ZUSE INSTITUTE
BERLIN

## Leveraging Combinatorial Symmetries in Flag Algebra-based SDP Formulations

Workshop on Recent Advances in Optimization, Fields Institute, CA

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6th of December 2022



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Tibor Szabó FU Berlin

## Combinatorial Symmetries in Flag Algebras

1. What are we interested in?
2. Where does Optimization come in?
3. Where can we go from here?
4. What are we interested in?

The Ramsey Multiplicity Problem
Theorem (Ramsey 1930)
For any $t \in \mathbb{N}$ there exists $R_{t, t} \in \mathbb{N}$ such that any 2-edge-coloring of the complete graph of order at least $R_{t, t}$ contains a monochromatic clique of size $t$.

## A well-known question:

Can we determine $R_{t_{1}, \ldots, t_{c}}$ ?

## A related question:

How many cliques do we need to have?

Letting $\chi: E\left(K_{n}\right) \rightarrow[c]$ denote a coloring of the complete graph, $\chi_{i}$ the graph given by color $i$ and $k_{t_{i}}\left(\chi_{i}\right)$ count all $t_{i}$-cliques in that color, we want to determine

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m_{t_{1}, \ldots, t_{c}}(n)=\min _{\chi} m_{t_{1}, \ldots, t_{c}}(\chi)=\min _{\chi} \frac{k_{t_{1}}\left(\chi_{1}\right)}{\binom{n}{t_{1}}}+\ldots \frac{k_{t_{c}}\left(\chi_{c}\right)}{\binom{n}{t_{c}}}
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The Ramsey Multiplicity Problem
Theorem (Ramsey 1930 - Multicolor Version)
For any $t_{1}, \ldots, t_{c} \in \mathbb{N}$ there exists $R_{t_{1}, \ldots, t_{c}} \in \mathbb{N}$ s.t. any c-edge-coloring of $K_{n}$ with $n \geq R_{t_{1}, \ldots, t_{c}} \in \mathbb{N}$ contains an clique of size $t_{i}$ with edges colored $i$ for some $1 \leq i \leq c$.

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## A connection to Ramsey Multiplicity Numbers

The two questions are related through the following inequality:

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\begin{equation*}
m_{t_{1}, \ldots, t_{c}}=\lim _{n \rightarrow \infty} m_{t_{1}, \ldots t_{c}}(n) \leq\left(R_{t_{1}, \ldots, t_{c-1}}-1\right)^{1-t_{c}} . \tag{1}
\end{equation*}
$$

Proof Write $R=R_{t_{1}, \ldots, t_{c-1}}$ and let $\chi$ be an extremal $c-1$-coloring of $K_{R-1}$.
Consider the sequence of $c$-colorings $\chi_{m}$ of $K_{m(R-1)}$ obtained by replacing each $v \in[R-1]$ by $m$ copies $v_{1}, \ldots, v_{m}$ and setting $\chi_{m}\left(v_{i} w_{j}\right)=\chi(v w)$. The edges $v_{i} v_{j}$ get colored with the additional color $c$.

The graphs $\chi_{m}^{i}$ avoid cliques of size $t_{i}$ for $1 \leq i \leq c-1$ and each of the $m$ large cliques in $\chi_{m}^{c}$ contains exactly an $(R-1)^{-t_{c}}$ proportion of all possible $t_{c}$-cliques.

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Proof Sketch Blow up $\chi$ while using the additional color $c$ for the cliques.

## Theorem (Goodman 1959)

Exact characterization of $m_{3,3}(n)$ for all $n \in \mathbb{N}$ implying $m_{3,3}=1 / 4=\left(R_{3}-1\right)^{1-3}$.

Proof Sketch The upper bound follows from Equation (1). The matching lower bound follows through double counting argument and an application of Cauchy-Schwarz.

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## Fixing two colors and growing the size of cliques

When $c=2$ and $t_{1}=t_{2}=t$, we have $R_{t}=t$ and a uniform random coloring beats (1).

