ABSTRACT

MISRA, PRATIK. Combinatorial Problems in Trees and Graphical Models. (Under the direction of Seth Sullivant.)

Algebraic statistics is a relatively new area of research which explores the connection between algebraic geometry and statistics. This thesis deals with problems based on the expected distance between phylogenetic trees and characterization of undirected and directed Gaussian graphical models having toric vanishing ideals. Although these problems seem disjoint at the surface, they can be considered as combinatorial problems at their core.

In phylogenetics, different tree reconstruction methods, and different datasets on the same set of species, can lead to the reconstruction of different trees. In such cases, it is important to measure the distance between different trees constructed. In Chapter 2, we focus on the maximum agreement subtree as a measure of discrepancy between trees. We study the distribution of the maximum agreement subtree of trees that are uniformly sampled from all trees with the same shape and prove that the expected size is of the order of $\sqrt{n}$ in this case. We also show results of simulations that suggest that our ideas based on "blobs" could be used to improve lower bounds on the expected value of the maximum agreement subtree for other distributions of random trees.

Gaussian graphical models are used throughout the natural sciences and computational biology as they explicitly capture the statistical relationships between the variables of interest in the form of a graph. Sturmfels and Uhler conjectured that the vanishing ideal of an undirected Gaussian graphical model is generated in degree at most 2 if and only if each connected component of the graph G is a 1-clique sum of complete graphs. We prove this conjecture in Chapter 3. We exploit the connection between the generating sets of toric ideals and connectivity properties of the fiber graphs to prove the conjecture. We also formulate a way to write the vanishing ideal of G in terms of smaller graphs G_1 and G_2 when G is a 1-clique sum of G_1 and G_2 where G_1 and G_2 are not necessarily complete.

In Chapter 4, we try to get a similar characterization as in Chapter 3 for Gaussian graphical models represented by directed acyclic graphs. The problem of characterizing DAGs having toric vanishing ideal is more complicated than its undirected counterpart as it is not only dependent on the structure of the graph but also depends on the direction of its edges. We develop three techniques to construct DAGs having toric vanishing ideal from smaller DAGs which have toric vanishing ideal. We call these techniques safe gluing, gluing at sinks and adding a new sink. We conjecture that if two DAGs have toric vanishing ideals, then any of the three operations would yield us a new DAG whose vanishing ideal is also toric. We further conjecture that every DAG whose vanishing ideal is toric can be obtained as a combination of these three operations on complete DAGs. We analyze an example and prove some other results which provide evidence to these conjectures.

Combinatorial Problems in Trees and Graphical Models

by
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DEDICATION

To my parents

BIOGRAPHY

Pratik Misra was born in Odisha, India, where he completed his entire schooling. He received his undergraduate degree in Mathematics from Institute of Mathematics and Applications, Bhubaneswar in 2014. He then joined the prestigious Indian Institute of Technology, Madras, to pursue his Master's degree in Mathematics. After completing his master's degree in 2016, Pratik moved to Raleigh, North Carolina where he joined the North Carolina State University and began his Doctoral research in Mathematics under the guidance of Prof. Sullivant. He will continue his mathematical career as a Postdoctoral Research fellow at KTH, Royal Institute of Technology, Stockholm. When he is not doing Mathematics, Pratik enjoys playing Cricket, Badminton and Soccer along with sketching and watching movies.

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The dream of receiving a doctoral degree is shared by many, but very few people get the opportunity to achieve it. That being said, I have been supported and encouraged throughout my career by some amazing people in my life. First and foremost is my advisor, Seth Sullivant, who has been incredibly patient with me throughout my graduate life. His detailed feedback and generosity with his time, attention and resources have made me achieve results which I never thought possible 5 years ago. Even with his busy schedule, he always had the time to meet me and guide me through my problems. He taught me how to approach various research problems, helped me improve my academic writing skills and encouraged me to collaborate with other researchers. It won't be wrong to say that everything I know about research is what I have learnt from him. Apart from research, he has also been my teaching mentor and has provided me with valuable tips and comments to improve my teaching skills. I feel privileged to have had him as my advisor and my mentor.

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The journey of a thousand miles begins with a single step, and for me, that first step into my mathematical career was joining Institute of Mathematics and Applications for my undergraduate studies. I am indebted to Prof. Swadhin Pattanayak, who mentored me during my undergraduate days and inspired me to pursue higher studies in Mathematics. I would also like to thank Sarang Sane and A.V. Jayanthan who introduced me to the world of commutative algebra during my Master's and wrote the letters of recommendation for my graduate applications.

I am grateful to my family for their constant support. My mother has been the pillar of support and encouragement throughout my life. My father's unconventional yet successful journey of becoming a lawyer has always been a source of inspiration for me. He has always encouraged me to aim big in life and work hard to achieve the goal. My elder sisters Sonali Misra and Monali Misra have always supported my career choices and have always been there for me. Working towards my goal would not have been possible without their love and support.

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Finally I thank NC State University for giving me the opportunity to grow as a mathematician and as a person.

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Introduction

Algebraic statistics is a relatively new area of research which explores the connection between algebraic geometry and statistics. The study of algebraic statistics began in 1990s with the work of Diaconis and Sturmfels [7] when they established a connection between random walks and generating sets of toric ideals. Since then, this area of research has developed rapidly [11; 35].

This thesis deals with problems based on the expected distance between phylogenetic trees and characterization of undirected and directed Gaussian graphical models having toric vanishing ideals. Although these problems seem disjoint at the surface, they can be considered as combinatorial problems at their core. Before going into the details of the chapters, we first provide the elementary background on a number of concepts that are used throughout this thesis.

1.1 Basic definitions and results in graph theory

In this section, we look at the basic definitions and results in graph theory which will be used extensively in the upcoming chapters. Graphs arise throughout this thesis in both phylogenetics and Gaussian graphical models. In phylogenetics, we use trees to represent the evolutionary processes of a set of species. In Gaussian graphical models, we use undirected and directed acyclic graphs to study the models and characterize them.

Definition 1.1.1. A *graph* $G = (V, E)$ is pair where V is the set of vertices or nodes and E is the set of edges. Each edge $e \in E$ is a set $e = \{v_1, v_2\}$ of two vertices $v_1, v_2 \in V$

with $v_1 \neq v_2$ (unless specified otherwise). When $e = \{v_1, v_2\} \in E$, we say that v_1 and v_2 are *adjacent* to each other.

In a graph G, a *path* of length n from vertex v_0 to vertex v_n is a sequence of distinct vertices $v_0, v_1, v_2, ..., v_n$ such that each v_i is adjacent to v_{i+1}. A graph is said to be *connected* if there is a path between any two distinct vertices. Similarly, a graph is said to be *complete* if there is an edge between any two vertices of G.

Definition 1.1.2. Let $G = (V, E)$ be a graph.

i) A set $C \subseteq V$ is called a *clique* of G if the subgraph induced by C is a complete graph.
ii) Let A, B, and C be disjoint subsets of the vertex set of G with $A \cup B \cup C = V$. Then C *separates* A and B if for any $a \in A$ and $b \in B$, any path from a to b passes through a vertex in C.
iii) The graph G is said to be a *c-clique sum* of smaller graphs G_1 and G_2 if there exists a partition (A, B, C) of its vertex set such that
    a) C is a clique with $|C| = c$,
    b) C separates A and B,
    c) G_1 and G_2 are the subgraphs induced by $A \cup C$ and $B \cup C$ respectively.

    In the case that G is a c-clique sum, we call the corresponding partition (A, B, C) a *c-clique partition* of G.

Definition 1.1.3. A graph G is called a *block graph* (also known as *1-clique sum of complete graphs*) if there exists a partition (A, B, C) of its vertex set such that

i) $|C| = 1$,
ii) C separates A and B,
iii) the subgraphs induced by $A \cup C$ and $B \cup C$ are either complete graphs or block graphs.

We illustrate the definitions above with an example.

Example 1.1.4. Let $G = ([6], E)$ be the block graph as shown in Figure 1.1. Clearly, the graph is connected as there exists a path between any two vertices of G. It is also a block graph as there exists a partition $(A, B, C) = (\{1, 2\}, \{4, 5, 6\}, \{3\})$ which satisfies the following conditions :

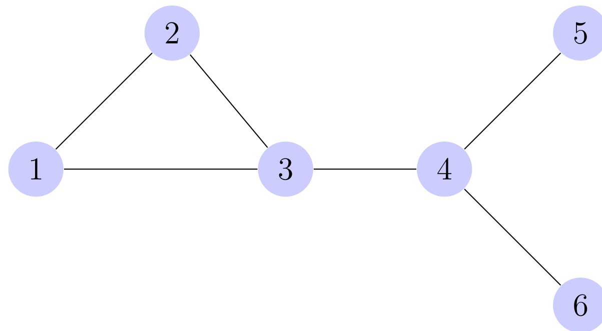


Figure 1.1: Example of a block graph G

i) $|C| = 1$,

ii) The vertex 3 separates $\{1, 2\}$ and $\{4, 5, 6\}$ as every path from $\{1, 2\}$ to $\{4, 5, 6\}$ passes through 3,

iii) The subgraph induced by $\{1, 2, 3\}$ is a complete graph of 3 vertices and the subgraph induced by $\{3, 4, 5, 6\}$ is also a block graph with $C = \{4\}$.

The graph G also has three more 1-clique partitions apart from the one already shown above:

$$\text{Partition 2}: A = \{1, 2, 3\}, B = \{5, 6\}, C = \{4\}$$
$$\text{Partition 3}: A = \{1, 2, 3, 5\}, B = \{6\}, C = \{4\},$$
$$\text{Partition 4}: A = \{1, 2, 3, 6\}, B = \{5\}, C = \{4\}.$$

We study block graphs and the Gaussian graphical models represented by them in Chapter 3. One of the important properties of block graphs which we use extensively throughout Chapter 3 is as follows :

Proposition 1.1.5. *If G is a block graph, then for any two vertices i and j there exists a unique shortest path in G connecting them. Further, if (A, B, C) is a 1-clique partition of G with $c \in C$ and if $i \in A$ and $j \in B$, then the unique shortest path from i to j can be decomposed into the unique shortest paths from i to c and c to j.*

Proof. We prove this by applying induction on the number of vertices in G. If i and j are connected by a single edge, then that is the unique shortest path. If they are not connected by a single edge, then there exists a 1-clique partition (A, B, C) with $C = \{c\}$

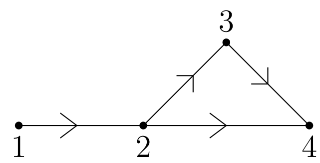


Figure 1.2: A Directed acyclic graph G

which separates them. But as $A \cup C$ and $B \cup C$ are also block graphs and have fewer vertices than G, by induction there exist unique shortest paths from i to c and from c to j. But as any path from i to j must pass through c, the concatenation of the unique shortest paths from i to c and c to j would be the unique shortest path from i to j.

The second part follows from a property of unique shortest paths that if c is a point on the path, then the subpaths from i to c and c to j are the unique shortest paths from i to c and c to j respectively. $\square$

We end this section by giving a brief description of *directed graphs*. So far we have only talked about graphs where there is no sense of direction. Directed graphs are the graphs where each edge has a specified direction. Each edge $\{i, j\}$ is denoted by either $i \to j$ or $j \to i$ depending on the direction.

Definition 1.1.6. Let G be a directed graph. A *directed path* is a path in G with directed edges. A directed graph which does not have any directed cyclic path of the form $i_1 \to i_2 \to \cdots \to i_n \to i_1$ is called a *directed acyclic graph* (commonly known as DAG).

Directed acyclic graphs arise in Chapter 4 where we find the vanishing ideal of Gaussian graphical models represented by DAGs. We use the properties of DAGs to characterize the models which have a toric vanishing ideal. Below is an example of a DAG with 4 vertices.

Example 1.1.7. Let G be a directed graph as shown in Figure 1.2. We observe that there is only one directed cycle in G, which is $2 \to 3 \to 4 \leftarrow 2$. As it is not of the form $i_1 \to i_2 \to \cdots \to i_n \to i_1$, G is a directed acyclic graph (DAG).

1.2 Basic definitions in phylogenetics

Rooted binary trees are used in evolutionary biology to represent the evolution of a set of species where the leaves denote the existing species and the internal nodes denote the unknown ancestors. The study of methods to reconstruct evolutionary trees from biological data is the area called *phylogenetics* [14; 27]. The major goal of phylogenetics is to reconstruct this evolutionary tree from the data obtained from the existing species at the leaves.

Before the development of sequencing technology, primary methods for reconstructing phylogenetic trees were to look for morphological similarities between species and group species together that had similar characteristics. Unfortunately, focusing only on morphological features resulted in grouping organisms together that developed similar characteristics through different pathways. Modern methods for reconstructing phylogenetic trees use sequencing technology to compare sequences for genes that appear in all species under consideration.

This section gives the necessary background on phylogenetics needed for Chapter 2. More details on this topic can be found in [2; 30]

Definition 1.2.1. Let $G = (V, E)$ be a graph with vertex set V and edge set E. A *cycle* is a sequence of vertices $v_0, v_1, ..., v_n = v_0$ which are distinct (other than $v_n = v_0$) with $n \geq 3$ and v_i adjacent to v_{i+1}. A *tree* $T = (V, E)$ is a connected graph with no cycles.

Theorem 1.2.2. *If v_0 and v_1 are any two vertices in a tree T, then there is a unique path from v_0 to v_1.*

If a vertex lies in two or more distinct edges of a tree, then it is called an *interior* vertex. If it lies in only one edge, then we call it a terminal vertex or a *leaf*. Further, trees can be categorized as *rooted* and *unrooted*. A rooted tree is a tree in which one of the nodes is specified to be the root. This allows us to determine a direction of ancestral relationship. An unrooted tree has no pre-determined root but can be turned into a rooted tree by inserting a new node which functions as the root.

In this thesis, we use rooted binary trees to represent evolutionary processes. The leaves represent the existing species, interior vertices represent the unknown ancestors and the edges indicate the lines of direct evolutionary relationships among the species. We explain this with an example.

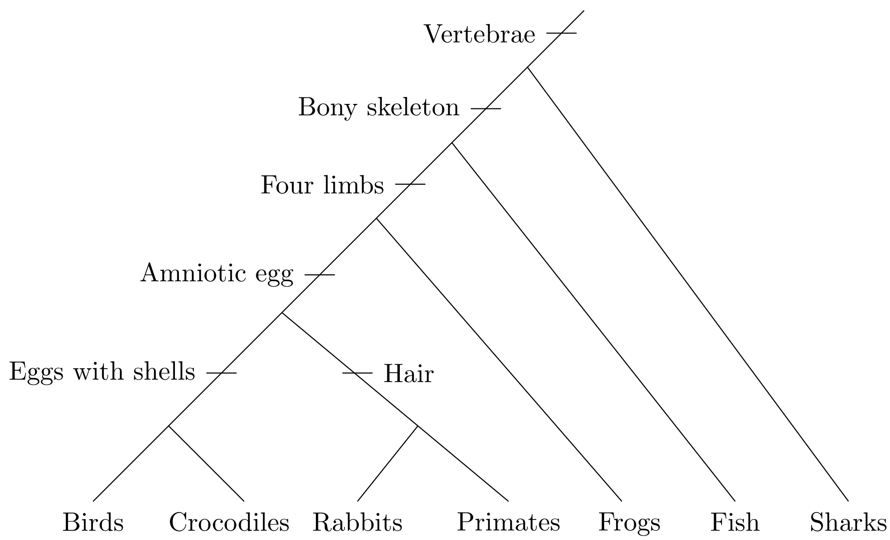


Figure 1.3: A Phlyogenetic tree depicting evolutionary processes [12]

Example 1.2.3. In Figure 1.3 we observe a phylogenetic tree representing the evolutionary processes of the existing species of Birds, Crocodiles, Rabbits, Primates, Frogs, Fish and Sharks. The classification of these species is done in the following way: All the existing species are vertebrates but at some point in time an ancestor evolved into two different species where one of the species did not have bony skeleton (sharks) and the other did have a bony skeleton. Later on, that species evolved into two different species where one did have four limbs and the other did not (fish), and so on.

1.2.1 Counting binary trees

Definition 1.2.4. Let X denote a finite set of labels. Then a *phylogenetic X-tree* is a tree $T = (V, E)$ together with a bijective correspondence $\varphi : X \to L$, where $L \subseteq V$ denotes the set of leaves of the tree. We call φ the labeling map. Such a tree is also called a *leaf-labeled tree.*

Example 1.2.5. In Figure 1.4, we see a rooted binary phylogenetic [6]-tree T where $X = [6]$ and $\varphi : [6] \to L$ is the map through which we label the leaves.

Definition 1.2.6. Two phylogenetic X-trees are *isomorphic* if there is a bijective correspondence between their vertices that respects adjacency and their leaf labeling.

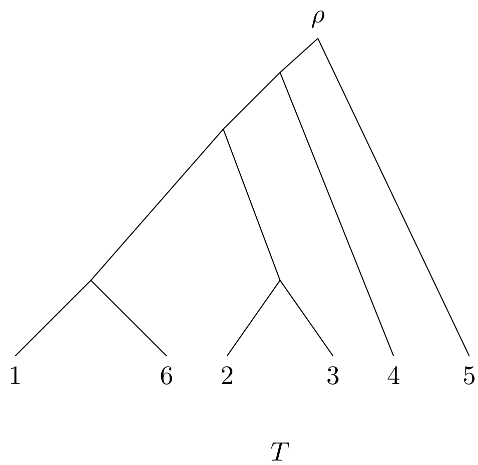


Figure 1.4: A rooted binary phylogenetic [6]-tree

Isomorphism between the trees is independent of the way the trees are drawn in the plane. Let $b(n)$ denote the number of distinct (up to isomorphism) unrooted binary trees with n leaves leaf labelled by $[n] = \{1, 2, \ldots, n\}$. Then we know that $b(2) = 1, b(3) = 1$, and $b(4) = 3$. To construct unrooted binary trees with 5 leaves, we can select any of the three trees of $b(4)$ and add a new edge to any of the 5 existing edges. This gives us that $b(5) = 3 \cdot 5 = 15$. So, in order to obtain a general formula for $b(n)$, we also need a formula for the number of edges in these trees.

Theorem 1.2.7. *An unrooted binary tree with $n \geq 2$ leaves has $2n-2$ vertices and $2n-3$ edges.*

Proof. We prove this by applying induction on the number of leaves. Clearly, the statement is true for $n = 2$. Let the statement be true for all trees with $n - 1$ leaves. Now, for any tree T with $n \geq 3$ leaves, let v_1 be one of the leaves of T. Then v_1 lies on a unique edge $\{v_1, v_2\}$ while v_2 lies on two other edges $\{v_2, v_3\}$ and $\{v_2, v_4\}$. Removing the vertex v_1 and suppressing the internal vertex v_2 gives us a new binary tree T' with $n-1$ leaves. Since both the number of vertices and edges have been decreased by 2, T must have $(2(n-1)-2)+2 = 2n-2$ vertices and $(2(n-1)-3)+2 = 2n-3$ edges. $\square$

Theorem 1.2.8. *For $n \geq 3$, there are $b(n) = (2n-5)!! = 1 \cdot 3 \cdot 5 \cdots (2n-5)$ number of distinct unrooted binary leaf labelled trees.*

Proof. We again use induction to prove this statement. The base case for $n = 3$ is clear. Now, let T be an unrooted tree with n leaves and let T' be the tree with $n-1$ leaves as constructed in Theorem 1.2.7. Then with v_1 fixed, the map $T \mapsto (T', \{v_3, v_4\})$ is a bijection from n-leaf trees to pairs of $(n-1)$-leaf trees and edges. Counting these pairs gives us that $b(n) = b(n-1) \cdot (2(n-1)-3) = b(n-1) \cdot (2n-5)$. But from the inductive hypothesis we know that $b(n-1) = (2(n-1)-5)!! = (2n-7)!!$. So, $b(n) = (2n-5)!!$. $\square$

The proof of the last theorem can be used to get a count for rooted binary trees as well. We observe that by adjoining a new edge at the root, we can form a bijective correspondence between rooted binary trees with n leaves and unrooted binary trees with $n+1$ leaves. Hence, we have the following result :

Corollary 1.2.9. *The number of rooted binary trees with n leaves leaf labelled by $[n] = \{1, 2, \ldots n\}$ is given by $b(n+1) = (2n-3)!! = 1 \cdot 3 \cdot 5 \cdots (2n-3)$.*

1.3 Basics of algebraic geometry

This section gives the necessary background on algebraic geometry. The concepts and results reviewed here are mainly used in Chapter 3 and 4 where we study the vanishing ideal of Gaussian graphical models. We use the tools from Algebraic Geometry to characterize the graphical models based on their vanishing ideals. More details on algebraic geometry can be found in [15].

All rings in this thesis are assumed to be commutative. Let $\mathbb{K}$ be a field and let $\mathbb{K}[x_1, \ldots, x_n]$ denote the polynomial ring over $\mathbb{K}$ in n indeterminates. We assume the field $\mathbb{K}$ to be algebraically closed for most parts the thesis and hence replace it with the field of complex numbers $\mathbb{C}$ in the later chapters. We use the notation $x^u := x_1^{u_1} \ldots x_n^{u_n}$ to denote monomials in $\mathbb{K}[x_1, \ldots, x_n]$.

1.3.1 Gröbner bases

In this subsection, we study the properties of the Gröbner basis of an ideal and focus on its construction.

Definition 1.3.1. Let R be any arbitrary ring. An *ideal* I in R is a subset of R which satisfies the following conditions :

i) I is a subring, and
ii) if $f \in I$ and $g \in R$, then $fg \in I$.

For a given subset F of R, the ideal generated by F is denoted by $\langle F \rangle$. Given an ideal I, any subset $F \subseteq \mathbb{K}[x_1, \ldots, x_n]$ for which $\langle F \rangle = I$ is called a *generating set* of I. The following theorem says that every ideal $I \subseteq \mathbb{K}[x_1, \ldots, x_n]$ has a finite generating set. A proof for this can be found in [15].

Theorem 1.3.2 (Hilbert basis theorem)**.** *Every ideal $I \in \mathbb{K}[x_1, \ldots, x_n]$ can be finitely generated.*

Definition 1.3.3. A *monomial order* $>$ on $\mathbb{K}[x_1, \ldots, x_n]$ is a total order on monomials which satisfy the following conditions :

i) If $x^\alpha > x^\beta$ then $x^\alpha x^\gamma > x^\beta x^\gamma$ for any α, β, γ.
ii) An arbitrary set of monomials $\{x^\alpha\}_{\alpha \in A}$ has a least element.

Definition 1.3.4. Let $f = \Sigma_\alpha c_\alpha x^\alpha$ be any polynomial in $\mathbb{K}[x_1, \ldots x_n]$. Then for a fixed monomial order, the *leading monomial* of f (denoted by $LM(f)$) is defined as the largest monomial x^α for which $c_\alpha \neq 0$. The *leading term* of f (denoted by $LT(f)$) is the corresponding term $c_\alpha x^\alpha$.

Example 1.3.5. Lexicographic order: In this ordering, we have $x^\alpha > x^\beta$ if the first nonzero entry of $(\alpha_1 - \beta_1, \alpha_2 - \beta_2, \ldots, \alpha_n - \beta_n)$ is positive. For example,

$$x_1 >_{\text{lex}} x_2^3 >_{\text{lex}} x_2 x_3 >_{\text{lex}} x_3^{100}.$$

A *monomial ideal* $I \subset \mathbb{K}[x_1, \ldots x_n]$ is an ideal generated by a set of monomials $\{x^\alpha\}_{\alpha \in A}$. For a fixed monomial order $>$ on $\mathbb{K}[x_1, \ldots x_n]$, the *ideal of leading terms* is defined as

$$LT(I) := \langle LT(g) : g \in I \rangle.$$

Let $>$ be a fixed monomial order on $\mathbb{K}[x_1, \ldots, x_n]$ and $f_1, \ldots, f_r \in \mathbb{K}[x_1, \ldots, x_n]$ be a set of nonzero polynomials. Then for any arbitrary polynomial $g \in \mathbb{K}[x_1, \ldots, x_n]$, we apply the *Division algorithm* (Algorithm 2.7, [15]) to determine if g lies in $\langle f_1, \ldots, f_r \rangle$. The algorithm is as follows :

Step 0 : Substitute $g_0 = g$. If there exists no f_j such that $LM(f_j) | LM(g_0)$, then we stop. Else, we pick such an f_{j_0} and cancel the leading terms by putting

$$g_1 = g_0 - f_{j_0} LT(g_0)/LT(f_{j_0}).$$

...

Step i : Given g_i, if there exists no f_j with $LM(f_j)|LM(g_i)$ then we stop. Else, we pick such an f_{j_i} and cancel the leading terms by putting

$$g_{i+1} = g_i - f_{j_i} LT(g_i)/LT(f_{j_i}).$$

If the procedure does not stop, then g_N must be 0 for some N and hence g lies in $\langle f_1, \ldots, f_r \rangle$. Unfortunately, this algorithm does not always work as even when $g \in \langle f_1, \ldots, f_r \rangle$, the leading monomial of g may not always be divisible by some $LM(f_j)$. We use this algorithm later while computing the Gröbner basis of an ideal.

Definition 1.3.6. Let $I \subset \mathbb{K}[x_1, \ldots, x_n]$ be any ideal. Then for a fixed monomial order $>$ on $\mathbb{K}[x_1, \ldots, x_n]$, a *Gröbner basis* for I is a collection of nonzero polynomials $\{f_1, \ldots, f_r\} \subset I$ such that $LT(f_1), \ldots, LT(f_r)$ generate $LT(I)$.

Although not mentioned in the definition, any Gröbner basis of I is also a generating set of I (Cor 2.14, [15]). The next theorem shows the existence of a Gröbner basis for any given ideal and any term order.

Theorem 1.3.7 (Existence theorem)**.** *Let $I \subset \mathbb{K}[x_1, \ldots, x_n]$ be any arbitrary nonzero ideal. Then for any fixed monomial order $>$, I admits a finite Gröbner basis.*

The Existence theorem can be seen as an application of the Hilbert Basis theorem. The proof follows from the Hilbert Basis theorem and Dickson's Lemma (Proposition 2.23, [15]) as it reduces the Existence theorem to the case of monomial ideals.

Now, for a given ideal $I \subset \mathbb{K}[x_1, \ldots, x_n]$, any arbitrary generating set of I is not necessarily a Gröbner basis. Thus, it is important to have an algorithm for finding a Gröbner basis for I. We describe the *Buchberger's algorithm* for constructing a Gröbner basis. But before that, we need to define the terms like *least common multiple* and *S-polynomial*. The *least common multiple* of two monomials x^α and x^β is defined as

$$LCM(x^\alpha, x^\beta) = x_1^{max(\alpha_1,\beta_1)} \ldots x_n^{max(\alpha_n,\beta_n)}.$$

For a fixed monomial order on $\mathbb{K}[x_1, \ldots, x_n]$, let f_1 and f_2 be two arbitrary polynomials. We set $x^{\gamma(12)} = LCM(LM(f_1), LM(f_2))$. Then the S-polynomial $S(f_1, f_2)$ is defined as

$$S(f_1, f_2) := (x^{\gamma(12)}/LT(f_1))f_1 - (x^{\gamma(12)}/LT(f_2))f_2.$$

The purpose of the construction of S-polynomial is to have the desired cancellations required in the division algorithm.

Example 1.3.8. Let $f_1 = 2x_1x_2 - x_3^2$ and $f_2 = 3x_1^2 - x_3$. Then the S-polynomial with respect to lexicographic order is

$$S(f_1, f_2) = \frac{x_1^2x_2}{2x_1x_2}(2x_1x_2 - x_3^2) - \frac{x_1^2x_2}{3x_1^2}(3x_1^2 - x_3) = \frac{-1}{2x_1x_3^2} + \frac{1}{3x_2x_3}.$$

Theorem 1.3.9 (Buchberger's Criterion). *Fix a monomial order and polynomials $f_1, \ldots, f_r$ in $\mathbb{K}[x_1, \ldots, x_n]$. Then the following are equivalent :*

i) $f_1, \ldots, f_r$ form a Gröbner basis for $\langle f_1, \ldots, f_r\rangle$.
ii) Each S-polynomial $S(f_i, f_j)$ gives remainder zero on applying division algorithm.

Corollary 1.3.10 (Corollary 2.29, [15]). *For a fixed monomial order and polynomials $f_1, \ldots, f_r \in \mathbb{K}[x_1, \ldots, x_n]$, a Gröbner basis for $\langle f_1, \ldots, f_r\rangle$ is obtained by iterating the following procedure :*

For each i, j we apply the diision algorithm to the S-polynomials to get the expressions

$$S(f_i, f_j) = \Sigma_{l=1}^{r} h(ij)_l f_l + r(ij), \qquad LM(S(f_i, f_j)) \geq LM(h(ij)_l f_l)$$

where each $LM(r(ij))$ is not divisible by any of the $LM(f_l)$. If all the remainders $r(ij) = 0$ then $f_1, \ldots, f_r$ are already a Gröbner basis. Else, let $f_{r+1}, \ldots, f_{r+s}$ denote the nonzero $r(ij)$ and adjoin these to get a new set of generators

$$\{f_1, \ldots, f_r, f_{r+1}, \ldots, f_{r+s}\}.$$

We illustrate this algorithm with an example.

Example 1.3.11. We compute the Gröbner basis of $I = \langle f_1, f_2\rangle = \langle x_1^2 - x_2, x_1^3 - x_3\rangle$ with respect to lexicographic order. Computing the first S-polynomial gives us

$$S(f_1, f_2) = x_1f_1 - f_2 = x_1(x_1^2 - x_2) - (x_1^3 - x_3) = -x_1x_2 + x_3.$$

We observe that its leading term is not contained in

$$\langle LM(f_1), LM(f_2)\rangle = \langle x_1^2\rangle.$$

Therefore, we add

$$f_3 = x_1x_2 - x_3$$

to the Gröbner basis. The next S-polynomial is given by

$$S(f_1, f_3) = x_2f_1 - x_1f_3 = x_1x_3 - x_2^2.$$

Again we see that its leading term is not contained in

$$\langle LM(f_1), LM(f_2), LM(f_3)\rangle = \langle x_1^2, x_1x_2\rangle.$$

So, we add

$$f_4 = x_1x_3 - x_2^2$$

to the Gröbner basis. Now, if we compute $S(f_3, f_4)$, we get

$$S(f_3, f_4) = x_3f_3 - x_2f_4 = x_2^3 - x_3^2.$$

As its leading term is not contained in

$$\langle LM(f_1), \ldots, LM(f_4)\rangle = \langle x_1^2, x_1x_2, x_1x_3\rangle,$$

we add

$$f_5 = x_2^3 - x_3^2$$

to the Gröbner basis. Computing all the S-polynomials involving f_5, we get

$$\begin{aligned}
S(f_1, f_5) &= (x_1x_3 + x_2^2)f_4 \\
S(f_2, f_5) &= x_1^2x_3f_3 + x_2x_3f_1 \\
S(f_3, f_5) &= x_3f_4 \\
S(f_4, f_5) &= x_3^2f_4 - x_2^2f_5.
\end{aligned}$$

Hence, by Buchberger's criterion we can conclude that $\{f_1, f_2, f_3, f_4, f_5\}$ is a Gröbner basis of I.

1.3.2 Varieties and ideals

In this subsection, we look at the concepts of "vanishing ideal" and "variety" and their properties. An *affine space* of dimension n over $\mathbb{K}$ is defined as

$$\mathbb{A}^n(\mathbb{K}) = \{(a_1, \ldots, a_n) : a_i \in \mathbb{K}\}.$$

Definition 1.3.12. For a given set $S \subset \mathbb{A}^n(\mathbb{K})$, the *vanishing ideal* of the set S is defined as

$$I(S) := \{f \in \mathbb{K}[x_1, \ldots, x_n] : f(s) = 0 \text{ for each } s \in S\}.$$

Similarly, for a given set of polynomials $F \subset \mathbb{K}[x_1, \ldots, x_n]$, the *affine variety* is defined as the collection of points where each $f \in F$ vanishes, i.e,

$$V(F) := \{a \in \mathbb{A}^n(\mathbb{K}) : f(a) = 0 \text{ for each } f \in F\}.$$

For the rest of the thesis, we use term 'variety' to denote affine variety. We look at an example to explain the two concepts.

Example 1.3.13. Let $S = \{(1, 1), (2, 3)\} \subset \mathbb{A}^2(\mathbb{Q})$. Then

$$I(S) = \langle (x - 1)(y - 3), (x - 1)(x - 2), (y - 1)(x - 2), (y - 1)(y - 3) \rangle.$$

Similarly, if $F = \{f_1, f_2\} = \{x^3 - x^2 + y^2, x - 2\}$, then $V(F) \subset \mathbb{A}^2(\mathbb{C})$ is the set of points where both f_1 and f_2 vanish. We substitute $x = 2$ in f_1 to get $y = \pm 2i$. So,

$$V(f_1, f_2) = \{(2, 2i), (2, -2i)\}.$$

From the definition above, we have two inclusion-reversing properties of vanishing ideals and varieties.

i) If S_1 and S_2 are two collection of points in $\mathbb{A}^n(\mathbb{K})$ with $S_1 \subset S_2$, then $I(S_2) \subset I(S_1)$.
ii) If F_1 and F_2 are two collection of polynomials in $\mathbb{K}[x_1, \ldots, x_n]$ with $F_1 \subset F_2$, then $V(F_2) \subset V(F_1)$.

It can be shown that the variety defined by a collection of polynomials only depends on the ideal they generate. Hence, we have the following proposition :

Proposition 1.3.14 (Proposition 3.8, [15]). *Let F be a collection of polynomials in $\mathbb{K}[x_1, \ldots, x_n]$. If I is the ideal generated by the polynomials in F, i.e, $I = \langle f : f \in F \rangle$, then $V(F) = V(I)$.*

From the definition, it follows that for any ideal $I \subset \mathbb{K}[x_1, \ldots, x_n]$,

$$I \subset I(V(I)).$$

But the equality depends on the field $\mathbb{K}$ and the properties of $V(I)$. We come back to this in Section 1.3.4 where we give a precise description of $I(V(I))$ in terms of I when $\mathbb{K}$ is algebraically closed.

1.3.3 Morphims and rational maps

A *morphism* ϕ of affine spaces is a map given by the rule

$$\begin{aligned} \phi \quad &: \quad \mathbb{A}^n(\mathbb{K}) \to \mathbb{A}^m(\mathbb{K}) \\ \phi(x_1, \ldots, x_n) \quad &= \quad (\phi_1(x_1, \ldots, x_n), \ldots, \phi_m(x_1, \ldots, x_n)), \end{aligned}$$

with each $\phi_i \in \mathbb{K}[x_1, \ldots, x_n]$. Now, for any $f \in \mathbb{K}[y_1, \ldots, y_m]$, the *pull-back* map of ϕ is defined as

$$\phi^* f = f \circ \phi = f(\phi_1(x_1, \ldots, x_n), \ldots, \phi_m(x_1, \ldots, x_n)).$$

This gives us a ring homomorphism

$$\begin{aligned} \phi^* : \mathbb{K}[y_1, \ldots, y_m] \quad &\to \quad \mathbb{K}[x_1, \ldots, x_n] \\ y_j \quad &\mapsto \quad \phi_j(x_1, \ldots, x_n), \end{aligned}$$

with the property that $\phi^*(c) = c$ for each constant $c \in \mathbb{K}$ (also called a $\mathbb{K}$-*algebra homomorphism*). Let $V \subset \mathbb{A}^n(\mathbb{K})$ be any subset with vanishing ideal $I(V)$. If we restrict polynomial functions on $\mathbb{A}^n(\mathbb{K})$ to V, then the elements of $I(V)$ are zero along V and hence can be identified with the quotient ring $\mathbb{K}[x_1, \ldots, x_n]/I(V)$ (also called the *coordinate ring*).

Example 1.3.15. Let $V = \{(x, y) : x^2 + y^2 = 1\} \subset \mathbb{A}^2(\mathbb{R})$ be the locus of the unit circle.

Then $I(V) = \langle x^2 + y^2 - 1 \rangle$ and hence the polynomials x^2 and $1 - y^2$ define the same function on the circle as

$$x^2 \equiv 1 - y^2 \bmod I(V).$$

Definition 1.3.16. Let $\mathbb{K}(x_1, \ldots, x_n)$ denote the fraction field of $\mathbb{K}[x_1, \ldots, x_n]$ which consists of quotients of the form f/g where $f, g \in \mathbb{K}[x_1, \ldots, x_n]$ and $g \neq 0$. Then a *rational map* $\rho : \mathbb{A}^n(\mathbb{K}) \dashrightarrow \mathbb{A}^m(\mathbb{K})$ is defined as

$$\rho(x_1, \ldots, x_n) = (\rho_1(x_1, \ldots, x_n), \ldots, \rho_m(x_1, \ldots, x_n)), \quad \rho_j \in \mathbb{K}(x_1, \ldots, x_n).$$

The rational map is represented by a dashed arrow as it is not a well-defined function from $\mathbb{A}^n(\mathbb{K})$ to $\mathbb{A}^m(\mathbb{K})$. Each component ρ_j is represented as a fraction f_j/g_j where $f_j, g_j \in \mathbb{K}[x_1, \ldots, x_n]$ and we assume that f_j and g_j do not have any common irreducible factors. Every rational map also induces a $\mathbb{K}$-algebra homomorphism

$$\begin{aligned} \rho^* : \mathbb{K}[y_1, \ldots, y_m] &\to \mathbb{K}(x_1, \ldots, x_n), \\ y_j &\mapsto \rho_j(x_1, \ldots, x_n). \end{aligned}$$

If $W \subset \mathbb{A}^m(\mathbb{K})$ is a variety, then a rational map $\rho : \mathbb{A}^n(\mathbb{K}) \dashrightarrow W$ is a rational map $\rho : \mathbb{A}^n(\mathbb{K}) \dashrightarrow \mathbb{A}^m(\mathbb{K})$ with $\rho^* I(W) = 0$. We illustrate this with an example.

Example 1.3.17. Let

$$\begin{aligned} W = \quad & \{(\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{22}, \sigma_{23}, \sigma_{33}) : \sigma_{11} = k_{22}k_{33} - k_{23}^2, \sigma_{12} = k_{12}k_{33}, \\ & \sigma_{13} = k_{12}k_{23}, \sigma_{22} = k_{11}k_{33}, \sigma_{23} = k_{11}k_{23}, \sigma_{33} = k_{11}k_{22} - k_{12}^2 : k_{ij} \in \mathbb{R}\}. \end{aligned}$$

The rational map ρ can be written as

$$\begin{aligned} \rho : \mathbb{A}^5 \quad &\dashrightarrow \quad W \\ \rho(K) \quad &= \quad (\rho_{11}(K), \rho_{12}(K), \rho_{13}(K), \rho_{22}(K), \rho_{23}(K), \rho_{33}(K)), \end{aligned}$$

where $K = (k_{11}, k_{12}, k_{22}, k_{23}, k_{33}) \subseteq \mathbb{A}^5$. Now, ρ^* is the map given by

$$\rho^*(p(\sigma_{11}, \ldots, \sigma_{33})) = p(k_{22}k_{33} - k_{23}^2, k_{12}k_{33}, \ldots, k_{11}k_{22} - k_{12}^2),$$

where $p(\sigma_{11}, \ldots, \sigma_{33})$ is any polynomial in variables $\sigma_{11}, \ldots, \sigma_{33}$. The ideal $I(W)$ is generated by $\langle \sigma_{12}\sigma_{23} - \sigma_{13}\sigma_{22} \rangle$. So, computing $\rho^* I(W)$ gives us

$$\rho^*(\sigma_{12}\sigma_{23} - \sigma_{13}\sigma_{22}) = (k_{12}k_{33})(k_{11}k_{23}) - (k_{12}k_{23})(k_{11}k_{33}) = 0.$$

We use a rational map ρ and its pullback ρ^* in Chapter 3 to express the vanishing ideal of the Gaussian graphical model as the kernel of ρ^*. We further use the pullback map as a motivation to construct a new monomial map which is used to prove the main results in Chapter 3.

1.3.4 More concepts on algebraic geometry

In this section we look at the definition of quotient ideal, saturation and some related concepts. We also state some known results based on these concepts which will be mainly used in Section 3.6 of Chapter 3 for formulating a way to write the vanishing ideal of an undirected graph in terms of smaller subgraphs.

Definition 1.3.18. Let $I \subset \mathbb{K}[x_1, \ldots, x_n]$ be any ideal. Then the *radical* of I is defined as

$$\sqrt{I} := \{g \in \mathbb{K}[x_1, \ldots, x_n] : g^N \in I \text{ for some } N \in \mathbb{N}\}.$$

It can be shown that the radical of any ideal is also an ideal. If $\mathbb{K}$ is algebraically closed, we have the following result :

Theorem 1.3.19 (Hilbert Nullstellensatz)**.** *If $\mathbb{K}$ is algebraically closed and $I \subset \mathbb{K}[x_1, \ldots, x_n]$ is an ideal then $I(V(I)) = \sqrt{I}$.*

Example 1.3.20. Let $I = \langle x^2 + y^2 + 1 \rangle$ be an ideal in $\mathbb{R}[x, y]$. Then $V(I) = \emptyset$ as there are no real solutions to $x^2 + y^2 = -1$. This implies that $I(V(I)) = \mathbb{R}[x, y]$. But as $1 \notin I$, we have $\sqrt{I} \neq \mathbb{R}[x, y]$ and hence

$$\sqrt{I} \subsetneq I(V(I)).$$

We now state a Corollary to Hilbert Nullstellensatz which we use in proving one of the main results in Section 3.6.

