Computational Combinatorics and the search for Uniquely K_r-Saturated Graphs

Derrick Stolee

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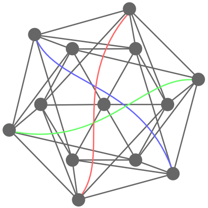
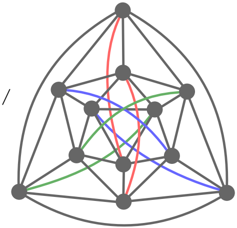
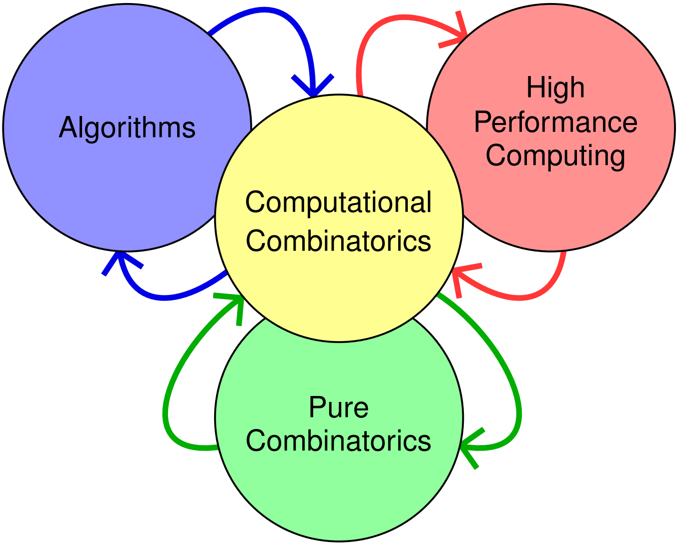




September 12, 2013

Joint work with Stephen G. Hartke, appeared in *Electronic Journal of Combinatorics*, 2012.

What is Computational Combinatorics?



What is Computational Combinatorics?

Using a combination of

- **pure mathematics**,
- **algorithms**, and
- **computational resources**

to solve problems in pure combinatorics by

- **providing evidence** for conjectures,
- finding **examples** and **counterexamples**, and
- **discovering and proving theorems**.

The Goal

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

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Examples:

1. Is there a **projective plane** of order 10?
2. When do **strongly regular graphs** exist?
3. How many **Steiner triple systems** are there of order 19?

The Goal

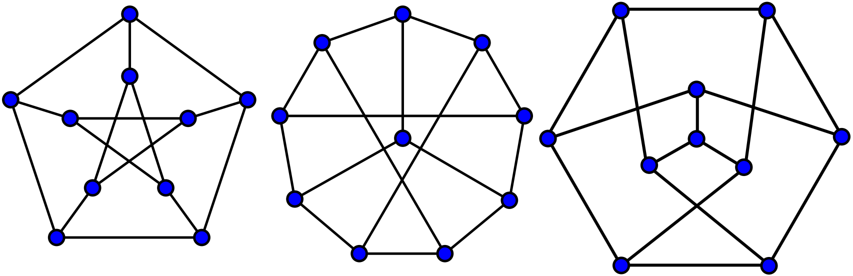
Determine if certain **combinatorial objects** exist with given **structural** or **extremal** properties.

Examples:

1. Is there a **projective plane** of order 10?
   (Lam, Thiel, Swiercz, 1989)
2. When do **strongly regular graphs** exist?
   (Spence 2000, Coolsaet, Degraer, Spence 2006, many others)
3. How many **Steiner triple systems** are there of order 19?
   (Kaski, Östergård, 2004)

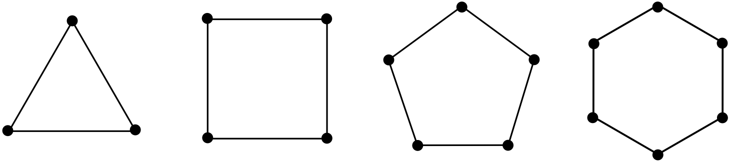
Combinatorial Object: Graphs

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.



Combinatorial Object: Graphs

Cycles C_k



C_3 C_4 C_5 C_6

Combinatorial Object: Graphs

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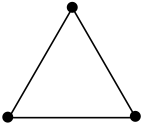
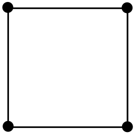
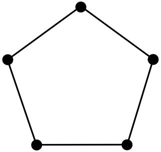


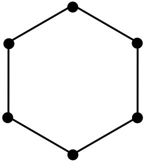
C_3



C_4

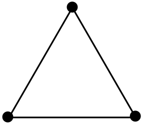


C_5

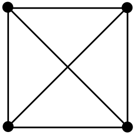


C_6

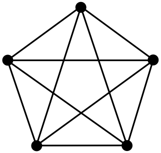
Complete Graphs K_r (cliques)



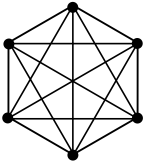
K_3



K_4



K_5



K_6

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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The computer performs a long, detailed case analysis.

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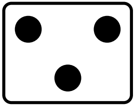
The computer performs a long, detailed case analysis.

Our job is to efficiently design the case analysis, using **algorithms**:

- Combinatorial Generation
- Combinatorial Optimization
- Graph Algorithms

Example: Generating Graphs by Edges

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



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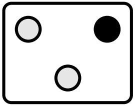

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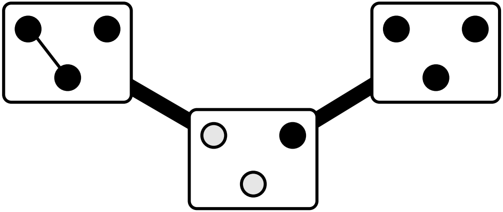

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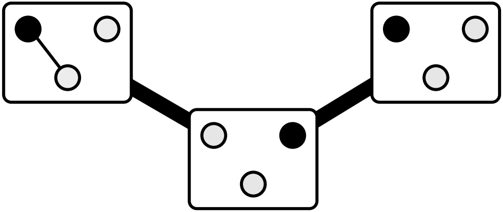

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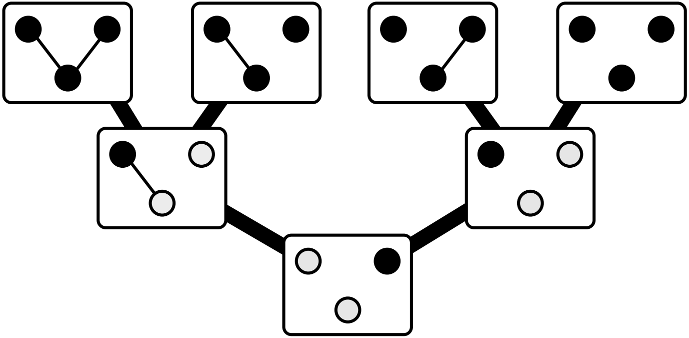

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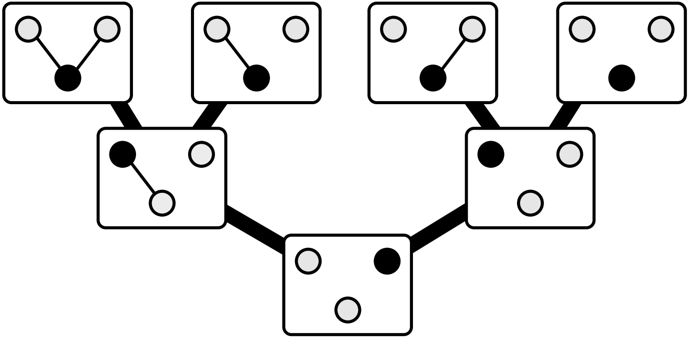

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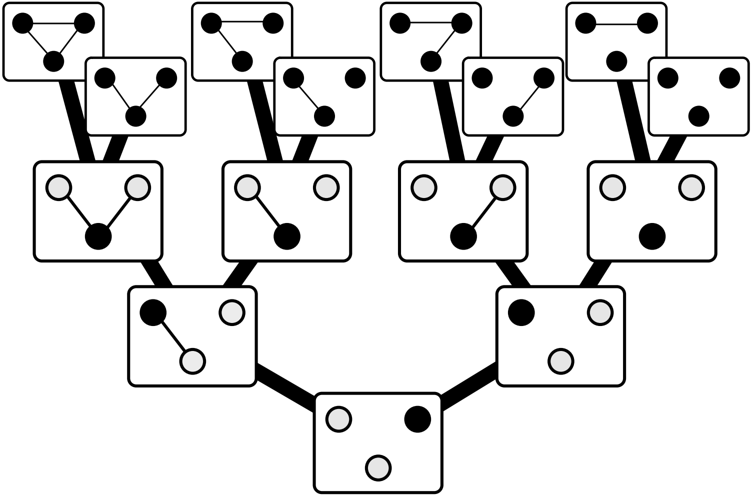

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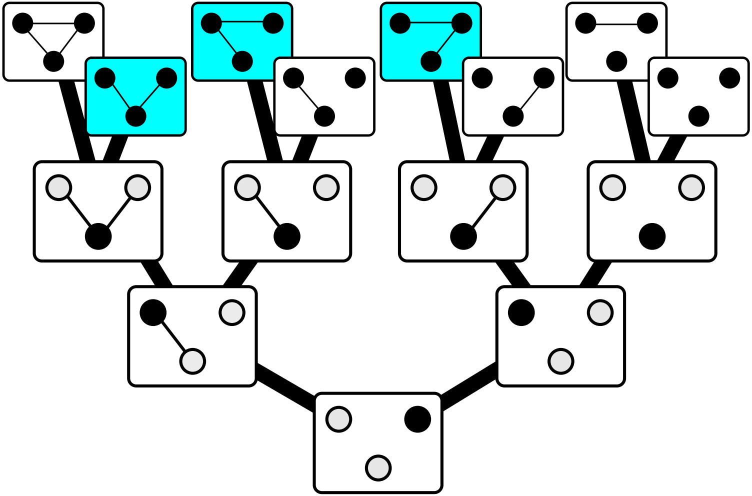

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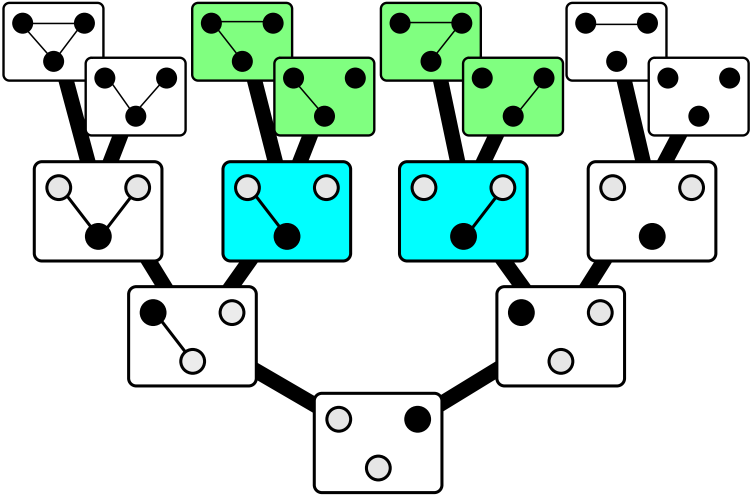

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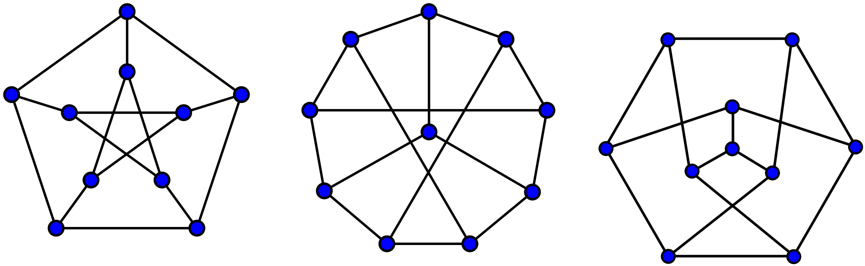

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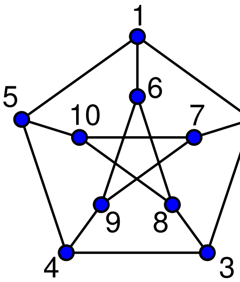
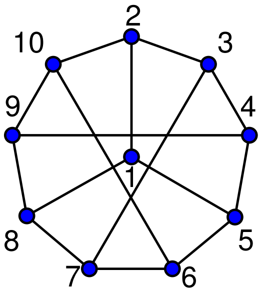
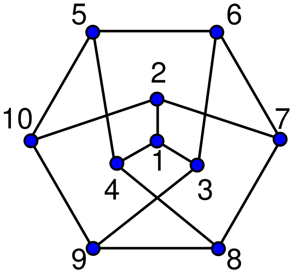
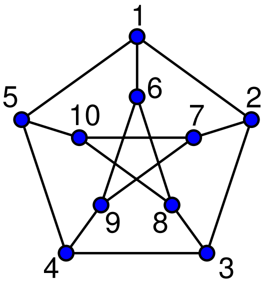


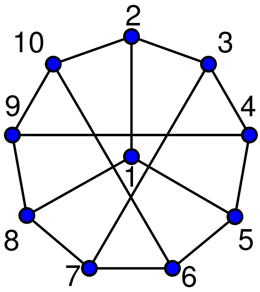


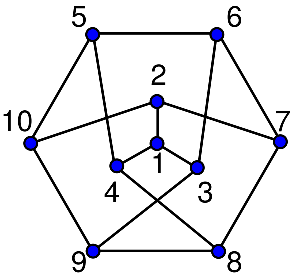


Example: Generating Graphs by Edges

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 $E(G_2)$.







Labeled Versus Unlabeled Objects

A **labeled** graph has a linear ordering on the vertices.

An **unlabeled** graph represents an isomorphism class of graphs.

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An **unlabeled** graph represents an isomorphism class of graphs.

Most interesting graph properties are **invariant under isomorphism**.

n	Labeled graphs of order n
6	32,768
7	2,097,152
8	268,435,456
9	68,719,476,736
10	35,184,372,088,832
11	36,028,797,018,963,968
12	73,786,976,294,838,206,464
13	302,231,454,903,657,293,676,544
14	2,475,880,078,570,760,549,798,248,448
15	40,564,819,207,303,340,847,894,502,572,032

$$2^{\binom{n}{2}} \approx 2^{\theta(n^2)}$$

n	Unlabeled connected graphs of order n
6	85
7	509
8	4,060
9	41,301
10	510,489
11	7,319,447
12	117,940,535
13	2,094,480,864
14	40,497,138,011
15	845,480,228,069

OEIS Sequence A002851 Grows $2^{\Omega(n^2)}$.

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Requires about **1 day** of CPU Time.

