Combinatorics Using Computational Methods

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The Goal

Determine if certain **combinatorial objects** exist with given **structural** or **extremal** properties.

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Examples:

Is there a projective plane of order 10?

When do strongly regular graphs exist?

How many Steiner triple systems are there of order 19?

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Determine if certain **combinatorial objects** exist with given **structural** or **extremal** properties.

Examples:

- Is there a projective plane of order 10? (Lam, Thiel, Swiercz, 1989)
- When do strongly regular graphs exist?
 (Spence 2000, Coolsaet, Degraer, Spence 2006, many others)

How many Steiner triple systems are there of order 19? (Kaski, Östergård, 2004)

Problems Tackled in This Thesis

- Which numbers are representable as the number of chains in a width-two poset?
- **2** Which colorings of $\{1, ..., n\}$ avoid monochromatic progressions?

Output the second se

What graphs are uniquely K_r-saturated?

Problems Tackled in This Thesis

- Which numbers are representable as the number of chains in a width-two poset? (with Kupin, Reiniger)
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- Which colorings of {1,..., n} avoid monochromatic progressions? (with Jobson, Kézdy)
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- How many edges can exist in a graph with p perfect matchings? (with Hartke, West, Yancey)
 Chapter 9
- What graphs are uniquely *K_r*-saturated?
 (with Hartke)
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Main Technique: Combinatorial Search

- **Goal:** Determine if certain combinatorial objects exist with given structural or extremal properties.
- **Idea:** Build objects *piece-by-piece* from *base examples* to enumerate all desired examples of a given order.

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- **Idea:** Build objects *piece-by-piece* from *base examples* to enumerate all desired examples of a given order.

Most interesting properties are invariant under isomorphism.

Combinatorial Object: Graphs

A graph *G* of order *n* is composed of a set V(G) of *n* vertices and a set E(G) of edges, where the edges are unordered pairs of vertices.



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Combinatorial Object: Graphs

An **isomorphism** between G_1 and G_2 is a bijection from $V(G_1)$ to $V(G_2)$ that induces a bijection from $E(G_1)$ to $E(G_2)$.



We can build graphs starting at $\overline{K_n}$ by adding edges.



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Two Techniques for Isomorphs

Canonical Deletion

- Removes all isomorphs.
- Not known how to integrate with constraint propagation.
- High cost per object.

2 Orbital Branching (Ostrowski, Linderoth, Rossi, Smriglio 2007)

- Removes some, but not all isomorphs.
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(McKay 1998)

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Overview in Chapter 6

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Overview in Chapter 10

(McKay 1998)

Search by Augmentations



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Implementation

My TreeSearch library enables parallelization in the Condor scheduler.

Executes on the **Open Science Grid**, a collection of supercomputers around the country.





Open Science Grid

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Chapter 11



A **perfect matching** is a set of edges which cover each vertex exactly once.

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Question (Dudek, Schmitt, 2010) What is the maximum number of edges in a graph with exactly *n* vertices and *p* perfect matchings?

Definition Let *n* be an even number and fix $p \ge 1$.

$$f(n,p) = \max\{|E(G)| : |V(G)| = n, \Phi(G) = p\}.$$

Graphs attaining this number of edges are *p*-extremal.

$$f(n,1)=\frac{n^2}{4}.$$



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The Form of f(n, p)

Theorem (Dudek, Schmitt, 2010) For each *p*, there exist constants

 n_p , c_p so that for all $n \ge n_p$,

$$f(n,p)=\frac{n^2}{4}+c_p.$$

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p	1	2	3	4	5	6			
Cp	0	1	2	2	2	3			
	Н	Dudek, Schmitt, 2010							

Structure Theorem

Theorem (Hartke, Stolee, West, Yancey, 2011) For a fixed *p*, every graph *G* with *n* vertices, *p* perfect matchings, and $f(n, p) = \frac{n^2}{4} + c_p$ edges is composed of a finite list of **fundamental graphs** combined in specified ways.