Corollary 1.3.21. *Let I and J be two ideals in $\mathbb{K}[x_1, \ldots, x_n]$. If $\mathbb{K}$ is algebraically closed and $V(I) = V(J)$, then I and J are equal up to radicals, i.e, $\sqrt{I} = \sqrt{J}$.*

The *Zariski closure* of a subset $S \subset \mathbb{A}^n(\mathbb{K})$ is defined as

$$\overline{S} = \{a \in \mathbb{A}^n(\mathbb{K}) : f(a) = 0 \text{ for each } f \in I(S)\} = V(I(S)).$$

A subset $S \subset \mathbb{A}^n(\mathbb{K})$ is *closed* if $S = \overline{S}$ and is *open* if its compliment is closed.

Definition 1.3.22. For any two ideals $I, J \subset \mathbb{K}[x_1, \ldots, x_n]$, the *quotient ideal* is defined as

$$I : J = \{f \in \mathbb{K}[x_1, \ldots, x_n] : fg \in I \text{ for each } g \in J\}.$$

A quotient ideal satisfies the following properties which we use in the later chapters :

i) $I : J \subset I(V(I) \setminus V(J))$;
ii) $V(I : J) \supset \overline{V(I) \setminus V(J)}$;
iii) $I(V) : I(W) = I(V \setminus W)$.

A nonzero polynomial $f = \Sigma_{\alpha_1,\ldots,\alpha_n} c_{\alpha_1,\ldots,\alpha_n} x_1^{\alpha_1} \ldots x_n^{\alpha_n}$ of degree d is said to be *homogeneous* if $c_{\alpha_1,\ldots,\alpha_n} = 0$ when $c_{\alpha_1\ldots\alpha_n} = 0$ whenever $\alpha_1 + \cdots + \alpha_n < d$. An ideal $I \subset \mathbb{K}[x_1, \ldots, x_n]$ is homogeneous if it has a generating set of homogeneous polynomials.

Definition 1.3.23. For any given variable x_i, *dehomogenization* with respect to x_i is defined as the homomorphism

$$\begin{aligned} \mu_i : \mathbb{K}[x_1, \ldots, x_n] &\rightarrow \mathbb{K}[y_0, \ldots, y_{i-1}, y_{i+1}, \ldots, y_n] \\ x_i &\rightarrow 1 \\ x_j &\rightarrow y_j, j \neq 1. \end{aligned}$$

Similarly, for any $f \in \mathbb{K}[y_0, \ldots, y_{i-1}, y_{i+1}, \ldots, y_n]$, the *homogenization* of f with respect to x_i is defined as

$$F(x_0, \ldots, x_n) := x_i^{deg(f)} f(x_0/x_i, \ldots, x_{i-1}/x_i, x_{i+1}/x_i, \ldots, x_n/x_i).$$

The homogenization of an ideal $I \subset \mathbb{K}[y_0, \ldots, y_{i-1}, y_{i+1}, \ldots, y_n]$ is defined as the ideal generated by the homogenizations of each $f \in I$.

For a given ideal $I = \langle f_1, \ldots, f_r \rangle$, the homogenization J is not necessarily generated by the homogenizations of f_is. We illustrate this with an example.

Example 1.3.24. Let

$$I = \langle y_2 - y_1^2, y_3 - y_1 y_2 \rangle = \langle f_1, f_2 \rangle$$

be an ideal in $\mathbb{K}[y_1, y_2, y_3]$ and let J be its homogenization. The homogenization of f_1 and f_2 gives us the ideal

$$\langle x_2 x_0 - x_1^2, x_3 x_0 - x_1 x_2 \rangle \subsetneq J.$$

If we consider the polynomial $h = x_2^2 - x_1 x_3$, then $h \in J$ as h is the homogenization of $y_2^2 - y_1 y_3$ with respect to x_0 and $y_2^2 - y_1 y_3 = y_2 f_1 - y_1 f_2 \in I$. But h is not contained in the ideal generated by the homogenizations of f_1 and f_2.

Theorem 1.3.25 (Theorem 9.6, [15])**.** *Let $I \subset \mathbb{K}[y_1, \ldots, y_n]$ be an ideal and $J \subset \mathbb{K}[x_0, \ldots, x_n]$ its homogenization with respect to x_0. Suppose that $f_1, \ldots, f_r$ is a Gröbner basis for I with respect to some graded order $>$. Then the homogenizations $F_1, \ldots, F_r$ of $f_1, \ldots, f_r$ generate J.*

Definition 1.3.26. For any two ideals $I, J \subset \mathbb{K}[x_1, \ldots, x_n]$, the *saturation* of I with respect to J is defined as the set of elements $f \in \mathbb{K}[x_1, \ldots, x_n]$ such that $J^N \cdot f$ is contained in I for some large value of N. The saturation forms an ideal and is denoted by $(I : J^\infty)$. For any variable x_i, the saturation of I with respect to x_i is given by $(I : x_i^\infty) = \{f \in \mathbb{K}[x_1, \ldots, x_n] : x_i^n f \in I \text{ for some } n \in \mathbb{N}\}$.

Example 1.3.27. Let $I = \langle x_1^3 - x_2 x_4^2, x_1^4 - x_3 x_4^3 \rangle$ be an ideal in $\mathbb{K}[x_1, x_2, x_3, x_4]$. Then saturating I with respect to x_4 gives us

$$(I : x_4^\infty) = \langle x_1 x_2 - x_3 x_4, x_1^2 x_3 - x_2^2 x_4, x_2^3 - x_1 x_3^2, x_1^3 - x_2 x_4^2 \rangle.$$

Now, if we want to introduce the inverse of any variable say x_1, in the ideal $I \subset \mathbb{K}[x_1, \ldots, x_n]$, then it same as adding a new generator of the form $z x_1 - 1$ and intersecting the new ideal with $\mathbb{K}[x_1, \ldots, x_n]$. We have the following lemma in which we write the new ideal in terms of saturation.

Lemma 1.3.28. *Let I be any ideal in $\mathbb{K}[x_1, \ldots, x_n]$. Then*

$$I + \langle zx_1 - 1\rangle \cap \mathbb{K}[x_1, \ldots, x_n] = (I : x_1^\infty).$$

Proof. Let r be any arbitrary element in $(I : x_1^\infty)$. Then $r \cdot x_1^n \in I$ for some $n \in \mathbb{N}$. This implies that $r \cdot x_1^n \cdot z^n \in I + \langle zx_1 - 1\rangle \subset \mathbb{K}[x_1, \ldots, x_n, z]$. But as $z \cdot x_1 = 1$, $r \in I + \langle zx_1 - 1\rangle \cap \mathbb{K}[x_1, \ldots, x_n]$.

Conversely, if $r \in I + \langle zx_1 - 1\rangle$, then

$$r = g_1(x_1, \ldots, x_n, z) \cdot h(x_1, \ldots, x_n) + g_2(x_1, \ldots, x_n, z) \cdot (zx_1 - 1) \in \mathbb{K}[x_1, \ldots, x_n, z],$$

where $g_1(x_1, \ldots, x_n, z), g_2(x_1, \ldots, x_n, z) \in \mathbb{K}[x_1, \ldots, x_n, z]$ and $h(x_1, \ldots, x_n) \in I$. Substituting $z = 1/x_1$, we get

$$r = \left(g_{11}(x_1, \ldots, x_n) + g_{12}(x_1, \ldots, x_n) \cdot \frac{1}{x_1} + \cdots + g_{1n}(x_1, \ldots, x_n) \cdot \frac{1}{x_1^n}\right) \cdot h(x_1, \ldots, x_n) + 0,$$

where $g_1(x_1, \ldots, x_n, z) = g_{11}(x_1, \ldots, x_n) + g_{12}(x_1, \ldots, x_n) \cdot z + ... + g_{1n}(x_1, \ldots, x_n) \cdot z^n$. This implies that

$$r \cdot x_1^n = (g_{11}(x_1, \ldots, x_n) \cdot x_1^n + g_{12}(x_1, \ldots, x_n) \cdot x_1^{n-1} + \cdots + g_{1n}(x_1, \ldots, x_n)) \cdot h(x_1, \ldots, x_n) \in I,$$

i.e $r \in (I : x_1^\infty)$. □

1.4 Toric ideals and SAGBI bases

In this section, we talk about toric ideals and the properties satisfied by these ideals. The results stated here are specifically used in Chapter 3 and 4 where we characterize the graphical models having toric vanishing ideals. More details on this topic can be found in [31].

1.4.1 Toric ideals

Definition 1.4.1. Let $\mathcal{A} = \{a_1, a_2, ..., a_n\}$ be a fixed subset of $\mathbb{Z}^d$. We consider the homomorphism

$$\pi : \mathbb{N}^n \to \mathbb{Z}^d, \qquad u = (u_1, ..., u_n) \mapsto u_1 a_1 + ... + u_n a_n.$$

This map π lifts to a homomorphism of subgroup algebras:

$$\hat{\pi} : \mathbb{R}[x_1, ..., x_n] \to \mathbb{R}[t_1, ..., t_d, t_1^{-1}, ..., t_d^{-1}], \qquad x_i \mapsto t^{a_i}.$$

The kernel of $\hat{\pi}$ is called the *toric ideal* of $\mathcal{A}$ and is denoted by $I_{\mathcal{A}}$.

Let u^+ be the vector which has the same positive entries as u and zero elsewhere, i.e,

$$u_i^+ = \begin{cases} u_i & u_i \geq 0 \\ 0 & u_i < 0. \end{cases}$$

Similarly, we define u^- as

$$u_i^- = \begin{cases} -u_i & u_i \leq 0 \\ 0 & u_i > 0. \end{cases}$$

So, we can write $u = u^+ - u^-$. Now, the following lemma gives us the structure of a generating set of any toric ideal.

Lemma 1.4.2 (Corollary 4.3, [31])**.** *The toric ideal $I_{\mathcal{A}}$ can be generated by the set of binomials of the form $x^{u^+} - x^{u^-}$ where $u \in \ker(\pi)$, i.e,*

$$I_{\mathcal{A}} = \langle x^{u^+} - x^{u^-} : u \in \mathbb{N}^n \text{ with } \pi(u) = 0 \rangle.$$

From the construction above we observe that any monomial map can be written as $\hat{\pi}$ for some given set of vectors $\mathcal{A}$. This gives us that the kernel of every monomial map is a toric ideal. We illustrate the construction of toric ideals with an example.

Example 1.4.3. Let

$$\mathcal{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

be a 8×10 matrix where $\{a_1, \ldots, a_{10}\}$ are the columns of $\mathcal{A}$. Computing the toric ideal $I_{\mathcal{A}}$ gives us that

$$I_{\mathcal{A}} = \langle x_{24}x_{33} - x_{23}x_{34}, x_{14}x_{33} - x_{13}x_{34}, x_{14}x_{23} - x_{13}x_{24} \rangle.$$

Observe that $x_{24}x_{33} - x_{23}x_{34}$ can be written as $x^{u_1^+} - x^{u_1^-}$ where

$$u_1 = (0, 0, 0, 0, 0, -1, 1, 1, -1, 0) \in \ker(\pi) = \ker(\mathcal{A}).$$

Similarly,

$$\begin{aligned} x_{14}x_{33} - x_{13}x_{34} &= x^{u_2^+} - x^{u_2^-}, \text{ where } u_2 = (0, 0, -1, 1, 0, 0, 0, 1, -1, 0) \text{ and} \\ x_{14}x_{23} - x_{13}x_{24} &= x^{u_3^+} - x^{u_3^-}, \text{ where } u_3 = (0, 0, -1, 1, 0, 1, -1, 0, 0, 0), \end{aligned}$$

where both $u_2, u_3 \in \ker(\mathcal{A})$.

If each a_i is assumed to be nonzero and non-negative, then the set $\pi^{-1}(b) = \{u \in \mathbb{N}^n : \pi(u) = b\}$ is finite for any $b \in \mathbb{N}^d$. The set $\pi^{-1}(b)$ is called the *fiber* of $\mathcal{A}$ over b. Now, let $\mathcal{F}$ be any finite subset of $\ker(\pi)$. Then the *fiber graph* of $\pi^{-1}(b)_{\mathcal{F}}$ is defined as follows : The nodes of this graph are the elements of $\pi^{-1}(b)$ and any two nodes are connected by an edge if $u - u' \in \mathcal{F}$ or $u' - u \in \mathcal{F}$. The following theorem gives a relation between the connectivity of fiber graphs and the generating set of $I_{\mathcal{A}}$.

Theorem 1.4.4 (Theorem 5.3, [31])**.** *Let $\mathcal{F} \subset \ker(\pi)$. The graphs $\pi^{-1}(b)_{\mathcal{F}}$ are connected for all $b \in \mathbb{N}\mathcal{A}$ if and only if the set $\{x^{v^+} - x^{v^-} : v \in \mathcal{F}\}$ generates the toric ideal $I_{\mathcal{A}}$.*

Let $\mathcal{A}_d = \{e_i + e_j : 1 \leq i < j \leq d\}$, where e_i are the standard basis vectors of $\mathbb{R}^d$. This can be considered as the column vectors of the vertex-edge incidence matrix of the complete graph K_d. The toric ideal $I_{\mathcal{A}_d}$ obtained from this matrix can be written as the kernel of the map

$$\Phi : \mathbb{K}[x_{ij} : 1 \leq i < j \leq d] \to \mathbb{K}[t_1, \ldots, t_d], \quad x_{ij} \mapsto t_i t_j.$$

The variables x_{ij} here correspond to the edges of the complete graph K_d. The vertices of K_d are identified with the vertices of a regular d-gon in the plane labelled clockwise from 1 to d. So, there are two paths between any two vertices of K_d which only use the edges of of the d-gon. The *circular distance* between any two vertices is defined as the length of the shorter path.

The term *edge* is used to denote the closed line segment joining any two vertices in the d-gon. The *weight* of the variable x_{ij} is defined as the number of edges of K_d which do not meet the edge (i, j). Let $\prec$ be any term order that refines the partial order on monomials specified by these weights. So for any given pair of non-intersecting edges $(i, j), (k, l)$ of K_d, one of two pairs $(i, k), (j, l)$ or $(i, l), (j, k)$ meet at a point. If $(i, l), (j, k)$ is the intersecting pair, then we associate the binomial $x_{ij}x_{kl} - x_{il}x_{jk}$ with the pair $(i, j), (k, l)$. Let $\mathcal{C}$ is the set of all such binomials obtained in this way. We show later in Chapter **??** that for each binomial $x_{ij}x_{kl} - x_{il}x_{jk}$ in $\mathcal{C}$, the initial term with respect to $\prec$ corresponds to the disjoint edges. We thus have the following theorem :

Theorem 1.4.5 (Theorem 2.1, [6])**.** *The set $\mathcal{C}$ is the reduced Gröbner basis of $I_{\mathcal{A}_d}$ with respect to $\prec$.*

1.4.2 SAGBI bases

In this section we look at the Subalgebra Analogue to Gröbner Bases for Ideals (commonly known as the SAGBI bases) and its connection with the toric ideals.

Definition 1.4.6. Let $\mathcal{R}$ be a finitely generated subalgebra of the polynomial ring $\mathbb{K}[t_1, \ldots, t_d]$. For a fixed term order $\prec$ on $\mathbb{K}[t_1, \ldots, t_d]$, the *initial algebra* $in_\prec(\mathcal{R})$ is the $\mathbb{K}$-vector space spanned by $\{in_\prec(f) : f \in \mathcal{R}\}$. A subset $\mathcal{C}$ of $\mathcal{R}$ is called a *SAGBI basis* if $in_\prec(\mathcal{R})$ is generated as a $\mathbb{K}$-algebra by the set of monomials $\{in_\prec(f) : f \in \mathcal{C}\}$.

The main difference between Gröbner bases for ideals and SAGBI bases for subalgebras is that the initial algebra $in_\prec(\mathcal{R})$ is not always finitely generated. If $in_\prec(\mathcal{R})$ is not finitely generated, then there is no SAGBI basis for $\mathcal{R}$ with respect to $\prec$. So, in this section we only consider the case where $in_{\prec}(\mathcal{R})$ is finitely generated.

We fix a set of polynomials $\mathcal{F} = \{f_1, \ldots, f_n\}$ in $\mathbb{K}[t_1, \ldots, t_d]$ and let $\mathcal{R} = \mathbb{K}[\mathcal{F}]$ be the subalgebra that they generate. Then for a fixed term order $\prec$ on $\mathbb{K}[t_1, \ldots, t_d]$, we are interested in finding a criterion for deciding if $\mathcal{F}$ forms a SAGBI basis for $\mathcal{R}$ with respect to $\prec$. Now, let $in_{\prec}(f_i) = t^{a_i}$ and $\mathcal{A} = \{a_1, \ldots, a_n\} \subset \mathbb{N}^d$. We introduce a new polynomial ring $\mathbb{K}[x_1, \ldots, x_n]$ and consider the epimorphism from $\mathbb{K}[x_1, \ldots, x_n]$ onto $\mathcal{R}$ which maps x_i to f_i for each $i = 1, \ldots, n$. We denote I to be the kernel of this map. Similarly, we consider another map from $\mathbb{K}[x_1, \ldots, x_n]$ onto $in_{\prec}(\mathcal{R})$ defined by $x_i \mapsto in_{\prec}(f_i) = t^{a_i}$. The kernel of this map is the toric ideal $I_{\mathcal{A}}$.

We select a weight vector $\omega \in \mathbb{R}^d$ which represents the term order $\prec$ for the polynomials in $\mathcal{F}$. If $\mathcal{A}$ is a $d \times n$ matrix, then $\mathcal{A}^T\omega$ is a vector in $\mathbb{R}^n$ which can be used as the weight vector for forming an initial ideal of $I \subset \mathbb{K}[x_1, \ldots, x_n]$. The following theorem gives us the required criterion for SAGBI basis :

Theorem 1.4.7 (Theorem 11.4, [31])**.** *The set $\mathcal{F} \subset \mathbb{K}[t_1, \ldots, t_d]$ is a SAGBI basis if and only if $in_{\mathcal{A}^T\omega}(I) = I_{\mathcal{A}}$.*

Example 1.4.8. Consider two polynomial rings $\mathbb{R}[x_{11}, x_{12}, ..., x_{44}]$ and $\mathbb{R}[k_{11}, k_{12}, ..., k_{44}]$. Let K be the matrix

$$\begin{bmatrix} k_{11} & k_{12} & k_{13} & 0 \\ k_{12} & k_{22} & k_{23} & 0 \\ k_{13} & k_{23} & k_{33} & k_{33} \\ 0 & 0 & k_{34} & k_{44} \end{bmatrix}$$

and $\mathcal{F} = \{f_{11}, f_{12}, ..., f_{44}\}$ where each f_{ij} is defined as

$$\begin{aligned}
f_{11} &= k_{22}k_{33}k_{44} - k_{22}k_{34}^2 - k_{23}^2k_{44} \\
f_{22} &= k_{11}k_{33}k_{44} - k_{11}k_{34}^2 - k_{13}^2k_{44} \\
f_{33} &= k_{11}k_{22}k_{44} - k_{44}k_{12}^2 \\
f_{44} &= k_{11}k_{22}k_{33} - k_{11}k_{23}^2 - k_{12}^2k_{33} \\
&\quad + k_{12}k_{13}k_{23} + k_{13}k_{12}k_{23} - k_{13}^2k_{22} \\
f_{12} &= k_{k12}k_{33}k_{44} - k_{12}k_{34}^2 - k_{23}k_{13}k_{44}
\end{aligned}
\qquad
\begin{aligned}
f_{13} &= -k_{13}k_{22}k_{44} + k_{12}k_{23}k_{44} \\
f_{14} &= -k_{13}k_{34}k_{22} + k_{12}k_{23}k_{34} \\
f_{23} &= k_{23}k_{11}k_{44} - k_{12}k_{13}k_{44} \\
f_{24} &= k_{23}k_{34}k_{11} - k_{34}k_{13}k_{12} \\
f_{34} &= k_{34}k_{11}k_{22} - k_{34}k_{12}^2
\end{aligned}$$

These f_{ij}s are obtained from the map $\mathbb{R}[x_{11}, x_{12}, ..., x_{44}] \mapsto \mathbb{R}[k_{11}, k_{12}, ..., k_{44}]$ which takes each x_{ij} to $det(K) \cdot ((ij)^{th}$ entry of $K^{-1})$. We fix the partial term order on $\mathbb{R}[k_{11}, k_{12}, ..., k_{44}]$

by defining the degree of a monomial as the number of diagonal elements k_{ii} in that monomial. Then the initial term of each f_{ij} is as follows:

$$
\begin{aligned}
&in_{\prec}(f_{11}) = k_{22}k_{33}k_{44}, && in_{\prec}(f_{12}) = k_{12}k_{33}k_{44}, && in_{\prec}(f_{13}) = k_{13}k_{22}k_{44},\\
&in_{\prec}(f_{14}) = k_{13}k_{34}k_{22}, && in_{\prec}(f_{22}) = k_{11}k_{33}k_{44}, && in_{\prec}(f_{23}) = k_{23}k_{11}k_{44},\\
&in_{\prec}(f_{24}) = k_{23}k_{34}k_{11}, && in_{\prec}(f_{33}) = k_{11}k_{22}k_{44}, && in_{\prec}(f_{34}) = k_{34}k_{11}k_{22},\\
& && in_{\prec}(f_{44}) = k_{11}k_{22}k_{33} &&
\end{aligned}
$$

Denoting the initial terms $in_{\prec}(f_{ij})$ as $k^{a_{ij}}$ where each a_{ij} are vectors in $\mathbb{N}^{10}$, we get the 8×10 matrix $\mathcal{A}$ as

$$
\mathcal{A} = \begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1\\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1\\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0\\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1\\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0\\
1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0
\end{bmatrix}
$$

The weight vector $\omega \in \mathbb{R}^8$ represents the term order $\prec$ for the polynomials in $\mathcal{F}$. In this case,

$$\omega = (1, 0, 0, 1, 0, 1, 0, 1).$$

So,

$$
\mathcal{A}^T\omega = \begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1\\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1\\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0\\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1\\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0\\
1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0
\end{bmatrix}^T
\begin{bmatrix} 1\\0\\0\\1\\0\\1\\0\\1 \end{bmatrix}
= \begin{bmatrix} 3\\2\\2\\1\\3\\2\\1\\3\\2\\3 \end{bmatrix}
$$

Computing the kernel of the map which takes each x_{ij} to f_{ij}, we get

$$I = \langle x_{24}x_{33} - x_{23}x_{34}, x_{14}x_{33} - x_{13}x_{34}, x_{14}x_{23} - x_{13}x_{24} \rangle.$$

Similarly, computing the toric ideal $I_{\mathcal{A}}$ gives us that $I_{\mathcal{A}} = I$. Now, if we compute the degree of each monomial in the generators of I using our new partial term order defined by $\mathcal{A}^T\omega$, we get

$$\begin{aligned}
d(\sigma_{24}\sigma_{33}) &= (0,0,0,0,0,0,1,1,0,0).A^T\omega = 4,\\
d(\sigma_{23}\sigma_{34}) &= (0,0,0,0,0,1,0,0,1,0).A^T\omega = 4,\\
d(\sigma_{14}\sigma_{33}) &= (0,0,0,1,0,0,0,1,0,0).A^T\omega = 4,\\
d(\sigma_{13}\sigma_{34}) &= (0,0,1,0,0,0,0,0,1,0).A^T\omega = 4,\\
d(\sigma_{14}\sigma_{23}) &= (0,0,0,1,0,1,0,0,0,0).A^T\omega = 3,\\
d(\sigma_{13}\sigma_{24}) &= (0,0,1,0,0,0,1,0,0,0).A^T\omega = 3,
\end{aligned}$$

where $d(\sigma_{ij})$ denotes the degree of σ_{ij}. We observe that the initial term of each of the generators of I is the entire term itself and hence $in_{A^T\omega}(I) = I = I_{\mathcal{A}}$ in this case. Hence, by Theorem 1.4.7 we can conclude that $\mathcal{F}$ is a SAGBI basis for $\mathbb{R}[\mathcal{F}]$.

1.5 Outline of the thesis

Now that we have all the necessary background, we give an outline of the upcoming chapters.

1.5.1 Bounds on expected size of the maximum agreement subtree for a given tree shape

Chapter 2 is based on the problem of determining the expected size of *maximum agreement subtree* for a given tree shape. The content of this chapter was joint work with Seth Sullivant and it was published in *SIAM Journal of Discrete Mathematics* [24].

In phylogenetics, different tree reconstruction methods, and different datasets on the same set of species, can lead to the reconstruction of different trees. In such cases, it is important to measure the distance between different trees constructed. There are various distances between trees that are used including Robinson-Foulds distance, distances based on tree rearrangements, and the geodesic distance. This chapter focuses on the maximum agreement subtree as a measure of discrepancy between trees.

Let $\mathrm{MAST}(T_1, T_2)$ (defined in chapter-2) denote the number of leaves of a maximum agreement subtree of T_1 and T_2. We study the distribution of $\mathrm{MAST}(T_1, T_2)$ where T_1 and T_2 are trees that are uniformly sampled from all trees with the same shape. In other words, T_2 is obtained from T_1 by applying a random permutation of the leaf labels. We prove that $E[\mathrm{MAST}(T_1, T_2)] = \Theta(\sqrt{n})$ in this case. Our proof of the lower bound is based on a structural result about general trees where we decompose arbitrary trees into substructures we call *blobs*. The proof of the upper bound is based on a strengthening of the previously mentioned result of [3].

1.5.2 Undirected Gaussian graphical models with toric vanishing ideals

Chapter 3 is concerned with the problem of characterizing the undirected Gaussian graphical models having toric vanishing ideals. We mainly focus on proving the conjecture of Sturmfels and Uhler [32] on undirected Gaussian graphical models. The results in this part was joint work with Seth Sullivant and it will be published in *Annals of the Institute of Statistical Mathematics* [25].

Gaussian graphical models are used throughout the natural sciences and especially in computational biology as seen in [20; 21]. These models explicitly capture the statistical relationships between the variables of interest in the form of a graph. Sturmfels and Uhler [32] conjectured that the vanishing ideal P_G of an undirected Gaussian graphical model is generated in degree at most 2 if and only if each connected component of the graph G is a 1-clique sum of complete graphs. We prove the conjecture in this chapter by using the connection between the generating sets of toric ideals and connectivity properties of the fiber graphs. We also formulate a way to write the vanishing ideal of G in terms of smaller graphs G_1 and G_2 when G is a 1-clique sum of G_1 and G_2 where G_1 and G_2 are not necessarily complete.

1.5.3 Directed acyclic Gaussian graphical models with toric vanishing ideals

In Chapter 4, we try to get a similar characterization as in Chapter 3 for Gaussian graphical models represented by directed acyclic graphs. The main objective in this chapter is to construct DAGs having toric vanishing ideal and understand the generating set of the ideal. We develop three techniques to construct such DAGs from smaller DAGs. These are called safe gluing, gluing at sinks and adding a new sink.

We conjecture that if two DAGs have toric vanishing ideals, then any of the three operations would yield us a new DAG whose vanishing ideal is also toric. Further, we conjecture that every DAG whose vanishing ideal is toric can be obtained as a combination of these three operations on complete DAGs. We analyze an example and prove some other results which provide evidence to these conjectures.

Chapter 2

Bounds on the expected size of the maximum agreement subtree for a given tree shape

Rooted binary trees are used in evolutionary biology to represent the evolution of a set of species where the leaves denote the existing species and the internal nodes denote the unknown ancestors. Different tree reconstruction methods, and different datasets on the same set of species, can lead to the reconstruction of different trees. In such cases, it is important to measure the distance between different trees constructed. In this chapter, we focus on the *maximum agreement subtree* as a measure of discrepancy between trees.

If T is a rooted binary tree with n leaves leaf labeled by $[n] = \{1, 2, \ldots, n\}$ and S is a subset of $[n]$, then the *binary restriction tree* $T|_S$ is defined as the subtree of T obtained after deleting all the leaves that are not in S and suppressing the internal nodes of degree 2. The new tree $T|_S$ is rooted at the most recent common ancestor of the set S. If T_1 and T_2 are two trees leaf labeled by X, then a subset $S \subseteq X$ is said to be an agreement set of T_1 and T_2 if $T_1|_S = T_2|_S$. A *maximum agreement subtree* is a subtree that is obtained from an agreement set of T_1 and T_2 and is of maximal size. Figures 2.1 and 2.2 give an example of two trees and a maximum agreement subtree.

A maximum agreement subtree of a pair of binary trees can be computed in polynomial time in n [29]. Let $\mathrm{MAST}(T_1, T_2)$ denote the number of leaves of a maximum agreement subtree of T_1 and T_2. We know from [22] that if T_1 and T_2 are any unrooted binary trees with n leaves, then $\mathrm{MAST}(T_1, T_2) = \Omega(\sqrt{\log n})$. This contrasts with the

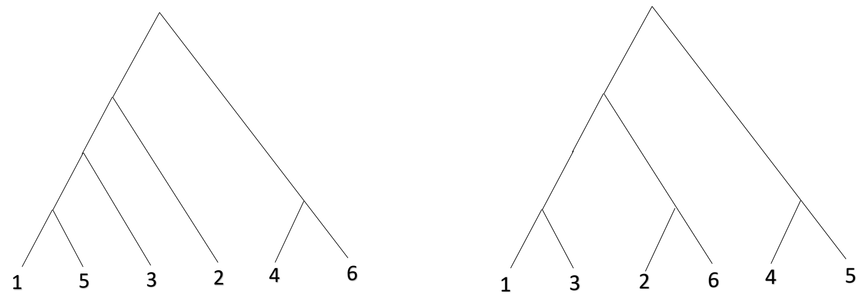


Figure 2.1: Two rooted trees T_1 and T_2

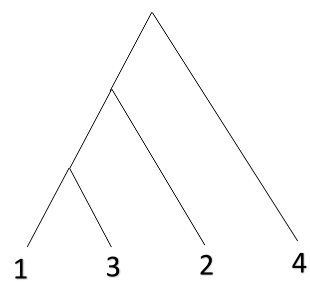


Figure 2.2: A maximum agreement subtree for T_1 and T_2

rooted case where there can be pairs of rooted trees where $\mathrm{MAST}(T_1, T_2) = 2$. For example, if we take T_1 and T_2 to be two comb trees with n leaves, then labeling the leaves of T_2 in the reverse order as that of T_1 gives us that $\mathrm{MAST}(T_1, T_2) = 2$. Martin and Thatte [22] also conjectured that if T_1 and T_2 are balanced rooted binary trees with n leaves, then $\mathrm{MAST}(T_1, T_2) \geq \sqrt{n}$. But in [4], Bordewich *et al.* disproved the conjecture by showing that for any $c > 0$, there exist two balanced rooted binary trees with n leaves such that any MAST for these two trees has size less than $c\sqrt{n}$.

For the purposes of hypothesis testing, it is important to understand the distribution of $\mathrm{MAST}(T_1, T_2)$ for trees generated from reasonable distributions of random trees. Simulations by Bryant, McKenzie, and Steel [5] suggest that under the uniform and Yule Harding distribution on the rooted binary trees with n leaves, the expected size of $\mathrm{MAST}(T_1, T_2)$ is of the order $\Theta(n^a)$ with $a \approx 1/2$. It is known that for any sampling consistent and exchangeable distribution on rooted binary trees with n leaves (including the uniform and Yule-Harding distributions), the expected size of the maximum agreement subtrees is less than $\lambda\sqrt{n}$ (for some constant $\lambda > e\sqrt{2}$) [3]. Lower bounds of order cn^α are also shown in [3] for the Yule-Harding and the uniform distribution. In [1], Aldous improved the lower bound of the expected size of the MAST to $n^{0.366}$ under the uniform distribution.

In this chapter, we study the distribution of $\mathrm{MAST}(T_1, T_2)$ where T_1 and T_2 are trees that are uniformly sampled from all trees with the same shape. In other words, T_2 is obtained from T_1 by applying a random permutation of the leaf labels. We prove that $\mathrm{E}[\mathrm{MAST}(T_1, T_2)] = \Theta(\sqrt{n})$ in this case, which provides some further evidence towards the problems posed in [5] for random trees. Our proof of the lower bound is based on a structural result about general trees where we decompose arbitrary trees into substructures we call *blobs*. The proof of the upper bound is based on a strengthening of the previously mentioned result of [3]. We also show results of simulations that suggest that our ideas based on blobs could be used to improve lower bounds on the expected value of $\mathrm{MAST}(T_1, T_2)$ for other distributions of random trees.

2.1 Lower bound: Blobification

In this section we derive a lower bound on the expected size of the maximum agreement subtree of two uniformly random trees on n leaves with same tree shape. We do this by dividing the trees into what we call as *blobs*, which helps us in constructing an agreement subtree between the two trees.

Let T be a rooted binary tree leaf-labeled by $[n]$. A *cherry blob* is a set of leaves in T consisting of all leaves below a vertex in the tree. Cherry blobs are also called clades in other phylogenetic contexts. An *edge blob* is a nonempty set of leaves of the form $C_1 \setminus C_2$ where C_1 and C_2 are two nonempty cherry blobs. A *blob* in T is either a cherry blob or an edge blob.

Definition 2.1.1. Given an integer k and a tree T, a *k-blobification* of T is a collection $\mathcal{B}$ of blobs of T such that, for all distinct blobs $B_1, B_2 \in \mathcal{B}$, $B_1 \cap B_2 = \emptyset$ and for all $B \in \mathcal{B}$, $k \leq |B| \leq 2k - 2$.

Definition 2.1.2. Let T be a binary tree, and $\mathcal{B}$ a k-blobification. Let S be a set of leaves consisting of one element from each of the blobs in $\mathcal{B}$. The *scaffold tree* of the blobification is the unlabelled tree T' obtained as the unlabelled version of the induced tree $T|_S$.

Let T be any rooted binary leaf-labeled tree with n leaves. We construct a k-blobification $\mathcal{B}$ of T using the following greedy procedure.

First, throw in as many cherry blobs into $\mathcal{B}$ as possible. Specifically, among all the cherry blobs C with $k \leq |C| \leq 2k-2$, we can take the set $\mathcal{C}$ to consist of all of those cherry blobs that are minimal, i.e., that do not contain any other cherry blobs that have between k and $2k-2$ leaves.

The set of cherry blobs $\mathcal{C}$, that we have constructed induces a labeled tree that we call the *prescaffold tree*. This tree has as leaves all the elements of $\mathcal{C}$, and can be obtained as an (unlabeled version of the) induced subtree $T|_S$ where S is any set of leaves that contain exactly one leaf from each of the cherry blobs in $\mathcal{C}$. If the root of $T|_S$ is not the root of T, then we also add an edge onto the prescaffold tree at the root. This is illustrated in Figure 2.4. Now we can think about the tree T as consisting of all the leaves grouped into blobs of various sizes, each of which attaches somewhere onto the prescaffold tree. The leaves that are not part of any of the cherry blobs will belong to blobs of size $k-1$ or less that connect onto the prescaffold tree.

On each edge of the prescaffold tree are some number of smaller blobs hanging off of size $k-1$ or less. Working up from the bottom edges of the prescaffold, we can group small blobs together until they produce an edge blob of size between k and $2k-2$. This is possible because each of the small blobs has size $< k$, so when we are grouping blobs together we have an edge blob with size $< k$ that we add $< k$ more elements to, we stop when we have formed an edge blob of size between k and $2k-2$. Let $\mathcal{E}$ be the resulting set of edge blobs that are produced, that all have size between k and $2k-2$. This *greedy k-blobification algorithm* stops with a blobification $\mathcal{B} = \mathcal{C} \cup \mathcal{E}$ where on each edge of the scaffold tree there are leftover small blobs whose total number of leftover leaves is at most $k-1$. The set $\mathcal{B} = \mathcal{C} \cup \mathcal{E}$ is called the *greedy k-blobification*.

Starting with the prescaffold tree T' and adding a leaf attached to an edge for each time an edge blob gets formed, we arrive at an unlabelled tree we call the scaffold tree.

Example 2.1.3. Consider the binary tree on 17 leaves pictured in Figure 2.3. We first consider the greedy 2-blobification. Note that the cherry blobs are exactly the cherries in this case. These are the sets $\{1,2\}, \{7,8\}, \{11,12\}, \{13,14\}$. The prescaffold tree is shown on the left of Figure 2.4. Note that there is an edge that hangs off the root. The edge blobs in this example are $\{3,4\}, \{5,6\}, \{15,16\}$. The resulting scaffold tree is the tree on the right in Figure 2.4. Note that leaves 9, 10, and 17 do not end up in any blob.

On the other hand, consider the greedy 3-blobification of the same tree. There are two cherry blobs, $\{1,2,3\}$ and $\{11,12,13,14\}$. The edge blobs are $\{4,5,6\}$, $\{7,8,9\}$, and

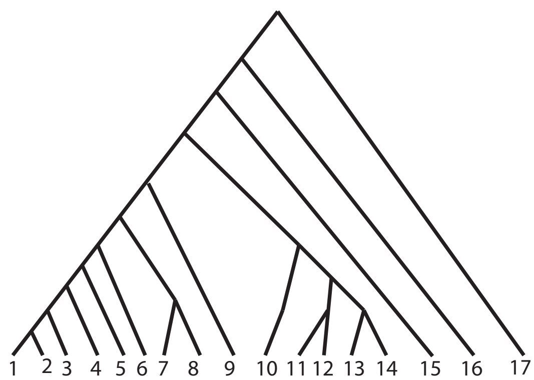


Figure 2.3: A tree

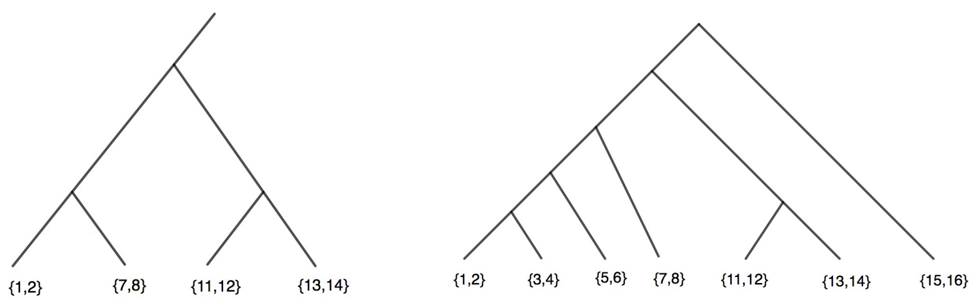


Figure 2.4: Prescaffold and scaffold tree for the 2-blobification (The labels indicate the cherry blobs on the prescaffold tree, and all blobs on the scaffold tree.)

$\{15, 16, 17\}$.

Proposition 2.1.4. *Let T be a rooted binary leaf-labeled tree with n leaves. Then for all $k \geq 2$, T has a k-blobification with at least $\frac{n}{4k}$ blobs.*

Proof. We apply the *k-blobification* algorithm on T. Let the final collection $\mathcal{B}$ of blobs contain a cherry blobs and b edge blobs. Since the prescaffold tree is a binary rooted tree with a leaves, there are at most $2a-1$ edges (potentially there is a root edge), each having at most $k-1$ leaves unassigned to any blob. Taking everything at its most extreme, we see that the total number of leaves, n is at most

$$n \leq (a+b)(2k-2) + (k-1)(2a-1) = (4a+2b-1)(k-1) \leq (4a+4b)k$$

where the first part comes from the contribution from each of the $a+b$ blobs, and the second term is the leftover leaves. The total number of blobs is $a+b$, which is greater than $n/4k$ from the above inequality. $\square$

Lemma 2.1.5. *Let S_1 and S_2 be uniformly random subsets of $[n]$, each of size at least $\sqrt{n}$. The probability that $S_1 \cap S_2 \neq \emptyset$ is at least $1-e^{-1}$.*

Proof. The probability that $S_1 \cap S_2 \neq \emptyset$ is clearly minimized when both S_1 and S_2 have $\sqrt{n}$ elements. In this case, the probability that $S_1 \cap S_2 = \emptyset$ is given by the formula

$$\begin{aligned} \frac{\binom{n-\sqrt{n}}{\sqrt{n}}}{\binom{n}{\sqrt{n}}} &= \prod_{i=1}^{\sqrt{n}} \left(1 - \frac{\sqrt{n}}{n-i+1}\right) \\ &\leq \left(1 - \frac{1}{\sqrt{n}}\right)^{\sqrt{n}} \\ &\leq e^{-1} \end{aligned}$$

This shows that the probability that $S_1 \cap S_2 \neq \emptyset$ is at least $1-e^{-1}$. $\square$

Theorem 2.1.6. *Let T_1 and T_2 be two uniformly random trees on n leaves among all trees with the same tree shape (i.e. T_2 is a random leaf relabeling of T_1). Then the expected size of* $\mathrm{MAST}(T_1, T_2)$ *is at least $\sqrt{n}(1-e^{-1})/4$.*

Proof. Consider the $\sqrt{n}$-blobification of T_1 and T_2, which we denote by $\mathcal{B}_1$ and $\mathcal{B}_2$. Since the trees have the same tree shape, this blobification has the same scaffold tree T'. We can order the blobs in $\mathcal{B}_1 = \{B_{11}, \ldots, B_{1s}\}$ and $\mathcal{B}_2 = \{B_{21}, \ldots, B_{2s}\}$ so that B_{1i} and B_{2i} correspond to the same leaf in the scaffold tree T'.

