'_1) = 2, \quad d_4(Γ_0, Γ_1) = d_4(Γ'_0, Γ'_1) = \frac{21}{11}$$

But it turns out that

$$d_5(Γ_0, Γ_1) = 1 + \frac{201}{253}, \quad d_5(Γ'_0, Γ'_1) = 1 + \frac{205}{253}.$$

As far as $d_6$ goes, we have the following result.

**Proposition 18** For every $Γ_1, Γ_2 ∈ S_n$,

$$d_6(Γ_1, Γ_2) = |Q_1 Δ Q_2| - \frac{1}{3} \left( (n+1)(2(|Q_1 ∪ Q_2|) - (|Q_1|) - (|Q_2|)) +2(|Q_2|) + 3 - |Q_1 ∪ Q_2| - (|Q_1 Δ Q_2| - λ_{≥2} - 2(n-1)λ_{≥3} + 2λ_{≥4} + 2(n-3)Θ^{(4)}) \right)$$

In a similar way, an explicit expression for $d_m$ on $S_n$ can be obtained for every $m ≥ 7$, yielding information about what these metrics measure: recall moreover that, for specific $Γ_1, Γ_2 ∈ S_n$, the value of $d_m(Γ_1, Γ_2)$ can be easily computed using a suitable computer algebra system. Unfortunately, we have not been able to produce a closed expression for all these metrics. Notice that, when finding an expression for $d_m$, the only new ingredient that is necessary to determine is the coefficient $SF_{m-1}(I_{Γ_1} ∪ I_{Γ_2})$, which can be done for each $m$ by counting carefully how many square-free monomials of total degree $m - 1$ belong to $I_{Γ_1} ∪ I_{Γ_2}$ as we do in this paper for $m = 4, 5, 6$. It is in this coefficient that new terms make their appearance in each $d_m$: when one balances the number of square-free monomials in $I_{Γ_1} ∪ I_{Γ_2}$ of the form

$$x_{i_1} \cdots x_{i_{m-1}}$$

such that $i_1, i_2, \ldots, i_{m-2}, i_{m-1} ∈ Q_1 ∪ Q_2$, the number $λ^{(m-2)}$ makes its first appearance, and if $m - 1$ is even, then to counterbalance the number of square-free monomials

$$x_{i_1} \cdots x_{i_{m-1}}$$

in $I_{Γ_1} ∪ I_{Γ_2}$ such that $\{i_1, \ldots, i_{m-1}\}$ is a cyclic orbit, the number $Ω^{(m-1)}$ must be used for the first time (cf. the proofs of Propositions 15 and 18 in the Appendix).
5 Conclusion

In the Discussion section of their paper [18], Reidys and Stadler, having pointed out that their group-based models and metrics cannot be used on arbitrary contact structures, ask “What if contacts are not unique as in the case of proteins?” Using edge ideals, we can represent arbitrary contact structures by means of monomial ideals of a polynomial ring, and we show that this representation generalizes the embedding of RNA secondary structures into the set of subgroups of $S_n$ proposed by Reidys and Stadler. We have used then this representation to define a family of edge ideal metrics on arbitrary contact structures, which can be easily computed using several freely available computer algebra systems, and we have studied their properties.

Edge ideals are not the unique possible monomial ideal representations of arbitrary contact structures. For instance, we could associate to every contact structure $\Gamma = ([n], Q)$ the clique ideal $J_{\Gamma}$ of $\mathbb{F}_2[x_1, \ldots, x_n]$ generated by the set of monomials consisting of one square-free monomial $x_{i_1} \cdots x_{i_k}$ for each non-trivial clique (complete subgraph) $\{i_1, \ldots, i_k\}$, with $k \geqslant 2$, of $\Gamma$. Notice that if $\Gamma$ is an RNA secondary structure, then $J_{\Gamma} = I_{\Gamma}$, but for arbitrary contact structures they can be different. For instance, if $\Gamma = ([5], \{1 \cdot 3, 3 \cdot 5, 1 \cdot 5\})$, then

$$I_{\Gamma} = \langle x_1x_3, x_1x_5, x_3x_5 \rangle \quad \text{while} \quad J_{\Gamma} = \langle x_1x_3x_5 \rangle.$$ 

We see that the clique ideal $J_{\Gamma}$ captures information on the clusters of monomers in three-dimensional structures (for instance, base triplets and quartets in RNA structures) in a way different to $I_{\Gamma}$. These ideals can be used to define new metrics on arbitrary contact structures of a fixed length similar to the edge ideal metrics introduced here. We shall report on them in a subsequent paper.

