

A new family of metrics for biopolymer contact structures¹

M. Llabrés^a F. Rosselló^{a,*}

^a*Department of Mathematics and Computer Science, Research Institute of Health Science (IUNICS), University of the Balearic Islands, E-07071 Palma de Mallorca, Spain.*

Abstract

Contact structures are simplified representations of biopolymers' three-dimensional structures. In this paper we introduce a new family of metrics $(d_m)_{m \geq 3}$ for contact structures of a fixed length, based on their representation by means of edge ideals of a polynomial ring, that generalize Reidys and Stadler's subgroup metric for RNA secondary structures. We study some abstract properties of these metrics, and we obtain explicit descriptions of them for some values of m .

Key words: Contact structure, RNA secondary structure, metric, distance, edge ideal.

1 Introduction

The three-dimensional structure of a biopolymer is often represented by means of its *contact structure* (Chan and Dill, 1989), the set of all pairs of monomers (nucleotides in RNA molecules, aminoacids in proteins) that are, in some specific sense, spatial neighbors in the three-dimensional structure. 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 $\{1, \dots, n\}$: 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

* Corresponding author; E-mail: cesc.rossello@uib.es

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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 simply impose that a contact can only exist between non-consecutive bases. A further restriction, called the *unique bonds condition*, is added to the definition of RNA secondary structure (Waterman and Smith, 1978): a base can only pair with at most one base. It is usual to impose a third 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 (Waterman and Smith, 1978; Zuker, 1989; Zuker and Sankoff, 1984). Real RNA structures can contain knots, which are moreover important structural elements in many RNA molecules, but they are regarded as “tertiary interactions” (Tinoco and Bustamante, 1999; Westhof and Jaeger, 1992).

Contact structures with unique bonds can also be used to represent the basic building blocks of protein structures, like α -helixes or β -sheets, often called protein secondary structures. But the full representation of the neighborhood in three-dimensional structures of RNA molecules and proteins needs contact structures without unique bonds. For one, the full spatial structure of RNA molecules may contain contacts that violate the unique bonds condition, like base triplets and guanine platforms (Batey et al, 1999; Moore, 1999). And in the tertiary structure of a protein, represented for instance by means of a self-avoiding walk in a lattice, one aminoacid can be spatial neighbor of several aminoacids (Chan and Dill, 1991; Dill et al, 1995). 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, because their spatial closeness is understood as a consequence of their position in the backbone.

The comparison of the three-dimensional structures of biopolymers is an important problem in molecular biology, as it is assumed that a preserved structure corresponds to a preserved function. 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 to the problem of determining the secondary structure of a given RNA molecule (Moulton et al, 2000; Zuker, 1989). 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 (G. Valiente, private communication). This similarity lies also at the basis of the study of the mapping that assigns to each RNA molecule or protein the structure it folds into (Fontana et al, 1993; Schuster et al, 1994) and it can be used in the study of phenotype spaces (Fontana and Schuster, 1998).

The similarity of contact structures can be quantified by means of metrics. Reidys and Stadler defined in their seminal paper (1996) on algebraic models of biopolymer structures three metrics on RNA secondary structures of fixed length, based on their representations as involutions and as permutation subgroups, and on Magarshak’s matrix representation (Magarshak and Benham, 1992), and they discussed their biophysical relevance. These metrics have been recently analyzed from the mathematical point of view (Casasnovas et al, 2003; Rosselló, 2003).

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 arbitrary contact structures of a fixed length. In this paper we overcome this drawback, by switching from permutation subgroups to monomial ideals. More specifically, we represent a contact structure of length n by means of its *edge ideal* in the polynomial ring $\mathbb{F}_2[x_1, \dots, x_n]$. Edge ideals are quite a popular tool in commutative algebra to represent graphs and to study their properties, as Villareal’s textbook (2001) evidences. By using them, we generalize Reidys and Stadler’s subgroup metric to a family of metrics $(d_m)_{m \geq 3}$ on the set of all contact structures of a fixed length n . These metrics can be expressed in terms of Hilbert functions, which makes them easily computable using several public domain computer algebra systems like, for instance, CoCoA (Capani et al) or Macaulay (Grayson and Stillman). We establish some global properties of these metrics and we obtain explicit expressions for several of them, which allow to grasp the notion of (dis)similarity they measure.

At the moment, it is not clear whether our metrics are useful or not, but we hope that they will increase the range of sensible metrics available in the applications of the comparison of structures of a fixed length mentioned above: as Moulton et al (2000, p. 290) point out, “[...] generally speaking, it is probably safest to try as many metrics as possible.”

2 Preliminaries

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

2.1 Contact structures

From now on, let $[n]$ denote the set $\{1, \dots, n\}$, for every positive integer n .

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 edges $\{i, j\} \in Q$, called *contacts*, satisfy the following condition (which translates the impossibility of a contact between two consecutive monomers): for every $i \in [n]$, $\{i, i+1\} \notin Q$.

A contact structure $\Gamma = ([n], Q)$ has *unique bonds* when it satisfies the following further condition: for every $i \in [n]$, if $\{i, j\}, \{i, k\} \in Q$, then $j = k$.

Contact structures and contact structures with unique bonds are also called, respectively, *diagrams* and *1-diagrams* (Haslinger and Stadler, 1999).

Let \mathcal{C}_n and \mathcal{U}_n denote the sets of all contact structures and of all contact structures with unique bonds of length n , respectively.

A contact structure $\Gamma = ([n], Q)$ is a *RNA secondary structure* when it has unique bonds and it satisfies moreover the following *no-pseudoknots* condition: if $\{i, j\}, \{k, l\} \in Q$ and $i < k < j$, then $i < l < j$.

We shall denote from now on a contact $\{j, k\}$ by $j \cdot k$ or $k \cdot j$, without distinction, and we shall say that a node is *isolated* in a contact structure when it is not involved in any contact.

Given two contact structures of the same length $\Gamma_1 = ([n], Q_1), \Gamma_2 = ([n], Q_2)$, their *union* is the contact structure $\Gamma_1 \cup \Gamma_2 = ([n], Q_1 \cup Q_2)$. The *empty contact structure* of length n is $([n], \emptyset)$.

From now on, and unless otherwise stated, given any contact structure Γ or Γ_i , $i = 1, 2, \dots$, we shall always denote its set of contacts by Q or Q_i , respectively.

We shall often represent specific RNA secondary structures by means of their *bracket representation* (Hofacker et al, 1994), 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,

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

represents the RNA secondary structure

$$\left([25], \{1 \cdot 25, 2 \cdot 14, 3 \cdot 13, 4 \cdot 12, 5 \cdot 11, 6 \cdot 10, 17 \cdot 23, 18 \cdot 22\} \right).$$

2.2 Reidys and Stadler's subgroup metric

For every $n \geq 1$, let S_n be the symmetric group of permutations of $[n]$. Reidys and Stadler (1996) associated to every contact structure with unique bonds $\Gamma \in \mathcal{U}_n$ the subgroup $G(\Gamma)$ of S_n generated by the set of the transpositions

corresponding to the contacts in Γ :

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

They also proved that the mapping $\Gamma \mapsto G(\Gamma)$ is an embedding of \mathcal{U}_n into the set $\text{Sub}(S_n)$ of subgroups of S_n , and they used this embedding to define the following *subgroup metric*:

$$d_{sgr} : \mathcal{U}_n \times \mathcal{U}_n \rightarrow \mathbb{R}$$

$$(\Gamma_1, \Gamma_2) \mapsto \ln \left| \frac{G(\Gamma_1) \cdot G(\Gamma_2)}{G(\Gamma_1) \cap G(\Gamma_2)} \right|$$

Rosselló (2003) showed 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 \mathcal{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 $\Gamma_1, \Gamma_2 \in \mathcal{C}_5$ be two contact structures with sets of contacts $Q_1 = \{1 \cdot 3, 3 \cdot 5\}$ and $Q_2 = \{1 \cdot 5, 3 \cdot 5\}$, respectively. Then $G(\Gamma_1) = \langle (1, 3), (3, 5) \rangle$ and $G(\Gamma_2) = \langle (1, 5), (3, 5) \rangle$ are both equal to

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

This entails in particular that the subgroup metric, when extended to \mathcal{C}_n , yields only a pseudometric: it is nonnegative and symmetric and satisfies the triangular inequality, but $d_{sgr}(\Gamma_1, \Gamma_2) = 0$ does not imply $\Gamma_1 = \Gamma_2$.

2.3 Orbits

Reidys and Stadler also represented a contact structure with unique bonds $\Gamma \in \mathcal{U}_n$ with set of contacts $Q = \{i_1 \cdot j_1, \dots, i_k \cdot j_k\}$ by the involution $\pi(\Gamma) = \prod_{t=1}^k (i_t, j_t) \in S_n$. They also proved that this construction yields an embedding $\pi : \mathcal{U}_n \hookrightarrow S_n$, which they used to induce metrics on \mathcal{U}_n from metrics on S_n (Haslinger and Stadler, 1999; Reidys and Stadler, 1996).

For every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$, 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 $\{i_1, i_2, \dots, i_m\} \subseteq [n]$, $m \geq 1$, such that

$$i_1 \cdot i_2, i_2 \cdot i_3, \dots, i_{m-1} \cdot i_m \in Q_1 \cup Q_2$$

and maximal with this property, i.e., such that the only other contact in $Q_1 \cup Q_2$ involving some element of this subset can possibly 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 $\{i_1, i_2, \dots, i_m\}$ is such an orbit, then $i_1 \cdot i_2, i_3 \cdot i_4, \dots$ belong to one of the sets Q_1 or Q_2 and $i_2 \cdot i_3, i_4 \cdot i_5, \dots$ to the other one.

Such an orbit is *closed* 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 *open* in all other cases: see Fig. 1. We shall call the cardinal of an orbit its *length*. The length of a closed orbit is always even: if $i_1 \cdot i_2 \in Q_1$ in a closed orbit $\{i_1, i_2, \dots, i_m\}$ with $m \geq 3$, then $i_1 \cdot i_m \in Q_2$ and hence $i_{m-1} \cdot i_m \in Q_1$.