If for each i, we had that $B_{1i} \cap B_{2i} \neq \emptyset$, we could take one leaf $\ell_i \in B_{1i} \cap B_{2i}$, and let $S = \{\ell_1, \ldots, \ell_s\}$, we would have $T_1|_S = T_2|_S$ and this common agreement subtree would have the same shape as the scaffold tree T'.

Note that, since our trees are uniformly random among all trees with a given fixed shape, the probability that $B_{1i} \cap B_{2i} \neq \emptyset$ is at least $1-e^{-1}$ by Lemma 2.1.5, so that the expected number of i where $B_{1i} \cap B_{2i} \neq \emptyset$ is at least $s(1-e^{-1})$. This set of index positions gives an agreement subtree of expected size at least $s(1-e^{-1})$, which will be isomorphic to an induced subtree of the scaffold tree. Since $s \geq \sqrt{n}/4$ by Proposition 2.1.4 we see that the expected size of $\mathrm{MAST}(T_1, T_2)$ is at least $\sqrt{n}(1-e^{-1})/4$. $\square$

The same argument can be used to show that if T_1 and T_2 are uniformly random trees among all trees that have the same $\sqrt{n}$-blobification, the expected value of $\mathrm{MAST}(T_1, T_2)$ will also be at least $\sqrt{n}(1 - e^{-1})/4$.

2.2 Upper bound: Eliminating sampling consistency

In this section we generalize the result obtained from [3] that if T_1 and T_2 are generated from any sampling consistent and exchangeable distribution on rooted binary trees with n leaves, the expected size of the MAST is less than $\lambda\sqrt{n}$ (for some constant $\lambda > e\sqrt{2}$). We show that the result holds true even if we remove sampling consistency as one of the conditions. Since the distribution of random trees with the same shape is exchangeable, this will prove an $O(\sqrt{n})$ bound on the expected size of the maximum agreement subtree for uniformly random trees with the same shape.

Let $RB(n)$ denote the set of all rooted binary trees with n leaves. For a set S let $RB(S)$ denote the set of all rooted binary trees with leaf label set S.

Definition 2.2.1. A distribution on $RB(n)$ is said to be *exchangeable* if any two trees which differ only by a permutation of leaves have the same probability.

For each $n = 1, 2, \ldots$, we can consider a probability distribution P_n on $RB(n)$. We denote the probability of a tree $t \in RB(n)$ by $P_n[t]$. The notion of sampling consistency is concerned with a probability model for random trees that describes probability distributions for random trees for all n. For example, the uniform distribution on trees gives a probability distribution P_n for each n, where $P_n[t] = \frac{1}{(2n-3)!!}$ for all $t \in RB(n)$. The property of sampling consistency is one that concerns the entire family of probability distributions P_n, $n = 1, 2, \ldots$.

Definition 2.2.2. A distribution of random trees is said to satisfy *sampling consistency* if for all n, all $s < n$, all $S \subseteq [n]$ with $|S| = s$, and all $t \in RB(S)$,

$$P_s[t] = \sum_{T \in RB(n): T|_S = t} P_n[T].$$

In other words, in a sampling consistent distribution if we take a random tree T and restrict to any subset of the leaves, the resulting tree has the same distribution as if we had just chosen a random tree on that subset of leaves, directly. Our goal in this section is to remove the restriction of sampling consistency for the following theorem from [3].

Theorem 2.2.3. *Consider an exchangeable and sampling consistent distribution on rooted binary trees. Then for any $\lambda > e\sqrt{2}$ there is a value m such that, for all $n \geq m$,*

$$\mathrm{E}[\mathrm{MAST}(T_1, T_2)] \leq \lambda\sqrt{n}$$

where T_1, T_2 are sampled from this distribution.

Let P_n be an exchangeable distribution on $RB(n)$. Since we do not have a family of distributions P_s for $s < n$, we can not talk about sampling consistency. To prove an analogue of Theorem 2.2.3 without sampling consistency depends on defining some new probability distributions on $RB(s)$ for $s < n$. Specifically, for any $s < n$, and $t \in RB(s)$ we define

$$P_s[t] = \sum_{T \in RB(n): T|_{[s]} = t} P_n[T].$$

We can also use the notation $P_s[t] = P_n[T|_{[s]} = t]$ to denote this same probability.

Proposition 2.2.4. *Let P_n be an exchangeable distribution defined on $RB(n)$. Then for any $s < n$, P_s satisfies exchangeability property on $RB(s)$.*

Proof. Let t and t' be two trees in $RB(s)$ with same tree shape, and let $s < n$. By definition, $P_s[t] = P_n[T|_{[s]} = t]$ and $P_s[t'] = P_n[T|_{[s]} = t']$. We define a bijection $\phi : [s] \to [s]$ from $[s]$ to itself such that $\phi(t) = t'$ and extend the map $\phi : [n] \to [n]$ from $[n]$ to itself with $\phi(a) = a$, for all $a > s$. This map can also be seen as a bijection between $RB(s)$ to $RB(s)$ (similarly between $RB(n)$ to $RB(n)$) by acting on the leaf set of the trees.

So, for any two trees T, T' in $RB(n)$ with $T|_{[s]} = t$ and $T'|_{[s]} = t'$, we have

$$\phi(T)|_{[s]} = \phi(t) = t' \text{ and } \phi^{-1}(T')|_{\{1,2,\ldots,s\}} = \phi^{-1}(t') = t.$$

Hence $T|_{[s]} = t$ if and only if $\phi(T)|_{[s]} = t'$ since any bijection from $[n]$ to $[n]$ induces a bijection from $RB(n)$ to $RB(n)$ by acting on the leaves of the trees. Also, as T and $\phi(T)$ have the same tree shape and P_n is exchangeable, we have $P_n[T] = P_n[\phi(T)]$. Hence we can conclude that $P_s[t] = P_s[t']$. $\square$

Lemma 2.2.5. *Suppose that phylogenetic trees T_1 and T_2 in $RB(n)$ are randomly generated under a model that satisfies exchangeability. Then*

$$P[MAST(T_1,T_2) \geq s] \leq \psi_{n,s} = \binom{n}{s} \sum_{t \in RB(s)} P_s[t]^2,$$

where $P_s[t]$ is defined as $P_s[t] = P_n[T|_{[s]} = t]$ for $t \in RB(s)$.

Proof. This theorem can be proved exactly the way Lemma 4.1 of [5] is proved with the last equality following from the way we have defined $P_s[t]$ instead of using sampling consistency. The details are included here for completeness.

Given a subset S of $[n]$ let

$$X_S = \begin{cases} 1, & \text{if } T_1|_S = T_2|_S \\ 0, & \text{otherwise.} \end{cases}$$

The number of agreement subtrees with s leaves for T_1 and T_2 is counted by

$$X^{(s)} = \sum_{S \subseteq [n]:|S|=s} X_S.$$

The event $MAST(T_1,T_2) \geq s$ is equivalent to the event $X^{(s)} \geq 1$, so

$$\begin{aligned} P[MAST(T_1,T_2) \geq s] &= P[X^{(s)} \geq 1] \\ &\leq E[X^{(s)}] \\ &= \sum_{S \subseteq [n]:|S|=s} E[X_S] \\ &= \sum_{S \subseteq [n]:|S|=s} P[X_S = 1] \\ &= \binom{n}{s} P[X_{[s]} = 1], \end{aligned}$$

where the last equality is by exchangeability. Now,

$$\begin{aligned} P[X_{[s]} = 1] &= P_n[T_1|_{[s]} = T_2|_{[s]}] \\ &= \sum_{t \in RB(s)} P_n[T_1|_{[s]} = t \text{ and } T_2|_{[s]} = t] \\ &= \sum_{t \in RB(s)} P_n[T_1|_{[s]} = t]^2 \\ &= \sum_{t \in RB(s)} P_s[t]^2 \end{aligned}$$

where the last equality follows from the way we have defined $P_s[t]$. Upon substituting back for this term, we obtain the upper bound as stated in the lemma. □

We now state a proposition from [3].

Proposition 2.2.6 (Proposition 4.2, [3]). *Let P_s be any exchangeable distribution on rooted binary trees with s leaves. Then*

$$\sum_{t \in RB(s)} P_s(t)^2 \leq \frac{2^{s-1}}{s!}.$$

Now we can combine these results to deduce the strengthened version of Theorem 2.2.3 that does not require sampling consistency.

Theorem 2.2.7. *Then for any $\lambda > e\sqrt{2}$ there is a value m such that, for all $n \geq m$,*

$$\mathrm{E}[\mathrm{MAST}(T_1, T_2)] \leq \lambda\sqrt{n}.$$

where T_1 and T_2 are sampled from any exchangeable distribution on $RB(n)$.

Proof. This theorem can be proved exactly the way as Theorem 4.3 in [3] is proved as we have already shown that P_s is exchangeable by Proposition 2.2.4.

We explore the asymptotic behaviour of the quantity $\phi_{n,s} = \binom{n}{s}\frac{2^{s-1}}{s!}$. Using the inequality $\binom{n}{s} \leq \frac{n^s}{s!}$ and Stirling's approximation, we have:

$$\phi_{n,s} \leq \frac{1}{4\pi s}\left(\frac{2e^2 n}{s^2}\right)^s \theta(s)$$

where $\theta(s) \sim 1$. Hence, $\phi_{n,s}$ tends to zero as an exponenential function of n as $n \to \infty$. Since $\phi_{n,s} \geq \psi_{n,s}$, we see that $P[\mathrm{MAST}(T_1, T_2) \geq \lambda\sqrt{n}]$ tends to zero as an exponential function of n. Since $\mathrm{MAST}(T_1, T_2) \leq n$, this implies that $E[\mathrm{MAST}(T_1, T_2)] \leq \lambda\sqrt{n}$. □

Now we can deduce the main result for trees with the same shape.

Corollary 2.2.8. *Let T_1 and T_2 be generated from the uniform distribution on rooted binary trees with n leaves with same tree shape (that is, T_2 is a random leaf relabeling of T_1). Then for any $\lambda > e\sqrt{2}$ there is a value m such that, for all $n \geq m$,*

$$E[\mathrm{MAST}(T_1, T_2)] \leq \lambda\sqrt{n}.$$

Proof. This follows immediately from Theorem 2.2.7 since the uniform distribution on trees with the same shape is exchangeable. □

Combining Theorem 2.1.6 and Corollary 2.2.8 we deduce the main result of the chapter.

Theorem 2.2.9. *Let T_1 and T_2 be generated from the uniform distribution on rooted binary trees with n leaves with same tree shape (that is, T_2 is a random leaf relabeling of T_1). Then*

$$E[\mathrm{MAST}(T_1, T_2)] = \Theta(\sqrt{n}).$$

2.3 Simulations with blobification

The blobification idea has the potential to be useful for proving lower bounds on the expected size of the maximum agreement subtree in other contexts. For example, suppose we have a model for random trees on n leaves and we can show that the scaffold tree of the $\sqrt{n}$-blobification of a random tree has depth $\geq f(n)$ with high probability $p > 0$ that does not depend on n. Then under this model, using Lemma 2.1.5, we see that two random trees will have an agreement subtree of expected size at least $f(n)(1 - e^{-1})p^2$. Such a tree would be obtained as a comb tree by comparing blobs that are matched along the path from the root to the deepest leaf in each scaffold tree. Hence, understanding the distribution of the depth of the scaffold trees in the $\sqrt{n}$-blobification could give improved lower bounds on the expected size of the maximum agreement subtree in some random tree models.

One specific application where this perspective might prove useful is for uniformly randomly trees. The current best lower bound for the expected size of the maximum agreement subtree for two uniformly random trees on n leaves is $\Omega(n^{0.366})$ [1]. To see if this blobification idea might be useful for improving the lower bound, we simulated a lower bound for the depth of the scaffold tree of a uniformly random tree using the following greedy procedure.

Algorithm 2.3.1 (Greedy Comb Scaffold)**.**

Input: A binary tree T and an integer k.

Output: A scaffold tree in shape of a comb, whose leaves correspond to blobs of size $\geq k$.

- Set $u = ()$.
- While T has more than one leaf Do:
  - Let T_1 and T_2 be the left and right subtrees of the root in T.
  - Append $\min(\#(T_1), \#(T_2))$ to u.
  - Set T equal to the larger of T_1 and T_2.
- Set $v = (0)$.
- While $u \neq ()$ do
  - If the last element of v is greater than or equal to k, append the last element of u to v.
    - Else, add the last element of u to the last element of v.
  - Delete the last element of u.
- Output v, a vector of sizes of blobs in T, all except the last one having size $\geq k$, which have a scaffold that is a comb tree.

Note that the length of the vector v (or possibly the length minus 1) gives the number of leaves in the greedy comb scaffold where all blobs will have size greater than k.

We applied the greedy comb scaffold algorithm to uniformly random binary trees with $k = \sqrt{n}$ on 2^n leaves for $n = 4, \ldots, 11$, with 1000 samples for each value of n. The results of these simulations are displayed in the log-log plot of Figure 2.5. The slope of the line of best fit is approximately .466. These data suggest that a strategy based on blobification could yield an $\Omega(n^{.466})$ lower bound on the size of the maximum agreement subtree for uniformly random trees. This would be a significant improvement on our estimates of the

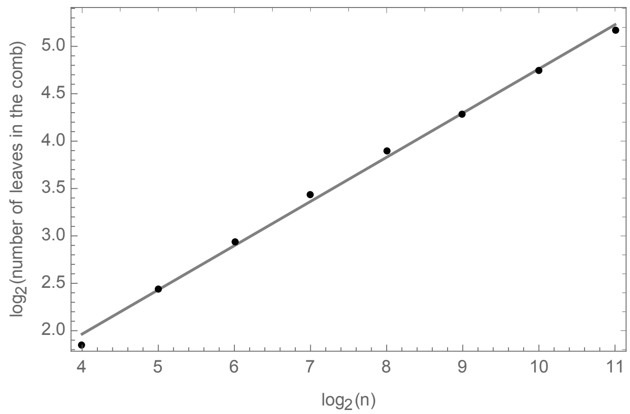


Figure 2.5: Log-log plot of the simulated expected size of the greedy comb scaffold

expected size of the maximal agreement subtree for uniformly random trees, given the current best known lower bound of $\Omega(n^{.366})$.

Chapter 3

Undirected Gaussian graphical models with toric vanishing ideals

Any positive definite $n \times n$ matrix Σ can be seen as the covariance matrix of a multivariate normal distribution in $\mathbb{R}^n$. The inverse matrix $K = \Sigma^{-1}$ is called the *concentration* matrix of the distribution, which is also positive definite. The statistical models where the concentration matrix K can be written as a linear combination of some fixed linearly independent symmetric matrices $K_1, K_2, ..., K_d$ are called *linear concentration* models.

Let $\mathbb{S}^n$ denote the vector space of real symmetric matrices and let $\mathcal{L}$ be a linear subspace of $\mathbb{S}^n$ generated by $K_1, K_2, ..., K_d$. The set $\mathcal{L}^{-1}$ is defined as

$$\mathcal{L}^{-1} = \{\Sigma \in \mathbb{S}^n : \Sigma^{-1} \in \mathcal{L}\}.$$

The homogeneous ideal of all the polynomials in $\mathbb{R}[\Sigma] = \mathbb{R}[\sigma_{11}, \sigma_{12}, ..., \sigma_{nn}]$ that vanish on $\mathcal{L}^{-1}$ is denoted by $P_{\mathcal{L}}$. Note that $P_{\mathcal{L}}$ is prime because it is the vanishing ideal of $\mathcal{L}^{-1}$, which is the image of the irreducible variety $\mathcal{L}$ under the rational inversion map. In this chapter, we study the problem of finding a generating set of $P_{\mathcal{L}}$ for the special case of Gaussian graphical models.

Gaussian graphical models are used throughout the natural sciences and especially in computational biology as seen in [20], [21]. These models explicitly capture the statistical relationships between the variables of interest in the form of a graph. The undirected Gaussian graphical model is obtained when the subspace $\mathcal{L}$ of $\mathbb{S}^n$ is defined by the vanishing of some off-diagonal entries of the concentration matrix K. We fix a graph $G = ([n], E)$

with vertex set $[n] = \{1, 2, ..., n\}$ and edge set E, which is assumed to contain all self loops. The subspace $\mathcal{L}$ is generated by the set $\{K_{ij} | (i, j) \in E\}$ of matrices K_{ij} with 1 entry at the $(i, j)^{th}$ and $(j, i)^{th}$ position and 0 in all other positions. We denote the ideal $P_{\mathcal{L}}$ as P_G in this model.

One way to compute P_G is to eliminate the entries of an indeterminate symmetric $n \times n$ matrix K from the following system of equations:

$$\Sigma \cdot K = Id_n, \quad K \in \mathcal{L},$$

where Id_n is the $n \times n$ identity matrix. However, this elimination is computationally expensive, and we would like methods to identify generators of P_G directly in terms of the graph.

Various methods have been proposed for finding some generators in the ideal P_G and for trying to build P_G from smaller ideals associated to subgraphs. These approaches are based on separation criteria in the graph G.

If G is a c-clique sum of G_1 and G_2, the ideal

$$P_{G_1} + P_{G_2} + \langle (c + 1) \times (c + 1)\text{-minors of } \Sigma_{A \cup C, B \cup C} \rangle \tag{3.1}$$

is contained in P_G. Here $\Sigma_{A \cup C, B \cup C}$ denotes the submatrix of Σ obtained by taking all rows indexed by $A \cup C$ and columns indexed by $B \cup C$, and so

$$\langle (c + 1) \times (c + 1)\text{-minors of } \Sigma_{A \cup C, B \cup C} \rangle$$

is the conditional independence ideal associated to the conditional independence statement $A \perp\!\!\!\perp B | C$. Though the ideal (3.1) fails to equal P_G, (or even have the same radical as that of P_G) for $c \geq 2$, [32] conjectured it to be equal to P_G for $c = 1$.

Conjecture 3.0.1 (Sturmfels-Uhler Conjecture, [32])**.** *Let G be a 1-clique sum of two smaller graphs G_1 and G_2. If (A, B, C) is the 1-clique partition of G where G_1 and G_2 are the subgraphs induced by $A \cup C$ and $B \cup C$ respectively, then*

$$P_G = P_{G_1} + P_{G_2} + \langle 2 \times 2\text{-}\mathit{minors\ of}\ \Sigma_{A \cup C, B \cup C} \rangle.$$

In Section 3.1, we give counterexamples to this conjecture, and even a natural strengthening of it. We also give a corrected version of the formula by using the idea of saturation in Section 3.6. However, the motivation for Conjecture 3.0.1 was to use it as a tool to prove a different conjecture characterizing the graphs for which the vanishing ideal P_G is generated in degree ≤ 2. To explain the details of this conjecture we need some further notions.

Let $X = (X_1, X_2, \ldots, X_n)$ be a Gaussian random vector. If $A, B, C \subseteq [n]$ are pairwise disjoint subsets, then from Proposition 4.1.9 of [35] we know that X_A is conditionally independent of X_B given X_C (i.e $A \perp\!\!\!\perp B|C$) if and only if the submatrix $\Sigma_{A\cup C, B\cup C}$ of the covariance matrix Σ has rank $|C|$. The *Gaussian conditional independence ideal* for the conditional independence statement $A \perp\!\!\!\perp B|C$ is given by

$$J_{A\perp\!\!\!\perp B|C} = \langle (|C|+1) \times (|C|+1) \text{ minors of } \Sigma_{A\cup C, B\cup C} \rangle.$$

If G is an undirected graph and (A, B, C) is a partition with C separating A from B, then the conditional independence statement $A \perp\!\!\!\perp B|C$ holds for all multivariate normal distributions where the covariance matrix Σ is obtained from G (by the global Markov property). The *conditional independence ideal* for the graph G is defined by

$$CI_G = \sum_{A\perp\!\!\!\perp B|C \text{ holds for } G} J_{A\perp\!\!\!\perp B|C}.$$

Proposition 3.0.2. *For any given graph G, $CI_G \subseteq P_G$.*

Proof. As the rank of the submatrices $\Sigma_{A\cup C, B\cup C}$ of the covariance matrix Σ is $|C|$ for all partitions (A, B, C) of G, the generators of CI_G vanish on the matrices in $\mathcal{L}^{-1}$. $\square$

The second conjecture in [32] which we prove in this chapter is as follows:

Theorem 3.0.3. *(Conjecture 4.4, [32]) The prime ideal P_G of an undirected Gaussian graphical model is generated in degree ≤ 2 if and only if each connected component of the graph G is a 1-clique sum of complete graphs.*

The "only if" part of the conjecture is proved in [32]. That is, it is shown there that a graph that is not the 1-clique sum of complete graphs (commonly known as block graphs) must have a generator of degree ≥ 3. Such a generator comes from a conditional independence statement with $\#C \geq 2$.

For block graphs, the conditional independence ideal can be written as

$$CI_G = \langle \bigcup_{(A,B,C)\in C_1(G)} 2\times 2 \text{ minors of } \Sigma_{A\cup C,B\cup C}\rangle,$$

where $C_1(G)$ denotes the set of all 1-clique partitions of G. In this chapter, our main result will be a proof that $CI_G = P_G$ when G is a block graph.

One important property of block graphs as shwon in Proposition 1.1.5 is that there is a unique locally shortest path between any pair of vertices in a connected component of a block graph.

Example 3.0.4. We illustrate the structure of Theorem 3.0.3 with an example. Let $G = ([6], E)$ be the block graph as shown in Figure 1.1. In Example 1.1.4, we saw that G has four 1-clique partitions. The matrices associated to each of the four partitions are as follows:

$$\text{For } 1 : \Sigma_{A\cup C,B\cup C} = \begin{bmatrix} \sigma_{13} & \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{23} & \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{33} & \sigma_{34} & \sigma_{35} & \sigma_{36} \end{bmatrix}, 2 : \Sigma_{A\cup C,B\cup C} = \begin{bmatrix} \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{34} & \sigma_{35} & \sigma_{36} \\ \sigma_{44} & \sigma_{45} & \sigma_{46} \end{bmatrix}$$

$$3 : \Sigma_{A\cup C,B\cup C} = \begin{bmatrix} \sigma_{14} & \sigma_{16} \\ \sigma_{24} & \sigma_{26} \\ \sigma_{34} & \sigma_{36} \\ \sigma_{44} & \sigma_{46} \\ \sigma_{45} & \sigma_{56} \end{bmatrix}, \qquad 4 : \Sigma_{A\cup C,B\cup C} = \begin{bmatrix} \sigma_{14} & \sigma_{15} \\ \sigma_{24} & \sigma_{25} \\ \sigma_{34} & \sigma_{35} \\ \sigma_{44} & \sigma_{45} \\ \sigma_{46} & \sigma_{56} \end{bmatrix}.$$

The ideal $CI_G = P_G$ is the ideal generated by the 2×2 minors of all four matrices:

$$
\begin{aligned}
CI_G = \langle & \sigma_{13}\sigma_{24} - \sigma_{14}\sigma_{23}, \sigma_{13}\sigma_{25} - \sigma_{15}\sigma_{23}, \sigma_{13}\sigma_{26} - \sigma_{16}\sigma_{23}, \sigma_{14}\sigma_{25} - \sigma_{15}\sigma_{24}, \sigma_{23}\sigma_{34} - \sigma_{24}\sigma_{33}, \\
& \sigma_{23}\sigma_{35} - \sigma_{25}\sigma_{33}, \sigma_{23}\sigma_{36} - \sigma_{26}\sigma_{33}, \sigma_{24}\sigma_{35} - \sigma_{25}\sigma_{34}, \sigma_{24}\sigma_{36} - \sigma_{26}\sigma_{34}, \sigma_{25}\sigma_{36} - \sigma_{26}\sigma_{35}, \\
& \sigma_{13}\sigma_{34} - \sigma_{14}\sigma_{33}, \sigma_{13}\sigma_{35} - \sigma_{15}\sigma_{33}, \sigma_{13}\sigma_{36} - \sigma_{16}\sigma_{33}, \sigma_{14}\sigma_{35} - \sigma_{15}\sigma_{34}, \sigma_{14}\sigma_{36} - \sigma_{16}\sigma_{34}, \\
& \sigma_{15}\sigma_{36} - \sigma_{16}\sigma_{35}, \sigma_{14}\sigma_{45} - \sigma_{15}\sigma_{44}, \sigma_{14}\sigma_{46} - \sigma_{16}\sigma_{44}, \sigma_{15}\sigma_{46} - \sigma_{16}\sigma_{45}, \sigma_{24}\sigma_{45} - \sigma_{25}\sigma_{44}, \\
& \sigma_{24}\sigma_{46} - \sigma_{26}\sigma_{44}, \sigma_{25}\sigma_{46} - \sigma_{26}\sigma_{45}, \sigma_{34}\sigma_{45} - \sigma_{35}\sigma_{44}, \sigma_{34}\sigma_{46} - \sigma_{36}\sigma_{44}, \sigma_{35}\sigma_{46} - \sigma_{36}\sigma_{45}, \\
& \sigma_{14}\sigma_{56} - \sigma_{16}\sigma_{45}, \sigma_{24}\sigma_{56} - \sigma_{26}\sigma_{45}, \sigma_{34}\sigma_{56} - \sigma_{36}\sigma_{45}, \sigma_{44}\sigma_{56} - \sigma_{46}\sigma_{45}, \sigma_{14}\sigma_{56} - \sigma_{15}\sigma_{46}, \\
& \sigma_{24}\sigma_{56} - \sigma_{25}\sigma_{46}, \sigma_{34}\sigma_{56} - \sigma_{35}\sigma_{46}, \sigma_{44}\sigma_{56} - \sigma_{45}\sigma_{46}, \sigma_{14}\sigma_{26} - \sigma_{16}\sigma_{24}, \sigma_{15}\sigma_{26} - \sigma_{16}\sigma_{25}\rangle.
\end{aligned}
$$

The history of trying to characterize constraints on the covariance matrices in Gaussian graphical models goes back to [19] and the discovery of the pentad constraints in the factor analysis model. Since then, the study of the constraints on Gaussian graphical models has seen many results including the deeper study of the factor analysis model in [10], the study of directed graphical models and characterization of tree models in [34], and the complete characterization of the determinantal constraints that apply to Gaussian graphical models in [36].

The study of the generators of the ideals P_G is an important problem for constraint-based inference for inferring the structure of the underlying graph from data. Elements of the vanishing ideal are tested to determine if the graph has certain underlying features, which are then used to reconstruct the entire graph. A prototypical example of this method is the TETRAD procedure in [28] which specifically tests the degree 2 generators (tetrads) of the vanishing ideals of Gaussian graphical models for directed graphs. Our main result in this chapter gives a characterization of which undirected graphs the tetrads are sufficient to characterize all distributions from the model, and is a key structural result for trying to use constraint based inference for undirected Gaussian graphical models. Developing characterizations of the vanishing ideals of Gaussian graphical models by higher order constraints (for example, determinantal constraints in [9] and [36]) has the potential to extend constraint-based inference beyond tetrad constraints.

This chapter is organized as follows. We give two counterexamples to Conjecture 3.0.1 in Section 3.1. In Section 3.2 we define a rational map ρ and its pullback map ρ^*, whose kernel is the ideal P_G. Using this uniqueness property of block graphs, we define the "shortest path map" ψ and the initial term map ϕ and show that the two maps have the

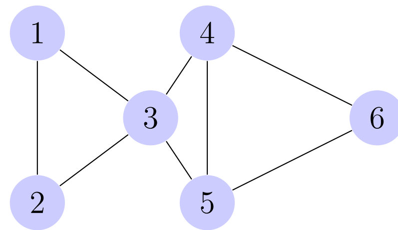


Figure 3.1: A counterexample to Conjecture 3.0.1

same kernel. We prove that the kernel of ψ is equal to the ideal CI_G for block graphs with one central vertex in Section 3.3. This result is generalized for all block graphs in Section 3.4. Finally, in Section 3.5 we put all the pieces together to prove Theorem 3.0.3 using the results proved in the previous sections. We also show that the set F forms a SAGBI basis (Subalgebra Analog to Gröbner Basis for Ideals) using the initial term map. We end this chapter with Section 3.6 where we give a rectified version of the formula given in Conjecture 3.0.1.

3.1 Counterexamples to the Sturmfels-Uhler Conjecture

We first begin with some counterexamples to Conjecture 3.0.1. Initial counterexamples suggest a modification of Conjecture 3.0.1 might be true, but we show that that strengthened version is also false. This last counterexample suggests that it is unlike that there is a repair for the conjecture.

Example 3.1.1. Let $G = ([6], E)$ be the graph as shown in Figure 3.1. Here $A = \{1, 2\}, B = \{4, 5, 6\}$ and $C = \{3\}$. Computing the ideals P_G and $P_{G_1} + P_{G_2} + \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C,B\cup C}\rangle$, we get

$$\begin{aligned} P_G \;=\; & \langle \sigma_{14}\sigma_{25}\sigma_{46} - \sigma_{14}\sigma_{26}\sigma_{45} - \sigma_{15}\sigma_{24}\sigma_{46} + \sigma_{15}\sigma_{26}\sigma_{44} + \sigma_{16}\sigma_{24}\sigma_{45} - \sigma_{16}\sigma_{25}\sigma_{44}, \\ & \sigma_{24}\sigma_{45}\sigma_{56} - \sigma_{24}\sigma_{46}\sigma_{55} - \sigma_{25}\sigma_{44}\sigma_{56} + \sigma_{25}\sigma_{46}\sigma_{45} + \sigma_{26}\sigma_{44}\sigma_{55} - \sigma_{26}\sigma_{45}^2\rangle \\ & + P_{G_1} + P_{G_2} + \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C,B\cup C}\rangle. \end{aligned}$$

Note that even for some small block graphs Conjecture 3.0.1 is false.

Example 3.1.2. Consider the graph $G = ([4], E)$ which is a path of length 4. Taking $c = \{3\}$, we get a decomposition of G into G_1 and G_2 which are paths of length 3 and 2 respectively. A quick calculation in Macaulay2 [13] shows that $P_G = CI_G$ is generated by 5 quadratic binomials. However,

$$P_{G_1} + P_{G_2} + \langle 2 \times 2\text{-minors of } \Sigma_{\{1,2,3\},\{3,4\}} \rangle$$

has only 4 minimal generators.

Although P_G is not equal to $P_{G_1} + P_{G_2} + \langle 2 \times 2 \text{ minors of } \Sigma_{A \cup C, B \cup C} \rangle$ in these examples, we observe that the extra generators of P_G are also determinantal conditions arising from submatrices of Σ. Furthermore, they can be seen as being implied by the original rank conditions in P_{G_1} and P_{G_2} plus the rank conditions that are implied by $\langle 2 \times 2 \text{ minors of } \Sigma_{A \cup C, B \cup C} \rangle$.

For instance, in Example 3.1.2, the ideal $R_G = P_{G_1} + P_{G_2} + \langle 2 \times 2\text{-minors of } \Sigma_{\{1,2,3\},\{3,4\}} \rangle$ is generated by the 2×2 minors of the two matrices

$$\begin{pmatrix} \sigma_{12} & \sigma_{13} \\ \sigma_{22} & \sigma_{23} \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} \sigma_{13} & \sigma_{14} \\ \sigma_{23} & \sigma_{24} \\ \sigma_{33} & \sigma_{34} \end{pmatrix}.$$

Whereas the P_G is generated by the 2×2 minors of the two matrices.

$$\begin{pmatrix} \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{22} & \sigma_{23} & \sigma_{24} \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} \sigma_{13} & \sigma_{14} \\ \sigma_{23} & \sigma_{24} \\ \sigma_{33} & \sigma_{34} \end{pmatrix}.$$

However, we can take the generators of R_G and assuming that σ_{33} is not zero (which is valid since Σ is positive definite), we observe that

$$\begin{pmatrix} \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{22} & \sigma_{23} & \sigma_{24} \end{pmatrix}$$

must be a rank 1 matrix.

Similarly, in Example 3.1.1, we know that $(\{3\}, \{6\}, \{4, 5\})$ is a separating partition for the subgraph G_2. So, the ideal $J_{\{3\} \perp\!\!\!\perp \{6\} | \{4,5\}}$ is contained in P_{G_2}, which implies that rank of the submatrix $\Sigma_{\{3,4,5\},\{4,5,6\}}$ is 2. Similarly, $(\{1,2\},\{4,5,6\},\{3\})$ is a separating partition of G, which implies that rank of the submatrix $\Sigma_{\{1,2,3\},\{3,4,5,6\}}$ is 1. Now, as $\Sigma_{\{1,2,3\},\{4,5,6\}}$ is a submatrix of $\Sigma_{\{1,2,3\},\{3,4,5,6\}}$, we can say that $\Sigma_{\{1,2,3\},\{4,5,6\}}$ also has rank 1. Hence, from these two rank constraints and the added assumption that σ_{33} is not zero we can conclude that the submatrix $\Sigma_{\{1,2,4,5\},\{4,5,6\}}$ has rank 2.

The details of these examples suggest that a better version of the conjecture might be

$$P_G = \mathrm{Lift}(P_{G_1}) + \mathrm{Lift}(P_{G_2}) + \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C, B\cup C}\rangle.$$

Here $\mathrm{Lift}(P_{G_1})$ denotes some operation that takes the generators of P_{G_1} and extends them to the whole graph, analogous to how the toric fiber product in [33] lifts generators for reducible hierarchical models on discrete variables [8; 17]. We do not make precise what this lifting operation could be, because if it preserves the degrees of generating sets the following example shows that no precise version of this notion could make this conjecture be true.

Example 3.1.3. Let $G = ([7], E)$ be the graph as shown in Figure 3.2 and let (A, B, C) be the partition $(\{1,2,3\},\{5,6,7\},\{4\})$. Computing the vanishing ideal, we get $P_G = CI_G$, but that among the minimal generators of P_G is one degree 4 polynomial m where

$$\begin{aligned} m \;=\;& \sigma_{17}^2\sigma_{23}\sigma_{56} - \sigma_{13}\sigma_{17}\sigma_{27}\sigma_{56} - \sigma_{12}\sigma_{17}\sigma_{37}\sigma_{56} + \sigma_{11}\sigma_{27}\sigma_{37}\sigma_{56} - \sigma_{16}\sigma_{17}\sigma_{23}\sigma_{57} \\ &+ \sigma_{13}\sigma_{16}\sigma_{27}\sigma_{57} + \sigma_{12}\sigma_{16}\sigma_{37}\sigma_{57} - \sigma_{11}\sigma_{26}\sigma_{37}\sigma_{57} - \sigma_{15}\sigma_{17}\sigma_{23}\sigma_{67} + \sigma_{13}\sigma_{15}\sigma_{27}\sigma_{67} \\ &+ \sigma_{12}\sigma_{15}\sigma_{37}\sigma_{67} - \sigma_{11}\sigma_{25}\sigma_{37}\sigma_{67} - \sigma_{12}\sigma_{13}\sigma_{57}\sigma_{67} + \sigma_{11}\sigma_{23}\sigma_{57}\sigma_{67} + \sigma_{15}\sigma_{16}\sigma_{23}\sigma_{77} \\ &- \sigma_{13}\sigma_{15}\sigma_{26}\sigma_{77} - \sigma_{12}\sigma_{15}\sigma_{36}\sigma_{77} + \sigma_{11}\sigma_{25}\sigma_{36}\sigma_{77} + \sigma_{12}\sigma_{13}\sigma_{56}\sigma_{77} - \sigma_{11}\sigma_{23}\sigma_{56}\sigma_{77}. \end{aligned}$$

As both P_{G_1} and P_{G_2} are generated by polynomials of degree 3, this degree 4 polynomial could not be obtained from a degree preserving lifting operation.

We come back to this problem in Section 3.6 where we give a revised formula for representing P_G in terms of P_{G_1} and P_{G_2}.

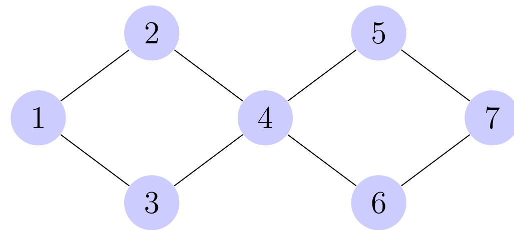


Figure 3.2: Graph with a degree 4 generator

3.2 Shortest path in block graphs

Our goal for the rest of the chapter is to prove Theorem 3.0.3. To do this, we need to phrase some parts in the language of commutative algebra. The vanishing ideal is the kernel of a certain ring homomorphism, or the presentation ideal of a certain $\mathbb{R}$-algebra. We will show that we can pass to a suitable initial algebra and analyze the combinatorics of the resulting toric ideal. This is proven in this section and those that follow.

We begin this section by defining a rational map ρ such that the kernel of its pullback map gives us the ideal P_G. We also use the existence of a unique shortest path between any two vertices of a block graph (as shown in Proposition 1.1.5) to define the "shortest path map".

Let $\mathbb{R}[K] = \mathbb{R}[k_{11}, k_{12}, ..., k_{nn}]$ denote the polynomial ring in the entries of the concentration matrix K, and $\mathbb{R}(K)$ its fraction field.

We define the rational map $\rho : \mathcal{L} \dashrightarrow \mathcal{L}^{-1}$ as follows:

$$\begin{aligned} \rho(K) &= \rho(k_{11}, k_{12}, \ldots, k_{nn}) \\ &= (\rho_{11}(k_{11}, k_{12}, \ldots, k_{nn}), \rho_{12}(k_{11}, k_{12}, \ldots, k_{nn}), ..., \rho_{nn}(k_{11}, k_{12}, \ldots, k_{nn})), \end{aligned}$$

where $\rho_{ij} \in \mathbb{R}(K)$ is the (i, j) coordinate of K^{-1}. The rational map does not yield a well defined function from $\mathcal{L}$ to $\mathcal{L}^{-1}$ as every matrix in $\mathcal{L}$ is not invertible (chapter 3, [15]). Also note that the definition of ρ depends on the underlying graph G, since the zero pattern of K is determined by G.

The *pull-back* map of ρ is

$$\rho^* : \mathbb{R}[\Sigma] \to \mathbb{R}(K), \quad \sigma_{ij} \mapsto \rho_{ij}(K).$$

So, for each $p \in \mathbb{R}[\Sigma]$ and $K \in \mathcal{L}$,

$$\rho^*(p)(K) = p \circ \rho(K) = p(\rho_{11}(K), \rho_{12}(K), ..., \rho_{nn}(K)).$$

Hence, we have

$$P_G = \mathcal{I}(\mathcal{L}^{-1}) = \ker(\rho^*).$$

For a given graph $G = ([n], E)$, let $f_{ij} \in \mathbb{R}[K]$ be the polynomial defined as $\det(K)$ times the (i, j) coordinate of the matrix K^{-1}. Let $F = \{f_{ij} : 1 \leq i \leq j \leq n\}$. So, the map ρ^* can be written as

$$\rho^* : \mathbb{R}[\Sigma] \to \mathbb{R}(K) \quad \rho^*(\sigma_{ij}) = \frac{1}{\det(K)} \cdot f_{ij}.$$

As $1/\det(K)$ is a constant which is present in the image of every σ_{ij}, removing that factor from every image would not change the kernel of ρ^*. Hence, we change the map ρ^* as

$$\rho^* : \mathbb{R}[\Sigma] \to \mathbb{R}[F], \quad \rho^*(\sigma_{ij}) = f_{ij},$$

where $\mathbb{R}[F] = \mathbb{R}[f_{11}, f_{12}, ..., f_{nn}] \subseteq \mathbb{R}[K]$.

