Maximum likelihood thresholds for colored Gaussian graphical models

Roser Homs Pons, Centre de Recerca Matemàtica

work *in progress* with Olga Kuznetsova, Bernadette Stolz, Danai Deligeorgaki, Joe Johnson, Bryson Kagy and Aida Maraj

New Directions in Algebraic Statistics
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Our models: Gaussian graphical models with additional vertex and edge symmetries

Start with an example

Table 1. Empirical concentrations (on or above the diagonal) and partial correlations (below the diagonal) for the examination marks in five mathematical subjects

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	Mechanics	*Vectors*	*Algebra*	*Analysis*	*Statistics*
Mechanics	5.24	−2.44	−2.74	0.01	−0.14
Vectors	0.33	10.43	−4.71	−0.79	−0.17
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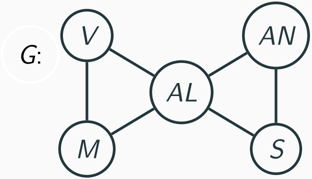

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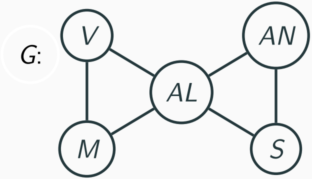

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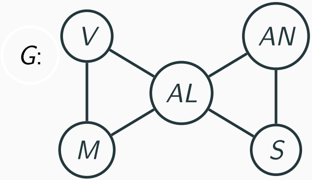

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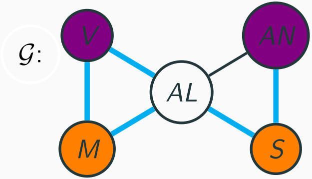

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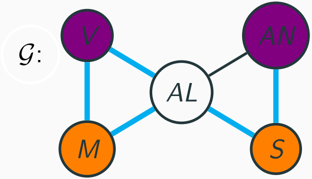

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$$\mathrm{wmlt}(G) = \mathrm{mlt}(G) = 3$$
$$\mathrm{wmlt}(\mathcal{G}) = \mathrm{mlt}(\mathcal{G}) = 1$$

And yet another example: Frets' heads

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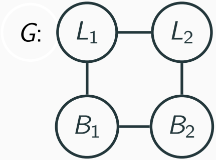

$$K_G = \begin{pmatrix} \lambda_1 & \lambda_5 & 0 & \lambda_8 \\ \lambda_5 & \lambda_2 & \lambda_6 & 0 \\ 0 & \lambda_6 & \lambda_3 & \lambda_7 \\ \lambda_8 & 0 & \lambda_7 & \lambda_4 \end{pmatrix}$$

$\mathrm{wmlt}(G) = 2,$
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Buhl, 1993

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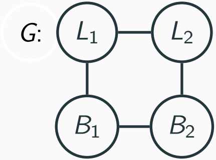

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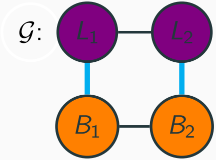

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$\mathrm{wmlt}(\mathcal{G}) = 1$,
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Uhler, 2012

Colored Gaussian graphical models

$G = (V, E)$ graph with vertex set $V = [m]$,
$\lambda : V \sqcup E \twoheadrightarrow [d]$ coloring of the vertices and edges of G for some $d \in \mathbb{N}$,
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$\mathcal{G}$:

$$\mathcal{L}_{\mathcal{G}} = \left\{ \begin{pmatrix} \lambda_1 & \lambda_2 \\ \lambda_2 & \lambda_1 \end{pmatrix} \in \mathrm{Sym}(2) \mid \lambda_1, \lambda_2 \in \mathbb{R} \right\}$$

Existence of the maximum likelihood estimate

$S = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^t$ sample covariance matrix, $x_1, \ldots, x_n \in \mathbb{R}^m$.

MLE for the covariance matrix $\hat{\Sigma} = \left(\hat{K}\right)^{-1}$

$$\hat{K} = \begin{array}{cc} \text{arg max}_K & \log\det K - \langle S, K\rangle, \\ \text{subject to} & K \in \mathcal{K}_G \end{array} \qquad \langle S, K\rangle := \mathrm{tr}(SK) = \sum_{1\le i,j\le m} s_{ij}k_{ij}$$

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Sufficient statistics:

$$\begin{array}{rccc} \pi_{\mathcal{G}}: & \mathrm{Sym}(m) & \longrightarrow & \mathbb{R}^d \\ & S & \longmapsto & (\langle S, K_1\rangle, \ldots, \langle S, K_d\rangle) \end{array}$$