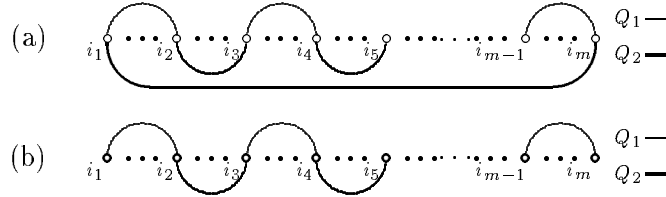


Fig. 1. A closed orbit (a) and an open orbit (b) of length m .

An orbit is *trivial* when it is a singleton: it is an open orbit consisting of a node isolated both in Γ_1 and Γ_2 . If $\{i_1, i_2, \dots, i_m\}$ is a non-trivial open orbit with $i_1 \cdot i_2, i_2 \cdot i_3, \dots, i_{m-1} \cdot i_m \in Q_1 \cup Q_2$ 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 an open orbit or in a closed orbit of length $m \geq 4$.

Let, for every $m \geq 2$, $\Omega^{(m)}$, $\Omega_{\geq m}$, and $\Theta^{(m)}$ denote, respectively, the number of open orbits of length m , the number of open orbits of length greater or equal than m , and the number of closed orbits of length m induced by the action of $D(\Gamma_1, \Gamma_2)$ on $[n]$. Since a closed orbit of length $m \geq 4$ involves m contacts and an open orbit of length m involves $m - 1$ contacts, we have that

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

3 Edge ideal metrics

Let n be from now on an integer greater than 2. Let $\mathcal{M}(x_1, \dots, x_n)$, or simply $\mathcal{M}(\underline{x})$, be the set of all monomials in the variables x_1, \dots, x_n . We shall denote a

monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n} \in \mathcal{M}(\underline{x})$ by $x^{(\alpha_1, \dots, \alpha_n)}$ or simply by $x^{\underline{\alpha}}$ if we let $\underline{\alpha}$ stand for the n -tuple $(\alpha_1, \dots, \alpha_n)$. The *total degree* of a monomial $x^{(\alpha_1, \dots, \alpha_n)}$ is $\sum_{i=1}^n \alpha_i$. For every $m \geq 0$, let $\mathcal{M}(\underline{x})^{(m)}$ and $\mathcal{M}(\underline{x})_m$ be the sets of all monomials in $\mathcal{M}(\underline{x})$ of total degree m and of total degree $\leq m$, respectively. Recall that $|\mathcal{M}(\underline{x})^{(m)}| = \binom{n+m-1}{n-1}$ and $|\mathcal{M}(\underline{x})_m| = \binom{n+m}{n}$.

Let \mathbb{F}_2 be the binary field² with elements $0, 1$ and $\mathbb{F}_2[x_1, \dots, x_n]$, or simply $\mathbb{F}_2[\underline{x}]$, the ring of polynomials in the variables x_1, \dots, x_n with coefficients in \mathbb{F}_2 . Let $Id(\mathbb{F}_2[\underline{x}])$ denote the set of ideals of $\mathbb{F}_2[\underline{x}]$. For every $I \in Id(\mathbb{F}_2[\underline{x}])$ and for every $m \geq 0$,

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

An ideal I of $\mathbb{F}_2[\underline{x}]$ is *monomial* when it is generated by a set of monomials. It should be recalled (Cox et al, 1997, §. 2.4) that, given a monomial ideal I generated by a set of monomials M , the monomials in $M(I)$ are exactly those 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 $\mathbb{F}_2[\underline{x}]$, $I = J$ if and only if $M(I) = M(J)$.

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

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

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

Proof. For every $\Gamma \in \mathcal{C}_n$, the monomials in I_Γ 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 Γ is uniquely determined by $M(I_\Gamma)^{(2)}$. \square

² To ease the task of the reader, in Appendix A we provide a reminder of the basic ring-theoretical definitions used in this paper.

Given two contact structures $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$, we have that

$$I_{\Gamma_1} + I_{\Gamma_2} = \left\langle \{x_i x_j \mid i \cdot j \in Q_1\} \cup \{x_i x_j \mid i \cdot j \in Q_2\} \right\rangle = I_{\Gamma_1 \cup \Gamma_2}.$$

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

$$\begin{aligned} & \{x_i x_j \mid i \cdot j \in Q_1 \cap Q_2\} \cup \{x_i x_j x_k \mid i \cdot j \in Q_1 - Q_2, j \cdot k \in Q_2 - Q_1\} \\ & \cup \{x_i x_j x_k x_l \mid i \cdot j \in Q_1 - Q_2, k \cdot l \in Q_2 - Q_1, \{i, j\} \cap \{k, l\} = \emptyset\}. \end{aligned}$$

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^α 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 $\mathbb{F}_2[\underline{x}]$.

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

$$R_{n,m} = \mathbb{F}_2[x_1, \dots, x_n] / \langle \mathcal{M}(\underline{x})^{(m)} \rangle,$$

and let $\pi_m : \mathbb{F}_2[x_1, \dots, x_n] \rightarrow R_{n,m}$ be the corresponding quotient ring homomorphism, which sends each polynomial in $\mathbb{F}_2[x_1, \dots, x_n]$ to its equivalence class modulo $\langle \mathcal{M}(\underline{x})^{(m)} \rangle$.

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

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

is a metric on \mathcal{C}_n .

Proof. When we perform the quotient $R_{n,m} = \mathbb{F}_2[\underline{x}] / \langle \mathcal{M}(\underline{x})^{(m)} \rangle$, all monomials with total degree greater or equal than m are cancelled. Then, each element of $R_{n,m}$ has a unique representative that is a linear combination with coefficients in \mathbb{F}_2 of monomials of total degree at most $m - 1$. Since \mathbb{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 $Sub(R_{n,m})$ denote its set of subgroups.

On the other hand, if $m \geq 3$, the quotient homomorphism π_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 $\pi_m \circ I : \mathcal{C}_n \rightarrow \text{Sub}(R_{n,m})$ sending every $\Gamma \in \mathcal{C}_n$ to $\pi_m(I_\Gamma)$, is an embedding.

Therefore, since by (Reidys and Stadler, 1996, 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 for every $m \geq 3$, as we claimed. \square

We have used \log_2 instead of \ln in the definition of d'_m in order to avoid unnecessary scalar factors: cf. (Rosselló, 2003, 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 $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,*

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

Proof. Notice that, for every $I \in \text{Id}(\mathbb{F}_2[\underline{x}])$, $\pi_m(I) = \pi_m(I + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)$. Then, for every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,

$$\begin{aligned} \frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} &= \frac{\pi_m(I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) + \pi_m(I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)}{\pi_m(I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) \cap \pi_m(I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)} \\ &= \frac{\pi_m\left((I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) + (I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)\right)}{\pi_m\left((I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) \cap (I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)\right)} \\ &\cong \frac{(I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) + (I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)}{(I_{\Gamma_1} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle) \cap (I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle)} \\ &= \frac{I_{\Gamma_1} + I_{\Gamma_2} + \langle \mathcal{M}(\underline{x})^{(m)} \rangle}{(I_{\Gamma_1} \cap I_{\Gamma_2}) + \langle \mathcal{M}(\underline{x})^{(m)} \rangle}, \end{aligned}$$

where the equality

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

used in the last step holds because I_{Γ_1} , I_{Γ_2} and $\langle \mathcal{M}(\underline{x})^{(m)} \rangle$ are monomial ideals.

To simplify the notations, set

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

so that

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

These ideals J and K are also monomial and

$$\begin{aligned} M(J) &= M(I_{\Gamma_1})_{m-1} \cup M(I_{\Gamma_2})_{m-1} \cup \bigcup_{r \geq m} \mathcal{M}(\underline{x})^{(r)}, \\ M(K) &= (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1}) \cup \bigcup_{r \geq m} \mathcal{M}(\underline{x})^{(r)}. \end{aligned}$$

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

$$\begin{aligned} M(J) - M(K) &= (M(I_{\Gamma_1})_{m-1} \cup M(I_{\Gamma_2})_{m-1}) - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1}) \\ &= M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1} \end{aligned}$$

is a finite set, this implies that

$$\left| \frac{\pi_m(I_{\Gamma_1}) + \pi_m(I_{\Gamma_2})}{\pi_m(I_{\Gamma_1}) \cap \pi_m(I_{\Gamma_2})} \right| = \left| \frac{J}{K} \right| = 2^{|M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1}|},$$

as we claimed. □

Proposition 5 allows us to express the metrics d'_m in terms of Hilbert functions. For every monomial ideal I of $\mathbb{F}_2[\underline{x}]$, let $H_I : \mathbb{N} \rightarrow \mathbb{N}$ be the mapping defined by $H_I(m) = |C(I)_m|$ for every $m \in \mathbb{N}$; 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 ; see (Cox et al, 1997, Chap. 9) for its basic properties. This function can be computed from any given finite set of generators of I (Bigatti, 1997), and, actually, several freely available computer algebra systems like, for instance, CoCoA (Capani et al) or Macaulay (Grayson and Stillman), compute Hilbert functions: see Example 10 below.