Proof involves several classic structure theorems from matching theory in an extremal setting.

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For $p \leq 10$, the graphs have order at most 12.

Using standard software (McKay's *geng*) we found the graphs and computed c_p .

Fundamental Graphs for $2 \le p \le 10$







p = 4



p = 5



p = 5









p = 7





p = 8







p = 8

p = 6





p = 8

c_p for small p

p	1	2	3	4	5	6	7	8	9	10
Cp	0	1	2	2	2	3	3	3	4	4
	H	Dudek, Schmitt 2010					HSWY 2011			

c_p for small p

p	1	2	3	4	5	6	7	8	9	10	
Cp	0	1	2	2	2	3	3	3	4	4	
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Q: Is c_p monotone in p?

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Computational Method

Developed a computational method from:

- 1. Augmentations: Lovász Two Ear Theorem.
- 2. Isomorphs: Canonical Deletion.

McKay

3. **Pruning:** Developed new structural and extremal theorems.

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Before: Stuck at $p \le 10$ when searching on most 12 vertices.

Now: Found graphs for all $p \le 27$ on up to 22 vertices.

Perfect Matchings

Fundamental Graphs for $11 \le p \le 27$



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Computational Combinatorics

Perfect Matchings

c_p for small p

p	1	2	3	4	5	6	7	8	9	10
Cp	0	1	2	2	2	3	3	3	4	4
	H	Du	dek, 🛛	Schm	nitt, 20	HSWY, 2011				

р	11	12	13	14	15	16	17	18	19	20	
Cp	3	5	3	4	6	4	4	5	4	5	
	Stolee, 2011										

р	21	22	23	24	25	26	27			
Cp	5	5	5	6	5	5	6			
	Stolee, 2011									

c_p for small p

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Cp	3	5	3	4	6	4	4	5	4	5	
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р	21	22	23	24	25	26	27			
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 c_p not monotonic in p ! Blue numbers match conjectured upper bound.

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Definition A graph G is H-saturated if

- G does not contain H as a subgraph. (H-free)
- For every $e \in E(\overline{G})$, G + e contains H as a subgraph.



Example: $H = K_3$ where K_r is the **complete graph** on *r* vertices.

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Turán's Theorem

Theorem (Turán, 1941) Let $r \ge 3$. If *G* is K_r -saturated on *n* vertices, then *G* has **at most** $\left(1 - \frac{1}{r-1}\right) \frac{n^2}{2}$ edges (asymptotically).

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Erdős, Hajnal, and Moon

Theorem (Erdős, Hajnal, Moon, 1964) Let $r \ge 3$. If *G* is K_r -saturated on *n* vertices, then *G* has at least $\binom{r-2}{2} + (r-2)(n-r+2)$ edges.

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Uniquely *H*-Saturated Graphs

The Turán graph has **many** copies of K_r when an edge is added.

The books have **exactly one** copy of K_r when an edge is added.

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Definition A graph *G* is **uniquely** *H***-saturated** if *G* does not contain *H* as a subgraph and for every edge $e \in \overline{G}$ admits **exactly one** copy of *H* in G + e.

We consider the case where $H = K_r$ (an *r*-clique).

Uniquely K₃-Saturated Graphs

Lemma (Cooper, Lenz, LeSaulnier, Wenger, West, 2011)

The uniquely K_3 -saturated graphs are either stars or Moore graphs of diameter 2 and girth 5.

Uniquely *K*₃-Saturated Graphs

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Theorem (Hoffman, Singleton, 1964) There are a **finite number** of Moore graphs of diameter 2 and girth 5.

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- •
- •







Adding a dominating vertex to a uniquely K_r -saturated graph creates a uniquely K_{r+1} -saturated graph.



Call uniquely K_r -saturated graphs without a dominating vertex

r-primitive.

A uniquely K_r -saturated graph with no dominating vertex is *r*-primitive.

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3-primitive graphs are Moore graphs of diameter 2 and girth 5.