Let us finally point out that another question of Reidys and Stadler’s remains open for our models as well as, to our knowledge, for theirs: “Is there any hope for extending or altering any of the above concepts in order to incorporate variable sizes of structures?”

Acknowledgments. We acknowledge with thanks X. Bordoy, J. Elias, J. Míró and G. Valiente for several discussions on the topic of this paper and for their comments on draft versions of it.

References

[1] R. T. Batey, R. P. Rambo, J. A. Doudna, Tertiary motifs and folding of RNA, Angew. Chem. Int. Ed. 38 (1999), 2326–2343.

[2] A. M. Bigatti, Computation of Hilbert-Poincaré series, J. Pure Appl. Alg. 119 (1997), 237-253.

[3] A. Capani, G. Niesi, L. Robbiano, CoCoA, a system for doing Computations in Commutative Algebra, available via anonymous ftp from cocoa.dima.unige.it.

[4] H. S. Chan, K. A. Dill, Compact polymers, Macromolecules 22, (1989), 4559–4573.

[5] H. S. Chan, K. A. Dill, Sequence space soup of proteins and copolymers, J. Chem. Phys. 95, (1991), 3775–3779.
[6] D. Cox, J. Little, D. O’Shea, *Ideals, Varieties, and Algorithms* (second ed.), Springer-Verlag (1997).

[7] K. A. Dill, S. Bromberg, K. Yue, K. M. Fiebig, D. P. Yeo, P. D. Thomas, H. S. Chan, Principles of protein folding: A perspective from simple exact models, *Prot. Sci.* 4 (1995), 561-602.

[8] J. Casasnovas, J. Miró, F. Rosselló, On the algebraic representation of RNA secondary structures with G.U pairs, to appear in *Journal of Mathematical Biology* (DOI: 10.1007/s00285-002-0188-0).

[9] W. Fontana, D. Konings, P. Stadler, P. Schuster, Statistics of RNA secondary structures, *Biopolymers* 33 (1993), 1389–1404.

[10] W. Fontana, P. Schuster, Shaping space: the possible and the attainable in RNA genotype-phenotype mapping, *J. Theor. Biol.* 194 (1998), 491–515.

[11] D. R. Grayson, M. Stillman, Macaulay 2, software system available at http://www.math.uiuc.edu/Macaulay2/.

[12] C. Haslinger, P. F. Stadler, RNA structures with pseudo-knots: Graph-theoretical, combinatorial, and statistical properties, *Bull. Math. Biol.* 61 (1999), 437–467.

[13] I. Hofacker, W. Fontana, P. Stadler, L. Bonhoeffer, M. Tacker, P. Schuster, Fast folding and comparison of RNA secondary structures, *Monatsh. Chem.* 125 (1994), 167–188.

[14] N. Madras, G. Sokal, *The self-avoiding walk*, Birkhäuser (1993).

[15] Y. Magarshak, C. J. Benham, An algebraic representation of RNA secondary structures, *J. of Biomol. Struct. & Dyn.* 10 (1992) 465–488.

[16] P. B. Moore, Structural motifs in RNA, *Annu. Rev. Biochem.*, 68 (1999), 287–300.

[17] V. Moulton, M. Zuker, M. Steel, R. Pointon, D. Penny, Metrics on RNA secondary structures, *J. Comp. Biol.* 7 (2000), 277–292.

[18] C. Reidys, P. F. Stadler, Bio-molecular shapes and algebraic structures, *Comp. & Chem.* 20 (1996), 85–94.

[19] F. Rosselló, On Reidys and Stadler’s metrics for RNA secondary structures, http://xxx.lanl.gov/pdf/math.GM/0305222, submitted.

[20] B. Shapiro, K. Zhang, Comparing multiple RNA secondary structures using tree comparisons, *CABIOS* 6 (1990), 309-318.