For every contact structure $\Gamma \in \mathcal{C}_n$, let H_Γ 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

$$\begin{aligned}
& |M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1}| \\
&= |M(I_{\Gamma_1})_{m-1} - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1})| \\
&\quad + |M(I_{\Gamma_2})_{m-1} - (M(I_{\Gamma_1})_{m-1} \cap M(I_{\Gamma_2})_{m-1})| \\
&= |M(I_{\Gamma_1} + I_{\Gamma_2})_{m-1} - M(I_{\Gamma_2})_{m-1}| + |M(I_{\Gamma_1} + I_{\Gamma_2})_{m-1} - M(I_{\Gamma_1})_{m-1}| \\
&= |C(I_{\Gamma_2})_{m-1} - C(I_{\Gamma_1 \cup \Gamma_2})_{m-1}| + |C(I_{\Gamma_1})_{m-1} - C(I_{\Gamma_1 \cup \Gamma_2})_{m-1}| \\
&= (|C(I_{\Gamma_2})_{m-1}| - |C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1}|) + (|C(I_{\Gamma_1})_{m-1}| - |C(I_{\Gamma_1} + I_{\Gamma_2})_{m-1}|) \\
&= (H_{\Gamma_2}(m-1) - H_{\Gamma_1 \cup \Gamma_2}(m-1)) + (H_{\Gamma_1}(m-1) - H_{\Gamma_1 \cup \Gamma_2}(m-1)),
\end{aligned}$$

as we claimed. \square

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 $\Gamma_0 = ([n], \emptyset)$ be the empty contact structure of length n and let Γ_1 be a contact 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

$$\begin{aligned}
H_{\Gamma_0}(m-1) &= |\mathcal{M}(\underline{x})_{m-1}| = \binom{n+m-1}{n} \\
H_{\Gamma_1}(m-1) &= \left| \{x^{\underline{a}} \in \mathcal{M}(\underline{x})_{m-1} \mid x_i x_j \text{ does not divide } x^{\underline{a}}\} \right| \\
&= |\mathcal{M}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)_{m-1}| \\
&\quad + |\mathcal{M}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n)_{m-1}| \\
&\quad - |\mathcal{M}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{j-1}, x_{j+1}, \dots, x_n)_{m-1}| \\
&= 2 \binom{n+m-2}{n-1} - \binom{n+m-3}{n-2},
\end{aligned}$$

$$\text{and hence } d'_m(\Gamma_0, \Gamma_1) = \binom{n+m-1}{n} - 2 \binom{n+m-2}{n-1} + \binom{n+m-3}{n-2} = \binom{n+m-3}{n}.$$

If we take 1 as the “natural” value for the distance between Γ_0 and Γ_1 , then instead of using the metrics d'_m on \mathcal{C}_n , we must divide them by $\binom{n+m-3}{n}$.

Definition 7. 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 , $d_3 = d'_3$, $d_4 = d'_4/(n+1)$, $d_5 = d'_5/\binom{n+2}{2}$, and so on.

After this normalization, these edge ideal metrics satisfy the following properties.

Proposition 8. *Let $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$ and $m \geq 3$.*

(i) $\frac{m-2}{n+m-2}d_m(\Gamma_1, \Gamma_2) \leq d_{m+1}(\Gamma_1, \Gamma_2) \leq d_m(\Gamma_1, \Gamma_2)$.

(ii) *If $\Gamma_1 \neq \Gamma_2$, then*

$$\lim_{m \rightarrow \infty} d_m(\Gamma_1, \Gamma_2) = \begin{cases} 0 & \text{if } \Gamma_1, \Gamma_2 \text{ are non-empty} \\ 1 & \text{if either } \Gamma_1 \text{ or } \Gamma_2 \text{ is empty} \end{cases}$$

(iii) *If $\Gamma_1^*, \Gamma_2^* \in \mathcal{C}_{n+1}$ are obtained from Γ_1, Γ_2 by adding the node $n+1$ isolated to both of them, then $d_m(\Gamma_1, \Gamma_2) \leq d_m(\Gamma_1^*, \Gamma_2^*)$.*

The proof of this proposition is quite long and it is not needed in the rest of this paper, therefore we postpone it until Appendix B. We only enlighten it here with a simple example.

Example 9. Let Γ_0 be an empty contact structure of some length $n \geq 6$ and let now $\Gamma_1 = ([n], \{1 \cdot 3, 4 \cdot 6\})$. 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 18 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,

$$\begin{aligned} d_m(\Gamma_0, \Gamma_1) &= \frac{1}{\binom{n+m-3}{n}}(2\binom{n+m-3}{n} - \binom{n+m-5}{n}) \\ &= 2 - \frac{(m-3)(m-4)}{(n+m-3)(n+m-4)} \end{aligned}$$

which increases with n and decreases with m .

Since we are only interested in comparing contact structures of the same length, the sensitiveness of the edge ideal metrics to the addition of isolated nodes is not a major drawback.

To end this section, we show an explicit computation of edge ideal metrics using the computer algebra system CoCoA 4.2, which can be freely downloaded

from its home page <http://cocoa.dima.unige.it>.

Example 10. Consider the following RNA secondary structures of length 76:

$$\Gamma_1 : (((((((...(((.....))))).((((.....)))))......((((.....)))..))))).....$$

$$\Gamma_2 : (((((((...(((...(((.....)))))......)).))))..))))).))))).))))).))))).$$

Γ_1 is the cloverleaf structure for yeast phenylalanine tRNA, while Γ_2 is a computer predicted minimum energy folding of the same molecule (Zuker, 1986, Fig. 6a). Their sets of contacts are, respectively,

$$Q_1 = \{(1, 72), (2, 71), (3, 70), (4, 69), (5, 68), (6, 67), (10, 25), (11, 24), \\ (12, 23), (13, 22), (27, 43), (28, 42), (29, 41), (30, 40), (31, 39), (50, 64), \\ (51, 63), (52, 62), (53, 61)\}$$

$$Q_2 = \{(1, 75), (2, 74), (3, 72), (4, 71), (5, 70), (9, 69), (10, 68), (11, 67), \\ (15, 64), (16, 63), (18, 62), (19, 61), (20, 60), (21, 59), (22, 56), (23, 55), \\ (24, 54), (25, 53), (26, 51), (27, 50), (28, 42), (29, 41), (30, 40), (31, 39)\}$$

The simple program shown in Fig. 2 computes their distances $d_m(\Gamma_1, \Gamma_2)$ for $m = 3, \dots, 10$. Its syntax is quite clear. The first lines are self explanatory: `N` (variables and functions in CoCoA must begin with a capital letter) is assigned the length of the molecules, 76, `L1` and `L2` are the lists of generators of I_{Γ_1} and I_{Γ_2} , respectively, obtained from their sets of contacts, and we declare that we shall work in the polynomial ring $R := \mathbb{F}_2[x_1, \dots, x_n]$ (note that the field \mathbb{F}_2 is entered as the quotient ring $\mathbb{Z}/\langle 2 \rangle$).

`Hilbert(R/I)` is the Hilbert function of an ideal `I` of `R`, that is conveniently defined in CoCoA, and `Ideal(L)` is a CoCoA function that defines the ideal generated by a set `L`. Hence, `H1`, `H2` and `H12` are the Hilbert functions H_{Γ_1} , H_{Γ_2} and $H_{\Gamma_1 \cup \Gamma_2}$, respectively, where `Concat` performs the union of the two lists. These functions are evaluated by `EvalHilbertFn`: thus, for instance, `EvalHilbertFn(H1, M-1)` corresponds to $H_{\Gamma_1}(m-1)$. In this way, the function `DP(L1, L2, M)` defined in the program computes the metric $d'_m(\Gamma_1, \Gamma_2)$ using the formula established in Corollary 6, and the function `D(L1, L2, N, M)` computes the edge ideal m -th metric $d_m(\Gamma_1, \Gamma_2)$. The last `For` loop makes the system compute $d_i(\Gamma_1, \Gamma_2)$ for $i = 3, \dots, 10$ and print the result. The output is given immediately below the last command line.

```

N:= 76;
Use R := Z/(2)[x[1..N]];

L1 := [x[1]x[72], x[2]x[71], x[3]x[70], x[4]x[69], x[5]x[68],
        x[6]x[67], x[10]x[25], x[11]x[24], x[12]x[23], x[13]x[22],
        x[27]x[43], x[28]x[42], x[29]x[41], x[30]x[40], x[31]x[39],
        x[50]x[64], x[51]x[63], x[52]x[62], x[53]x[61]];
L2 := [x[1]x[75], x[2]x[74], x[3]x[72], x[4]x[71], x[5]x[70],
        x[9]x[69], x[10]x[68], x[11]x[67], x[15]x[64], x[16]x[63],
        x[18]x[62], x[19]x[61], x[20]x[60], x[21]x[59], x[22]x[56],
        x[23]x[55], x[24]x[54], x[25]x[53], x[26]x[51], x[27]x[50],
        x[28]x[42], x[29]x[41], x[30]x[40], x[31]x[39]];

Define DP(L1,L2,M)
  H1 := Hilbert(R/Ideal(L1));
  H2 := Hilbert(R/Ideal(L2));
  H12 := Hilbert(R/Ideal(Concat(L1,L2)));
  Return (EvalHilbertFn(H1,M-1) + EvalHilbertFn(H2,M-1)
          - 2 EvalHilbertFn(H12,M-1));
EndDefine;

Define D(L1,L2,N,M)
  Return (DP(L1,L2,M)/Bin(N+M-3,N));
EndDefine;

For I:=3 To 10 Do D(L1,L2,N,I);
PrintLn;
EndFor;
35
2610/77
32553/1001
349406/11297
11536621/395395
8332585/305019
8893966751/350161812
48710089009/2075959314

```

Fig. 2. A computation of edge ideal metrics with CoCoA.

4 Some computations

In this section we compute explicitly some edge ideal metrics on \mathcal{C}_n and \mathcal{U}_n , for low values of m , and we discuss their meaning. We begin with $m = 3$.

Proposition 11. *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

$$\begin{aligned} M(I_{\Gamma_1})_2 \Delta M(I_{\Gamma_2})_2 &= M(I_{\Gamma_1})^{(2)} \Delta M(I_{\Gamma_2})^{(2)} \\ &= \{x_i x_j \mid i \cdot j \in (Q_1 - Q_2) \cup (Q_2 - Q_1)\} \end{aligned}$$

and hence $|M(I_{\Gamma_1})_2 \Delta M(I_{\Gamma_2})_2| = |Q_1 \Delta Q_2|$. \square

Actually, it is not difficult to prove that, for every $\Gamma \in \mathcal{U}_n$, the mapping $G(\Gamma) \rightarrow \pi_3(I_\Gamma)$ sending every permutation $\sigma = (i_1, j_1) \cdots (i_l, j_l) \in G(\Gamma)$, with $i_1 \cdot j_1, \dots, i_l \cdot j_l \in Q$, to the equivalence class of the polynomial $x_{i_1} x_{j_1} + \cdots + x_{i_l} x_{j_l} \in I_\Gamma$ modulo $\langle \mathcal{M}(\underline{x})^{(3)} \rangle$, 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 $\pi_3 \circ I : \mathcal{C}_n \hookrightarrow \text{Sub}(R_{n,3})$ generalizes the embedding $G : \mathcal{U}_n \hookrightarrow \text{Sub}(S_n)$, 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 explicit computation we can use the following lemma; notice that the edge ideals of contact structures are radical.

