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Learning the Linear Relations of Undirected Gaussian Graphical Models with Symmetries

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Thesis for the attainment of the academic degree

Bachelor of Science

at the TUM School of Computation, Information and Technology of the Technical University of Munich

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Submitted:
Munich, January 15, 2025

I hereby declare that this thesis is entirely the result of my own work except where otherwise indicated. I have only used the resources given in the list of references.

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Zusammenfassung

Gaußsche Graphenmodelle repräsentieren bedingte Unabhängigkeitsbeziehungen in multivariaten Gaußschen Verteilungen durch ungerichtete Graphen. Frühere Arbeiten zu diesem Thema haben die algebraische Struktur der Erzeuger des verschwindenden Ideals für bestimmte Grapharten mit einer bestimmten Färbung untersucht. Auf dieser Grundlage untersucht diese Arbeit zyklische Graphen im Detail und berücksichtigt dabei alle möglichen Färbungen dieses Graphentyps. Das Hauptziel besteht darin, die Gültigkeit einer Vermutung zu überprüfen, die besagt, dass in zyklischen Graphen die binomischen Linearformen im verschwindenden Ideal genau dann existieren, wenn es eine entsprechende Symmetrie im Graphen gibt. Durch rechnerische Studien und theoretische Analysen wird die hinreichende Bedingung der Vermutung für alle n-Zyklen bestätigt, wobei gezeigt wird, dass, wenn eine Symmetrie in einem zyklischen Graphen existiert, die binomischen Linearformen, die durch diese Symmetrie induziert werden, im verschwindenden Ideal enthalten sind. Die notwendige Bedingung dagegen kann nur für 3- und 5-Zyklen bewiesen werden. Indem wir Gegenbeispiele konstruieren, widerlegen wir, dass die notwendige Bedingung der Vermutung für alle n-Zyklen gilt. Das zeigt, dass nicht in allen n-Zyklen alle binomischen Linearformen durch Symmetrien im Graphen entstehen. Des Weiteren untersuchen wir nicht-binomische Linearformen im verschwindenden Ideal und schlagen eine Vermutung über ihre strukturellen Eigenschaften vor, die noch vollständig verstanden werden müssen. Alle Berechnungen für diese Arbeit werden mit Macaulay2 durchgeführt, wobei der Code im Anhang bereitgestellt wird, um weitere Forschungen zu unterstützen.

Abstract

Gaussian graphical models represent conditional independence relationships in multivariate Gaussian distributions through undirected graphs. Previous studies have explored the algebraic structures of the generators of the vanishing ideal for certain graph types with a specific coloring. Building on this foundation, this thesis investigates cycle graphs in detail, considering all possible colorings of this graph type. The primary objective is to evaluate the validity of a conjecture stating that, in cycle graphs, binomial linear forms are elements of the vanishing ideal if and only if there exists a corresponding symmetry in that graph. Through computational studies and theoretical analyses, the sufficient part of the conjecture is confirmed for all n-cycles, demonstrating that whenever a symmetry exists in a cyclic graph, all binomial linear forms induced by that symmetry lie in the vanishing ideal. The necessary condition, however, is proven only for 3- and 5-cycles. By constructing counterexamples, we show that the necessary condition of the conjecture does not hold for all n-cycles, demonstrating that not all binomial linear elements of the vanishing ideal arise from graph symmetries for all n-cycles. Furthermore, we examine non-binomial linear forms within the vanishing ideal and propose a conjecture regarding their structural properties, which remain to be fully understood. All computations for this thesis are performed using Macaulay2, with the code provided in the appendix to support further research.

Contents

1 Introduction

Gaussian graphical models provide a powerful framework for understanding the conditional dependence relationships in multivariate Gaussian distributions through graph theory. These models use graphs to encode dependencies among variables, with vertices representing variables and edges indicating direct conditional dependencies. They find applications in diverse fields such as genomics, finance, and social network analysis, where understanding the interactions between variables is critical for uncovering underlying structures. A central object of study in these models is the covariance matrix, which captures the direction and strength of the linear relationships between variables. The algebraic study of this matrix, particularly its constraints, has become a crucial aspect of understanding Gaussian graphical models. These constraints directly impact the vanishing ideal, since it encounters for all polynomial relations that need to be satisfied by the entries of the covariance matrix in order to preserve the underlying structure of the graph. This thesis extends the foundational analysis of Gaussian graphical models by examining the connection between graph symmetries and the vanishing ideal arising from these models. In particular, we investigate how symmetries in the graph influence the binomial linear elements of the vanishing ideal with a specific focus on cyclic graphs. Cyclic graphs are of major importance since they can represent complex, bidirectional, and recursive dependencies in systems, enabling the modeling of feedback loops, joint distributions, and real-world phenomena that exhibit cyclic, non-hierarchical behavior. A central question in this investigation is the validity of the following conjecture, proposed by Davies and Marigliano [3]:

Conjecture 1.0.1. [3, Conjecture 4.2] Let G be a colored n-cycle. All binomial linear forms in the vanishing ideal $I(\mathcal{L}^{-1})$ are induced by symmetries.

This conjecture establishes a precise relationship between algebraic structures and graph theoretic properties. If it proves correct, it provides a powerful tool for characterizing binomial linear forms in the vanishing ideal purely through the symmetries of the graph. This connection would not only simplify the study of the algebraic structure of reciprocal varieties but also enable more efficient computational analyses of Gaussian graphical models, especially in applications where model parameters need to be estimated or tested on large datasets. Despite the promise of this conjecture, its general validity remains an open question. Prior research, including the work by Davies and Marigliano [3], has explored specific cases, but a complete proof remains unknown. This thesis aims to address this gap by focusing on cyclic graphs. Through computational studies and theoretical analysis, we examine whether Conjecture 1.0.1 holds for all n-cycles. The thesis is structured as follows: Chapter 2 introduces Gaussian graphical models, discussing the concentration matrix and its role in defining the vanishing ideal. Therefore, a method for explicitly calculating the inverse of the concentration matrix, the covariance matrix, is presented, providing a way to find the elements of the vanishing ideal. Chapter 3 introduces the concept of graph colorings, which enable the examination of graph symmetries. This chapter includes an analysis of specific graphs with a particular coloring configuration: uniformly colored graphs. Chapter 4 is the main and most important part of this thesis. It begins with a computational study on binomial linear generators of the vanishing ideal for cyclic graphs with three, four, and five vertices. This chapter presents a detailed analysis of graph symmetries and their impact on the generators of the vanishing ideal. Furthermore, we investigate the binomial linear forms within this ideal, allowing us to address the main goal of this thesis: determining whether Conjecture 1.0.1 holds for all n-cycles. Chapter 5 extends the discussion to non-binomial linear forms. It includes a computational study of these forms for cyclic graphs with four and five vertices and proposes a conjecture explaining aspects of their structural properties. The chapter concludes by posing an open question for future research.

2 Preliminaries on Gaussian graphical models

Gaussian graphical models arise from the statistical framework for modeling multivariate Gaussian distributions, where the goal is to understand the conditional dependencies between random variables. By representing these dependencies through the structure of an undirected graph, Gaussian graphical models enable an intuitive and mathematically rigorous way to study relationships in high-dimensional data. This section introduces the core concepts of these models, laying the groundwork for their theoretical and practical applications.

2.1 Setup of a Gaussian graphical model

We setup a Gaussian graphical model by following the framework and its application to graph-based modeling of conditional dependencies established by Sullivant [9]. Let $X = (X_1, X_2, ..., X_n) \in \mathbb{R}^n$ be a random vector, which is distributed according to a multivariate Gaussian, $X \sim \mathcal{N}(\mu, \Sigma)$, where $\mu = (\mu_1, \mu_2, \ldots, \mu_n) \in \mathbb{R}^n$ is the vector of means and $\Sigma \in \mathbb{R}^{n\times n}$ is the symmetric matrix, capturing the covariances between all variables in X. For the Gaussian Graphical Model to be well-defined, we require the covariance matrix Σ to be positive definite, ensuring that it is invertible. To model the conditional dependencies and independencies among the components of X, we construct a Gaussian graphical model. In this framework, we define an undirected graph $G = (V, E)$, where the vertex set $V := \{1, 2, \ldots, n\}$ and the edge set E are determined as follows: each random variable X_i is associated with a vertex $i \in V$. An edge is placed between vertices i and j if and only if the corresponding random variables X_i and X_j are dependent. Conversely, if X_i and X_j are conditionally independent given all other variables, then there is no edge between i and j. Thus, the edge set is given by $E = \{\{i, j\} \mid i, j \in V \text{ and } X_i \text{ and } X_j \text{ are dependent}\}$.

2.2 Introduction of the concentration and adjacency matrices and the reciprocal variety

In the context of Gaussian graphical models, two matrices are of major importance: the *concentration matrix* and the *adjacency matrix*.

As described in [9], the conditional dependencies represented by the edge structure of the graph are encoded in the symmetric *concentration matrix* $K = (k_{ij}) \in \mathbb{R}^{n\times n}$, where K is the inverse of the covariance matrix. For $i, j \in V$, the entry ij-th and ji-th entries of K represents the conditional dependence between the random variables X_i and X_j. Formally:

$$k_{ij} \neq 0 \iff \text{there is an edge between the vertices } i \text{ and } j \text{ in the graph } G \iff X_i \text{ and } X_j \text{ are dependent.}$$

Conversely, if X_i and X_j are conditionally independent, given all other variables, which corresponds to the absence of an edge between i and j in G, it holds $k_{ij} = 0$. Due to the positive definiteness of Σ, its inverse K is also positive definite and therefore, $k_{ii} \neq 0$ for all vertices $i \in V$.

The concentration matrix K can be expressed as a linear combination of linearly independent symmetric matrices:

$$K = \sum_{\{i,j\}\in E} K_{ij} + \sum_{i\in V} K_{ii},$$

where each K_{ij} is defined as the symmetric matrix with the ij-th and ji-th entries corresponding to the partial correlation between X_i and X_j, and all other entries being zero. The collection of these matrices induces a linear subspace of the space of real symmetric matrices $\mathbb{S}^n$, as outlined in [9], defined as:

$$\mathcal{L} = \text{span}\{K_{ij} \mid \{i, j\} \in E \text{ or } i = j\}.$$

The *reciprocal variety* $\mathcal{L}^{-1}$ is the set of all symmetric matrices $\Sigma \in \mathbb{S}^n$ whose inverses belong to $\mathcal{L}$ [9]:

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

The vanishing ideal of $\mathcal{L}^{-1}$, denoted $I(\mathcal{L}^{-1})$, is the set of all polynomials in the polynomial ring $\mathbb{R}[\Sigma]$ that vanish on $\mathcal{L}^{-1}$. This ideal encodes the algebraic constraints that the matrix Σ must satisfy for its inverse to lie in $\mathcal{L}$.

The *adjacency matrix* $A = (a_{ij}) \in \mathbb{R}^{n\times n}$, as defined in [1], has a similar structure to the concentration matrix K. It is also symmetric and all off-diagonal, non-zero entries of K are set to be one in A. The main difference between K and A is that the diagonal entries of A are set to zero. Specifically, for $i, j \in V$ with $i \neq j$, the ij-th and ji-th entry of A is 1 if and only if there is an edge between i and j, i.e. $\{i, j\} \in E$.

2.3 Relating the concentration and covariance matrices

Our goal is to find the linear elements among the generators of the ideal $I(\mathcal{L}^{-1})$, especially the binomial linear ones. To do so, we are interested in representing the entries of the covariance matrix Σ by the entries of the concentration matrix K, which can be directly inferred from the graph. This requires a function that maps the entries of K to the entries of the covariance matrix Σ.

Sullivant established such a connection by introducing the *pull-back* map ρ in [9], which arises from the identity $K\cdot\Sigma^{-1} = \mathrm{Id}$. Let $\mathbb{R}[K] = \mathbb{R}[k_{11}, k_{12}, \dots, k_{nn}]$ be the polynomial ring in the entries of the concentration matrix K, and $\mathbb{R}(K)$ be its fraction field. Then the *pull-back* map is defined as:

$$\rho : \mathbb{R}[\Sigma] \to \mathbb{R}(K), \qquad \rho(\sigma_{ij}) = \rho_{ij}(K) = \left(K^{-1}\right)_{ij} = \frac{1}{\det(K)} \cdot \mathrm{Cofactor}(K)_{ji} = \frac{1}{\det(K)}(-1)^{j+i} \det\left(K^{ji}\right),$$

where K^{ji} is the submatrix of K obtained by deleting the j-th row and i-th column. The value $\rho_{ij} \in \mathbb{R}(K)$ thus represents the ij-th entry of K^{-1}. This map is well-defined since it only inserts invertible elements of $\mathcal{L}$. For any polynomial $f \in \mathbb{R}[\Sigma]$ and any $K \in \mathcal{L}$, we have the following composition:

$$\rho(f)(K) = f \circ \rho(K) = f(\rho_{11}(K), \rho_{12}(K), \dots, \rho_{nn}(K)).$$

Hence, the kernel of this map consists of the polynomial elements in $\mathbb{R}[\Sigma]$ that vanish when evaluated at $K^{-1} = \Sigma$:

$$\ker(\rho) = \{f \in \mathbb{R}[\Sigma] \mid f(K^{-1}) = f(\Sigma) = 0\}.$$

Therefore, the elements of the kernel correspond to polynomial relations between the entries of the covariance matrix Σ, that vanish. Since $\Sigma \in \mathcal{L}^{-1}$, the kernel of ρ is equal to the vanishing ideal, as outlined in [9]:

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

Any entry in K^{-1} can be expressed as the product of $1/\det(K)$ and a polynomial. Since the determinant is a constant scalar, the map defined by

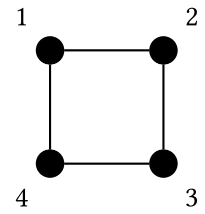
$$\rho^* : \mathbb{R}[\Sigma] \to \mathbb{R}(K), \qquad \rho^*(\sigma_{ij}) = \det(K) \cdot \rho_{ij}(K) = \mathrm{Cofactor}(K)_{ji},$$

has the same kernel as ρ [9]. Therefore, it also holds that

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

To illustrate the practical application of the *pull-back* map, we consider the following example:

Example 2.3.1. Let G be the uncolored 4-cycle.



The corresponding concentration matrix of this graph is

$$K = \begin{pmatrix} k_{11} & k_{12} & 0 & k_{14} \\ k_{12} & k_{22} & k_{23} & 0 \\ 0 & k_{23} & k_{33} & k_{34} \\ k_{14} & 0 & k_{34} & k_{44} \end{pmatrix}.$$

By applying the second version of the *pull-back* map, p^*, we can compute the covariance matrix Σ multiplied by the determinant of K, from which we obtain the generators of the vanishing ideal $I(\mathcal{L}^{-1})$. For example,

$$\rho^*(\sigma_{11}) = \det(K) \cdot \sigma_{11} = \det(K) \cdot \left(K^{-1}\right)_{11} = (-1)^{1+1} \cdot \det \begin{pmatrix} k_{22} & k_{23} & 0 \\ k_{23} & k_{33} & k_{34} \\ 0 & k_{34} & k_{44} \end{pmatrix} = k_{22}k_{33}k_{44} - k_{22}k_{34}^2 - k_{23}^2 k_{44},$$

$$\rho^*(\sigma_{12}) = \det(K) \cdot \sigma_{12} = \det(K) \cdot \left(K^{-1}\right)_{12} = (-1)^{2+1} \cdot \det \begin{pmatrix} k_{12} & 0 & k_{14} \\ k_{23} & k_{33} & k_{34} \\ 0 & k_{34} & k_{44} \end{pmatrix} = -k_{14}k_{23}k_{34} + k_{12}k_{34}^2 - k_{12}k_{33}k_{44}.$$

In this uncolored 4-cycle, no linear relations vanish on Σ since all entries of the concentration matrix K are distinct. With 8 degrees of freedom in K, the dimension of $I(\mathcal{L}^{-1})$ is 8.