[21] P. Schuster, W. Fontana, P. Stadler, I. Hofacker, From sequences to shapes and back: a case study in RNA secondary structures, *Proc. Roy. Soc. B* 255 (1994), 279–284.

[22] P. Schuster, P. F. Stadler, Discrete models of biopolymers, to appear in *Handbook of Computational Chemistry* (M.J.C. Crabbé, M. Drew and A. Konopka, eds.), Marcel Dekker (in press); see also Univ. Wien TBI Preprint No. pks-99-012 (1999).
[23] A. Simis, W. Vasconcelos, R. Villarreal, On the ideal theory of graphs, *J. Algebra* **167** (1994), 389–416.

[24] R. Villarreal, *Monomial ideals*, Marcel-Dekker (2000).

[25] M. S. Waterman, T. F. Smith, RNA secondary structure: a complete mathematical analysis, *Math. Biosci.* **42** (1978), 257–266.

[26] M. Zuker, On finding all suboptimal foldings of an RNA molecule, *Science* **244** (1989), 48–52.

[27] M. Zuker, The use of dynamic programming algorithms in RNA secondary structure prediction, In *Mathematical methods for DNA sequences* (M. Waterman, ed.), CRC Press (1989), 159–184.

[28] M. Zuker, D. Sankoff, RNA secondary structures and their prediction, *Bull. Math. Biol.* **46** (1984), 591–621.

**Appendix: Proof of Propositions 15 and 18**

To simplify the proofs, we establish first a lemma that we shall use several times and that generalizes the computation of $A(\Gamma_1 \cup \Gamma_2)$ carried on in the proof of Proposition 11.

For every $\Gamma_1, \Gamma_2 \in S_n$ and for every $k \geq 2$, let

$$M_k = \{\{i_1 \cdot i_2, i_2 \cdot i_3, \ldots, i_k \cdot i_{k+1}\} \subseteq Q_1 \cup Q_2 \mid i_1, \ldots, i_k \text{ pairwise different}\},$$

and let $A_k$ be its cardinal. Notice that $A_2$ is equal to the number of angles $A(\Gamma_1 \cup I_{\Gamma_2})$ in $\Gamma_1 \cup \Gamma_2$. To simplify the notations, from now on we shall systematically write $A_2$ instead of $A(\Gamma_1 \cup I_{\Gamma_2})$.

**Lemma A** For every $\Gamma_1, \Gamma_2 \in S_n$ and for every $k \geq 2$,

$$A_k = |Q_1 \Delta Q_2| - \sum_{m=4}^{k} m\Theta^{(m)} - \sum_{i=2}^{k} \Lambda_{2i}.$$

**Proof.** If $\{i_1 \cdot i_2, \ldots, i_k \cdot i_{k+1}\} \in M_k$, then the nodes $i_1, i_2, \ldots, i_{k+1}$ belong to the same orbit, whose length will be at least $k + 1$. Therefore, every cyclic orbit of length $m \leq k$ contributes no element to $M_k$, while every cyclic orbit of length $m \geq k + 1$ adds $m$ new elements to it. On the other hand, each linear orbit of length $m \leq k$ contributes no element to $M_k$, while every linear orbit of length $m \geq k + 1$ adds $m - k$ new elements to this set.

This shows that

$$A_k = \sum_{m=k}^{\infty} m\Theta^{(m)} + \sum_{m>k} (m-k)\Lambda^{(m)}$$

$$= \sum_{m>k} m\Theta^{(m)} + \sum_{m>k} (m-1)\Lambda^{(m)} - (k-1) \sum_{m=k}^{\infty} \Lambda^{(m)}$$

$$= |Q_1 \Delta Q_2| - \sum_{m=4}^{k} m\Theta^{(m)} - \sum_{i=2}^{k} (m-1)\Lambda^{(m)} - (k-1) \sum_{m=k}^{\infty} \Lambda^{(m)}$$

$$= |Q_1 \Delta Q_2| - \sum_{m=4}^{k} m\Theta^{(m)} - \sum_{i=2}^{k} \Lambda_{2i}.$$

\[ \blacksquare \]
In particular, we obtain again that \( A_2 = |Q_1 \Delta Q_2| - \Lambda_{\geq 2} \), as we already saw in the proof of Proposition 11.

