## Fully <br> Computer-Assisted Proofs in Extremal Combinatorics

37th AAAI Conference on Artificial Intelligence Christoph Spiegel (Zuse Institute Berlin)

February 2023



Olaf Parczyk<br>Freie Universität Berlin



Sebastian Pokutta Zuse Institute Berlin


Tibor Szabó
Freie Universität Berlin

Research partially funded through Math+ project EF1-12

## Computer-Assisted Proofs in Combinatorics

1. The Ramsey Multiplicity Problem
2. Search Heuristics for Constructive Bounds
3. Beyond the Ramsey multiplicity of quadrangles

Theorem (Ramsey 1930)
For any $s, t \in \mathbb{N}$ there exists $R_{s, t} \in \mathbb{N}$ such that any graph of order at least $R_{s, t}$ contains either a clique of size $s$ or an independent set of size $t$.

A well-known question
Can we determine the Ramsey numbers $R_{s, t}$ or their asymptotic behavior?

A related question
How many cliques and independent sets do we need to have?

Theorem (Goodman 1959 - asymptotic version)
Asymptotically at least $1 / 4$ of all triangles are either cliques or independent sets.
There has been little progress towards an answer for any $\{s, t\} \neq\{3\}$

Theorem (Ramsey 1930)
For any $s, t \in \mathbb{N}$ there exists $R_{s, t} \in \mathbb{N}$ such that any graph of order at least $R_{s, t}$ contains either a clique of size $s$ or an independent set of size $t$.

## A well-known question

Can we determine the Ramsey numbers $R_{s, t}$ or their asymptotic behavior?

A related question
How many cliques and independent
sets do we need to have?

Theorem (Goodman 1959 - asymptotic version)
Asymptotically at least $1 / 4$ of all triangles are either cliques or independent sets.
There has been little progress towards an answer for any $\{s, t\} \neq\{3\}$

Theorem (Ramsey 1930)
For any $s, t \in \mathbb{N}$ there exists $R_{s, t} \in \mathbb{N}$ such that any graph of order at least $R_{s, t}$ contains either a clique of size $s$ or an independent set of size $t$.

## A well-known question

Can we determine the Ramsey numbers $R_{s, t}$ or their asymptotic behavior?

## A related question

How many cliques and independent
sets do we need to have?

Theorem (Goodman 1959 - asymptotic version)
Asymptotically at least $1 / 4$ of all triangles are either cliques or independent sets.
There has been little progress towards an answer for any $\{s, t\} \neq\{3\}$

## 1. The Ramsey Multiplicity Problem

## The Ramsey Multiplicity Problem

Theorem (Ramsey 1930)
For any $s, t \in \mathbb{N}$ there exists $R_{s, t} \in \mathbb{N}$ such that any graph of order at least $R_{s, t}$ contains either a clique of size $s$ or an independent set of size $t$.

## A well-known question

Can we determine the Ramsey numbers $R_{s, t}$ or their asymptotic behavior?

## A related question

How many cliques and independent
sets do we need to have?

Theorem (Goodman 1959 - asymptotic version)
Asymptotically at least $1 / 4$ of all triangles are either cliques or independent sets.

There has been little progress towards an answer for any $\{s, t\} \neq\{3\}$

## 1. The Ramsey Multiplicity Problem

## The Ramsey Multiplicity Problem

## Theorem (Ramsey 1930)

For any $s, t \in \mathbb{N}$ there exists $R_{s, t} \in \mathbb{N}$ such that any graph of order at least $R_{s, t}$ contains either a clique of size $s$ or an independent set of size $t$.

## A well-known question

Can we determine the Ramsey numbers $R_{s, t}$ or their asymptotic behavior?

## A related question

How many cliques and independent
sets do we need to have?

Theorem (Goodman 1959 - asymptotic version)
Asymptotically at least $1 / 4$ of all triangles are either cliques or independent sets.
There has been little progress towards an answer for any $\{s, t\} \neq\{3\}$.