Lemma 12. *Let I be a radical monomial ideal of $\mathbb{F}_2[\underline{x}]$ and, for every $k \geq 0$, let $SF(I)^{(k)}$ be the number of square-free monomials of total degree k belonging to $M(I)$. Then, for every $m \geq 0$,*

$$H_I(m) = \binom{n+m}{n} - \sum_{k=0}^m \binom{m}{k} SF(I)^{(k)}.$$

Proof. If I is a radical monomial ideal, a monomial of the form $x_{i_1}^{\alpha_{i_1}} \cdots x_{i_k}^{\alpha_{i_k}}$, with i_1, \dots, i_k pairwise different and each $\alpha_{i_t} \geq 1$, 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 $SF(I)^{(k)}$ square-free monomials $x_{i_1} \cdots x_{i_k}$ of total degree k in $M(I)$ adds as many monomials $x_{i_1}^{\alpha_{i_1}} \cdots x_{i_k}^{\alpha_{i_k}}$ to $M(I)_m$ as vectors $(\alpha_{i_1}, \dots, \alpha_{i_k}) \in (\mathbb{N} - \{0\})^k$ such that $\sum_{t=1}^k \alpha_{i_t} \leq m$ 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, this proves that

$$|M(I)_m| = \sum_{k=0}^m \binom{m}{k} SF(I)^{(k)},$$

and hence

$$|C(I)_m| = |\mathcal{M}(\underline{x})_m| - |M(I)_m| = \binom{n+m}{n} - \sum_{k=0}^m \binom{m}{k} SF(I)^{(k)},$$

as we claimed. \square

Notice that if $\Gamma \in \mathcal{C}_n$, then $SF(I_\Gamma)^{(0)} = SF(I_\Gamma)^{(1)} = 0$ and $SF(I_\Gamma)^{(2)} = |Q|$, and thus

$$H_\Gamma(m) = \binom{n+m}{n} - \binom{m}{2}|Q| - \sum_{k=3}^m \binom{m}{k} SF(I_\Gamma)^{(k)}.$$

Let us compute now d_4 on \mathcal{C}_n . For every contact structure $\Gamma \in \mathcal{C}_n$, let

$$\begin{aligned} A(\Gamma) &= \left| \left\{ \{i \cdot j, j \cdot k\} \subseteq Q \mid j \neq k \right\} \right| \\ T(\Gamma) &= \left| \left\{ \{i, j, k\} \subseteq [n] \mid i \cdot j, j \cdot k, i \cdot k \in Q \right\} \right| \end{aligned}$$

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

Proposition 13. *For every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$,*

$$\begin{aligned} d_4(\Gamma_1, \Gamma_2) &= |Q_1 \Delta Q_2| \\ &\quad - \frac{1}{n+1} \left(2A(\Gamma_1 \cup \Gamma_2) - A(\Gamma_1) - A(\Gamma_2) - 2T(\Gamma_1 \cup \Gamma_2) + T(\Gamma_1) + T(\Gamma_2) \right). \end{aligned}$$

Proof. For every $\Gamma \in \mathcal{C}_n$ we have that $H_\Gamma(3) = \binom{n+3}{n} - 3|Q| - SF(I_\Gamma)^{(3)}$. It remains to compute $SF(I_\Gamma)^{(3)}$:

- (1) For every $i \cdot j \in Q$, there are $(n-2)$ square-free monomials $x_i x_j x_k$ in $M(I_\Gamma)$: this makes $(n-2)|Q|$ such monomials.
- (2) Now, if $i \cdot j, j \cdot k \in Q$ 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 Γ , 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 $SF(I_\Gamma)^{(3)} = (n-2)|Q| - A(\Gamma) + T(\Gamma)$, and hence

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

We have then

$$\begin{aligned}
d'_4(\Gamma_1, \Gamma_2) &= H_{\Gamma_1}(3) + H_{\Gamma_2}(3) - 2H_{\Gamma_1 \cup \Gamma_2}(3) \\
&= \binom{n+3}{n} - (n+1)|Q_1| + A(\Gamma_1) - T(\Gamma_1) \\
&\quad + \binom{n+3}{n} - (n+1)|Q_2| + A(\Gamma_2) - T(\Gamma_2) \\
&\quad - 2 \left(\binom{n+3}{n} - (n+1)|Q_1 \cup Q_2| + A(\Gamma_1 \cup \Gamma_2) - T(\Gamma_1 \cup \Gamma_2) \right) \\
&= (n+1)|Q_1 \Delta Q_2| \\
&\quad - (2A(\Gamma_1 \cup \Gamma_2) - A(\Gamma_1) - A(\Gamma_2) - 2T(\Gamma_1 \cup \Gamma_2) + T(\Gamma_1) + T(\Gamma_2));
\end{aligned}$$

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. \square

Example 14. Let $\Gamma_0 = ([9], \{1 \cdot 3, 4 \cdot 6\})$, and consider the following “modifications” of it:

$$\begin{aligned}
\Gamma_1 &= ([9], \{1 \cdot 3, 4 \cdot 6, 7 \cdot 9\}), \quad \Gamma_2 = ([9], \{1 \cdot 3, 4 \cdot 6, 6 \cdot 9\}), \\
\Gamma_3 &= ([9], \{1 \cdot 3, 4 \cdot 6, 1 \cdot 6\}) \quad \Gamma_4 = ([9], \{1 \cdot 3, 4 \cdot 7\}), \\
\Gamma_5 &= ([9], \{1 \cdot 3, 3 \cdot 6\}), \quad \Gamma_6 = ([9], \{1 \cdot 3, 3 \cdot 5\}), \quad \Gamma_7 = ([9], \{1 \cdot 3, 5 \cdot 7\})
\end{aligned}$$

The contact structures Γ_1, Γ_2 and Γ_3 are obtained by adding a contact to Γ_0 in three ways, Γ_4 and Γ_5 are obtained by shifting the contact $4 \cdot 6$ in two ways, and Γ_6 and Γ_7 are obtained by displacing this contact in two ways. Notice that $\Gamma_0, \Gamma_1, \Gamma_4$ and Γ_7 have unique bonds, but the others do not.

We have that

$$\begin{aligned}
d_3(\Gamma_0, \Gamma_1) &= d_3(\Gamma_0, \Gamma_2) = d_3(\Gamma_0, \Gamma_3) = 1, \\
d_3(\Gamma_0, \Gamma_4) &= d_3(\Gamma_0, \Gamma_5) = d_3(\Gamma_0, \Gamma_6) = d_3(\Gamma_0, \Gamma_7) = 2,
\end{aligned}$$

while

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

The expression for d_4 on contact structures with unique bonds is much simpler. Recall that, for every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$, $\Omega_{\geq 2}$ stands for the number of open orbits of length ≥ 2 , i.e., of non-trivial open orbits induced by the action of $D(\Gamma_1, \Gamma_2)$ on $[n]$. It is also equal to half the number of nodes that are isolated in one structure but not in the other.

Proposition 15. For every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$,

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

Proof. The unique bonds condition implies in this case that

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

and hence

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

It remains to prove that if $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$, then $A(\Gamma_1 \cup \Gamma_2) = |Q_1 \Delta Q_2| - \Omega_{\geq 2}$. To do it, notice that if $\{i \cdot j, j \cdot k\}$ forms an angle in $\Gamma_1 \cup \Gamma_2$, then, again by the unique bonds condition, one of these contacts belongs 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, which will be of length at least 3. Now, each closed orbit of length $m > 2$ contains m angles, while any open orbit of length $m \geq 2$ contains $m - 2$ angles. Then

$$\begin{aligned} A(\Gamma_1 \cup \Gamma_2) &= \sum_{m \geq 4} m \Theta^{(m)} + \sum_{m \geq 2} (m - 2) \Omega^{(m)} \\ &= \sum_{m \geq 4} m \Theta^{(m)} + \sum_{m \geq 2} (m - 1) \Omega^{(m)} - \sum_{m \geq 2} \Omega^{(m)} = |Q_1 \Delta Q_2| - \Omega_{\geq 2}, \end{aligned}$$

as we wanted to prove. \square

Therefore, on \mathcal{U}_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 one, and only one, node. Notice moreover that

$$0 \leq A(\Gamma_1 \cup \Gamma_2) = |Q_1 \Delta Q_2| - \Omega_{\geq 2} \leq |Q_1 \Delta Q_2|;$$

the lower bound is achieved when all non-trivial orbits are open of length 2, i.e., when $\Gamma_1 \cup \Gamma_2$ has also unique bonds, and the upper bound when all non-trivial orbits are closed, i.e., when Γ_1 and Γ_2 have exactly the same isolated nodes.

Example 16. According to Schuster and Stadler (1999, §5.3.2), most RNA AU-sequences of length 16 do not fold at all, i.e., they form the empty contact structure. But some of these sequences (about a 3% of them) do fold, forming one of the following three hairpins:

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

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 , Γ_1 and Γ_2 are closer to Γ_3 than to each other.

Example 17. Let us consider the hairpin with an interior loop

$$\Gamma_0 : ((.(((....))))....))$$

One possible rearrangement of this RNA secondary structure splits the hairpin into a multibranch loop by means of two shift moves:

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

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

$$\begin{aligned} \Gamma_0 : ((.(((....))))....)) &\implies \Gamma'_1 : (((.(((....))))....)) \implies \Gamma'_2 : (((((....))))....)) \\ &\implies \Gamma'_3 : (((((....)))(...)) \implies \Gamma'_4 : ((((((....))))....)) \end{aligned}$$

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

$$d_4(\Gamma_0, \Gamma_1) = d_4(\Gamma_0, \Gamma'_1) = \frac{21}{11},$$

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 , Γ'_2 is closer to Γ_0 than Γ_2 . This could translate the fact that it is “easier” to move a bulge than to split a hairpin. We believe that this kind of arguments could be applied in the study of RNA folding kinetics (Flamm et al, 2000); we hope to report on it elsewhere.