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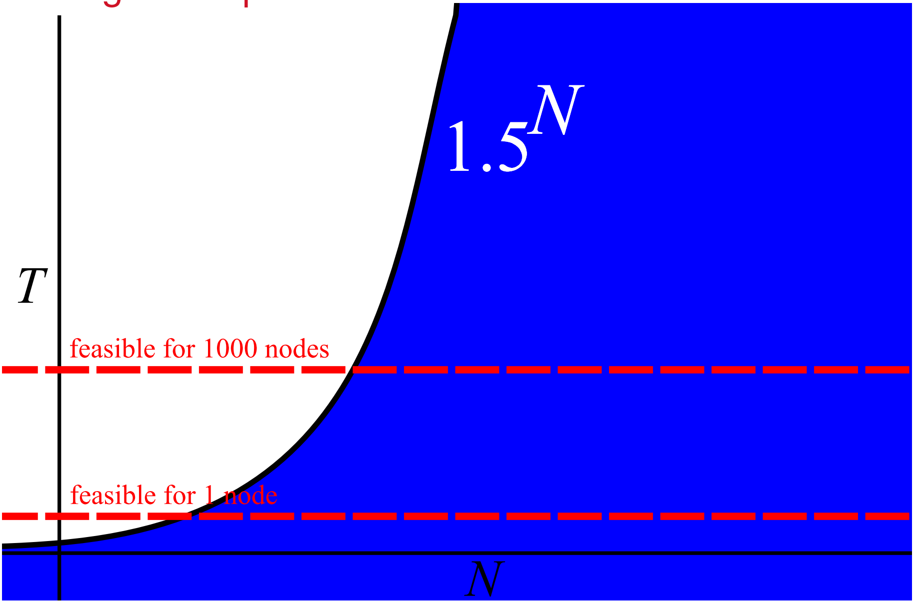
Requires over **1 year** of CPU Time.

Shifting the Exponent



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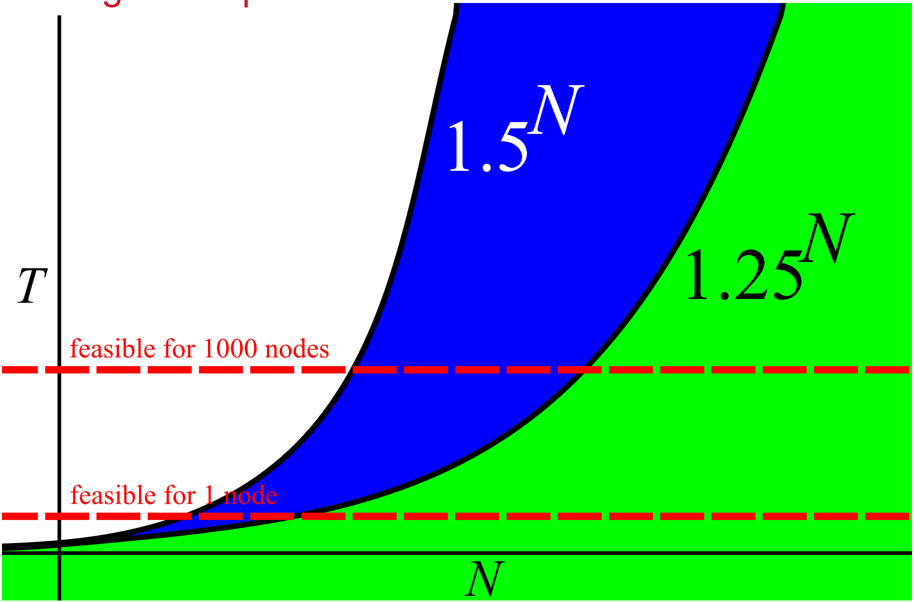
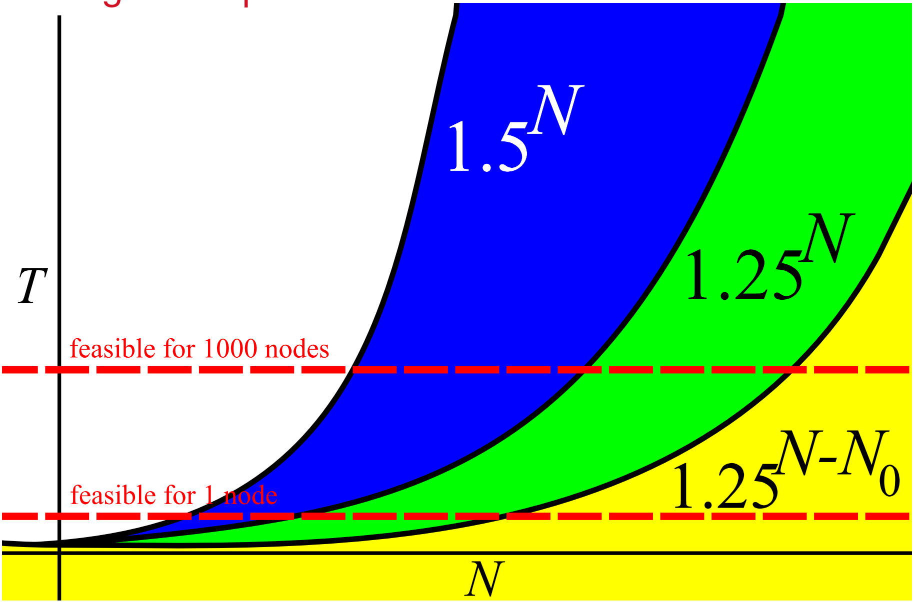


Shifting the Exponent



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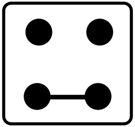
Unlabeled Graphs 

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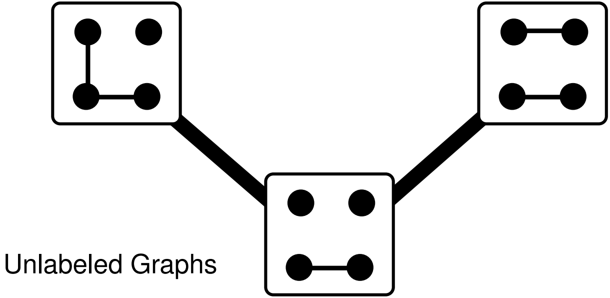

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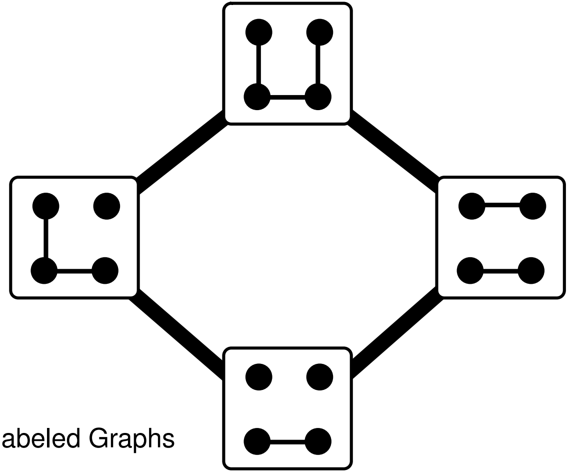

Unlabeled Graphs

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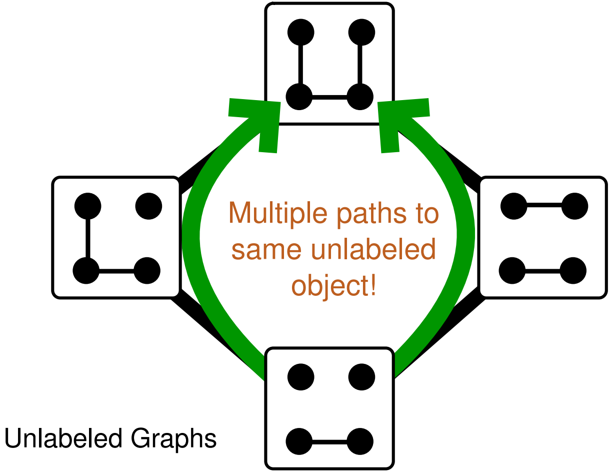
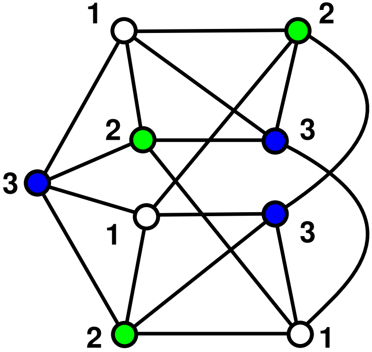
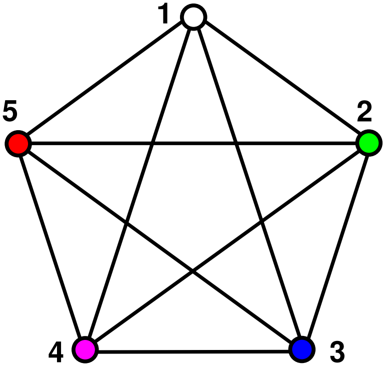


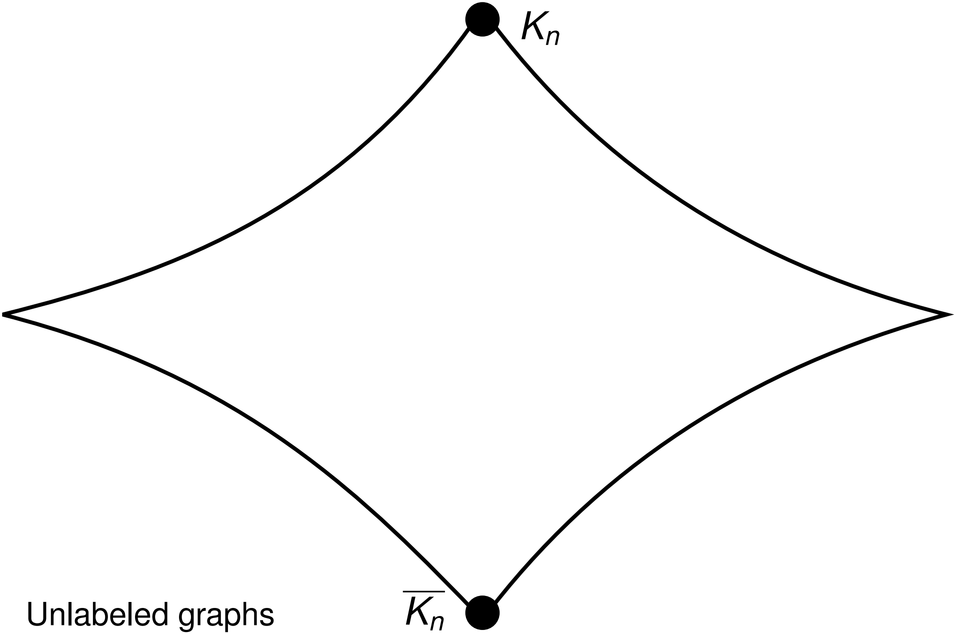
Toy Example

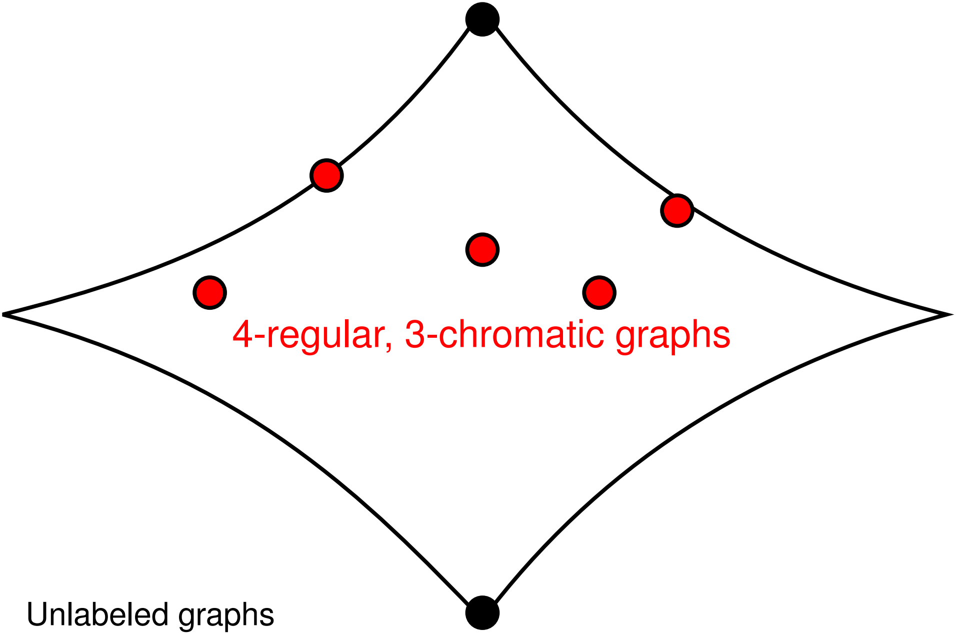
Suppose we are searching for graphs which are:

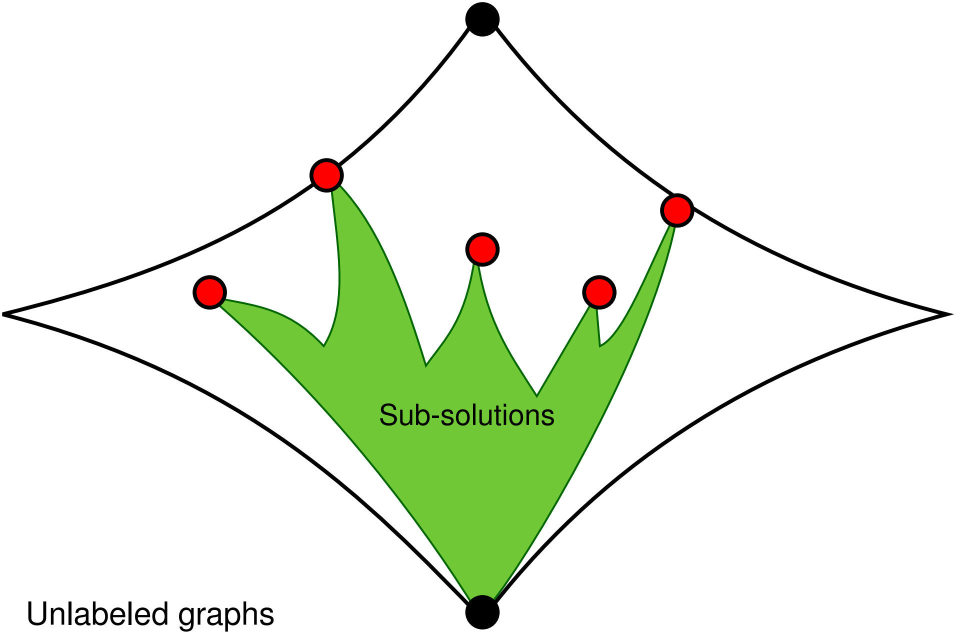
1. **4-regular**: All vertices have 4 incident edges.
2. **3-colorable**: The vertices can be colored with three colors so that no edge is monochromatic.