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of $s$-cliques in $G$.

## Problem (Ramsey Multiplicity)

What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?

So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

Conjecture (Erdős 1962)

```
m}\mp@subsup{m}{t,t}{}=\mp@subsup{2}{}{1-(\begin{array}{c}{t}\\{2}\end{array})}\mathrm{ for any }t\geq2
    False for t\geq4 (Thomason 1989)
```

How can we use computers to find bounds beyond human intuition?

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.
Problem (Ramsey Multiplicity)
What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

## Conjecture (Erdós 1962)

$$
m_{t, t}=2^{1-\binom{t}{2}} \text { for any } t \geq 2 .
$$

$\square$

How can we use computers to find bounds beyond human intuition?

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.

## Problem (Ramsey Multiplicity)

What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

## Conjecture (Erdós 1962)

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.

## Problem (Ramsey Multiplicity)

What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

## Conjecture (Erdős 1962)

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.

## Problem (Ramsey Multiplicity)

What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

Conjecture (Erdős 1962)

$$
m_{t, t}=2^{1-\binom{t}{2}} \text { for any } t \geq 2 .
$$

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of $s$-cliques in $G$.
Problem (Ramsey Multiplicity)
What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

Conjecture (Erdős 1962)
$m_{t, t}=2^{1-\binom{t}{2}}$ for any $t \geq 2$.
False for $t \geq 4$ (Thomason 1989)

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.
Problem (Ramsey Multiplicity)
What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

Conjecture (Erdős 1962)
$m_{t, t}=2^{1-\binom{t}{2}}$ for any $t \geq 2$.
False for $t \geq 4$ (Thomason 1989)

How can we use computers to find bounds beyond human intuition?

## Beyond Goodman's Result

Notation. Let $\mathcal{G}_{n}$ denote all graphs of order $n$ and $k_{s}(G)$ the fraction of s-cliques in $G$.
Problem (Ramsey Multiplicity)
What is the value of $m_{s, t}=\lim _{n \rightarrow \infty} \min _{G \in \mathcal{G}_{n}} k_{s}(G)+k_{t}(\bar{G})$ ?
So far studied for $s=t$, though recently Behague et al. (2022+) also considered the off-diagonal case. For $s, t=3$ tight upper bound given by the binomial random graph.

Conjecture (Erdős 1962)
$m_{t, t}=2^{1-\binom{t}{2}}$ for any $t \geq 2$.
False for $t \geq 4$ (Thomason 1989)

How can we use computers to find constructive bounds beyond human intuition?

## Computer-Assisted Proofs in Combinatorics

1. The Ramsey Multiplicity Problem
2. Search Heuristics for Constructive Bounds
3. Beyond the Ramsey multiplicity of quadrangles
4. Search Heuristics for Constructive Bounds

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=U_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in $G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}(\overline{G \times m})=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Corollary (Relating Ramsey numbers and Ramsey multiplicity)
By blowing up Ramsey graphs, we get $m_{s, t} \leq\left(R_{s, t}-1\right)^{1-t}$
2. Search Heuristics for Constructive Bounds

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in G. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}(\overline{G \times m})=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Corollary (Relating Ramsey numbers and Ramsey multiplicity)
By blowing up Ramsey graphs, we get $m_{s, t} \leq\left(R_{s, t}-1\right)^{1-t}$

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in $G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}(G \times m)=k_{s}^{0}(G)+k_{t}^{0}(\bar{G})$.

Corollary (Relating Ramsey numbers and Ramsey multiplicity)
By blowing up Ramsey graphs, we get $m_{s, t} \leq\left(R_{s, t}-1\right)^{1-t}$.