As m grows, the description of d_m on \mathcal{C}_n gets more and more involved or, if we want it to remain simple, more and more uninformative. The same happens on \mathcal{U}_n , but at a lower pace. Moreover, obtaining explicit descriptions for edge ideal m th metrics on \mathcal{U}_n is easier, because of the availability of the following explicit formula for the Hilbert function of the edge ideal of a contact structure with unique bonds, which seems to be new in the literature. In it we use the convention that $\binom{0}{0} = 1$ and $\binom{0}{j} = 0$ if $j > 0$, and $\lfloor x \rfloor$ stands for the greatest integer number smaller or equal than x .

Proposition 18. *For every $\Gamma \in \mathcal{U}_n$ 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. Notice that if $\Gamma \in \mathcal{U}_n$, then the Hilbert function H_Γ depends only on $|Q|$ because, for every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$ 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 $m \geq 0$. So, for every $k \geq 0$, let H_k denote the Hilbert function of the edge ideal of any $\Gamma \in \mathcal{U}_n$ with $|Q| = k$.

Now, if $\Gamma = ([n], Q) \in \mathcal{U}_n$ with $Q = \{i_1 \cdot j_1, \dots, i_k \cdot j_k\}$, then no monomial $x_{i_t} x_{j_t}$, for $t = 1, \dots, k$, is a zero divisor modulo the ideal $\langle x_{i_1} x_{j_1}, \dots, x_{i_{t-1}} x_{j_{t-1}} \rangle$. This implies (by (Cox et al, 1997, §9.4, Cor. 5) or, rather, its proof) that

$$H_{k+1}(m) = H_k(m) - H_k(m-2), \text{ for every } k \geq 0, m \geq 2,$$

and hence

$$H_{k+1}(m) = H_0(m) - \sum_{i=0}^k H_i(m-2), \text{ for every } k \geq 0, m \geq 2.$$

We use this recursion to prove the expression in the statement by induction on m .

To begin with, we know that, for every $m \geq 0$, $H_0(m) = |\mathcal{M}(\underline{x})_m| = \binom{n+m}{n}$, which clearly satisfies the expression in the statement (with $|Q| = 0$). Moreover, for every $k \geq 0$, $H_k(0) = 1$ and $H_k(1) = n+1$, because, for every $\Gamma \in \mathcal{U}_n$, $C(I_\Gamma)_0 = \{1\}$ and $C(I_\Gamma)_1 = \{1, x_1, \dots, x_n\}$. These values for $H_k(0)$ and $H_k(1)$ clearly satisfy the expression given in the statement. Now, as induction hypothesis, assume that

$$H_k(m_0) = \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{k}{j} \binom{n+m_0-2j}{n} \text{ for every } k \geq 0.$$

Then, for every $k \geq 1$,

$$\begin{aligned} H_k(m_0+2) &= H_0(m_0+2) - \sum_{i=0}^{k-1} H_i(m_0) \\ &= \binom{n+m_0+2}{n} - \sum_{i=0}^{k-1} \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^j \binom{i}{j} \binom{n+m_0-2j}{n} \\ &= \binom{n+m_0+2}{n} + \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^{j+1} \binom{n+m_0-2j}{n} \left(\sum_{i=0}^{k-1} \binom{i}{j} \right) \\ &= \binom{n+m_0+2}{n} + \sum_{j=0}^{\lfloor m_0/2 \rfloor} (-1)^{j+1} \binom{n+m_0-2j}{n} \binom{k}{j+1} \\ &= (-1)^0 \binom{k}{0} \binom{n+m_0+2}{n} + \sum_{j=1}^{\lfloor m_0/2 \rfloor + 1} (-1)^j \binom{k}{j} \binom{n+m_0+2-2j}{n} \\ &= \sum_{j=0}^{\lfloor (m_0+2)/2 \rfloor} (-1)^j \binom{k}{j} \binom{n+m_0+2-2j}{n}, \end{aligned}$$

where the second equality uses the induction hypothesis and the fourth equality uses that $\sum_{i=0}^{k-1} \binom{i}{j} = \binom{k}{j+1}$. Since we knew the expression in the statement to be true for $m = 0, 1$, this proves it by induction for all $m \geq 0$. \square

Thus, for instance, for every $\Gamma = ([n], Q) \in \mathcal{U}_n$,

$$\begin{aligned} H_\Gamma(2) &= \binom{n+2}{2} - |Q| \\ H_\Gamma(3) &= \binom{n+3}{3} - (n+1)|Q| \\ H_\Gamma(4) &= \binom{n+4}{4} - \binom{n+2}{2}|Q| + \binom{|Q|}{2} \\ H_\Gamma(5) &= \binom{n+5}{5} - \binom{n+3}{3}|Q| + (n+1)\binom{|Q|}{2} \\ H_\Gamma(6) &= \binom{n+6}{6} - \binom{n+4}{4}|Q| + \binom{n+2}{2}\binom{|Q|}{2} - \binom{|Q|}{3} \end{aligned}$$

and so on. Unfortunately, we do not have a similar explicit expression for the Hilbert function of arbitrary contact structures, even for unions of contact structures with unique bonds.

To close this paper, we provide explicit descriptions of d_5 and d_6 on the set \mathcal{U}_n just to grasp what they measure. Their proof is similar to that of Proposition 13, but longer and more involved, so we postpone it until Appendix C.

Proposition 19. *For every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$,*

$$\begin{aligned} d_5(\Gamma_1, \Gamma_2) &= |Q_1 \Delta Q_2| - \frac{1}{\binom{n+2}{2}} \left(2 \binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} - \binom{|Q_2|}{2} \right) \\ &\quad + 2(n-1)(|Q_1 \Delta Q_2| - \Omega_{\geq 2}) + 2(\Omega_{\geq 3} + \Theta^{(4)}). \\ d_6(\Gamma_1, \Gamma_2) &= |Q_1 \Delta Q_2| - \frac{1}{\binom{n+3}{3}} \left((n+1) \left(2 \binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} - \binom{|Q_2|}{2} \right) \right. \\ &\quad \left. + 2 \left(\binom{n+1}{2} - |Q_1 \cup Q_2| \right) (|Q_1 \Delta Q_2| - \Omega_{\geq 2}) \right. \\ &\quad \left. + 2(n-1)(\Omega_{\geq 3} + \Theta^{(4)}) - 2\Omega_{\geq 4} - 4\Theta^{(4)} \right). \end{aligned}$$

It is interesting to observe that, contrary to what happens with d_3 and d_4 , the term $2 \binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} - \binom{|Q_2|}{2}$ makes the value of $d_5(\Gamma_1, \Gamma_2)$ and $d_6(\Gamma_1, \Gamma_2)$ to depend not only on the cardinal and structure of the set $Q_1 \Delta Q_2$, but also on $|Q_1 \cap Q_2|$. For instance, it is not difficult to check that if $\Gamma_1, \Gamma_2, \Gamma'_1, \Gamma'_2 \in \mathcal{U}_n$ are such that $Q_1 - Q_2 = Q'_1 - Q'_2$ and $Q_2 - Q_1 = Q'_2 - Q'_1$, then

$$d_5(\Gamma_1, \Gamma_2) < d_5(\Gamma'_1, \Gamma'_2) \iff |Q_1 \cap Q_2| > |Q'_1 \cap Q'_2|;$$

i.e., the greater the set of contacts they share, the smaller their distance.

Example 20. Consider again the hairpin with an interior loop Γ_0 and its rearrangement Γ_1 given in Example 17

$$\Gamma_0 : ((.(((....))))....)) \quad \Gamma_1 : ((..(((....)))(...).))$$

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:

$$\Gamma'_0 : \dots((((...))))\dots\dots\dots \quad \Gamma'_1 : \dots((((...)))(\dots)\dots$$

Since $Q_1 \Delta Q_2 = Q'_1 \Delta Q'_2 = \{4 \cdot 14, 14 \cdot 18\}$, we have that

$$d_3(\Gamma_0, \Gamma_1) = d_3(\Gamma'_0, \Gamma'_1) = 2, \quad d_4(\Gamma_0, \Gamma_1) = d_4(\Gamma'_0, \Gamma'_1) = \frac{21}{11}.$$

But it turns out that

$$d_5(\Gamma_0, \Gamma_1) = 1 + \frac{199}{253}, \quad d_5(\Gamma'_0, \Gamma'_1) = 1 + \frac{203}{253}.$$

Notice moreover that in d_5 and d_6 new terms appear: $\Omega_{\geq 3}$ and $\Theta^{(4)}$ in d_5 and $\Omega_{\geq 4}$ in d_6 .

Example 21. Consider the RNA secondary structures of length 13

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

Then

$$d_3(\Gamma_1, \Gamma_2) = d_3(\Gamma_1, \Gamma_3) = 7, \quad d_4(\Gamma_1, \Gamma_2) = d_4(\Gamma_1, \Gamma_3) = 45/7, \\ d_5(\Gamma_1, \Gamma_2) = d_5(\Gamma_1, \Gamma_3) = 5 + 77/105$$

but

$$d_6(\Gamma_1, \Gamma_2) = 4 + \frac{346}{560}, \quad d_6(\Gamma_1, \Gamma_3) = 4 + \frac{344}{560}.$$

5 Discussion

In the Discussion section of their paper (1996), 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 this representation generalizes the embedding of contact structures with unique bonds into the set of subgroups of the symmetric group S_n proposed by these authors. We have used then this representation to define a family of *edge ideal metrics* on arbitrary contact structures. 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 have derived explicit descriptions for d_3 and d_4 on \mathcal{C}_n and for d_5 and d_6 on \mathcal{U}_n . Similar (but more involved) computations provide explicit expressions for d_m for each m , which could be used to study the notion of similarity it measures. Unfortunately, we have not been able to produce a closed expression for all these metrics. Recall moreover that, for specific $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$ and $m \geq 3$, the value of $d_m(\Gamma_1, \Gamma_2)$ can be easily computed using several computer algebra systems.