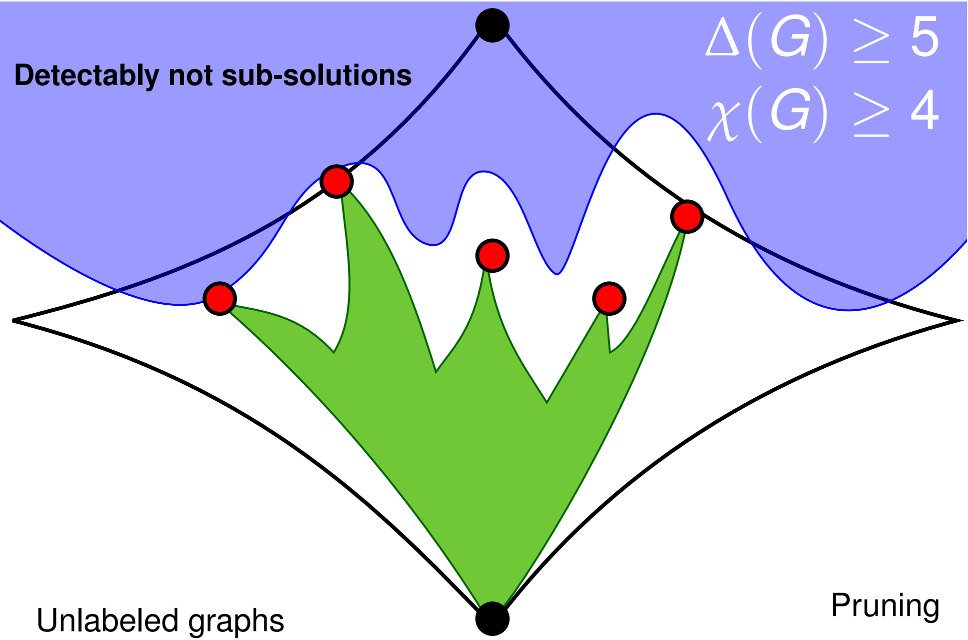




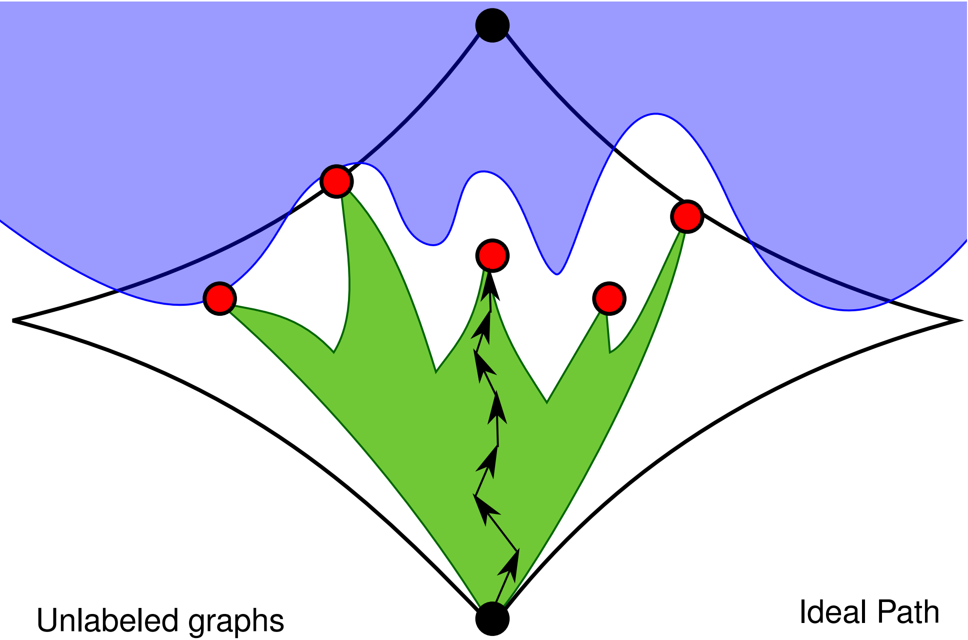

K_n
$\overline{K_n}$
Unlabeled graphs

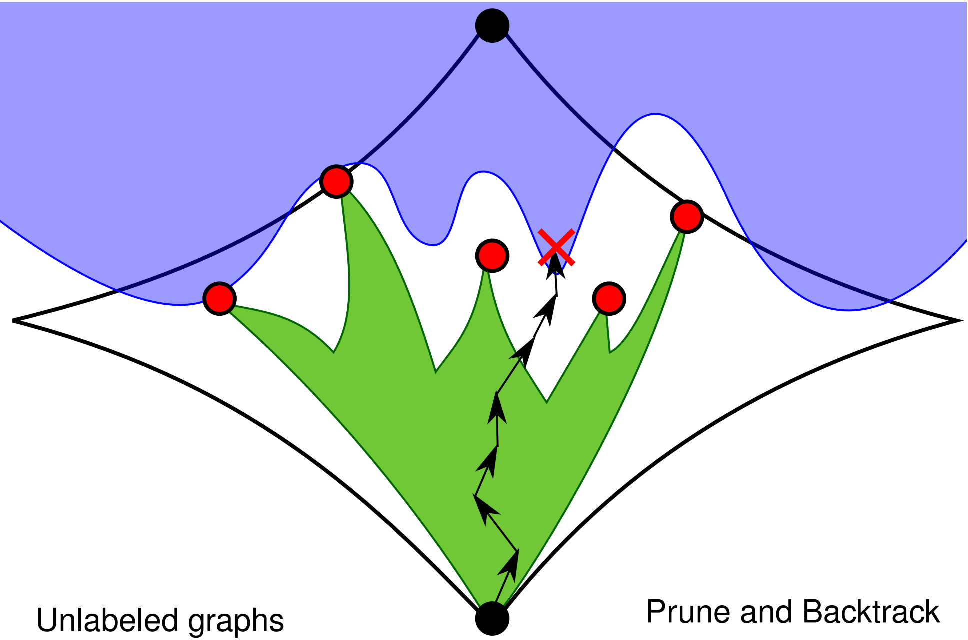

4-regular, 3-chromatic graphs
Unlabeled graphs

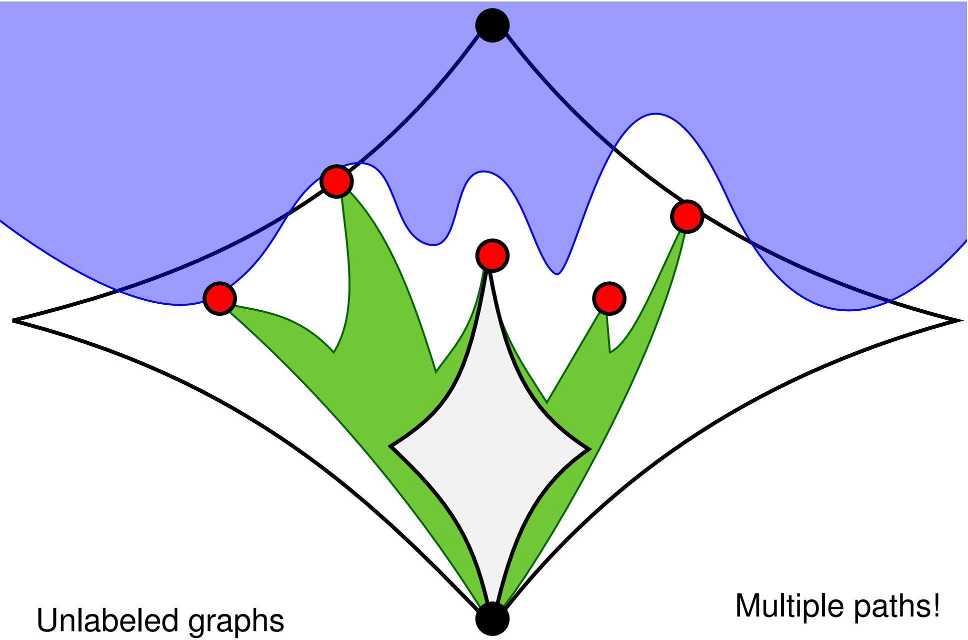

Sub-solutions
Unlabeled graphs

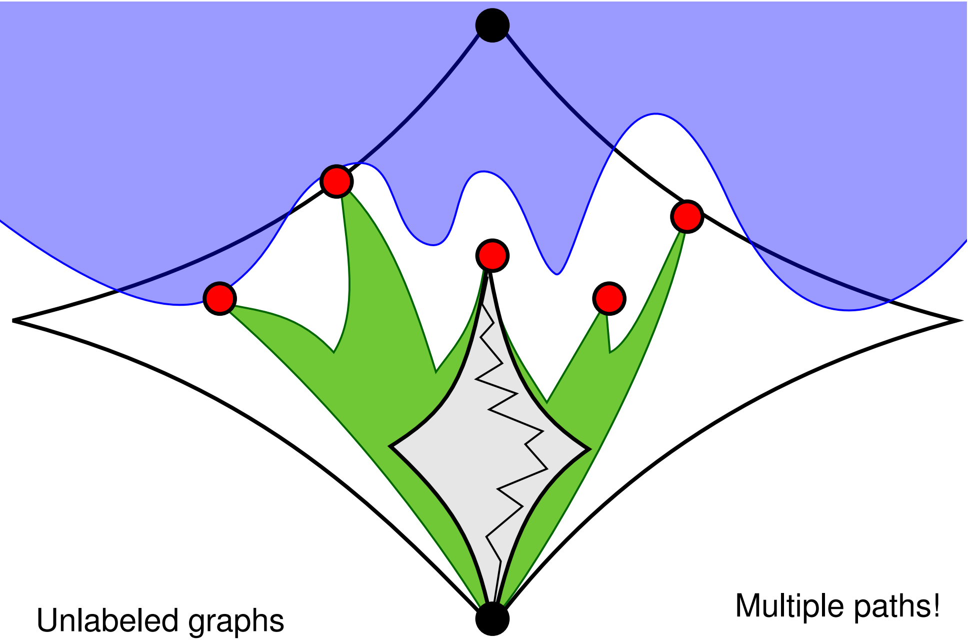


Detectably not sub-solutions
$\Delta(G) \geq 5$
$\chi(G) \geq 4$
Unlabeled graphs
Pruning


Unlabeled graphs
Ideal Path


Unlabeled graphs
Prune and Backtrack


Unlabeled graphs
Multiple paths!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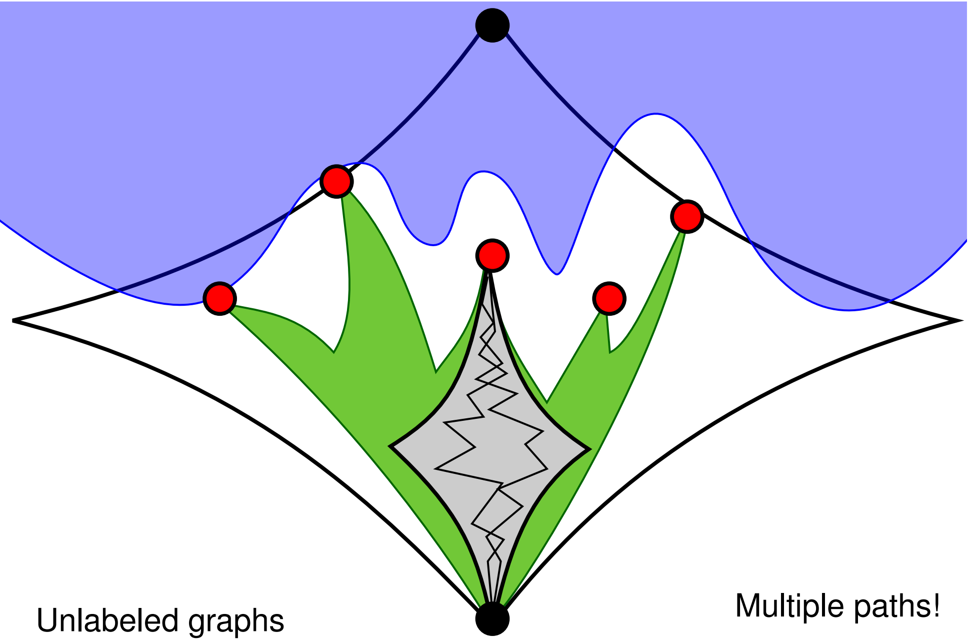