**Proof of Proposition 15.** To simplify the notations, we shall denote each \( SF_i(I_{\Gamma_1 \cup \Gamma_2}) \) simply by \( SF_i \). We shall use the expression

\[
d_5(\Gamma_1, \Gamma_2) = \frac{1}{\binom{n}{2}^2} \left( H_{\Gamma_1}(4) + H_{\Gamma_2}(4) - 2H_{\Gamma_1 \cup \Gamma_2}(4) \right),
\]

where we already know that

\[
H_{\Gamma_1}(4) = \binom{n+4}{4} - \binom{n+2}{2}|Q_1| + \binom{|Q_1|}{2} + \binom{|Q_1|}{2}, \quad i = 1, 2,
\]

\[
H_{\Gamma_1 \cup \Gamma_2}(4) = \binom{n+4}{n} - (4SF_1 + 6SF_2 + 4SF_3 + SF_4)
\]

with

\[
SF_1 = 0, \quad SF_2 = |Q_1 \cup Q_2|, \quad SF_3 = (n-2)|Q_1 \cup Q_2| - A_2;
\]

the value of \( SF_3 \) was obtained in the proof of Proposition 9; notice that \( T(\Gamma_1 \cup \Gamma_2) = 0 \) and recall that \( A(\Gamma_1 \cup \Gamma_2) = A_2 \). It remains to compute \( SF_4 \):

1. For every \( i, j \in Q_1 \cup Q_2 \), there are \( \binom{n-2}{2} \) square free monomials \( x_i x_j x_k x_l \in M(I_{\Gamma_1 \cup \Gamma_2}) \). This makes \( \binom{n-2}{2}|Q_1 \cup Q_2| \) such monomials.
2. Now, if \( i, j, k, l \in Q_1 \cup Q_2 \) with \( \{i, j\} \cap \{k, l\} = \emptyset \), then the monomial \( x_i x_j x_k x_l \) is counted twice in (1). Therefore, we must subtract \( \binom{|Q_1 \cup Q_2|}{2} - A_2 \) to the value given in (1).
3. If \( i, j, k \in Q_1 \cup Q_2 \) form an angle in \( \Gamma_1 \cup \Gamma_2 \), then for every \( l \notin \{i, j, k\} \) the monomial \( x_i x_j x_k x_l \) is counted twice in (1). Thus, we must also subtract \( (n-3)A_2 \).
4. If \( i, j, k, l \in Q_1 \cup Q_2 \), with \( i, j, k, l \) pairwise different, then the monomial \( x_i x_j x_k x_l \) is counted three times in (1), then it is subtracted once in (2) and it is subtracted twice in (3). Therefore, to retrieve these monomials, we must add \( A_3 \).
5. Finally, if \( i, j, k, l \in Q_1 \cup Q_2 \), so that if \( \{i, j, k, l\} \) form a cyclic orbit of length 4, then the monomial \( x_i x_j x_k x_l \) is counted four times in (1), it is subtracted twice in (2), it is subtracted four more times in (3) and it is added four times in (4). To balance these operations, we must subtract \( \Theta(4) \).

In all, this shows that

\[
SF_4 = \left( \binom{n-2}{2} \right) |Q_1 \cup Q_2| - \binom{|Q_1 \cup Q_2|}{2} - (n-4)A_2 + A_3 - \Theta(4)
\]

and hence

\[
H_{\Gamma_1 \cup \Gamma_2}(4) = \binom{n+4}{4} - \left( \binom{n+2}{2} \right) |Q_1 \cup Q_2| + \binom{|Q_1 \cup Q_2|}{2} + nA_2 - A_3 + \Theta(4).
\]

A simple computation shows then that

\[
d_5(\Gamma_1, \Gamma_2) = H_{\Gamma_1}(4) + H_{\Gamma_2}(4) - 2H_{\Gamma_1 \cup \Gamma_2}(4)
\]

\[
= 2\binom{n+4}{4} - \binom{n+2}{2}(|Q_1| + |Q_2|) + \binom{|Q_1|}{2} + \binom{|Q_1|}{2} - 2\binom{n+2}{2}|Q_1 \cup Q_2| + \left( |Q_1 \cup Q_2| \right) + nA_2 - A_3 + \Theta(4)
\]

\[
= \binom{n+2}{2}|Q_1 \Delta Q_2| - 2\left( \binom{|Q_1 \cup Q_2|}{2} \right) - \binom{|Q_1|}{2} - \binom{|Q_1|}{2} + 2nA_2 - 2A_3 + 2\Theta(4)
\]