We want to point out that, when finding an expression for d_m , the only new ingredient that is necessary to determine is the value of $SF(I_{\Gamma_1 \cup \Gamma_2})^{(m-1)}$, which can be done for each m by counting carefully how many square-free monomials of total degree $m-1$ belong to $I_{\Gamma_1 \cup \Gamma_2}$; notice moreover that $SF(I_{\Gamma_1 \cup \Gamma_2})^{(k)} = 0$ if $k > n$ and $SF(I_{\Gamma_1 \cup \Gamma_2})^{(n)} = 1$ if $\Gamma_1 \neq \Gamma_2$ (see the proof of Proposition 8.(ii) in Appendix B). It is when computing $SF(I_{\Gamma_1 \cup \Gamma_2})^{(m-1)}$ that new terms make their appearance in each d_m for $m \leq n$: when one compensates in this computation the number of square-free monomials in $I_{\Gamma_1 \cup \Gamma_2}$ of the form $x_{i_1} \cdots x_{i_{m-1}}$ such that $i_1 \cdot i_2, \dots, i_{m-2} \cdot i_{m-1} \in Q_1 \cup Q_2$, the term $\Omega_{\geq m-2}$ makes its first appearance, and if $m-1$ is even, then when one compensates the number of square-free monomials $x_{i_1} \cdots x_{i_{m-1}}$ in $I_{\Gamma_1 \cup \Gamma_2}$ such that $\{i_1, \dots, i_{m-1}\}$ is a closed orbit, the term $\Theta^{(m-1)}$ must be used for the first time (cf. Appendix C).

Edge ideals are not the unique monomial ideal possible representations of arbitrary contact structures. For instance, we could associate to every contact structure $\Gamma = ([n], Q)$ the *clique ideal* J_Γ of $\mathbb{F}_2[x_1, \dots, x_n]$ generated by the set of monomials consisting of one square-free monomial $x_{i_1} \cdots x_{i_k}$ for each non-trivial *maximal clique* (maximal complete subgraph) $\{i_1, \dots, i_k\}$, with $k \geq 2$, of Γ . Notice that if Γ has unique bonds, 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 $I_\Gamma = \langle x_1 x_3, x_1 x_5, x_3 x_5 \rangle$, while $J_\Gamma = \langle x_1 x_3 x_5 \rangle$. The clique ideal J_Γ 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_Γ . These ideals can be used to define new metrics on arbitrary contact structures of a fixed length similar in spirit to the edge ideal metrics. We shall report on them in a subsequent paper. Other algebraic objects, like toric or path ideals (Villarreal, 2001), could also be used with this purpose.

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?"

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Appendix A: Rings and ideals

A *ring* is an algebraic structure consisting of a set R and two binary operations $+$ and \cdot on it such that:

- R together with the operation $+$ is a *commutative group*: i.e., the operation $+$ is *commutative* ($a+b = b+a$ for every $a, b \in R$), *associative* ($a+(b+c) = (a+b)+c$ for every $a, b, c \in R$), it has a *zero element* (an element $0 \in R$ such that $a+0 = a$ for every $a \in R$), and, for every $a \in R$, there exists an element $-a$ such that $a+(-a) = 0$.
- The operation \cdot is also associative and there exists an element $1 \in R$, called the *unit element*, such that $1 \cdot a = a \cdot 1 = a$ for every $a \in R$.

- The operations $+$ and \cdot satisfy the *distributive law*:

$$a \cdot (b + c) = a \cdot b + a \cdot c, \quad (b + c) \cdot a = b \cdot a + c \cdot a \quad \text{for every } a, b, c \in R.$$

A ring is said to be *commutative* when the operation \cdot is also commutative. A ring is a *field* when, for every $a \in R - \{0\}$, there exists an element $a' \in R$ such that $a \cdot a' = a' \cdot a = 1$.

For instance, the set \mathbb{Z} of integer numbers with the usual addition $+$ and multiplication \cdot is a commutative ring, while the set \mathbb{R} of real numbers, again with the usual addition $+$ and multiplication \cdot , is a commutative field. In the main body of the paper we use the *binary field* \mathbb{F}_2 , which consists of the set $\{0, 1\}$ together with the operations $+$ and \cdot defined by the following tables:

$$\begin{array}{c|cc} + & 0 & 1 \\ \hline 0 & 0 & 1 \\ 1 & 1 & 0 \end{array} \quad \begin{array}{c|cc} \cdot & 0 & 1 \\ \hline 0 & 0 & 0 \\ 1 & 0 & 1 \end{array}$$

This is the smallest possible field, and it is commutative.

Given n variables x_1, \dots, x_n , a *monomial* in these variables is a product of the form $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ with $\alpha_1, \dots, \alpha_n \in \mathbb{N}$, with the convention that if $\alpha_i = 0$, then $x_i^{\alpha_i} = 1$; in particular, $x_1^0 \cdots x_n^0 = 1$. We shall denote a monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ by $x^{(\alpha_1, \dots, \alpha_n)}$ or simply by $x^{\underline{\alpha}}$ if we let $\underline{\alpha}$ stand for the n -tuple $(\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$.

Given a commutative field \mathbb{K} , a *polynomial* in x_1, \dots, x_n with coefficients in \mathbb{K} is a finite linear combination of monomials with coefficients in \mathbb{K} : we can understand it as a sum

$$\sum_{\underline{\alpha} \in \mathbb{N}^n} a_{\underline{\alpha}} x^{\underline{\alpha}}, \quad a_{\underline{\alpha}} \in \mathbb{K}$$

with $a_{\underline{\alpha}} = 0$ for every $\underline{\alpha} \in \mathbb{N}^n$ but a finite set of them.

Let $\mathbb{K}[x_1, \dots, x_n]$ denote the set of all polynomials in x_1, \dots, x_n with coefficients in \mathbb{K} . On this set we define the following addition and multiplication operations:

- $\left(\sum_{\underline{\alpha} \in \mathbb{N}^n} a_{\underline{\alpha}} x^{\underline{\alpha}} \right) + \left(\sum_{\underline{\alpha} \in \mathbb{N}^n} b_{\underline{\alpha}} x^{\underline{\alpha}} \right) = \sum_{\underline{\alpha} \in \mathbb{N}^n} (a_{\underline{\alpha}} + b_{\underline{\alpha}}) x^{\underline{\alpha}}$
- $\left(\sum_{\underline{\alpha} \in \mathbb{N}^n} a_{\underline{\alpha}} x^{\underline{\alpha}} \right) \cdot \left(\sum_{\underline{\alpha} \in \mathbb{N}^n} b_{\underline{\alpha}} x^{\underline{\alpha}} \right) = \sum_{\underline{\alpha} \in \mathbb{N}^n} \left(\sum_{\underline{\beta} + \underline{\gamma} = \underline{\alpha}} a_{\underline{\beta}} \cdot b_{\underline{\gamma}} \right) x^{\underline{\alpha}}$

These operations define $\mathbb{K}[x_1, \dots, x_n]$ as a commutative ring, called the *polynomial ring* in the variables x_1, \dots, x_n with coefficients in \mathbb{K} . Its zero and unit elements are those of \mathbb{K} .

From now on, let R denote a commutative ring. An *ideal* of R is a non-empty subset $I \subseteq R$ that satisfies the following conditions:

- $0 \in I$
- If $a \in I$, then $-a \in I$
- If $a, b \in I$, then $a + b \in I$.
- If $a \in I$ and $r \in R$, then $r \cdot a \in I$.

Actually, the first two conditions are a consequence of the last condition and the fact that $I \neq \emptyset$.

Given a subset X of R , the ideal $\langle X \rangle$ *generated* by X is the smallest ideal of R that contains X . It is equal to the set of all finite linear combinations of elements of X with coefficients in R , i.e., to the set of those elements of R of the form

$$r_1 \cdot a_1 + \cdots + r_k \cdot a_k$$

with $\{a_1, \dots, a_k\}$ any finite subset of X and r_1, \dots, r_k any elements of R .

The *sum* $I_1 + I_2$ of two ideals I_1, I_2 of R is the ideal generated by their union $I_1 \cup I_2$. If I_1 is generated by $X_1 \subseteq R$ and I_2 by $X_2 \subseteq R$, then $I_1 + I_2$ is generated by $X_1 \cup X_2$.

For every $a \in R$ and for every $n \geq 1$, let $a^n = \overbrace{a \cdots a}^n$: this product makes sense because \cdot is associative. An ideal I of R is *radical* when, for every $a \in R$, if $a^n \in I$ for some $n \geq 1$, then $a \in I$.

An ideal I of R defines the following equivalence relation on R , called the *equivalence modulo I* :

$$a \equiv_I b \text{ if and only if } a - b \in I.$$

Let R/\equiv_I denote the quotient set whose elements are the equivalence classes $[x]_I$ modulo I of the elements x of R . On this set we can define the following operations:

$$[a]_I + [b]_I = [a + b]_I, [a]_I \cdot [b]_I = [a \cdot b]_I.$$

These operations turn out to be well-defined (in the sense that if $[a]_I = [c]_I$ and $[b]_I = [d]_I$, then $[a + b]_I = [c + d]_I$ and $[a \cdot b]_I = [c \cdot d]_I$) and the quotient set R/\equiv_I , together with the operations $+$ and \cdot defined in this way, turns out to be a commutative ring. Its zero element is the equivalence class $[0]_I$ modulo I of the zero element 0 of R and its unit element is the equivalence class $[1]_I$ modulo I of the unit element 1 of R . This ring is called the *quotient ring* of R modulo I and it is simply denoted by R/I . Roughly speaking, the overall effect of performing the quotient of a commutative ring R modulo an ideal I is to make all elements in I equal to 0 and to redefine the operations in order to take into account this identification.

For instance, the quotient ring $\mathbb{Z}/\langle 2 \rangle$ of the ring \mathbb{Z} of integer numbers by the ideal $\langle 2 \rangle$ generated by $\{2\}$ (which consists of all multiples of 2) has only two elements, the equivalence classes of 0 and 1 modulo $\langle 2 \rangle$, and it can be identified with (it is *isomorphic* to) the binary field \mathbb{F}_2 .

We call the mapping $\pi_I : R \rightarrow R/I$ that sends every $a \in R$ to its equivalence class $[a]_I$ modulo I the *quotient ring homomorphism* corresponding to I .

Given any ideal J of R with $I \subseteq J$, we denote by J/I the subset $\pi_I(J)$ of R/I : it is an ideal of this quotient ring. Given *any* ideal J of R , the set $\pi_I(J)$ is equal to the set $\pi_I(J + I)$ and in particular it is also an ideal of R/I .