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
$G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.
Corollary (Relating Ramsey numbers and Ramsey multiplicity)
By blowing up Ramsey graphs, we get $m_{s, t} \leq\left(R_{s, t}-1\right)^{1-t}$

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The m-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
G. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Corollary (Relating Ramsey numbers and Ramsey multiplicity)
By blowing up Ramsey graphs, we get $m_{s, t} \leq\left(R_{s, t}-1\right)^{1-t}$.

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

Proposition (Bounds from any graph)
We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The m-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in $G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Question: How can we find better candidates for $G$ ?

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

Proposition (Bounds from any graph)
We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
$G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}(\overline{G \times m})=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

## Theorem (Thomason 1989)

$m_{4,4} \leq 0.3050$ and $m_{5,5} \leq 0.001770$.

Explicit by-hand construction with local search improvements.

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

Proposition (Bounds from any graph)
We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
$G$. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Theorem (Franek and Rödl 1993)
$m_{4,4} \leq 0.03052$ (not an improvement)

Exhaustive search over specific powerset constructions.

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The m-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
G. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

## Theorem (Thomason 1997)

$m_{4,4} \leq 0.03031$ and $m_{5,5} \leq 0.001720$.

Exhaustive search over small XOR graph products.

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
G. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Theorem (Even-Zohar and Linial '15)
$m_{4,4} \leq 0.03028$.

Iterating the construction of Thomason (1997).

## How to blow up graphs

Notation. Let $\mathcal{G}_{n}^{\circ}$ denote all possibly looped graphs of order $n$ and $k_{s}^{\circ}(G)$ the fraction of not nec. injective maps from $K_{s}$ to $G$ that are strong graph homomorphisms.

## Proposition (Bounds from any graph)

We have $m_{s, t} \leq k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for any $G \in \mathcal{G}^{\circ}=\bigcup_{n} \mathcal{G}_{n}^{\circ}$.
Proof. The $m$-fold blow-up $G^{\times m} \in \mathcal{G}_{n m}$ of $G$ is obtained by replacing each vertex $v$ in $G$ with $m$ copies $v_{1}, \ldots, v_{m}$ and connecting $v_{i}$ with $w_{j}$ in $G^{\times m}$ if $v$ is adjacent to $w$ in
G. By definition $m_{s, t} \leq \lim _{m \rightarrow \infty} k_{s}\left(G^{\times m}\right)+k_{t}\left(\overline{G^{\times m}}\right)=k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$.

Theorem (Parczyk, Pokutta, S., and Szabó 2022+)
$m_{4,4} \leq 0.03012$ and $m_{5,5} \leq 0.001707$.

Search heuristics over Cayley graph search space ...

## Constructing graphs through search heuristics

We phrased the problem through binary representations and applied Metaheuristics, i.e., Simulated Annealing (Kirkpatrick et al. 1983) and Tabu search (Glover 1986):

For any binary vector $\mathbf{x}=\left(x_{1}, \ldots, x_{\binom{n}{2}+n}\right) \in\{0,1\}^{\binom{n}{2}+n}$ let the graph $G_{\mathbf{x}} \in \mathcal{G}_{n}^{\circ}$ be given by connecting any two vertices $1 \leq i \leq j \leq n$ if $x_{\binom{j}{2}+i}=1$. We want to determine

$$
\begin{equation*}
\min _{x} k_{s}^{\circ}\left(G_{x}\right)+k_{t}^{\circ}\left(\overline{G_{x}}\right) \tag{1}
\end{equation*}
$$

## Disadvantages. Problem structure is ignored. No guarantees of optimality.

Advantages. Applicable to many problems. Optimality through matching bounds.
SA and TS have previously proven successful in finding Ramsey numbers. Recently learning-based approaches have also been suggested (Wagner 2021; Bello et al. 2016).

