Colored Graphical Models and Their Symmetries

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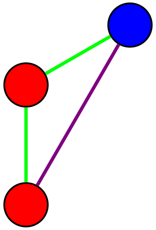
Colored Graphs

Let $G = (V, E)$ be a graph. A *coloring* if G is a partition of V together with a partition of E. A *color* is an equivalence class with respect to one of these partitions.



Adjacency Matrices

Let γ_k be a color of the graph G with n vertices and d colors. We define the matrix A_k associated to γ_k as follows: if γ_k is a vertex color then

$$(A_k)_{ij} = \begin{cases} 1 & i = j \text{ and vertex } i \text{ has color } \gamma_k \\ 0 & \text{else} \end{cases}.$$

If γ_k is an edge color then

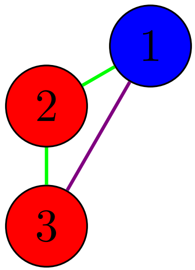
$$(A_k)_{ij} = \begin{cases} 1 & \text{edge } (i,j) \text{ has color } \gamma_k \\ 0 & \text{else} \end{cases}.$$

Then the *adjacency matrix* for the colored graph G is given by

$$\sum_{k=1}^{d} \lambda_k A_k \in \mathbb{Z}[\lambda_1, \ldots, \lambda_d]^{n \times n}.$$

Example

With the previous graph G:



We have

$$A = \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_2 & \lambda_4 & \lambda_2 \\ \lambda_3 & \lambda_2 & \lambda_4 \end{pmatrix}.$$

Linear Space of Symmetric Matrices

Let G be a graph with n vertices and d colors. Then the associated linear subspace of symmetric matrices is

$$\mathcal{L} = \left\{ \sum_{k=1}^{d} \lambda_k A_k : \lambda_1, \ldots, \lambda_d \in \mathbb{C} \right\} \subseteq \mathbb{S}^n$$

where $\mathbb{S}^n$ is the space of symmetric $n \times n$ matrices.

The Reciprocal Variety and its Ideal

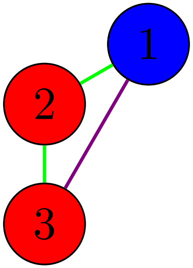
Let G be a colored graph with an associated linear space $\mathcal{L}$. Then the *reciprocal variety* of $\mathcal{L}$ is given by

$$\mathcal{L}^{-1} = \text{cl}_{\mathbb{S}^n} \left\{ M^{-1} : M \in \mathcal{L},\, M \text{ invertible} \right\}.$$

Note a generic element of $\mathcal{L}^{-1}$ has the form $\text{adj}(A)$ for the adjacency matrix A.
Its ideal is denoted $I(\mathcal{L}^{-1})$. Davies and Marigliano are interested in finding the generators of this ideal.

Example

In the graph G,



the reciprocal variety $\mathcal{L}^{-1}$ consists of matrices of the form

$$\begin{pmatrix} -\lambda_2^2+\lambda_4^2 & \lambda_2\lambda_3-\lambda_2\lambda_4 & \lambda_2^2-\lambda_3\lambda_4 \\ \lambda_2\lambda_3-\lambda_2\lambda_4 & -\lambda_3^2-\lambda_1\lambda_4 & -\lambda_1\lambda_2+\lambda_2\lambda_3 \\ \lambda_2^2-\lambda_3\lambda_4 & -\lambda_1\lambda_2+\lambda_2\lambda_3 & -\lambda_2^2+\lambda_1\lambda_4 \end{pmatrix}.$$

Proposition 2.2

Let A be the adjacency matrix of a colored graph G. A *symmetry* of G is an $n \times n$ permutation matrix B such that $BAB^{-1} = A$.

Proposition 2.2: Let B be a symmetry of the graph G and let $X \in \mathbb{S}^n$ be a generic matrix. The binomial linear forms defined by the distinct entries of $BXB^{-1} - X$ belong to the ideal $I(\mathcal{L}^{-1})$.

Proof.

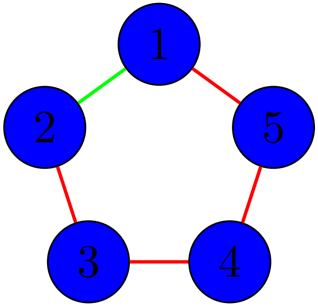
Since $AB = BA$, we know

$$\mathrm{adj}(A)B\det(A) = \mathrm{adj}(A)BA\mathrm{adj}(A) = \det(A)B\mathrm{adj}(A).$$

Since $\det(A) \neq 0$, $B\mathrm{adj}(A)B^{-1} - \mathrm{adj}(A) = 0$. Since $X \in \mathcal{L}^{-1}$ has the form $\mathrm{adj}(A)$, we have $BXB^{-1} - X = 0$. □

Example

Consider the graph G:



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The only nontrivial symmetry is $B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$.