## Conjecture (Erdős 1962)

$\square$
$m_{t, t}(n)=2^{1-\binom{t}{2}}$ for any $t \in \mathbb{N}$. False for $t \geq 4$ (Thomason 1989)

Theorem (Thomason 1989)
$m_{4,4} \leq 0.03050$ and $m_{5,5} \leq 0.001770$.

```
Theorem (Giraud 1976)
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m_{4,4} \geq 0.02172
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## Theorem (Parczyk, Pokutta, S., Szabó 2022)

$m_{3,4}=689 / 3^{8}$ and the extremal constructions are based on the Schläfli graph.

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Theorem (Thomason 1997)
$m_{4,4} \leq 0.03032$ and $m_{5,5} \leq 0.001721$.

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Theorem (Even-Zohar, Linial 2016)
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Theorem (Parczyk, Pokutta, S., Szabó 2022)
$m_{4,4} \leq 0.03013$ and $m_{5,5} \leq 0.001707$.

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Theorem (Sperfeld / Niess 2011)
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Fixing triangles and growing the number of colors
Theorem (Goodman 1959)
$m_{3,3}=1 / 4=1 /\left(R_{3}-1\right)^{2}$ and there are many extremal constructions.

Theorem (Cummings et al. 2013)
$m_{3,3,3}=1 / 25=1 /\left(R_{3,3}-1\right)^{2}$ and the only extremal constructions are based on $R_{3,3}$.

## Theorem (Kiem, Pokutta, S. 2022 + )

$m_{3,3,3,3}=1 / 256=1 /\left(R_{3,3,3}-1\right)^{2}$

Open Problem: $\quad m_{3, \ldots, 3}=\left(R_{3, \ldots, 3}-1\right)^{-2}$ for all $c$ or $m_{3, \ldots, 3} \cdot\left(R_{3, \ldots, 3}-1\right)^{2}=o(1)$ ?

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4. Where does Optimization come in?

## Upper bounds through Discrete Optimization

Using blow-ups, we can derive an upper bound for $m_{t_{1}, \ldots, t_{c}}$ from any coloring

$$
\chi: E\left(K_{n}\right) \cup\{n\} \rightarrow[c]
$$

of the looped complete graph through

$$
m_{t_{1}, \ldots, t_{c}} \leq m_{t_{1}, \ldots, t_{c}}^{\prime}(\chi)=\frac{k_{t_{1}}^{\prime}\left(\chi_{1}\right)}{n^{t_{1}}}+\ldots+\frac{k_{t_{c}}^{\prime}\left(\chi_{c}\right)}{n^{t_{c}}}
$$

where $k_{t_{i}}^{\prime}\left(\chi_{i}\right)$ counts not necessarily injective copies of $t_{i}$-cliques in $\chi_{i}$.
So we have found a discrete optimization problem! How to solve it?

## Approach 0. Check some obvious existing constructions.

2. Where does Optimization come in?

## Upper bounds through Discrete Optimization

Using blow-ups, we can derive an upper bound for $m_{t_{1}, \ldots, t_{c}}$ from any coloring

$$
\chi: E\left(K_{n}\right) \cup\{n\} \rightarrow[c]
$$

of the looped complete graph through

$$
m_{t_{1}, \ldots, t_{c}} \leq m_{t_{1}, \ldots, t_{c}}^{\prime}(\chi)=\frac{k_{t_{1}}^{\prime}\left(\chi_{1}\right)}{n^{t_{1}}}+\ldots+\frac{k_{t_{c}}^{\prime}\left(\chi_{c}\right)}{n^{t_{c}}}
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Approach 1 Check colorings $\chi$ exhaustively.
2. Where does Optimization come in?

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Using blow-ups, we can derive an upper bound for $m_{t_{1}, \ldots, t_{c}}$ from any coloring

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where $k_{t_{i}}^{\prime}\left(\chi_{i}\right)$ counts not necessarily injective copies of $t_{i}$-cliques in $\chi_{i}$.
So we have found a discrete optimization problem! How to solve it?
Approach 1.5 Check colorings $\chi$ exhaustively up to isomorphism.
2. Where does Optimization come in?

## Upper bounds through Discrete Optimization

Using blow-ups, we can derive an upper bound for $m_{t_{1}, \ldots, t_{c}}$ from any coloring