## Constructing graphs through search heuristics

We phrased the problem through binary representations and applied Metaheuristics, i.e., Simulated Annealing (Kirkpatrick et al. 1983) and Tabu search (Glover 1986):

For any binary vector $\mathbf{x}=\left(x_{1}, \ldots, x_{\binom{n}{2}+n}\right) \in\{0,1\}^{\binom{n}{2}+n}$ let the graph $G_{\mathbf{x}} \in \mathcal{G}_{n}^{\circ}$ be given by connecting any two vertices $1 \leq i \leq j \leq n$ if $x_{\binom{j}{2}+i}=1$. We want to determine

$$
\begin{equation*}
\min _{\mathrm{x}} k_{s}^{\circ}\left(G_{\mathrm{x}}\right)+k_{t}^{\circ}\left(\overline{G_{\mathrm{x}}}\right) . \tag{1}
\end{equation*}
$$

Disadvantages. Problem structure is ignored. No guarantees of optimality.
Advantages. Applicable to many problems. Optimality through matching bounds.
SA and TS have previously proven successful in finding Ramsey numbers. Recently learning-based approaches have also been suggested (Wagner 2021; Bello et al. 2016).

## Constructing graphs through search heuristics

We phrased the problem through binary representations and applied Metaheuristics, i.e., Simulated Annealing (Kirkpatrick et al. 1983) and Tabu search (Glover 1986):

For any binary vector $\mathbf{x}=\left(x_{1}, \ldots, x_{\binom{n}{2}+n}\right) \in\{0,1\} \begin{gathered}\binom{n}{2}+n \\ \text { let the graph } \\ G_{\mathbf{x}}\end{gathered} \in \mathcal{G}_{n}^{\circ}$ be given by connecting any two vertices $1 \leq i \leq j \leq n$ if $x_{\binom{j}{2}+i}=1$. We want to determine

$$
\begin{equation*}
\min _{\mathrm{x}} k_{s}^{\circ}\left(G_{\mathrm{x}}\right)+k_{t}^{\circ}\left(\overline{G_{\mathrm{x}}}\right) . \tag{1}
\end{equation*}
$$

Disadvantages. Problem structure is ignored. No guarantees of optimality.
Advantages. Applicable to many problems. Optimality through matching bounds.
SA and TS have previously proven successful in finding Ramsey numbers. Recently learning-based approaches have also been suggested (Wagner 2021; Bello et al. 2016).

## Constructing graphs through search heuristics

We phrased the problem through binary representations and applied Metaheuristics, i.e., Simulated Annealing (Kirkpatrick et al. 1983) and Tabu search (Glover 1986):

For any binary vector $\mathbf{x}=\left(x_{1}, \ldots, x_{\binom{n}{2}+n}\right) \in\{0,1\}^{\binom{n}{2}+n}$ let the graph $G_{\mathbf{x}} \in \mathcal{G}_{n}^{\circ}$ be given by connecting any two vertices $1 \leq i \leq j \leq n$ if $x_{\binom{j}{2}+i}=1$. We want to determine

$$
\begin{equation*}
\min _{\mathrm{x}} k_{s}^{\circ}\left(G_{\mathrm{x}}\right)+k_{t}^{\circ}\left(\overline{G_{\mathrm{x}}}\right) . \tag{1}
\end{equation*}
$$

Disadvantages. Problem structure is ignored. No guarantees of optimality.
Advantages. Applicable to many problems. Optimality through matching bounds.
SA and TS have previously proven successful in finding Ramsey numbers. Recently learning-based approaches have also been suggested (Wagner 2021; Bello et al. 2016)

## Constructing graphs through search heuristics

We phrased the problem through binary representations and applied Metaheuristics, i.e., Simulated Annealing (Kirkpatrick et al. 1983) and Tabu search (Glover 1986):

For any binary vector $\mathbf{x}=\left(x_{1}, \ldots, x_{\binom{n}{2}+n}\right) \in\{0,1\}^{\binom{n}{2}+n}$ let the graph $G_{\mathbf{x}} \in \mathcal{G}_{n}^{\circ}$ be given by connecting any two vertices $1 \leq i \leq j \leq n$ if $x_{\binom{j}{2}+i}=1$. We want to determine

$$
\begin{equation*}
\min _{\mathrm{x}} k_{s}^{\circ}\left(G_{\mathrm{x}}\right)+k_{t}^{\circ}\left(\overline{G_{\mathrm{x}}}\right) \tag{1}
\end{equation*}
$$