Example

Now consider $X = \begin{pmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\ x_{12} & x_{22} & x_{23} & x_{24} & x_{25} \\ x_{13} & x_{23} & x_{33} & x_{34} & x_{35} \\ x_{14} & x_{24} & x_{34} & x_{44} & x_{45} \\ x_{15} & x_{25} & x_{35} & x_{45} & x_{55} \end{pmatrix} \in \mathbb{S}^5$. Then

$$BXB^{-1} - X = \begin{pmatrix} -x_{11} + x_{22} & 0 & -x_{13} + x_{25} & -x_{14} + x_{24} & -x_{15} + x_{23} \\ 0 & x_{11} - x_{22} & x_{15} - x_{23} & x_{14} - x_{24} & x_{13} - x_{25} \\ -x_{13} + x_{25} & x_{15} - x_{23} & -x_{33} + x_{55} & -x_{34} + x_{45} & 0 \\ -x_{14} + x_{24} & x_{14} - x_{24} & -x_{34} + x_{45} & 0 & x_{34} - x_{45} \\ -x_{15} + x_{23} & x_{13} - x_{25} & 0 & x_{34} - x_{45} & x_{33} - x_{55} \end{pmatrix}.$$

Thus
$x_{11} - x_{22}, x_{13} - x_{25}, x_{14} - x_{24}, x_{23} - x_{15}, x_{33} - x_{55}, x_{34} - x_{45} \in I(\mathcal{L}^{-1})$.

Open Problems

But also $x_{14} + x_{44} - x_{35} - x_{55} \in I(\mathcal{L}^{-1})$, which is not a linear combination of the aforementioned linear forms.

This leads to some open problems in [DM]:

Conjecture 4.2: Let G be a colored n-cycle. All *binomial* linear forms in $I(\mathcal{L}^{-1})$ can be found using Proposition 2.2.

Question 4.3: Let G be a colored n-cycle. Is there a graphical explanation for all generators of the linear part of $I(\mathcal{L}^{-1})$?

Theorem 3.6

A *uniform colored n-cycle* is the colored n-cycle G with only one edge color γ_1 and one vertex color γ_2.

Theorem 3.6: For a uniform colored n-cycle, the linear part of $I(\mathcal{L}^{-1})$ is generated by the linear forms

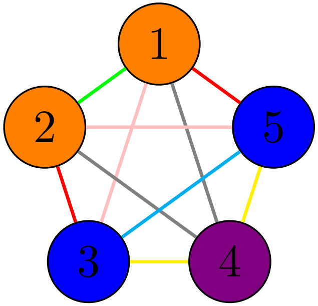
$$x_{i,i+d} - x_{1,1+d}$$

where $2 \leq i \leq n$ and $0 \leq d \leq \lfloor n/2 \rfloor$ and all indices are modulo n and x_{ji} for $j > i$ is taken to mean x_{ij}.

Induced Graphs

Let I' be the ideal generated only by the linear forms found by applying Proposition 2.2. Then the linear space $\mathcal{L}' = V(I')$ is associated to a colored graph G'.

In the previous example, G induces the following colored graph G':



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Maximum Likelihood Degree

For a given space $\mathcal{L} \subseteq \mathbb{S}^n$, the *maximum likelihood degree* of $\mathcal{L}$ is defined by

$$\operatorname{mld}(\mathcal{L}) = \#(\mathcal{L}^{-1} \cap (\mathcal{L}^{\perp} + S)),$$

where S is a general element of $\mathbb{S}^n$, $\mathcal{L}^{\perp}$ is the orthogonal complement of $\mathcal{L}$ under the trace inner product, and $\mathcal{L}^{\perp} + S = \{X + S : X \in \mathcal{L}^{\perp}\}$.

Proposition 2.7

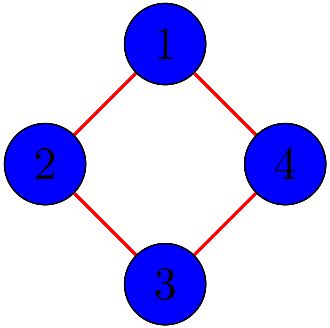
With $\mathcal{L} \subseteq \mathcal{L}' \subseteq \mathbb{S}^n$, we can use $\mathcal{L}'$ as a smaller ambient space to compute the ML degree of $\mathcal{L}$.

Proposition 2.7: Let S' be a general matrix of $\mathcal{L}'$, and let $(\mathcal{L}^\perp)' = \mathcal{L}^\perp \cap \mathcal{L}'$. Then

$$\text{mld}(\mathcal{L}) = \#(\mathcal{L}^{-1} \cap ((\mathcal{L}^\perp)' + S')).$$

Quadratic Forms

The reciprocal variety is not always generated by linear forms. For example, let G be the following uniform colored 4-cycle:



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Then $\mathcal{L}^{-1}$ consists of matrices of the form

$$\begin{pmatrix} \lambda_1^3 - 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 & 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 \\ -\lambda_1^2\lambda_2 & \lambda_1^3 - 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 & 2\lambda_1\lambda_2^2 \\ 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 & \lambda_1^3 - 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 \\ -\lambda_1^2\lambda_2 & 2\lambda_1\lambda_2^2 & -\lambda_1^2\lambda_2 & \lambda_1^3 - 2\lambda_1\lambda_2^2 \end{pmatrix}$$

and so $x_{13}^2 - 2x_{12}^2 + x_{13}x_{11} \in I(\mathcal{L}^{-1})$.

Table

Davies and Marigliano give the following table for uniform colored n-cycles:

	n even	n odd
$\mathrm{mld}(\mathcal{L})$	$n/2$	$(n-1)/2$
$\mathrm{rmld}(\mathcal{L})$	$n-1$	$n-2$
$\deg(\mathcal{L}^{-1})$	$n/2$	$(n-1)/2$
no. linear forms	$(n^2-2)/2$	$(n^2-1)/2$
no. quadratic forms	$n(n-2)/8$	$(n-1)(n-3)/8$

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Bibliography

Davies, Marigliano. *Coloured Graphical Models and Their Symmetries.* `ArXiV:2012.01905`. 3 Dec. 2020.