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So we have found a discrete optimization problem! How to solve it?
Approach 2 Bounded Tree search taking the parameter into account.
2. Where does Optimization come in?

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So we have found a discrete optimization problem! How to solve it?
Approach 3 Search Heuristics $\rightarrow$ upper bounds for $m_{4,4}, m_{5,5}$ and $m_{3,4}$
2. Where does Optimization come in?

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Using blow-ups, we can derive an upper bound for $m_{t_{1}, \ldots, t_{c}}$ from any coloring

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So we have found a discrete optimization problem! How to solve it?
Approach 4? Good source of benchmark problems...
2. Where does Optimization come in?

## Lower bounds through Semidefinite Programming

Razborov (2007) introduced Flag Algebras to study the limits of discrete objects. They allow one to apply a Cauchy-Schwarz-argument by solving a concrete SDP formulation.

Can be seen as an improvement over a trivial computational bound:

Letting $d_{\varphi}(\chi)$ denote the density of $\varphi$ in $\chi$, double counting gives us

$$
m_{t_{1}, \ldots, t_{c}}(\chi)=\sum_{\varphi \text { of order } N} d_{\varphi}(\chi) m_{t_{1}, \ldots, t_{c}}(\varphi)
$$

for $t_{1}, \ldots, t_{c} \leq N \leq v(\chi)$. This implies a trivial lower bound of

$$
m_{t_{1}, \ldots, t_{c}} \geq \min _{\varphi \text { of order } N} m_{t_{1}, \ldots, t_{c}}(\varphi) .
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## Lower bounds through Semidefinite Programming

Razborov (2007) introduced Flag Algebras to study the limits of discrete objects. They allow one to apply a Cauchy-Schwarz-argument by solving a concrete SDP formulation. Can be seen as an improvement over a trivial computational bound:

Letting $D_{\varphi}$ denote a particular, computable matrix of density values, any $Q \succeq 0$ satisfies

$$
\sum_{\varphi} d_{\varphi}(\chi)\left\langle Q, D_{\varphi}\right\rangle \leq O(1 / v(\chi))
$$

for any coloring $\chi$. This implies the following strengthening:

$$
\begin{equation*}
m_{t_{1}, \ldots, t_{c}} \geq \max _{\boldsymbol{Q} \succeq 0} \min _{\varphi \text { of order } N} m_{t_{1}, \ldots, t_{c}}(\varphi)-\left\langle\boldsymbol{Q}, \boldsymbol{D}_{\varphi}\right\rangle \tag{2}
\end{equation*}
$$

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2. Where does Optimization come in?

## Leveraging Symmetries

Increasing $N$ both improves the bound and makes the SDP more difficult to solve:

| $N$ | value | time | memory |
| :--- | :--- | :--- | :--- |
| 6 | 0.02875 | $0.2 \mathrm{~s} \pm 0.0$ | $81.2_{\mathrm{MB}} \pm 24.7$ |
| 7 | 0.02918 | $4.9 \mathrm{~s} \pm 0.1$ | $126.9_{\mathrm{MB} \pm 26.3}$ |
| 8 | 0.02942 | $1.8 \mathrm{~h} \pm 0.1$ | $1.8 \mathrm{~GB} \pm 0.0$ |
| 9 | $? ? ?$ | - | - |

Table: Complexity of SDP problem formulations for $m_{4,4}$ using CSDP

How can we use combinatorial information to reduce these SDP formulations?
2. Where does Optimization come in?

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| baseline |  |  |  | ours |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $N$ | value | time | memory | time | memory |
| 6 | 0.02875 | $0.2 \mathrm{~s}_{ \pm 0.0}$ | $81.2_{\mathrm{MB}}^{ \pm 24.7}$ | $0.2 \mathrm{~s}_{ \pm 0.0}$ | $69.8 \mathrm{MB} \pm 25.1$ |
| 7 | 0.02918 | $4.9 \mathrm{~s}_{ \pm 0.1}$ | $126.9_{\mathrm{MB}} \pm 26.3$ | $2.4 \mathrm{~s}_{ \pm 0.0}$ | $100.7 \mathrm{MB} \pm 28.0$ |