We define an uncolored graph as one where all partial correlations are distinct. For such graphs, no linear forms exist in the vanishing ideal, except for those originating from disconnected components. This result follows from the proposition established in [3]:

Proposition 2.3.2. *[3, Prop. 2.5] Let G be a colored graph, and let the vertices i and j belong to different connected components of G. Then, $\sigma_{ij} \in I(\mathcal{L}^{-1})$.*

Proof. When i and j belong to different components in G, the graph G can be decomposed into m disjoint subgraphs $G_1, G_2, ..., G_m$, where i is in one component and j is in another component. By reordering the vertices of G in a way such that the vertices of each connected component are grouped together, the concentration matrix K of the underlying uncolored graph can be written in a block-diagonal form:

$$K = \begin{pmatrix} K_1 & 0 & \cdots & 0 \\ 0 & K_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & K_m \end{pmatrix},$$

where K_l corresponds to the subgraph G_l for $l \in \{1, 2, \ldots, m\}$. Since K is block-diagonal, its inverse $\Sigma = K^{-1}$ also exhibits block-diagonal structure:

$$\Sigma = \begin{pmatrix} \Sigma_1 & 0 & \cdots & 0 \\ 0 & \Sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_m \end{pmatrix}.$$

Here, $\Sigma_l = K_l^{-1}$ is the covariance matrix corresponding to the subgraph G_l. Since i and j belong to different connected components and the off-diagonal blocks of Σ are zero, $\sigma_{ij} = 0$ for all i, j in different connected components. □

For any uncolored graph, where all edges and vertices have distinct partial correlations, the vanishing ideal $I(\mathcal{L}^{-1})$ has dimension $|V| + |E|$, since there are as many distinct entries in K that determine Σ, and thus the vanishing ideal. Consequently, calculating the generators of this ideal can become algebraic complex, even for relatively small graphs. To address this, we introduce graph colorings as a tool to reduce the dimension of the vanishing ideal and the computational complexity in the next chapter.

3 Obtaining binomial linear forms from symmetries

This chapter explores methods to reduce the dimension of the vanishing ideal $I(\mathcal{L}^{-1})$ and therefore simplify the computation of the linear generators of $I(\mathcal{L}^{-1})$. To achieve this, we introduce graph colorings, which enable the analysis of graph symmetries. These symmetries offer a powerful technique for identifying specific linear generators, the binomial linear ones. Finally, we provide an explicit characterization of all binomial linear generators of the vanishing ideal for specific types of graphs with specific color configurations.

3.1 Graph colorings

Partial correlations between distinct vertices in a graph can be equal, reflecting structural equivalences in the graph. When such partial correlations are equal, this reduces the complexity of the calculation of the generators of the vanishing ideal $I(\mathcal{L}^{-1})$. To formalize and make use of these equivalences, we introduce the concept of graph coloring. Graph coloring is based on the idea of grouping variables, vertices or edges, with approximately equal partial concentrations into equivalence classes. If two partial correlations are equal, the corresponding vertices or edges in the graph are assigned the same color [3].

To describe this formally, let $\lambda(i)$ and $\lambda(\{i,j\})$ denote the colors of a vertex $i \in V$ and an edge $\{i,j\} \in E$, respectively. The relationship between the colorings and the concentration matrix is then as described in [2]:

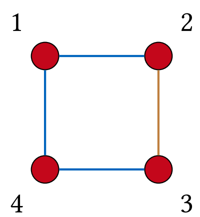
Definition 3.1.1 (Concentration matrix of a colored graph). Let $G = (V, E)$ be an undirected graph with associated concentration matrix K. The matrix K has the following properties:

1. If the vertices $i \in V$ and $j \in V$ have the same partial correlation and are therefore in the same equivalence class, then $\lambda(i) = \lambda(j)$ and $k_{ii} = k_{jj}$.

2. If the edges $\{i,j\} \in E$ and $\{l,m\} \in E$ have the same partial correlation, then $\lambda(\{i,j\}) = \lambda(\{l,m\})$ and $k_{ij} = k_{lm}$.

This approach not only reduces the number of free parameters in the concentration matrix but also influences the structure of the vanishing ideal $I(\mathcal{L}^{-1})$. Specifically, the dimension of the vanishing ideal is directly tied to the number of distinct entries in the concentration matrix, which corresponds to the number of distinct colors used in the graph. Fewer colors correspond to a lower dimensional linear subspace, offering a more compact representation of the ideal and reducing the computational time required to calculate the generators of the vanishing ideal. The benefits of graph coloring are illustrated in the following example, which is a colored version of Example 2.3.1:

Example 3.1.2. Let G be the 4-cycle defined in Example 2.3.1, with the following specific coloring:



In this example, all vertices are in the same equivalence class, so all diagonal entries of the concentration matrix are equal. Furthermore, the edges $\{1,2\}$, $\{3,4\}$, and $\{1,4\}$ share the same color, leading to the following concentration matrix:

$$K = \begin{pmatrix} k_{11} & k_{12} & 0 & k_{12} \\ k_{12} & k_{11} & k_{23} & 0 \\ 0 & k_{23} & k_{11} & k_{12} \\ k_{12} & 0 & k_{12} & k_{11} \end{pmatrix}.$$

Calculating the *pull-back* map yields the covariance matrix Σ, enabling us to find the generators of the ideal of the reciprocal variety $I(\mathcal{L}^{-1})$. In this case, the dimension of the ideal is 3, since there are 3 distinct entries in the concentration matrix K. Compared to the uncolored version of this graph, the degrees of freedom are reduced by 5, significantly simplifying the system. This coloring also results in some binomial linear forms within the vanishing ideal:

$$\sigma_{22} - \sigma_{33}, \quad \sigma_{13} - \sigma_{24}, \quad \sigma_{12} - \sigma_{34}, \quad \sigma_{11} - \sigma_{44}.$$

In the next section, we provide an explanation of the origin of these binomial linear forms.

3.2 Graph symmetries and induced binomial linear forms

Specific graph coloring configurations naturally reveal graph symmetries. Intuitively, a graph symmetry refers to a rearrangement, or permutation, of the vertices and edges of a graph such that the graph remains unchanged after the transformation, preserving the relationships between all vertices and edges. In other words, a symmetry is a way of shuffling the graph while maintaining its structure and the connections between its elements. These graph symmetries have an interesting role in determining the algebraic relations among the entries of Σ and consequently the generators of the $I(\mathcal{L}^{-1})$. To begin this investigation, we first recall the definition of a graph symmetry as stated in [3]:

Definition 3.2.1 (Graph symmetry). A symmetry of a graph G is a permutation matrix $P \in GL(n, \mathbb{R})$, the general linear group of invertible matrices, for which the following equation holds:

$$PKP^{-1} = K,$$

where K is the concentration matrix associated with G.

Remark 3.2.2. Whenever a permutation matrix P meets this condition for the concentration matrix K, it also holds that $PAP^{-1} = A$ for the corresponding adjacency matrix A of G. This is because A has the same structure as K, where all non-zero entries are equal to one, except for the diagonal, which is zero in A.

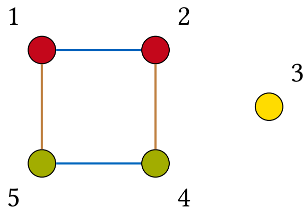
Using these symmetries, one can derive the binomial linear generators of the vanishing ideal $I(\mathcal{L}^{-1})$:

Proposition 3.2.3. *[3, Prop. 2.2] Let G be a colored graph and $P \in GL(n, \mathbb{R})$ be a symmetry of that graph. Then, the entries of the matrix $P\Sigma P^{-1} - \Sigma$, where Σ is the covariance matrix of G, vanish on $\mathcal{L}^{-1}$, and the distinct entries form binomial linear generators of the ideal $I(\mathcal{L}^{-1})$.*

Proof. If P is a symmetry of G, then by Definition 3.2.1, $PKP^{-1} = K$ for the concentration matrix $K \in \mathcal{L}$ of the graph. Since $\Sigma = K^{-1} \in \mathcal{L}^{-1}$, it also holds that $P\Sigma P^{-1} = \Sigma$. Subtracting Σ from both sides yields $P\Sigma P^{-1} - \Sigma = 0$, which implies that the entries of $P\Sigma P^{-1} - \Sigma$ vanish on $\mathcal{L}^{-1}$. Since P is a permutation matrix, the entries of this difference are binomial linear forms. □

Following the terminology introduced in [3], we refer to these linear forms as *induced by symmetries*, and we say that the ideal $I(\mathcal{L}^{-1})$ is *induced by symmetries* if the entire linear part of the ideal is generated by these forms. To illustrate the connection between graph symmetries and the generation of binomial linear forms, consider the following example:

Example 3.2.4. Let G be the following disconnected graph:



Since the graph consists of two disconnected components, we can apply Proposition 2.3.2, which ensures that the following linear forms vanish on the reciprocal variety and are therefore elements of $I(\mathcal{L}^{-1})$:

$$\sigma_{13}, \quad \sigma_{23}, \quad \sigma_{34}, \quad \sigma_{35}.$$

Moreover, the only non-trivial symmetry of this graph is the permutation swapping vertices 1 and 2 as well as 5 and 6. The associated permutation matrix P is:

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

By Proposition 3.2.3, all binomial linear forms defined by the distinct entries of $P\Sigma P^{-1} - \Sigma$ belong to the ideal $I(\mathcal{L}^{-1})$. The covariance matrix $\Sigma \in \mathcal{L}^{-1}$ has the following generic structure:

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} & \sigma_{15} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} & \sigma_{24} & \sigma_{25} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} & \sigma_{34} & \sigma_{35} \\ \sigma_{14} & \sigma_{24} & \sigma_{34} & \sigma_{44} & \sigma_{45} \\ \sigma_{15} & \sigma_{25} & \sigma_{35} & \sigma_{45} & \sigma_{55} \end{pmatrix}.$$

We compute $P\Sigma P^{-1} - \Sigma$ as follows:

$$P\Sigma P^{-1} - \Sigma = \begin{pmatrix} -\sigma_{11} + \sigma_{22} & 0 & -\sigma_{13} + \sigma_{23} & -\sigma_{14} + \sigma_{25} & -\sigma_{15} + \sigma_{24} \\ 0 & \sigma_{11} - \sigma_{22} & \sigma_{13} - \sigma_{23} & \sigma_{15} - \sigma_{24} & \sigma_{14} - \sigma_{25} \\ -\sigma_{13} + \sigma_{23} & \sigma_{13} - \sigma_{23} & 0 & -\sigma_{34} + \sigma_{35} & \sigma_{34} - \sigma_{35} \\ -\sigma_{14} + \sigma_{25} & \sigma_{15} - \sigma_{24} & -\sigma_{34} + \sigma_{35} & -\sigma_{44} + \sigma_{55} & 0 \\ -\sigma_{15} + \sigma_{24} & \sigma_{14} - \sigma_{25} & \sigma_{34} - \sigma_{35} & 0 & \sigma_{44} - \sigma_{55} \end{pmatrix}.$$

Thus, by Proposition 3.2.3, we conclude that the following binomial linear forms belong to the vanishing ideal $I(\mathcal{L}^{-1})$:

$$\sigma_{11} - \sigma_{22}, \quad \sigma_{15} - \sigma_{24}, \quad \sigma_{44} - \sigma_{55}, \quad \sigma_{14} - \sigma_{25}.$$

Using the *pull-back* map approach outlined in Section 2.3, we can verify whether these linear forms provide a complete description of the linear part of the ideal. By executing the Macaulay2 code provided in Appendix A.1, we conclude that all linear generators of $I(\mathcal{L}^{-1})$ are given by:

$$\sigma_{13}, \quad \sigma_{23}, \quad \sigma_{34}, \quad \sigma_{35}, \quad \sigma_{11} - \sigma_{22}, \quad \sigma_{15} - \sigma_{24}, \quad \sigma_{44} - \sigma_{55}, \quad \sigma_{14} - \sigma_{25}.$$

Thus, in this example, all binomial linear forms are induced by symmetries.

3.3 Uniform colored graphs

Uniform colored graphs represent a specific class of colored graphs for which Davies and Marigliano provided deeper insights into the structure of the linear generators of the vanishing ideal. As defined in [3], a uniform colored graph is a graph where all vertices have the same partial correlation and all edges share a different, uniform partial correlation. Consequently, the symmetric concentration matrix of a uniform colored graph exhibits a special structure [3]:

$$K = k_{11} Id + k_{12} A,$$

where k_{11} is the partial correlation of all vertices and Id is the $n \times n$ identity matrix. Similarly, k_{12} is the partial correlation of all edges and A the adjacency matrix of the underlying graph. The special properties of such graphs are illustrated in the graph by assigning a single color to all vertices and a different color to all edges. Examples of such graphs are shown in Figure 3.1.

To characterize the linear generators of the ideal $I(\mathcal{L}^{-1})$ for uniform colored graphs, we first need an important intermediate result. The following corollary introduced in [3] provides crucial information on the number of linearly independent linear forms, which is essential for the analysis.

Corollary 3.3.1. *[3, Corollary 3.3] Let G be an undirected uniform colored graph with vertex set V. The number of linearly independent linear forms in the vanishing ideal $I(\mathcal{L}^{-1})$ that are induced by symmetries is $\binom{n+1}{2} - s$, where s denotes the number of orbits of the entrywise action of $Aut(G)$ on the set of unordered pairs of vertices $V \times V$.*

Proof. The set of unordered pairs of vertices is $V \times V = \{(1,1), (1,2), \ldots, (1,n), (2,2), (2,3), \ldots, (n,n)\}$, which has $\binom{n+1}{2}$ elements. The automorphism group $\mathrm{Aut}(G)$ acts on $V \times V$ by permuting vertices in a way that preserves the adjacency structure of the graph. This action partitions $V \times V$ into s orbits, denoted by $Y_1, \ldots, Y_s$, such that: $\sum_{i=1}^{s} |Y_i| = \binom{n+1}{2}$. For each orbit Y_i, any pair of vertices in that orbit can be mapped to any other pair in Y_i to produce a binomial linear form. Thus, for each orbit Y_i, there are $|Y_i| - 1$ linearly independent binomial linear forms in the vanishing ideal $I(\mathcal{L}^{-1})$. Summing over all orbits, the total number of linearly independent binomial linear forms in $I(\mathcal{L}^{-1})$ is:

$$\sum_{i=1}^{s} (|Y_i| - 1) = \sum_{i=1}^{s} |Y_i| - s = \binom{n+1}{2} - s.$$

The forms are induced by symmetries since they arise from applying an element of the automorphism group to a pair in the set $V \times V$. This action corresponds to a permutation of the vertices in that pair, preserving the adjacency structure of the graph. Thus, by Definition 3.2.1 and Proposition 3.2.3 we complete the proof. □

Let r denote the number of distinct eigenvalues of the adjacency matrix A. According to [4], the total number of linearly independent linear generators of the vanishing ideal is given by $\binom{n+1}{2} - r$. Comparing the total number of linear forms in the vanishing ideal $I(\mathcal{L}^{-1})$ with those induced by symmetries, we conclude that, for uniform colored graphs, the entire linear part of $I(\mathcal{L}^{-1})$ is induced by symmetries if and only if $r = s$ [3]. In this context, Davies and Marigliano examined four types of graphs:

1. The first one is the *cycle graph* C_n, which is formed by arranging n vertices in a circular sequence. Each vertex is connected to exactly two others, creating a closed loop.