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r-Primitive Graphs

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Uniquely K₄-Saturated Graphs



Previously known 4-primitive graphs (Collins, Cooper, Kay, 2010)

Two Questions

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1. Fix $r \ge 3$. Are there a **finite number** of *r*-primitive graphs?

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1. Fix $r \ge 3$. Are there a **finite number** of *r*-primitive graphs?

2. Is every *r*-primitive graph regular?

Edges and Non-Edges

Non-edges are crucial to the structure of *r*-primitive graphs.

Computational Method

Edges and Non-Edges

Non-edges are crucial to the structure of *r*-primitive graphs.



K_r-Completions

For every non-edge we add, we add a K_r -completion:

ij a non-edge **if and only if** there exists a set $S \subset [n]$, |S| = r - 2, so that *ia*, *ja*, and *ab* are edges for all $a, b \in S$.



Computational Method

Developed a computational method from:

- 1. **Augmentations:** *K*_{*r*}-Completions.
- 2. Isomorphs: Orbital Branching.

Ostrowsky et al.

3. **Pruning:** Contains K_r or double-completion.

Exhaustive Search Times

n	<i>r</i> = 4	<i>r</i> = 5	<i>r</i> = 6	<i>r</i> = 7	<i>r</i> = 8
10	0.10 s	0.37 s	0.13 s	0.01 s	0.01 s
11	0.68 s	5.25 s	1.91 s	0.28 s	0.09 s
12	4.58 s	1.60 m	25.39 s	1.97 s	1.12 s
13	34.66 s	34.54 m	6.53 m	59.94 s	20.03 s
14	4.93 m	10.39 h	5.13 h	20.66 m	2.71 m
15	40.59 m	23.49 d	10.08 d	12.28 h	1.22 h
16	6.34 h	1.58 y	1.74 y	34.53 d	1.88 d
17	3.44 d			8.76 y	115.69 d
18	53.01 d				
19	2.01 y				
20	45.11 y				

Total CPU times using Open Science Grid.





Empty graphs



Empty graphs Cycle complements



Empty graphs Cycle complements Old examples



Empty graphs Cycle complements Old examples

New examples



Empty graphs Cycle complements Old examples

New examples

4-Primitive Graphs

4-Primitive Graphs n = 13





Paley(13)

5-Primitive Graph

5-Primitive Graph $n = 16: G_{16}^{(A)}$



5-Primitive Graph

5-Primitive Graph $n = 16: G_{16}^{(A)}$



5-Primitive Graph $n = 16: G_{16}^{(A)}$



Not all *r*-primitive graphs are regular!

5-Primitive Graph

7-Primitive Graph $n = 17: G_{17}^{(A)}$



5-Primitive Graph

7-Primitive Graph $n = 17: G_{17}^{(A)}$



Let Γ be a group and $S \subseteq \Gamma$ a set of generators.

The undirected **Cayley graph** $C(\Gamma, S)$ has vertex set Γ and for all $a \in \Gamma$ and $b \in S$, there is an edge between *a* and *ab*.

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For
$$r \ge 1$$
, $\overline{C}(\mathbb{Z}_{2r-1}, \{1\}) \cong \overline{C_{2r-1}}$ is *r*-primitive.



Two or Three Generators

S	r	n	S	r	n		
{1,4}	7	17	$\{1, 5, 6\}$	9	31		
{1,6}	16	37	$\{1, 8, 9\}$	22	73		
{1,8}	29	65	{1, 11, 12 }	41	133		
{1,10}	46	101	$\{1, 14, 15\}$	66	211		
{1,12}	67	145	{1, 17, 18}	97	307		
g= 2			g =	g= 3			

Infinite Families

Conjecture (Hartke, Stolee, 2012) Let $t \ge 1$, $n = 4t^2 + 1$, and $r = 2t^2 - t + 1$.

The Cayley complement $\overline{C}(\mathbb{Z}_n, \{1, 2t\})$ is *r*-primitive.