Disadvantages. Problem structure is ignored. No guarantees of optimality.
Advantages. Applicable to many problems. Optimality through matching bounds.
SA and TS have previously proven successful in finding Ramsey numbers. Recently learning-based approaches have also been suggested (Wagner 2021; Bello et al. 2016).
2. Search Heuristics for Constructive Bounds

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?

Turns out all previous constructions are actually graphs with very specific symmetries:
Definition (Cayley graphs)
Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let $\mathbf{x}$ now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?
Turns out all previous constructions are actually graphs with very specific symmetries:

## Definition (Cayley graphs)

Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let $\mathbf{x}$ now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?

Turns out all previous constructions are actually graphs with very specific symmetries:

## Definition (Cayley graphs)

Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let $\mathbf{x}$ now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?

Turns out all previous constructions are actually graphs with very specific symmetries:
Definition (Cayley graphs)
Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let x now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?

Turns out all previous constructions are actually graphs with very specific symmetries:
Definition (Cayley graphs)
Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let $\mathbf{x}$ now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Constructing Cayley graphs through search heuristics

Unfortunately does not scale beyond $n \approx 40$, barely disproving Erdős' original conjecture for $m_{4,4}$. Can we bias the search space using combinatorial insights?

Turns out all previous constructions are actually graphs with very specific symmetries:
Definition (Cayley graphs)
Given an abelian group $G$ and set $S \subseteq G^{\star}$ satisfying $S^{-1}=S$, the associated Cayley graph has vertex set $G$ and $g_{1}, g_{2} \in G$ are adjacent if and only if $g_{1}^{-1} g_{2} \in S$.

Let $\mathbf{x}$ now represent the generating set $S$. Since $|G| / 2<|S|<|G|$ the number of binary variables is linear (instead of quadratic) in the number of vertices!

The groups $C_{3} \times C_{2}^{\times 8}$ and $C_{3} \times C_{2}^{\times 6}$ give the improved upper bounds for $m_{4,4}$ and $m_{5,5}$.

## Computer-Assisted Proofs in Combinatorics

1. The Ramsey Multiplicity Problem
2. Search Heuristics for Constructive Bounds
3. Beyond the Ramsey multiplicity of quadrangles
4. Beyond the Ramsey multiplicity of quadrangles

## Off-diagonal Ramsey Multiplicity

Question. Determining $m_{3,3}$ is easy, but even $m_{4,4}$ has been unresolved for over 60 years. Can we say more when studying the off-diagonal variant where $s \neq t$ ?

A famous result of Reiher from 2016 implies that $m_{2, t}=1 /(t-1)$.

## Theorem (Parczyk, Pokutta, S., and Szabó 2022+)

$m_{3,4}=689 \cdot 3^{-8}$ and any large enough graph $G$ admits a strong homomorphism into the Schläfli graph after changing at most $O\left(k_{3}(\bar{G})+k_{4}(G)-m_{3,4}\right) v(G)^{2}$ edges.

The fact that we can show stability proves that the search heuristic found a unique global optimum over all graphs of order 27 !
3. Beyond the Ramsey multiplicity of quadrangles

## Off-diagonal Ramsey Multiplicity

Question. Determining $m_{3,3}$ is easy, but even $m_{4,4}$ has been unresolved for over 60 years. Can we say more when studying the off-diagonal variant where $s \neq t$ ?

A famous result of Reiher from 2016 implies that $m_{2, t}=1 /(t-1)$.