2. The second type is the *complete graph* K_n, where every vertex is directly connected to every other vertex, resulting in the maximum number of edges.

3. The third type is the *complete bipartite graph* $K_{n,n}$, formed by splitting the vertices into two groups of size n, where every vertex in one group is connected to every vertex in the other group. No edges connect vertices within the same group.

4. Finally, the *hyperoctahedral graph* H_n is based on the complete graph K_{2n}, but the edges $\{\{2k-1, 2k\} \mid k \in \{1, 2, \ldots, n\}\}$ are removed.

The following figure shows examples of these four types of graphs with 6 vertices and uniform coloring:

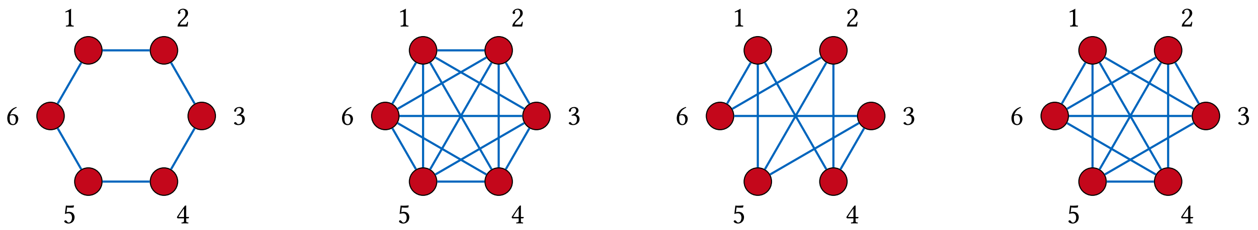


Figure 3.1 (a) Cycle graph C_6, (b) Complete graph K_6, (c) Complete bipartite graph $K_{3,3}$, (d) Hyperoctahedral graph H_3.

For these types of graphs with uniform coloring, Davies and Marigliano provided a total description of the linear part of the ideal $I(\mathcal{L}^{-1})$, which is given by the following theorem:

Theorem 3.3.2. *[3, Theorem 3.4] The linear part of $I(\mathcal{L}^{-1})$ is induced by symmetries for the following uniform colored graph types and precisely characterized as follows:*

1. *For a cycle graph C_n, the linear part of $I(\mathcal{L}^{-1})$ consists of the relations:*

$$\sigma_{11+d} - \sigma_{ii+d}, \qquad \text{for } i \in \{2, \ldots, n\} \text{ and } d \in \{0, \ldots, \left\lfloor \frac{n}{2} \right\rfloor\},$$

   where all indices are taken modulo n.

2. *For a complete graph K_n, the linear part of $I(\mathcal{L}^{-1})$ is generated by:*

$$\sigma_{11} - \sigma_{ii}, \qquad \text{for } i \in V,$$
$$\sigma_{12} - \sigma_{ij}, \qquad \text{for } \{i, j\} \in E.$$

3. *For a complete bipartite graph $K_{n,n}$, the linear part of $I(\mathcal{L}^{-1})$ is given by:*

$$\sigma_{11} - \sigma_{ii}, \qquad \text{for } i \in V,$$
$$\sigma_{12} - \sigma_{ij}, \qquad \text{for } \{i, j\} \in E,$$
$$\sigma_{13} - \sigma_{ij}, \qquad \text{for } \{i, j\} \in E^c.$$

4. *For a hyperoctahedral graph H_n, the linear part of $I(\mathcal{L}^{-1})$ is generated by:*

$$\sigma_{11} - \sigma_{ii}, \qquad \text{for } i \in V,$$
$$\sigma_{13} - \sigma_{ij}, \qquad \text{for } \{i, j\} \in E,$$
$$\sigma_{12} - \sigma_{ij}, \qquad \text{for } \{i, j\} \in E^c.$$

Proof. The result follows from comparing the number of eigenvalues r of the adjacency matrix A of the underlying graph with the number of orbits s under the action of $\mathrm{Aut}(G)$ on pairs of vertices. The eigenvalue results are provided by [1, pp. 11, 17]. We analyze each graph type separately:

1. The eigenvalues of the adjacency matrix of C_n are given by:

$$2\cos\left(\frac{2k\pi}{n}\right), \qquad \text{for } k \in \{0, \ldots, \left\lfloor \frac{n}{2} \right\rfloor\}.$$

   Thus, $r = \lfloor \frac{n}{2} \rfloor + 1$. The automorphism group $\mathrm{Aut}(C_n)$ generates the following orbits: V, E and $E_d^c = \{\{i, i+d\} \mid i \in V\}$ for $d \in \{2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. Therefore, $s = 2 + (\lfloor \frac{n}{2} \rfloor - 1) = \lfloor \frac{n}{2} \rfloor + 1 = r$.

2. The eigenvalues of the adjacency matrix of K_n are $n-1$ and -1, so $r = 2$. Since the graph contains the maximum number of edges, the automorphism group $\mathrm{Aut}(K_n)$ acts on the orbits V and E. Thus, $s = r = 2$.

3. The eigenvalues of the adjacency matrix of $K_{n,n}$ are $-\lambda$, 0 and λ for some $\lambda > 0$, giving $r = 3$. The automorphism group $\text{Aut}(K_{n,n})$ partitions into three orbits: V, E, and E^c. Thus, $s = r = 3$.

4. The eigenvalues of the adjacency matrix of H_n are $2n - 1$, 0 and -2. The automorphism group $\text{Aut}(H_n)$ acts on three orbits: V, E, and $E^c = \{\{2k-1, 2k\} \mid k \in \{1, \ldots, n\}\}$. Thus, $s = r = 3$.

Since $r = s$ in all cases, all binomial linear forms in $I(\mathcal{L}^{-1})$ are induced by symmetries. □

For these four graph types with uniform coloring, the entire linear part of the vanishing ideal $I(\mathcal{L}^{-1})$ is induced by symmetries, confirming the validity of Conjecture 1.0.1 through Theorem 3.3.2. However, uniform coloring represents only one of many possible color configurations. In the subsequent chapters, we aim to examine the validity of Conjecture 1.0.1 for all possible colorings within one of the graph classes discussed in this section. We focus on cycle graphs because their simple, periodic structure allows symmetries to be easily identified and analyzed. Therefore, they are particularly suitable for understanding the relationship between graph symmetries and the linear generators of $I(\mathcal{L}^{-1})$, allowing for a more systematic and detailed study.

4 Binomial linear forms in the vanishing ideal of cyclic graphs

This chapter addresses the main objective of this thesis, which is evaluating whether Conjecture 1.0.1, proposed in [3], holds for all n-cycles. The conjecture, previously introduced in Chapter 1, states:

Conjecture 4.0.1. [3, Conjecture 4.2] Let G be a colored n-cycle. All binomial linear forms in $I(\mathcal{L}^{-1})$ are induced by symmetries.

Building on the insights from [3], revisited in the previous chapter, this conjecture can be equivalently reformulated as an *if and only if* statement:

Conjecture 4.0.2. Let G be a colored n-cycle. Then a linear binomial exists in the vanishing ideal $I(\mathcal{L}^{-1})$ if and only if there is a corresponding symmetry in the graph G.

To investigate the validity of this conjecture, we performed a computational study of the binomial linear relations associated with n-cycles of size $n = 3, 4$ and 5, using the Macaulay2 code provided in Appendix A.2. Representative examples of 5-cycles are provided in Section 4.1. We also analyzed graph symmetries to better understand their role in generating binomial linear forms and examined the implications of these forms being elements of the vanishing ideal. This systematic approach aims to determine whether the conjecture holds true for all n-cycles.

4.1 Computational study on binomial linear generators for the 5-cycle

To systematically investigate the role of coloring configurations in the emergence of binomial linear forms, we developed an algorithm that computes the binomial linear forms in $I(\mathcal{L}^{-1})$ for any coloring configuration of an n-cycle, where $n \in \mathbb{N}$, on a set of n distinct vertex colors and a disjoint set of n distinct edge colors. The implementation of this algorithm is provided in Appendix A.2. For $n = 5$, the computation required significant time, limiting our study to cycles of size 3, 4, and 5. While all three cycles exhibit binomial linear forms, we focus on providing examples from various scenarios of the 5-cycle. This is because the 5-cycle is the largest cycle for which we were able to fully compute the linear part of the vanishing ideal. These examples highlight how the specific coloring configurations influence the appearance of binomial linear forms in the ideal $I(\mathcal{L}^{-1})$.

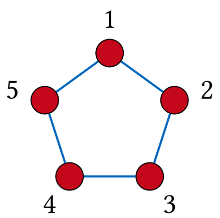
Graph	**Binomial linear forms in $I(\mathcal{L}^{-1})$**
	$\sigma_{44} - \sigma_{55}$ $\sigma_{34} - \sigma_{45}$ $\sigma_{33} - \sigma_{55}$ $\sigma_{25} - \sigma_{35}$ $\sigma_{24} - \sigma_{35}$ $\sigma_{23} - \sigma_{45}$ $\sigma_{22} - \sigma_{55}$ $\sigma_{15} - \sigma_{45}$ $\sigma_{14} - \sigma_{35}$ $\sigma_{13} - \sigma_{35}$ $\sigma_{12} - \sigma_{45}$ $\sigma_{11} - \sigma_{55}$

Table 4.1 Binomial linear generators of $I(\mathcal{L}^{-1})$ for colored 5-cycles. The left column presents the colored cycles and the right column lists the corresponding binomial linear forms.

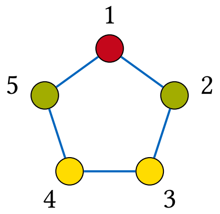
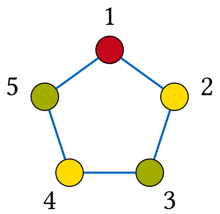
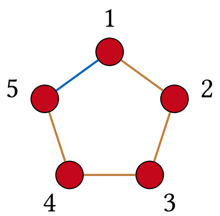
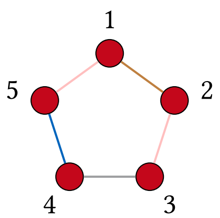
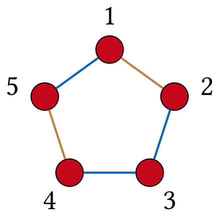
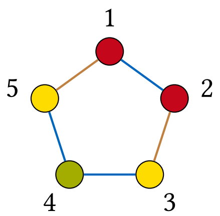
Graph	**Binomial linear forms in $I(\mathcal{L}^{-1})$**
	$\sigma_{33}-\sigma_{44}$ $\sigma_{24}-\sigma_{35}$ $\sigma_{23}-\sigma_{45}$ $\sigma_{22}-\sigma_{55}$ $\sigma_{13}-\sigma_{14}$ $\sigma_{12}-\sigma_{15}$
	None.
	$\sigma_{23}-\sigma_{34}$ $\sigma_{22}-\sigma_{44}$ $\sigma_{14}-\sigma_{25}$ $\sigma_{13}-\sigma_{35}$ $\sigma_{12}-\sigma_{45}$ $\sigma_{11}-\sigma_{55}$
	None.
	$\sigma_{23}-\sigma_{34}$ $\sigma_{22}-\sigma_{44}$ $\sigma_{14}-\sigma_{25}$ $\sigma_{13}-\sigma_{35}$ $\sigma_{12}-\sigma_{45}$ $\sigma_{11}-\sigma_{55}$
	$\sigma_{34}-\sigma_{45}$ $\sigma_{33}-\sigma_{55}$ $\sigma_{15}-\sigma_{23}$ $\sigma_{14}-\sigma_{24}$ $\sigma_{13}-\sigma_{25}$ $\sigma_{11}-\sigma_{22}$

Table 4.2 Continuation of Table 4.1

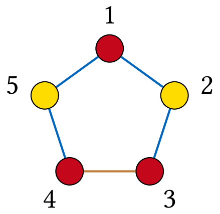
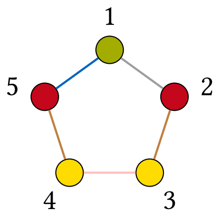
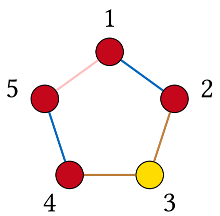
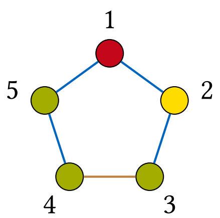
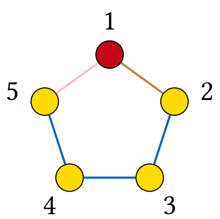
Graph	Binomial linear forms in $I(\mathcal{L}^{-1})$
	$\sigma_{33}-\sigma_{44}$ $\sigma_{24}-\sigma_{35}$ $\sigma_{23}-\sigma_{45}$ $\sigma_{22}-\sigma_{55}$ $\sigma_{13}-\sigma_{14}$ $\sigma_{12}-\sigma_{15}$
	None.
	$\sigma_{23}-\sigma_{34}$ $\sigma_{22}-\sigma_{44}$ $\sigma_{14}-\sigma_{25}$ $\sigma_{13}-\sigma_{35}$ $\sigma_{12}-\sigma_{45}$ $\sigma_{11}-\sigma_{55}$
	None.
	None.

Table 4.3 Continuation of Table 4.2

The results of the conducted computational study for the 3- and 5-cycles suggest that the presence or absence of binomial linear forms in $I(\mathcal{L}^{-1})$ is likely to be dependent on the existence of an axis of symmetry in the graph, providing evidence in support of Conjecture 4.0.2. However, specific colorings of the 4-cycle seem to give rise to binomial linear forms in the vanishing ideal, even in the absence of symmetry. These observations motivate a deeper investigation into the interplay between graph symmetries and binomial linear forms, with the aim of determining whether Conjecture 4.0.2 holds for all n-cycles or if a counterexample can be constructed.

A key insight, directly following from the results established in [3], is that the sufficient condition of the conjecture holds universally, regardless of n. This leads to the following theorem:

Theorem 4.1.1. *Let G be a colored n-cycle. If there exists a symmetry in the graph G, then all binomial linear forms obtained from that symmetry are contained in $I(\mathcal{L}^{-1})$.*

Proof. If a symmetry exists in the graph, then, by Definition 3.2.1, there is a permutation matrix P such that $PKP^{-1} - K = 0$ for the concentration matrix K of the graph. By Proposition 3.2.3, all distinct binomial linear forms arising from the equation $P\Sigma P^{-1} - \Sigma = 0$ are contained in $I(\mathcal{L}^{-1})$. Thus, all binomial linear forms obtained from a symmetry are contained in $I(\mathcal{L}^{-1})$. □

To evaluate the necessary condition of Conjecture 4.0.2, we first delve into a detailed study of graph symmetries. Following this, we analyze the implications of a binomial linear form being an element of the vanishing ideal $I(\mathcal{L}^{-1})$, aiming to uncover its relationship with a potential underlying symmetry of the graph.