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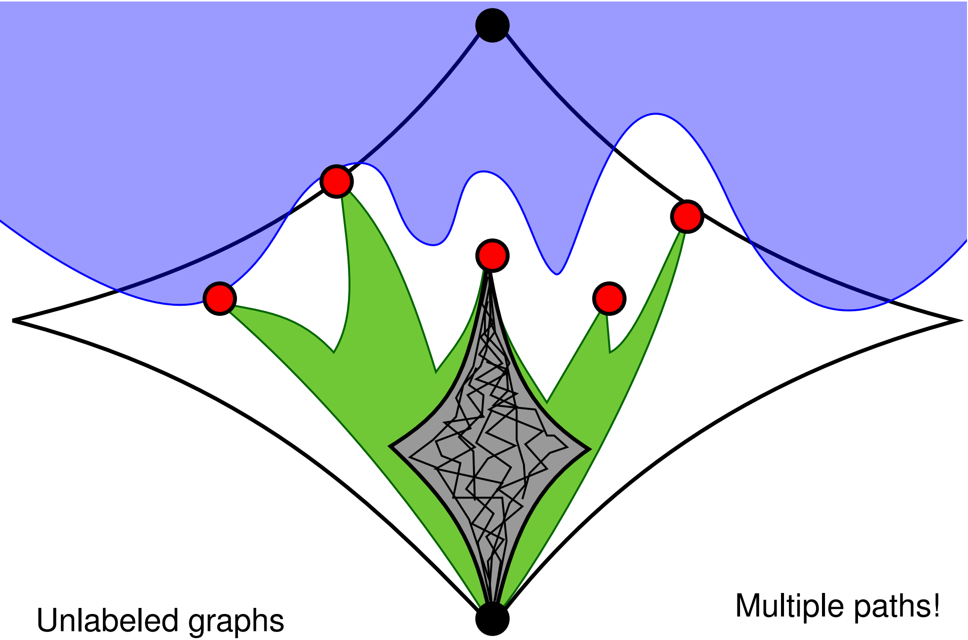
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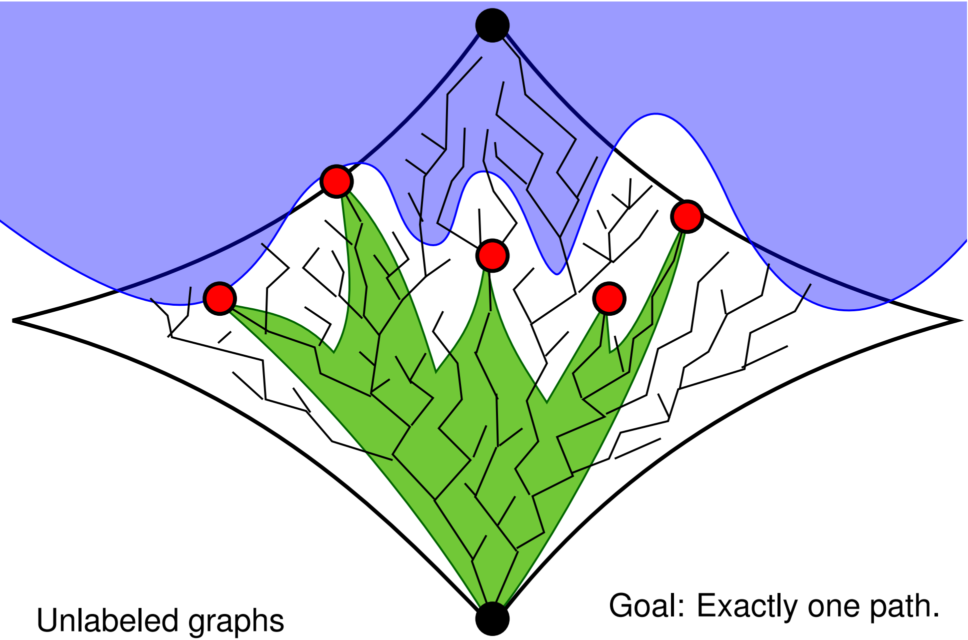
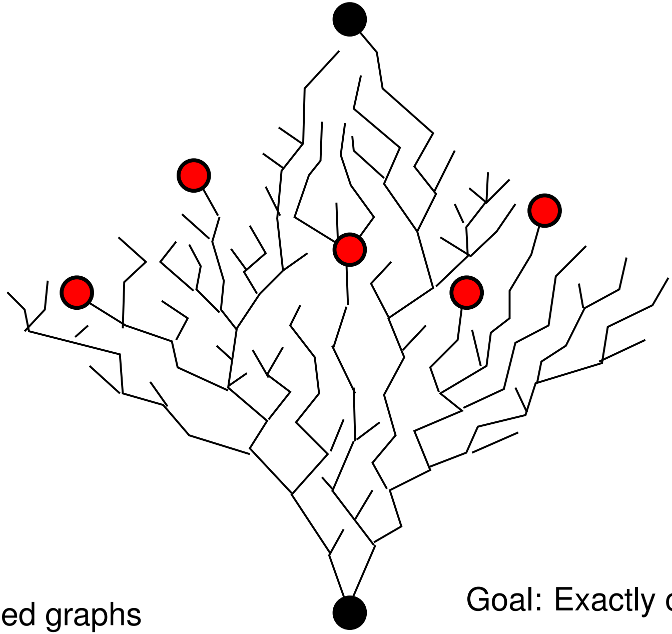

Unlabeled graphs
Goal: Exactly one path.



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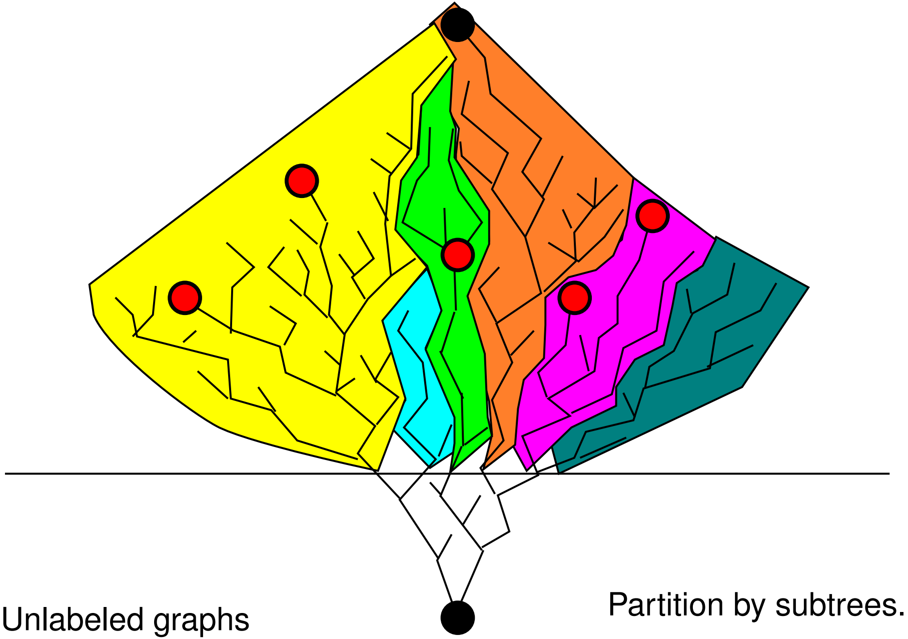
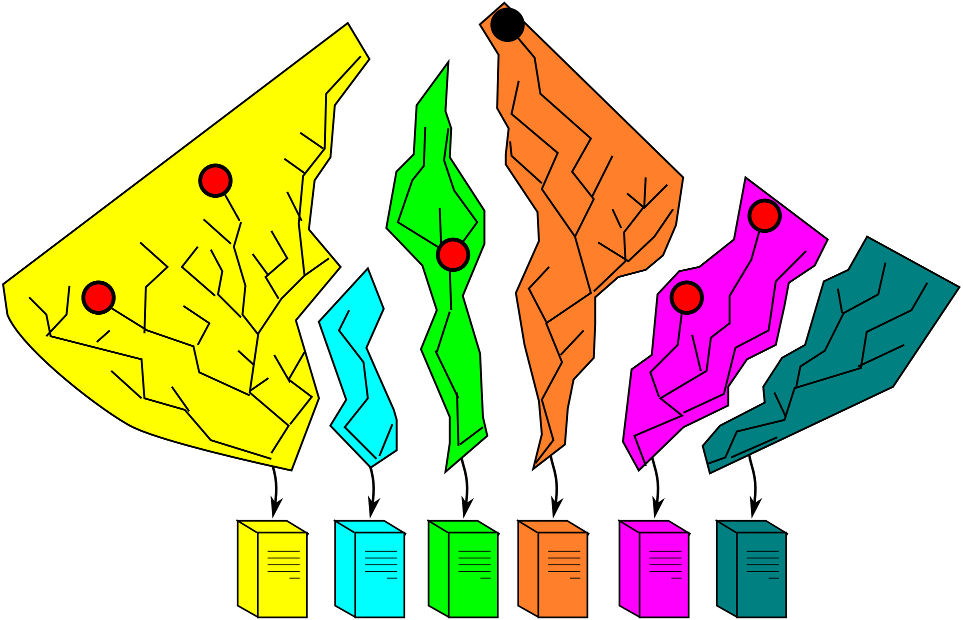

Unlabeled graphs
Partition by subtrees.



Parallelize!

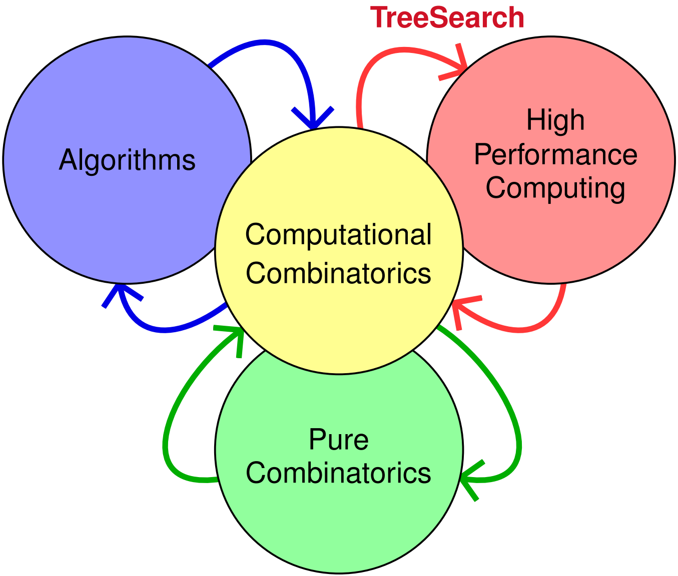
Implementation

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

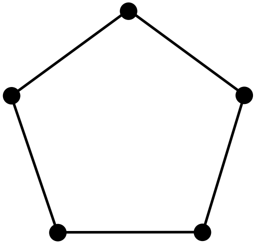
Computational Combinatorics



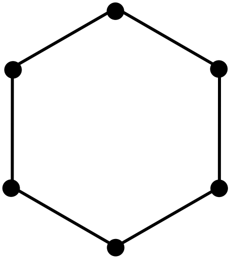
H-Saturated Graphs

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.



5-cycle



6-cycle

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

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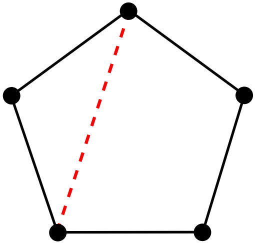
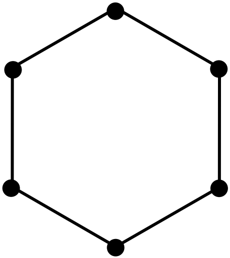


5-cycle
is K_3-saturated



6-cycle

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

H-Saturated Graphs

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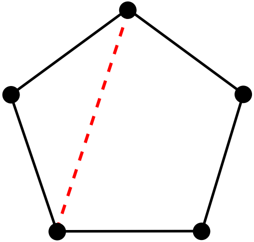

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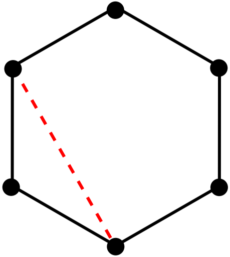

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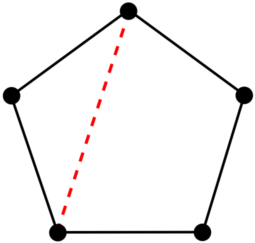

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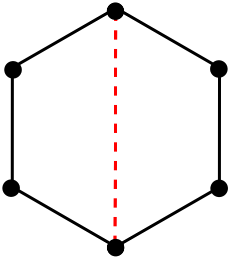

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Turán's Theorem

Theorem (Turán, 1941) Let $r \geq 3$. 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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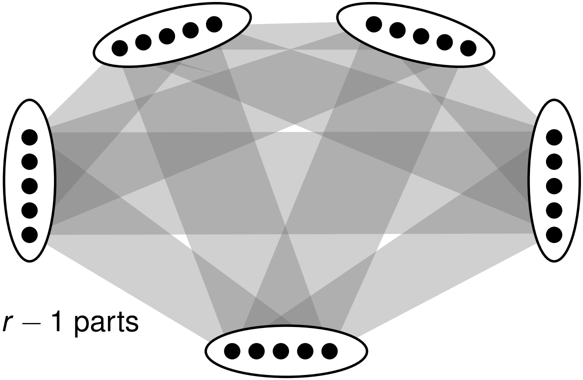

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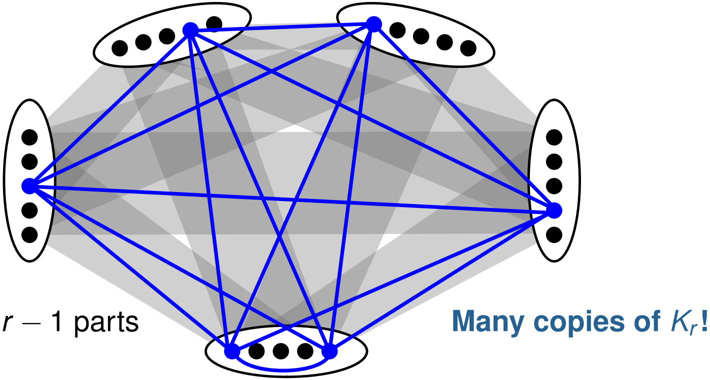

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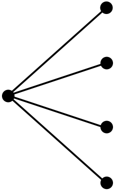
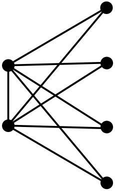
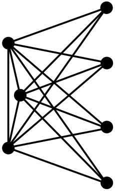


1-book



2-book



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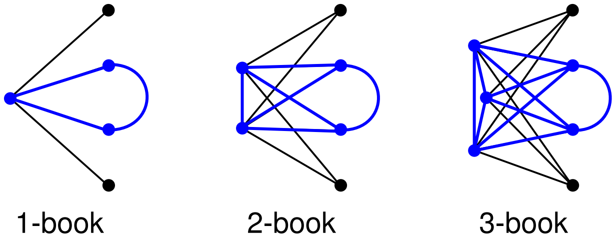

Exactly one copy of K_r!

Uniquely H-Saturated Graphs

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The uniquely C_3-saturated graphs are either **stars** or **Moore graphs** of diameter 2 and girth 5.

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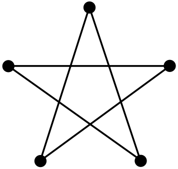
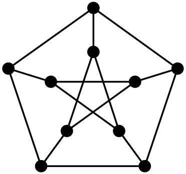


C_5



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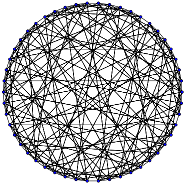

Hoffman–Singleton

?

57-Regular
Order 3250

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Theorem (Wenger, 2010)
For $k \in \{6, 7, 8\}$, no uniquely C_k-saturated graph exists.