Now, we know from Lemma A that

\[
A_2 = |Q_1 \Delta Q_2| - \Lambda_{\geq 2}, \quad A_3 = |Q_1 \Delta Q_2| - \Lambda_{\geq 2} - \Lambda_{\geq 3}.
\]
Replacing them in the expression obtained above for \( d_5(\Gamma_1, \Gamma_2) \), and dividing the resulting expression by \( \binom{n+2}{2} \), we finally obtain

\[
d_5(\Gamma_1, \Gamma_2) = \binom{n}{2}\left(2\binom{Q_1 \cup Q_2}{2} - \binom{Q_1}{2} - \binom{Q_2}{2} + 2(n-1)(|Q_1\Delta Q_2| - \Lambda_{\geq 2}) + 2(\Lambda_{\geq 3} + \Theta^{(4)})\right),
\]

as we wanted to prove.

**Proof of Proposition 18.** To simplify the notations, we shall denote again \( SF(I_{\Gamma_1 \cup \Gamma_2}) \) simply by \( SF \).

In the expression

\[
d_6(\Gamma_1, \Gamma_2) = \frac{1}{\binom{n+3}{3}} \left(H_{\Gamma_1}(5) + H_{\Gamma_2}(5) - 2H_{\Gamma_1 \cup \Gamma_2}(5)\right),
\]

we already know that

\[
H_{\Gamma_1}(5) = \binom{n+5}{5} - \binom{n+3}{3}|Q_1| + (n+1)\binom{|Q_1|}{2}, \quad i = 1, 2
\]

\[
H_{\Gamma_1 \cup \Gamma_2}(5) = \binom{n+5}{5} - (5SF_1 + 10SF_2 + 10SF_3 + 5SF_4 + SF_5)
\]

with

\[
SF_1 = 0, \quad SF_2 = |Q_1 \cup Q_2|, \quad SF_3 = (n-2)|Q_1 \cup Q_2| - A_2
\]

\[
SF_4 = \binom{n-2}{2}|Q_1 \cup Q_2| - 2\binom{|Q_1 \cup Q_2|}{2} - (n-4)A_2 + A_3 - \Theta^{(4)}
\]

Let us compute now \( SF_5 \):

1. For every \( i \cdot j \in Q_1 \cup Q_2 \), there are \( \binom{n-2}{2} \) square free monomials \( x_i x_j x_k x_l x_m \in M(I_{\Gamma_1 \cup \Gamma_2}) \). This makes \( \binom{n+2}{2}|Q_1 \cup Q_2| \) such monomials.

2. Now, if \( i \cdot j, k \cdot l \in Q_1 \cup Q_2 \) with \( \{i, j\} \cap \{k, l\} = \emptyset \), then for every \( m \notin \{i, j, k, l\} \) the monomial \( x_i x_j x_k x_l x_m \) is counted twice in (1). Therefore, we must subtract \( (n-4)\binom{|Q_1 \cup Q_2|}{2} - A_2 \) to (1).

3. If \( i \cdot j, k \cdot l \in Q_1 \cup Q_2 \), then for every \( l, m \notin \{i, j, k\} \) the monomial \( x_i x_j x_k x_l x_m \) is counted twice in (1). Therefore, we must also subtract \( \binom{n-3}{2}A_2 \) to (1).

4. If \( i \cdot j, k \cdot l \in Q_1 \cup Q_2 \) with \( \{i, j\} \cap \{k, l\} = \emptyset \), the monomial \( x_i x_j x_k x_l x_m \) is counted 3 times in (1), then it is subtracted twice in (2) and it is subtracted once again in (3). Therefore, to retrieve these monomials we must add

\[
\left\{\{i \cdot j, j \cdot k, l \cdot m\} \mid i \cdot j, j \cdot k, l \cdot m \in Q_1 \cup Q_2, \{i, j, k\} \cap \{l, m\} = \emptyset\right\}.
\]

Let us call for the moment \( X \) this number.