Example 3.2.1. Let $G = ([4], E)$ be a graph with 4 vertices as shown in Fig 3.3. The matrices Σ and K for this graph are:

$$\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} & \sigma_{34} \\ \sigma_{14} & \sigma_{24} & \sigma_{34} & \sigma_{44} \end{bmatrix}, \qquad K = \begin{bmatrix} k_{11} & k_{12} & k_{13} & 0 \\ k_{12} & k_{22} & k_{23} & 0 \\ k_{13} & k_{23} & k_{33} & k_{34} \\ 0 & 0 & k_{34} & k_{44} \end{bmatrix}.$$

The ideal P_G can be calculated by using the equation $\Sigma \cdot K = Id_4$ and eliminating the K variables.

$$\begin{aligned} \langle \Sigma \cdot K - Id_4 \rangle &= \langle \sigma_{11}k_{11} + \sigma_{12}k_{12} + \sigma_{13}k_{13} - 1, \sigma_{11}k_{12} + \sigma_{12}k_{22} + \sigma_{13}k_{23}, \ldots, \\ &\qquad \sigma_{14}k_{13} + \sigma_{24}k_{23} + \sigma_{34}k_{33} + \sigma_{44}k_{34}, \sigma_{34}k_{33} + \sigma_{44}k_{44} - 1\rangle. \end{aligned}$$

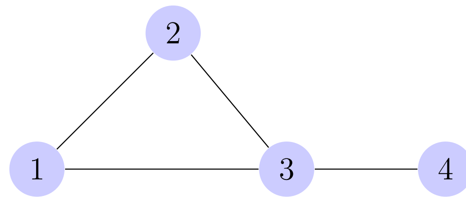


Figure 3.3: A block graph with 4 vertices

Eliminating the K variables, we get

$$P_G \;=\; \langle \Sigma \cdot K - Id_4 \rangle \cap \mathbb{R}[\Sigma] \;=\; \langle \sigma_{13}\sigma_{34} - \sigma_{14}\sigma_{33}, \sigma_{23}\sigma_{34} - \sigma_{24}\sigma_{33}, \sigma_{14}\sigma_{23} - \sigma_{13}\sigma_{24} \rangle.$$

From the map ρ^*, we have

$$\begin{aligned} f_{11} &= \underline{k_{22}k_{33}k_{44}} - k_{22}k_{34}^2 - k_{23}^2k_{44} \\ f_{22} &= \underline{k_{11}k_{33}k_{44}} - k_{11}k_{34}^2 - k_{13}^2k_{44} \\ f_{33} &= \underline{k_{11}k_{22}k_{44}} - k_{44}k_{12}^2 \\ f_{44} &= \underline{k_{11}k_{22}k_{33}} - k_{11}k_{23}^2 - k_{12}^2k_{33} \\ &\quad + k_{12}k_{13}k_{23} + k_{13}k_{12}k_{23} - k_{13}^2k_{22} \end{aligned} \qquad \begin{aligned} f_{12} &= -\underline{k_{12}k_{33}k_{44}} - k_{12}k_{34}^2 - k_{23}k_{13}k_{44} \\ f_{13} &= -\underline{k_{13}k_{22}k_{44}} + k_{12}k_{23}k_{44} \\ f_{14} &= \quad \underline{k_{13}k_{34}k_{22}} - k_{12}k_{23}k_{34} \\ f_{23} &= -\underline{k_{23}k_{11}k_{44}} + k_{12}k_{13}k_{44} \\ f_{24} &= \quad \underline{k_{23}k_{34}k_{11}} - k_{34}k_{13}k_{12} \\ f_{34} &= -\underline{k_{34}k_{11}k_{22}} + k_{34}k_{12}^2 \end{aligned} \tag{3.2}$$

where f_{ij} is $\det(K)$ times the (i, j) coordinate of K^{-1}. Evaluating the kernel of ρ^*, we get

$$\ker(\rho^*) \;=\; \langle \sigma_{13}\sigma_{34} - \sigma_{14}\sigma_{33}, \sigma_{23}\sigma_{34} - \sigma_{24}\sigma_{33}, \sigma_{14}\sigma_{23} - \sigma_{13}\sigma_{24} \rangle$$

which is same as the ideal P_G. Note that G is a block graph with a single 1-clique sum decomposition. As the generators of P_G are the 2×2 minors of $\Sigma_{\{1,2,3\},\{3,4\}}$, the conjecture holds for this example.

Observe that in Example 3.2.1, each f_{ij} contains a monomial which corresponds to the shortest path from i to j in the graph G along with loops at the vertices not in the path. For example, f_{24} has the monomial $k_{23}k_{34}k_{11}$ where $k_{23}k_{34}$ corresponds to the shortest path from 2 to 4 and k_{11} corresponds to the loop at the vertex 1. In (3.2), the underlined terms are this special terms. This turns out to be important in our proofs, and we formalize this observation in Proposition 3.2.3.

For the rest of the chapter, we assume that G is a block graph and the shortest path from i to j in G is denoted by $i \leftrightarrow j$. We use $(i', j') \in i \leftrightarrow j$ to indicate that the edge (i', j') appears in the path $i \leftrightarrow j$. We let $\ell(i, j)$ denote the length of the shortest path from i to j. We now state a result from [18] which will be used to prove Proposition 3.2.3.

Theorem 3.2.2. *(Theorem 1, [18]) Consider an $n-$dimensional multivariate normal distribution with a finite and non-singular covariance matrix Σ, with precision matrix $K = \Sigma^{-1}$. Let K determine the incidence matrix of a finite, undirected graph on vertices $\{1, ..., n\}$, with nonzero elements in K corresponding to edges. The element of K corresponding to the covariance between variables x and y can be written as a sum of path weights over all paths in the graph between x and y:*

$$\sigma_{xy} = \sum_{P \in \mathscr{P}_{xy}} (-1)^{m+1} k_{p_1 p_2} k_{p_2 p_3} ... k_{p_{m-1} p_m} \frac{\det(K_{\setminus P})}{\det(K)},$$

where $\mathscr{P}_{xy}$ represents the set of paths between x and y, so that $p_1 = x$ and $p_m = y$ for all $P \in \mathscr{P}_{xy}$ and $K_{\setminus P}$ is the matrix with rows and columns corresponding to variables in the path P omitted, with the determinant of a zero-dimensional matrix taken to be 1.

Proposition 3.2.3. *Let $G = ([n], E)$ be a block graph with the corresponding concentration matrix K. If f_{xy} denote* $\det(K)$ *times the (x, y) coordinate of K^{-1}, then f_{xy} has the monomial*

$$(-1)^{\ell(i,j)} \prod_{(x',y') \in x \leftrightarrow y} k_{x'y'} \prod_{t \notin x \leftrightarrow y} k_{tt}$$

as one of its terms. Furthermore, this term has the highest number of diagonal entries k_{tt} among all the monomials of f_{xy}.

Proof. From Theorem 3.2.2, we have

$$f_{xy} = \det(K) \cdot \sigma_{xy} = \sum_{P \in \mathscr{P}_{xy}} (-1)^{m+1} k_{p_1 p_2} k_{p_2 p_3} ... k_{p_{m-1} p_m} \det(K_{\setminus P}).$$

From Proposition 1.1.5 we know that if G is a block graph, then for any two vertices x and y, there exists a unique shortest path between x and y. If $z \in x \leftrightarrow y$ with $z \neq x, y$, then there exists a 1-clique partition (A, B, C) of G with $C = \{z\}$ and $x \in A, y \in B$. By the definition of 1-clique partition we know that any path from x to y must pass through z. As z is arbitrarily chosen, any path in G from x to y must pass through all the vertices in $x \leftrightarrow y$. This gives us that the unique shortest path has the least number of vertices among all the other paths from x to y. So, the matrix $K_{\backslash x\leftrightarrow y}$ has the highest dimension among all the other matrices $K_{\backslash P}, P \in \mathscr{P}_{xy}$.

Now, for any $P \in \mathscr{P}_{xy}$, $\det(K_{\backslash P})$ contains the monomial $\prod_{t\notin P} k_{tt}$ as G is assumed to have self loops. This monomial has the highest number of diagonals among all the monomials in $\det(K_{\backslash P})$ as the degree of $\det(K_{\backslash P})$ is same as the degree of $\prod_{t\notin P} k_{tt}$. So, the monomial

$$\prod_{(x',y')\in P} k_{x'y'} \prod_{t\notin P} k_{tt}$$

has the highest number of diagonal terms among all the monomials in $\prod_{(x',y')\in P} k_{x'y'} \det(K_{\backslash P})$. As $K_{\backslash x\leftrightarrow y}$ has the highest dimension, we can conclude that the monomial

$$\prod_{(x',y')\in x\leftrightarrow y} k_{x'y'} \prod_{t\notin x\leftrightarrow y} k_{tt}$$

has the maximum number of diagonal terms among all the monomials in f_{xy}. $\square$

We call the monomial defined above as the *shortest path monomial* of f_{ij}. As the shortest path monomial in each f_{ij} has the highest power of diagonals k_{tt} among all the other monomials in f_{ij}, we can define a weight order on $\mathbb{R}[K]$ where the weight of any monomial is the number of diagonal entries of the monomial. The initial term of f_{ij} in this order will be precisely the shortest path monomial.

Definition 3.2.4. Let G be a block graph. Define the $\mathbb{R}$-algebra homomorphism

$$\phi : \mathbb{R}[\Sigma] \to \mathbb{R}[K], \quad \sigma_{ij} \mapsto \prod_{(i',j')\in i\leftrightarrow j} k_{i'j'} \prod_{t\notin i\leftrightarrow j} k_{tt}.$$

This monomial homomorphism is called the *initial term map*.

The map ϕ is the initial term map of ρ^*, but with the sign $(-1)^{\ell(i,j)}$ omitted. We will use this to show that the set F forms a SAGBI basis of $\mathbb{R}[F]$ by using this term order, as part of our proof of Theorem 3.0.3. This appears in Section 3.5. To do this we must spend some time proving properties of ϕ and $\ker\phi$.

Note that the kernel of ϕ is the same with or without the signs $(-1)^{\ell(i,j)}$. This is because the monomials that appear are graded by the number of diagonal terms that appear, which is also counted by the $(-1)^{\ell(i,j)}$. Any binomial relation $\sigma^u - \sigma^v \in \ker \phi$ much also lead to the same power of negative one on both sides of the equation.

From the standpoint of proving results about this monomial map based on shortest paths in a block graph, it turns out to be easier to work with a related map that we call the shortest path map.

Definition 3.2.5. Let $G = ([n], E)$ be a block graph. The *shortest path map* ψ is defined as

$$\begin{aligned} \psi \quad &: \quad \mathbb{R}[\Sigma] \to \mathbb{R}[a_1, ..., a_n, k_{12}, ..., k_{n-1,n}] = \mathbb{R}[A, K] \\ \psi(\sigma_{ij}) \quad &= \quad \begin{cases} a_i a_j \prod_{(i',j') \in i \leftrightarrow j} k_{i'j'} & i \neq j \\ a_i^2 & i = j. \end{cases} \end{aligned}$$

Example 3.2.6. Let G be the graph in Example 3.2.1. Let ψ be the shortest path map and ϕ the initial monomial map as given in Definitions 3.2.4 and 3.2.5. So for example,

$$\phi(\sigma_{11}) = k_{22}k_{33}k_{44}, \phi(\sigma_{12}) = k_{12}k_{33}k_{44}, \ldots$$

$$\psi(\sigma_{11}) = a_1^2, \psi(\sigma_{12}) = a_1 a_2 k_{12}, \ldots.$$

As is typical for monomial parametrizations, we can represent them by matrices whose columns are the exponent vectors of the monomials appearing in the parametrization. In this case, we get the following matrices corresponding to ϕ and ψ respectively.

$$M_\phi = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix} \qquad M_\psi = \begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 2 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 2 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}.$$

The rows of M_ϕ are ordered as $\{k_{11}, k_{22}, k_{33}, k_{44}, k_{12}, k_{13}, k_{23}, k_{34}\}$ and the rows of M_ψ are ordered as $\{a_1, a_2, a_3, a_4, k_{12}, k_{13}, k_{23}, k_{34}\}$.

In fact, these two monomial maps have the same kernel for block graphs.

Proposition 3.2.7. *Let G be a block graph and let ϕ and ψ be the initial term map and the shortest path map, respectively. Then* $\ker(\psi) = \ker(\phi)$.

Proof. Both $\ker(\phi)$ and $\ker(\psi)$ are toric ideals. To show that they have the same kernel, it suffices to show that the associated matrices of exponent vectors have the same kernel, or equivalently, that they have the same row span. Let M_ϕ and M_ψ denote those matrices. As $\psi(\sigma_{ij}) = a_i a_j \prod_{(i',j') \in i \leftrightarrow j} k_{i'j'}$ and $\phi(\sigma_{ij}) = \prod_{(i',j') \in i \leftrightarrow j} k_{i'j'} \prod_{s \notin i \leftrightarrow j} k_{ss}$, the rows corresponding to k_{ij} with $i \neq j$ remain the same in both the matrices. So, we only need to write the k_{ii} rows of M_ϕ as a linear combination of the rows of M_ψ and vice versa.

The row vector corresponding to k_{ii} in M_ϕ is 1 at the σ_{pq} coordinates where $i \notin p \leftrightarrow q$ and is 0 elsewhere. Similarly, the row vector corresponding to a_i in M_ψ is 2 at the σ_{ii} coordinate, 1 at the σ_{pq} coordinates where either of the end points is i (either $p = i$ or $q = i$) and 0 elsewhere.

We observe that the k_{ii} rows of M_ϕ can be written as a linear combination of the rows of M_ψ using the following relation:

$$2k_{ii} = \sum_{j \neq i} a_j - \sum_{s : i \leftrightarrow s \text{ is an edge}} k_{is}. \tag{3.3}$$

Here we are using k_{ii} to denote the row vector of M_ϕ corresponding to the indeterminate k_{ii}, and similarly for a_j and k_{is}. We have

$$\begin{aligned} \sum_{j \neq i} a_j &= \text{ paths ending at } i + 2(\text{ paths not ending at } i) - i \leftrightarrow i, \\ \sum_{s : i \leftrightarrow s \text{ is an edge}} k_{is} &= \text{ paths ending at } i + 2(\text{ paths containing } i \text{ but not ending at } i) - i \leftrightarrow i. \end{aligned}$$

So,

$$\sum_{j \neq i} a_j - \sum_{s : i \leftrightarrow s \text{ is an edge}} k_{is} = 2(\text{ paths not containing } i) = 2k_{ii}.$$

As this relation is true for any i, the row space of M_ϕ is contained in the row space of M_ψ. So, $\ker(\psi) \subseteq \ker(\phi)$.

To get the reverse containment, we need to write the a_i rows of M_ψ as a linear combination of the rows of M_ϕ. From (3.3), we get

$$\sum_{j \neq i} a_j = 2k_{ii} + \sum_{s : i \leftrightarrow s \text{ is an edge}} k_{is}.$$

Writing these n equations in the matrix form, we get an $n \times n$ matrix in the left hand side which has 0 in its diagonal entries and 1 elsewhere. As this matrix is invertible for any $n > 1$, we can conclude that the row space of M_ψ is contained in the row space of A. Hence, $\ker(\psi) = \ker(\phi)$. $\square$

Our goal in the next two sections will be to characterize the vanishing ideal of the shortest path map for block graphs.

Definition 3.2.8. Let G be a block graph. Let $SP_G = \ker(\psi) = \ker(\phi)$ be the kernel of the shortest path map. This ideal is called the *shortest path ideal.*

As the shortest path map is a monomial map, we know that the shortest path ideal is a toric ideal. We will eventually show that $SP_G = CI_G = P_G$, however we find it useful to have different notation for these ideals while we have not yet proven the equality.

3.3 Shortest path map for block graphs with 1 central vertex

In this section we show that $SP_G = CI_G$ in the case that G is a block graph with only one central vertex. This will be an important special case and tool for proving that $SP_G = CI_G$ for all block graphs, which we do in Section 3.4. Our proof for graphs with only one central vertex depends on reducing the study of the ideal SP_G in this case to related notions of edge rings in [6] and [16].

Definition 3.3.1. If G is a block graph, a vertex c in G is called a *central vertex* if there exists a 1-clique partition (A, B, C) of G such that $C = \{c\}$.

Example 3.3.2. Let G be the block graph with 5 vertices as in Figure 3.4. There are three possible 1-clique partitions of G,

$$(\{1,2\},\{4,5\},\{3\}), \ \ (\{1,2,4\},\{5\},\{3\}) \text{ and } \ (\{1,2,5\},\{4\},\{3\}).$$

We see that 3 is the only central vertex of G as $C = \{3\}$ for all the three partitions. Now

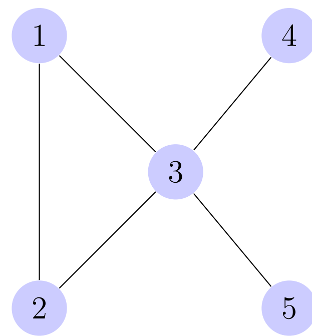


Figure 3.4: A block graph with 1 central vertex

computing SP_G for this graph, we get

$$\begin{aligned}\ker(\psi) = \langle &\sigma_{34}\sigma_{35} - \sigma_{33}\sigma_{45}, \sigma_{24}\sigma_{35} - \sigma_{23}\sigma_{45}, \sigma_{14}\sigma_{35} - \sigma_{13}\sigma_{45}, \sigma_{25}\sigma_{34} - \sigma_{23}\sigma_{45},\\ &\sigma_{15}\sigma_{34} - \sigma_{13}\sigma_{45}, \sigma_{25}\sigma_{33} - \sigma_{23}\sigma_{35}, \sigma_{24}\sigma_{33} - \sigma_{23}\sigma_{34}, \sigma_{15}\sigma_{33} - \sigma_{13}\sigma_{35},\\ &\sigma_{14}\sigma_{33} - \sigma_{13}\sigma_{34}, \sigma_{15}\sigma_{24} - \sigma_{14}\sigma_{25}, \sigma_{15}\sigma_{23} - \sigma_{13}\sigma_{25}, \sigma_{14}\sigma_{23} - \sigma_{13}\sigma_{24}\rangle.\end{aligned}$$

We observe that in Example 3.3.2, none of the generators of SP_G contain the terms $\sigma_{12}, \sigma_{11}, \sigma_{22}, \sigma_{44}$ and σ_{55}. These terms correspond to the edges in G which cannot be separated by any 1-clique partition of G. This property is true for all block graphs with one central vertex as we prove it in the next Lemma.

Lemma 3.3.3. *Let G be a block graph with one central vertex c and let D be the set of variables σ_{pq}, where the shortest path $p \leftrightarrow q$ does not intersect c. Then none of the variables appearing in D appear in any of the minimal generators of the kernel of ψ.*

Proof. Since ψ is a monomial parametrization, the kernel of ψ is a homogeneous binomial ideal. Let

$$f = \sigma^u - \sigma^v$$

be an arbitrary binomial in any generating set for the kernel of SP_G. In particular, this implies that σ^u and σ^v have no common factors. Suppose by way of contradiction that σ_{pq} is some variable in D that divides one of the terms of f, say σ^u. Then $\psi(\sigma^u)$ would have k_{pq} as a factor. But k_{pq} appears only in the image of σ_{pq} as no other shortest path between any two vertices in G contains the edge (p, q). This would imply that σ_{pq} is also a factor of σ^v contradicting the fact that σ^u and σ^v have no common factors.

Similarly, if σ_{pp} is a factor of σ^u where p is not the central vertex, then $\psi(\sigma^u)$ would have a_p^2 as a factor. In order to have a_p^2 as a factor of $\psi(\sigma^v)$, it would require two variables in σ^v to have p as one of their end points. As p is not a central vertex, we will have k_{cp}^2 as a factor of $\psi(\sigma^v)$. But then this means that there must be two variables in σ^u that touch vertex p. Which in turn forces another factor of a_p^2 to divide $\psi(\sigma^u)$. Which in turn forces another two variables in σ^v to touch vertex p, and so on. This process never terminates, showing that it is impossible that σ_{pp} is a factor of σ^u.

Hence we can conclude that none of the variables in D appear in any of the generators of SP_G. $\square$

Note that the proof of Lemma 3.3.3 also applies to any block graph with multiple central vertices. Hence, we can eliminate some of the variables in the computation of the shortest path ideal.

We let $\mathbb{R}[\Sigma \setminus D]$ denote the polynomial ring with the variables D eliminated. Here we are always taking D to the be set of variables corresponding to paths that do not touch the central vertex x. Lemma 3.3.3 shows that it suffices to consider the problem of finding a generating set of SP_G inside of $\mathbb{R}[\Sigma \setminus D]$.

The next step in our analysis of SP_G for block graphs with one central vertex will be to relate this ideal to a simplified parametrization which we can then relate to edge ideals.

Let G be a block graph with one central vertex. Consider the map

$$\hat{\psi} : \mathbb{R}[\Sigma \setminus D] \to \mathbb{R}[a], \quad \sigma_{ij} \mapsto a_i a_j.$$

Proposition 3.3.4. *Let G be a block graph with one central vertex. Then* $\ker \hat{\psi} = \ker \psi$.

Proof. Note that because we only consider $\sigma_{pq} \in \mathbb{R}[\Sigma \setminus D]$ then any time $\psi(\sigma_{pq})$ contains k_{pc} it will automatically contain a_p as well, and vice versa. Hence, the $a_p k_{pc}$ always occurs as a factor together in $\psi(\sigma_{pq})$. So we can eliminate the k_{pc} from the parametrization without affecting the kernel of the homomorphism. $\square$

In order to analyze $SP_G = \ker \hat{\psi} = \ker \psi$, we find it useful to first extend the map to all of $\mathbb{R}[\Sigma]$, where the kernel is well understood. In particular, we associate an edge in the graph K_n° to each variable in $\mathbb{R}[\Sigma]$, where K_n° denotes the complete graph K_n with a loop added to each vertex. We embed K_n° in the plane so that the vertices are arranged to lie on a circle. We consider the map

$$\hat{\psi} : \mathbb{R}[\Sigma] \to \mathbb{R}[a], \quad \sigma_{ij} = a_i a_j$$

and its kernel $SP_{K_n^\circ} = \ker \hat{\psi}$. We describe a Gröbner basis for this ideal, based on the combinatorics of the embedding of the graph K_n°. We consider a pair of edges $(i,j),(k,l)$ to be *intersecting* if the two edges share a vertex or the edges intersect each other in the circular embedding of K_n°.

The *circular distance* between two vertices of K_n is defined as the length of the shorter path among the two paths present along the edges of the n-gon. We define the *weight* of the variable σ_{ij} as the number of edges of K_n° that do not intersect the edge (i,j). Let $\prec$ denote any term order that refines the partial order on monomials specified by these weights. Now, for any pair of non-intersecting edges $(i,j),(k,l)$ of K_n°, one of the pairs $(i,k),(j,l)$ or $(i,l)(j,k)$ is intersecting. If $(i,k),(j,l)$ is the intersecting pair, we associate the binomial $\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}$ with the non intersecting pair of edges $(i,j),(k,l)$. We denote by S' the set of all binomials obtained in this way.

Lemma 3.3.5. *For any binomial $\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}$, where $(i,j),(k,l)$ are non-intersecting edges and $(i,k),(j,l)$ intersect, the initial term with respect to $\prec$ corresponds to the non intersecting edges in K_n°.*

Proof. We divide the set of vertices in K_n° into four different parts (excluding the vertices i,j,k and l). Let P_1 denote the set of vertices that are present in the path between i and j along the edges of the n-gon that do not contain k and l. Similarly, let P_2, P_3 and P_4 denote the set of vertices between j and k, k and l and l and i respectively. Let the cardinality of each P_i be p_i for $i = 1,2,3,4$. Then, the weight of the four variables are as follows:

$$\begin{aligned}
w(\sigma_{ij}) &= \sum_{i=1}^{4}\binom{p_i}{2}+p_2p_3+p_2p_4+p_3p_4+2(p_2+p_3+p_4)+1+(n-2)\\
w(\sigma_{kl}) &= \sum_{i=1}^{4}\binom{p_i}{2}+p_1p_2+p_1p_4+p_2p_4+2(p_1+p_2+p_4)+1+(n-2)\\
w(\sigma_{ik}) &= \sum_{i=1}^{4}\binom{p_i}{2}+p_1p_2+p_3p_4+p_1+p_2+p_3+p_4+(n-2)\\
w(\sigma_{jl}) &= \sum_{i=1}^{4}\binom{p_i}{2}+p_1p_4+p_2p_3+p_1+p_2+p_3+p_4+(n-2).
\end{aligned}$$

This gives us

$$w(\sigma_{ij})+w(\sigma_{kl})-(w(\sigma_{ik})+w(\sigma_{jl}))=2p_2p_4+2(p_2+p_4)+2>0.$$

Hence, the initial term of $\sigma_{ij}\sigma_{kl}-\sigma_{ik}\sigma_{jl}$ with respect to $\prec$ is $\sigma_{ij}\sigma_{kl}$. Further, if $k=l$ then we have the binomial $\sigma_{ij}\sigma_{kk}-\sigma_{ik}\sigma_{jk}$ where

$$\begin{aligned}
w(\sigma_{kk}) &= \binom{n-1}{2}+n-1 \text{ and}\\
w(\sigma_{jk}) &= \sum_{i=1}^{4}\binom{p_i}{2}+p_1p_4+p_1p_3+p_3p_4+2(p_1+p_3+p_4)+1+(n-2).
\end{aligned}$$

This gives us

$$\begin{aligned}
w(\sigma_{ij})+w(\sigma_{kk})-(w(\sigma_{ik})+w(\sigma_{jk})) &= \sum_{i=2}^{4}\frac{p_i}{2}+2(p_2p_3+p_2p_4)+\frac{3}{2}(p_2+p_3+p_4)\\
&\quad +p_2+4>0.
\end{aligned}$$

So, the initial term of $\sigma_{ij}\sigma_{kk}-\sigma_{ik}\sigma_{jk}$ with respect to $\prec$ is $\sigma_{ij}\sigma_{kk}$. □

Lemma 3.3.6. *Let S' be the set of binomials obtained from all the pairs of non-intersecting edges of K_n°. Then S' is the reduced Gröbner basis of $SP_{K_n^\circ}$ with respect to $\prec$.*

Proof. By lemma 3.3.5 we know that for any binomial $\sigma_{ij}\sigma_{kl}-\sigma_{il}\sigma_{jk}\in S'$, where $(i,j),(k,l)$ are non-intersecting edges and $(i,l),(j,k)$ intersect, the initial term with respect to $\prec$ corresponds to the non intersecting edges in K_n°. Clearly, $\sigma_{ij}\sigma_{kl}-\sigma_{il}\sigma_{jk}\in SP_{K_n^\circ}$.

The proof follows the basic outline as the proof of Theorem 9.1 in [31]. For any even closed walk $\Gamma = (i_1, i_2, ..., i_{2k-1}, i_{2k}, i_1)$ in K_n° we associate the binomial

$$b_\Gamma := \prod_{l=1}^{k} \sigma_{i_{2l-1},i_{2l}} - \prod_{l=1}^{k} \sigma_{i_{2l},i_{2l+1}}$$

which belongs to $SP_{K_n^\circ}$. To prove that S' is a Gröbner basis, it is enough to prove that the initial monomial of any binomial b_Γ is divisible by some monomial $\sigma_{ij}\sigma_{kl}$ which is the initial term of some binomial in S', where (i, j) and (k, l) are a pair of non intersecting edges. Let there exist a binomial $b_\Gamma = \sigma^u - \sigma^v \in SP_{K_n^\circ}$ with $in_\prec(b_\Gamma) = \sigma^u$ which contradicts the assertion. Then assuming that b_Γ has minimal weight, we can say that each pair of edges appearing in σ^v intersects.

The edges of the walk are labeled as even or odd, where even edges look like (i_{2r}, i_{2r+1}) and the odd edges are of the form (i_{2r-1}, i_{2r}). We pick an edge (s, t) of the walk Γ which has the least circular distance between s and t. The edge (s, t) separates the vertices of K_n° except s and t into two disjoint sets P and Q where $|P| \geq |Q|$. We start Γ at $(s, t) = (i_1, i_2)$. From our assertion on b_Γ we have that each pair of odd (resp. even) edges intersect. Also, it can be proved that if P contains an odd vertex i_{2r-1}, then it contains all the subsequent odd vertices $i_{2r+1}, i_{2r+3}, ..., i_{2k-1}$. As the circular distance between s and t is the least, we need to have i_3 to be in P. So, all the odd vertices except i_1 lie in P and all the even vertices lie in $Q \cup \{i_1, i_2\}$. This gives us that the two even edges (i_2, i_3) and (i_{2k}, i_1) do not intersect, which is a contradiction. □

Our goal next is to use Lemma 3.3.6, to prove that $SP_G = CI_G$ for block graphs with one central vertex. Recall that the set D consisted of all variables σ_{ij} such that in the graph G $i \leftrightarrow j$ does not touch the central vertex. As the σ_{ij} appearing in D do not appear in any generators of SP_G, let us construct an associated subgraph of K_n° without those edges. Specifically, let G° be the graph obtained by removing the edges (i, j) from K_n° such that $\sigma_{ij} \in D$. Note that we choose an embedding of G° so that each maximal clique minus c forms a contiguous block on the circle. The placement of c can be anywhere that is between the maximal blocks.

Figure 3.5 illustrates the construction of the graph G° in an example.

Example 3.3.7. Let G be a block graph with 5 vertices in Figure 3.5. There are 3 possible 1-clique partitions of G, each of them having $C = \{3\}$. The edges in K_5° which cannot

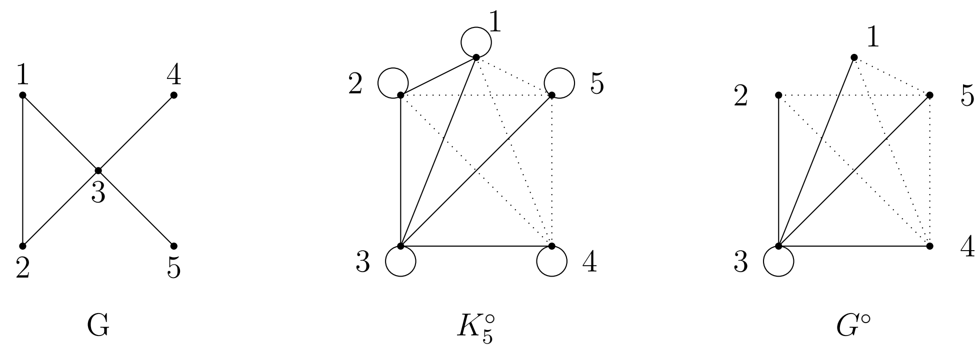


Figure 3.5: Construction of the graph G°. The dark lines in K_5° correspond to the edges in G whereas a dotted line between i and j tells us that there is no edge between i and j in G. The dotted line basically corresponds to the shortest path between the two vertices in G. Note that the addition of extra edges gives us K_5° and the deletion of some edges gives us G°.

be separated by any 1-clique partition of G are $D = \{(1,2),(1,1),(2,2),(4,4),(5,5)\}$. So we remove them from K_5° to get G°.

Lemma 3.3.8. *For any non intersecting pair of edges $(i,j),(k,l)$ in G°, there exists a 1-clique partition (A,B,C) of G such that $i,l \in A \cup C$ and $j,k \in B \cup C$.*

Proof. We first prove this for the non intersecting edges $(i,j),(k,l)$ with $i,j,k,l \neq c$. Without loss of generality we can assume that $i < j < k < l$. We know that for each edge (i,j) in G° there exists a 1-clique partition (A,B,C) of G such that $i \in A \cup C$ and $j \in B \cup C$. This implies that i and j (similarly k and l) lie in different maximal cliques of G. As the vertices of G° are labeled counter-clockwise, there are only three ways how the vertices i,j,k,l can be placed:

$$\begin{aligned} &i) \quad i,l \in C_1, j,k \in C_2, \qquad ii) \quad i,l \in C_1, j \in C_2, k \in C_3, \\ &iii) \quad i \in C_1, j \in C_2, k \in C_3, l \in C_4, \end{aligned}$$

where C_i are the different maximal cliques of G. In all the three cases i and k (similarly j and l) are in different maximal cliques. Hence there exists a 1-clique partition (A,B,C) such that $i,l \in A \cup C$ and $k,j \in B \cup C$.

A similar argument can be given for the non intersecting edges $(i,c),(k,l)$ and $(c,c),(i,j)$. $\square$

Lemma 3.3.9. *Let S' be the Gröbner basis for $SP_{K_n^\circ} \subseteq \mathbb{R}[\Sigma]$ as defined in Lemma 3.3.6. Then the set $S' \cap \mathbb{R}[\Sigma \setminus D]$ forms a Gröbner basis for SP_G.*

Proof. Let $g = \sigma^u - \sigma^v$ be an arbitrary binomial in $SP_G = \ker \hat{\psi}$. This implies that the initial term of g is contained in $\mathbb{R}[\Sigma \setminus D]$. Since S' is a Gröbner basis for $SP_{K_n^\circ}$ with respect to $\prec$, there must exist some $f \in S'$ such that $\text{in}_\prec(f)$ divides $in_\prec(g)$. This gives us that the initial term of f is contained in $\mathbb{R}[\Sigma \setminus D]$.

So it is enough to show that for every $f \in S'$ whose leading term is in $\mathbb{R}[\Sigma \setminus D]$ is actually contained in $\mathbb{R}[\Sigma \setminus D]$. Let

$$f = \sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}$$

be a binomial in S' whose leading term is contained in $\mathbb{R}[\Sigma \setminus D]$. Let $\sigma_{ij}\sigma_{kl}$ be the leading term. Then the edges $(i, j), (k, l)$ are non intersecting as the initial term of each binomial in S' corresponds to the non intersecting edges. So by Lemma 3.3.8, there must exist a 1-clique partition (A, B, C) of G which separates the edges (i, j) and (k, l), that is, $i, l \in A \cup C$ and $j, k \in B \cup C$. This implies that (A, B, C) also separates the edges (i, k) and (j, l). Hence we can say that $\sigma_{ik}, \sigma_{jl} \notin D$ and $\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl} \in \mathbb{R}[\Sigma \setminus D]$. $\square$

Now that we have all the required results, we prove the main result of this section.

Theorem 3.3.10. *Let G be a block graph with n vertices having only one central vertex. Then the set of all 2×2 minors of $\Sigma_{A\cup C, B\cup C}$ for all possible 1-clique partitions (A, B, C) of G form a Gröbner basis for SP_G. In particular, $SP_G = CI_G$.*

Proof. We rearrange the graph by placing the vertices in K_n° such that there is no intersection among the edges of G in $A \cup C$ and $B \cup C$ for any 1-clique partition (A, B, C) (with $C = \{c\}$). We complete the graph by drawing the remaining edges with dotted lines.

The complete graph K_n° gives us a partial term order on $\mathbb{R}[\Sigma]$ by defining the weight of the variable σ_{ij} as the number of edges of K_n° which do not intersect the edge (i, j). Let $\prec$ denote the term order that refines the partial order on monomials specified by the weights. Let S be the set of all 2×2 minors of $\Sigma_{A\cup C,B\cup C}$ for all possible 1-clique partitions of G. Any binomial in S has one of the three forms:

i) $\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}$ with $i, l \in A \cup C$ and $j, k \in B \cup C$

ii) $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{jk}$ with $i, k \in A \cup C$ and $j, l \in B \cup C$

iii) $\sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl}$ with $i, j \in A \cup C$ and $k, l \in B \cup C$.

Here $(i,j),(k,l)$ and $(i,l),(j,k)$ are the non intersecting pairs of edges and $(i,k)(j,l)$ is the intersecting pair in G°. So any binomial in S of the form (i) or (iii) is contained in S'. If the binomial $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{jk}$ (of form (ii)) is in S, then by Lemma 3.3.8 we know that the binomials $\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}$ and $\sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl}$ are also in S. As

$$\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{jk} = \sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl} - (\sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl}),$$

we can conclude that S and $S \cap S'$ generate the same ideal. Furthermore, the set $S \cap S'$ has the same initial terms as $S' \cap \mathbb{R}[\Sigma \setminus D]$ so this guarantees that S is a Gröbner basis for SP_G as well. $\square$

3.4 The shortest path ideal for an arbitrary block graph

To generalize the statement in Theorem 3.3.10 for any arbitrary block graph, we further exploit the toric structure of the ideal SP_G. As SP_G is the kernel of a monomial map, it is a toric ideal, a prime ideal generated by binomials. Finding a generating set of SP_G is equivalent to finding a set of binomials that make some associated graphs connected. We use this perspective to prove that $SP_G = CI_G$.

From the shortest path map ψ, we can obtain the matrix M_ψ as shown in Example 3.2.6. So $SP_G = \ker(\psi)$ is the toric ideal of the matrix M_ψ as

$$\psi(\sigma^u) = t^{M_\psi u},$$

where $\sigma = (\sigma_{11}, \sigma_{12}, ..., \sigma_{nn})$ and $t = (a_1, a_2, ..., a_n, k_{12}, ..., k_{n-1n})$.

Let $G = ([n], E)$ be a block graph. For any vector $b \in \mathbb{N}^{(n+|E|)}$, the fiber of M_ψ over b is the set

$$M_\psi^{-1}(b) = \{u \in \mathbb{N}^{(n^2+n)/2} : M_\psi u = b\}.$$

As the columns of M_ψ are non-zero and non-negative, $M_\psi^{-1}(b)$ is always finite for any $b \in \mathbb{N}^{(n+|E|)}$. Let $\mathcal{F}$ be any finite subset of $\ker_{\mathbb{Z}}(M_\psi)$. The fundamental theorem of Markov bases (Theorem 1.4.4) connects the generating sets of toric ideals to connectivity properties of the fiber graphs. We state the Theorem explicitly for the shortest path maps.

Theorem 3.4.1. *(Thm 5.3, [31]) Let $\mathcal{F} \subset \ker_{\mathbb{Z}}(M_\psi)$. The graphs $M_\psi^{-1}(b)_{\mathcal{F}}$ are connected for all $b \in \mathbb{N}M_\psi = \{\lambda_1 M_{\psi 1} + ... + \lambda_{n+|E|} M_{\psi n+|E|} : \lambda_i \in \mathbb{N}, M_{\psi i}$ are columns of $M_\psi\}$ if and only if the set $\{\sigma^{v^+} - \sigma^{v^-} : v \in \mathcal{F}\}$ generates the toric ideal SP_G.*

As we proved in Theorem 3.3.10 that the set of all 2×2 minors of $\Sigma_{A\cup C, B\cup C}$ for all possible 1-clique partitions of G form a Gröbner basis for $\ker(\psi)$ for all block graphs with one central vertex, by using Theorem 4.4.2 we can say that the graph $M_\psi^{-1}(b)_{\mathcal{F}}$ is connected for all $b \in \mathbb{N}M_\psi$. Here $\mathcal{F}$ is the set of all 2×2 minors of $\Sigma_{A\cup C, B\cup C}$ in the vector form, for all possible 1-clique partitions of G.

So, to generalize the result in Theorem 3.3.10 for all block graphs, we need to show that $M_\psi^{-1}(b)_{\mathcal{F}}$ is connected for any $b \in \mathbb{N}M_\psi$. For a fixed b, let $u, v \in M_\psi^{-1}(b)_{\mathcal{F}}$. This implies that both $M_\psi u$ and $M_\psi v$ are equal to b, which gives us $\psi(\sigma^u - \sigma^v) = 0$. Therefore, it is enough to show that for any $f = \sigma^u - \sigma^v \in SP_G$, σ^u and σ^v are connected by the moves in $\mathcal{F}$.

Let G be a block graph with n vertices. Let $u \in \mathbb{N}^{(n^2+n)/2}$ which is a node in the graph of $M_\psi^{-1}(b)_{\mathcal{F}}$. We represent this u, or equivalently σ^u, as a graph in the following way: For each factor σ_{ij} of σ^u we draw the shortest path $i \leftrightarrow j$ along G with end points at i and j. For each σ_{ii} we draw a loop at the vertex i. Let $\deg_i(\sigma^u)$ denote the *degree* of a vertex i in σ^u which is defined to be the number of end points of paths in σ^u. We count the loops corresponding to σ_{ii} as having two endpoints at i.

If $f = \sigma^u - \sigma^v$ is a homogeneous binomial in SP_G, then $\psi(\sigma^u) = \psi(\sigma^v)$ if and only if the following conditions are satisfied:

i) The graphs of σ^u and σ^v both have the same number of paths (as f is homogeneous),
ii) The graphs of σ^u and σ^v have the same number of edges between any two adjacent vertices i and j (as the exponent of k_{ij} in $\psi(\sigma^u)$ gives the number of edges between i and j in the graph of σ^u),
iii) The degree of any vertex in both the graphs is the same (as the exponent of a_i in $\psi(\sigma^u)$ gives us the degree of the vertex i in the graph of σ^u).

Next we show how to use the results from Section 3.3 to make moves that bring σ^u and σ^v closer together. This approach works by localizing the computations at each central vertex in the graph.

Let c be a central vertex in G. We define a map ρ_c between the set of vertices as follows:

$$\rho_c(i) = \begin{cases} c & i = c \\ i & i \text{ is adjacent to } c \\ i' & i' \text{ is adjacent to } c \text{ and lies in } i \leftrightarrow c. \end{cases}$$

Let G_c be the graph obtained by applying ρ_c to the vertices of G. Note that G can have multiple vertices mapped to a single vertex in G_c. The map ρ_c can also be seen as a map between $\mathbb{R}[\Sigma]$ to itself by the rule $\rho_c(\sigma_{ij}) = \sigma_{\rho_c(i)\rho_c(j)}$.

For a vector $u \in \mathbb{N}^{n(n+1)/2}$ and c a central vertex let u_c be the vector that extracts all the coordinates that correspond to shortest paths that touch c. That is,

$$u_c(ij) = \begin{cases} u(ij) & c \in i \leftrightarrow j \\ 0 & \text{otherwise.} \end{cases}$$

Proposition 3.4.2. *Suppose that* $\sigma^u - \sigma^v \in SP_G$ *and let* c *be a central vertex of* G*. Then* $\psi_{G_c}(\rho_c(\sigma^{u_c})) - \psi_{G_c}(\rho_c(\sigma^{v_c})) = 0$.

Note that we use the notation ψ_{G_c} to denote that we use the ψ map associated to the graph G_c. However, the map ψ associated to G can be used since that will give the same result.