## Theorem (Parczyk, Pokutta, S., and Szabó 2022+)

$m_{3.4}=689 \cdot 3^{-8}$ and any large enough graph $G$ admits a strong homomorphism into the Schläfli graph after changing at most $O\left(k_{3}(\bar{G})+k_{4}(G)-m_{3,4}\right) v(G)^{2}$ edges.

The fact that we can show stability proves that the search heuristic found a unique global optimum over all graphs of order 27 !
3. Beyond the Ramsey multiplicity of quadrangles

## Off-diagonal Ramsey Multiplicity

Question. Determining $m_{3,3}$ is easy, but even $m_{4,4}$ has been unresolved for over 60 years. Can we say more when studying the off-diagonal variant where $s \neq t$ ?

A famous result of Reiher from 2016 implies that $m_{2, t}=1 /(t-1)$.
Theorem (Parczyk, Pokutta, S., and Szabó 2022+)
$m_{3,4}=689 \cdot 3^{-8}$ and any large enough graph $G$ admits a strong homomorphism into the Schläfli graph after changing at most $O\left(k_{3}(\bar{G})+k_{4}(G)-m_{3,4}\right) v(G)^{2}$ edges.

The fact that we can show stability proves that the search heuristic found a unique global optimum over all graphs of order 27 !
3. Beyond the Ramsey multiplicity of quadrangles

## Off-diagonal Ramsey Multiplicity

Question. Determining $m_{3,3}$ is easy, but even $m_{4,4}$ has been unresolved for over 60 years. Can we say more when studying the off-diagonal variant where $s \neq t$ ?

A famous result of Reiher from 2016 implies that $m_{2, t}=1 /(t-1)$.

## Theorem (Parczyk, Pokutta, S., and Szabó 2022+)

$m_{3,4}=689 \cdot 3^{-8}$ and any large enough graph $G$ admits a strong homomorphism into the Schläfli graph after changing at most $O\left(k_{3}(\bar{G})+k_{4}(G)-m_{3,4}\right) v(G)^{2}$ edges.

The fact that we can show stability proves that the search heuristic found a unique global optimum over all graphs of order 27 !
3. Beyond the Ramsey multiplicity of quadrangles

## Remarks and Open Problems

- One can also study other variants of the Ramsey multiplicity problem, for example for hypergraphs, additive structures, structures in finite geometry ...
- For many other problems the (current best) upper bounds come from blow-up-esque constructions: the capset problem, the Sunflower conjecture, Turán's (3,4)-conjecture, the Shannon Capacity of odd cycles
- One can more fundamentally ask when such constructions are optimal, e.g., do we always have $m_{s, t}=\min _{G \in \mathcal{G}^{\circ}} k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for the Ramsey multiplicity problem?

3. Beyond the Ramsey multiplicity of quadrangles

## Remarks and Open Problems

- One can also study other variants of the Ramsey multiplicity problem, for example for hypergraphs, additive structures, structures in finite geometry ...
- For many other problems the (current best) upper bounds come from blow-up-esque constructions: the capset problem, the Sunflower conjecture, Turán's (3, 4)-conjecture, the Shannon Capacity of odd cycles ...
- One can more fundamentally ask when such constructions are optimal, e.g., do we always have $m_{s, t}=\min _{G \in \mathcal{G}} \circ k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for the Ramsey multiplicity problem?


## Remarks and Open Problems

- One can also study other variants of the Ramsey multiplicity problem, for example for hypergraphs, additive structures, structures in finite geometry ...
- For many other problems the (current best) upper bounds come from blow-up-esque constructions: the capset problem, the Sunflower conjecture, Turán's (3, 4)-conjecture, the Shannon Capacity of odd cycles..
- One can more fundamentally ask when such constructions are optimal, e.g., do we always have $m_{s, t}=\min _{G \in \mathcal{G}^{\circ}} k_{s}^{\circ}(G)+k_{t}^{\circ}(\bar{G})$ for the Ramsey multiplicity problem?

Thank you for your attention!