5. If \( i \cdot j, k \cdot l \in Q_1 \cup Q_2 \), for every \( m \notin \{i, j, k, l\} \) the monomial \( x_i x_j x_k x_l x_m \) is counted 3 times in (1), then it is subtracted once in (2) and it is subtracted twice in (3). Therefore, to retrieve these monomials we must also add \( (n-4)A_3 \) monomials.

Notice now that

\[
X + A_3 = \left|\left\{i \cdot j, j \cdot k, l \cdot m \mid i \cdot j, j \cdot k, l \cdot m \in Q_1 \cup Q_2\right\}\right| = (|Q_1 \cup Q_2| - 2)A_2.
\]

Therefore, (4) and (5) add jointly

\[
(|Q_1 \cup Q_2| - 2)A_2 + (n-5)A_3
\]

monomials.
(6) If $i, j, k, l \in Q_1 \cup Q_2$, i.e., if $\{i, j, k, l\}$ form a cyclic orbit of length 4, then for every $m \notin \{i, j, k, l\}$ the monomial $x_ix_jx_kx_m$ is counted four times in (1), it is subtracted twice in (2), it is subtracted four more times in (3) and it is added four times in (5). Therefore, we must subtract $(n - 4)\Theta^{(4)}$.

(7) Finally, if $i, j, k, l, m \in Q_1 \cup Q_2$, then the monomial $x_ix_jx_kx_lx_m$ is counted four times in (1), it is subtracted three times in (2), it is subtracted three more times in (3) and it is added twice in (4) and twice in (5). Therefore, we must subtract $A_4$.

In all, this shows that
\[
SF_3 = \binom{n}{3}|Q_1 \cup Q_2| - (n - 4)(\binom{|Q_1 \cup Q_2|}{2} - A_2) - \binom{n}{2}A_2 \\
+ (|Q_1 \cup Q_2| - 2)A_2 + (n - 5)A_3 - (n - 4)\Theta^{(4)} - A_4
\]

and hence
\[
H_{\Gamma_1 \cup \Gamma_2}(5) = \binom{n+5}{5} - \binom{n+3}{3}|Q_1 \cup Q_2| + (n + 1)(\binom{|Q_1 \cup Q_2|}{2} + \binom{|Q_2|}{2}) \\
- 2\binom{n+5}{5} - \binom{n+3}{3}|Q_1 \cup Q_2| + (n + 1)(\binom{|Q_1 \cup Q_2|}{2} + \binom{|Q_2|}{2}) \\
+ (\binom{n+1}{2} - |Q_1 \cup Q_2| + 2)A_2 - nA_3 + (n + 1)\Theta^{(4)} + A_4 \\
= \binom{n+3}{3}|Q_1\Delta Q_2| - (n + 1)\left(2\binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} + \binom{|Q_2|}{2}\right) - 2\binom{n+1}{2} + 2 - |Q_1 \cup Q_2|A_2 \\
+ 2nA_3 - 2(n + 1)\Theta^{(4)} - 2A_4.
\]

Since we already know, by Lemma A, that
\[
A_2 = |Q_1\Delta Q_2| - \Lambda_{\geq 2}, \quad A_3 = |Q_1\Delta Q_2| - \Lambda_{\geq 2} - \Lambda_{\geq 3} \\
A_4 = |Q_1\Delta Q_2| - \Lambda_{\geq 2} - \Lambda_{\geq 3} - \Lambda_{\geq 4} - 4\Theta^{(4)}
\]

when we replace these values in the expression obtained above for $d_6(\Gamma_1, \Gamma_2)$ and we divide the resulting expression by $\binom{n+3}{3}$, we finally obtain
\[
d_6(\Gamma_1, \Gamma_2) = |Q_1\Delta Q_2| - \frac{1}{\binom{n+3}{3}}\left((n + 1)(2\binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2}) - \binom{|Q_2|}{2}\right) \\
+ 2\binom{n+1}{2} + 2 - |Q_1 \cup Q_2|(|Q_1\Delta Q_2| - \Lambda_{\geq 2}) - 2(n - 1)\Lambda_{\geq 3} + 2\Lambda_{\geq 4} + 2(n - 3)\Theta^{(4)}
\]