4.2 Analysis of graph symmetries

Definition 4.2.1. The automorphism group of a graph $G = (V, E)$ is defined as:

$$\mathrm{Aut}(G) = \{\pi : G \mapsto G \mid \{\pi(i), \pi(j)\} \in E \text{ for } \{i, j\} \in E \text{ and } \pi \text{ is bijective}\}.$$

Theorem 4.2.2. *[8, Theorem 4.5] The automorphism group of a cycle graph C_n is isomorphic to the dihedral group D_n.*

Proof. The dihedral group D_n consists of n rotation and n reflection. We define a map $\varphi : D_n \mapsto \mathrm{Aut}(C_n)$, where each rotation $r_k \in D_n$ maps to the vertex permutation $\varphi(r_k)(i) = (k + i) \mod n$, and each reflection $s_k \in D_n$ maps to $\varphi(s_k)(i) = (k - i) \mod n$. For any $\{i, j\} \in E$ and any rotation $r_k \in D_n$, the vertices $\varphi(r_k)(i) = (i + k) \mod n$ and $\varphi(r_k)(j) = (j + k) \mod n$ are still adjacent due to the adjacency structure of the cyclic graph. Therefore, the edge is preserved, $\{\varphi(r_k)(i), \varphi(r_k)(j)\} \in E$, and thus $\varphi(r_k) \in \mathrm{Aut}(C_n)$. Similarly, for any $\{i, j\} \in E$, the reflected vertices $\varphi(s_k)(i) = (k - i) \mod n$ and $\varphi(s_k)(j) = (k - j) \mod n$ are still adjacent, ensuring that $\{\varphi(s_k)(i), \varphi(s_k)(j)\}$ is an element of E. Thus, $\varphi(s_k) \in \mathrm{Aut}(C_n)$. Hence, the map φ is well-defined.
For any $r_q, r_r, s_u, s_v \in D_n$ and $i \in V$, we verify that φ respects the group operation:

$$\begin{aligned}
\varphi(r_q \circ r_r)(i) &= \varphi(r_{q+r})(i) = (i + q + r) \mod n = \varphi(r_q)((i + r) \mod n) = \varphi(r_q)(i) \circ \varphi(r_r)(i),\\
\varphi(r_q \circ s_u)(i) &= \varphi(s_{q+u})(i) = (q + u - i) \mod n = \varphi(r_q)((u - i) \mod n) = \varphi(r_q)(i) \circ \varphi(s_u)(i),\\
\varphi(s_u \circ r_q)(i) &= \varphi(s_{u-q})(i) = (u - q - i) \mod n = \varphi(s_u)((q + i) \mod n) = \varphi(s_u)(i) \circ \varphi(r_q)(i),\\
\varphi(s_u \circ s_v)(i) &= \varphi(r_{u-v})(i) = (i + u - v) \mod n = \varphi(s_u)((v - i) \mod n) = \varphi(s_u)(i) \circ \varphi(s_v)(i).
\end{aligned}$$

Thus, φ is a homomorphism, as per Definition 1.3 in [8]. The dihedral group D_n consists of distinct rotations and reflections, and φ assigns a unique automorphism in $\mathrm{Aut}(C_n)$ to each element of D_n. Hence, φ is injective. Consider an automorphism $\pi \in \mathrm{Aut}(C_n)$. The image of i under π can be any vertex $j \in V$, giving n possible choices for j. Since π preserves the adjacency structure of C_n, the image of the adjacent vertex $i + 1 \mod n$ must be either $j + 1 \mod n$ or $j - 1 \mod n$. These two choices for the adjacency preserving action determine two unique automorphisms. Thus, $\mathrm{Aut}(C_n)$ has $2n$ elements, matching that also D_n has $2n$ elements. Hence, φ is also surjective. Therefore, φ is a bijective homomorphism and thus an isomorphism by Definition 1.4 in [8]. We conclude that $\mathrm{Aut}(C_n) \cong D_n$. □

Theorem 4.2.3. *A permutation matrix $P \in \mathbb{R}^{n\times n}$ satisfies $PAP^{-1} = A$, where A is the adjacency matrix of a graph G with n vertices, if and only if P corresponds to an element in D_n.*

Proof. This is a well-known result in algebraic graph theory. Nevertheless, we include the proof for completeness. Additional details can be found in [6]. We prove the statement by showing both implications:

First, assume that the permutation matrix $P = (p_{ij})$ satisfies $PAP^{-1} = A$, where $A = (a_{ij})$ is the adjacency matrix of a graph G. Let $f : \{1, 2, \dots, n\} \to \{1, 2, \dots, n\}$ be the map defined by $f(i) = j$ if and only if $p_{ij} = 1$. Since P is a permutation matrix, each row and each column of P contains exactly one 1, implying that f is a bijection. Now, consider a vector $x \in \mathbb{R}^n$. The i-th entry of the vector Px is given by

$$(Px)_i = \sum_{j=1}^{n} p_{ij} x_j = x_{f(i)},$$

since $p_{ij} = 0$ for all $j \neq f(i)$ and $p_{if(i)} = 1$. Therefore, we can express the result of multiplying P by x as:

$$Px = \begin{pmatrix} x_{f(1)} \\ x_{f(2)} \\ \vdots \\ x_{f(n)} \end{pmatrix}. \tag{4.1}$$

Therefore,

$$PA = \begin{pmatrix} a_{f(1)1} & a_{f(1)2} & \cdots & a_{f(1)n} \\ a_{f(2)1} & a_{f(2)2} & \cdots & a_{f(2)n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{f(n)1} & a_{f(n)2} & \cdots & a_{f(n)n} \end{pmatrix},$$

and by the transposed version of (4.1):

$$PAP^{-1} = PAP^{\mathrm{T}} = \begin{pmatrix} a_{f(1)f(1)} & a_{f(1)f(2)} & \cdots & a_{f(1)f(n)} \\ a_{f(2)f(1)} & a_{f(2)f(2)} & \cdots & a_{f(2)f(n)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{f(n)f(1)} & a_{f(n)f(2)} & \cdots & a_{f(n)f(n)} \end{pmatrix}.$$

This holds since P is a permutation matrix, implying that $P^T = P^{-1}$. For $PAP^{-1} = A$ to hold, it must be true that for all $i, j \in V$, the entries a_{ij} and $a_{f(i)f(j)}$ are equal. This implies that the map f preserves the adjacency relation and since f is bijective, $f \in \mathrm{Aut}(G)$. Thus, by Theorem 4.2.2, P corresponds to an element of D_n, as required.

Next, let P be the permutation matrix corresponding to the element $\pi \in D_n$. By Definition 4.2.1 and Theorem 4.2.2, for $i, j \in V$, we have $a_{ij} = 1$ if and only if $a_{\pi(i)\pi(j)} = 1$. Consider $B := P^{-1}AP$. For any $i, j \in V$, we compute:

$$a_{ij} = e_i^{\mathrm{T}} A e_j = e_{\pi(i)}^{\mathrm{T}} A e_{\pi(j)} = (Pe_i)^{\mathrm{T}} A (Pe_j) = e_i^{\mathrm{T}} (P^{\mathrm{T}} AP) e_j = e_i^{\mathrm{T}} (P^{-1} AP) e_j = e_i^{\mathrm{T}} B e_j = b_{ij}.$$

Therefore, $A = B = P^{-1}AP$. □

Theorem 4.2.4. *Every symmetry of an n-cycle is either a reflection or a rotation.*

Proof. By Remark 3.2.2, any symmetry of C_n is a permutation matrix $P \in \mathbb{R}^{n \times n}$ that satisfies $PAP^{-1} = A$ for the adjacency matrix A of C_n. Therefore, according to Theorem 4.2.3, P corresponds to an element in the dihedral group D_n, which consists of rotations and reflections only. Thus, P must be either a rotation or a reflection. □

4.3 Reflections and rotations under the parametrization

To deepen our understanding of the role symmetry plays in a graph, we continue by exploring its implications. A key tool in this exploration is a theorem established by Jones and West. Before presenting the theorem, it is essential to recall the definition of a path:

Definition 4.3.1. A path P is a graph with vertex set $V(P) = \{1, 2, \ldots, n\}$ and edge set $E(P) = \{\{i, i+1\} \mid 1 \leq i \leq n-1\}$, which is connected and acyclic.

Considering this, we now investigate the following theorem by Jones and West, which provides valuable insight into the relationship between the edge structure of a graph and the entries of its associated covariance matrix. Specifically, it shows how the entries of the covariance matrix can be expressed as sums over paths in the graph, with weights determined by the entries of the concentration matrix:

Theorem 4.3.2. *[5, Theorem 1] Consider an n-dimensional multivariate normal distribution with a finite and non-singular covariance matrix Σ, and concentration matrix $K = \Sigma^{-1}$. The element of Σ corresponding to the covariance between vertices i and j can be written as a sum of path weights over all paths in the graph between i and j:*

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

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

Proof. The proof of this theorem is omitted here, as it is rigorously established in [5]. □

We will apply this theorem to our object of interest: cyclic graphs.

Corollary 4.3.3. *Let G be an n-cycle with concentration matrix K and let i and j be vertices in G. Then, there exist precisely two distinct paths connecting i and j: a shorter path, denoted by $i \leftrightarrow j$, and a complementary path, denoted by $i \overset{c}{\leftrightarrow} j$. The covariance between the vertices i and j is then given by:*

$$\sigma_{ij} = \frac{1}{\det(K)} \Big((-1)^{n_{i \leftrightarrow j} + 1} \prod_{\{i',j'\} \in i \leftrightarrow j} k_{i'j'} \quad \det\left(K_{\setminus i \leftrightarrow j}\right) \quad + \quad (-1)^{n_{i \overset{c}{\leftrightarrow} j} + 1} \prod_{\{i'_c, j'_c\} \in i \overset{c}{\leftrightarrow} j} k_{i'_c j'_c} \quad \det\left(K_{\setminus i \overset{c}{\leftrightarrow} j}\right) \Big).$$

Here, $n_{i \leftrightarrow j}$ denotes the number of vertices on the path $i \leftrightarrow j$, and $K_{\setminus i \leftrightarrow j}$ is the submatrix of the concentration matrix K, with rows and columns corresponding to variables used in the path $i \leftrightarrow j$ omitted.

Proof. Due to the structure of a cycle, there are only two distinct paths connecting any two vertices in V. As a result, the formula in Theorem 4.3.2 simplifies to the expression given in this corollary. □

For the rest of this thesis, we assume $G = (V, E)$ to be a colored n-cycle, with V as the set of n vertices and E as the set of edges. We will continue the convention established in Corollary 4.3.3 and denote the shorter path between two vertices $i, j \in V$ by $i \leftrightarrow j$, and the complementary path by $i \overset{c}{\leftrightarrow} j$. Thus, both the shorter and the complementary paths include the vertices i and j. Additionally, we will denote $n_{i \leftrightarrow j}$ as the number of vertices on the path $i \leftrightarrow j$. Note that the shorter path may not be unique, since in a cycle with an even number of vertices the two paths could be of the same length for specific $i, j \in V$. Nevertheless, it is always true that $n_{i \leftrightarrow j} \leq n_{i \overset{c}{\leftrightarrow} j}$.

Since the path on vertices $V \setminus V(i \leftrightarrow j)$ is equal to the one on the vertices of the complementary path without i and j, denoted by $V\big(i \overset{c}{\leftrightarrow} j \setminus \{i, j\}\big)$, the concentration matrix $K_{\setminus i \leftrightarrow j}$ is equal to the concentration matrix induced by the complementary path, with rows and columns corresponding to the vertices i and j omitted, which is $K_{i \overset{c}{\leftrightarrow} j \setminus \{i,j\}}$. Since the concentration matrix of paths has a specific pattern, we can derive an explicit formula to efficiently compute the determinants required in Corollary 4.3.3.

Lemma 4.3.4. *Let P be a colored path in a graph $G = (V, E)$ with $m \leq |V|$ vertices such that $K_P \in \mathbb{R}^{m \times m}$ is the concentration matrix that contains all rows and columns corresponding to the variables used in that path. Then K_P is a tridiagonal matrix and its determinant is given by:*

$$\det(K_P) = \sum_{\substack{|S|=0, \\ S \subseteq E \text{ disjoint}}}^{\lfloor \frac{m}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\} \in S} k_{ij}^2 \prod_{v \in V \setminus V(S)} k_{vv},$$

where $V(S)$ is the set of vertices incident to the edges in S.

Proof. The concentration matrix induced by a path P is tridiagonal since, by Definition 4.3.1, every vertex i for $i \in \{2, \dots, m-1\}$ is connected to its two neighbors $i-1$ and $i+1$, while the vertices 1 and m are only connected to 2 and $m-1$, respectively. Let $K^{m\times m}$ denote the concentration matrix K_P and E_m the edge set of the path P including $m-1$ edges and V_m the corresponding set of m vertices. To prove the formula by induction on m, the size of the matrix, we use the well-know recurrence relation for the determinant of a tridiagonal matrix, which is given by:

$$\det\left(K^{m\times m}\right) = k_{mm}\det\left(K^{m-1\times m-1}\right) - k_{m-1m}^2\det\left(K^{m-2\times m-2}\right).$$

Base Case: Since $m = 1$ is the trivial case, we start with $m = 2$. The concentration matrix K is symmetric, therefore, the formula in this lemma gives:

$$\det\left(K^{2\times 2}\right) = \sum_{\substack{|S|=0,\\ S\subseteq E_2 \text{ disjoint}}}^{1} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_2\setminus V(S)} k_{vv} = k_{11}k_{22} - k_{12}^2.$$

One can easily verify that this determinant is correct.

Induction hypothesis: Assume the formula holds for all subpaths of P of length smaller or equal to $m-1$.