Conjecture (Wenger, 2010)
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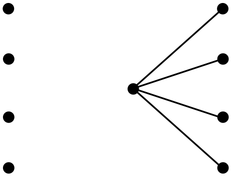

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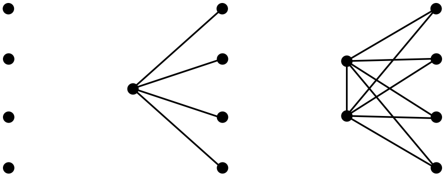

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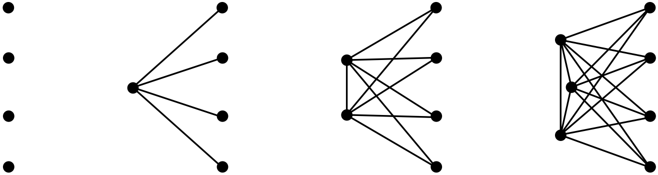

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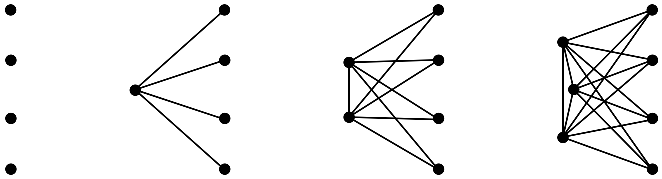

Call uniquely K_r-saturated graphs without a dominating vertex

***r*-primitive**.

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

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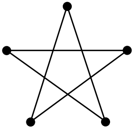

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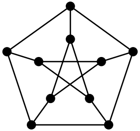

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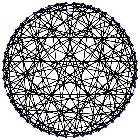

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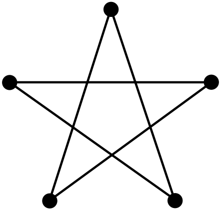
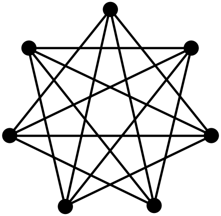


$\overline{C_5}$



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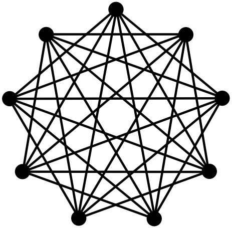

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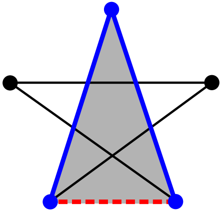

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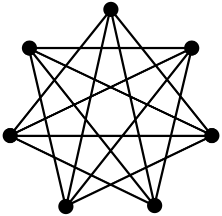

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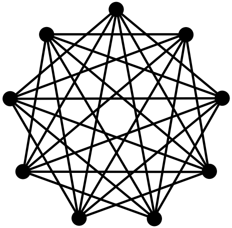

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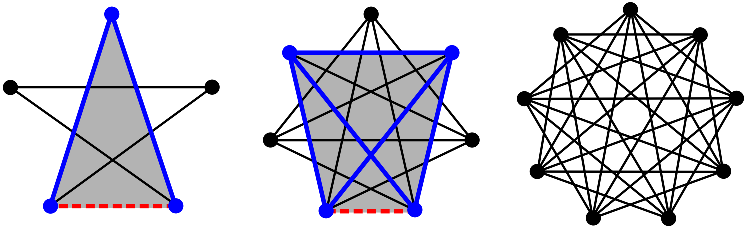

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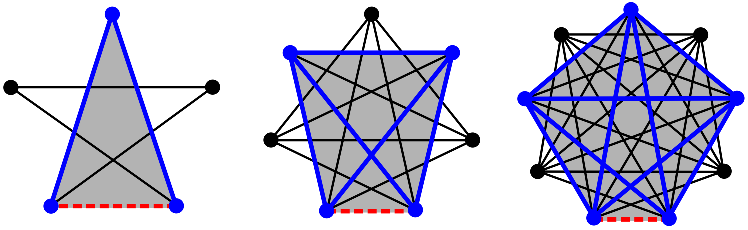

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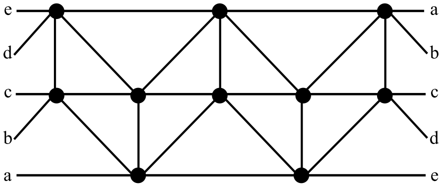
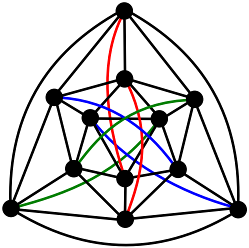


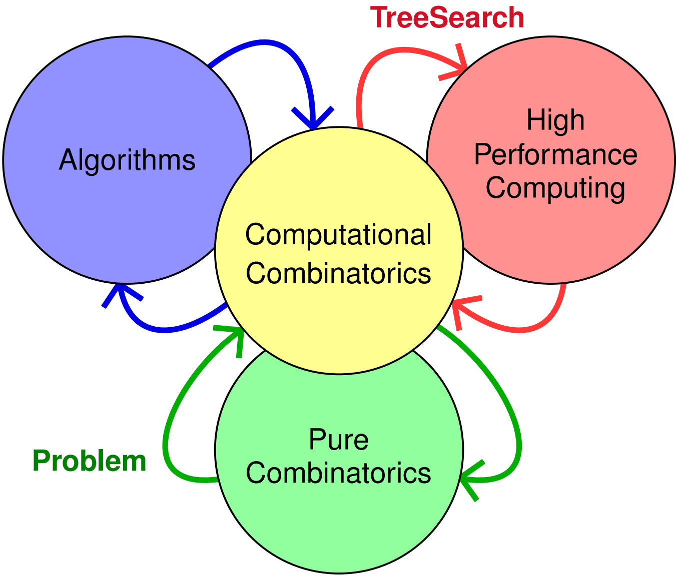
10 vertices



12 vertices

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

Computational Combinatorics



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Goal: Characterize uniquely K_r-saturated graphs.

First Step: Reduce to r-primitive graphs.

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

Edges and Non-Edges

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

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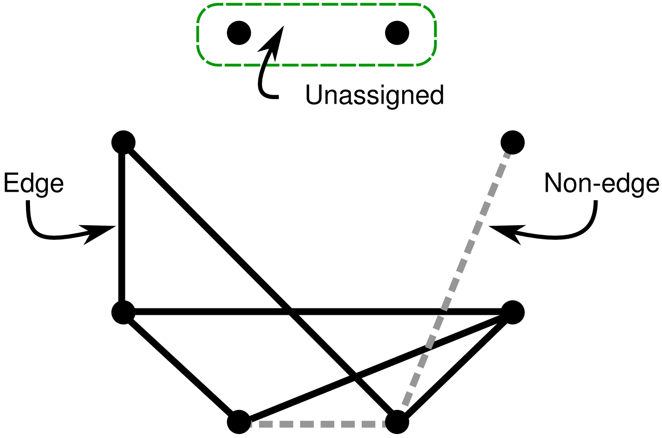

Tricolored graph

Edges, Non-Edges, and Variables

Fix a vertex set $\{v_1, v_2, \dots, v_n\}$.

For $i, j \in \{1, \dots, n\}$, let

$$x_{i,j} = \begin{cases} 1 & v_iv_j \in E(G) \\ 0 & v_iv_j \notin E(G) \\ * & v_iv_j \text{ unassigned} \end{cases}.$$

A vector $\mathbf{x} = (x_{i,j} : i, j \in \{1, \dots, n\})$ is a **variable assignment**.

Symmetries of the System

The constraints

- There is no r-clique in G.
- Every non-edge e of G has exactly one r-clique in $G + e$.

are independent of vertex labels.

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Automorphisms of the tricolored graph define **orbits** on variables $x_{i,j}$.

Orbital Branching

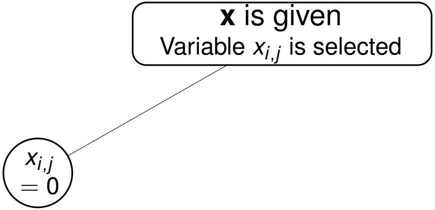
Orbital branching reduces the number of isomorphic duplicates.
(Ostrowski, Linderoth, Rossi, Smriglio, 2007)

Generalizes **branch-and-bound** strategy from Integer Programming.

Branch-and-Bound

x is given
Variable $x_{i,j}$ is selected

Branch-and-Bound



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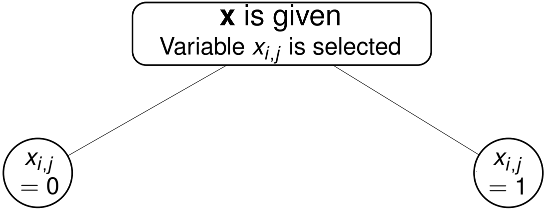

Orbital Branching

$\mathbf{x}$ is given
Orbit $\mathcal{O}$ is selected

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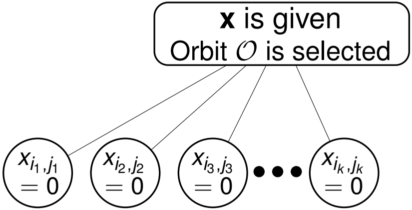

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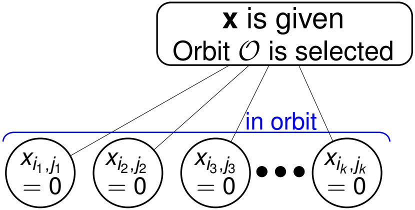

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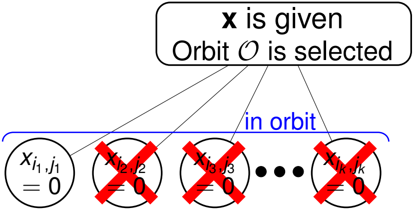

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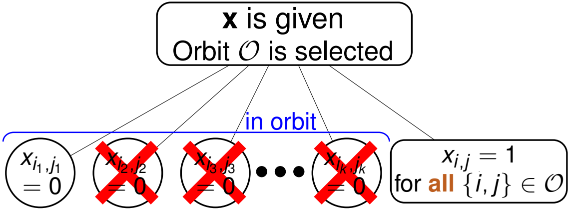

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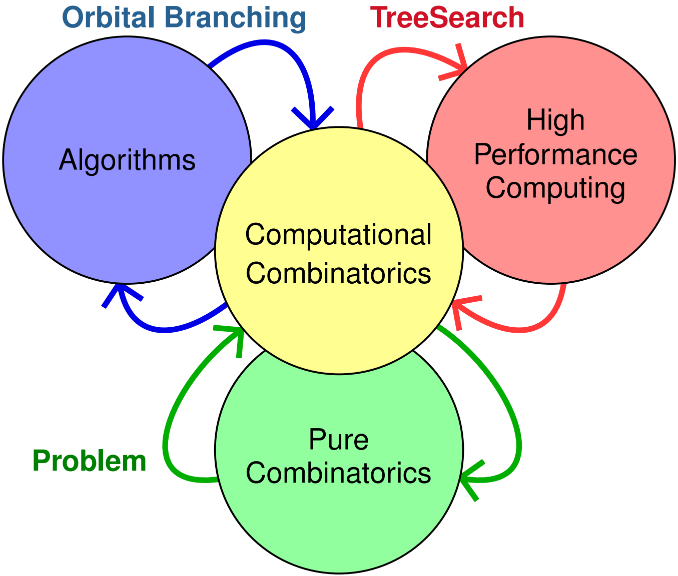
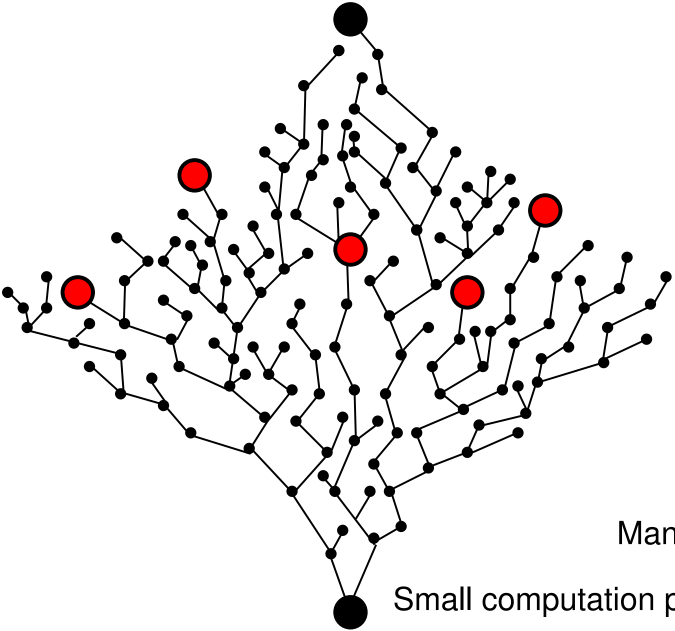
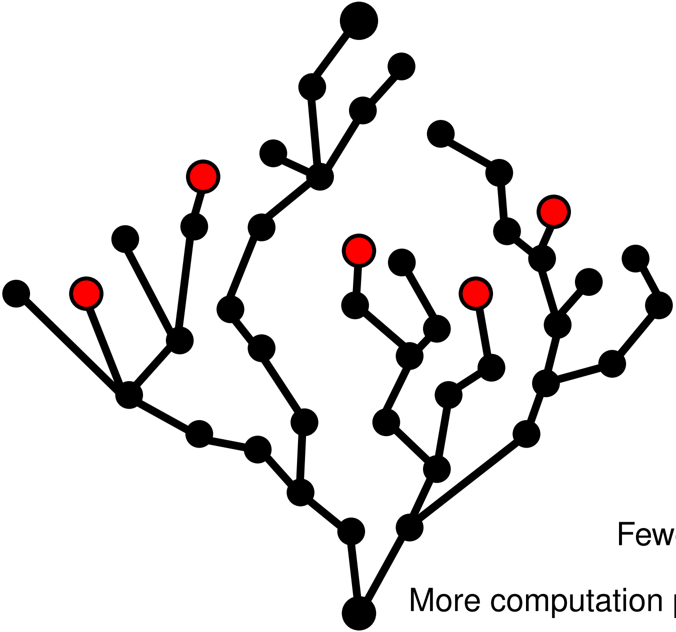




Many nodes.

Small computation per node.



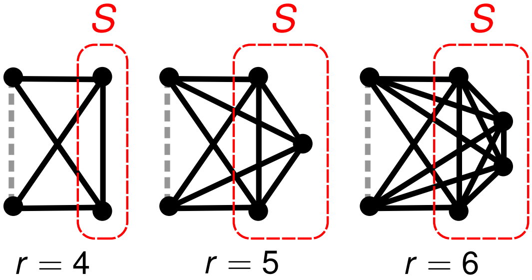
Fewer nodes.

More computation per node.

K_r-Completions

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

$x_{i,j} = 0$ **if and only if** there exists a set $S \subset [n]$, $|S| = r - 2$, so that $x_{i,a} = x_{j,a} = x_{a,b} = 1$ for all $a, b \in S$.