An element $a \in R$ is a *zero divisor modulo I* when $a \notin I$ and there exists some element $b \in R - I$ such that $a \cdot b \in I$. Equivalently, when $[a]_I \neq [0]_I$ and there exists some $[b]_I \neq [0]_I$ such that $[a]_I \cdot [b]_I = [0]_I$ in R/I .

Appendix B: Proof of Proposition 8

To begin with, we have the following two inequalities.

Lemma B *For every $\Gamma_1, \Gamma_2 \in \mathcal{C}_n$ and for every $m \geq 3$:*

$$(a) \quad (m - 2) |M(I_{\Gamma_1})^{(m)} \Delta M(I_{\Gamma_2})^{(m)}| \leq n d'_m(\Gamma_1, \Gamma_2).$$

$$(b) \quad (m - 3) d'_m(\Gamma_1, \Gamma_2) \leq (n + 1) \sum_{k=3}^{m-1} d'_k(\Gamma_1, \Gamma_2).$$

Proof. (a) Let

$$N = \{(x^\alpha, x_i^{m-|\alpha|}) \mid x^\alpha \in M(I_{\Gamma_1})_{m-1} \Delta M(I_{\Gamma_2})_{m-1}, i = 1, \dots, n\},$$

and consider the mapping $\Phi : N \rightarrow \mathcal{M}(\underline{x})^{(m)}$ defined by $\Phi(x^\alpha, x_i^{m-|\alpha|}) = x^\alpha \cdot x_i^{m-|\alpha|}$.

It turns out that each element of $M(I_{\Gamma_1})^{(m)} \Delta M(I_{\Gamma_2})^{(m)}$ has at least $m-2$ preimages under this mapping. Indeed, if, say, $x^\beta \in M(I_{\Gamma_1})^{(m)} - M(I_{\Gamma_2})^{(m)}$, then we can decompose $x^\beta = x_i x_j \cdot x^\gamma$ with $i \cdot j \in Q_1 - Q_2$ and $x^\gamma \in \mathcal{M}(\underline{x})^{(m-2)}$. Then, for every s such that $\gamma_s > 0$ and for every $t = 1, \dots, \gamma_s$,

$$x_i x_j \cdot x^{(\gamma_1, \dots, \gamma_s - t, \dots, \gamma_n)} \in M(I_{\Gamma_1})^{(m-t)} - M(I_{\Gamma_2})^{(m-t)}$$

and $(x_i x_j \cdot x^{(\gamma_1, \dots, \gamma_s - t, \dots, \gamma_n)}, x_s^t) \in N$ is a preimage of x^β under Φ . These preimages of x^β are pairwise different and there are $m-2$ of them.

This clearly entails that $(m-2) |M(I_{\Gamma_1})^{(m)} \Delta M(I_{\Gamma_2})^{(m)}| \leq |N| = n d'_m(\Gamma_1, \Gamma_2)$.

(b) We prove it by induction on m . The case $m = 3$ is obvious, since both sides of the inequality are equal to 0. Assume now the inequality to be true for m , and let

us prove it for $m + 1$:

$$\begin{aligned}
(m-2)d'_{m+1}(\Gamma_1, \Gamma_2) &= (m-2)d'_m(\Gamma_1, \Gamma_2) + (m-2)|M(I_{\Gamma_1})^{(m)}\Delta M(I_{\Gamma_2})^{(m)}| \\
&\leq (n+1)\sum_{k=3}^{m-1}d'_k(\Gamma_1, \Gamma_2) + d'_m(\Gamma_1, \Gamma_2) + nd'_m(\Gamma_1, \Gamma_2) \\
&\quad \text{(by the induction hypothesis and (a))} \\
&= (n+1)\sum_{k=3}^m d'_k(\Gamma_1, \Gamma_2).
\end{aligned}$$

□

We can proceed now to prove Proposition 8.

(i) Since $d'_{m+1}(\Gamma_1, \Gamma_2) = d'_m(\Gamma_1, \Gamma_2) + |M(I_{\Gamma_1})^{(m)}\Delta M(I_{\Gamma_2})^{(m)}|$, using Lemma B.(a), we have that

$$d'_m(\Gamma_1, \Gamma_2) \leq d'_{m+1}(\Gamma_1, \Gamma_2) \leq d'_m(\Gamma_1, \Gamma_2) + \frac{n}{m-2}d'_m(\Gamma_1, \Gamma_2) = \frac{n+m-2}{m-2}d'_m(\Gamma_1, \Gamma_2).$$

Dividing all terms in these inequalities by $\binom{n+m-2}{n}$, and using that $\frac{n+m-2}{m-2}\binom{n+m-3}{n} = \binom{n+m-2}{n}$, we obtain the inequalities in the statement.

(ii) For every monomial ideal I and for every $k \geq 1$, let $SF(I)^{(k)}$ be the number of square-free monomials belonging to $M(I)^{(k)}$; see Lemma 12. To simplify the notations, for every $k \geq 1$ let $SF^{(k)} = 2SF(I_{\Gamma_1 \cup \Gamma_2})^{(k)} - SF(I_{\Gamma_1})^{(k)} - SF(I_{\Gamma_2})^{(k)}$; this is the number of square-free monomials belonging to $M(I_{\Gamma_1})^{(k)}\Delta M(I_{\Gamma_2})^{(k)}$. Then, by Corollary 6 and Lemma 12,

$$d_m(\Gamma_1, \Gamma_2) = \sum_{k=2}^{m-1} \frac{\binom{m-1}{k}}{\binom{n+m-3}{n}} SF^{(k)}.$$

In this expression we have that:

- $SF^{(k)} = 0$ if $k > n$, because there does not exist any square-free monomial with n variables of total degree greater than n .
- $SF^{(n)} = 1$ if Γ_1 or Γ_2 is empty (and then the other one is non-empty), because if, say, Γ_2 is empty, then $SF(I_{\Gamma_2})^{(n)} = 0$ and hence $SF^{(n)} = SF(I_{\Gamma_1})^{(n)} = 1$ (if $I_{\Gamma_1} \neq (0)$, then $x_1 \cdots x_n \in I_{\Gamma_1}$, and it is the unique square-free monomial of total degree n).
- $SF^{(n)} = 0$ if Γ_1 and Γ_2 are non-empty, because in this case $SF(I_{\Gamma_1})^{(n)} = SF(I_{\Gamma_2})^{(n)} = SF(I_{\Gamma_1 \cup \Gamma_2})^{(n)} = 1$.

Now, a simple application of Stirling's formula $p! \sim \sqrt{2\pi}p^{p+\frac{1}{2}}e^{-p}$ yields for every $k > 0$

$$\frac{\binom{m-1}{k}}{\binom{n+m-3}{n}} \sim \frac{n^{n+\frac{1}{2}}}{k^{k+\frac{1}{2}}} m^{k-n}$$

and hence

$$\lim_{m \rightarrow \infty} \frac{\binom{m-1}{k}}{\binom{n+m-3}{n}} = \lim_{m \rightarrow \infty} \frac{n^{n+\frac{1}{2}}}{k^{k+\frac{1}{2}}} m^{k-n} = \begin{cases} 0 & \text{if } 0 < k < n \\ 1 & \text{if } k = n \end{cases}$$

Therefore, if Γ_1 and Γ_2 are non-empty,

$$d_m(\Gamma_1, \Gamma_2) = \sum_{k=2}^{n-1} \frac{\binom{m-1}{k}}{\binom{n+m-3}{n}} S F^{(k)} \xrightarrow{m \rightarrow \infty} 0$$

while if one, and only one, of them is empty, then

$$d_m(\Gamma_1, \Gamma_2) = \sum_{k=2}^{n-1} \frac{\binom{m-1}{k}}{\binom{n+m-3}{n}} S F^{(k)} + \frac{\binom{m-1}{n}}{\binom{n+m-3}{n}} \xrightarrow{m \rightarrow \infty} 1.$$

(iii) Notice that, for every $i = 1, 2$ and for every $k \geq 2$, $x^{(\alpha_1, \dots, \alpha_{n+1})} \in M(I_{\Gamma_i^*})^{(k)}$ if and only if $x^{(\alpha_1, \dots, \alpha_n)} \in M(I_{\Gamma_i})^{(k-\alpha_{n+1})}$. This implies that

$$M(I_{\Gamma_1^*})^{(k)} \Delta M(I_{\Gamma_2^*})^{(k)} = \bigcup_{j=2}^k (M(I_{\Gamma_1})^{(j)} \Delta M(I_{\Gamma_2})^{(j)}) \cdot x_{n+1}^{k-j},$$

from where we obtain that

$$\begin{aligned} |M(I_{\Gamma_1^*})^{(k)} \Delta M(I_{\Gamma_2^*})^{(k)}| &= \sum_{j=2}^k |M(I_{\Gamma_1})^{(j)} \Delta M(I_{\Gamma_2})^{(j)}| \\ &= |M(I_{\Gamma_1})_k \Delta M(I_{\Gamma_2})_k| = d'_{k+1}(\Gamma_1, \Gamma_2) \end{aligned}$$

and hence

$$\begin{aligned} d'_m(\Gamma_1^*, \Gamma_2^*) &= \sum_{k=2}^{m-1} |M(I_{\Gamma_1^*})^{(k)} \Delta M(I_{\Gamma_2^*})^{(k)}| \\ &= \sum_{k=2}^{m-1} d'_{k+1}(\Gamma_1, \Gamma_2) = \sum_{k=3}^m d'_k(\Gamma_1, \Gamma_2). \end{aligned}$$

Finally,

$$\begin{aligned} d_m(\Gamma_1, \Gamma_2) &= \frac{1}{\binom{n+m-3}{n}} d'_m(\Gamma_1, \Gamma_2) = \frac{n+m-2}{(n+1)\binom{n+m-2}{n+1}} d'_m(\Gamma_1, \Gamma_2) \\ &\leq \frac{1}{\binom{n+m-2}{n+1}} \sum_{k=3}^m d'_k(\Gamma_1, \Gamma_2) = \frac{1}{\binom{n+m-2}{n+1}} d'_m(\Gamma_1^*, \Gamma_2^*) = d_m(\Gamma_1^*, \Gamma_2^*), \end{aligned}$$

where the inequality $\frac{n+m-2}{n+1} d'_m(\Gamma_1, \Gamma_2) \leq \sum_{k=3}^m d'_k(\Gamma_1, \Gamma_2)$ is obtained by adding $(n+1)d'_m(\Gamma_1, \Gamma_2)$ to both sides of inequality (b) in Lemma B and then dividing it by $(n+1)$.