Induction step: Applying the recurrence relation and substituting the inductive hypothesis for $\det\left(K^{m-1\times m-1}\right)$ and $\det\left(K^{m-2\times m-2}\right)$, we find:

$$\det\left(K^{m\times m}\right) = k_{mm}\det\left(K^{m-1\times m-1}\right) - k_{m-1m}^2\det\left(K^{m-2\times m-2}\right)$$

$$= k_{mm} \sum_{\substack{|S|=0,\\ S\subseteq E_{m-1} \text{ disjoint}}}^{\lfloor \frac{m-1}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_{m-1}\setminus V(S)} k_{vv} \; - \; k_{m-1m}^2 \sum_{\substack{|S|=0,\\ S\subseteq E_{m-2} \text{ disjoint}}}^{\lfloor \frac{m-2}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_{m-2}\setminus V(S)} k_{vv}$$

For $S \subseteq E_{m-1}$, the vertex m is never included in $v \in V_{m-1} \setminus V(S)$. Hence, multiplying the product k_{vv} over these vertices by k_{mm} is equivalent to taking the product of k_{vv} over $v \in V_m \setminus V(S)$. Moreover, multiplying the second sum by k_{m-1m}^2 corresponds to summing over all edge sets $S \subseteq E_{m-2}$ that additionally include the edge $\{m-1, m\}$. Since S then contains one more edge than in the previous sum, the upper bound of the sum increases by 1 and the sign switches. This new S ensures that the vertices $m-1$ and m are always included in $V(S)$. Consequently, we can rewrite the equation as:

$$= \sum_{\substack{|S|=0,\\ S\subseteq E_{m-1} \text{ disjoint}}}^{\lfloor \frac{m-1}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_m\setminus V(S)} k_{vv} \; + \sum_{\substack{|S|=0,\\ S\subseteq E_{m-2} \text{ disjoint},\\ \{m-1,m\}\in S}}^{\lfloor \frac{m}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_m\setminus V(S)} k_{vv}$$

In the first sum, since $E_{m-1} = E_m \setminus \{m-1, m\}$, we can rewrite $S \subseteq E_{m-1}$ disjoint as $S \subseteq E_m$ disjoint with the additional condition that $\{m-1, m\} \notin S$. Furthermore, the upper bound of that sum can be increased by 1 since, for $|S| = \left\lfloor \frac{m}{2} \right\rfloor$, the sum is empty as the edges in S need to be disjoint, and $\{m-1, m\} \notin S$. In the second sum, requiring $\{m-1, m\} \in S$, we avoid the edge $\{m-2, m-1\}$ in all summand due to the disjointness condition. Thus, we can rewrite $S \subseteq E_{m-2}$ disjoint with $\{m-1, m\} \in S$ as $S \subseteq E_m$ disjoint with $\{m-1, m\} \in S$:

$$= \sum_{\substack{|S|=0,\\ S\subseteq E_m \text{ disjoint},\\ \{m-1,m\}\notin S}}^{\lfloor \frac{m}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_m\setminus V(S)} k_{vv} \; + \sum_{\substack{|S|=0,\\ S\subseteq E_m \text{ disjoint},\\ \{m-1,m\}\in S}}^{\lfloor \frac{m}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_m\setminus V(S)} k_{vv}$$

Thus, we arrive at the desired formula:

$$= \sum_{\substack{|S|=0,\\ S\subseteq E_m \text{ disjoint}}}^{\lfloor \frac{m}{2} \rfloor} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V_m\setminus V(S)} k_{vv}$$

□

Example 4.3.5. Consider a path P with $m = 4$ vertices, where its concentration matrix is given by:

$$K_P = \begin{pmatrix} k_{11} & k_{12} & 0 & 0 \\ k_{12} & k_{22} & k_{23} & 0 \\ 0 & k_{23} & k_{33} & k_{34} \\ 0 & 0 & k_{34} & k_{44} \end{pmatrix}.$$

By applying the formula from Lemma 4.3.4, we can calculate the determinant of this matrix as follows:

$$\begin{aligned} \det(K^{4\times4}) &= \sum_{\substack{|S|=0,\\ S\subseteq E \text{ disjoint}}}^{2} (-1)^{|S|} \prod_{\{i,j\}\in S} k_{ij}^2 \prod_{v\in V\setminus V(S)} k_{vv} \\ &= \underbrace{k_{11}k_{22}k_{33}k_{44}}_{\text{for } |S|=0} \underbrace{- k_{12}^2k_{33}k_{44} - k_{23}^2k_{11}k_{44} - k_{34}^2k_{11}k_{22}}_{\text{for } |S|=1} \underbrace{+ k_{12}^2k_{34}^2}_{\text{for } |S|=2}. \end{aligned}$$

One can easily verify that this determinant is correct.

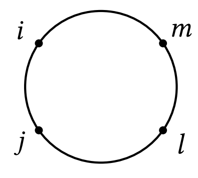
Now that we have established an efficient way to calculate the determinants in the covariance formula in Corollary 4.3.3, we proceed to analyze the possible symmetries in a cycle graph C_n. By Theorem 4.2.4, every symmetry in a cycle graph is either a reflection or a rotation. Therefore, we analyze each type of symmetry separately:

4.3.1 Reflection symmetry

Assume there exists a symmetry in the graph, which is a reflection. Suppose it maps the vertices $i \longrightarrow m$ and $j \longrightarrow l$ for some $i, j, l, m \in V$, where i, j, l, m are not all the same (since this would correspond the trivial case). The reflection symmetry preserves the structure of the graph, including adjacency and cyclic ordering by Theorems 4.2.3 and 4.2.2. As a result, the relative positions of i and j are mirrored by m and l, and the sequence of edges in $i \leftrightarrow j$ maps directly onto $m \leftrightarrow l$, ensuring that the shortest paths $i \leftrightarrow j$ and $m \leftrightarrow l$ are identical.
We analyze this symmetry by examining the structure of the paths between the vertices separately. In this context, we denote $P \sim Q$ to mean that the paths P and Q are graphically identical.

Case 1: Suppose m and l lie on the complementary path between i and j.
In this scenario, the complementary paths are given by:

$$\begin{aligned} i \overset{c}{\leftrightarrow} j &= i \leftrightarrow m \leftrightarrow l \leftrightarrow j, \\ m \overset{c}{\leftrightarrow} l &= m \leftrightarrow i \leftrightarrow j \leftrightarrow l. \end{aligned}$$



The reflection symmetry in the graph yields $i \leftrightarrow j \sim m \leftrightarrow l$, so it follows directly that $i \overset{c}{\leftrightarrow} j \sim m \overset{c}{\leftrightarrow} l$.

According to Corollary 4.3.3, for any pair of vertices $i, j \in V$, the ij-th entry of the covariance matrix Σ can be expressed as the sum of contributions from the shortest path and its complementary path between i and j:

$$\sigma_{ij} = \frac{1}{\det(K)}\Big((-1)^{n_{i\leftrightarrow j}+1} \prod_{\{i',j'\}\in i\leftrightarrow j} k_{i'j'} \ \det\big(K_{\setminus i\leftrightarrow j}\big) \ + \ (-1)^{n_{i\overset{c}{\leftrightarrow} j}+1} \prod_{\{i'_c,j'_c\}\in i\overset{c}{\leftrightarrow} j} k_{i'_cj'_c} \ \det\big(K_{\setminus i\overset{c}{\leftrightarrow} j}\big)\Big),$$

$$\sigma_{ml} = \frac{1}{\det(K)}\Big((-1)^{n_{m\leftrightarrow l}+1} \prod_{\{m',l'\}\in m\leftrightarrow l} k_{m'l'} \ \det\big(K_{\setminus m\leftrightarrow l}\big) \ + \ (-1)^{n_{m\overset{c}{\leftrightarrow} l}+1} \prod_{\{m'_c,l'_c\}\in m\overset{c}{\leftrightarrow} l} k_{m'_cl'_c} \ \det\big(K_{\setminus m\overset{c}{\leftrightarrow} l}\big)\Big),$$

where $K_{\setminus i\leftrightarrow j}$ is the concentration matrix of the cycle with rows and columns corresponding to variables used in the path $i \leftrightarrow j$ omitted. From the reflection $i \leftrightarrow j \sim m \leftrightarrow l$ and $i \overset{c}{\leftrightarrow} j \sim m \overset{c}{\leftrightarrow} l$, we observe:

- The path on the vertices $V \setminus V(i \leftrightarrow j)$ is identical to the one on $V\big(i \overset{c}{\leftrightarrow} j \setminus \{i, j\}\big)$, which is isomorphic to the path on the vertices $V\big(m \overset{c}{\leftrightarrow} l \setminus \{m, l\}\big)$, and this path is identical to the one on the vertices $V \setminus V(m \leftrightarrow l)$. Therefore, the corresponding submatrices $K_{\setminus i\leftrightarrow j} = K_{i\overset{c}{\leftrightarrow} j\setminus\{i,j\}}$ and $K_{\setminus m\leftrightarrow l} = K_{m\overset{c}{\leftrightarrow} l\setminus\{m,l\}}$ are equal, which implies $\det\left(K_{\setminus i\leftrightarrow j}\right) = \det\left(K_{\setminus m\leftrightarrow l}\right)$.
- The reflection symmetry also ensures that $n_{i\leftrightarrow j} = n_{m\leftrightarrow l}$.
- The product of edge weights along the paths is preserved:

$$\prod_{\{i',j'\}\in i\leftrightarrow j} k_{i'j'} = \prod_{\{m',l'\}\in m\leftrightarrow l} k_{m'l'}.$$

Thus, the terms corresponding to the shorter paths in σ_{ij} and σ_{ml} are identical.
Using analogous reasoning, we also have $\det\left(K_{\setminus i\overset{c}{\leftrightarrow} j}\right) = \det\left(K_{\setminus m\overset{c}{\leftrightarrow} l}\right)$ and $n_{i\overset{c}{\leftrightarrow} j} = n_{m\overset{c}{\leftrightarrow} l}$, along with:

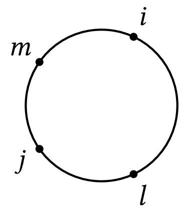
$$\prod_{\{i'_c,j'_c\}\in i\overset{c}{\leftrightarrow} j} k_{i'_c j'_c} = \prod_{\{m'_c,l'_c\}\in m\overset{c}{\leftrightarrow} l} k_{m'_c l'_c}.$$

Thus, the terms corresponding to the complementary paths in σ_{ij} and σ_{ml} are also identical.
Combining these results, all contributions from both the shortest paths and their complementary paths in the expressions for σ_{ij} and σ_{ml} are identical. Therefore, we conclude:

$$\sigma_{ij} = \sigma_{ml}.$$

Case 2: Suppose, without loss of generality, m lies on the shortest path from i to j and j lies on the shortest path from m to l.
Given the symmetry in the graph, the paths satisfy:

$$i \leftrightarrow j \sim m \leftrightarrow l \quad \Leftrightarrow \quad i \leftrightarrow m \leftrightarrow j \sim m \leftrightarrow j \leftrightarrow l.$$



This path equality implies $i \leftrightarrow m \sim j \leftrightarrow l$.
Furthermore, the complementary pathsare given by:

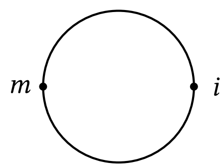
$$i \overset{c}{\leftrightarrow} j = i \leftrightarrow l \leftrightarrow j$$
$$m \overset{c}{\leftrightarrow} l = m \leftrightarrow i \leftrightarrow l.$$

Therefore, we conclude $i \overset{c}{\leftrightarrow} j \sim m \overset{c}{\leftrightarrow} l$.
Since the equivalence relations in this case are analogous to the ones in Case 1, we immediately obtain:

$$\sigma_{ij} = \sigma_{ml}.$$

Case 3: Assume $i = j$ and $m = l$.

In this case, the shortest paths from i to j and m to l collapse into single vertices. Since the symmetry in in the graph implies that the corresponding subgraphs induced by $V \setminus \{i\}$ and $V \setminus \{m\}$ are identical, the contributions from both the shortest and complementary paths to σ_{ij} and σ_{ml} are trivially identical. Hence, we conclude:



$$\sigma_{ij} = \sigma_{ml}.$$

After considering all possible cases, we conclude that $\sigma_{ij} = \sigma_{ml}$ for all possible $i, j, l, m \in V$.

Next, we investigate the second type of symmetry in a cycle: rotation symmetries.

4.3.2 Rotation symmetry

For a graph C_n a rotation symmetry corresponds to rotating the cycle by an angle $\theta = k \cdot \frac{360°}{n}$ for $k \in \{1, 2, \dots, n\}$, with each vertex mapping to the next in a cyclic order. Suppose the rotation maps the vertices $i \to l$ and $j \to m$ through a fixed angle of rotation. Under the rotation symmetry, both the shorter path $i \leftrightarrow j$ and its complementary path $i \overset{c}{\leftrightarrow} j$ will undergo the same rotation. Since the rotation preserves the relative positions of vertices and the adjacency structure of the graph, and since i is mapped to l and j is mapped to m, it follows that $i \leftrightarrow j \sim m \leftrightarrow l$ and $i \overset{c}{\leftrightarrow} j \sim m \overset{c}{\leftrightarrow} l$. Thus, by the same reasoning as established for reflection symmetries, the terms in the formulas for σ_{ij} and σ_{ml} from Corollary 4.3.3 corresponding to the shorter paths are identical under the rotation, as are the terms corresponding to the complementary paths. Therefore, we conclude:

$$\sigma_{ij} = \sigma_{ml}.$$

By analyzing the two types of symmetries in a cyclic graph C_n, we have gained a deeper understanding of why the existence of a symmetry in a cycle graph forces the covariance matrix entries corresponding to pairs of symmetrically related vertices to be equal. This insight enables us to proceed with the analysis of the covariance matrix and its algebraic relations.

4.4 Analysis of binomial linear elements of the vanishing ideal

Suppose there exists a binomial linear form in $I(\mathcal{L}^{-1})$, specifically $\sigma_{ij} - \sigma_{ml} = 0$ for some $i, j, l, m \in V$. By Corollary 4.3.3, the formulas for σ_{ij} and σ_{ml} each consist of two summands: one containing terms arising from the shorter path and the other containing terms arising from the complementary path. Comparing the number of vertices on these paths, it holds that $n_{i\leftrightarrow j} \le n_{i\overset{c}{\leftrightarrow} j}$ and $n_{m\leftrightarrow l} \le n_{m\overset{c}{\leftrightarrow} l}$. From the equation $\sigma_{ij} - \sigma_{ml} = 0$, it follows that $n_{i\leftrightarrow j} = n_{m\leftrightarrow l}$ and $n_{i\overset{c}{\leftrightarrow} j} = n_{m\overset{c}{\leftrightarrow} l}$, and consequently, the terms arising from the shorter paths between i, j and m, l match, and the ones arising from the complementary paths. Therefore, the product of weights along the shorter paths are equal, as well as the product of weights along the complementary paths. Additionally, the determinants used in the formula of Corollary 4.3.3 satisfy in this case $\det(K_{\setminus i\leftrightarrow j}) = \det(K_{\setminus m\leftrightarrow l})$ and $\det(K_{\setminus i\overset{c}{\leftrightarrow} j}) = \det(K_{\setminus m\overset{c}{\leftrightarrow} l})$. The path on the vertices $V \setminus V(i \leftrightarrow j)$ is isomorphic to the one on $V(i \overset{c}{\leftrightarrow} j \setminus \{i, j\})$, and similarly, the path on the vertices $V \setminus V(i \overset{c}{\leftrightarrow} j)$ is isomorphic to the one on $V(i \leftrightarrow j \setminus \{i, j\})$. Thus, the the determinant equalities can be rewritten as $\det(K_{i\leftrightarrow j\setminus\{i,j\}}) = \det(K_{m\leftrightarrow l\setminus\{m,l\}})$ and $\det(K_{i\overset{c}{\leftrightarrow} j\setminus\{i,j\}}) = \det(K_{m\overset{c}{\leftrightarrow} l\setminus\{m,l\}})$. There are various possibilities for when these determinants of concentration matrices of paths can be equal. We want to analyze them in the following subsection.

4.4.1 Conditions on when two tridiagonal matrices have the same determinant

When P and Q are of the same length, there are several cases in which the determinants of the tridiagonal concentration matrices of these two paths are equal:

1. P is equal to Q.
2. P is the reflection of Q.
3. Third and special case.

Before discussing these cases, which are sufficient for the purposes of this thesis, it is important to acknowledge the possibility of other configurations of paths that could also result in equal determinants. Therefore we state the following question, which remains open for further investigation.

Question 4.4.1. Are there any additional conditions under which the determinants of the concentration matrices of two paths are equal?

To begin with examining the three given cases, we first want to provide an important result, which is based on the first and second case.