$K_1, \ldots, K_d$ basis of $\mathcal{L}_G$

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$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ basis of $\mathcal{L}_G$

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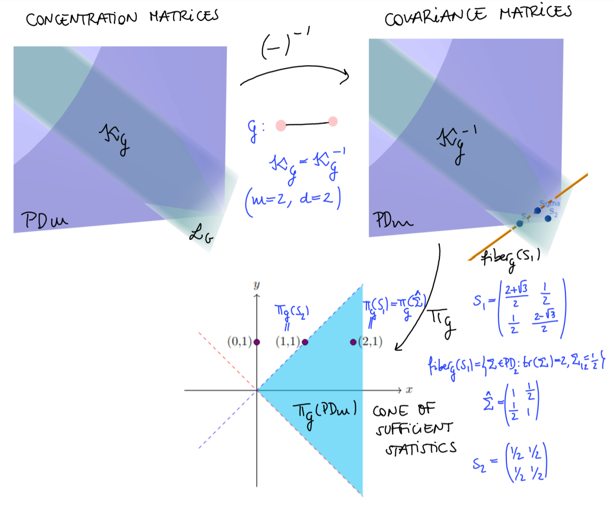
Theorem The MLE $\hat{\Sigma}$ exists for a sample covariance matrix S iff

$$\text{fiber}_{\mathcal{G}}(S) := \{\Sigma \in \mathrm{PD}_m \mid \pi_{\mathcal{G}}(\Sigma) = \pi_{\mathcal{G}}(S)\} \neq \emptyset.$$

Then the MLE $\hat{\Sigma}$ is the unique matrix in $\text{fiber}_{\mathcal{G}}(S)$ such that $\hat{\Sigma}^{-1} \in \mathcal{K}_G$.


CONCENTRATION MATRICES
COVARIANCE MATRICES
PDm
PDm
(0,1)
(1,1)
(2,1)
CONE OF SUFFICIENT STATISTICS

An algebraic relaxation: the generic completion rank

Let $\mathcal{G}$ be a colored graph on $[m]$. The *generic completion rank* $\mathrm{gcr}(\mathcal{G})$ is the smallest n such that $\dim \pi_{\mathcal{G}}(\mathrm{Sym(m, n)}) = d$.

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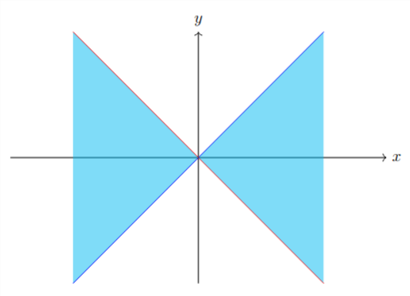

Figure 1: $\pi_{\mathcal{G}}(\mathrm{Sym}(2, 1))$ for the 2-cycle with a single vertex color.

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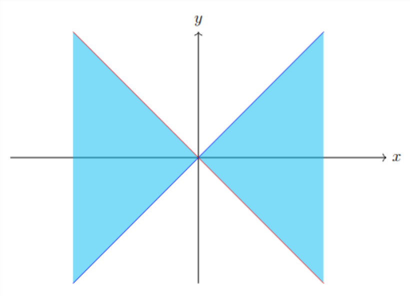

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Theorem (Uhler, 2012) $\mathrm{mlt}(\mathcal{G}) \leq \mathrm{gcr}(\mathcal{G})$

Matrix completion problems

For $S = \begin{pmatrix} s_{11} & 1/2 \\ 1/2 & s_{22} \end{pmatrix}$, the MLE is $\hat{\Sigma} = \begin{pmatrix} \mathrm{tr}(S)/2 & 1/2 \\ 1/2 & \mathrm{tr}(S)/2 \end{pmatrix}$ if it exists.

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Positive definite completions:

- $\mathrm{tr}(S) = 2$: $\text{fiber}_{\mathcal{G}}(S) = \left\{ \begin{pmatrix} 1 \pm a & 1/2 \\ 1/2 & 1 \mp a \end{pmatrix} : 0 \leq a < \sqrt{3}/2 \right\}$
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Matrix completion problems

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Low rank completions (rank 1):

- $\mathrm{tr}(S) = 2$: $\begin{pmatrix} (2 \pm \sqrt{3})/2 & 1/2 \\ 1/2 & (2 \mp \sqrt{3})/2 \end{pmatrix}$
- $\mathrm{tr}(S) = 1$: $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$
- $\mathrm{tr}(S) = 0$: no real rank 1 completion but $\begin{pmatrix} \pm i/2 & 1/2 \\ 1/2 & \mp i/2 \end{pmatrix}$

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- Trivial case: If $\mathrm{gcr}(\mathcal{G}) = 1$, then $\mathrm{mlt}(\mathcal{G}) = 1$.