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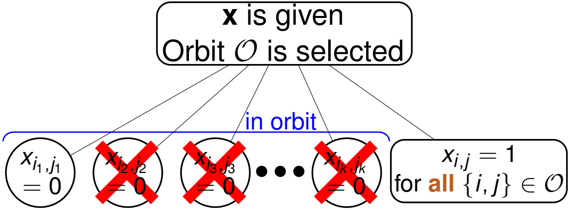

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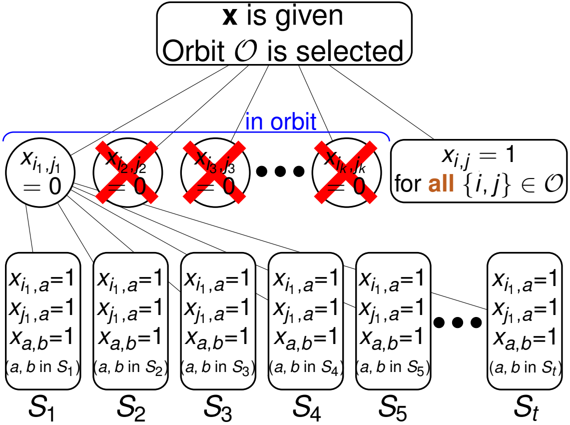
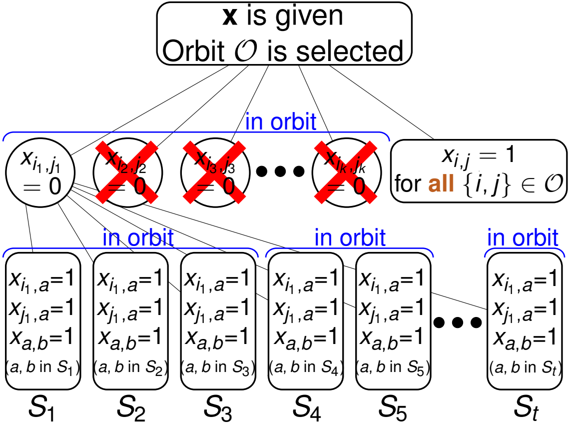
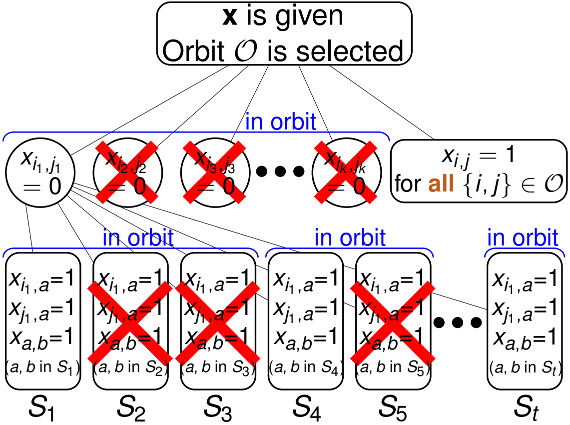


Orbital Branching with K_r-Completions



Orbital Branching with K_r-Completions



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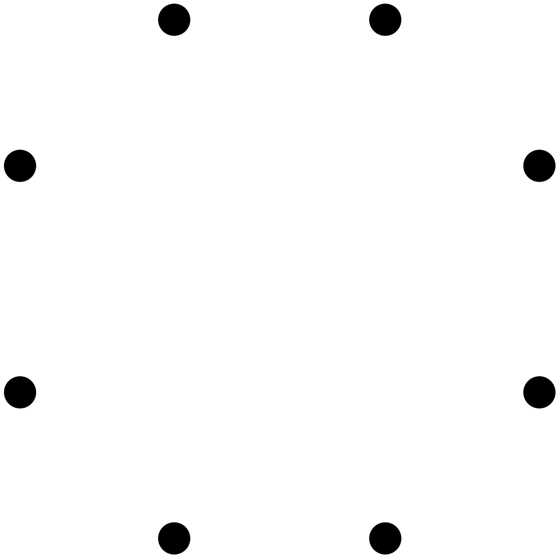
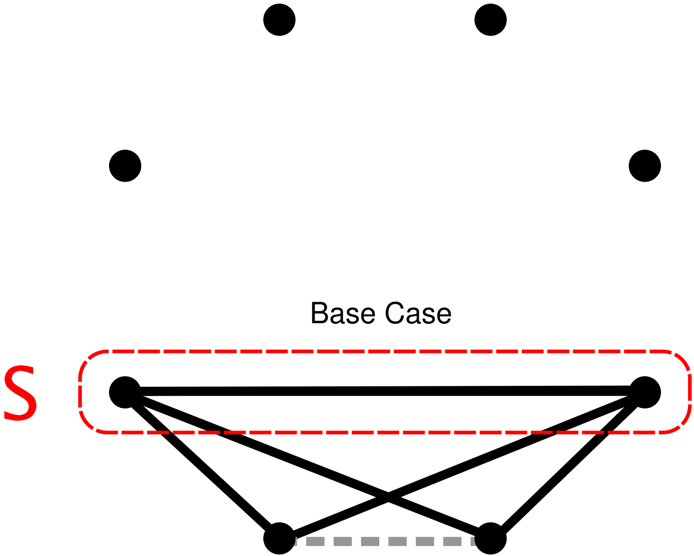


Orbital Branching with K_r-Completions



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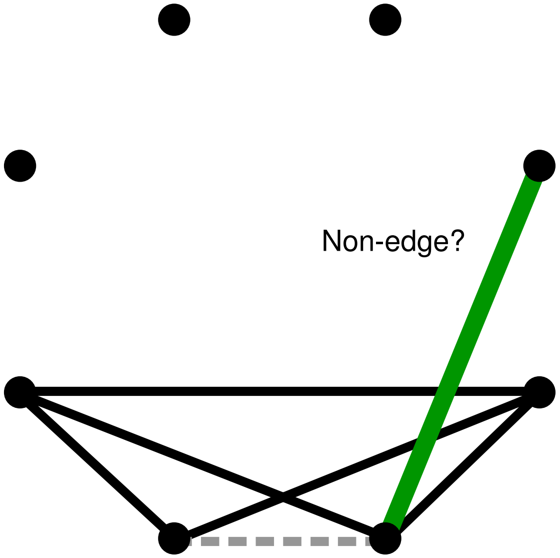

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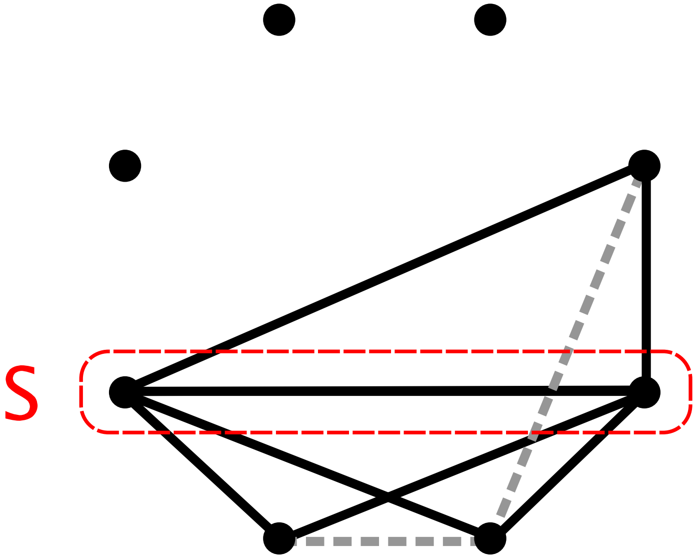

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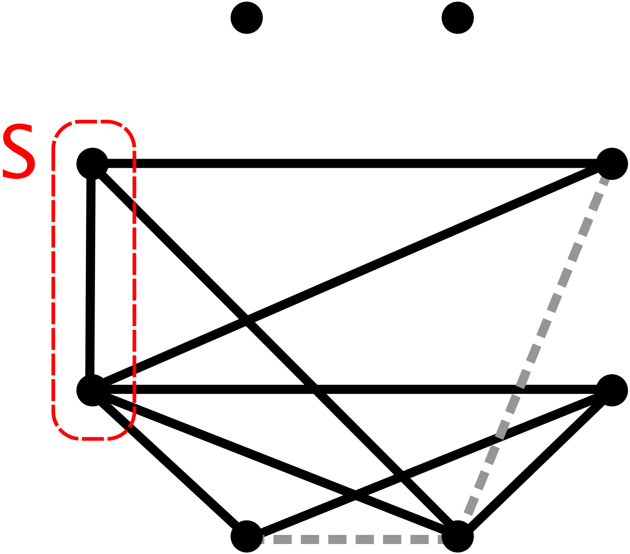

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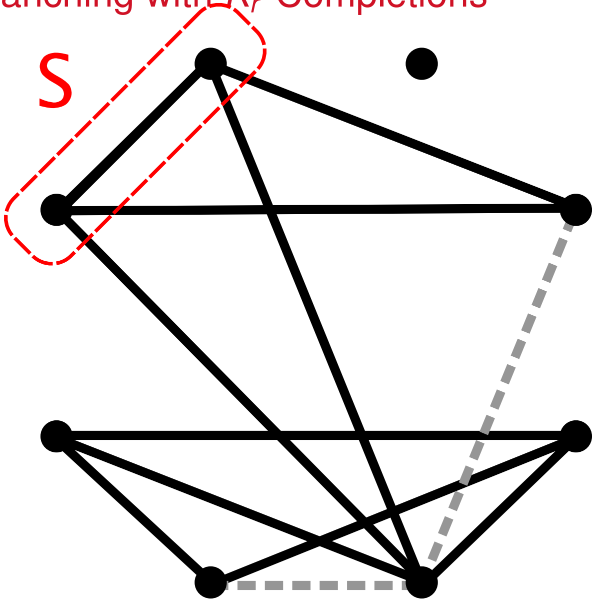
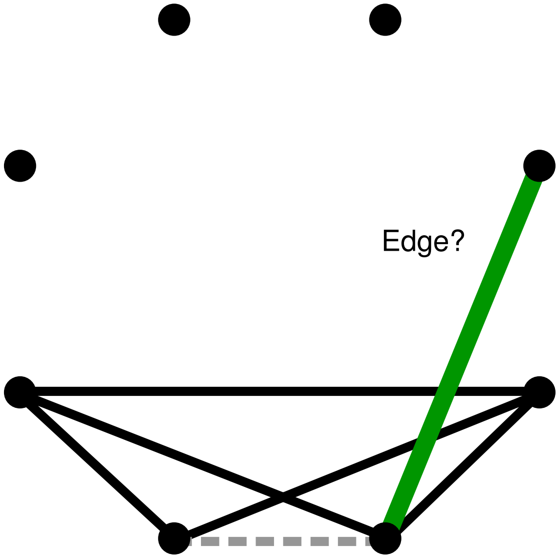
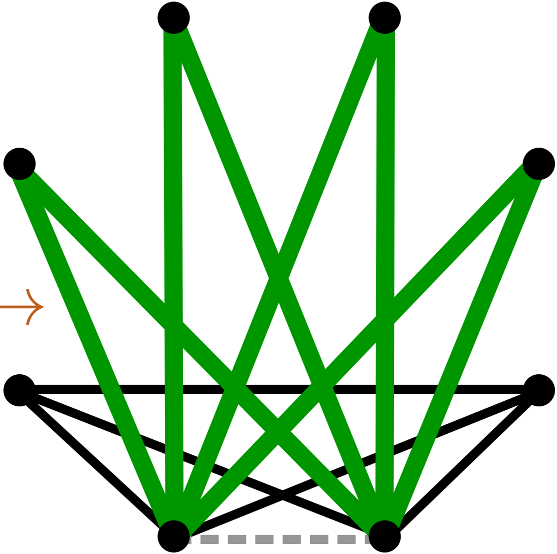


Orbital Branching with K_r-Completions

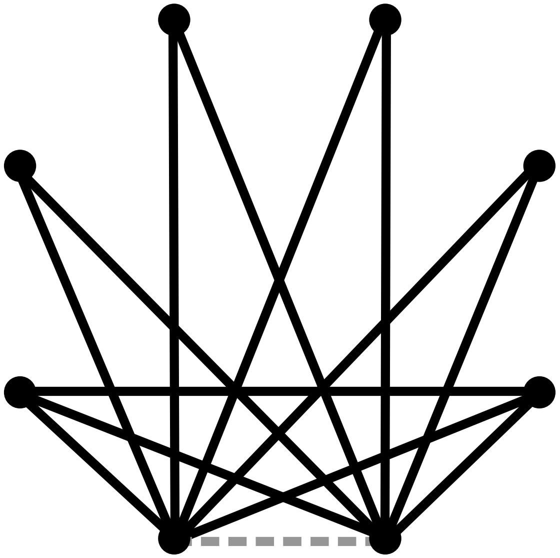


Orbital Branching with K_r-Completions

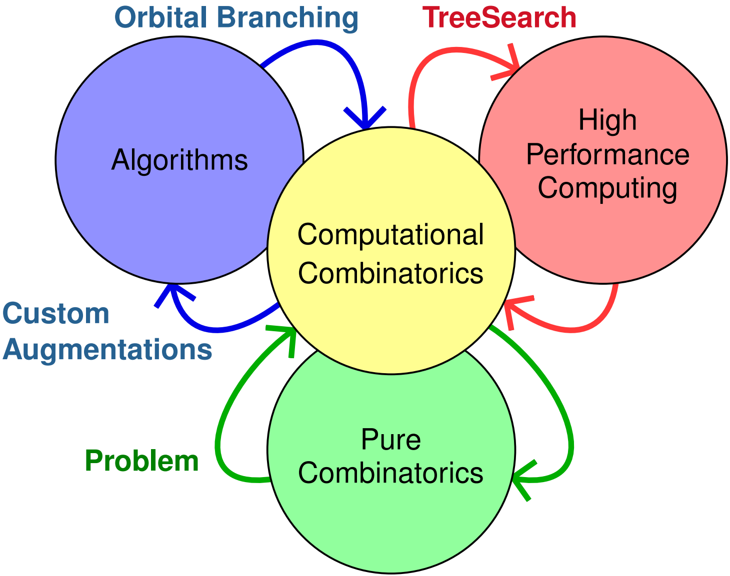
in orbit $\longrightarrow$



Orbital Branching with K_r-Completions



Computational Combinatorics



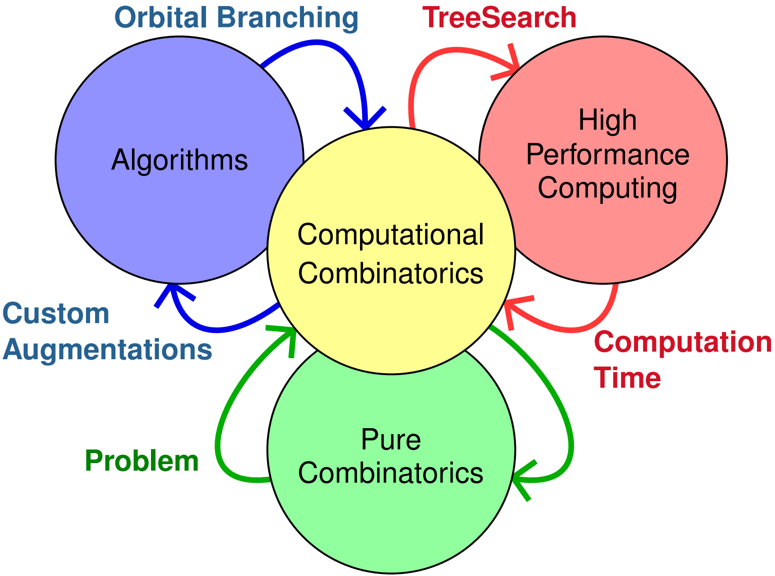
Exhaustive Search Times

n	$r = 4$	$r = 5$	$r = 6$	$r = 7$	$r = 8$
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.