Proof. We have

$$\rho_c(\sigma_{ij}) = \begin{cases} \sigma_{ij} & i, j \text{ are adjacent to } c \\ \sigma_{ic} & i \text{ is adjacent to } c, j = c \\ \sigma_{cj} & j \text{ is adjacent to } c, i = c \\ \sigma_{i'c} & i' \text{ is adjacent to } c \text{ and } i' \in i \leftrightarrow c, j = c \\ \sigma_{cj'} & j' \text{ is adjacent to } c \text{ and } j' \in j \leftrightarrow c, i = c \\ \sigma_{ij'} & i, j' \text{ are adjacent to } c \text{ and } j' \in c \leftrightarrow j \\ \sigma_{i'j} & i', j \text{ are adjacent to } c \text{ and } i' \in i \leftrightarrow c \\ \sigma_{i'j'} & i', j' \text{ are adjacent to } c \text{ and } i' \in i \leftrightarrow c, j' \in j \leftrightarrow c_1 \\ \sigma_{i'i'} & i' \text{ is adjacent to } c \text{ and } i' \in i \leftrightarrow c \text{ and } j \leftrightarrow c. \end{cases}$$

We know that σ^u and σ^v have the same number of paths. Also, the degree of each vertex and the number of edges between any two adjacent vertices is the same. So, it is enough to show that $\rho_c(\sigma^{u_c})$ and $\rho_c(\sigma^{v_c})$ have the same number of paths and the degree of each vertex, number of edges between any two adjacent vertices is also the same.

$$\begin{aligned}
\text{Number of paths in } \sigma^{u_c} &= \text{number of paths in } \sigma^u \text{ ending at } c + \\
&\quad \text{number of paths containing } c \text{ but not ending at } c \\
&= \text{degree of } a_c \text{ in } \psi(\sigma^u) + 1/2(\text{ number of variables of} \\
&\quad \text{the form } k_{ic} \text{ in } \psi(\sigma^u) - \text{ degree of } a_c \text{ in } \psi(\sigma^u)) \\
&= \text{number of paths in } \sigma^{v_c}
\end{aligned}$$

The number of paths in σ^{u_c} and $\rho_c(\sigma^{u_c})$ are the same as ρ_c maps monomials of degree 1 to monomials of degree 1.

For any vertex s which is adjacent to c, the degree of s in $\rho_c(\sigma^{u_c})$ is

$$\begin{aligned}
\deg_s(\rho_c(\sigma^{u_c})) &= \text{number of edges } s \leftrightarrow c \text{ in } \sigma^u \\
&= \text{number of edges } s \leftrightarrow c \text{ in } \sigma^v \\
&= deg_s(\rho_c(\sigma^{v_c})).
\end{aligned}$$

Now, for any two vertices i' and j' adjacent to c, the number of edges $i' \leftrightarrow j'$ in $\rho_c(\sigma^{u_c})$ is 0 as every path in $\rho_c(\sigma^{u_c})$ contains c. The number of edges $i' \leftrightarrow c$ in $\rho_c(\sigma^{u_c})$ is equal to the number of edges $i' \leftrightarrow c$ in σ^u, which is equal to the number of edges $i' \leftrightarrow c$ in σ^v.

Hence, we can conclude that $\psi_{G_c}(\rho_c(\sigma^{u_c})) - \psi_{G_c}(\rho_c(\sigma^{v_c})) = 0$. $\square$

By Theorem 4.4.2 we know that we can reach from $\rho_c(\sigma^{u_c})$ to $\rho_c(\sigma^{v_c})$ by making a finite set of moves from the set of 2×2 minors of $\Sigma_{A\cup C,B\cup C}$, for all possible 1-clique partitions of G_c. But from the map ρ_c we have that for each move $\sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'}$ in G_c there exists a corresponding move $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$ in G, where $i' \leftrightarrow j' \subseteq i \leftrightarrow j$ and $k' \leftrightarrow l' \subseteq k \leftrightarrow l$. In fact, there are many such corresponding moves corresponding to all the ways to pull back ρ_c.

Definition 3.4.3. Let G be a block graph and let c be a central vertex. We call two monomials σ^u and σ^v in the same fiber to be *similar at a vertex c* if the subgraph over

c and its adjacent vertices is the same for both the monomials.

For a given block graph G and a central vertex c, let S_c denote the set of all 2×2 minors of all matrices $\Sigma_{A \cup C, B \cup C}$ where (A, B, C) is a separation condition that is valid for G with $C = \{c\}$.

Proposition 3.4.4. *If a sequence of moves in G_c take $\rho_c(\sigma^{u_c})$ to $\rho_c(\sigma^{v_c})$, then there exist a corresponding sequence of moves in S_c which takes σ^u to a monomial which is similar to σ^v at c.*

Proof. We know that $\rho_c(\sigma^{u_c})$ and σ^u are similar at c by construction. So, it is enough to show that if m is a move in G_c and m' is the corresponding move in G, then m applied to $\rho_c(\sigma^{u_c})$ and m' applied to σ^u are similar at c. Let $m = \sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'}$ be a move in G_c acting on the paths $\sigma_{i'j'}, \sigma_{k'l'}$ in $\rho_c(\sigma^{u_c})$. Let $m' = \sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$ be its corresponding move in S_c acting on the paths σ_{ij}, σ_{kl} in σ^u. As $i' \leftrightarrow j' \subseteq i \leftrightarrow j$, $k' \leftrightarrow l' \subseteq k \leftrightarrow l$ and $c \in i' \leftrightarrow j'$ and $k' \leftrightarrow l'$, m and m' make the same changes at c in both the graphs. So, we can conclude that m applied to $\rho_c(\sigma^{u_c})$ and m' applied to σ^u are similar at c. $\square$

Once we have the set of moves which takes σ^u to a monomial which is similar to σ^v at c, we can apply the same procedure at the other central vertices as well. To show that this ends up producing two monomials that are similar at every central vertex it is necessary to check that the moves obtained for a different central vertex c' do not affect the structure previously obtained at c.

Proposition 3.4.5. *Let $m = \sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$ be a move obtained from a partition with $C = \{c\}$. Let V be the set of vertices in G. Then σ^u and m applied to σ^u are similar at $V \setminus c$.*

Proof. If s is any vertex which is not in $i \leftrightarrow j$ or $k \leftrightarrow l$, then σ^u and m applied to σ^u remain similar at s as the move does not make any change at s. If $s \neq c$ is a vertex in $i \leftrightarrow j$, we then consider 2 cases:

Case 1: $s \in i \leftrightarrow j$ and $s \notin k \leftrightarrow l$

Let $s \in i \leftrightarrow c$. As m converts $i \leftrightarrow c \leftrightarrow j$ to $i \leftrightarrow c \leftrightarrow l$, $i \leftrightarrow c$ is contained in $i \leftrightarrow l$. This implies that s and all the vertices in $i \leftrightarrow j$ adjacent to s are also present in $i \leftrightarrow l$. A similar argument applies for $s \in c \leftrightarrow j$.

Case 2: $s \in i \leftrightarrow j$ and $s \in k \leftrightarrow l$

Let $s \in i \leftrightarrow c$ and $s \in k \leftrightarrow c$. As m converts $i \leftrightarrow c \leftrightarrow j$ to $i \leftrightarrow c \leftrightarrow l$ and $k \leftrightarrow c \leftrightarrow l$ to $k \leftrightarrow c \leftrightarrow j$, $i \leftrightarrow c$ is contained in $i \leftrightarrow l$ and $k \leftrightarrow c$ is contained in $k \leftrightarrow j$. So s and all the vertices in $i \leftrightarrow j$ ($k \leftrightarrow l$) adjacent to s are present in $i \leftrightarrow l$ ($k \leftrightarrow j$). A similar argument applies for $s \in c \leftrightarrow j, c \leftrightarrow l$.

In both the cases, m preserves the structure of σ^u around the vertex s. Hence, σ^u and m applied to σ^u are similar at all the vertices in $V \setminus c$. □

Note an important key feature that follows from the proof of Proposition 4.4.13: If m can be obtained from two partitions (A_1, B_1, C_1) and (A_2, B_2, C_2) with different central vertices, then σ^u and m applied to σ^u are similar at the central vertices as well.

We now give a proof for the generalized version of Theorem 3.3.10.

Theorem 3.4.6. *Let G be a block graph. Then the shortest path ideal SP_G is generated by the set of all 2×2 minors of $\Sigma_{A \cup C, B \cup C}$, for all possible 1-clique partitions of G, i.e, $SP_G = CI_G$.*

Proof. Suppose that $c_1, \ldots, c_k$ are the central vertices of G. Let $S_1, \ldots S_k$ be the corresponding quadratic moves associated to each central vertex. Let $f = \sigma^u - \sigma^v \in SP_G$. By applying Proposition 3.4.4 and Proposition 4.4.13 together with Theorem 3.3.10, we can assume that σ^u and σ^v are similar at every vertex after applying moves from $S_1, \ldots, S_k$.

We can assume that σ^u and σ^v have no variables in common, otherwise we could delete this variable from both monomials and do an induction on dimension. So consider an arbitrary path $i \leftrightarrow j$ in σ^u which is not present in σ^v. We select the path in σ^v which has the highest number of common edges with $i \leftrightarrow j$. Let that path be $i' \leftrightarrow j'$ and let $s \leftrightarrow t$ be the common path in both the paths. Let s_1 and t_1 be the vertices adjacent to s and t respectively in $i \leftrightarrow j$. Similarly, let s' and t' be the vertices adjacent to s and t respectively in $i' \leftrightarrow j'$. Let p be the vertex in $s \leftrightarrow t$ adjacent to t (see Figure 4.13 for an illustration of the idea).

If we apply the map ρ_t on both the monomials, we get that there exists a path $p \leftrightarrow t_1$ in $\rho_t(\sigma^u)$ which is not in $\rho_t(\sigma^v)$. But as σ^u and σ^v are similar at t, there must exist a path $x \leftrightarrow y$ in σ^v containing $p \leftrightarrow t_1$. So, the move $m = \sigma_{i'j'}\sigma_{xy} - \sigma_{i'y}\sigma_{xj'}$ is a valid move as none of the vertices in $i' \leftrightarrow p$ can be adjacent to any vertex in $t_1 \leftrightarrow y$ (as it would form a closed circuit implying that $i' \leftrightarrow t$ is not the shortest path). Similarly, none of the vertices in $x \leftrightarrow p$ can be adjacent to any vertex in $t' \leftrightarrow j'$. Further, this move can be obtained from two different partitions with central vertices p and t respectively. So, by Proposition

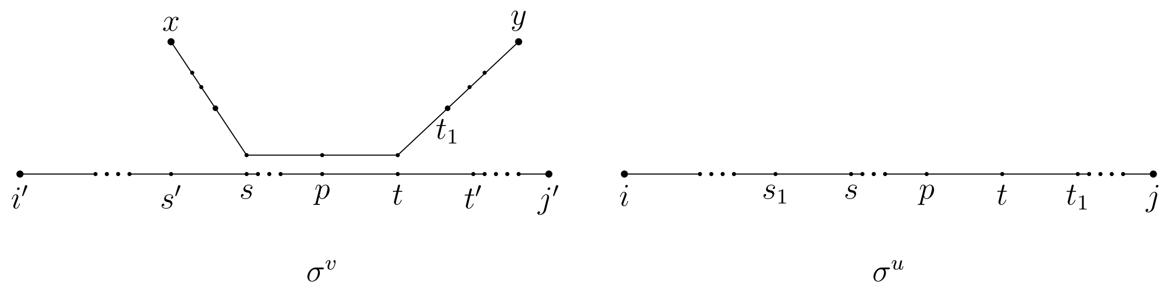


Figure 3.6: σ^v and σ^u and the construction of a move which brings them closer.

4.4.13 and the comment after its proof, we know that the move $\sigma_{i'j'}\sigma_{xy} - \sigma_{i'y}\sigma_{xj'}$ preserves the similarity of all the vertices.

Applying m on σ^v increases the length of the common path between $i \leftrightarrow j$ and $i' \leftrightarrow j'$ by at least 1, while keeping the monomials σ^u and m applied to σ^v similar at all the vertices. Repeating this process again, we can continue to shorten the length of the disagreement until the resulting monomials have a common monomial, in which case induction implies that we can use moves to connect these smaller degree monomials.

This implies that the set of binomials $S_1 \cup \cdots \cup S_k$ generates SP_G and hence $CI_G = SP_G$.

□

3.5 Initial term map and SAGBI bases

In this section we put all our previous results on shortest path maps together to prove Theorem 3.0.3. We also show that the set of polynomials $\{f_{ij} : 1 \leq i \leq j \leq n\}$ obtained from the inverse of K are a SAGBI basis for the $\mathbb{R}$-algebra they generate in the case of block graphs.

Proof of Theorem 3.0.3. We have already seen that $SP_G = CI_G \subseteq P_G$. We just need to show that $SP_G = P_G$ to complete the proof. Note that both SP_G and P_G are prime ideals so it suffices to show that they have the same dimension.

In both SP_G and P_G an upper bound on the dimension is equal to the number of vertices plus the number of edges in the graph. This follows because that is the number of free parameters in both parametrizations. In the case of P_G this upper bound is tight, because the map that sends $\Sigma \mapsto \Sigma^{-1}$ is the inverse map that recovers the entries of

K. Since $SP_G \subseteq P_G$ we have the $\dim SP_G \geq \dim P_G$. Hence they must have the same dimension. $\square$

Finally, we can show the SAGBI basis property for the polynomials $\{f_{ij} : 1 \leq i \leq j \leq n\}$. Recall the definition of a SAGBI basis (which stands for Subalgebra Analogue of Gröbner Basis for Ideals) as given in 1.4.6. See Chapter 11 of [31] for more details.

Let G be a block graph and let $F = \{f_{ij} : 1 \leq i \leq j \leq n\}$ be the polynomials appearing as the numerators in K^{-1}. To prove that F forms a SAGBI basis, we will use some key result on SAGBI bases. Note that if $\prec$ is a term order on $\mathbb{R}[K]$ induced by a weight vector ω, then this induces a partial term order on $\mathbb{R}[\Sigma]$ by declaring that the weight of the variable σ_{ij} is the weight of the largest monomial appearing in f_{ij}. Denote by ω^* this induced weight order on $\mathbb{R}[\Sigma]$.

Both the algebras $\mathbb{R}[F]$ and $\mathbb{R}[\{\mathrm{in}_\prec(f) : f \in F\}]$ have presentation ideals in $\mathbb{R}[\Sigma]$. In the first case, this presentation ideal is exactly P_G, the vanishing ideal of the Gaussian graphical model. That is, $\mathbb{R}[F] = \mathbb{R}[\Sigma]/P_G$. In the second case, this presentation is exactly SP_G, the shortest path ideal, since that is the ideal of relations among the shortest path monomials. That is, $\mathbb{R}[\{\mathrm{in}_\prec(f) : f \in F\}] = \mathbb{R}[\Sigma]/SP_G$.

A fundamental theorem on SAGBI bases applied in the specific case of these ideals says the following.

Theorem 3.5.1. *(Thm 11.4, [31]) The set $F \subseteq \mathbb{R}[K]$ is a SAGBI basis if and only if $\mathrm{in}_{\omega^*}(P_G) = SP_G$.*

Corollary 3.5.2. *Let G be a block graph. Then the set $F \subseteq \mathbb{R}[K]$ is a SAGBI basis of $\mathbb{R}[F]$.*

Proof. We have already shown that $SP_G = P_G$. By construction, every one of the binomials in SP_G is homogeneous with respect to the weighting ω^*. Indeed, this weighting is exactly the weighting that counts the multiplicity of each edge of σ^u and the $\deg_i(\sigma^u)$ as used in Section 3.4. But then $\mathrm{in}_{\omega^*}(P_G) = \mathrm{in}_{\omega^*}(SP_G) = SP_G$ as desired. By Theorem 3.5.1, this shows that F is a SAGBI basis. $\square$

3.6 Revised version of the Sturmfels-Uhler conjecture

In this section, we give the correct expression for the vanishing ideal of a graph G when it can be written as a 1-clique sum of two smaller graphs G_1 and G_2. The revised version of Conjecture 3.0.1 is as follows :

Theorem 3.6.1. *Let G be a 1-clique sum of two smaller graphs G_1 and G_2 attached at the vertex $\{c\}$. Then*

$$P_G = (P_{G_1} + P_{G_2} + \langle 2 \times 2 \textit{ minors of } \Sigma_{A\cup C, B\cup C}\rangle) : \langle \sigma_{cc}\rangle^{\infty}.$$

We first go through some necessary results required to prove this theorem. Let R_G denote the ideal

$$R_G = P_{G_1} + P_{G_2} + \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C, B\cup C}\rangle.$$

Then, we know that

$$R_G \subseteq (R_G : \sigma_{cc}^{\infty}) \subseteq P_G.$$

This implies that

$$\mathcal{L}^{-1} \subseteq V(P_G) \subseteq V(R_G : \sigma_{cc}^{\infty}) \subseteq V(R_G).$$

So, to prove that $(R_G : \sigma_{cc}^{\infty}) = P_G$, we first need to show that $V(R_G : \sigma_{cc}^{\infty}) = V(P_G)$. This would give us that the two ideals are same at least up to radical (by Corollary 1.3.21).

Now, $V(R_G : \sigma_{cc}^{\infty})$ can be written as $\overline{V(R_G) \setminus V(\sigma_{cc}^{\infty})}$. Let $M \in V(R_G) \setminus V(\sigma_{cc}^{\infty})$ be any arbitrary matrix. Then M satisfies all the polynomials in P_{G_1}, P_{G_2} and the rank constraints obtained from the 2×2 minors of $\Sigma_{A\cup C, B\cup C}$, along with the condition that $m_{cc} \neq 0$, where m_{cc} is the $(c, c)^{th}$ entry of M. As $CI_G \subseteq P_G$, we first prove the following:

Lemma 3.6.2. *Let G be a 1-clique sum of two graphs G_1 and G_2 attached at the vertex $\{c\}$. Then every matrix $M \in V(R_G) \setminus V(\sigma_{cc}^{\infty})$ satisfies all the conditional independence statements of CI_G.*

Proof. Let $A' \perp\!\!\!\perp B' | C'$ be a conditional independence statement of G where A', B', C' are disjoint subsets of $[n]$. Then C' separates A' from B' in G. Let (A, B, C) be the partition which separates G_1 from G_2, i.e $A = \{\text{vertices in } G_1 \setminus c\}$, $B = \{\text{vertices in } G_2 \setminus c\}$ and $C = \{c\}$.

Case 1: $c \in C'$

We write the sets A', B', C' as

$$A' = A_1 \cup A_2, \;\; B' = B_1 \cup B_2 \text{ and } \;\; C' = C_1 \cup C_2 \cup \{c\},$$

where A_1, B_1, C_1 are vertices in G_1 and A_2, B_2, C_2 are vertices in G_2. Assuming none of the sets A_i, B_i, C_i are empty, we arrange the rows of the submatrix $M_{A'\cup C', B'\cup C'}$ as (A_1, C_1, c, C_2, A_2) and the columns as (B_1, C_1, c, C_2, B_2). This divides the submatrix $M_{A'\cup C', B'\cup C'}$ into four blocks as

$$\begin{gathered} M_{\{A_1\cup C_1\cup c\},\{B_1\cup C_1\cup c\}}, \;\; M_{\{A_1\cup C_1\cup c\},\{c\cup C_2\cup B_2\}}, \\ M_{\{c\cup C_2\cup A_2\},\{B_1\cup C_1\cup c\}} \text{ and } M_{\{c\cup C_2\cup A_2\},\{c\cup C_2\cup B_2\}}. \end{gathered}$$

The blocks $M_{\{A_1\cup C_1\cup c\},\{c\cup C_2\cup B_2\}}$ and $M_{\{c\cup C_2\cup A_2\},\{B_1\cup C_1\cup c\}}$ are submatrices of $M_{A\cup C, B\cup C}$, which is of rank 1 (as it corresponds to the partition $(A, B, \{c\})$). So, the two blocks have rank ≤ 1. Now, as C' separates A' from B', we can say that $C_1 \cup \{c\}$ separates A_1 from B_1 in G_1 and $C_2 \cup \{c\}$ separates A_2 from B_2 in G_2. This gives us that the block $M_{\{A_1\cup C_1\cup c\},\{B_1\cup C_1\cup c\}}$ has rank $\leq |C_1| + 1$ and the block $M_{\{c\cup C_2\cup A_2\},\{c\cup C_2\cup B_2\}}$ has rank $\leq |C_2| + 1$ as they correspond to conditional independent statements in G_1 and G_2 respectively.

We now use the condition that $m_{cc} \neq 0$. As the blocks $M_{\{A_1\cup C_1\cup c\},\{c\cup C_2\cup B_2\}}$ and $M_{\{c\cup C_2\cup A_2\},\{B_1\cup C_1\cup c\}}$ have rank ≤ 1, all the entries of these two blocks (except the $(c, c)-$entry) can be turned into 0 by performing row and column operations. This would give us that the block $M_{\{A_1\cup C_1\},\{B_1\cup C_1\}}$ has rank $\leq |C_1|$ (as the column $M_{\{A_1\cup C_1\cup c\},\{c\}}$ cannot be generated by the remaining columns of $M_{\{A_1\cup C_1\cup c\},\{B_1\cup C_1\cup c\}}$). Similarly, the block $M_{\{C_2\cup A_2\},\{C_2\cup B_2\}}$ has rank $\leq |C_2|$. Hence, we can conclude that the submatrix $M_{A'\cup C', B'\cup C'}$ has rank $\leq |C_1| + 1 + |C_2| = |C'|$ and that M satisfies the conditional independence statement $A' \perp\!\!\!\perp B' | C'$.

Case 2: $c \notin C'$

Let $c \in A'$. To show that the submatrix $M_{A'\cup C', B'\cup C'}$ has rank $\leq |C'|$, we look at the vectors $M_{c, B_1\cup C_1}$ and $M_{c, C_2\cup B_2}$. If the vector $M_{c, B_1\cup C_1}$ is non zero, then we can say

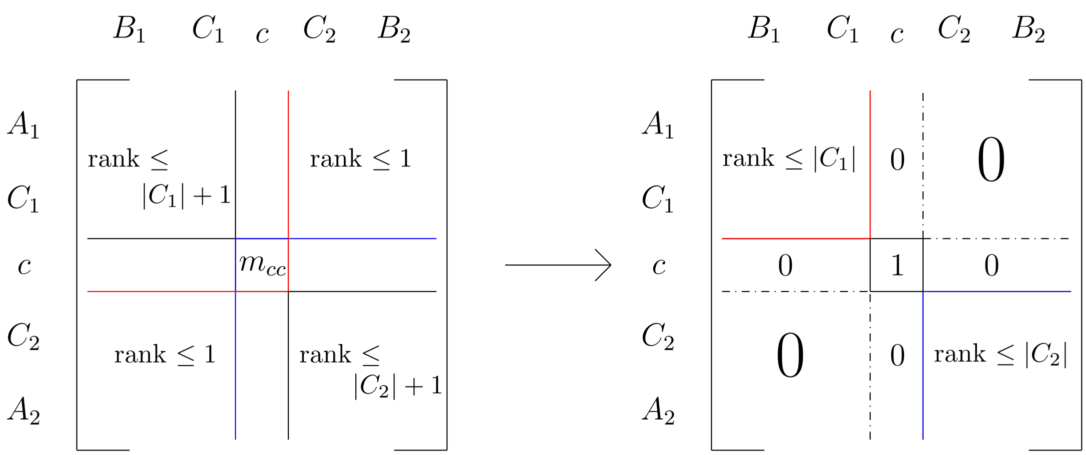


Figure 3.7: The matrix M and the possible ranks of each submatrix

that $M_{A'\cup C',B_1\cup C_1}$ has rank $\leq |C_1|$ as $M_{A_1\cup C_1\cup c,B_1\cup C_1}$ has rank $\leq |C_1|$. Similar argument follows for the submatrix $M_{A'\cup C',C_2\cup B_2}$ if the vector $M_{c,C_2\cup B_2}$ is non zero. Now, if the vector $M_{c,B_1\cup C_1}$ is a zero vector, we look at the submatrix $M_{A'\cup C',c\cup B'\cup C'}$. As the block $M_{c\cup C_2\cup A_2,B_1\cup C_1\cup c}$ has rank ≤ 1, we can conclude that all the entries in $M_{C_2\cup A_2,B_1\cup C_1}$ are zero (as $m_{cc} \neq 0$). Thus we can say that $M_{A'\cup C',B_1\cup C_1}$ has rank $\leq |C_1|$. Using the same argument on $M_{c,C_2\cup B_2}$, we can say that $M_{A'\cup C',C_2\cup B_2}$ has rank $\leq |C_2|$ and hence $M_{A'\cup C',B'\cup C'}$ has rank $\leq |C_1| + |C_2| = |C'|$.

The cases $c \in A_2, B_1, B_2$ and $c \notin A' \cup B'$ follow in the similar way. In either case if any of the set is empty, say $A_2 = \emptyset$, then the block $M_{c\cup C_2\cup A_2,c\cup C_2\cup B_2}$ is a $|C_2|+1 \times |C_2|+1+|B_2|$ matrix which always has rank $\leq |C_2| + 1$. $\square$

So, by Lemma 3.6.2 we can conclude that $V(R_G : \sigma_{cc}^{\infty}) \subseteq V(CI_G)$, which implies

$$CI_G \subseteq (R_G : \sigma_{cc}^{\infty}).$$

We now state a Proposition from [34].

Proposition 3.6.3. *(Proposition 6.1, [34]) Let $I \subseteq \mathbb{C}[\mu, \Sigma]$ be the vanishing ideal for a Gaussian model. Let $H \cup O = [n]$ be a partition of the random variables into hidden and observed variables H and O. Then*

$$I_O := I \cap \mathbb{C}[\mu_i, \sigma_{ij} | i, j \in O]$$

is the vanishing ideal for the partially observed model.

If G is a 1-clique sum of G_1 and G_2 with central vertex c, then marginalizing over the vertices in $G_2 \setminus \{c\}$ gives us G_1 as there are no edges between the vertices of $G_1 \setminus \{c\}$ and $G_2 \setminus \{c\}$. So, if we take H as the vertices in $G_2 \setminus \{c\}$ and O as the vertices in G_1, then by Proposition 3.6.3 we can conclude that

$$P_{G_1} = P_G \cap \mathbb{C}[\sigma_{ij} | i, j \in G_1],$$

i.e, P_{G_1} is an elimination ideal of P_G. A similar result follows for P_{G_2} by interchanging the sets H and O and we get

$$P_{G_2} = P_G \cap \mathbb{C}[\sigma_{ij} | i, j \in G_2].$$

In the next proposition we show that the two ideals P_G and $(R_G : \sigma_{cc}^{\infty})$ have the same varieties.

Proposition 3.6.4. *If G is a 1-clique sum of two smaller graphs G_1 and G_2 with central vertex c, then $V(P_G) = V(R_G : \sigma_{cc}^{\infty})$.*

Proof. Let n be the number of vertices in G and n_1, n_2 be the number of vertices in G_1 and G_2 respectively. Then, $n_1 + n_2 = n + 1$. Now, as $(R_G : \sigma_{cc}^{\infty}) \subseteq P_G$, $V(P_G) \subseteq V(R_G : \sigma_{cc}^{\infty})$. So, we only need to show that $V(R_G : \sigma_{cc}^{\infty}) \subseteq V(P_G)$. We use the fact that $P_G = I(\mathcal{L}^{-1})$, which implies $V(P_G)$ is equal to $V(I(\mathcal{L}^{-1})) = \overline{\mathcal{L}^{-1}}$, the Zariski closure of $\mathcal{L}^{-1}$. If $M \in V(R_G) \setminus V(\sigma_{cc}^{\infty})$ be any arbitrary matrix, then we have the following two cases :

Case I: M is invertible:

Let i and j be two vertices of G which do not have an edge between them. Then $i \perp\!\!\!\perp j | n \setminus \{i, j\}$ is a conditional independence statement of G. So, the $n-1$ minors of all the non edges in G lie in CI_G. As $CI_G \subseteq P_G$, by Lemma 3.6.2 all the non edge positions of M^{-1} are 0. Then M^{-1} can be written as a linear combination of the basis matrices in $\mathcal{L}$. So, $M \in \mathcal{L}^{-1} \subseteq V(P_G)$.

Case II: M is not invertible:

Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be the subspaces obtained from the subgraphs G_1 and G_2 respectively. Then every matrix in $V(R_G) \setminus V(\sigma_{cc}^{\infty})$ is of the form of M as shown in Figure 3.8, where $A_{n_1 \times n_1} \in V(P_{G_1}) = \overline{\mathcal{L}_1^{-1}}$, $B_{n_2 \times n_2} \in V(P_{G_2}) = \overline{\mathcal{L}_2^{-1}}$ and $m_{cc} \neq 0$. Again by Lemma 3.6.2, we know that M satisfies all the conditional independence statements of the form $i \perp\!\!\!\perp j | c$ for all $i \in G_1 \setminus \{c\}, j \in G_2 \setminus \{c\}$. Using the fact that $m_{cc} \neq 0$, we can replace every entry m_{ij} with the relation

$$m_{ij} = \frac{m_{ic} m_{cj}}{m_{cc}},$$

for all $i \in G_1 \setminus \{c\}, j \in G_2 \setminus \{c\}$. Now, expanding the determinant of M along the first column (when $n_1 < n_2$) or the last column (when $n_2 < n_1$), we get that

$$\det M = \frac{\det A \cdot \det B}{m_{cc}}.$$

So, if M is non invertible, then either of A or B has to be non-invertible. Let B be the non-invertible matrix. Then for any given $\epsilon_2 > 0$, there exists a matrix S_2 with $||S_2||_\infty = \epsilon_2$ such that $B + S_2 \in \mathcal{L}_2^{-1}$.

Adding S_2 with B changes the (n_1, n_1) position of A. But as A is an interior point of $\mathcal{L}_1^{-1}$, for any given $\epsilon_1 > 0$, there must exist a matrix S_1 with $||S_1||_\infty = \epsilon_1$ such that $A + S_1 \in \mathcal{L}_1^{-1}$. We select the matrix S_1 such that $S_1(n_1, n_1) = S_2(1, 1)$.

For any given $\epsilon > 0$, our objective is to construct an $n \times n$ matrix S with block diagonals S_1 and S_2 (as shown in Figure 3.8) and $||S||_\infty \leq \epsilon$ such that $M + S \in \mathcal{L}^{-1}$. This would imply that any neighbourhood of M will contain a matrix from $\mathcal{L}^{-1}$ and M could be approximated by that matrix. As $A + S_1 \in \mathcal{L}_1^{-1}$, its (n_1, n_1) entry cannot be zero. So, we construct the matrix S_3 using the fact that $C + S_3$ has rank one. Equating all the 2×2 minors of $C + S_3$ which contains the nonzero term $C(1, n_1) + S_3(1, n_1)$(which is equal to $A(n_1, n_1) + S_1(n_1, n_1)$) to zero, we get

$$\begin{aligned} S_3(i,j) &= \frac{(A(i,n_1) + S_1(i,n_1)) \cdot S_2(1, j+1) + S_1(i,n_1) \cdot B(1, j+1) - C(i,j) \cdot S_1(n_1,n_1)}{A(n_1,n_1) + S_1(n_1,n_1)} \\ &\leq \frac{(||A||_\infty + \epsilon_1) \cdot \epsilon_2 + \epsilon_1 \cdot ||D||_\infty + ||B||_\infty \cdot \epsilon_1}{||A||_\infty} \\ &< \epsilon, \end{aligned}$$

for all $1 \leq i \leq n - n_1$ and $1 \leq j \leq n - n_2$. So, for any given M and $\epsilon > 0$, we can select ϵ_1 and ϵ_2 accordingly such that the above inequality holds and $||S||_\infty \leq \epsilon$. Hence, we can conclude that M is a limit point of $\mathcal{L}^{-1}$, which implies that $M \in \overline{\mathcal{L}^{-1}}$. □

Next, we prove that the ideal $P_{G_1} + P_{G_2}$ is a prime ideal. In order to prove this, we first state a few results.

$$M = \begin{bmatrix} A & & C \\ & m_{cc} & \\ C^T & & B \end{bmatrix} \qquad S = \begin{bmatrix} S_1 & & S_3 \\ & & \\ S_3^T & & S_2 \end{bmatrix}$$

Figure 3.8: Non invertible matrix M and perturbation matrix S

Proposition 3.6.5. *(Proposition 5.17, [23]) Let $\mathbb{K}$ be an algebraically closed field and let A, B be $\mathbb{K}$-algebras with A finitely generated. If A and B are integral domains, then so is $A \otimes_{\mathbb{K}} B$.*

Proposition 3.6.6. *Let $\mathbb{K}$ be an algebraically closed field and P, Q be finitely generated prime ideals in the polynomial rings $\mathbb{K}[x_1, x_2, ..., x_m]$ and $\mathbb{K}[y_1, y_2, ..., y_n]$ respectively. Then $P + Q$ is a prime ideal in $\mathbb{K}[x_1, x_2, ..., x_m, y_1, y_2, ..., y_n]$.*

Proof. We know that $\mathbb{K}[x_1, x_2, ..., x_m, y_1, y_2, ..., y_n] \cong \mathbb{K}[x_1, x_2, ..., x_m] \otimes \mathbb{K}[y_1, y_2, ..., y_n] = \mathbb{K}[\overline{x}] \otimes \mathbb{K}[\overline{y}]$. Under this isomorphism, the ideal $P + Q \subset \mathbb{K}[\overline{x}, \overline{y}]$ corresponds to the ideal $P \otimes \mathbb{K}[\overline{y}] + \mathbb{K}[\overline{x}] \otimes Q$. Since $P \otimes \mathbb{K}[\overline{y}] + \mathbb{K}[\overline{x}] \otimes Q$ is the kernel of the canonical map

$$\begin{aligned} \mathbb{K}[\overline{x}] \otimes \mathbb{K}[\overline{y}] &\rightarrow \mathbb{K}[\overline{x}]/P \otimes \mathbb{K}[\overline{y}]/Q \\ (f(\overline{x}) \otimes g(\overline{y})) &\rightarrow (f(\overline{x}) + P \otimes g(\overline{y}) + Q), \end{aligned}$$

$P \otimes \mathbb{K}[\overline{y}] + \mathbb{K}[\overline{x}] \otimes Q$ is a prime ideal if and only if $\mathbb{K}[\overline{x}]/P \otimes \mathbb{K}[\overline{y}]/Q$ is an integral domain. As P and Q are prime ideals, $\mathbb{K}[\overline{x}]/P$ and $\mathbb{K}[\overline{y}]/Q$ are integral domains. So, by Proposition 3.6.5 we can conclude that $\mathbb{K}[\overline{x}]/P \otimes \mathbb{K}[\overline{y}]/Q$ is an integral domain and hence $P + Q$ is a prime ideal. $\square$

Theorem 3.6.7. *(Theorem 9.6, [15]) Let $I \subset \mathbb{K}[y_1, ..., y_n]$ be an ideal and $J \subset \mathbb{K}[x_0, ..., x_n]$ be its homogenization with respect to x_0. Suppose that $f_1, ..., f_r$ is a Gröbner basis for I with respect to some graded order $>$. Then the homogenizations $F_1, ..., F_r$ of $f_1, ..., f_r$ generate J.*

Proposition 3.6.8. *If G is a 1-clique sum of G_1 and G_2 with central vertex c, then $P_{G_1} + P_{G_2}$ is a prime ideal.*

Proof. Let P_1 and P_2 be the dehomogenizations of P_{G_1} and P_{G_2} respectively with respect to σ_{cc}. As P_{G_1} and P_{G_2} are prime ideals, so are P_1 in $\mathbb{C}[\sigma_{ij} : i \in G_1, j \in G_1 \setminus c]$ and P_2 in $\mathbb{C}[\sigma_{ij} : i \in G_2, j \in G_2 \setminus c]$. Since P_1 and P_2 are contained in rings with disjoint variables and $\mathbb{C}$ is algebraically closed, by Proposition 3.6.6 we know that $P_1 + P_2$ is a prime ideal in $\mathbb{C}[\sigma_{ij} : i, j \in G]$.

We now homogenize the ideal P_1+P_2 with respect to σ_{cc}. We need to show that homogenizing P_1+P_2 gets us back to $P_{G_1}+P_{G_2}$. Let $\{f_1, \dots, f_r\}$ and $\{g_1, \dots, g_s\}$ be the Gröbner bases of P_1 and P_2 respectively. As P_1 and P_2 lie in disjoint rings, $\{f_1, \dots, f_r, g_1, \dots, g_s\}$ forms a Gröbner basis of $P_1 + P_2$. Let $\bar{f}_i$ and $\bar{g}_j$ be the homogenizations of f_is and g_js respectively. Then each $\bar{f}_i$ and $\bar{g}_j$ lies in P_{G_1} and P_{G_2} respectively (as P_{G_1} and P_{G_2} are both prime ideals). If J is the homogenization of $P_1 + P_2$, then we know that J is a prime ideal contained in $P_{G_1} + P_{G_2}$ and is generated by $\{\bar{f}_1, \dots, \bar{f}_r, \bar{g}_1, \dots, \bar{g}_s\}$ (by Theorem 3.6.7).

On the other hand, the homogenization of the dehomoginization of an ideal is always contains the ideal. Thus, $P_{G_1} + P_{G_2}$ is contained in J. This proves that $J = P_{G_1} + P_{G_2}$, and so $P_{G_1} + P_{G_2}$ is prime. □

Now that we have all the necessary results, we give a proof for Theorem 3.6.1.

Proof of Theorem 3.6.1. From Proposition 3.6.4 we know that the two ideals are same up to radicals, i.e, $P_G = \sqrt{(R_G : \sigma_{cc}^{\infty})}$. Now, let $f \in P_G$ be any arbitrary polynomial. We need to show that $f \in (R_G : \sigma_{cc}^{\infty})$. If f has variables of the form σ_{ij} where $i \in G_1 \setminus \{c\}$ and $j \in G_2 \setminus \{c\}$, then by multiplying enough powers of σ_{cc} to f, we can replace each $\sigma_{ij}\sigma_{cc}$ with $\sigma_{ic}\sigma_{cj}$ as the 2×2 minors of $\Sigma_{A\cup C, B\cup C}$ lie in P_G. This gives us that

$$f \cdot \sigma_{cc}^n + g = h \in P_G,$$

where $g \in \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C, B\cup C}\rangle$ and h is a polynomial in P_G which does not have any variable of the form σ_{ij} with $i \in G_1 \setminus \{c\}$ and $j \in G_2 \setminus \{c\}$.

By the definition of radicals and saturation, we know that $h^m \cdot \sigma_{cc}^m \in R_G$ for some $m > 0$. But as $h^m \cdot \sigma_{cc}^m$ does not have any variable of the form σ_{ij} with $i \in G_1 \setminus \{c\}$ and $j \in G_2 \setminus \{c\}$, we can say that $h^m \cdot \sigma_{cc}^m \in P_{G_1} + P_{G_2}$. Now, by Proposition 3.6.8, we know that $P_{G_1} + P_{G_2}$ is a prime ideal. So h must lie in $P_{G_1} + P_{G_2}$ as $\sigma_{cc}^m \notin P_{G_1} + P_{G_2}$. Thus, we have

$$h \in P_{G_1} + P_{G_2} \subset R_G \text{ and } g \in \langle 2 \times 2 \text{ minors of } \Sigma_{A\cup C, B\cup C}\rangle \subseteq R_G,$$

which implies that

$$f \cdot \sigma_{cc}^{n} = h - g \in R_G.$$

Hence, we can conclude that $f \in (R_G : \sigma_{cc}^{\infty})$. $\square$

Chapter 4

Directed acyclic Gaussian graphical models with toric vanishing ideals

Graphical models can be defined by undirected graphs, directed acyclic graphs, or graphs that use a mixture of different types of edges. In this chapter, we only consider those models which can be defined by directed acyclic graphs (DAGs). A DAG specifies a graphical model in two ways. The first way is via a combinatorial parametrization of covariance matrices that belong to the model and the second way is via conditional independence statements implied by the graph. The factorization theorem (Theorem 3.27,[21]) says that these two methods yield the same family of probability distribution functions.

The combinatorial parametrization of the covariance matrices for a Gaussian DAG model is also known as the *simple trek rule* (see e.g. [36]). The vanishing ideal of the Gaussian DAG model, I_G, is equal to the set of polynomials in the covariances that are zero when evaluated at the simple trek rule. The algebraic interpretation of the second method, i.e., the conditional independence statements, give us the conditional independence ideal CI_G. An important question that arises in the algebraic study of graphical models is to determine the DAGs where the vanishing ideal and the conditional independence ideal are the same. Although it is still an open problem, some past work and computational study [34] has been done in this direction.