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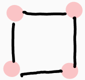

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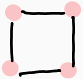

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  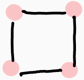

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  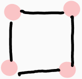

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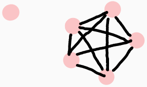
  Question posed in the uncolored setting by Bleckherman-Sinn

  If $\mathcal{G}$ is the disjoint union of a vertex and an m-complete graph with $|\Lambda(V)| = 1$ and $|\Lambda(E)| = |E|$,

  - $\mathrm{gcr}(\mathcal{G}) \geq \lceil (m-2)/2 \rceil$,
  - $\mathrm{mlt}(\mathcal{G}) = 1$.

Which colorings give $\mathrm{gcr}(\mathcal{G}) = 1$?

For $i \in V$ and $c \in \Lambda(E)$, $N(i, c) := \{j \in V \mid \lambda(i, j) = c\} \subset N(i)$.

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MLE existence via the ideal of the projection

Ideal of the projection via $\pi_{\mathcal{G}}$ of rank n matrices:

$$I_{\mathcal{G},n} := \left(I_{n+1}(S) + \left\langle \{t_i - \langle S, K_i \rangle\}_{1 \leq i \leq d} \right\rangle \right) \cap \mathbb{R}[t_1, \ldots, t_d].$$

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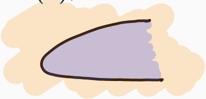

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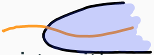

4-cycle with single vertex color for $n = 1$

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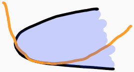
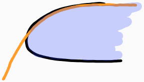


$\mathrm{mlt}(\mathcal{G}) > n$, $\mathrm{wmlt}(\mathcal{G}) \le n$

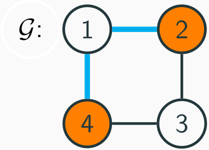
3-cycle with single vertex color for $n = 1$

- ...never exists $\mathrm{mlt}(\mathcal{G}) \ge \mathrm{wmlt}(\mathcal{G}) > n$



3-cycle with two vertex color for $n = 1$

Computing MLT via elimination ideal - an example



Sufficient statistics: $t_1 = s_{1,1}$,
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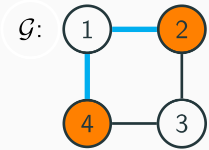

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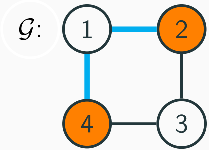

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Cholesky decomposition $S = LL^t$:

$$\begin{aligned} f_2(l_{ij}) = 4(-l_{13}l_{22} + l_{12}l_{23})^2 + 4(l_{12}l_{33})^2 + 4(-l_{14}l_{23} + l_{13}l_{24})^2 \\ + 4(-l_{14}l_{33} + l_{13}l_{34})^2 + 4(l_{13}l_{44})^2 + 4(l_{22}l_{33})^2 \\ + 4(-l_{24}l_{33} + l_{23}l_{34})^2 + 4(l_{23}l_{44})^2 + 4(l_{33}l_{44})^2 > 0. \end{aligned}$$

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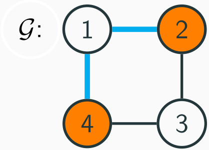

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$$I_{\mathcal{G},1} = \langle t_3 t_4^2 - t_1 t_5^2 - 2t_1 t_5 t_6 - t_1 t_6^2, 4t_2 t_3 - t_5^2 - t_6^2 \rangle.$$

Cholesky decomposition $S = LL^t$:

$$\begin{aligned} f_2(l_{ij}) = {} & 4(-l_{13}l_{22} + l_{12}l_{23})^2 + 4(l_{12}l_{33})^2 + 4(-l_{14}l_{23} + l_{13}l_{24})^2 \\ & + 4(-l_{14}l_{33} + l_{13}l_{34})^2 + 4(l_{13}l_{44})^2 + 4(l_{22}l_{33})^2 \\ & + 4(-l_{24}l_{33} + l_{23}l_{34})^2 + 4(l_{23}l_{44})^2 + 4(l_{33}l_{44})^2 > 0. \end{aligned}$$

$$\mathrm{wmlt}(\mathcal{G}) = \mathrm{mlt}(\mathcal{G}) = \mathrm{gcr}(\mathcal{G}) = 2$$

Reinterpretation of thresholds: generalizing Bleckherman-Sinn

generic completion rank

Theorem The maximum likelihood threshold of $\mathcal{G}$ is the smallest

weak maximum likelihood threshold

$\mathcal{L}_{\mathcal{G}}$

n for which there is no matrix $K \neq 0$ in $\mathcal{L}_{\mathcal{G}} \cap \mathrm{PSD}_m$ such that

$\mathcal{L}_{\mathcal{G}} \cap \mathrm{PSD}_m$

some l.i.