($\approx 8.83 \times 10^{18}$ connected graphs of order 20)

Computational Combinatorics



clique size

vertices

$n \setminus r$		2	3	4	5	6	7	8	
2									
3									
4									
5									
6									
7									
8									
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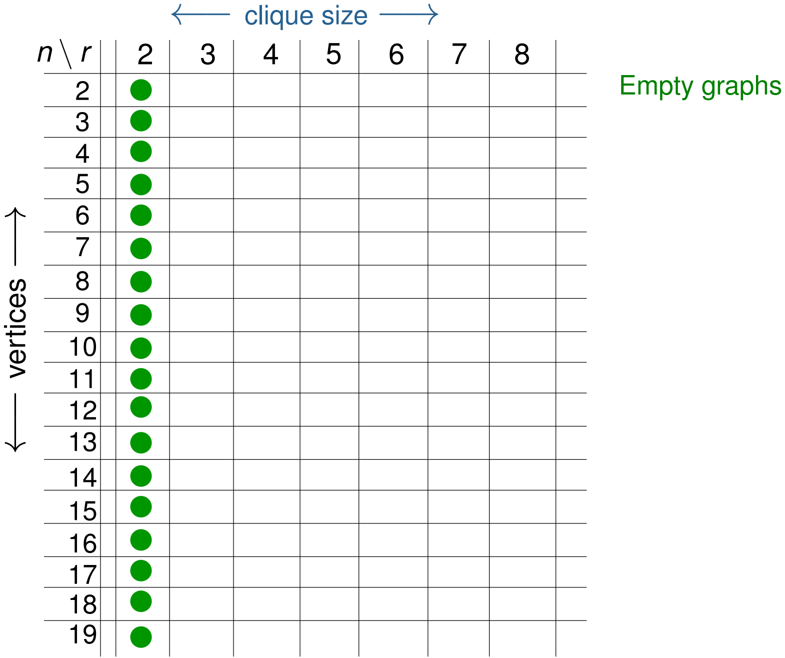
19									


clique size
n \ r
2
3
4
5
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7
8
vertices
9
10
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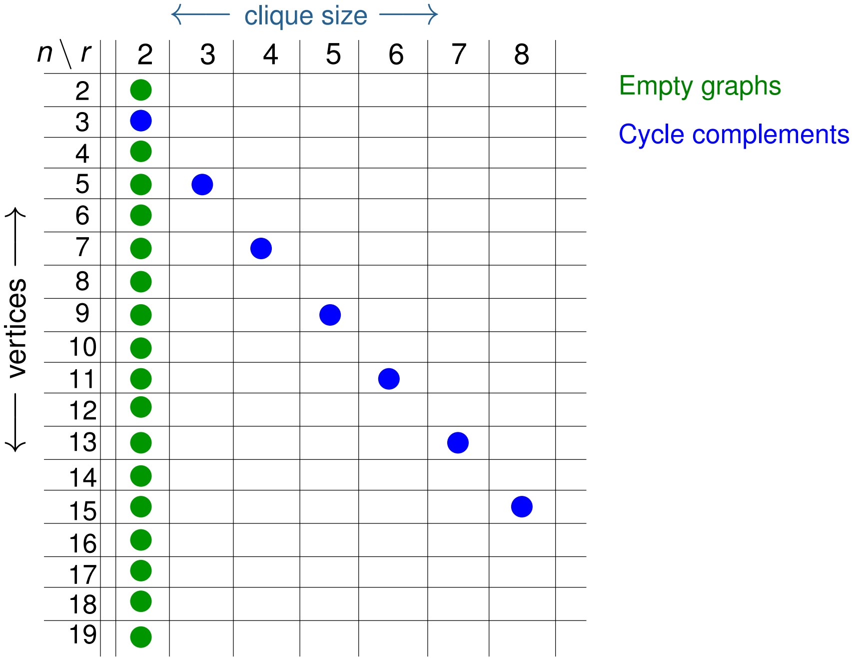
16
17
18
19
Empty graphs


clique size
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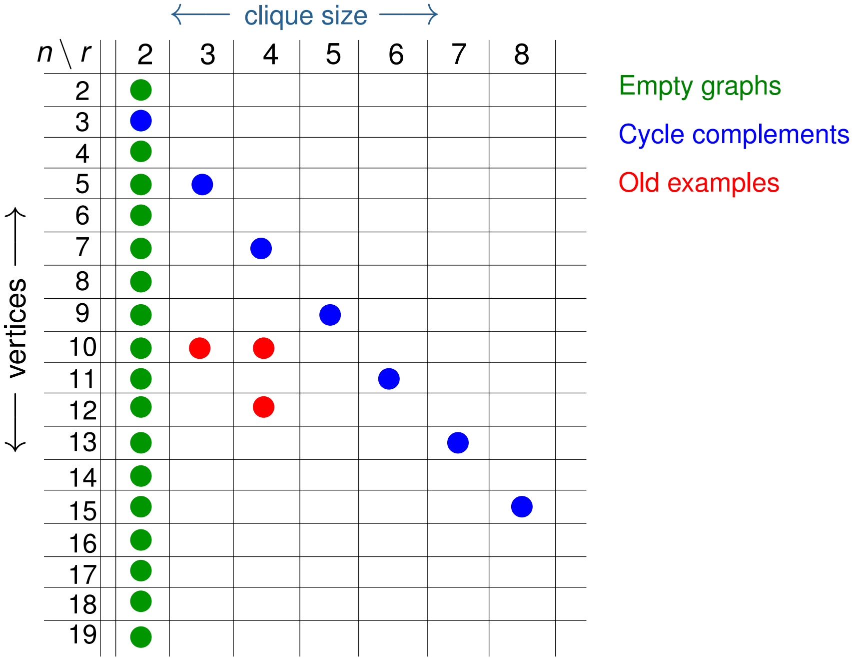
vertices
Empty graphs
Cycle complements


clique size
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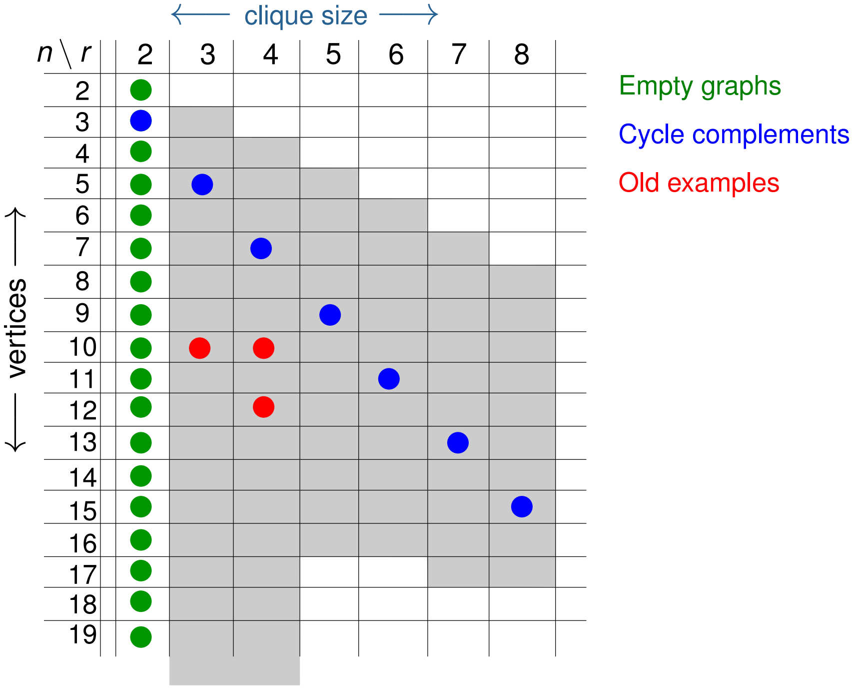
vertices
Empty graphs
Cycle complements
Old examples


clique size
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vertices
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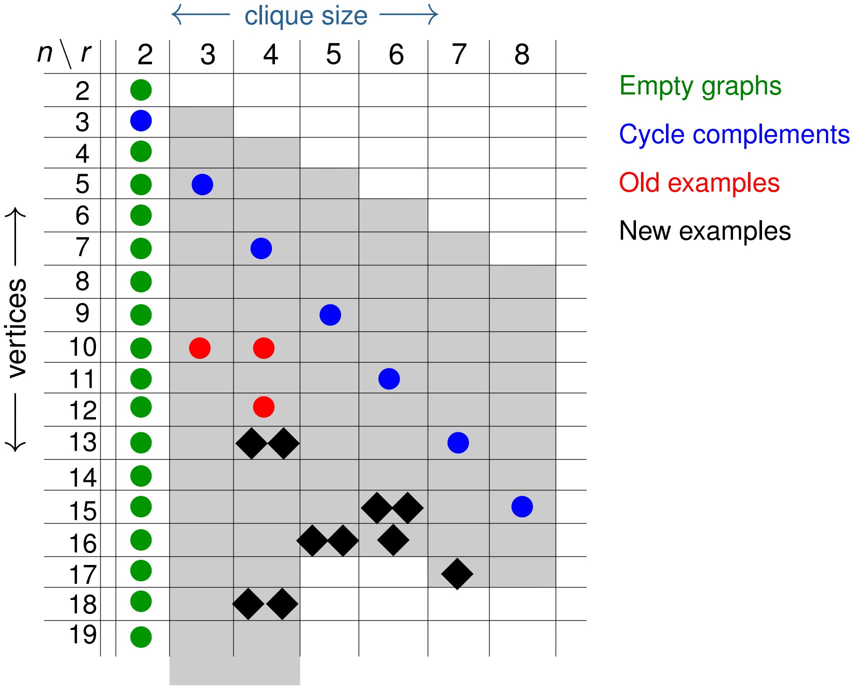
Empty graphs
Cycle complements
Old examples



clique size
n \ r
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5
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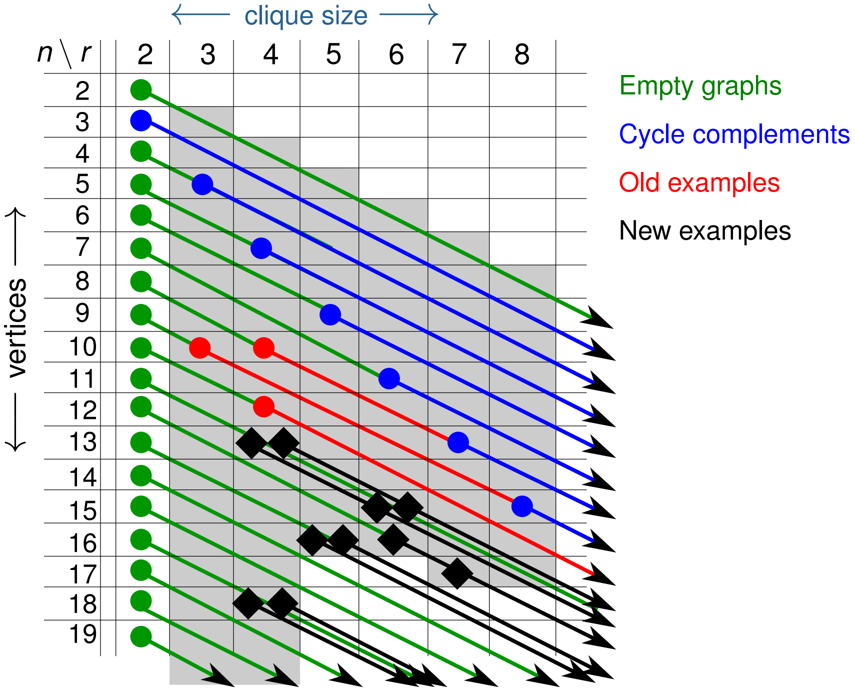
vertices
Empty graphs
Cycle complements
Old examples
New examples



clique size
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vertices
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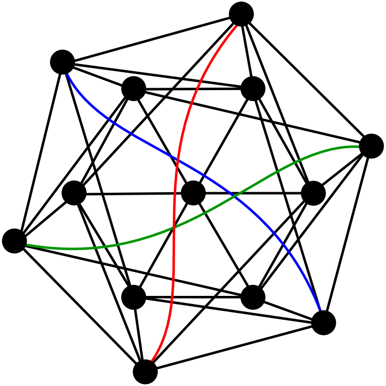
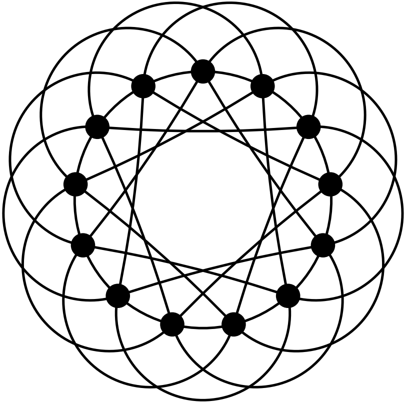
18
19
Empty graphs
Cycle complements
Old examples
New examples

4-Primitive Graphs

$n = 13$



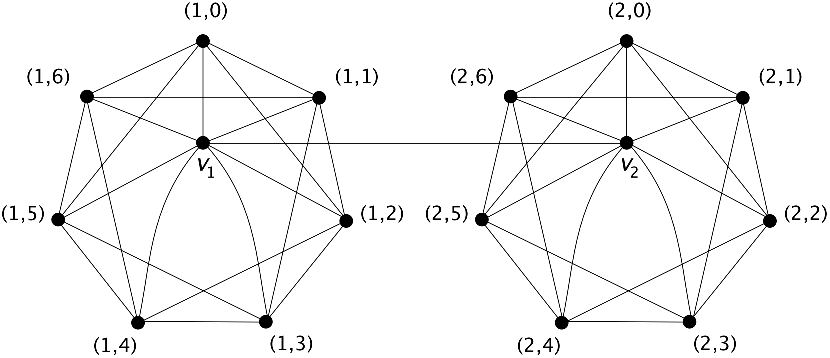
$G_{13}^{(A)}$



Paley(13)