Appendix C: Proof of Proposition 19

We establish first a lemma that generalizes the computation of $A(\Gamma_1 \cup \Gamma_2)$ carried out in the proof of Proposition 15. For every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$ and for every $k \geq 2$, let

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

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

Lemma C *For every $\Gamma_1, \Gamma_2 \in \mathcal{U}_n$ and for every $k \geq 2$,*

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

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

$$\begin{aligned} A_k &= \sum_{m>k} m \Theta^{(m)} + \sum_{m>k} (m - k) \Omega^{(m)} \\ &= \sum_{m>k} m \Theta^{(m)} + \sum_{m>k} (m - 1) \Omega^{(m)} - (k - 1) \sum_{m>k} \Omega^{(m)} \\ &= |Q_1 \Delta Q_2| - \sum_{m=4}^k m \Theta^{(m)} - \sum_{m=2}^k (m - 1) \Omega^{(m)} - (k - 1) \sum_{m>k} \Omega^{(m)} \\ &= |Q_1 \Delta Q_2| - \sum_{m=4}^k m \Theta^{(m)} - \sum_{i=2}^k \Omega_{\geq i}. \end{aligned}$$

□

In particular, we obtain again that $A_2 = |Q_1 \Delta Q_2| - \Omega_{\geq 2}$, as we already saw in the proof of Proposition 15.

We can proceed now to prove Proposition 19. To simplify the notations, we shall denote each $SF(I_{\Gamma_1 \cup \Gamma_2})^{(i)}$ simply by $SF^{(i)}$. We use the expressions

$$\begin{aligned} d_5(\Gamma_1, \Gamma_2) &= \frac{1}{\binom{n+2}{2}} \left(H_{\Gamma_1}(4) + H_{\Gamma_2}(4) - 2H_{\Gamma_1 \cup \Gamma_2}(4) \right) \\ d_6(\Gamma_1, \Gamma_2) &= \frac{1}{\binom{n+3}{3}} \left(H_{\Gamma_1}(5) + H_{\Gamma_2}(5) - 2H_{\Gamma_1 \cup \Gamma_2}(5) \right), \end{aligned}$$

where we already know that

$$\begin{aligned} H_{\Gamma_i}(4) &= \binom{n+4}{4} - \binom{n+2}{2} |Q_i| + \binom{|Q_i|}{2}, \quad i = 1, 2 \\ H_{\Gamma_i}(5) &= \binom{n+5}{5} - \binom{n+3}{3} |Q_i| + (n+1) \binom{|Q_i|}{2}, \quad i = 1, 2 \\ H_{\Gamma_1 \cup \Gamma_2}(4) &= \binom{n+4}{4} - (6|Q_1 \cup Q_2| + 4SF^{(3)} + SF^{(4)}) \\ H_{\Gamma_1 \cup \Gamma_2}(5) &= \binom{n+5}{5} - (10|Q_1 \cup Q_2| + 10SF^{(3)} + 5SF^{(4)} + SF^{(5)}) \end{aligned}$$

with $SF^{(3)} = (n-2)|Q_1 \cup Q_2| - A_2$, as we saw in the proof of Proposition 13: notice that $T(\Gamma_1 \cup \Gamma_2) = 0$ and recall that $A(\Gamma_1 \cup \Gamma_2) = A_2$. It remains to compute $SF^{(4)}$ and $SF^{(5)}$.

As far as $SF^{(4)}$ goes:

- (1) For every $i \cdot j \in Q_1 \cup Q_2$, there are $\binom{n-2}{2}$ square-free monomials $x_i x_j x_k x_l \in M(I_{\Gamma_1 \cup \Gamma_2})$. 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 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 $i \cdot j, j \cdot k \in Q_1 \cup Q_2$ 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 $i \cdot j, j \cdot k, k \cdot l \in Q_1 \cup Q_2$, 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 $i \cdot j, j \cdot k, k \cdot l, l \cdot i \in Q_1 \cup Q_2$, so that if $\{i, j, k, l\}$ form a closed 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

$$SF^{(4)} = \binom{n-2}{2} |Q_1 \cup Q_2| - \binom{|Q_1 \cup Q_2|}{2} - (n-4)A_2 + A_3 - \Theta^{(4)}.$$

And as far as $SF^{(5)}$ goes:

- (1) For every $i \cdot j \in Q_1 \cup Q_2$, there are $\binom{n-2}{3}$ square-free monomials $x_i x_j x_k x_l x_m \in M(I_{\Gamma_1 \cup \Gamma_2})$. This makes $\binom{n-2}{3} |Q_1 \cup Q_2|$ 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 $(n-4) \left(\binom{|Q_1 \cup Q_2|}{2} - A_2 \right)$ to (1).
- (3) If $i \cdot j, j \cdot k \in Q_1 \cup Q_2$, 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 $i \cdot j, j \cdot k, l \cdot m \in Q_1 \cup Q_2$ with $\{i, j, k\} \cap \{l, m\} = \emptyset$, 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

$$\left| \left\{ \{i \cdot j, j \cdot k, l \cdot m\} \mid i \cdot j, j \cdot k, l \cdot m \in Q_1 \cup Q_2, \{i, j, k\} \cap \{l, m\} = \emptyset \right\} \right|;$$

let us call for the moment X this number.

- (5) If $i \cdot j, j \cdot k, k \cdot l \in Q_1 \cup Q_2$, 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 $i \cdot j, j \cdot k, k \cdot l, l \cdot i \in Q_1 \cup Q_2$, i.e., if $\{i, j, k, l\}$ form a closed orbit of length 4, then for every $m \notin \{i, j, k, l\}$ the monomial $x_i x_j x_k x_l x_m$ 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 $i \cdot j, j \cdot k, k \cdot l, l \cdot m \in Q_1 \cup Q_2$, then the monomial $x_i x_j x_k x_l x_m$ 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

$$\begin{aligned} SF^{(5)} &= \binom{n-2}{3} |Q_1 \cup Q_2| - (n-4) \left(\binom{|Q_1 \cup Q_2|}{2} - A_2 \right) - \binom{n-3}{2} A_2 \\ &\quad + (|Q_1 \cup Q_2| - 2) A_2 + (n-5) A_3 - (n-4) \Theta^{(4)} - A_4 \end{aligned}$$

Using these values for $SF^{(4)}$ and $SF^{(5)}$, a simple computation shows that

$$\begin{aligned} H_{\Gamma_1 \cup \Gamma_2}(4) &= \binom{n+4}{4} - \binom{n+2}{2} |Q_1 \cup Q_2| + \binom{|Q_1 \cup Q_2|}{2} + n A_2 - A_3 + \Theta^{(4)} \\ H_{\Gamma_1 \cup \Gamma_2}(5) &= \binom{n+5}{5} - \binom{n+3}{3} |Q_1 \cup Q_2| + (n+1) \binom{|Q_1 \cup Q_2|}{2} \\ &\quad + \left(\binom{n+2}{2} - |Q_1 \cup Q_2| - 2 \right) A_2 - n A_3 + (n+1) \Theta^{(4)} + A_4. \end{aligned}$$

Let us compute now d_5 . We have that

$$\begin{aligned} d_5'(\Gamma_1, \Gamma_2) &= H_{\Gamma_1}(4) + H_{\Gamma_2}(4) - 2H_{\Gamma_1 \cup \Gamma_2}(4) \\ &= 2 \binom{n+4}{4} - \binom{n+2}{2} (|Q_1| + |Q_2|) + \binom{|Q_1|}{2} + \binom{|Q_2|}{2} \\ &\quad - 2 \left(\binom{n+4}{4} - \binom{n+2}{2} |Q_1 \cup Q_2| + \binom{|Q_1 \cup Q_2|}{2} + n A_2 - A_3 + \Theta^{(4)} \right) \\ &= \binom{n+2}{2} |Q_1 \Delta Q_2| - \left(2 \binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} - \binom{|Q_2|}{2} \right) + 2n A_2 - 2A_3 + 2\Theta^{(4)} \end{aligned}$$

Now, we know from Lemma C that

$$A_2 = |Q_1 \Delta Q_2| - \Omega_{\geq 2}, \quad A_3 = |Q_1 \Delta Q_2| - \Omega_{\geq 2} - \Omega_{\geq 3}.$$

Replacing them in the expression obtained above for $d_5'(\Gamma_1, \Gamma_2)$, and dividing the result by $\binom{n+2}{2}$, we obtain the expression for d_5 given in the statement.

As far as d_6 goes, we have that

$$\begin{aligned} d_6'(\Gamma_1, \Gamma_2) &= H_{\Gamma_1}(5) + H_{\Gamma_2}(5) - 2H_{\Gamma_1 \cup \Gamma_2}(5) \\ &= 2 \binom{n+5}{5} - \binom{n+3}{3} (|Q_1| + |Q_2|) + (n+1) \left(\binom{|Q_1|}{2} + \binom{|Q_2|}{2} \right) \\ &\quad - 2 \left(\binom{n+5}{5} - \binom{n+3}{3} |Q_1 \cup Q_2| + (n+1) \binom{|Q_1 \cup Q_2|}{2} \right) \\ &\quad + \left(\binom{n+2}{2} - 2 - |Q_1 \cup Q_2| \right) A_2 - n A_3 + (n+1) \Theta^{(4)} + A_4 \\ &= \binom{n+3}{3} |Q_1 \Delta Q_2| - (n+1) \left(2 \binom{|Q_1 \cup Q_2|}{2} - \binom{|Q_1|}{2} - \binom{|Q_2|}{2} \right) \\ &\quad - 2 \left(\binom{n+2}{2} - 2 - |Q_1 \cup Q_2| \right) A_2 + 2n A_3 - 2(n+1) \Theta^{(4)} - 2A_4. \end{aligned}$$

If we replace in this expression A_2 , A_3 and A_4 by their values provided by Lemma C and we divide the result by $\binom{n+3}{3}$, we obtain the expression for d_6 given in the statement.