| 8 | 0.02942 | $1.8 \mathrm{~h} \pm 0.1$ | $1.8 \mathrm{~GB} \pm 0.0$ | $0.3 \mathrm{~h}_{ \pm 0.0}$ | $642 . \mathrm{MB}^{2} \pm 18.1$ |
| 9 | $\mathbf{0 . 0 2 9 6 1}$ | - | - | weeks | less than 1.5 TB |

Table: Complexity of SDP problem formulations for $m_{4,4}$ using CSDP

How can we use combinatorial information to reduce these SDP formulations?
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## Leveraging Symmetries

Increasing $N$ both improves the bound and makes the SDP more difficult to solve:

| baseline |  |  |  | ours |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $N$ | value | time | memory | time | memory |
| 4 | 0.0 | $0.06 \mathrm{~s} \pm 0.0$ | $79.39 \mathrm{MB} \pm 21.0$ | $0.02 \mathrm{~s} \pm 0.0$ | $3.61 \mathrm{MB} \pm 0.0$ |
| 5 | 0.002938 | $1.5 \mathrm{~m} \pm 0.0$ | $1.1 \mathrm{~GB} \pm 0.0$ | $1.1 \mathrm{~s} \pm 0.0$ | $86.9 \mathrm{MB} \pm 22.8$ |
| 6 | $\mathbf{0 . 0 0 3 9 0 6}$ | - | - | 1 day | less than 128GB |

Table: Complexity of SDP problem formulations for $m_{3,3,3,3}$ using CSDP

How can we use combinatorial information to reduce these SDP formulations?

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2. Where does Optimization come in?

## Leveraging Symmetries

How can we use combinatorial information to reduce these SDP formulations?
Observation The $D_{\varphi}$ have a block-diagonal structure with many symmetries.


Figure: The SDP formulation for $m_{3,3}$

Method 1 Reduce the number of constraints and blocks by combining constraints.
Method 2 Reduce the number of variables by block diagonalization.
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## Leveraging Symmetries

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Observation The $D_{\varphi}$ have a block-diagonal structure with many symmetries.

$$
\max _{Q \succeq 0} \min \left\{1-\left\langle Q,\left(\begin{array}{ll}
1 & 0 \\
0 & 0
\end{array}\right)\right\rangle,-\left\langle Q,\binom{1 / 31 / 3}{1 / 3}\right\rangle,-\left\langle Q,\left(\begin{array}{cc}
0 & 1 / 3 \\
1 / 3 & 1 / 3
\end{array}\right)\right\rangle, 1-\left\langle Q,\left(\begin{array}{ll}
0 & 0 \\
0 & 1
\end{array}\right)\right\rangle\right\},
$$

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## Leveraging Symmetries

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$$
\max _{Q \succeq 0} \min \left\{1-\left\langle Q,\left(\begin{array}{cc}
1 / 2 & 0 \\
0 & 1 / 2
\end{array}\right)\right\rangle,-\left\langle Q,\left(\begin{array}{c}
1 / 6 \\
1 / 3 / 3 \\
1 / 6
\end{array}\right)\right\rangle\right\},
$$

Figure: The SDP formulation for $m_{3,3}$

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## Leveraging Symmetries

How can we use combinatorial information to reduce these SDP formulations?
Observation The $D_{\varphi}$ have a block-diagonal structure with many symmetries.

$$
\max _{x, y \geq 0} \min \left\{1-\frac{x}{2}-\frac{y}{2},-\frac{x}{2}+\frac{y}{6}\right\} .
$$

Figure: The SDP formulation for $m_{3,3}$

Method 1 Reduce the number of constraints and blocks by combining constraints.
Method 2 Reduce the number of variables by block diagonalization.

1. What are we interested in?
2. Where does Optimization come in?
3. Where can we go from here?
4. Where can we go from here?

## Outlook

We have...
...optimized the computation and formulation of the SDP problems.

Can we...
...improve the solution process
and extend the approach to new domains?

Thank you for your attention!