The study of generators of the vanishing ideal I_G is an important problem for constraint-based inference for inferring the structure of the underlying graph from data. For example, the TETRAD procedure [28] specifically tests the degree 2 generators (tetrads) of the vanishing ideal for directed graphs to determine if the graphs have certain underlying features. For the undirected case, we showed in chapter 3 that the vanishing ideal is generated by polynomials of degree at most 2 if and only if G is a 1-clique sum of complete graphs [25]. Our goal in the present chapter is to study the analogous problem for Gaussian DAG models. While we are not able to give a complete characterization of the DAGs that have degree two generators, and are toric, we develop methods to construct DAGs having toric vanishing ideals and understand the generating set of the vanishing ideal when it is toric. In particular, we develop three techniques to construct such DAGs with toric vanishing ideals from smaller DAGs with the same property. These are called *safe gluing, gluing at sinks* and *adding a new sink.*

One of the important tools that we use throughout the chapter is the *shortest trek map* ψ_G. We show that in some instances, the shortest trek map and the simple trek map have the same kernel, namely the ideal I_G. Being a monomial map, the kernel of ψ_G, which we denote by ST_G, is always a toric ideal. Although I_G, CI_G and ST_G are not always equal, we are interested in characterizing the DAGs where these three ideals are the same. This not only tells us when the vanishing ideals are toric but we also get to know the structure of the generators of I_G from ST_G. We show that when two DAGs G_1 and G_2 have toric vanishing ideals then gluing at sinks and adding a new sink always produces a new graph G with toric vanishing ideal. We also conjecture that the same is true for the safe gluing of G_1 and G_2, and prove a number of partial results towards this conjecture. Further, we conjecture that every DAG whose vanishing ideal is toric can be obtained as a combination of these three operations starting with complete DAGs.

The chapter is organized as follows. Section 4.1 gives an explicit description of the simple trek rule. We recall the notion of *directed separation*, which is used in defining the conditional independence ideal. We also introduce the shortest trek map, and the shortest trek ideal ST_G.

In Section 4.2 we look at some existing results from [21; 25; 34], about gluing graphs where that preserve nice properties of the vanishing ideals. Using those results as inspiration, we construct a general operation which we call the "*safe gluing*" of DAGs. Safe gluing is a type of clique sum for DAGs such that most of the vertices in the clique are colliders along any paths passing through the clique. We conjecture that when the vanishing ideals of two DAGs are the same as the kernel of their shortest trek maps, then a safe gluing of the two DAGs would also have a toric vanishing ideal. We prove this conjecture in some special cases.

In Section 4.3 we look at two more ways to construct new DAGs where the toric property is preserved, which we call *gluing at sinks* and *adding a new sink*. We analyze the generators of ST_G in Section 4.4 and show that the safe gluing action preserves the toric property when ST_G equals CI_G for the smaller DAGs, which further provides evidence for our Conjecture 4.2.14. In Section 4.5, we conclude with some conjectures which may be used to formulate a complete characterization of all possible DAGs having toric vanishing ideal.

4.1 Preliminaries

This section primarily is concerned with preliminary definitions that we will use throughout the chapter. We introduce the Gaussian DAG models, and their vanishing ideals I_G. We explain the concept of d-separation and how this leads to the conditional independence ideal CI_G. Finally, we introduce the shortest trek map, and the corresponding shortest trek ideal ST_G.

Let $G = (V, E)$ be a directed acyclic graph with vertex set $V(G)$ and edge set $E(G)$. As there are no directed cycles in the graph, we assume that the vertices are numerically ordered, i.e, $i \to j \in E(G)$ only if $i < j$. A *parent* of a vertex j is a node $i \in V(G)$ such that $i \to j$ is an edge in G. We denote the set of all parents of a vertex j by $\mathrm{pa}(j)$. Given such a directed acyclic graph, we introduce a family of normal random variables that are related to each other by recursive regressions.

To each node i in the graph, we introduce two random variables X_i and ε_i. The ε_i are independent normal variables $\varepsilon_i \sim \mathcal{N}(0, \omega_i)$ with $\omega_i > 0$. For simplicity, we assume that all our random variables have mean zero. The recursive regression property of the DAG gives an expression for each X_j in terms of ε_j, X_i with $i < j$ and some regression parameters $\lambda_{ij} \in \mathbb{R}$ assigned to the edges $i \to j$ in the graph,

$$X_j = \sum_{i \in pa(j)} \lambda_{ij} X_i + \varepsilon_j.$$

From this recursive sequence of regressions, we can solve for the covariance matrix Σ of the jointly normal random vector X. This covariance matrix is given by a simple matrix factorization in terms of the regression parameters λ_{ij} and the variance parameters ω_i.

Let D be the diagonal matrix D =diag$(\omega_1, \omega_2, \ldots, \omega_m)$ and let L be the $m \times m$ upper triangular matrix with $L_{ij} = \lambda_{ij}$ if $i \to j$ is an edge in G and $L_{ij} = 0$ otherwise.

Proposition 4.1.1. *([26], Section 8). The covariance matrix of the normal random variable $X = \mathcal{N}(0, \Sigma)$ is given by the matrix factorization*

$$\Sigma = (I - L)^{-T} D (I - L)^{-1}. \tag{4.1}$$

The vanishing ideal of the Gaussian graphical model is denoted by I_G and it is an ideal in the polynomial ring $\mathbb{C}[\Sigma] = \mathbb{C}[\sigma_{ij} : 1 \leq i \leq j \leq n]$. This is the ideal of all polynomials in the entries of the covariance matrix Σ, that evaluate to zero for every choice of the parameters ω_i and λ_{ij}. That is:

$$I_G = \left\{ f \in \mathbb{C}[\Sigma] : f((I - L)^{-T} D (I - L)^{-1}) = 0 \right\}.$$

One way to obtain I_G is to eliminate the variables ω_i and λ_{ij} from the following system of equations:

$$\Sigma - (I - L)^{-T} D (I - L)^{-1} = 0.$$

Using elimination is computationally expensive, and we are interested in theoretical results that characterize the generators of I_G when possible.

A variant on the parametrization (4.1) is the *simple trek rule* which is a common and useful representation of the covariances in a Gaussian DAG model. In order to explain the simple terk rule, we first need to go through a few definitions. A *collider* is a pair of edges $i \to k$, $j \to k$ with the same head. If a path contains the edges $i \to k$ and $j \to k$, then the vertex k is called the *collider vertex* within that path. A path that does not repeat any vertex is called a *simple path*. Let $T(i, j)$ be a collection of simple paths P in G from i to j such that there is no collider in P. Such a colliderless path is called a *simple trek*. For the rest of the chapter, we consider treks to be simple treks. We will often use the notation $i \rightleftharpoons j$ to denote a specific trek between i and j, as this helps to call attention to the endpoints. When we speak generically of a trek, we often denote it by P.

Each trek P has a unique *topmost* element top(P), which is the point where orientation of the path changes. A trek P between i and j can also be represented by a pair of sets (P_i, P_j), where P_i corresponds to the path from top(P) to i and P_j corresponds to the path from top(P) to j. The vertex top(P) is also called the *common source* of P_i and P_j.

To get the simple trek rule, we introduce an alternate parameter a_i associated to each node i in the graph and is defined as the variance of X_i, i.e. $\sigma_{ii} = a_i$. We expand the matrix product for Σ in Proposition 4.1.1 by taking the sum over all treks $P \in T(i, j)$. Using this expansion along with the alternate parameters a_i, we get the following definition :

Definition 4.1.2. For a given DAG G, the *simple trek rule* is defined as the rule in which the covariance σ_{ij} is mapped to the sum of all possible simple treks from i to j in G. We represent the rule as a ring homomorphism ϕ_G where

$$\begin{aligned} \phi_G : \mathbb{C}[\sigma_{ij} : 1 \leq i \leq j \leq n] &\rightarrow \mathbb{C}[a_i, \lambda_{ij} : i, j \in [n], i \rightarrow j \in E(G)], \\ \sigma_{ij} &\mapsto \sum_{P \in T(i,j)} a_{\mathrm{top}(P)} \prod_{k \rightarrow l \in P} \lambda_{kl}. \end{aligned}$$

By Proposition 2.3 [34] we know that the kernel of the homomorphism ϕ_G equals the vanishing ideal I_G of the model. We illustrate the simple trek rule with an example.

Example 4.1.3. Let G_1 be a directed graph on four vertices with edges $1 \rightarrow 2, 1 \rightarrow 3, 1 \rightarrow 4, 2 \rightarrow 3$ and $2 \rightarrow 4$ (this is graph G_1 in Figure 4.3). The homomorphism ϕ_G is given by

$$\begin{aligned} &\sigma_{11} \mapsto a_1 && \sigma_{23} \mapsto a_2\lambda_{23} + a_1\lambda_{12}\lambda_{13} \\ &\sigma_{12} \mapsto a_1\lambda_{12} && \sigma_{24} \mapsto a_2\lambda_{24} + a_1\lambda_{12}\lambda_{14} \\ &\sigma_{13} \mapsto a_1\lambda_{13} + a_1\lambda_{12}\lambda_{23} && \sigma_{33} \mapsto a_3 \\ &\sigma_{14} \mapsto a_1\lambda_{14} + a_1\lambda_{12}\lambda_{24} && \sigma_{34} \mapsto a_2\lambda_{23}\lambda_{24} + a_1\lambda_{13}\lambda_{14} \\ &\sigma_{22} \mapsto a_2 && \sigma_{44} \mapsto a_4 \end{aligned}$$

The ideal I_G is generated by a degree 3 polynomial given by

$$I_G = \langle \sigma_{13}\sigma_{14}\sigma_{22} - \sigma_{12}\sigma_{14}\sigma_{23} - \sigma_{12}\sigma_{13}\sigma_{24} + \sigma_{11}\sigma_{23}\sigma_{24} + \sigma_{12}^2\sigma_{34} - \sigma_{11}\sigma_{22}\sigma_{34} \rangle.$$

We now look at the notion of *directed separation* (also known as d-separation). The d-separation criterion is used to construct the *conditional independence* ideal CI_G.

Definition 4.1.4. Let G be a DAG with n vertices. Let A, B and C be disjoint subsets of $[n]$. Then C *d-separates* A and B if every path in G connecting a vertex $i \in A$ to a vertex $j \in B$ contains a vertex k that is either

i) a non-collider that belongs to C or
ii) a collider that does not belong to C and has no descendants that belong to C.

A key result for DAG models relates conditional independence to d-separation (see e.g. Sec. 3.2.2, [21]).

Proposition 4.1.5. *The conditional independence statement $A \perp\!\!\!\perp B | C$ holds for the directed Gaussian model associated to G if and only if C d-separates A from B in G.*

Let A, B and C be disjoint subsets of $[n]$. The normal random vector $X \sim \mathcal{N}(\mu, \Sigma)$ satisfies the conditional independence constraint $A \perp\!\!\!\perp B | C$ if and only if the submatrix $\Sigma_{A\cup C, B\cup C}$ has rank less than or equal to $|C|$. Combining this result with the definition of d-separation, we have the following:

Definition 4.1.6. The *conditional independence ideal* of G is defined as the ideal generated by the set of all d-separations in G, that is,

$$CI_G = \langle (\#C + 1) \text{ minors of } \Sigma_{A\cup C, B\cup C} |\ C\ d\text{-separates } A \text{ from } B \text{ in } G \rangle.$$

Note that every covariance matrix in the Gaussian DAG model satisfies the conditional independence constraints obtained by d-separation. This means that $CI_G \subseteq I_G$. In fact, the variety of CI_G defines the model inside the cone of positive definite matrices. Still, one would like to understand when $CI_G = I_G$. Towards this end, we study the related question of when I_G and, hence, CI_G are toric.

Example 4.1.7. Let G be a DAG with 4 vertices as shown in Figure 4.1. Observe that there exists no trek between the vertices 1 and 2 as the path $1 \to 3 \leftarrow 2$ has a collider at 3 and the other path $1 \to 3 \to 4 \leftarrow 2$ has a collider at 4. So, we have that $\sigma_{12} \in CI_G$.

We now look at the two paths $1 \to 3 \to 4$ and $1 \to 3 \leftarrow 2 \to 4$ between 1 and 4. In the first path, 3 is the only vertex in the path, which is also a non-collider. So, any d-separating set of 1 and 4 must contain 3. But $\{3\}$ is not enough to d-separate 1 from 4 as 3 is a collider vertex in the second path. So, we add the vertex 2 to the d-separating set which gives us that $\{2, 3\}$ d-separates 1 from 4. This implies that the 3×3 minors of $\Sigma_{\{1,2,3\},\{2,3,4\}} \in CI_G$.

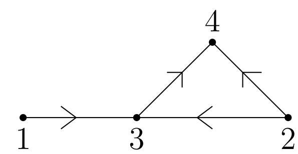


Figure 4.1: A DAG G with 4 vertices

Computing I_G and CI_G gives us that

$$I_G = CI_G = \langle \sigma_{12}, \sigma_{12}\sigma_{23}\sigma_{34} - \sigma_{12}\sigma_{33}\sigma_{24} - \sigma_{13}\sigma_{22}\sigma_{34} + \sigma_{13}\sigma_{23}\sigma_{24} + \sigma_{14}\sigma_{22}\sigma_{33} - \sigma_{14}\sigma_{23}^2 \rangle,$$

where the second generator of CI_G is the determinant of $\Sigma_{\{1,2,3\},\{2,3,4\}}$.

Proposition 4.1.8. *Let G be a DAG such that there exists a unique simple trek (or no trek) between any two vertices of G. Then the simple trek rule is a monomial map hence I_G is toric.*

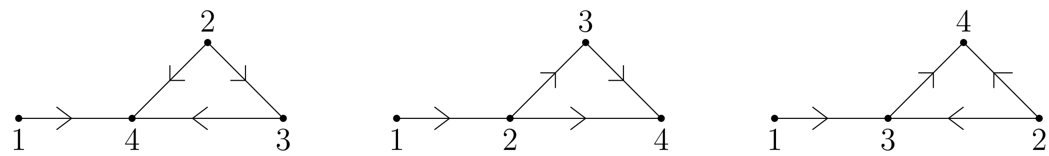
Proof. As shown in Definition 4.1.2, the simple trek rule maps σ_{ij} to the sum of all the treks between i and j. So, if there exists a unique trek (or no trek) between any two vertices of G, then the simple trek rule becomes a monomial map and hence I_G is toric. $\square$

Proposition 4.1.8 already shows that the DAGs where I_G is a toric ideal can be quite complicated.

Example 4.1.9. Let G be an undirected graph, and form a DAG by replacing each undirected edge $i - j$ with two directed edges $v_{i,j} \to i$ and $v_{i,j} \to j$, where $v_{i,j}$ is a new vertex. The resulting DAG $\hat{G}$, has a unique simple trek between any pair of vertices, or no trek, and so the ideal $I_{\hat{G}}$ is toric.

A second natural source of DAGs which have a toric vanishing ideal are DAGs that have a natural connection to undirected graphs. In the previous chapter, we characterized the undirected Gaussian graphical models which have toric vanishing ideals (Theorem 3.0.3).

Recall that a *clique sum* of graphs G_1 and G_2 is a new graph obtained by identifying two cliques of the same size in G_1 and G_2. In a k-clique sum, the cliques identified each have size k. While Theorem 3.0.3 is a good starting point for the analysis of DAG models,



(i) G_1 (ii) G_2 (iii) G_3

Figure 4.2: 3 different DAGs having the same underlying undirected graph.

the underlying undirected structure is not enough to characterize whether a DAG yields a toric vanishing ideal.

Example 4.1.10. Consider the three DAGs as given in Figure 4.2. Computing the vanishing ideals I_{G_i}, we get

$$\begin{aligned}
I_{G_1} &= \langle \sigma_{12}, \sigma_{13} \rangle \\
I_{G_2} &= \langle \sigma_{12}\sigma_{23} - \sigma_{13}\sigma_{22}, \sigma_{12}\sigma_{24} - \sigma_{14}\sigma_{22}, \sigma_{13}\sigma_{24} - \sigma_{14}\sigma_{23} \rangle \\
I_{G_3} &= \langle \sigma_{12}, \sigma_{12}\sigma_{23}\sigma_{34} - \sigma_{12}\sigma_{33}\sigma_{24} - \sigma_{13}\sigma_{22}\sigma_{34} + \sigma_{13}\sigma_{23}\sigma_{24} + \sigma_{14}\sigma_{22}\sigma_{33} - \sigma_{14}\sigma_{23}^2 \rangle.
\end{aligned}$$

Note that all three DAGs have the same underlying undirected graph, which is a 1-clique sum of complete graphs. But only the first two DAGs have toric vanishing ideals. In G_2, the generators of I_{G_2} correspond to the 2×2 minors of $\Sigma_{12,234}$ as $\{2\}$ d-separates $\{1\}$ from $\{3,4\}$. Similarly, one of the generators of I_{G_3} is the determinant of $\Sigma_{123,234}$ as $\{2,3\}$ d-separates $\{1\}$ from $\{4\}$. Observe that the vertex $\{3\}$ in G_3 is a collider within the path $1 \leftarrow 3 \rightarrow 2 \leftarrow 4$ and is a non collider within the trek $1 \leftarrow 3 \leftarrow 4$. This is an important observation for defining safe gluing later in the chapter.

One thing that should be apparent in Example 4.1.10 is that the existence of a unique simple trek between pairs of vertices is not a necessary condition for I_G to be toric. Indeed, in the DAG G_1, there are two simple treks in $T(3, 4)$ and yet the ideal I_{G_1} is still toric. So in other cases when I_G is toric, one way to demonstrate this is to find an alternate parametrization for the ideal I_G that is monomial. Our candidate for this new map is the *shortest trek map*. This is defined in a similar manner as the *shortest path map* which played an important role in our proof of Theorem 3.0.3.

Definition 4.1.11. Let G be a DAG with n vertices. Suppose that G satisfies the property that between any two vertices there is a unique shortest trek connecting them (or

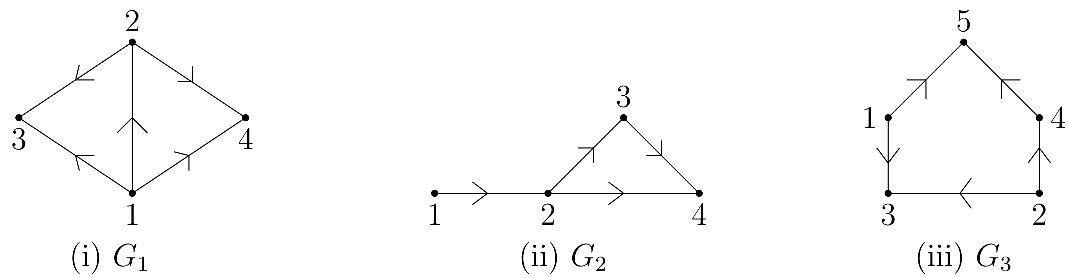


Figure 4.3: Existence of a shortest trek map

no trek connecting them). For vertices i and j in G, let $i \leftrightarrow j$ denote the shortest trek from i to j (if it exists). Then the *shortest trek map* ψ_G is given by

$$\psi_G \quad : \quad \mathbb{C}[\sigma_{ij} : 1 \leq i \leq j \leq n] \to \mathbb{C}[a_i, \sigma_{ij} : i, j \in [n], i \to j \in E(G)]$$

$$\psi_G(\sigma_{ij}) \quad = \quad \begin{cases} 0 & \text{if there is no trek from } i \text{ to } j \\ a_{\text{top}(i \leftrightarrow j)} \prod_{i' \to j' \in i \leftrightarrow j} \lambda_{i'j'} & \text{if shortest trek from } i \text{ to } j \text{ exists} \\ a_i & i = j. \end{cases}$$

The shortest trek map is defined only on those DAGs where there exists a unique shortest trek (or no trek) between any two vertices of G. We call the kernel of ψ_G the *shortest trek ideal* and denote it by ST_G. We illustrate this with an example.

Example 4.1.12. Let G_1 and G_2 be two DAGs as in Figure 4.3. In G_1, there are exactly two treks of the same length from $\{3\}$ to $\{4\}$. So, the shortest trek map is not defined for G_1. But as there exists a unique shortest trek between any two vertices in G_2, the shortest trek map ψ_{G_2} is given by

$$\begin{array}{ll} \sigma_{11} \mapsto a_1 & \sigma_{23} \mapsto a_2\lambda_{23} \\ \sigma_{12} \mapsto a_1\lambda_{12} & \sigma_{24} \mapsto a_2\lambda_{24} \\ \sigma_{13} \mapsto a_1\lambda_{12}\lambda_{23} & \sigma_{33} \mapsto a_3 \\ \sigma_{14} \mapsto a_1\lambda_{12}\lambda_{24} & \sigma_{34} \mapsto a_2\lambda_{34} \\ \sigma_{22} \mapsto a_2 & \sigma_{44} \mapsto a_4. \end{array}$$

Computing the vanishing ideal of G_1 gives us that I_{G_1} is not toric as there exists a degree 3 minor in the generating set ($\{1,2\}$ d-separates $\{3\}$ from $\{4\}$). But computing the kernel of the shortest trek map of G_2 gives us that

$$\ker(\psi_{G_2}) = ST_{G_2} = \langle \sigma_{12}\sigma_{23} - \sigma_{13}\sigma_{22}, \sigma_{12}\sigma_{24} - \sigma_{14}\sigma_{22}, \sigma_{13}\sigma_{24} - \sigma_{14}\sigma_{23} \rangle,$$

which equals I_{G_2} in Example 4.1.10. On the other hand, if we compute ST_{G_3}, we get

$$ST_{G_3} = \langle \sigma_{14}, \sigma_{12}, \sigma_{13}\sigma_{15} - \sigma_{11}\sigma_{35}, \sigma_{23}\sigma_{24} - \sigma_{22}\sigma_{34}, \sigma_{24}\sigma_{45} - \sigma_{44}\sigma_{25} \rangle,$$

which does not equal I_{G_3} which has a generator of degree 3 corresponding to a 3×3 minor (as $\{1, 2\}$ d-separates $\{3\}$ from $\{5\}$).

In the example above we see that the shortest trek map does not exist for G_1. Although the existence of the shortest trek map does not ensure that I_G would be toric (as seen in G_3), we do believe that I_G cannot be toric when the shortest trek map is not well defined. We look into this in more detail in Section 4.5.

The main problem of our interest is to find a characterization of the DAGs which have toric vanishing ideal and also understand the structure of its generators. In this context, it is also an important problem to understand when I_G equals CI_G as that would give us a definite structure of a generating set in terms of d-separations and minors. The ideal ST_G comes into play here as we believe that I_G is generated by monomials and binomials of degree at most 2 if and only if I_G is equal to ST_G. In the next two sections, we find ways to construct DAGs where $I_G = ST_G$.

4.2 Safe gluing of DAGs

As mentioned in the end of Section 4.1, we are interested in those DAGs where I_G equals ST_G. In this section we look at a specific way to construct such DAGs from smaller DAGs having the same property. Given two DAGs G_1 and G_2 whose vanishing ideal is toric, there are various ways to glue G_1 and G_2 together. But the resultant DAG does not always have a toric vanishing ideal. We are interested in those particular types of gluing operations which give us a toric vanishing ideal for the new DAG. We use the term “safe gluing” of two DAGs to denote a particular construction which we conjecture to always preserve the toric property. Considering complete DAGs as the base case (as $I_G = 0$ in that case), this method can be used to construct many DAGs which have toric vanishing ideal. The goal of this section is to explain the construction. To motivate the concept of safe gluing, we first look at some existing results from the literature that give gluing operations on DAGs that preserve the property of having a toric vanishing ideal.

Definition 4.2.1. Let G be a DAG. A vertex s in G is called a *sink* if all the edges adjacent to s are directed towards s.

Proposition 4.2.2 (Proposition 3.7, [34])**.** *Let G_1 and G_2 be two DAGs having a common vertex m that is a sink in both G_1 and G_2. If G is the new DAG obtained after gluing G_1 and G_2 at m, then I_G can be written as*

$$I_G = I_{G_1} + I_{G_2} + \langle \sigma_{ij} : i \in V(G_1) \setminus \{m\}, j \in V(G_2) \setminus \{m\} \rangle.$$

The vertex m in G is a collider vertex within any path from $V(G_1) \setminus \{m\}$ to $V(G_2) \setminus \{m\}$. Further, if I_{G_1} and I_{G_2} are toric, then from Proposition 4.2.2 we can conclude that gluing G_1 and G_2 at a vertex m such that m is a collider within any path from $V(G_1) \setminus \{m\}$ to $V(G_2) \setminus \{m\}$ produces a new DAG G whose vanishing ideal is also toric. In other words, we have the following corollary.

Corollary 4.2.3. *Let G_1 and G_2 be two DAGs having a common vertex m that is a sink in both G_1 and G_2. Let G be the new DAG obtained after gluing G_1 and G_2 at m. If I_{G_1} and I_{G_2} are toric, then so is I_G. Furthermore, if $I_{G_1} = ST_{G_1}$ and $I_{G_2} = ST_{G_2}$ then $I_G = ST_G$.*

An example where this can be seen to occur is the graph G_1 in Example 4.1.10. In G_1, $\{4\}$ is a collider between any path from $\{1\}$ to $\{2, 3\}$ and the resultant vanishing ideal I_{G_1} is toric. We will generalize Corollary 4.2.3 in two ways. One is the safe gluing concept which is a combined generalization of Proposition 4.2.2 and Corollary 4.2.6. The other is the concept of *gluing at sinks* which we discuss in Section 4.3.

A second situation where existing results in the literature can give us DAGs with toric vanishing ideals concerns situations where a DAG gives the same independence structures as an undirected graph. This is incapsulated in the concept of a perfect DAG.

Definition 4.2.4. Let i, j, k be 3 vertices in a DAG G containing the edges $i \to k$ and $j \to k$. Then k is said to be an *unshielded collider* in G if i and j are not adjacent. A DAG G is said to be *perfect* if there are no unshielded colliders in G.

Using the above definition, we state a result from [21].

Proposition 4.2.5 (Proposition 3.28, [21]). *Let G be a perfect DAG and $G^{\sim}$ be its undirected version. Then the probability distribution P admits a recursive factorization with respect to G if and only if it factorizes according to $G^{\sim}$.*

In other words, when G is a perfect DAG, the directed Markov property on G and the factorization Markov property on its undirected version $G^{\sim}$ coincide. In particular, this implies that

$$I_G = P_{G^{\sim}}$$

for perfect DAGs (where P_H denotes the vanishing ideal of Gaussian graphical model associated to the undirected graph H as seen in chapter 3). On the other hand, we know from 3 that in the undirected case, P_H is toric if H is a block graph. Hence, we have the following result :

Corollary 4.2.6. *Let G be a DAG whose undirected version $G^{\sim}$ is a block graph. If G is perfect then I_G is toric.*

We call a DAG G where $G^{\sim}$ is a block graph and G is perfect a *perfect block DAG*. Note that perfect block DAGs can be obtained by gluing smaller perfect block DAGs together at a single vertex in such a way that no unshielded colliders are created.

Corollaries 4.2.3 and 4.2.6 give two different ways to glue DAGs together that have toric vanishing ideals that preserve the toric property. Both methods consist of gluing the graphs at cliques of size one, subject to some extra conditions. We generalize these criteria to obtain the safe gluing criteria in which a DAG is obtained as an n-clique sum of two smaller DAGs so that the vanishing ideal is toric. To give the general definition of safe gluing, we first need to recall the definition of a choke point.

Definition 4.2.7 (Definition 4.1, [34]). A vertex $c \in V(G)$ is a *choke point* between the sets I and J if every trek from a vertex in I to a vertex in J contains c and either

i) c is on the I-side of every trek from I to J, or
ii) c is on the J-side of every trek from I to J.

Definition 4.2.8. Let G_1 and G_2 be two DAGs. Suppose that G_1 and G_2 share a common set of vertices $C = \{c\} \cup D$ such that the induced subgraphs $G_1|_C$ and $G_2|_C$ are the same and this common subgraph is a complete DAG (hence a clique). The clique sum of G_1 and G_2 at C is called a *safe gluing* if

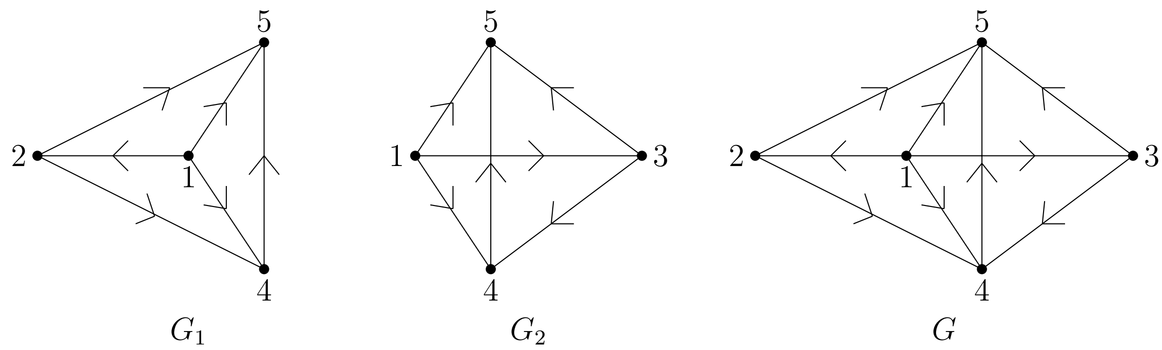


Figure 4.4: Safe gluing of G_1 and G_2 at a 3-clique

i) c is a choke point between the sets $V(G_1) \setminus D$ and $V(G_2) \setminus D$ and
ii) none of the treks between the vertices in $V(G_1) \setminus D$ and $V(G_2) \setminus D$ contain a vertex in D.

Remark 4.2.9. Using the definition above, the gluing of G_1 and G_2 where there are no treks between the vertices of $V(G_1) \setminus C$ and $V(G_2) \setminus C$ can also be considered as a safe gluing. Thus, both types of gluing operations implied by Corollaries 4.2.3 and 4.2.6 are safe gluings.

We further illustrate the definition of safe gluing with an example.

Example 4.2.10. Let G_1 and G_2 be two DAGs having a common 3-clique at $\{1, 4, 5\}$ as shown in the figure 4.4. Thus, G is the DAG obtained after a safe gluing of G_1 and G_2 at the 3-clique. Note that there is a single trek from $\{2\}$ to $\{3\}$ and that passes through $\{1\}$. Any other path from $\{2\}$ to $\{3\}$ containing $\{4\}, \{5\}$ or both has a collider at $\{4\}$ or $\{5\}$. Computing the vanishing ideal of G gives us that $I_G = \langle \sigma_{12}\sigma_{13} - \sigma_{11}\sigma_{23} \rangle$, which is a toric ideal.

We now look at some properties obtained from the safe gluing construction.

Definition 4.2.11. Let G_1 and G_2 be two DAGs, and suppose that G is obtained from G_1 and G_2 by a safe gluing at $C = \{c\} \cup D$. This safe gluing is called a *minimal safe gluing* if we cannot find two other DAGs G_1' and G_2' such that G is the safe gluing of G_1' and G_2' at $\{c\} \cup D'$ with D' a proper subset of D.

Example 4.2.12. Let G be the DAG as shown in Figure 4.5. If we take $G_1 = \{1 \to 3, 1 \to 5, 3 \to 5\}$ and $G_2 = \{2 \to 3, 2 \to 5, 3 \to 5, 4 \to 5\}$, then G is a safe gluing of

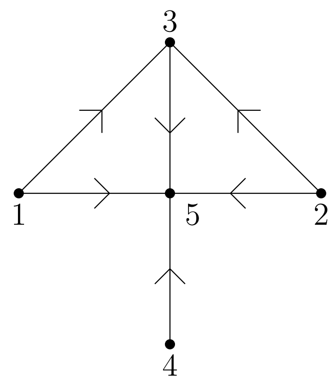


Figure 4.5: Example of a non minimal gluing

G_1 and G_2 with $C = \{3, 5\}$. But this gluing is not minimal as we can take $G_1' = \{1 \to 3, 1 \to 5, 2 \to 3, 2 \to 5, 3 \to 5\}$ and $G_2' = \{4 \to 5\}$ such that G is a safe gluing of G_1' and G_2' with $C' = \{5\} \subset C$.

One useful consequence of having a minimal safe gluing is that for any $d \in D$, there must exist a vertex $i \in V(G_1) \setminus C$ such that $i \to d$ is an edge (and analogously there is a $j \in V(G_2) \setminus C$). This is because if for some vertex $d \in D$ there does not exist any vertex in $V(G_1) \setminus C$ such that $i \to d$ is an edge, then it would mean that we can write G as a safe gluing of G_1' and G_2 at $C' = \{c\} \cup D \setminus \{d\}$ where $V(G_1') = V(G_1) \setminus \{d\}$. We use this observation for proving part (ii) of Lemma 4.2.13.

Lemma 4.2.13. *Let G_1 and G_2 be two DAGs and G be the resultant DAG obtained after a safe gluing of G_1 and G_2 at an n-clique. Let $C = \{c\} \cup D$ be the vertices in the n-clique.*

i) Every trek from a vertex in $V(G_1) \setminus D$ to a vertex in $V(G_2) \setminus D$ must have the topmost vertex (i.e, the source vertex) either always in G_1 or always in G_2.

ii) For each $d \in D$, we must have the edge $c \to d$.

Proof. **i)** To show this, let us assume that there are two treks $i_1 \rightleftharpoons j_1$ and $i_2 \rightleftharpoons j_2$ with $i_1, i_2 \in V(G_1) \setminus D$ and $j_1, j_2 \in V(G_2) \setminus D$ such that $\text{top}(i_1 \rightleftharpoons j_1)$ lies in $V(G_1) \setminus D$ and $\text{top}(i_2 \rightleftharpoons j_2)$ lies in $V(G_2) \setminus D$. Since c must lie in these treks, since it is a choke point, this would imply that c lies in the G_2-side of $i_1 \rightleftharpoons j_1$ and the G_1-side of $i_2 \rightleftharpoons j_2$. That contradicts that c is a choke point.

ii) Let us assume by way of contradiction that $d \to c$ is an edge for some $d \in D$. Since G is obtained from a safe gluing, there are no edges that go from d to any vertex in $V(G_1) \setminus C$ or $V(G_2)\setminus$. For if there were such an edge $d \to i$, there would be a trek $c \leftarrow d \to i$ contradicting the definition of safe gluing.

Now without loss of generality we can assume that the gluing is minimal. Thus, there must be vertices s_1 and s_2 in $G_1 \setminus C$ and $G_2 \setminus C$, respectively, such that $s_1 \to d$ and $s_2 \to d$ are two edges in $E(G)$. By the definition of safe gluing, we know that c must be a choke point between the sets $\{s_1, c\}$ and $\{s_2, c\}$. We consider the treks $s_1 \rightleftharpoons c$ and $c \rightleftharpoons s_2$. As $s_1 \to d \to c$ is already a trek, we cannot have any trek of the form $c \to t_1 \to t_2 \to \cdots \to s_1$ (else it would form a cycle). So, c always lies in the G_2-side of any trek $s_1 \rightleftharpoons c$. Similarly, as $s_2 \to d \to c$ is already a trek, we cannot have any trek of the form $c \to r_1 \to r_2 \to \cdots \to s_2$. So, c lies in the G_1-side of the treks $c_1 \rightleftharpoons s_2$, which is a contradiction. □

The observations in Lemma 4.2.13 are helpful for ruling out various bad scenarios as we work to prove results about the preservation of the toric property for DAGs under safe gluing.

Our main aim in this section is to check that if G_1 and G_2 have toric vanishing ideals then a safe gluing of G_1 and G_2 would give us a DAG G whose vanishing ideal is also toric. From the structure of G we know that every trek between a vertex $i \in G_1 \setminus C$ and $j \in G_2 \setminus C$ passes through the choke point c. This allows us to decompose the treks $i \rightleftharpoons j$ as $i \rightleftharpoons c \cup c \rightleftharpoons j$. So, if we assume that $I_{G_1} = ST_{G_1}$ and $I_{G_2} = ST_{G_2}$, then this would imply that the shortest trek map is well defined for G as well. Thus, we give the following conjecture :

Conjecture 4.2.14. *Let G_1 and G_2 be two DAGs having toric vanishing ideals such that I_{G_1} equals ST_{G_1} and I_{G_2} equals ST_{G_2}. If G is the DAG obtained by a safe gluing of G_1 and G_2 at an n-clique, then I_G is equal to ST_G and hence is toric.*

Although we do not have a proof of Conjecture 4.2.14, we provide a proof when I_{G_1} and I_{G_2} satisfy an extra condition.

Theorem 4.2.15. *Let G_1 and G_2 be two DAGs such that I_{G_1} equals ST_{G_1} and I_{G_2} equals ST_{G_2}. Let G be the DAG obtained by a safe gluing of G_1 and G_2 at an n-clique and c be the choke point. If the generators of I_{G_1} and I_{G_2} have at most one common variable σ_{cc}, then I_G is equal to ST_G and hence is toric.*

Proof. Let $C = \{c\} \cup D$ be the n-clique where G_1 and G_2 are glued. We break the problem into two cases: The first case is when the vertex c lies on some treks from $V(G_1) \setminus C$ to $V(G_2) \setminus C$. The second case is when there are no such treks.

Case I : The choke point $c \in C$ is on some trek from $V(G_1) \setminus C$ to $V(G_2) \setminus C$. In particular, it will be a non-collider vertex along that path.

As c is the only vertex in C that can be on some trek from $V(G_1) \setminus C$ to $V(G_2) \setminus C$, no trek between any two vertices in $V(G_1) \setminus C$ passes through a vertex in $V(G_2) \setminus C$ (and similarly similarly for vertices in $V(G_2) \setminus C$). Further, ST_{G_1} equals I_{G_1}, which implies that there exists a unique shortest trek (or no trek) between any two vertices in G_1 (similarly for G_2). Now, from the structure of G we know that every trek between a vertex in $V(G_1) \setminus C$ and $V(G_2) \setminus C$ must pass through c. So, we can write the shortest trek map of G as follows :

$$\psi_G(\sigma_{ij}) = \begin{cases} \psi_{G_1}(\sigma_{ij}) & : i, j \in V(G_1) \\ \psi_{G_2}(\sigma_{ij}) & : i, j \in V(G_2) \\ \frac{\psi_{G_1}(\sigma_{ic}) . \psi_{G_2}(\sigma_{cj})}{a_c} & : i \in V(G_1) \setminus C, j \in V(G_2) \setminus C. \end{cases}$$

Also, we know that the conditional independence statement $i \perp\!\!\!\perp j | c$ holds for all $i \in V(G_1) \setminus C$ and $j \in V(G_2) \setminus C$. So $\sigma_{ic}\sigma_{cj} - \sigma_{ij}\sigma_{cc}$ lies in both I_G and ST_G for all $i \in V(G_1) \setminus C$ and $j \in V(G_2) \setminus C$.

The vanishing ideals I_{G_1} and I_{G_2} lie in the polynomial rings $\mathbb{C}[\sigma_{ij} : i, j \in V(G_1)]$ and $\mathbb{C}[\sigma_{ij} : i, j \in V(G_2)]$ respectively, where the common variables are of the form $\sigma_{c_i c_j}, c_i, c_j \in C$. But from the assumption, we know that σ_{cc} can be the only common variable among the generators of I_{G_1} and I_{G_2}. So, without loss of generality, we can treat the ideals I_{G_1} and I_{G_2} as if they lie in other rings, that contain enough variables for all their generators. In particular, we can treat the ideals as belong to:

$$\begin{aligned} I_{G_1} &\subseteq \mathbb{C}[\sigma_{ij} : i, j \in V(G_1) \setminus D] \text{ and} \\ I_{G_2} &\subseteq \mathbb{C}[\sigma_{ij} : i, j \in V(G_2)]. \end{aligned}$$

Note that there is only the variable σ_{cc} common between the two rings $\mathbb{C}[\sigma_{ij} : i, j \in V(G_1) \setminus D]$ and $\mathbb{C}[\sigma_{ij} : i, j \in V(G_2)]$.

Now, let $f = \sigma^u - \sigma^v$ be any binomial in a generating set of ST_G consisting of primitive binomials. Suppose that $i \in V(G_1) \setminus C$ and $j \in V(G_2) \setminus C$. We can replace σ_{ij} with $\frac{\sigma_{ic}\sigma_{cj}}{\sigma_{cc}}$

in both σ^u and σ^v. Multiplying enough powers of σ_{cc}, we get

$$\sigma_{cc}^n f = \sigma^{u_1}\sigma^{u_2} - \sigma^{v_1}\sigma^{v_2}\sigma_{cc}^m,$$

(modulo the quadratic generators $\sigma_{ic}\sigma_{cj} - \sigma_{ij}\sigma_{cc}$ that belong to I_G), where $\sigma^{u_1}, \sigma^{v_1} \in \mathbb{C}[\sigma_{ij} : i,j \in V(G_1) \setminus D]$ and $\sigma^{u_2}, \sigma^{v_2} \in \mathbb{C}[\sigma_{ij} : i,j \in V(G_2)]$, but none of $\sigma^{u_1}, \sigma^{v_1}, \sigma^{u_2}, \sigma^{v_2}$ involve the variable σ_{cc}.

We can split the monomial $\sigma_{cc}^m = \sigma_{cc}^{m_1}\sigma_{cc}^{m_2}$ so that the two binomials

$$\sigma^{u_1} - \sigma^{v_1}\sigma_{cc}^{m_1} \qquad \text{and} \qquad \sigma^{u_2} - \sigma^{v_2}\sigma_{cc}^{m_2}$$

are homogeneous. Since all the variables appearing in σ^{u_1} and σ^{v_1} involve parameters from the graph G_1 with no overlap with parameters from G_2 (except possibly a_{cc}) we see that if $\sigma^{u_1}\sigma^{u_2} - \sigma^{v_1}\sigma^{v_2}\sigma_{cc}^m$ belongs to ST_G, it must be the case that $\sigma^{u_1} - \sigma^{v_1}\sigma_{cc}^{m_1}$ belongs to ST_{G_1}. Then if $\sigma^{u_1}\sigma^{u_2} - \sigma^{v_1}\sigma^{v_2}\sigma_{cc}^m$ is to belong to ST_G, then it must also be the case that $\sigma^{u_2} - \sigma^{v_2}\sigma_{cc}^{m_2}$ belongs to ST_{G_2}.