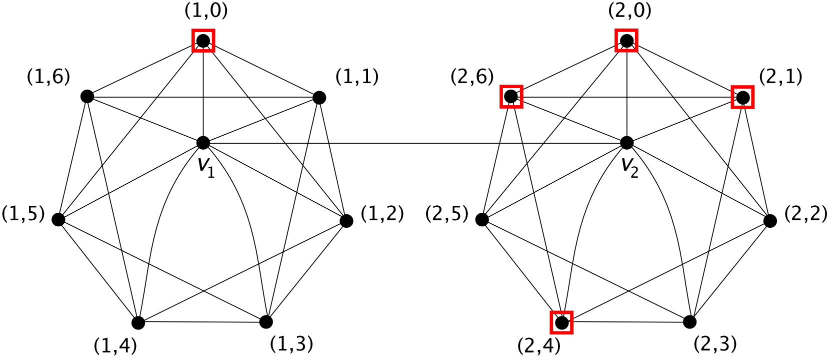
5-Primitive Graph

$n = 16 : G_{16}^{(A)}$



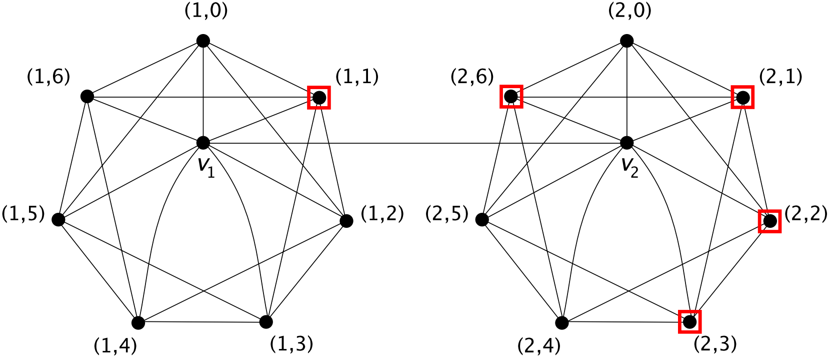
5-Primitive Graph

$n = 16 : G_{16}^{(A)}$



5-Primitive Graph

$n = 16 : G_{16}^{(A)}$



5-Primitive Graph

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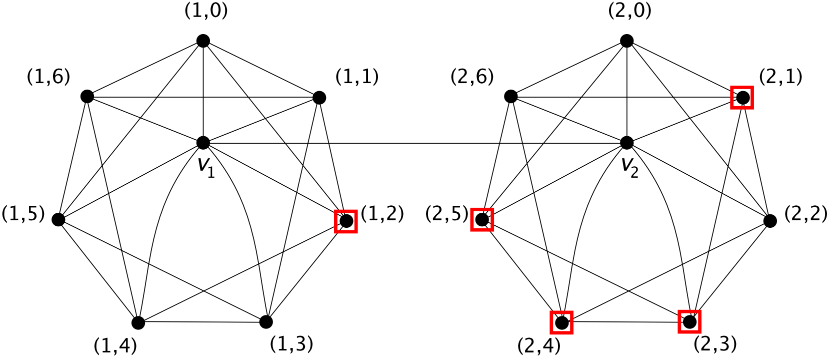

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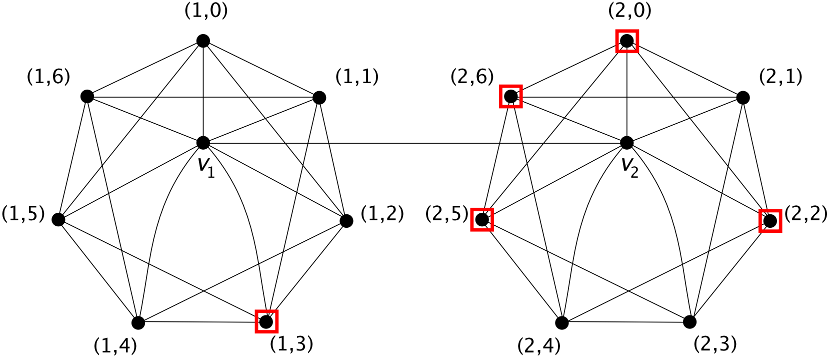

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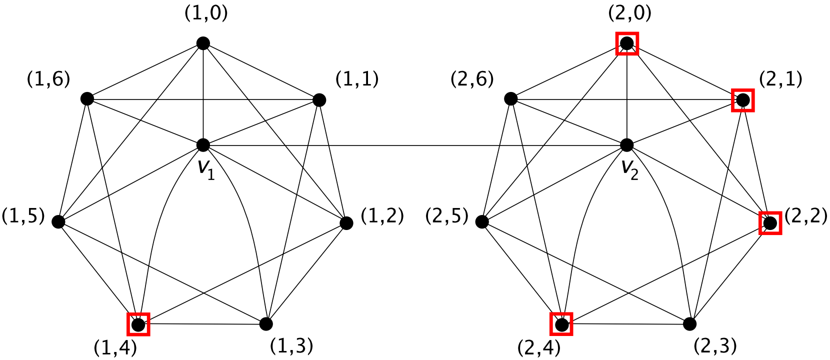
$n = 16 : G_{16}^{(A)}$



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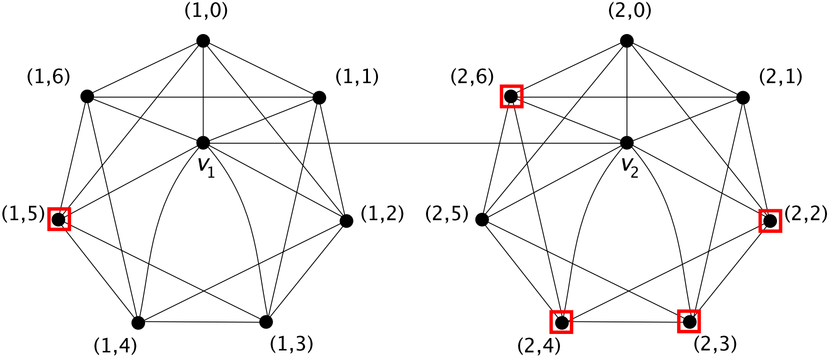

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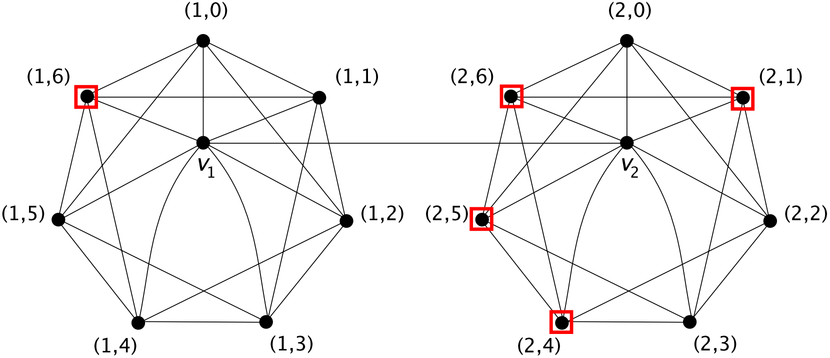

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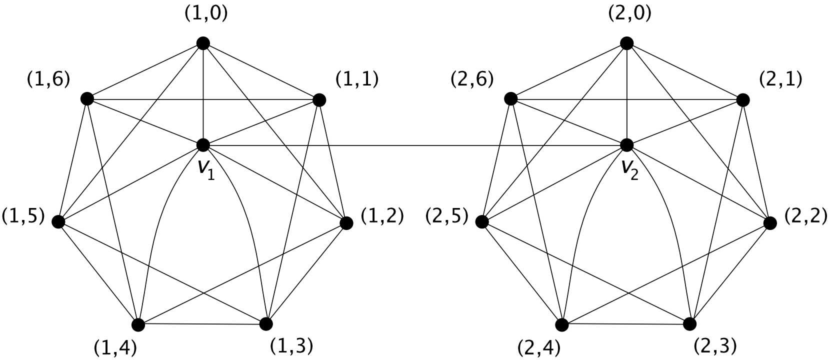
$n = 16 : G_{16}^{(A)}$



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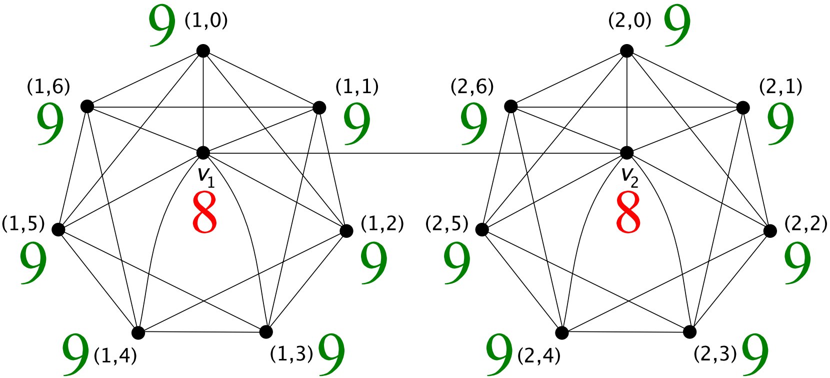
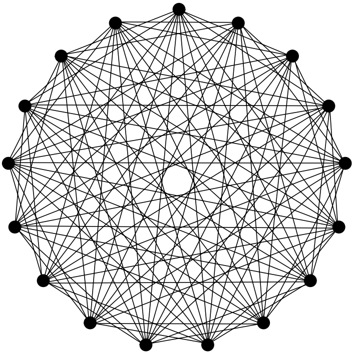


Not all *r*-primitive graphs are regular!

7-Primitive Graph

$n = 17 : G_{17}^{(A)}$



7-Primitive Graph

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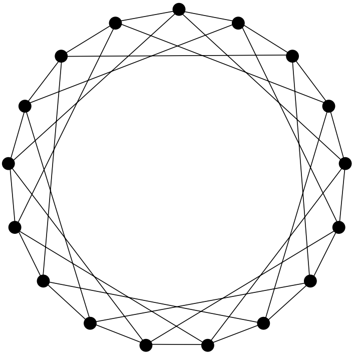

The **Cayley complement** $\overline{C}(\mathbb{Z}_n, S)$ has vertex set $\{0, 1, \dots, n-1\}$ and an edge ij if and only if $|i - j| \pmod{n} \notin S$.

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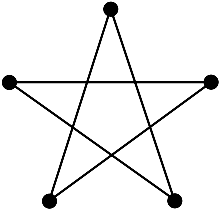
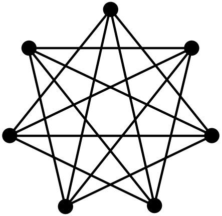
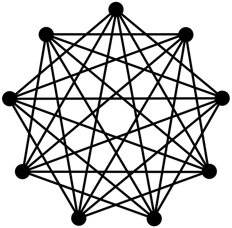
For $r \geq 1$, $\overline{C}(\mathbb{Z}_{2r-1}, \{1\}) \cong \overline{C_{2r-1}}$ is r-primitive.



$\overline{C_5}$



$\overline{C_7}$



$\overline{C_9}$

Searching for r-Primitive Cayley Complements

To search for Cayley complements $\overline{C}(\mathbb{Z}_n, S)$ with $|S| = g$:

1. Select a generator set $S = \{a_1 = 1 < a_2 < a_3 < \cdots < a_g\} \subseteq \mathbb{Z}$.

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4. Check if $\overline{C}(\mathbb{Z}_n, S) + \{0, a_i\}$ has a unique r-clique for all $a_i \in S$.

Used Niskanen and Östergård's *cliquer* software to compute $\omega(G)$.

Two or Three Generators

S	r	n
$\{1,4\}$	7	17
$\{1,6\}$	16	37
$\{1,8\}$	29	65
$\{1,10\}$	46	101
$\{1,12\}$	67	145

$g = 2$

S	r	n
$\{1,5,6\}$	9	31
$\{1,8,9\}$	22	73
$\{1,11,12\}$	41	133
$\{1,14,15\}$	66	211
$\{1,17,18\}$	97	307

$g = 3$

Infinite Families

Conjecture (Hartke, Stolee, 2012) Let $t \geq 1$,

$$n = 4t^2 + 1, \qquad \text{and} \qquad r = 2t^2 - t + 1.$$

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

Conjecture (Hartke, Stolee, 2012) Let $t \geq 1$,

$$n = 9t^2 - 3t + 1 \qquad \text{and} \qquad r = 3t^2 - 2t + 1.$$

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

Infinite Families

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Proof uses **counting** method.

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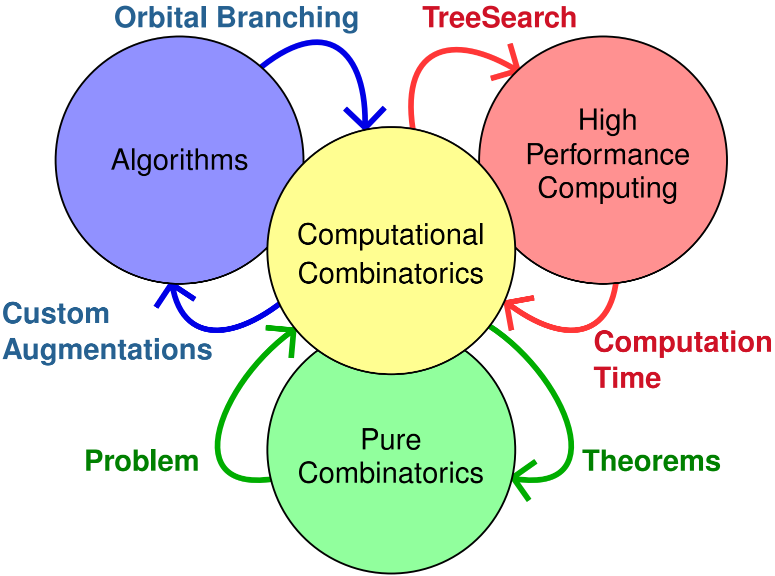
Proof uses **discharging** method.

Computational Combinatorics



What Next?

Technique-specific

1. **Orbital Branching:** Formalize custom augmentations for arbitrary constraint systems.
2. **Discharging:** Automate process so computer can discover and write proofs.
3. **More Techniques:** Find, Adapt, or Develop.

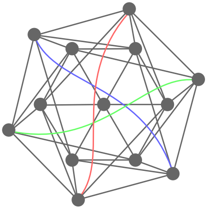
Computational Combinatorics and the search for Uniquely K_r-Saturated Graphs

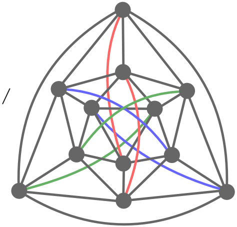
Derrick Stolee

Iowa State University

dstolee@iastate.edu

http://www.math.iastate.edu/dstolee/





September 12, 2013

Joint work with Stephen G. Hartke, appeared in *Electronic Journal of Combinatorics*, 2012.