4.4.2 Proof of the conjecture for 3- and 5-cycles

The computational study conducted in Section 4.1 provides evidence in support of the necessary condition of Conjecture 4.0.2 for 3- and 5-cycles, which claims that for every binomial linear form in $I(\mathcal{L}^{-1})$, there exists a corresponding symmetry in the graph that induces this form. Demonstrating that all relevant paths between any two vertices in 3- and 5-cycles fall into the first or second cases described in Section 4.4.1 allows us to establish a key result that confirms this evidence for these cycles. To achieve this, we require the following lemma:

Lemma 4.4.2. *Let P and Q be two colored paths in a graph G, which are either both of length one or both of length two. If $\det(K_P) = \det(K_Q)$, then P and Q are either identical or reflections of each other.*

Proof. We analyze the two possible path lengths separately:

Length one: Suppose P and Q are paths of length one, and assume $\det(K_P) = \det(K_Q)$. Let the vertices of path P be v and w and those of path Q be x and y. The associated concentration matrices are given by:

$$K_P = \begin{pmatrix} k_{vv} & k_{vw} \\ k_{vw} & k_{ww} \end{pmatrix}, \quad K_Q = \begin{pmatrix} k_{xx} & k_{xy} \\ k_{xy} & k_{yy} \end{pmatrix}.$$

Equating the determinants, we have:

$$\det(K_P) = \det(K_Q) \quad \Rightarrow \quad k_{vv}k_{ww} - k_{vw}^2 = k_{xx}k_{yy} - k_{xy}^2.$$

This implies $k_{vw} = k_{xy}$. Two cases arise:

1. If $k_{vv} = k_{xx}$ and $k_{ww} = k_{yy}$, then P and Q are identical.
2. If $k_{vv} = k_{yy}$ and $k_{ww} = k_{xx}$, the P and Q are reflections of each other.

Length two: Suppose P and Q are paths of length two, and assume $\det(K_P) = \det(K_Q)$. Let the vertices of P be u, v, w, and those of Q be x, y, z. The associated concentration matrices are given by:

$$K_P = \begin{pmatrix} k_{uu} & k_{uv} & 0 \\ k_{uv} & k_{vv} & k_{vw} \\ 0 & k_{vw} & k_{ww} \end{pmatrix}, \quad K_Q = \begin{pmatrix} k_{xx} & k_{xy} & 0 \\ k_{xy} & k_{yy} & k_{yz} \\ 0 & k_{yz} & k_{zz} \end{pmatrix}.$$

Thus, by Lemma 4.3.4:

$$\det(K_P) = \det(K_Q) \quad \Rightarrow \quad k_{uu}k_{vv}k_{ww} - k_{uv}^2 k_{ww} - k_{vw}^2 k_{uu} = k_{xx}k_{yy}k_{zz} - k_{xy}^2 k_{zz} - k_{yz}^2 k_{xx}.$$

Since the degrees need to match, we conclude $k_{uu}k_{vv}k_{ww} = k_{xx}k_{yy}k_{zz}$. Two possible cases follow:

1. If $k_{uv}^2 k_{ww} = k_{xy}^2 k_{zz}$ and $k_{vw}^2 k_{uu} = k_{yz}^2 k_{xx}$, it follows that $k_{uv} = k_{xy}$ and $k_{ww} = k_{zz}$. Additionally, $k_{vw} = k_{yz}$ and $k_{uu} = k_{xx}$. Since $k_{uu}k_{vv}k_{ww} = k_{xx}k_{yy}k_{zz}$, we have $k_{vv} = k_{yy}$, and therefore P and Q are identical.
2. If $k_{uv}^2 k_{ww} = k_{yz}^2 k_{xx}$ and $k_{vw}^2 k_{uu} = k_{xy}^2 k_{zz}$, we deduce $k_{uv} = k_{yz}$, $k_{ww} = k_{xx}$ and $k_{vw} = k_{xy}$, $k_{uu} = k_{zz}$, which implies $k_{vv} = k_{yy}$. In this case, the paths P and Q are reflections of each other. □

This lemma assists in proving the validity of Conjecture 4.0.2 for 3- and 5-cycles:

Theorem 4.4.3. *Let G be a colored 3-cycle or 5-cycle. Then a binomial linear form exists in $I(\mathcal{L}^{-1})$ if and only if there is a corresponding symmetry in G.*

Proof. The sufficient condition of this theorem is already established in Theorem 4.1.1 for all n-cycles, so we focus on proving the necessary condition. Let $\sigma_{ij} - \sigma_{ml} = 0$ be a binomial linear form in $I(\mathcal{L}^{-1})$, where $i, j, m, l \in V$. Our previous results in the beginning of Section 4.4 have shown that in this case, the shorter paths between i, j and m, l are of the same length, as well as their complementary paths. Moreover, we have the following determinant equalities: $\det\left(K_{i\leftrightarrow j\setminus\{i,j\}}\right) = \det\left(K_{m\leftrightarrow l\setminus\{m,l\}}\right)$ and $\det\left(K_{i\overset{c}{\leftrightarrow} j\setminus\{i,j\}}\right) = \det\left(K_{m\overset{c}{\leftrightarrow} l\setminus\{m,l\}}\right)$. Our goal is to show that there exists a symmetry in the graph that induces the binomial linear form. We analyze the two graph types, 3-cycles and 5-cycles, separately:

3-cycle: In a 3-cycle, the shorter path between any two distinct vertices is of length one, and the complementary path is of length two. Since the numbering of the vertices can be chosen arbitrarily, we assume without loss of generality that $\sigma_{ij} - \sigma_{ml} = \sigma_{12} - \sigma_{23} \in I(\mathcal{L}^{-1})$. Any other binomial linear form in $I(\mathcal{L}^{-1})$, where exactly two of the variables i, j, m, l are equal, can be obtained by appropriately renumbering the vertices. By Corollary 4.3.3, this linear form yields:

$$\begin{aligned} k_{12} \det\left(K_{1 \overset{c}{\leftrightarrow} 2 \setminus \{1,2\}}\right) = k_{23} \det\left(K_{2 \overset{c}{\leftrightarrow} 3 \setminus \{2,3\}}\right) \quad &\Rightarrow \quad k_{12}k_{33} = k_{23}k_{11}, \\ k_{23}k_{13} \det\left(K_{1 \leftrightarrow 2 \setminus \{1,2\}}\right) = k_{13}k_{12} \det\left(K_{2 \leftrightarrow 3 \setminus \{2,3\}}\right) \quad &\Rightarrow \quad k_{23}k_{13} = k_{13}k_{12}. \end{aligned}$$

Therefore, $k_{23} = k_{12}$ and $k_{33} = k_{11}$, which implies that there exists a reflection symmetry mapping vertex 1 to vertex 3.

A binomial linear form in the vanishing ideal of a 3-cycle can also take the form $\sigma_{ii} = \sigma_{mm}$. Assume, without loss of generality, that $\sigma_{11} = \sigma_{22} \in I(\mathcal{L}^{-1})$. Then, the following holds by Corollary 4.3.3:

$$\begin{aligned} \det\left(K_{\setminus 1}\right) = \det\left(K_{\setminus 2}\right) \quad &\Rightarrow \quad \det\left(K_{2 \leftrightarrow 3}\right) = \det\left(K_{3 \leftrightarrow 1}\right), \\ k_{12}k_{23}k_{13} \det\left(K_{1 \leftrightarrow 1 \setminus 1}\right) = k_{23}k_{13}k_{12} \det\left(K_{2 \leftrightarrow 2 \setminus 2}\right) \quad &\Rightarrow \quad k_{12}k_{23}k_{13} = k_{23}k_{13}k_{12}. \end{aligned}$$

By Lemma 4.4.2, the paths on vertices $V(2 \leftrightarrow 3)$ and $V(3 \leftrightarrow 1)$ are either identical or reflections of each other:

1. If the paths are identical, it follows $k_{22} = k_{33} = k_{11}$ and $k_{23} = k_{13}$. Thus, there exists a reflection symmetry mapping vertex 1 to vertex 2.
2. If the paths are reflections of each other, it holds $k_{22} = k_{11}$ and $k_{23} = k_{13}$. In this case, there also exists a reflection symmetry mapping vertex 1 to vertex 2.

Since the symmetries in all these cases exist independent of the unconstrained entries of K, in a 3-cycle, all binomial linear forms in $I(\mathcal{L}^{-1})$ are induced by symmetries of G.

5-cycle: In a 5-cycle, either the shorter path between any two distinct vertices is of length one and the complementary path is of length four, or the shorter path is of length two and the complementary path is of length three.

For the first case, assume without loss of generality $\sigma_{12} - \sigma_{45} \in I(\mathcal{L}^{-1})$. Then, by Corollary 4.3.3, we have:

$$\begin{aligned} k_{12} \det\left(K_{1 \overset{c}{\leftrightarrow} 2 \setminus \{1,2\}}\right) = k_{45} \det\left(K_{4 \overset{c}{\leftrightarrow} 5 \setminus \{4,5\}}\right) \quad &\Rightarrow \quad k_{12} \det\left(K_{3 \leftrightarrow 5}\right) = k_{45} \det\left(K_{1 \leftrightarrow 3}\right), \\ k_{23}k_{34}k_{45}k_{15} \det\left(K_{1 \leftrightarrow 2 \setminus \{1,2\}}\right) = k_{15}k_{12}k_{23}k_{34} \det\left(K_{4 \leftrightarrow 5 \setminus \{4,5\}}\right) \quad &\Rightarrow \quad k_{23}k_{34}k_{45}k_{15} = k_{15}k_{12}k_{23}k_{34}. \end{aligned}$$

Therefore, $k_{12} = k_{45}$. Since the paths on $V(3 \leftrightarrow 5)$ and $V(1 \leftrightarrow 3)$ are both of length two, by Lemma 4.4.2, they are either identical or reflections of each other.

1. If the paths on $V(3 \leftrightarrow 5)$ and $V(1 \leftrightarrow 3)$ are equal to each other, it follows $k_{33} = k_{11}$, $k_{44} = k_{22}$, $k_{55} = k_{33}$, and $k_{34} = k_{12}$, $k_{45} = k_{23}$. Thus, there is a reflection symmetry in the graph mapping vertex 1 to vertex 5 and vertex 2 to vertex 4.
2. If the paths $V(3 \leftrightarrow 5)$ and $V(1 \leftrightarrow 3)$ are reflections of each other, it holds $k_{44} = k_{22}$, $k_{55} = k_{11}$, and $k_{34} = k_{23}$. In this case, there exists a reflection symmetry mapping vertex 1 to vertex 5 and vertex 2 to vertex 4.

For the second case, assume without loss of generality $\sigma_{13} = \sigma_{24} \in I(\mathcal{L}^{-1})$. Then, it holds by Corollary 4.3.3:

$$\begin{aligned} k_{12}k_{23} \det\left(K_{1 \overset{c}{\leftrightarrow} 3 \setminus \{1,3\}}\right) = k_{23}k_{34} \det\left(K_{2 \overset{c}{\leftrightarrow} 4 \setminus \{2,4\}}\right) \quad &\Rightarrow \quad k_{12}k_{23} \det\left(K_{4 \leftrightarrow 5}\right) = k_{23}k_{34} \det\left(K_{5 \leftrightarrow 1}\right), \\ k_{34}k_{45}k_{15} \det\left(K_{1 \leftrightarrow 3 \setminus \{1,3\}}\right) = k_{45}k_{15}k_{12} \det\left(K_{2 \leftrightarrow 4 \setminus \{2,4\}}\right) \quad &\Rightarrow \quad k_{34}k_{45}k_{15}k_{22} = k_{45}k_{15}k_{12}k_{33}. \end{aligned}$$

Thus, $k_{12} = k_{34}$ and $k_{22} = k_{33}$. Since the paths on $V(4 \leftrightarrow 5)$ and $V(5 \leftrightarrow 1)$ are both of length 1, we can apply Lemma 4.4.2 to find two cases:

1. If the paths on $V(4 \leftrightarrow 5)$ and $V(5 \leftrightarrow 1)$ are equal, it follows $k_{44} = k_{55} = k_{11}$ and $k_{45} = k_{15}$. Then there exists a reflection symmetry in the cycle mapping vertex 1 to 4 and vertex 2 to 3.
2. If the paths on $V(4 \leftrightarrow 5)$ and $V(5 \leftrightarrow 1)$ are reflections of each other, it holds $k_{44} = k_{11}$ and $k_{45} = k_{15}$. Thus, there exists a reflection symmetry mapping vertex 1 to 4 and vertex 2 to 3.

A binomial linear form in the vanishing ideal of a 5-cycle can also take the form $\sigma_{ii} - \sigma_{mm}$. Assume, without loss of generality, that $\sigma_{11} - \sigma_{33} \in I(\mathcal{L}^{-1})$. By Corollary 4.3.3, it holds that

$$\begin{aligned} \det\left(K_{\setminus 1}\right) = \det\left(K_{\setminus 3}\right) \quad &\Rightarrow \quad \det\left(K_{\overset{c}{2\leftrightarrow 5}}\right) = \det\left(K_{\overset{c}{4\leftrightarrow 2}}\right), \\ k_{12}k_{23}k_{34}k_{45}k_{15}\det\left(K_{1\leftrightarrow 1\setminus 1}\right) = k_{34}k_{45}k_{15}k_{12}k_{23}\det\left(K_{3\leftrightarrow 3\setminus 3}\right) \quad &\Rightarrow \quad k_{12}k_{23}k_{34}k_{45}k_{15} = k_{34}k_{45}k_{15}k_{12}k_{23}. \end{aligned}$$

To compute the determinant in the first equation, we apply Lemma 4.3.4, obtaining:

$$\begin{aligned} &k_{22}k_{33}k_{44}k_{55} - k_{23}^2k_{44}k_{55} - k_{34}^2k_{22}k_{55} - k_{45}^2k_{22}k_{33} + k_{23}^2k_{45}^2 \\ &= k_{44}k_{55}k_{11}k_{22} - k_{45}^2k_{11}k_{22} - k_{15}^2k_{44}k_{22} - k_{12}^2k_{44}k_{55} + k_{45}^2k_{12}^2. \end{aligned}$$

From the first terms, we deduce $k_{33} = k_{11}$ and from the last terms, we conclude $k_{23} = k_{12}$. Additionally, the equality $k_{34}^2k_{22}k_{55} = k_{15}^2k_{44}k_{22}$ implies that $k_{34} = k_{15}$ and $k_{44} = k_{55}$. Therefore, there exists a reflection symmetry mapping vertex 1 to vertex 3 and vertex 5 to vertex 4.