Now we have that, modulo the quadratic generators $\sigma_{ic}\sigma_{cj} - \sigma_{ij}\sigma_{cc}$ that belong to I_G, we have that

$$\begin{aligned} \sigma_{cc}^n f &= \sigma^{u_1}(\sigma^{u_2} - \sigma_{cc}^{m_2}\sigma^{v_2}) + \sigma_{cc}^{m_2}\sigma^{v_2}(\sigma^{u_1} - \sigma_{cc}^{m_1}\sigma^{v_1}) \\ &\in ST_{G_1} + ST_{G_2} \\ &= I_{G_1} + I_{G_2} \subseteq I_G. \end{aligned}$$

Thus, $\sigma_{cc}^n f \in I_G$. As I_G is a prime ideal, that does not contain σ_{cc}, we deduce that $f \in I_G$. This implies that $ST_G \subseteq I_G$. The vanishing ideal I_G is well-known to have dimension $n + e$, as the model is identifiable. The dimension of ST_G equals $n + e$ by Proposition 4.4.1. But as the dimension of I_G equals the dimension of ST_G, both ideals are prime, and $ST_G \subseteq I_G$, we can conclude that $I_G = ST_G$.

Case II: There are no treks between the vertices of $V(G_1) \setminus C$ and $V(G_2) \setminus C$: In this case, the shortest trek map ψ_G can be written as :

$$\psi_G(\sigma_{ij}) = \begin{cases} \psi_{G_1}(\sigma_{ij}) : i, j \in V(G_1) \\ \psi_{G_2}(\sigma_{ij}) : i, j \in V(G_2) \\ \quad 0 \qquad : i \in V(G_1) \setminus C, j \in V(G_2) \setminus C. \end{cases}$$

We claim that ST_G in this case is

$$ST_G = ST_{G_1} + ST_{G_2} + \langle \sigma_{ij} : i \in V(G_1) \setminus C, j \in V(G_2) \setminus C \rangle.$$

We prove this equality in the same way as the proof of Proposition 4.2.2. We have $\psi_G(\sigma_{ij}) = 0$ for all $i \in V(G_1) \setminus C$ and $j \in V(G_2) \setminus C$. By our assumption we know that none of the variables of the form σ_{cd} or $\sigma_{d,d'}$, with $d, d' \in D$ can appear among any of the generators of ST_{G_1}. Also in this case, σ_{cc} cannot appear in ST_{G_1} or ST_{G_2} as $\psi_{G_1}(\sigma_{cc}) = \psi_{G_2}(\sigma_{cc}) = a_c$ and no treks involving $i \in V(G_1) \setminus C$ or $j \in V(G_2) \setminus C$ can have c as its source. So, for any $\sigma_{ij}, i \in V(G_1) \setminus C, j \in V(G_1)$ and $\sigma_{kl}, k \in V(G_2), l \in V(G_2) \setminus \{c\}$ which appear in ST_G, $\psi_G(\sigma_{ij})$ and $\psi_G(\sigma_{kl})$ are monomials in two polynomial rings having disjoint variables. Thus, we have a partition of the variables σ_{ij} into three sets

$$\begin{aligned} A_1 &= \{\sigma_{ij} : i \in V(G_1), j \in V(G_1) \setminus C\}, \\ A_2 &= \{\sigma_{ij} : i, j \in V(G_2)\} \text{ and} \\ A_3 &= \{\sigma_{ij} : i \in V(G_1) \setminus C, j \in V(G_2) \setminus C\}, \end{aligned}$$

in which the image $\psi_G(\sigma_{ij})$ appears in disjoint sets of variables. Further, there can be no nontrivial relations involving two or more of these three sets of variables. So, the equality in the above equation holds.

But then, $ST_{G_1} = I_{G_1}$ and $ST_{G_2} = I_{G_2}$. Thus, we have

$$\begin{aligned} ST_G &= I_{G_1} + I_{G_2} + \langle \sigma_{ij} : i \in V(G_1) \setminus C, j \in V(G_2) \setminus C \rangle \\ &\subseteq I_G. \end{aligned}$$

As both the ideals are prime and have the same dimension, $ST_G = I_G$. □

Although Theorem 4.2.15 uses the assumption that only σ_{cc} appears among the generators of both I_{G_1} and I_{G_2}, we believe that the safe gluing would yield a toric vanishing

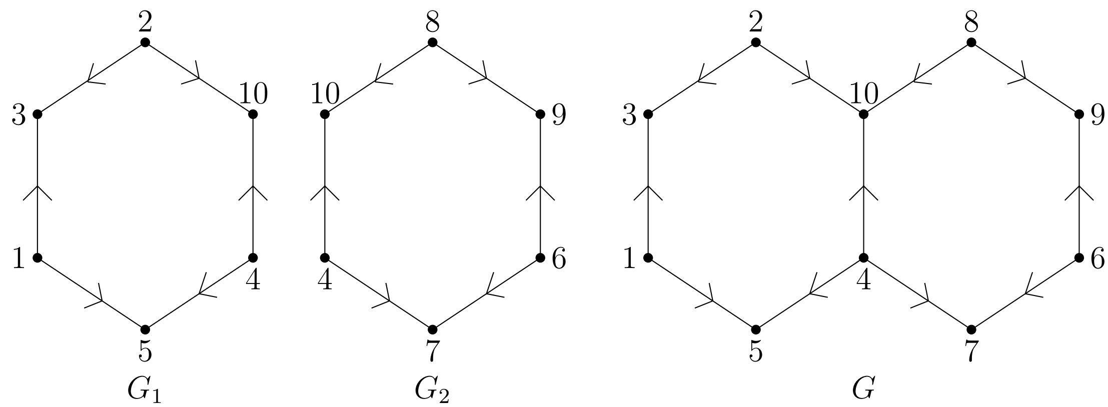


Figure 4.6: Safe gluing of G_1 and G_2 at a 2-clique

ideal even without that assumption. We illustrate this point with an example.

Example 4.2.16. Let G_1 and G_2 be two non chordal cycles as shown in Figure 4.6. Computing the vanishing ideals I_{G_1} and I_{G_2}, we get

$$\begin{aligned} I_{G_1} &= \langle \sigma_{24}, \sigma_{14}, \sigma_{12}, \sigma_{1,10}, \sigma_{25}, \sigma_{34}, \sigma_{23}\sigma_{2,10} - \sigma_{22}\sigma_{3,10}, \sigma_{13}\sigma_{15} - \sigma_{11}\sigma_{35}, \sigma_{45}\sigma_{4,10} - \sigma_{44}\sigma_{5,10}\rangle, \\ I_{G_2} &= \langle \sigma_{6,10}, \sigma_{78}, \sigma_{68}, \sigma_{49}, \sigma_{48}, \sigma_{46}, \sigma_{89}\sigma_{8,10} - \sigma_{88}\sigma_{9,10}, \sigma_{67}\sigma_{69} - \sigma_{66}\sigma_{79}, \sigma_{47}\sigma_{4,10} - \sigma_{44}\sigma_{7,10}\rangle, \end{aligned}$$

which are both toric ideals. Now, if we perform a safe gluing of G_1 and G_2 at the 2-clique $C = \{4, 10\}$, we get the resultant DAG G as in the figure. Observe that the variable $\sigma_{4,10}$ appears in the vanishing ideal of both G_1 and G_2. Computing the vanishing ideal I_G gives us

$$\begin{aligned} I_G = \; & \langle \sigma_{14}, \sigma_{12}, \sigma_{6,10}, \sigma_{68}, \sigma_{49}, \sigma_{48}, \sigma_{29}, \sigma_{46}, \sigma_{28}, \sigma_{27}, \sigma_{26}, \sigma_{25}, \sigma_{24}, \sigma_{78}, \sigma_{59}, \sigma_{58}, \sigma_{39}, \sigma_{56}, \sigma_{38}, \\ & \sigma_{1,10}, \sigma_{19}, \sigma_{37}, \sigma_{18}, \sigma_{36}, \sigma_{17}, \sigma_{16}, \sigma_{34}, \sigma_{13}\sigma_{15} - \sigma_{11}\sigma_{35}, \sigma_{89}\sigma_{8,10} - \sigma_{88}\sigma_{9,10}, \\ & \sigma_{67}\sigma_{69} - \sigma_{66}\sigma_{79}, \sigma_{4,10}\sigma_{57} - \sigma_{47}\sigma_{5,10}, \sigma_{4,10}\sigma_{57} - \sigma_{45}\sigma_{7,10}, \sigma_{47}\sigma_{4,10} - \sigma_{44}\sigma_{7,10}, \\ & \sigma_{45}\sigma_{4,10} - \sigma_{44}\sigma_{5,10}, \sigma_{45}\sigma_{47} - \sigma_{44}\sigma_{57}, \sigma_{23}\sigma_{2,10} - \sigma_{22}\sigma_{3,10}\rangle, \end{aligned}$$

which is still a toric ideal.

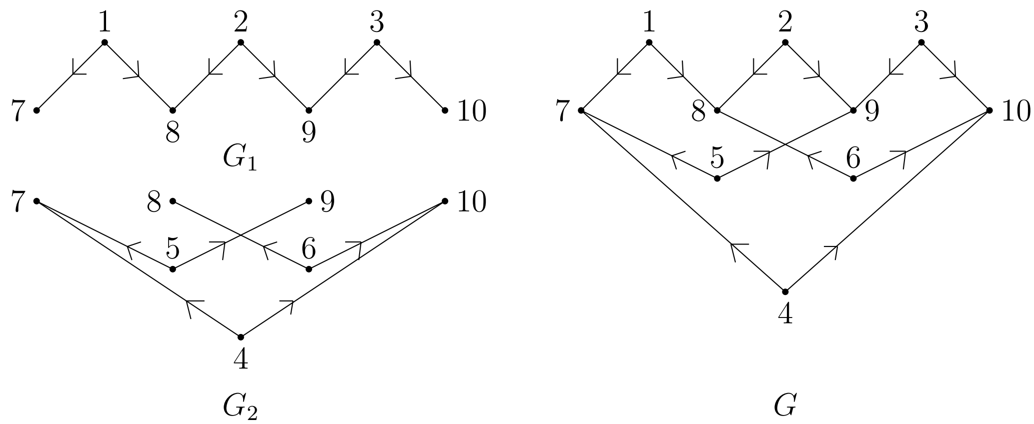


Figure 4.7: Gluing G_1 and G_2 at the sinks

4.3 Gluing at sinks and adding a new sink

We now look at two more ways of constructing DAGs which have toric vanishing ideals. Both methods involve sinks in the DAGs. The first construction we analyze is gluing the two graphs together at the sinks. The second concept involves adding new sinks to the DAG.

Definition 4.3.1. Let G_1 and G_2 be two DAGs and S_1, S_2 be the set of sinks in G_1 and G_2 respectively. If S is the set of all the common vertices in S_1 and S_2, then *gluing* G_1 *and* G_2 *at the sinks* refers to the construction of a new DAG G with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$.

We illustrate this construction of gluing at sinks with an example.

Example 4.3.2. Let G_1 and G_2 be two DAGs as shown in Figure 4.7. Here, the set of sinks in both G_1 and G_2 are $S_1 = S_2 = S = \{7, 8, 9, 10\}$. We glue G_1 and G_2 at the sinks to form G.

Theorem 4.3.3. *Let G_1 and G_2 be two DAGs. Let S be the set of common sinks in G_1 and G_2. Let G be the DAG obtained after gluing G_1 and G_2 at the sinks. Suppose that for each pair of vertices $i, j \in S$, either all treks between i and j lie in G_1 or all treks* *between i and j lie in G_2. Then*

$$\begin{aligned} I_G &= \langle \textit{ generators of } I_{G_1} \setminus \{\sigma_{ij} : i,j \in S\}\rangle \\ &\quad + \langle \textit{ generators of } I_{G_2} \setminus \{\sigma_{ij} : i,j \in S\}\rangle \\ &\quad + \langle \sigma_{ij} : i \in V(G_1) \setminus S, j \in V(G_2) \setminus S\rangle \\ &\quad + \langle \sigma_{ij} : i,j \in S \textit{ such that there is no trek between } i \textit{ and } j\rangle. \end{aligned}$$

Remark 4.3.4. From the condition mentioned in the statement, we know that at least one of $\phi_{G_1}(\sigma_{ij})$ or $\phi_{G_2}(\sigma_{ij})$ is zero for all $i, j \in S, i \neq j$. So, "$\langle$ generators of $I_{G_1} \setminus \{\sigma_{ij} : i, j \in S\}\rangle$", refers to forming a homogeneous generating set of I_{G_1} that includes those variables in $\{\sigma_{ij} : i, j \in S\}$ which are mapped to zero under ϕ_{G_1} and then removing those variables from the generating set. Similarly, for "$\langle$ generators of $I_{G_2} \setminus \{\sigma_{ij} : i, j \in S\}\rangle$".

Proof. From the assumption that S is a set of sinks of G, we know that there is no trek in G between the vertices of $G_1 \setminus S$ and $G_2 \setminus S$. This implies that $\sigma_{ij} \in I_G$ for all $i \in V(G_1) \setminus S, j \in V(G_2) \setminus S$. Further, no two sinks i, j in S can have treks $i \rightleftharpoons j$ in both G_1 and G_2. So, the map ϕ_G can be written as

$$\phi_G(\sigma_{ij}) = \begin{cases} \phi_{G_1}(\sigma_{ij}) : i \in V(G_1), j \in V(G_1) \setminus S \\ \phi_{G_2}(\sigma_{ij}) : i \in V(G_2), j \in V(G_2) \setminus S \\ \phi_{G_1}(\sigma_{ij}) + \phi_{G_2}(\sigma_{ij}) : i, j \in S \\ \quad 0 \qquad : i \in V(G_1) \setminus S, j \in V(G_2) \setminus S. \end{cases}$$

This allows us to partition the variables σ_{ij} into four sets A_1, A_2, A_3, A_4 where

$$\begin{aligned} A_1 &= \{\sigma_{ij} : i \in V(G_1), j \in V(G_1) \setminus S \text{ or } i, j \in S \text{ such that the treks } i \rightleftharpoons j \text{ lie in } G_1\} \\ A_2 &= \{\sigma_{ij} : i \in V(G_2), j \in V(G_2) \setminus S \text{ or } i, j \in S \text{ such that the treks } i \rightleftharpoons j \text{ lie in } G_2\} \\ A_3 &= \{\sigma_{ij} : i \in V(G_1) \setminus S, j \in V(G_2) \setminus S\} \\ A_4 &= \{\sigma_{ij} : i, j \in S \text{ such that there is no trek between } i \text{ and } j\}. \end{aligned}$$

In these four sets, $\phi_G(\sigma_{ij})$ appear in disjoint sets of variables and there can be no nontrivial relations involving two or more of these sets of variables. So,

$$\begin{aligned} I_G &= \ker \phi_G \\ &= \langle \text{ generators of } I_{G_1} \setminus \{\sigma_{ij} : i,j \in S\} \rangle + \langle \text{ generators of } I_{G_2} \setminus \{\sigma_{ij} : i,j \in S\} \rangle \\ &\quad + \langle \sigma_{ij} : \sigma_{ij} \in A_3 \cup A_4 \rangle. \end{aligned}$$

This completes the proof. □

Example 4.3.5. Going back to Example 4.3.2, we compute the vanishing ideals of the three DAGs G_1, G_2, and G. That gives us

$$\begin{aligned} I_{G_1} &= \langle \sigma_{23}, \sigma_{13}, \sigma_{12}, \sigma_{8,10}, \sigma_{7,10}, \sigma_{79}, \sigma_{2,10}, \sigma_{38}, \sigma_{1,10}, \sigma_{37}, \sigma_{19}, \sigma_{27}, \sigma_{39}\sigma_{3,10} - \sigma_{33}\sigma_{9,10}, \\ &\quad \sigma_{28}\sigma_{29} - \sigma_{22}\sigma_{89}, \sigma_{17}\sigma_{18} - \sigma_{11}\sigma_{78} \rangle, \\ I_{G_2} &= \langle \sigma_{9,10}, \sigma_{89}, \sigma_{78}, \sigma_{69}, \sigma_{5,10}, \sigma_{67}, \sigma_{49}, \sigma_{58}, \sigma_{48}, \sigma_{56}, \sigma_{46}, \sigma_{45}, \sigma_{68}\sigma_{6,10} - \sigma_{66}\sigma_{8,10}, \\ &\quad \sigma_{47}\sigma_{4,10} - \sigma_{44}\sigma_{7,10}, \sigma_{57}\sigma_{59} - \sigma_{55}\sigma_{79} \rangle, \\ I_G &= \langle \sigma_{15}, \sigma_{14}, \sigma_{13}, \sigma_{12}, \sigma_{69}, \sigma_{67}, \sigma_{49}, \sigma_{48}, \sigma_{2,10}, \sigma_{46}, \sigma_{45}, \sigma_{27}, \sigma_{26}, \sigma_{25}, \sigma_{24}, \sigma_{23}, \sigma_{5,10}, \\ &\quad \sigma_{58}, \sigma_{56}, \sigma_{38}, \sigma_{1,10}, \sigma_{19}, \sigma_{37}, \sigma_{36}, \sigma_{35}, \sigma_{16}, \sigma_{34}, \sigma_{68}\sigma_{6,10} - \sigma_{66}\sigma_{8,10}, \sigma_{28}\sigma_{29} - \sigma_{22}\sigma_{89}, \\ &\quad \sigma_{47}\sigma_{4,10} - \sigma_{44}\sigma_{7,10}, \sigma_{57}\sigma_{59} - \sigma_{55}\sigma_{79}, \sigma_{39}\sigma_{3,10} - \sigma_{33}\sigma_{9,10}, \sigma_{17}\sigma_{18} - \sigma_{11}\sigma_{78} \rangle \end{aligned}$$

Observe that the variables $\sigma_{27}, \sigma_{79}, \sigma_{37}, \sigma_{7,10}, \sigma_{12}, \sigma_{19}, \sigma_{13}, \sigma_{1,10}, \sigma_{38}, \sigma_{8,10}, \sigma_{23}$, and $\sigma_{2,10}$ are mapped to zero by ϕ_{G_1} and the variables $\sigma_{9,10}, \sigma_{89}, \sigma_{78}, \sigma_{69}, \sigma_{5,10}, \sigma_{67}, \sigma_{49}, \sigma_{58}, \sigma_{48}, \sigma_{56}, \sigma_{46}$ and σ_{45} are mapped to zero by ϕ_{G_2}. Further, the treks $7 \rightleftharpoons 8, 8 \rightleftharpoons 9$ and $9 \rightleftharpoons 10$ lie within G_1 whereas $7 \rightleftharpoons 9, 7 \rightleftharpoons 10$ and $8 \rightleftharpoons 10$ lie within G_2. Also, no two sinks have treks between them in both G_1 and G_2. Hence we are in a position where we can apply Theorem 4.3.3.

Analyzing the generating set of I_G, we see that the variables

$$\begin{aligned} &\{\sigma_{13}, \sigma_{12}, \sigma_{2,10}, \sigma_{27}, \sigma_{23}, \sigma_{38}, \sigma_{1,10}, \sigma_{19}, \sigma_{37}\} \text{ and the binomials} \\ &\{\sigma_{28}\sigma_{29} - \sigma_{22}\sigma_{89}, \sigma_{39}\sigma_{3,10} - \sigma_{33}\sigma_{9,10}, \sigma_{17}\sigma_{18} - \sigma_{11}\sigma_{78}\} \end{aligned}$$

in the generating set of I_G are obtained from the generating set of I_{G_1} after removing the variables of the form $\{\sigma_{ij} : i, j \in S\}$. Similarly, the variables

$$\{\sigma_{69}, \sigma_{67}, \sigma_{49}, \sigma_{48}, \sigma_{46}, \sigma_{45}, \sigma_{5,10}, \sigma_{58}, \sigma_{56}\} \text{ and the binomials}$$
$$\{\sigma_{68}\sigma_{6,10} - \sigma_{66}\sigma_{8,10}, \sigma_{47}\sigma_{4,10} - \sigma_{44}\sigma_{7,10}, \sigma_{57}\sigma_{59} - \sigma_{55}\sigma_{79}\}$$

are obtained from the generating set of I_{G_2} after removing the variables $\{\sigma_{ij} : i, j \in S\}$. The variables

$$\{\sigma_{15}, \sigma_{14}, \sigma_{26}, \sigma_{25}, \sigma_{24}, \sigma_{36}, \sigma_{35}, \sigma_{16}, \sigma_{34}\}$$

correspond to the third set of generators which are variables of the form $\{\sigma_{ij} : i \in V(G_1) \setminus S, j \in V(G_2) \setminus S\}$. In this example, there are no generators of the form

$$\langle \sigma_{ij} : i, j \in S \text{ such that there is no trek between } i \text{ and } j \rangle.$$

If we add the extra condition in Theorem 4.3.3 that both I_{G_1} and I_{G_2} are toric, then we get the following result :

Corollary 4.3.6. *Let G_1 and G_2 be two DAGs. Let S be the set of common sinks in G_1 and G_2. Let G be the DAG obtained after gluing G_1 and G_2 at the sinks. Suppose that for each pair of vertices $i, j \in S$, either all treks between i and j lie in G_1 or all treks between i and j lie in G_2.*

i) If I_{G_1} and I_{G_2} are toric, then I_G is also toric.
ii) If $I_{G_1} = ST_{G_1}$ and $I_{G_2} = ST_{G_2}$, then I_G is also equal to ST_G.

Proof. Part i) follows directly from Theorem 4.3.3, since the generating set will be a union of a set of variables and a collection of binomials. For part ii), the shortest trek map ψ_G has the same structure as ϕ_G as shown in the proof of Theorem 4.3.3. $\square$

We now look at a simple construction where instead of gluing two DAGs at the sinks, we add a new sink vertex to an existing DAG G. We show that the new DAG G' has the same vanishing ideal as the existing one.

Theorem 4.3.7. *Let G be any arbitrary DAG. Construct a new DAG G' from G, where we add another vertex s and all edges $i \to s$ for $i \in V(G)$. Then*

$$I_{G'} = I_G \cdot \mathbb{C}[\sigma_{ij} : i, j \in V(G) \cup \{s\}].$$

Proof. Let G have n vertices and e edges. From the construction, we know that G' has $n+1$ vertices and $e+n$ edges. Since the new vertex s is a sink, none of the treks between any two vertices $i, j \in V(G') \setminus \{s\}$ can pass through s. Further, as s is connected to every vertex of G, the image of σ_{is} has a monomial of the form $a_i\lambda_{is}$ for all $i \in G$. Thus, the map $\phi_{G'}$ can be written as

$$\phi_{G'}(\sigma_{ij}) = \begin{cases} \phi_G(\sigma_{ij}) : i, j \in V(G) \\ a_i\lambda_{is} + \text{ other terms } : i \in V(G), j = s \\ \quad a_s \quad : i = j = s. \end{cases}$$

Since $\phi_G(\sigma_{ij}) = \phi_{G'}(\sigma_{ij})$ for all $i, j \in V(G') \setminus \{s\}$, it is clear that $I_G \subseteq I_{G'}$.

In order to show that $I_{G'} = I_G \cdot \mathbb{C}[\sigma_{ij} : i, j \in V(G) \cup \{s\}]$, we look at the dimension of the two ideals. We know that the dimension of I_G is $n + e$, whereas the dimension of $I_{G'} \subseteq \mathbb{C}[\sigma_{ij} : i, j \in V(G')]$ is $(n+1)+(e+n) = 2n+e+1$. The only new variables present in $\mathbb{C}[\sigma_{ij} : i, j \in V(G')]$ are the variables of the form $\sigma_{is} : i \in V(G')$. So, the dimension of I_G in $\mathbb{C}[\sigma_{ij} : i, j \in V(G')]$ is $n + e + (n + 1)$, which equals the dimension of $I_{G'}$. But as $I_G \subseteq I_{G'}$ and both ideals are prime, we can conclude that $I_G = I_{G'}$. $\square$

Again, if we add the extra condition that I_G is toric in Theorem 4.3.7, then we get the following result :

Corollary 4.3.8. *Let G be any arbitrary DAG. Construct a new DAG G' from G, where we add another vertex s and all edges $i \to s$ for $i \in V(G)$.*

i) If I_G is toric, then $I_{G'}$ is also toric.
ii) If $I_G = ST_G$, then $I_{G'}$ is also equal to $ST_{G'}$ and hence is toric.

Proof. For part i), since the two ideals have the same generating set, then they are both toric.

For part ii), using the same argument as in the Proof of Theorem 4.3.7, the shortest trek map $\psi_{G'}$ can be written as

$$\psi_{G'}(\sigma_{ij}) = \begin{cases} \psi_G(\sigma_{ij}) : i, j \in V(G) \\ \quad a_i\lambda_{is} \quad : i \in V(G), j = s \\ \quad a_s \quad : i = j = s. \end{cases}$$

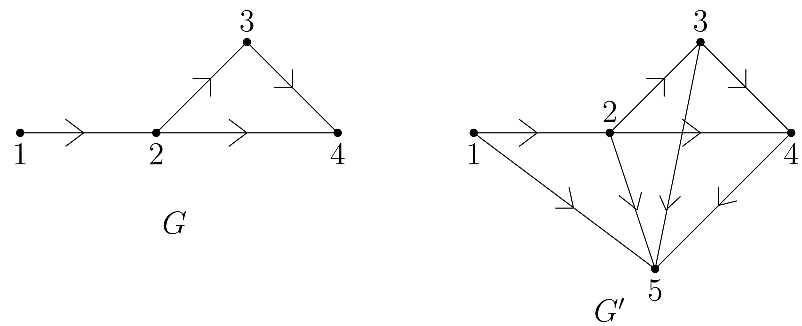


Figure 4.8: Introducing a new sink in G to get G'

So it is clear that $ST_G \subseteq ST_{G'}$. Now, the variable λ_{is} only appears in the image of σ_{is} for all $i \in V(G)$. Similarly, the variable a_s only appears in the image of σ_{ss}. This implies that the variables of the form $\sigma_{is}, i \in V(G')$ can not appear in any generators of $ST_{G'}$. Thus $ST_{G'} = ST_G \cdot \mathbb{C}[\sigma_{ij} : i, j \in V(G) \cup \{s\}]$ as well, so $I_{G'} = ST_{G'}$. □

Example 4.3.9. Let G be a DAG with four vertices as shown in Figure 4.8. From Example 4.1.10, we know that I_G is a toric ideal. Now, we add another vertex $\{5\}$ to G and connect all the existing vertices to 5 by edges pointing towards 5. Here 5 is the sink in the new DAG G'. Computing the vanishing ideal of G' gives us that $I_{G'}$ has the same generating set as I_G.

To this point, we have described three ways to construct DAGs from smaller DAGs that preserve the toric property: safe gluing, gluing at sinks, and adding a new sink. We believe that these are the only possible operations that could be done to construct such DAGs. We know that the vanishing ideal of a complete DAG is zero and hence is toric. So starting with those examples as a base case, we can combine these three operations to get many more examples of DAGs with toric vanishing ideals. We explain this idea with an example.

Example 4.3.10. Let G be the DAG as shown in Figure 4.9. Computing the vanishing

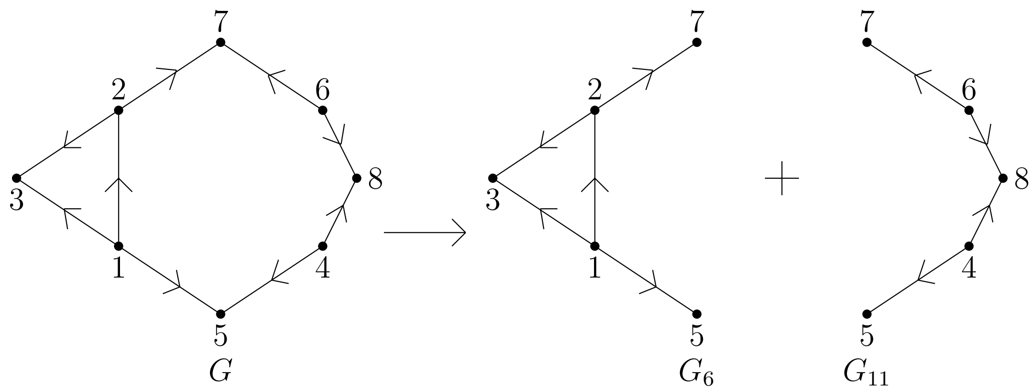


Figure 4.9: Constructing G as a combination of safe gluing, gluing at sinks and adding a new sink to complete DAGs

ideal gives us that

$$\begin{aligned} I_G &= \langle \sigma_{5,6}, \sigma_{4,7}, \sigma_{4,6}, \sigma_{3,8}, \sigma_{3,6}, \sigma_{3,4}, \sigma_{2,8}, \sigma_{2,6}, \sigma_{2,4}, \sigma_{1,8}, \sigma_{1,6}, \sigma_{1,4}, \sigma_{6,7}\sigma_{6,8} - \sigma_{6,6}\sigma_{7,8}, \\ &\quad \sigma_{4,5}\sigma_{4,8} - \sigma_{4,4}\sigma_{5,8}, \sigma_{2,5}\sigma_{3,7} - \sigma_{2,3}\sigma_{5,7}, \sigma_{1,7}\sigma_{3,5} - \sigma_{1,3}\sigma_{5,7}, \sigma_{2,5}\sigma_{2,7} - \sigma_{2,2}\sigma_{5,7}, \\ &\quad \sigma_{2,3}\sigma_{2,7} - \sigma_{2,2}\sigma_{3,7}, \sigma_{1,7}\sigma_{2,5} - \sigma_{1,2}\sigma_{5,7}, \sigma_{1,3}\sigma_{2,5} - \sigma_{1,2}\sigma_{3,5}, \sigma_{1,7}\sigma_{2,3} - \sigma_{1,2}\sigma_{3,7}, \\ &\quad \sigma_{1,7}\sigma_{2,2} - \sigma_{1,2}\sigma_{2,7}, \sigma_{1,5}\sigma_{1,7} - \sigma_{1,1}\sigma_{5,7}, \sigma_{1,3}\sigma_{1,5} - \sigma_{1,1}\sigma_{3,5}, \sigma_{1,2}\sigma_{1,5} - \sigma_{1,1}\sigma_{2,5}\rangle. \end{aligned}$$

Now, we show that G can be obtained as a combination of safe gluing, gluing at sinks, and adding a new sink starting from complete DAGs. Let G_1 be the DAG with vertices $\{1,2\}$. Then the vertex 3 can be considered as adding a new sink to G_1 to form G_2. So, G_2 is the DAG with vertices $\{1,2,3\}$ and I_{G_2} is toric.

Let G_3 be the complete DAG with vertices $\{2,7\}$. Then we can make a safe gluing of G_2 with G_3 to get G_4 as 2 is a choke point between $\{1,2,3\}$ and $\{2,7\}$. Similarly, if G_5 is the complete DAG with vertices $\{1,5\}$, then we can make another safe gluing of G_4 with G_5 to form G_6. Observe that G_6 has three sinks, which are $3, 7$, and 5.

Let G_7, G_8, G_9 and G_{10} be the complete DAGs with vertices $\{6,7\}, \{6,8\}, \{4,8\}$ and $\{4,5\}$ respectively. Then we can perform multiple safe gluing of these four DAGs to get G_{11} with vertices $\{4,5,6,7,8\}$. It can be seen that 5 and 7 are the two sinks in G_{11}. So, finally we can glue G_6 and G_{11} at the set of common sinks, i.e., 5 and 7. As there exist only trek between 5 and 7 and that lies in G_6, we can conclude that the final DAG G obtained after gluing G_6 and G_{11} at the sinks must have a toric vanishing ideal.

4.4 The shortest trek ideal

The shortest trek ideal ST_G appears to play an important role in the problem of classifying those DAGs whose vanishing ideal is toric. For this reason, we focus on purely combinatorial properties of this ideal in this section. In particular, we prove our main result, Theorem 4.4.15, that if ST_{G_1} equals CI_{G_1} and ST_{G_2} equals CI_{G_2}, then ST_G eqauls CI_G where G is a safe gluing of G_1 and G_2. This result provides further evidence for Conjecture 4.2.14.

We begin with exploring the structure of the shortest trek map.

Proposition 4.4.1. *Let G be a DAG such that the shortest trek ideal ST_G exists. Then the dimension of ST_G is $n + e$, the number of vertices plus the number of edges.*

Proof. The number of parameters in the ring $\mathbb{C}[a, \lambda]$ is $n + e$, so $n + e$ is an upper bound on the dimension. On the other hand, for each i, $\psi_G(\sigma_{ii}) = a_i$ and for edge edge $i \to j$, $\psi_G(\sigma_{ij}) = a_i\lambda_{ij}$. This collection of expressions

$$\{a_i : i \in V(G)\} \cup \{a_i\lambda_{ij} : i \to j \in E(G)\}$$

is algebraically independent, and has cardinality $n + e$ which gives a lower bound for the dimension of ST_G. □

As ψ_G is a monomial map, there is a corresponding matrix M, whose columns are the exponent vectors in the monomials $\psi_G(\sigma_{ij})$. So ST_G is the toric ideal of the matrix M as

$$\psi_G(\sigma^u) = t^{Mu},$$

where $\sigma = (\sigma_{11}, \sigma_{12}, \ldots, \sigma_{nn})$ and $t = (a_1, a_2, \ldots, a_n, \lambda_{12}, \ldots, \lambda_{n-1n})$. This matrix will be useful in proving some properties of the ideal ST_G.

To prove results about the generating sets of toric ideals we look the fiber graph of $M^{-1}(b)_{\mathcal{F}}$ where $\mathcal{F} \subset \ker_{\mathbb{Z}}(M)$. The fundamental theorem of Markov bases (Theorem 1.4.4) connects the generating sets of toric ideals to connectivity properties of the fiber graphs. We state the result again explicitly in the case of the fiber graphs for the shortest trek maps.

Theorem 4.4.2 (Theorem 1.4.4). *Let $\mathcal{F} \subset \ker_{\mathbb{Z}}(M)$. The graphs $M^{-1}(b)_{\mathcal{F}}$ are connected for all b such that $M^{-1}(b)$ is nonempty, if and only if the set $\{\sigma^{v^+} - \sigma^{v^-} : v \in \mathcal{F}\}$ generates the toric ideal ST_G.*

Now we relate the toric ideal ST_G to some other familiar toric ideals that are studied in the combinatorial algebra literature. These results will be useful for proving results on the generators of ST_G.

Definition 4.4.3. We define a map called the *end point map* η_G as follows:

$$\begin{aligned} \eta_G : \mathbb{C}[\sigma_{ij} : 1 \leq i \leq j \leq n] &\rightarrow \mathbb{C}[d_1, \ldots, d_n] \\ \sigma_{ij} &\mapsto \begin{cases} d_i d_j & \text{if there is a trek from } i \text{ to } j \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

As η_G is also a monomial map, $\ker(\eta_G)$ is a toric ideal.

Lemma 4.4.4. *For any given DAG G where the shortest trek map ψ_G is well defined,*

$$ST_G \subseteq \ker(\eta_G).$$

Proof. Let M and N be the matrices corresponding to the maps ψ_G and η_G respectively. Note that we can ignore all pairs i, j where there is no trek between i and j, as these σ_{ij}s are mapped to zero under both the end point map and the shortest trek map. It is enough to show that the row space of N is contained in the row space of M. We construct a matrix M_1 as follows:

i) M_1 is an $n \times (n + |E|)$ matrix, where the rows correspond to the vertices of G (i.e, the variables d_i) and the columns correspond to the vertices and edges of G (i.e, the variables a_i and λ_{ij}).
ii) For every vertex variable a_i, the corresponding column is $2e_i$ and for every edge variable λ_{ij}, the corresponding column is $-e_i + e_j$, where e_i is the ith standard unit vector.

Now, let $\psi_G(\sigma_{ij}) = a_k \lambda_{ki_1} \lambda_{i_1 i_2} \cdots \lambda_{i_s i} \lambda_{kj_1} \lambda_{j_1 j_2} \cdots \lambda_{j_t j}$, where k is the topmost vertex within the shortest trek $i \leftrightarrow j$. As $\psi_G(\sigma_{ij}) = t^{Mu_{ij}}$ where $\sigma^{u_{ij}} = \sigma_{ij}$, we have

$$\begin{aligned}
M_1 M u_{ij} &= 2e_k - e_k + e_{i_1} - e_{i_1} + e_{i_2} - \cdots - e_{i_s} + e_i - e_k + e_{j_1} - e_{j_1} + e_{j_2} - \cdots - e_{j_t} + e_j \\
&= e_i + e_j \\
&= N u_{ij},
\end{aligned}$$

for all $\sigma_{ij}, 1 \le i \le j \le n$. This implies that $N = M_1 M$, which shows that N is contained in the row space of M and thus completes the proof. □

A consequence of Lemma 4.4.4 is that the ideal ST_G is homogeneous with respect to the grading by indices. So, if $\sigma^u - \sigma^v$ is in ST_G, and all variables involved correspond to actual treks, then, for each i, the index i appears the same number of times in both σ^u and σ^v. For example, it is not possible that $\sigma_{11}\sigma_{23} - \sigma_{13}\sigma_{24}$ is in any shortest trek ideal (unless some of these variables correspond to pairs of vertices that are not connected by treks, i.e, some of the variables are mapped to zero).

Remark 4.4.5. Since the σ_{ij} corresponding to pairs of vertices i and j with no trek between them always appear as generators in the ideal ST_G, we need a way to ignore those terms when speaking about binomials in ST_G. Henceforth, when we speak of a binomial $\sigma^u - \sigma^v$ in ST_G, we assume that all variables appearing in this binomial actually correspond to treks in G.

For a DAG G if we want to show that ST_G equals CI_G, it is enough to show that the set of 2×2 minors of $\Sigma_{A \cup C, B \cup C}$ for all possible d-separations of G form a generating set for ST_G. By using Theorem 4.4.2 this is equivalent to show that the graphs $M^{-1}(b)_{\mathcal{F}}$ is connected for all b, where $\mathcal{F}$ is the set of all 2×2 minors of $\Sigma_{A \cup C, B \cup C}$ in the vector form, for all possible d-separations of G. Now, for a fixed b, let $u, v \in M^{-1}(b)_{\mathcal{F}}$. This implies that both Mu and Mv are equal to b, which gives us $\psi_G(\sigma^u - \sigma^v) = 0$. Therefore, it is enough to show that for any $f = \sigma^u - \sigma^v \in ST_G$, σ^u and σ^v are connected by the moves in $\mathcal{F}$.

Now, for a DAG G with n vertices, let $u \in \mathbb{N}^{(n^2+n)/2}$ be a node in the graph of $M^{-1}(b)_{\mathcal{F}}$. We in turn, represent this u, or equivalently the monomial σ^u, as a multi-digraph in the following way: For each factor σ_{ij} of σ^u we draw all edges in the shortest trek $i \leftrightarrow j$ along G with highlighting the top vertices. For each σ_{ii} we highlight that it is a top vertex.

Let $\deg_i(\sigma^u)$ denote the *degree* of a vertex i in σ^u which is defined to be the number of end points of paths in σ^u. We count the loops corresponding to σ_{ii} as having two endpoints at i. If $f = \sigma^u - \sigma^v$ is a homogeneous binomial in ST_G, then $\psi_G(\sigma^u) = \psi_G(\sigma^v)$ if and only if the following conditions are satisfied:

i) The graphs of σ^u and σ^v both have the same number of treks (as f is homogeneous),
ii) The graphs of σ^u and σ^v have the same number of edges between any two adjacent vertices i and j (as the exponent of λ_{ij} in $\psi_G(\sigma^u)$ gives the number of edges between i and j in the graph of σ^u),
iii) The multiset of top vertices in both graphs is the same.
iv) The degree of any vertex in both the graphs is the same (as ST_G is contained in the kernel of η_G by Lemma 4.4.4).

Example 4.4.6. Let G be the DAG as shown in Figure 4.10. From Example 4.1.12 (ii), we know that

$$I_G = ST_G = CI_G = \langle \sigma_{12}\sigma_{23} - \sigma_{13}\sigma_{22}, \sigma_{12}\sigma_{24} - \sigma_{14}\sigma_{22}, \sigma_{13}\sigma_{24} - \sigma_{14}\sigma_{23}\rangle.$$

So, by Theorem 4.4.2, we know that σ^u and σ^v are connected by the moves in $\mathcal{F}$ for any $\sigma^u - \sigma^v \in ST_G$, where $\mathcal{F}$ is the set of 2×2 minors of $\Sigma_{A\cup C,B\cup C}$ in the vector form for all possible d-separations of G. Now, let

$$f = \sigma^u - \sigma^v = \sigma_{12}^2\sigma_{24}\sigma_{23} - \sigma_{22}^2\sigma_{13}\sigma_{14} \in ST_G.$$

The multi-digraphs of σ^u and σ^v are as shown in Figure 4.11. Observe that the graphs of both σ^u and σ^v four treks each. The number of edges $1 \to 2$, $2 \to 3$ and $2 \to 4$ are 2,1 and 1 respectively in both the graphs. Further, the degree of each vertex $\{1\}, \{2\}, \{3\}$ and $\{4\}$ are also 2,4,1 and 1 respectively in both the graphs.