Conjecture (Hartke, Stolee, 2012) Let $t \ge 1$, $n = 9t^2 - 3t + 1$ and $r = 3t^2 - 2t + 1$.

The Cayley complement $\overline{C}(\mathbb{Z}_n, \{1, 3t - 1, 3t\})$ is *r*-primitive.

Infinite Families

Theorem (Hartke, Stolee, 2012) Let $t \ge 1$,

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Proof uses **counting** method.

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The Cayley complement $\overline{C}(\mathbb{Z}_n, \{1, 3t - 1, 3t\})$ is *r*-primitive.

Proof uses **discharging** method.

Computational Combinatorics









Complexity Results in This Thesis



Chapter 13

 Reachability in surface-embedded acyclic digraphs. (with Vinodchandran)
Chapter 14

Space-Bounded Complexity

A language is in L if there is a **deterministic** Turing machine that decides the language using at most $O(\log(n))$ work cells.

Space-Bounded Complexity

A language is in L if there is a **deterministic** Turing machine that decides the language using at most $O(\log(n))$ work cells.

A language is in NL if there is a **non-deterministic** Turing machine that decides the language using at most $O(\log(n))$ work cells.

$\mathsf{L}\subseteq\mathsf{N}\mathsf{L}$
If *M* is an $O(\log(n))$ -space non-deterministic Turing machine and $\mathbf{x} \in \{0, 1\}^*$, the **configuration graph** $G_{M, \mathbf{x}}$ has

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Vertices are configurations: assignments of state, work cell contents, and tape head positions.
(Requires O(log n) bits to describe.)

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Vertices are configurations: assignments of state, work cell contents, and tape head positions.

(Requires $O(\log n)$ bits to describe.)

2 An edge $C \rightarrow C'$ exists if there is a transition function of M whose operation on C results in C'.

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 $G_{M,\mathbf{x}}$ has poly-size and can be written using log-space.

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Every space-bounded complexity problem can be reduced to some form of the **reachability problem** in digraphs.

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Reach = { $\langle G, s, t \rangle$: *G* is a directed graph with a path from *s* to *t*}

$\mathsf{L}\subseteq\mathsf{N}\mathsf{L}\subseteq\mathsf{P}$

Complexity Results in This Thesis



Chapter 13

 Reachability in surface-embedded acyclic digraphs. (with Vinodchandran)
Chapter 14

Complexity Results in This Thesis



ReachFewL = ReachUL.

Reachability in surface-embedded acyclic digraphs. 2 (with Vinodchandran) Chapter 14

Log-space Classes and Reachability



Undirected Reach (Reingold 08)

Derrick Stolee (UNL)

Log-space Classes and Reachability



Complete: Undirected Reach (Reingold 08)



Complete: Directed Reach

Log-space Classes and Reachability



(Reingold 08)

Dir. Planar Reach (Bourke, Tewari, Vinodchandran 09) **Directed Reach**

NL 1 UL

Derrick Stolee (UNL)











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Surface-embedded graphs

We also extend to graphs embedded in *surfaces of low genus*.



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Let $\mathcal{G}(m, g)$ denote the **acyclic** digraphs with *m* **sources** and embedded in a **genus** *g* **surface**.

Reduction with Compression

Theorem (Stolee, Vinodchandran, '12) Given a graph $G \in \mathcal{G}(m, g)$ and $s, t \in V(G)$, we can compute in **log-space** a graph G' with vertices s', t' so that

There is a path from s to t in G if and only if there is a path from s' to t' in G'.

2
$$G'$$
 has $O(m+g)$ vertices.













Computational Combinatorics

Our Results (Stolee, Vinodchandran, '12)

Theorem (Sub-Savitch) Reachability for graphs of order *n* in $\mathcal{G}(m, g)$ is in SPACE[log $n + \log^2(m + g)$].
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Theorem (Time-Space) Reachability for graphs of order *n* in $\mathcal{G}(m, g)$ is in TISP[poly(*n*), log n + m + g].

Our Results





Combinatorics Using Computational Methods

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