In all the cases outlined, the symmetries exist independent of the unconstrained entries of K. Thus, in a 5-cycle, all binomial linear forms in $I(\mathcal{L}^{-1})$ are induced by symmetries of G, and we complete the proof. □

4.5 Counterexamples to the conjecture

The analyses conducted so far have enabled the identification of counterexamples to the necessary condition of Conjecture 4.0.2. These counterexamples are presented and discussed in the following subsections:

4.5.1 Counterexample of size 4

When analyzing small cycles for Theorem 4.4.3, we observed that binomial linear forms with shorter paths of length one in the vanishing ideal of 4-cycles can lead to problems in identifying a corresponding symmetry. The reason for this issue is as follows:

Assume without loss of generality $\sigma_{12} - \sigma_{34} \in I(\mathcal{L}^{-1})$. Then, by Corollary 4.3.3:

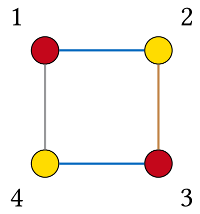
$$\begin{aligned} k_{12}\det\left(K_{\overset{c}{1\leftrightarrow 2}\setminus\{1,2\}}\right) = k_{34}\det\left(K_{\overset{c}{3\leftrightarrow 4}\setminus\{3,4\}}\right) \quad &\Rightarrow \quad k_{12}\det\left(K_{3\leftrightarrow 4}\right) = k_{34}\det\left(K_{1\leftrightarrow 2}\right), \\ k_{23}k_{34}k_{14}\det\left(K_{1\leftrightarrow 2\setminus\{1,2\}}\right) = k_{14}k_{12}k_{23}\det\left(K_{3\leftrightarrow 4\setminus\{3,4\}}\right) \quad &\Rightarrow \quad k_{23}k_{34}k_{14} = k_{14}k_{12}k_{23}. \end{aligned}$$

From this, we deduce that $k_{12} = k_{34}$. Since the paths on $V(3 \leftrightarrow 4)$ and $V(1 \leftrightarrow 2)$ are both of length 1, we can apply Lemma 4.4.2, which yields two possible cases:

1. If the paths on $V(3 \leftrightarrow 4)$ and $V(1 \leftrightarrow 2)$ are identical, we obtain the equalities $k_{33} = k_{11}$ and $k_{44} = k_{22}$.
2. If the paths on $V(3 \leftrightarrow 4)$ and $V(1 \leftrightarrow 2)$ are reflections of each other, we derive the equalities $k_{33} = k_{22}$ and $k_{44} = k_{11}$. In this case, the graph exhibits a reflection symmetry mapping vertex 1 to vertex 4 and vertex 2 to vertex 3.

In both cases, no constraints are required on k_{23} and k_{14}. In the second case, where the paths on $V(3 \leftrightarrow 4)$ and $V(1 \leftrightarrow 2)$ are reflections of each other, the symmetry exists regardless of the values of k_{23} and k_{14}. In the first case, however, where the paths are identical, the symmetry condition requires that $k_{23} = k_{14}$. Thus, whenever a 4-cycle of the first type does not satisfy this extra constraint, there will be a binomial linear form in the vanishing ideal that is not induced by symmetry. This observation leads us to the following counterexample to Conjecture 4.0.2:

Example 4.5.1. Let G be the following colored 4-cycle:



The Macaulay2 code provided in Appendix A.3 verifies that there is no symmetry within this graph. However, the code confirms the existence of the following binomial linear element in the vanishing ideal $I(\mathcal{L}^{-1})$:

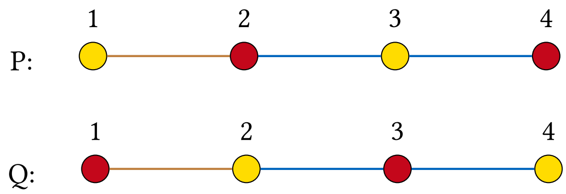
$$\sigma_{12} - \sigma_{34}.$$

In this example, the binomial linear form is not obtained from a symmetry in the graph, thereby disproving that the necessary condition of Conjecture 4.0.2 holds for all n-cycles with $n \in \mathbb{N}$.

4.5.2 Counterexample of size 6

Investigating the third and special case discussed in Section 4.4.1 leads us to another interesting counterexample to Conjecture 4.0.2 of larger size. To begin, we illustrate the third type path with the following example:

Example 4.5.2. Let P and Q be two paths both with vertex set $V = \{1, 2, 3, 4\}$ and coloring as follows:

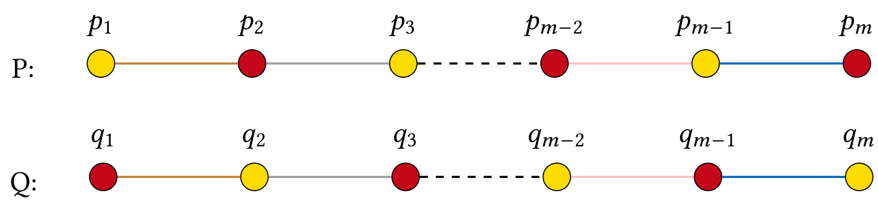


Calculating the determinants of K_P and K_Q using Lemma 4.3.4 yields $\det(K_P) = \det(K_Q)$.

Building on this example, we are able to generalize the third type path for any even length m:

Lemma 4.5.3. *Let P and Q be two even sized paths with vertices $V_P = \{p_1, p_2, \ldots, p_m\}$ and $V_Q = \{q_1, q_2, \ldots, q_m\}$, where $\lambda(\{p_i, p_j\}) = \lambda(\{q_i, q_j\})$ for all edges $\{p_i, p_j\} \in E_P$ and $\{q_i, q_j\} \in E_Q$. Additionally, suppose that $\lambda(p_1) = \lambda(p_3) = \cdots = \lambda(p_{m-1}) = \lambda(q_2) = \lambda(q_4) = \cdots = \lambda(q_m)$ and $\lambda(p_2) = \lambda(p_4) = \cdots = \lambda(p_m) = \lambda(q_1) = \lambda(q_3) = \cdots = \lambda(q_{m-1})$. Then, $\det(K_P) = \det(K_Q)$.*

Proof. The paths have the following structure:



We assign the odd vertices of P the partial correlation k_{11} and the even vertices of P the partial correlation k_{22}. By the color constraints specified in the lemma, the concentration matrices $K_P = (p_{ij})$ and $K_Q = (q_{ij})$ meet the following conditions:

$$\begin{aligned} p_{ii} &= k_{11} \text{ and } q_{ii} = k_{22}, && \text{if } i \in \{1, 2, \ldots, m\} \text{ is odd,} \\ p_{ii} &= k_{22} \text{ and } q_{ii} = k_{11}, && \text{if } i \in \{1, 2, \ldots, m\} \text{ is even,} \\ p_{ij} &= q_{ij} = k_{ij}, && \text{for all } \{p_i, p_j\} \in E_P \text{ and } \{q_i, q_j\} \in E_Q. \end{aligned}$$

The concentration matrices of P and Q are then given by:

$$K_P = \begin{pmatrix} k_{11} & k_{12} & 0 & \cdots & 0 \\ k_{12} & k_{22} & k_{23} & \ddots & \vdots \\ 0 & k_{23} & k_{11} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & k_{m-1m} \\ 0 & \cdots & 0 & k_{m-1m} & k_{22} \end{pmatrix}, \qquad K_Q = \begin{pmatrix} k_{22} & k_{12} & 0 & \cdots & 0 \\ k_{12} & k_{11} & k_{23} & \ddots & \vdots \\ 0 & k_{23} & k_{22} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & k_{m-1m} \\ 0 & \cdots & 0 & k_{m-1m} & k_{11} \end{pmatrix}.$$

To calculate the determinants of K_P and K_Q, we apply the well-known Leibniz formula:

$$\det(K_P) = \sum_{\tau \in \mathbb{S}^m} \operatorname{sgn}(\tau) \prod_{i=1}^{m} p_{i\tau(i)}, \qquad \det(K_Q) = \sum_{\tau \in \mathbb{S}^m} \operatorname{sgn}(\tau) \prod_{i=1}^{m} q_{i\tau(i)}.$$

For the tridiagonal matrices K_P and K_Q, any permutation τ where $\tau(i)$ maps i to an index not adjacent to i results in a product term that is zero, since the corresponding matrix entries $p_{i\tau(i)}$ and $q_{i\tau(i)}$ are zero for non-adjacent indices. Consequently, only permutations that are either the identity or disjoint compositions of 2-cycles, which permute adjacent indices, contribute to the determinant. Let $\mathcal{T} \subseteq \mathbb{S}^m$ denote the set of such permutations. Then:

$$\det(K_P) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau) \prod_{i=1}^{m} p_{i\tau(i)}, \qquad \det(K_Q) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau) \prod_{i=1}^{m} q_{i\tau(i)}.$$

The products in these formulas can be decomposed into two components: the product of variables corresponding to indices permuted under the permutation τ, and the product of variables corresponding to indices fixed by τ:

$$\det(K_P) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau) \prod_{\substack{i=1,\\ \tau(i)\neq i}}^{m} p_{i\tau(i)} \prod_{\substack{i=1,\\ \tau(i)=i}}^{m} p_{i\tau(i)}, \qquad \det(K_Q) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau) \prod_{\substack{i=1,\\ \tau(i)\neq i}}^{m} q_{i\tau(i)} \prod_{\substack{i=1,\\ \tau(i)=i}}^{m} q_{i\tau(i)}.$$

Let $t_\tau \in \{0, 1, \ldots, \frac{m}{2}\}$ denote the number of 2-cycles within the permutation $\tau \in \mathcal{T}$. The first product in $\det(K_P)$ corresponds to the off-diagonal entries of K_P. Any $\tau \in \mathcal{T}$ permutes an even amount of $2t_\tau$ off-diagonal entries, which are equal in K_P and K_Q. Since m is even, τ fixes an even amount of diagonal entries. Specifically, τ fixes $\frac{m}{2} - t_\tau$ diagonal entries corresponding to even indices i, and $\frac{m}{2} - t_\tau$ diagonal entries corresponding to odd indices i. Thus, the second product in the determinant formula includes $\frac{m}{2} - t_\tau$ factors of k_{11} and $\frac{m}{2} - t_\tau$ factors of k_{22}. Thus, the determinant of K_P simplifies as:

$$\det(K_P) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau)\, k_{11}^{\frac{m}{2}-t_\tau}\, k_{22}^{\frac{m}{2}-t_\tau} \prod_{\substack{i=1,\\ \tau(i)\neq i}}^{m} k_{i\tau(i)}.$$

Similarly, for K_Q, the fixed diagonal entries contribute $\frac{m}{2} - t_\tau$ factors of k_{22} and $\frac{m}{2} - t_\tau$ factors of k_{11} for each $\tau \in \mathcal{T}$:

$$\det(K_Q) = \sum_{\tau \in \mathcal{T}} \operatorname{sgn}(\tau)\, k_{22}^{\frac{m}{2}-t_\tau}\, k_{11}^{\frac{m}{2}-t_\tau} \prod_{\substack{i=1,\\ \tau(i)\neq i}}^{m} k_{i\tau(i)}.$$

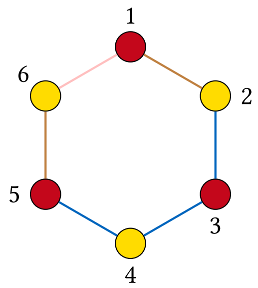
Hence, we conclude:

$$\det(K_P) = \det(K_Q).$$

□

From Example 4.5.2, which illustrates a path of the third type, we constructed a larger cycle that serves as another counterexample to Conjecture 4.0.2, thereby preventing its verification for all n-cycles.

Example 4.5.4. Let G be the 6-cycle, which is colored as follows:



The only potential symmetry in this 6-cycle would require a reflection along the symmetry axis passing through the edges $\{1, 6\}$ and $\{3, 4\}$, due to the unique pink edge. However, this cannot be a valid symmetry since vertex 1 is not equivalent to vertex 6. Therefore, the graph has no symmetry. To support this conclusion, Macaulay2 code is provided in Appendix A.4, which computes all permutation matrices satisfying the symmetry condition. Running this code confirms that the graph possesses no symmetry.
The concentration matrix associated with this 6-cycle graph is given by:

$$K = \begin{pmatrix} k_{11} & k_{12} & 0 & 0 & 0 & k_{16} \\ k_{12} & k_{22} & k_{23} & 0 & 0 & 0 \\ 0 & k_{23} & k_{11} & k_{23} & 0 & 0 \\ 0 & 0 & k_{23} & k_{22} & k_{23} & 0 \\ 0 & 0 & 0 & k_{23} & k_{11} & k_{12} \\ k_{16} & 0 & 0 & 0 & k_{12} & k_{22} \end{pmatrix}.$$

Calculating its inverse using the *pull-back* map approach defined in Section 2.3, we obtain the following binomial linear forms, which are contained in the ideal $I(\mathcal{L}^{-1})$:

$$\sigma_{23} - \sigma_{45}, \quad \sigma_{14} - \sigma_{36}, \quad \sigma_{12} - \sigma_{56}.$$

This counterexample is directly related to the third case path described in Example 4.5.2. Specifically, the cycle was constructed such that the paths P and Q from Example 4.5.2 are embedded within it. These paths directly yield the third binomial linear form, $\sigma_{12} - \sigma_{56}$. To see this, note that the path on $V(1 \overset{c}{\leftrightarrow} 2 \setminus \{1, 2\})$ corresponds to the path on the vertices $\{3, 4, 5, 6\}$, which is the reflection of path P in Example 4.5.2. Similarly, the path on $V(5 \overset{c}{\leftrightarrow} 6 \setminus \{5, 6\})$ corresponds to the path on the vertices $\{1, 2, 3, 4\}$, which is equal to path Q in the same example. By the results of Section 4.4, the determinants of the concentration matrices of path P and its reflection are equal. Therefore, by Example 4.5.2, we have:

$$\det\left(K_{1 \overset{c}{\leftrightarrow} 2 \setminus \{1,2\}}\right) = \det\left(K_{5 \overset{c}{\leftrightarrow} 6 \setminus \{5,6\}}\right).$$

Moreover, the construction of the cycle ensures that the weights along the shorter paths and the complementary paths are identical. Consequently, all terms in the formulas for σ_{12} and σ_{56} given in Corollary 4.3.3 are equal, resulting in the binomial linear form $\sigma_{12} - \sigma_{56} \in I(\mathcal{L}^{-1})$. This demonstrates that a binomial linear form can arise in a cycle that lacks symmetry.

Note that using a similar argument, the linear form $\sigma_{23} - \sigma_{45}$ also arises from a determinant equality induced by a third case path, demonstrating the generality of this construction.

5 Non-binomial linear forms in the vanishing ideal of cyclic graphs

After completing the computation of the entire linear part of the vanishing ideal for the study presented in Section 4.1, we observed the presence of non-binomial linear elements within the vanishing ideal of the 4- and 5-cycles. In contrast, 3-cycles, which were also considered in the computational study, do not exhibit non-binomial linear generators. Consequently, the 4-cycle is the smallest graph with an even number of vertices where non-binomial linear forms appear, while the 5-cycle is the smallest such graph with an odd number of vertices. These observations suggest that the structure of the linear part of the vanishing ideal can exhibit significant complexity beyond the binomial case. To further illustrate these findings, we present examples of the 4- and 5-cycle, emphasizing the algebraic properties that arise from specific color configurations:

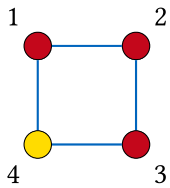
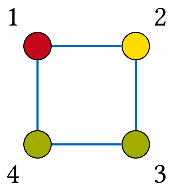
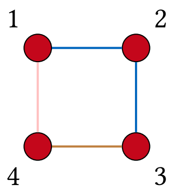
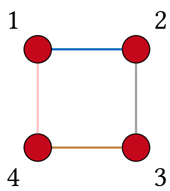
<table>
<tr><th>Graph</th><th>Non-binomial linear forms in $I(\mathcal{L}^{-1})$</th></tr>
<tr><td>
</td><td>$\sigma_{13} - \sigma_{22} - \sigma_{24} + \sigma_{33}$</td></tr>
<tr><td>
</td><td>$\sigma_{13} - \sigma_{24} + \sigma_{33} - \sigma_{44}$</td></tr>
<tr><td>
</td><td>$\sigma_{11} - \sigma_{22} + \sigma_{33} - \sigma_{44}$</td></tr>
<tr><td>
</td><td>$\sigma_{11} - \sigma_{22} + \sigma_{33} - \sigma_{44}$</td></tr>
</table>

Table 5.1 Non-binomial linear generators of $I(\mathcal{L}^{-1})$ for colored cycles. The left column of the table presents the colored cycle and the right column the corresponding non-binomial linear forms.