We can reach from σ^u to σ^v by first applying the move which takes $\sigma_{12}\sigma_{24}$ to $\sigma_{22}\sigma_{14}$ and then applying the move which takes $\sigma_{12}\sigma_{23}$ to $\sigma_{13}\sigma_{22}$.

Lemma 4.4.7. *Let G be a safe gluing of G_1 and G_2 such that $ST_{G_1} = CI_{G_1}$ and $ST_{G_2} = CI_{G_2}$. Then the set of all the 2×2 minors of $\Sigma_{A\cup c,B\cup c}$ lie in ST_G, where $A = V(G_1) \setminus C$ and $B = V(G_2) \setminus C$.*

Proof. Let M be the set of all the 2×2 minors of $\Sigma_{A\cup c,B\cup c}$. These minors correspond to the separation criterion that $\{c\}$ d-separates A from B. Every element in M is of the

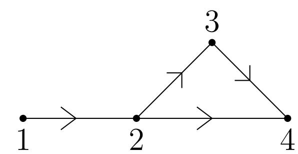


Figure 4.10: A DAG G where $I_G = ST_G$

Figure 4.11: The multi-digraphs of σ^u and σ^v

form $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$, where $i, l \in A \cup c$ and $j, k \in B \cup c$. Now, if all the four shortest treks $i \leftrightarrow j, k \leftrightarrow l, i \leftrightarrow l$ and $k \leftrightarrow j$ contain c, then each of these four treks can be decomposed as

$$\begin{aligned} i \leftrightarrow j &= i \leftrightarrow c \cup c \leftrightarrow j, \\ k \leftrightarrow l &= k \leftrightarrow c \cup c \leftrightarrow l, \\ i \leftrightarrow l &= i \leftrightarrow c \cup c \leftrightarrow l, \\ k \leftrightarrow j &= k \leftrightarrow c \cup c \leftrightarrow j. \end{aligned}$$

From this decomposition, it is clear that $\sigma_{ij}\sigma_{kl}$ covers the same set of edges as $\sigma_{il}\sigma_{kj}$ and hence $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj} \in ST_G$.

If one of these four shortest treks does not pass through c, then we cannot have a decomposition as above and hence cannot imply that the binomial lies in ST_G. Thus, we need to show that such a binomial does not appear in M.

Let $f = \sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$, where $i, l \in A \cup c, k, j \in B \cup c$ and the shortest trek $i \leftrightarrow l$ does not pass through c. Then the two monomials $\sigma_{ij}\sigma_{kl}$ and $\sigma_{il}\sigma_{kj}$ do not preserve the number of edges between adjacent vertices. To illustrate this, let us consider the vertex c' which is adjacent to c and lies in $i \leftrightarrow c$ (Fig 4.12 (i)). (The shortest trek $i \leftrightarrow l$ here passes through the dashed line.) We observe that the multi-digraph of $\sigma_{ij}\sigma_{kl}$ contains the edge $c' \to c$ but the multi-digraph of $\sigma_{il}\sigma_{kj}$ does not contain $c' \to c$ as $i \leftrightarrow l$ does not

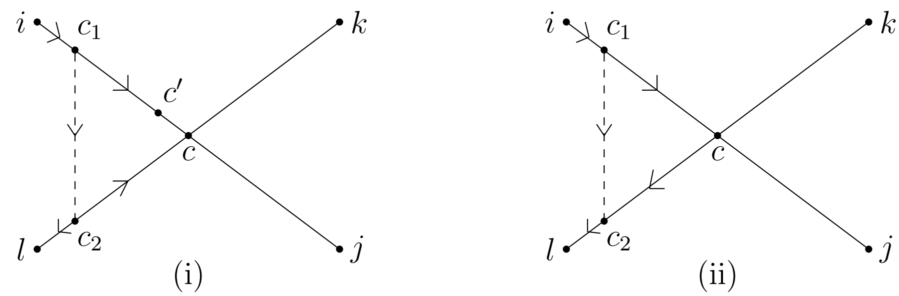


Figure 4.12: Two possible types of cases where an invalid move is possible

pass through c. So, we need to show that $f \notin M$.

Now, all the possible options for DAGs which could fit in the above situation can be classified into two categories. This categorization is independent of the directions in $c \leftrightarrow k$ and $c \leftrightarrow j$ and is as follows :

Case I : The path between i and j containing c has a collider at c :

We illustrate this case in Fig 4.12, (i). Here, the shortest trek $i \leftrightarrow l$ is the trek which passes through the dashed line. Observe that c can d-separate i from j and k from l but it cannot d-separate i from l. Similarly, any vertex which lies in $c_1 \leftrightarrow c_2$ can d-separate i from l but they cannot d-separate i from j and k from l simultaneously. So, there does not exist any 2×2 minor in M where σ_{il} and σ_{ij} or σ_{kl} can occur together.

Case II: The path between i and j containing c does not have a collider at c :

In this case (Fig 4.12, (ii)), we see that c alone cannot d-separate i and l. So, we cannot have a binomial in M with σ_{il} as one of its terms.

Hence we can conclude that every element in M lies in ST_G. $\square$

Suppose that G can be written as a safe gluing of G_1 and G_2 at an n-clique. We define a map $\rho_{G_1} : V(G) \to V(G_1)$ as follows:

$$\rho_{G_1}(i) = \begin{cases} i & i \in V(G_1) \\ c & i \in V(G_2) \setminus C \end{cases}$$

where C is the clique at which G_1 and G_2 are glued and c is the special vertex (choke point) in C. We can lift ρ_{G_1} as a map between from $\mathbb{C}[\Sigma]$ to itself by the rule $\rho_{G_1}(\sigma_{ij}) = \sigma_{\rho_{G_1}(i)\rho_{G_1}(j)}$.

For a vector $u \in \mathbb{N}^{n(n+1)/2}$, let u_{G_1} be the vector that extracts all the coordinates that correspond to the shortest treks that do not lie within G_2. That is,

$$u_{G_1}(ij) = \begin{cases} 0 & i, j \in G_2 \setminus C \\ u(ij) & \text{otherwise.} \end{cases}$$

Then we have the following result.

Proposition 4.4.8. *Let G be a safe gluing of G_1 and G_2, with the map ρ_{G_1} defined as above. Suppose that $\sigma^u - \sigma^v \in ST_G$ and this binomial only involves σ_{ij} variables corresponding to treks. Then*

$$\psi_{G_1}(\rho_{G_1}(\sigma^{u_{G_1}})) - \psi_{G_1}(\rho_{G_1}(\sigma^{v_{G_1}})) = 0.$$

Note that we use the notation ψ_{G_1} to denote the shortest trek map associated to the graph G_1. However, the map ψ_G can also be used since that will give the same result.

Proof. We have

$$\rho_{G_1}(\sigma_{ij}) = \begin{cases} \sigma_{ij} & i, j \in V(G_1) \\ \sigma_{ic} & i \in V(G_1) \text{ and } j \in V(G_2) \setminus C \end{cases}$$

We know that σ^u and σ^v have the same number of treks. Also, the degree of each vertex and the number of edges between any two adjacent vertices is the same. Moreover, the power of each a_i (which corresponds to the source of every trek) is also the same. So, it is enough to show that $\rho_{G_1}(\sigma^{u_{G_1}})$ and $\rho_{G_1}(\sigma^{v_{G_1}})$ have the same number of treks (which corresponds to the sum of all the powers of $a_i, i \in V(G_1)$ in the image) and the number of edges between any two adjacent vertices (which we refer to as the degree of the edge) is also the same.

From the vector u_{G_1} and the map ρ_{G_1}, we see that the treks in σ^u of the form $i \leftrightarrow j$ are converted to $i \leftrightarrow c$, where $i \in V(G_1)$ and $j \in V(G_2) \setminus C$. As $i \leftrightarrow j$ and $i \leftrightarrow c$ have the same edges within G_1, they do not change the degree of any edge within G_1. So, the degree of each edge in G_1 is the same in both σ^u and $\rho_{G_1}(\sigma^{u_{G_1}})$ and hence is the same in $\rho_{G_1}(\sigma^{v_{G_1}})$.

Now all we need to show is that the power of each a_i is the same in both $\rho_{G_1}(\sigma^{u_{G_1}})$ and $\rho_{G_1}(\sigma^{v_{G_1}})$ for each $i \in G_1$. We observe that for every vertex $i \in V(G_1) \setminus \{c\}$, the number of treks in $\rho_{G_1}(\sigma^{u_{G_1}})$ with source a_i remain the same as that in σ^u. The only change that can occur in $\rho_{G_1}(\sigma^{u_{G_1}})$ is the number of treks with source c. There are four types of treks in which c can be the source:

i) treks of the form $c \leftrightarrow i$, where $i \in V(G_1) \setminus C$,
ii) treks of the form $c \leftrightarrow j$, where $j \in V(G_2) \setminus C$,
iii) treks of the form $i \leftrightarrow j$, where $i \in V(G_1) \setminus C$ and $j \in V(G_2) \setminus C$,
iv) $c \leftrightarrow c_i, c_i \in C$.

Case I : The source of each trek of the form $i \leftrightarrow j$ with $i \in G_1$ and $j \in G_2$ lies in G_1 :

In this case, the treks of the form (i) and (iv) remain as it is whereas the treks of the form (ii) and (iii) are converted into $c \leftrightarrow c$ and $c \leftrightarrow i$ respectively, keeping the source of the treks as c. As all the sources lie within G_1, there are no treks of the form $i \leftrightarrow j, i \in G_1, j \in V(G_2) \setminus C$ with source in G_2 which could increase the power of a_c in the image. Hence, the power of a_c is preserved.

Case II : The source of each trek of the form $i \leftrightarrow j$ with $i \in G_1$ and $j \in G_2$ lies in G_2 :

In this case, the existing treks with source c continue to contribute to the power of a_c as in Case I. But, there is a possibility of increasing the power of a_c in $\rho_{G_1}(\sigma^{u_{G_1}})$ as the treks of the form $i \leftrightarrow j, i \in V(G_1), j \in V(G_2) \setminus C$ with source in $V(G_2) \setminus C$ are converted to $c \leftrightarrow i$ with source c. So, we need to show here that the increase in the power of a_c remains the same in both $\rho_{G_1}(\sigma^{u_{G_1}})$ and $\rho_{G_1}(\sigma^{v_{G_1}})$.

We count the number of variables of the form λ_{dc} (i.e, $d < c$) in the image of σ^u. This precisely gives us the number of the treks of the form $i \leftrightarrow j, i \in V(G_1), j \in V(G_2) \setminus C$ with source in $V(G_2) \setminus C$. This is because of the fact that if λ_{ic} occurs in the image of σ^u with $i \in V(G_1) \setminus C$, then it would imply that σ^u has a trek which has an edge $i \to c, i \in V(G_1)$. This would mean the of treks of the form $i \leftrightarrow j, i \in V(G_1), j \in V(G_2) \setminus C$ cannot have source in G_2. As the number of variables of the form λ_{dc} is the same in both σ^u and σ^v, we can conclude that the increase in the power of a_c remains the same in $\rho_{G_1}(\sigma^{u_{G_1}})$ and $\rho_{G_1}(\sigma^{v_{G_1}})$.

So, $\psi_{G_1}(\rho_{G_1}(\sigma^{u_{G_1}})) - \psi_{G_1}(\rho_{G_1}(\sigma^{v_{G_1}})) = 0$. □

Definition 4.4.9. Let G be a safe gluing of G_1 and G_2 with $ST_{G_1} = CI_{G_1}$ and $ST_{G_2} = CI_{G_2}$. Then the *lifting* of any binomial $f = \sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'} \in CI_{G_1}$ is defined as the set of binomials having the following form :

$$\text{lift}(f) = \begin{cases} \sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'} & i', j', k', l' \in V(G_1) \setminus \{c\} \\ \sigma_{i'j}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j} & j' = c \text{ and for any } j \in V(G_2) \setminus D \text{ with } i' \leftrightarrow c \subseteq i' \leftrightarrow j \\ \sigma_{i'j'}\sigma_{k'l} - \sigma_{i'l}\sigma_{k'j'} & l' = c \text{ and for any } l \in V(G_2) \setminus D \text{ with } k' \leftrightarrow c \subseteq k' \leftrightarrow l \\ \sigma_{i'p}\sigma_{ql'} - \sigma_{i'l'}\sigma_{pq} & j' = k' = c \text{ and for any } p, q \in V(G_2) \setminus D \text{ with} \\ & i' \leftrightarrow c \subseteq i' \leftrightarrow q, c \leftrightarrow l' \subseteq p \leftrightarrow l \text{ and } c \in p \leftrightarrow q \end{cases}$$

We can similarly define the lift operation for binomials in CI_{G_2}. From the definition above, lift(f) is not necessarily unique and can be lifted to multiple binomials. The lift operation can be seen as an inverse of the map ρ_{G_1} (or ρ_{G_2}, although the ρ_{G_i} maps are not invertible). In the next lemma, we show that the set of all binomials in lift(f) lies in CI_G and also in ST_G for any $f = \sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'} \in CI_{G_1}$.

Lemma 4.4.10. *Let f be any binomial in CI_{G_1} of the form $\sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'} \in CI_{G_1}$. Then the set of all the binomials in lift(f) lies in both CI_G and ST_G.*

Proof. **i)** We first show that lift$(f) \in CI_G$ for all the four cases given in the definition of lift.

a) In the first case, as $CI_{G_1} \subseteq CI_G$, $\sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'} \in CI_G$ when $i', j', k', l' \in V(G_1) \setminus \{c\}$.

b) When $j' = c$ and $i', k', l' \in V(G_1) \setminus \{c\}$, then $f \in CI_{G_1}$ implies that $\{l'\}$ d-separates $\{i', k'\}$ from $\{c\}$ (or $\{i'\}$ d-separates $\{k'\}$ from $\{l', c\}$). Now, as every trek from i' and k' to any vertex in $V(G_2) \setminus C$ passes through $\{c\}$, we can conclude that $\{l'\}$ d-separates $\{i', k'\}$ from $V(G_2) \setminus D$. So, $\sigma_{i'j}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j} \in CI_G$ for any $j \in V(G_2) \setminus D$. (Similar argument follows when $\{i'\}$ d-separates $\{k'\}$ from $\{l', c\}$.)

c) A similar argument as in (b) follows here.

d) When $j' = k' = c$ and $c \in p \leftrightarrow q$, then we know that every trek from i' to q passes through c. Similarly, every trek from l' to p passes through c. Further, as $\sigma_{i'c}\sigma_{cl'} - \sigma_{i'l'}\sigma_{cc} \in CI_{G_1}$, we know that $\{c\}$ d-separates $\{i\}'$ from $\{l'\}$. From the definition of lift, we know that c lies in $p \leftrightarrow q$. But as $CI_{G_2} = SP_{G_2}$, we can also say that $\{c\}$ d-separates $\{p\}$ from $\{q\}$. Combining all the separations, we have that $\{c\}$ d-separates $\{i', p\}$ from $\{l', q\}$ and hence $\sigma_{i'p}\sigma_{ql'} - \sigma_{i'l'}\sigma_{pq} \in CI_G$.

ii) In each case above, the d-separation criterion forces all the four shortest treks of each binomial to pass through a particular vertex. So, a decomposition similar to the one shown in the proof of Lemma 4.4.7 is always possible and hence lift(f)$\in ST_G$ for all the four cases. $\square$

Lemma 4.4.11. *Let G be a safe gluing of G_1 and G_2, with the map ρ_{G_1} defined as above. Suppose that $\sigma^u - \sigma^v \in ST_G$ and this binomial only involves σ_{ij} variables corresponding to treks. Suppose that $ST_{G_1} = CI_{G_1}$. Then, there is a set of quadratic moves in CI_G that will transform σ^u into a monomial $\sigma^{u'}$ such that $\rho_{G_1}(\sigma^{u'}) = \rho_{G_1}(\sigma^v)$.*

Proof. Since ST_{G_1} equals CI_{G_1}, by Theorem 4.4.2 we know that either $\rho_{G_1}(\sigma^{u_{G_1}})$ is equal to $\rho_{G_1}(\sigma^{v_{G_1}})$ or we can reach from $\rho_{G_1}(\sigma^{u_{G_1}})$ to $\rho_{G_1}(\sigma^{v_{G_1}})$ by making a finite set of moves from the set of 2×2 minors of $\Sigma_{A\cup C,B\cup C}$, for all possible d-separations of G_1.

By using the map ρ_{G_1} we lift each move each move $\sigma_{i'j'}\sigma_{k'l'} - \sigma_{i'l'}\sigma_{k'j'}$ in G_1 to a corresponding move $\sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$ in G, where

$$\rho_{G_1}(\sigma_{ij}) = \sigma_{i'j'},\ \ \rho_{G_1}(\sigma_{kl}) = \sigma_{k'l'},\ \ \rho_{G_1}(\sigma_{il}) = \sigma_{i'l'} \text{ and } \ \rho_{G_1}(\sigma_{kj}) = \sigma_{k'j'}.$$

These moves take σ^u to $\sigma^{u'}$ for some u' such that $\sigma^{u'}$ and σ^v have the same subgraph within G_1. $\square$

We illustrate the technique used in the proof with an example.

Example 4.4.12. Let $G = \{1\to 2, 1\to 4, 1\to 6, 1\to 8, 2\to 3, 4\to 5, 6\to 7, 8\to 9\}$ be a DAG with $V(G_1) = \{1,2,3,6,7\}$ and $V(G_2) = \{1,4,5,8,9\}$. Let

$$f = \sigma^u - \sigma^v = \sigma_{56}\sigma_{47}\sigma_{67}\sigma_{28} - \sigma_{66}\sigma_{27}\sigma_{57}\sigma_{48} \in ST_G.$$

Then $\rho_{G_1}(\sigma^{u_{G_1}}) = \sigma_{16}\sigma_{17}\sigma_{67}\sigma_{12}$. We take

$$m_1 = \sigma_{16}\sigma_{67} - \sigma_{66}\sigma_{17} \in CI_{G_1}$$

as the first move which takes $\rho_{G_1}(\sigma^{u_{G_1}})$ to $\sigma_{66}\sigma_{17}^2\sigma_{12}$. As

$$\rho_{G_1}(\sigma_{56}\sigma_{67} - \sigma_{66}\sigma_{57}) = \sigma_{16}\sigma_{67} - \sigma_{66}\sigma_{17},$$

we lift m_1 to $m_1' = \sigma_{56}\sigma_{67} - \sigma_{66}\sigma_{57} \in CI_G$. Now, we take

$$m_2 = \sigma_{17}\sigma_{12} - \sigma_{27}\sigma_{11} \in CI_{G_1}$$

as the second move which takes $\sigma_{66}\sigma_{17}^2\sigma_{12}$ to $\sigma_{66}\sigma_{17}\sigma_{27}\sigma_{11}$. Further, as

$$\rho_{G_1}(\sigma_{47}\sigma_{28} - \sigma_{27}\sigma_{48}) = \sigma_{17}\sigma_{12} - \sigma_{27}\sigma_{11},$$

we lift m_2 to $m_2' = \sigma_{47}\sigma_{28} - \sigma_{27}\sigma_{48}$. Observe that applying m_1' and then m_2' on σ^u takes σ^u to σ^v.

In a similar way, we can define the map ρ_{G_2} and get a set of moves which would take $\rho_{G_2}(\sigma^{u'})$ to $\rho_{G_2}(\sigma^v)$. This in turn would give us a corresponding set of moves in G which would take $\sigma^{u'}$ to $\sigma^{v'}$ for some v' such that $\sigma^{v'}$ and σ^v have the same subgraph within G_2. But before that, it is important to check that the second set of lifted moves obtained from ρ_{G_2} does not affect the structure of $\sigma^{u'}$ within G_1.

Proposition 4.4.13. *Let $m = \sigma_{ij}\sigma_{kl} - \sigma_{il}\sigma_{kj}$ be a move obtained as a lift of one of the moves in CI_{G_2} which takes $\rho_{G_2}(\sigma^{u'})$ closer to $\rho_{G_2}(\sigma^v)$. Then $\rho_{G_1}(\sigma^{u'}) = \rho_{G_1}(m(\sigma^{u'}))$.*

Proof. As $\rho_{G_1}(\sigma^{u'}) = \rho_{G_1}(\sigma^v)$, the move m corresponds to a d-separation by a vertex in $V(G_2) \setminus C$. Let that vertex be c'. Now, if $i, j, k, l \in V(G_2) \setminus C$, then clearly m does not affect the structure of $\sigma^{u'}$. So, let $i, k \in V(G_1) \setminus C$ and $j, l \in V(G_2) \setminus C$. Then we have

$$\begin{aligned} i \leftrightarrow j &= i \leftrightarrow \cup\, c \leftrightarrow c' \cup c' \leftrightarrow j \\ k \leftrightarrow l &= k \leftrightarrow \cup\, c \leftrightarrow c' \cup c' \leftrightarrow l \\ i \leftrightarrow l &= i \leftrightarrow \cup\, c \leftrightarrow c' \cup c' \leftrightarrow l \\ k \leftrightarrow j &= k \leftrightarrow \cup\, c \leftrightarrow c' \cup c' \leftrightarrow j. \end{aligned}$$

This gives us that the multi-digraph of both $\rho_{G_1}(\sigma_{ij}\sigma_{kl})$ and $\rho_{G_1}(\sigma_{il}\sigma_{kj})$ are same. So, we can conclude that m does not affect the structure of $\rho_{G_1}(\sigma^{u'})$ and hence $\rho_{G_1}(\sigma^{u'}) = \rho_{G_1}(m(\sigma^{u'}))$. ☐

As the moves obtained from ρ_{G_2} do not change the structure of $\rho_{G_1}(\sigma^{u_{G_1}})$ (and vice versa), we see that $\sigma^{v'}$ and σ^v have the same subgraph within G_1 as well. This brings us to the next lemma.

Lemma 4.4.14. *Let G be a safe gluing of G_1 and G_2, with the maps ρ_{G_1} and ρ_{G_2} defined as above. Suppose that $\sigma^u - \sigma^v \in ST_G$ and this binomial only involves σ_{ij} variables corresponding to treks. Suppose that $\rho_{G_1}(\sigma^u) = \rho_{G_1}(\sigma^v)$ and $\rho_{G_2}(\sigma^u) = \rho_{G_2}(\sigma^v)$. Then σ^u and σ^v can be connected by quadratic binomials in CI_G.*

Proof. We can assume that σ^u and σ^v have no variables in common. Since σ^u and σ^v have the same image under ρ_{G_1} and ρ_{G_2} this implies that we cannot have any variables of the form $\sigma_{ij}, i, j \in V(G_1) \setminus \{c\}$ or $i, j \in V(G_2) \setminus \{c\}$ in the monomial factors. This is because the variables of this form are mapped to itself by either of the two maps which would mean that σ^u and σ^v would still have some more common factors between them. So, all the variables appearing in the two factors need to contain c as an end point or as a vertex in their corresponding shortest treks and both end points not lying within the same subgraph (i.e, G_1 or G_2).

Consider an arbitrary trek $i \leftrightarrow j$ in σ^u which is not present in σ^v. We select the trek in σ^v which has the highest number of common edges with $i \leftrightarrow j$. Let that trek be $i' \leftrightarrow j'$ and let $s \leftrightarrow t$ be the common trek in both the treks. Let s_1 and t_1 be the vertices adjacent to s and t respectively in $i \leftrightarrow j$. Similarly, let s' and t' be the vertices adjacent to s and t respectively in $i' \leftrightarrow j'$. Let p be the vertex in $s \leftrightarrow t$ adjacent to t (see Figure 4.13 for an illustration of the idea).

As $\psi_G(\sigma^{v'} - \sigma^v) = 0$ there must exist a path $x \leftrightarrow y$ in σ^v containing the edge $t \leftrightarrow t_1$. We know that all the variables appearing in both the monomial factors need to contain c. This implies that c must lie within the common trek $s \leftrightarrow t$. Let i, i' and x be in $V(G_1) \setminus C$ and j, j', y be in $V(G_2) \setminus C$. The move $m = \sigma_{i'j'}\sigma_{xy} - \sigma_{i'y}\sigma_{xj'}$ is now a valid move as none of the vertices in $i' \leftrightarrow p$ can have a shorter connection to any vertex in $t_1 \leftrightarrow y$ (as every shortest trek from a vertex in $V(G_1) \setminus C$ to $V(G_2) \setminus C$ must pass through c).

Applying m on σ^v increases the length of the common trek between $i \leftrightarrow j$ and $i' \leftrightarrow j'$ by at least 1. As any move preserves the kernel of ψ_G, $m(\sigma^u) - \sigma^v$ still lies in ST_G. Repeating this process again, we can continue to shorten the length of the disagreement until the resulting monomials are the same. $\square$

Using all the results and observations that we have so far, we give a proof of the main result of this section, which shows that quadratic generation of the shortest trek ideals is preserved under the safe gluing operation.

Theorem 4.4.15. *Let G_1 and G_2 be two DAGs such that $ST_{G_1} = CI_{G_1}$ and $ST_{G_2} = CI_{G_2}$. If G is the DAG obtained after a safe gluing of G_1 and G_2 at an n-clique, then ST_G is equal to CI_G and I_G is toric.*

Proof of Theorem 4.4.15. Let $\sigma^u - \sigma^v$ be an arbitrary binomial in ST_G. Then in order to prove that $ST_G = CI_G$, we need to show that σ^u and σ^v are connected by the moves in $\mathcal{F}$, where $\mathcal{F}$ is the set of all the generators of CI_G.

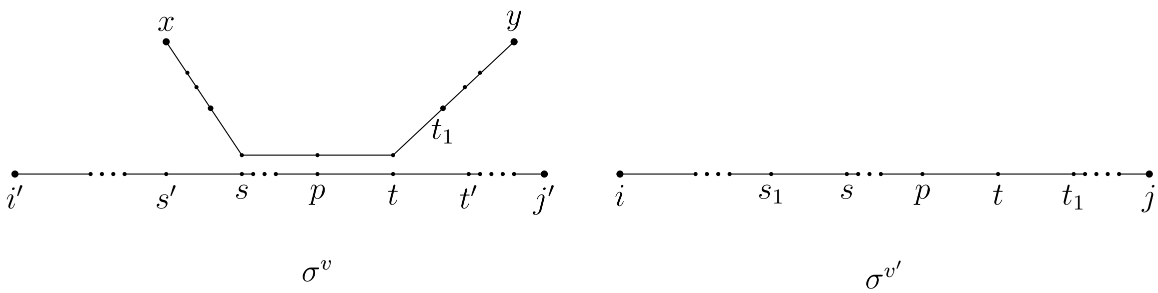


Figure 4.13: Graphs of σ^v and $\sigma^{v'}$. We use undirected treks in the figure to represent treks of unknown direction as the proof is independent of the direction of the treks.

Lemma 4.4.11 shows that we can apply quadratic moves in CI_G to transform σ^u into a monomial $\sigma^{u'}$ such that $\rho_{G_1}(\sigma^{u'}) = \rho_{G_1}(\sigma^v)$. Applying the analogous result for G_2, we see that we can apply quadratic movies in CI_G to transform $\sigma^{u'}$ into $\sigma^{v'}$ such that $\rho_{G_1}(\sigma^{v'}) = \rho_{G_1}(\sigma^v)$ and $\rho_{G_2}(\sigma^{v'}) = \rho_{G_2}(\sigma^v)$. Then applying Lemma 4.4.14, we see that $\sigma^{v'}$ and σ^v can be connected using binomials in CI_G. This shows that $ST_G \subseteq CI_G \subseteq I_G$. But as I_G and ST_G are both prime ideals of the same dimension, this shows that all three ideals are equal. $\square$

4.5 Conjectures

We close the chapter by giving some conjectures about the Gaussian DAGs with toric vanishing ideals. These include some main conjectures, and also conjectures of a more technical nature that would be important tools for proving the main conjectures. We also discuss some consequences of these auxiliary conjectures.

Our first main conjecture relates with a running theme throughout the chapter, identifying the underlying combinatorics of the toric structure when I_G is actually a toric ideal.

Conjecture 4.5.1. *A DAG G has a toric vanishing ideal if and only if $I_G = ST_G$.*

Note, as mentioned previously, there are DAGs G such that ST_G exists, but it not equal to I_G. Our second main conjecture concerns the combinatorial construction of the DAGs for which I_G is toric.

Conjecture 4.5.2. *If G is a DAG such that I_G is toric, then either:*

1. *G is a complete DAG,*
2. *G is either a safe gluing or the gluing at sinks of two smaller DAGs that also have toric vanishing ideals, or*
3. *G is obtained by adding a sink to a smaller DAG.*

Important auxialiary conjectures that we have seen so far in the chapter concern the safe gluing operation, in particular, Conjecture 4.2.14, that safe gluing preserves the property of I_G being equal to ST_G. Another conjecture that seems key to proving classification results for toric vanishing ideals is the following conjecture, that would rule out many graphs from having toric vanishing ideals.

Conjecture 4.5.3. *Let G be a DAG and i, j be two vertices in G such that the minimal size of a d-separating set of i and j is 2 or larger. Then I_G is not toric.*

Assuming the conjecture is true, we have two results on when the vanishing ideal is not toric.

Lemma 4.5.4. *Suppose that Conjecture 4.5.3 is true. Let G be a DAG and i, j be two vertices in G having at least 2 different paths P_1 and P_2 between them. If P_2 is a trek containing the vertex c and P_1 is a path having exactly one collider at c, then I_G is not toric if Conjecture 4.5.3 is true.*

Proof. **Case I:** P_1 and P_2 have no common vertices except i, c and j :

The proof follows from the d-separation of i and j. As c is the only collider within P_1, any set C which contains c and d-separates i from j has to contain at least one more vertex from P_1. This is because $C = \{c\}$ is not enough to d-separate i and j. Hence, by using Conjecture 4.5.3 we can conclude that I_G is not toric.

Case II: P_1 and P_2 have more than 3 common vertices :

Let i_1 be the last common vertex before c and j_1 be the first common vertex after c within the two paths. Then following Case I by replacing i and j with i_1 and j_1 respectively completes the proof. □

Lemma 4.5.5. *Suppose that Conjecture 4.5.3 is true. Let G be a DAG where the shortest trek map cannot be defined. Then I_G is not toric.*

Proof. The shortest trek map in G is not defined when there is no unique shortest trek between two vertices. Let i and j be two vertices in G having two treks P_1 and P_2 between them of the same length and have no other trek whose length is smaller.

Case I: There is no common vertex between P_1 and P_2 except i and j :

In this case, we will have to select at least one vertex from each of the two treks to d-separate i and j. Hence by Conjecture 4.5.3 we can conclude that I_G is not toric.

Case II: P_1 and P_2 have at least one common vertex :

Without loss of generality, we can assume that $i < j$. Let c be the first common vertex between P_1 and P_2. Then the treks P_1 and P_2 can be written as

$$\begin{aligned} P_1 &= P_1(i \rightleftharpoons c) \cup P_1(c \rightleftharpoons j) \text{ and} \\ P_2 &= P_2(i \rightleftharpoons c) \cup P_2(c \rightleftharpoons j), \end{aligned}$$

where $P_1(i \rightleftharpoons c)$ and $P_2(i \rightleftharpoons c)$ denote the trek between i and c within the treks P_1 and P_2 respectively. Let the lengths of $P_1(i \rightleftharpoons c), P_1(c \rightleftharpoons j), P_2(i \rightleftharpoons c)$ and $P_2(c \rightleftharpoons j)$ be r_1, s_1, r_2 and s_2 respectively. Then we have

$$r_1 + s_1 = r_2 + s_2. \tag{4.2}$$

This gives us two new paths between i and j, namely $P_3 = P_1(i \rightleftharpoons c) \cup P_2(c \rightleftharpoons j)$ and $P_4 = P_2(i \rightleftharpoons c) \cup P_1(c \rightleftharpoons j)$. If either of P_3 or P_4 has a collider at c, then by Lemma 4.5.4 we know that I_G is not toric. So, we can assume that P_3 and P_4 are also treks.

Now, let $r_1 < r_2$. Then by equation 4.2, we know that $s_2 < s_1$. From these inequalities, we get that the trek P_3 is of length $r_1 + s_2$ which is smaller than $r_1 + s_1$, a contradiction. (Similar argument follows for $r_2 < r_1$). Thus, we have $r_1 = r_2$ and $s_1 = s_2$. Now replacing j with c, we can follow the same argument as that in Case I. Hence, I_G is not toric. □

Recall that an undirected graph is *chordal* if it has no induced cycles of length ≥ 4. For the remainder of the section, we consider DAGs G whose undirected version $G^{\sim}$ is a chordal graph. In Theorem 4.2.15 we used the condition that I_{G_1} and I_{G_2} can have at most one common variable σ_{cc}. In the next Lemma we show that if Conjecture 4.5.3 is true, then the above condition of Theorem 4.2.15 is satisfied when at least one of G_1 or G_2 is a chordal DAG. So this provides further evidence in favor of Conjecture 4.2.14.

Lemma 4.5.6. *Suppose that Conjecture 4.5.3 is true. Let G_1 and G_2 be two DAGs with $I_{G_1} = ST_{G_1}$ and $I_{G_2} = ST_{G_2}$. Let G be the resultant DAG obtained after a safe gluing of G_1 and G_2 at an n-clique. Let $C = \{c\} \cup D$ be the vertices in the n-clique where c is the choke point. Let $c' \in C$ and $d \in D$. If G_1 is chordal and p_1 is a vertex in $G_1 \setminus C$ such* *that the shortest trek $p_1 \leftrightarrow c'$ contains the edge $c' \to d$ then G can be constructed by safe gluing two DAGs at an $(n-1)$-clique.*

Proof. Let $p_1 - p_2 - \cdots - p_m - c' \to d$ be the shortest trek between p_1 and d, where $p_1 - p_2$ denotes the edge between p_1 and p_2 of unknown direction. Then $p_m - c' \to d$ is also the shortest trek between p_m and d. Let us assume that G cannot be constructed by safe gluing two DAGs at an $(n-1)$-clique. Then there must exist another path from p_m to d not containing the edge $c' \to d$. We select that path whose vertices are adjacent to either p_m, c' or d. Let $p_m - q_1 - \cdots - q_r \to d$ be such a path. As G_1 is chordal, either $p_m \to d$ is an edge or there exists an edge between q_r and c'. If $p_m \to d$ is an edge, then $p_m \to d$ becomes a shorter trek than $p_m - c' \to d$, which is a contradiction. If there is an edge between q_r and c', there must also be an edge between p_m and q_r (again as G_1 is chordal and I_{G_1} is toric). Independent of the direction of these two edges $q_r - c'$ and $p_m - q_r$, we can say that p_m is d-separated from d by at least two vertices c' and q_r. Thus by using Conjecture 4.5.3 we can imply that I_{G_1} is not toric, which is a contradiction. $\square$

So far we have shown that safe gluing preserves the toric property of the vanishing ideals. But it is an interesting problem to check if a DAG G with toric vanishing ideal can always be obtained as a safe gluing of smaller DAGs with toric vanishing ideals. We end this chapter with the conjecture that such a decomposition always exist for chordal graphs if Conjecture 4.5.3 is true.

Conjecture 4.5.7. *Suppose that Conjecture 4.5.3 is true. Let G be a chordal DAG with toric vanishing ideal. Then there exist G_1 and G_2 with toric vanishing ideals such that G can be obtained as a safe gluing of G_1 and G_2 at an n-clique.*

REFERENCES

[1] Aldous, D. J. (2020). On the Largest Common Subtree of Random Leaf-Labeled Binary Trees. *https://arxiv.org/abs/2006.10545*

[2] Allman., E. S., and John A. Rhodes., J. A. (2005). *Lecture Notes: The Mathematics of Phylogenetics*

[3] Bernstein., D. I., Tung Ho., L. S., Long, C., Steel, M., John, K., and Sullivant, S. (2015). Bounds on the expected size of the maximum agreement subtree. *SIAM J. Discrete Math*, 29(4): 2065–2074.

[4] Bordewich, M., Linz, S., Owen, M., John, K. S., Semple, C., and Wicke, K. (2020). On the maximum agreement subtree conjecture for balanced trees. *https://arxiv.org/abs/2005.07357*.

[5] Bryant, D., McKenzie, A., and Steel, M. (2003). The size of a Maximum agreement subtree for random binary trees. in BioConsensus, *DIMACS Ser. Discrete Math. Theoret. Comput. Sci.*, 61:55–65. AMS, Providence, RI.

[6] DeLoera, J. A., Sturmfels, B., and Thomas, R. R. (1995). Gröbner bases and triangulations of the second hypersimplex. *Combinatorica*, 15(3):409–424.

[7] Diaconis, P. and Sturmfels, B. (1998). Algebraic algorithms for sampling from conditional distributions. *Ann. Statist.* 26(1):363–397.

[8] Dobra, A. and Sullivant, S. (2004). A divide-and-conquer algorithm for generating Markov bases of multi-way tables. *Computational Statistics*, 19(3):347–366.

[9] Drton, M., Massam, H., and Olkin, I. (2008). Moments of minors of Wishart matrices. *The Annals of Statistics*, 36(5):2261–2283.

[10] Drton, M., Sturmfels, B., and Sullivant, S. (2007). Algebraic factor analysis: tetrads, pentads and beyond. *Probability Theory and Related Fields*, 138(3-4):463–493.

[11] Drton, M., Sturmfels, B., and Sullivant, S. (2009). *Lectures on algebraic statistics.* Oberwolfach Seminars, Vol 39, Birkhäuser Verlag, Basel.

[12] Examples of Phylogenetic trees : https://www.pinterest.com/pin/560064903645773178/

[13] Grayson, D. R. and Stillman, M. E. (2017). Macaulay2, a software system for research in algebraic geometry. `https://faculty.math.illinois.edu/Macaulay2/`.

[14] Felsenstein, J. (2004). *Inferring Phylogenies.* Sinauer Associates, Inc.

[15] Hassett, B. (2007). *Introduction to algebraic geometry.* Cambridge University Press, Cambridge.

[16] Herzog, J., Hibi, T., and Ohsugi, H. (2018). *Binomial ideals*, volume 279 of *Graduate Texts in Mathematics.* Springer, Cham.

[17] Hoşten, S. and Sullivant, S. (2002). Gröbner bases and polyhedral geometry of reducible and cyclic models. *Journal of Combinatorial Theory. Series A*, 100(2):277–301.

[18] Jones, B. and West, M. (2005). Covariance decomposition in undirected Gaussian graphical models. *Biometrika*, 92(4):779–786.

[19] Kelley, T. (1935). *Essential Traits of Mental Life*, volume 26 of *Harvard Studies in Education.* Harvard University Press, Cambridge, MA.

[20] Koller, D. and Friedman, N. (2009). *Probabilistic graphical models.* Adaptive Computation and Machine Learning. MIT Press, Cambridge, MA.

[21] Lauritzen, S. L. (1996). *Graphical models*, volume 17 of *Oxford Statistical Science Series*. Oxford University Press, New York.

[22] Martin, D. M., and Thatte, B. D. (2013). The maximum agreement subtree problem. *Discrete Appl. Math.*, 161:1805-1817.

[23] Milne, J. S. (2017) Algebraic Geometry, Version 6.02. *www.jmilne.org/math/*

[24] Misra, P. and Sullivant, S. (2019). Bounds on the expected size of the maximum agreement subtree for a given shape. *SIAM Journal on Discrete Mathematics*, 33(4): 2316–2325

[25] Misra, P. and Sullivant, S. (2020). Gaussian graphical models with toric vanishing ideals. *Annals of the Institute of Statistical Mathematics*, DOI 10.1007/s10463-020-00765-0.

[26] T.S. Richardson, T. S. and P. Spirtes, P. (2002) Ancestral graph Markov models. *Ann. Statist*, 30: 962-1030.

[27] Semple, C. and Steel, M. (2003). *Phylogenetics.* Oxford University Press.

[28] Spirtes, P., Glymour, C., and Scheines, R. (2000). *Causation, prediction, and search.* Adaptive Computation and Machine Learning. MIT Press, Cambridge, MA, second edition.

[29] Steel, M. and Warnow, T. (1993). Kaikoura tree theorems: computing the maximum agreement subtree. *Information Processing Letters* 48:77-82

[30] Steel., M. (2016). *Phylogeny — discrete and random processes in evolution*, volume 89 CBMS-NSF Regional Conference Series in Applied Mathematics, *Society for Industrial and Applied Mathematics (SIAM)* . Philadelphia, PA.

[31] Sturmfels, B. (1996). *Gröbner bases and convex polytopes*, Volume 8 of *University Lecture Series*. American Mathematical Society, Providence, RI.

[32] Sturmfels, B. and Uhler, C. (2010). Multivariate Gaussian, semidefinite matrix completion, and convex algebraic geometry. *Annals of the Institute of Statistical Mathematics*, 62(4):603–638.

[33] Sullivant, S. (2007). Toric fiber products. *Journal of Algebra*, 316(2):560–577.

[34] Sullivant, S. (2008). Algebraic geometry of Gaussian Bayesian networks. *Advances in Applied Mathematics*, 40(4):482–513.

[35] Sullivant, S. (2018). *Algebraic statistics*, Volume 194 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI.

[36] Sullivant, S., Talaska, K., and Draisma, J. (2010). Trek separation for Gaussian graphical models. *The Annals of Statistics*, 38(3):1665–1685.