$x_i \in \ker(K)$ for generic observations $x_1, \ldots, x_n \in \mathbb{R}^m$.

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$$I_{\mathcal{G}} := \langle \{(y_1 \; \ldots \; y_m) K_i (y_1 \; \ldots \; y_m)^t\}_{d+1<i\leq m(m-1)/2} \rangle, \; R := \mathbb{R}[y_1, \ldots, y_m]/I_{\mathcal{G}},$$

$K_{d+1}, \ldots, K_{m(m-1)/2}$ basis of $\mathcal{L}_G^\perp$

$\ell_i = x_i^{(1)} y_1 + \cdots + x_i^{(m)} y_m \in R_1$ for some $x_i^{(j)} \in \mathbb{R}$

$\langle \ell_1, \ldots, \ell_n \rangle_2 \in R_2 \simeq \mathrm{Sym}(m)/\mathcal{L}_{\mathcal{G}}^\perp$,

$x_i = \left(x_i^{(1)}, \ldots, x_i^{(m)} \right)^t \in \mathbb{R}^m$.

4-cycle with a single vertex color

Proposition (H., Kuznetsova, Stolz 25+)
If $\mathcal{G}$ is a colored *m*-cycle with $|\Lambda(V)| = 1$, then $\mathrm{gcr}(\mathcal{G}) = 2$.

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  - Rewrite $K(a_1 \dots a_m)^t = 0$ as $A\left(\lambda_1 \dots \lambda_{m+1}\right)^t = 0$.
  - If $a_1 \neq 0$, $\left(\sum_i^m (-1)^{i+1} a_i^2\right)\lambda_1 = 0$ for m even: $\lambda_1 = 0$.

Summary of techniques

For gcr:

- Compute ideal of the projection.

For mlt or wmlt:

- Studying the sign of the generators of the ideal of the projection.
- Studying the algebraic boundary of the cone of sufficient statistics.

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Local persistence homology

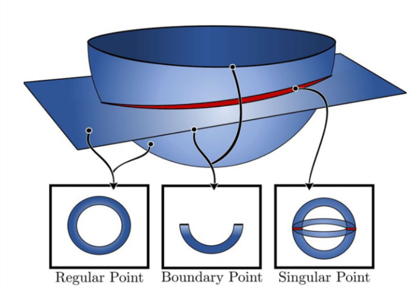
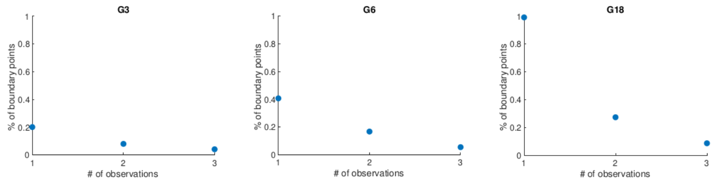


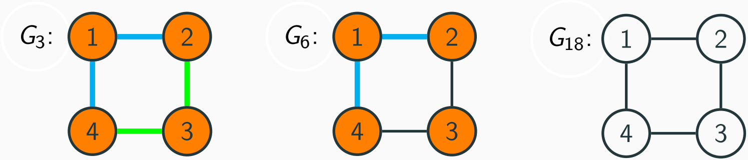
Figure 2: *Geometric anomaly detection in data*, Bernadette Stolz et al. PNAS (2020)

Performance



(A) Dim 1 homology (B) Dim 1&2 homology (C) Dim 2 homology

Figure 3: Percentage of boundary points in two colored 4-cycles and the uncolored 4-cycle. Points with less than 4 neighbours in their annular neighbourhoods are excluded.



$\text{wmlt}(G_3) = \text{mlt}(G_3) = 1$ $\text{wmlt}(G_6) = \text{mlt}(G_6) = 1$ $\text{wmlt}(G_{18}) = 2, \text{mlt}(G_{18}) = 3$

Thanks a lot!
Moltes gràcies!