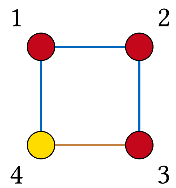
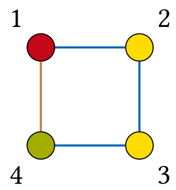
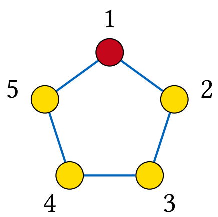
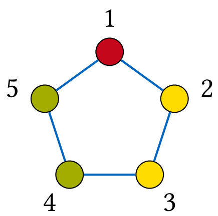
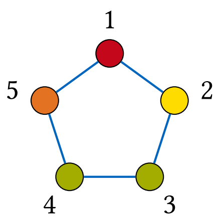
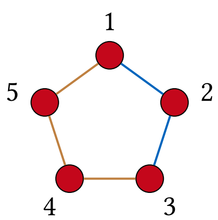
Graph	Non-binomial linear forms in $I(\mathcal{L}^{-1})$
	$\sigma_{11} + \sigma_{13} - \sigma_{22} - \sigma_{24}$
	$\sigma_{13} - \sigma_{22} - \sigma_{24} + \sigma_{33}$
	$\sigma_{25} - \sigma_{34} - \sigma_{35} + \sigma_{44} + \sigma_{45} - \sigma_{55}$ $\sigma_{14} - \sigma_{35} + \sigma_{44} - \sigma_{55}$ $\sigma_{13} - \sigma_{35} + \sigma_{44} - \sigma_{55}$
	$\sigma_{14} - \sigma_{35} + \sigma_{44} - \sigma_{55}$ $\sigma_{13} - \sigma_{22} - \sigma_{24} + \sigma_{33}$
	$\sigma_{24} - \sigma_{33} - \sigma_{35} + \sigma_{44}$
	$\sigma_{13} - \sigma_{33} + \sigma_{34} - \sigma_{35} - \sigma_{45} + \sigma_{55}$

Table 5.2 Continuation of Table 5.1

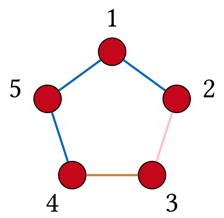
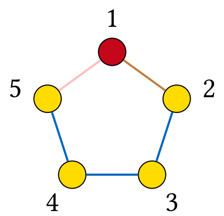
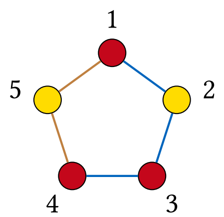
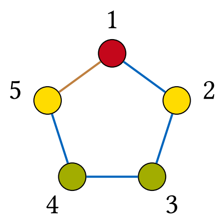
Graph	**Non-binomial linear forms in $I(\mathcal{L}^{-1})$**
	$\sigma_{11} + \sigma_{14} - \sigma_{25} - \sigma_{55}$
	$\sigma_{24} - \sigma_{33} - \sigma_{35} + \sigma_{44}$
	$\sigma_{12} + \sigma_{14} - \sigma_{23} - \sigma_{24} + \sigma_{33} - \sigma_{44}$
	$\sigma_{24} - \sigma_{33} - \sigma_{35} + \sigma_{44}$

Table 5.3 Continuation of Table 5.2.

Based on our observations of non-binomial generators of the vanishing ideal $I(\mathcal{L}^{-1})$ for 4- and 5-cycles, we propose the following conjecture:

Conjecture 5.0.1. Let G be a colored n-cycle. In any linear form in $I(\mathcal{L}^{-1})$, the number of non-zero terms with positive coefficients is equal to the number of non-zero terms with negative coefficients.

The computational study also raises the question of whether there is an underlying pattern in the way the non-binomial linear generators are defined. As explained in Chapter 4, when symmetry exists in the graph, the binomial linear forms arise from projecting edges and nodes along the symmetry axis of the graph or rotating them by a specific angle. This behavior, induced by symmetries, is well understood and leads to predictable structures for the corresponding linear forms. However, for non-binomial linear forms, we were unable to identify a structural pattern within the time available. This motivates the following question:

Question 5.0.2. Let G be a colored n-cycle. What is the underlying pattern of the non-binomial linear forms in $I(\mathcal{L}^{-1})$?

6 Conclusion

This thesis was motivated by previous work on Gaussian graphical models, with the aim of investigating whether Conjecture 1.0.1 presented by Davies and Marigliano in [3] holds for all n-cycles. The conjecture states that binomial linear forms exists in the vanishing ideal $I(\mathcal{L}^{-1})$ if and only if they are obtained from a corresponding symmetry of the graph.

To address this question, we began by reviewing key concepts of Gaussian graphical models and their algebraic properties, with a focus on the vanishing ideal $I(\mathcal{L}^{-1})$ [3, 9]. We introduced the *pull-back* map [9], a powerful tool for computing the generators of this ideal. In order to simplify these calculations, we discussed the concept of graph colorings based on the work of [3, 2], which allowed us to define symmetries within graphs. Furthermore, we revisited the description of the entire linear part of $I(\mathcal{L}^{-1})$ for certain uniform colored graphs [3].

Focusing on cycle graphs, we conducted a computational study of the entire linear part of the vanishing ideal $I(\mathcal{L}^{-1})$ for small cycles. This study provided preliminary evidence supporting the conjecture for 3- and 5-cycles. In Section 4.1, we successfully verified the sufficient condition of the conjecture for all n-cycles, proving that whenever a symmetry exists within a graph, all binomial linear forms obtained from that symmetry are contained in the vanishing ideal. After thoroughly analyzing the types of symmetries present in cycle graphs and the properties they imply, we focused on studying the binomial linear elements of the vanishing ideal. Building on a key theorem by [5], we confirmed the necessary condition for 3- and 5-cycles, proving that in these cases, all binomial linear forms in the vanishing ideal are indeed obtained from corresponding symmetries in the graph. However, we found specific colorings of the 4- and 6-cycle, where binomial linear forms are elements of the vanishing ideal, but no symmetry exists in the graph. Thus, by Counterexamples 4.5.1 and 4.5.4, we disproved that the necessary condition of Conjecture 1.0.1 holds for all n-cycles.

In addition to resolving the conjecture, our study revealed that the linear part of $I(\mathcal{L}^{-1})$ contains numerous non-binomial linear forms, whose structural patterns remain unexplained. While we provided illustrative examples of 4- and 5-cycles in Chapter 5, a comprehensive characterization of these forms remains as an open question.

In conclusion, this thesis has verified the sufficient condition of Conjecture 1.0.1 for all n-cycles, but disproved that the necessary condition holds for all n-cycles. This clarifies the relationship between graph symmetries and binomial linear forms in the vanishing ideal. We believe this thesis lays the groundwork for deeper explorations of the algebraic and combinatorial properties of Gaussian graphical models.

A Appendix: Macaulay2 implementations

A.1 Code for Example 3.2.4

The following code demonstrates how to find all symmetries of the underlying graph and the corresponding binomial linear elements of the vanishing ideal for Example 3.2.4. Additionally, the *pull-back* map is implemented to ensure that no binomial linear forms exist beyond those induced by the symmetry. This implementation provides a clear computational framework for analyzing linear generators of the vanishing ideal.

```
S=QQ[x11,x12,x13,x14,x15,x22,x23,x24,x25,x33,x34,x35,x44,x45,x55];
R=frac(QQ[k11,k12,k15,k33,k44]);

--Define the concentration matrix of the underlying graph
K=matrix{{k11,k12,0,0,k15},{k12,k11,0,k15,0},{0,0,k33,0,0},{0,k15,0,
   k44,k12},{k15,0,0,k12,k44}};

--Find all permutation matrices meeting the symmetry condition
n=5;
Id = map(ZZ^n);
for p in permutations(n) list(
     P := Id_p;
     if (P*K*transpose(P) - K ) == 0  then p
     else continue
)

--This ensures that the following matrix is the only non-trivial
   permutation:
P = matrix
   {{0,1,0,0,0},{1,0,0,0,0},{0,0,1,0,0},{0,0,0,0,1},{0,0,0,1,0}};

--Calculate the linear forms induced by this symmetry
X=matrix{{x11,x12,x13,x14,x15},{x12,x22,x23,x24,x25},{x13,x23,x33,x34
   ,x35},{x14,x24,x34,x44,x45},{x15,x25,x35,x45,x55}};
P * X * inverse(P) - X

--Use the pull-back map approach for verification of the linear forms
N = inverse K * det K;

--Define the pull-back map
f = map(R,S,{N_(0,0),N_(0,1),N_(0,2),N_(0,3),N_(0,4),N_(1,1),N_(1,2),
   N_(1,3),N_(1,4),N_(2,2),N_(2,3),N_(2,4),N_(3,3),N_(3,4),N_(4,4)});

--Get the generators of the ideal as a list of polynomials
I = ker f;
gen = flatten entries gens I;
--The linear generators of I are given by:
linearGens = select(gen, f -> sum degree f == 1)
```

A.2 Code for the computational study on 3-, 4- and 5-cycles

The following Macaulay2 code was used to perform the computational study described in Section 4.1. It provides the results for the binomial and non-binomial linear forms for all examples presented in Section 4.1 and Chapter 5. It is important to note that whenever the number of vertices in the graph is modified, the sets of vertex colors and edge colors must be updated to contain the same number of elements as the number of vertices in the graph. Additionally, the code may require a relatively long computational time, primarily due to the matrix operations and the computation of the entire ideal. Suggestions for optimizing or simplifying this program are welcome.

```
numNodes = 5;                --number of vertices; adjust accordingly
SetVertexColors = {a, b, c, d, e};
SetEdgeColors = {v, w, x, y ,z};
colorings = {};
combinedColorings = {};
results = {};
R=frac(QQ[flatten(SetVertexColors, SetEdgeColors)]);

GenerateAllLinearForms = (numNodes, fractionF, vertexColors,
   edgeColors) -> (
    S=QQ[createVariables(numNodes)];
    colorings = {};
    combinedColorings = {};
    verticesCombinations = calculateAllCombinations({}, 0,
       vertexColors);
    colorings = {};
    combinedColorings = {};
    edgesCombinations = calculateAllCombinations({}, 0, edgeColors);

    for vCombi in verticesCombinations do(
        for eCombi in edgesCombinations do(
            K = createConcentrationMatrix(numNodes, vCombi, eCombi);
            linearGenerators = applyMathematicalOperations(numNodes,
               K, fractionF, S);
            if length(linearGenerators) > 0 then(
                results = append(results, {vCombi, eCombi,
                   linearGenerators});
            );
        );
    );
    return results;
);

--Function that calculates all possible color combinations
calculateAllCombinations = (currentCombination, GraphDepth, colors)
   -> (
    if GraphDepth == numNodes then (
        colorings = append(colorings, currentCombination);
        return ();
    );
    for color in colors do (
    calculateAllCombinations(append(currentCombination, color),
       GraphDepth + 1, colors);
    );
    return colorings;
);

--Function that creates the colored concentration matrix
```

```
createConcentrationMatrix = (numNodes, vertexEntryList, edgeEntryList
   ) -> (
    K = matrix( for i from 1 to numNodes list(
    for j from 1 to numNodes list(
        if i==j then k_(i,j) = vertexEntryList_(i-1)
        else if i==(j+1) or j==(i+1) then k_(i,j) = edgeEntryList_(
           max(i,j)-2)
        else if (i==1 and j==numNodes) or (j==1 and i==numNodes) then
            k_(i,j) = edgeEntryList_(max(i,j)-1)
        else 0
            )
        )
    )
)

--Function that creates the variables of the corresponding ring
createVariables = (numNodes) ->(
    sVars = flatten for i from 1 to numNodes list(
    for j from i to numNodes list(
        if i <= j  then s_(i,j)
        else continue
        )
    )
)

--Function that computes all linear generators of the vanishing ideal
applyMathematicalOperations = (numNodes, concentrationMatrix,
   fractionField, givenRing) -> (
    N = det(concentrationMatrix) * inverse(concentrationMatrix);
    mapping = flatten for i from 0 to (numNodes - 1) list (
                for j from i to (numNodes - 1) list (
                    N_(i, j)
                    )
                );
    f = map(fractionField, givenRing, mapping);
    I = ker f;
    gen = flatten entries gens I;
    linearGenerators = select(gen, f -> sum degree f == 1);
    return linearGenerators
)

--Generate all linear forms by running the code:
GenerateAllLinearForms(5, R, {a, b, c, d, e}, {v, w, x, y, z})
```

A.3 Code for Counterexample 4.5.1

This implementation verifies that the 4-cycle in Counterexample 4.5.1 has no symmetry and computes the linear part of the vanishing ideal, uncovering the presence of a binomial linear form within the ideal.

```
S=QQ[s11,s12,s13,s14,s22,s23,s24,s33,s34,s44];
R=frac(QQ[k11,k12,k15,k33,k14,k44,k22,k23]);

--Encode the concentration matrix of the underlying 4-cycle
K=matrix{{k11,k12,0,k14},{k12,k22,k23,0},{0,k23,k11,k12},{k14,0,k12,
   k22}};
```

```
--Test if any non-trivial permutation matrix meets the symmetry
   condition
n=4;
Id = map(ZZ^n);
for p in permutations(n) list(
    P := Id_p;
    if (P*K*transpose(P) - K ) == 0  then p
    else continue
)

--Check for linear elements of the vanishing ideal
N = inverse K * det K;
f = map(R,S,{N_(0,0),N_(0,1),N_(0,2),N_(0,3),N_(1,1),N_(1,2),N_(1,3),
   N_(2,2),N_(2,3),N_(3,3)});
I= ker f;
gen = flatten entries gens I;
linearGens= select(gen, f -> sum degree f == 1)
```

A.4 Code for Counterexample 4.5.4

This implementation verifies that the 6-cycle in Example 4.5.4 has no symmetry and computes the entire linear part of the vanishing ideal, revealing the presence of binomial linear elements within the ideal.

```
S=QQ[s11,s12,s13,s14,s15,s16,s22,s23,s24,s25,s26,s33,s34,s35,s36,s44,
   s45,s46,s55,s56,s66];
R=frac(QQ[k11,k12,k16,k22,k23]);

--Define the concentration matrix of the 6-cycle in this
   counterexample
K = matrix{{k11,k12,0,0,0,k16},{k12,k22,k23,0,0,0}, {0,k23,k11,k23
   ,0,0},{0,0,k23,k22,k23,0},{0,0,0,k23,k11,k12},{k16,0,0,0,k12,k22
   }};

--Test if any non-trivial permutation matrix meets the symmetry
   condition
n=6;
Id = map(ZZ^n);
for p in permutations(n) list(
    P := Id_p;
    if (P*K*transpose(P) - K ) == 0  then p
    else continue
)

--Check for linear elements of the vanishing ideal
N = inverse K * det K;
f = map(R,S,{N_(0,0),N_(0,1),N_(0,2),N_(0,3),N_(0,4),N_(0,5),N_(1,1),
   N_(1,2),N_(1,3),N_(1,4),N_(1,5),N_(2,2),N_(2,3),N_(2,4),N_(2,5),N_
   (3,3),N_(3,4),N_(3,5),N_(4,4),N_(4,5),N_(5,5)});
I= ker f;
gen = flatten entries gens I;
linearGens= select(gen, f -> sum degree f == 1)
```

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