

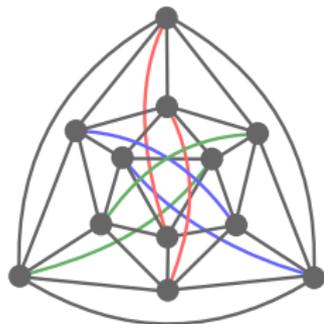
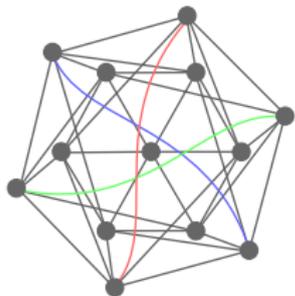
Computational Combinatorics and the search for Uniquely K_r -Saturated Graphs

Stephen G. Hartke

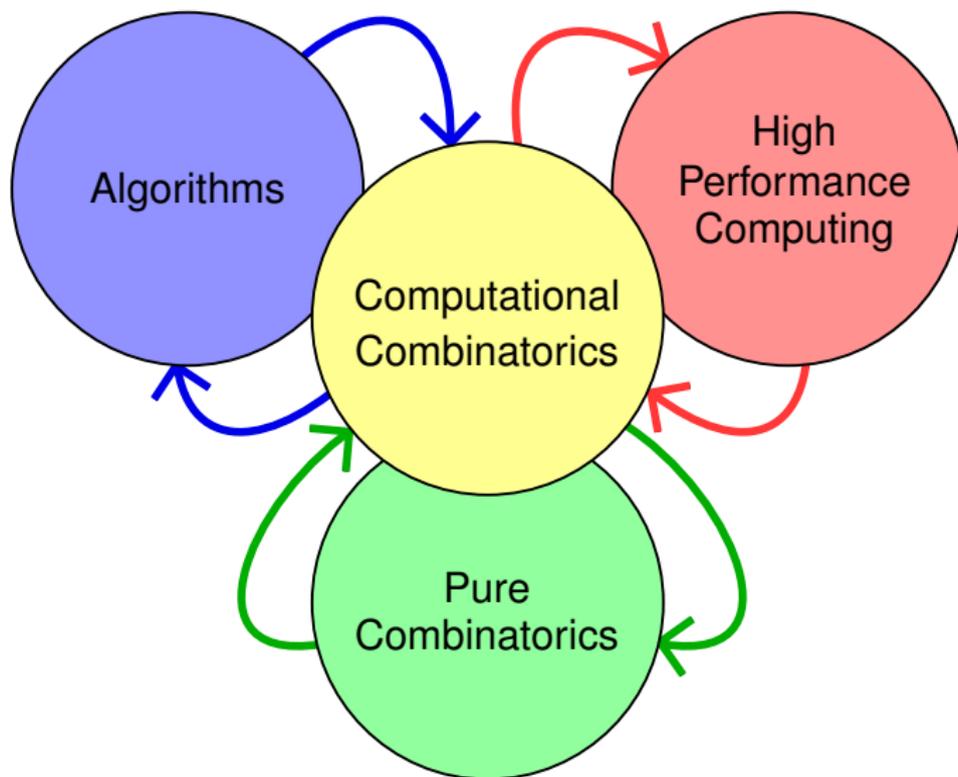
University of Nebraska–Lincoln, USA

hartke@math.unl.edu

<http://www.math.unl.edu/~shartke2/>



What is Computational Combinatorics?



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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

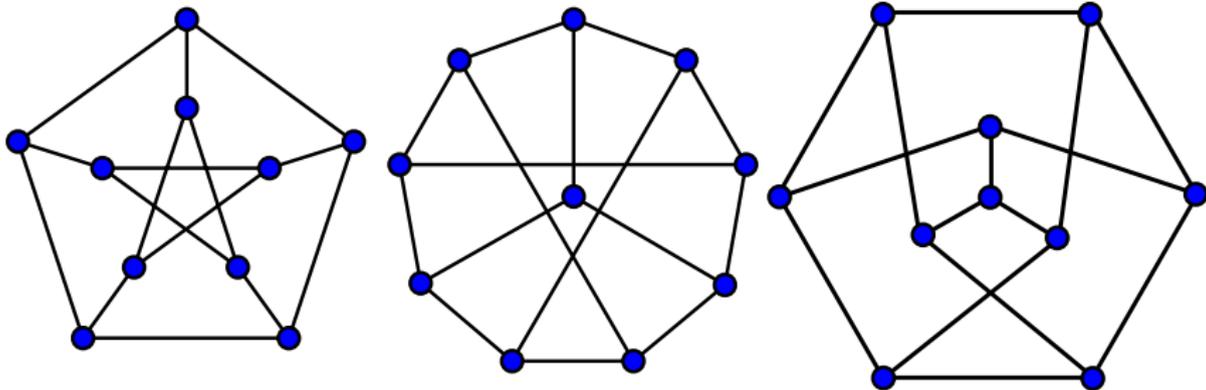
Determine if certain **combinatorial objects** exist with given **structural** or **extremal** properties.

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)

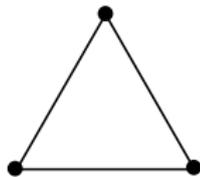
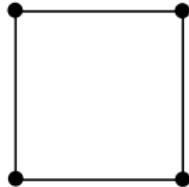
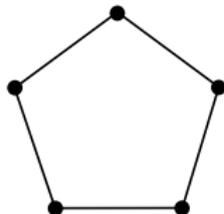
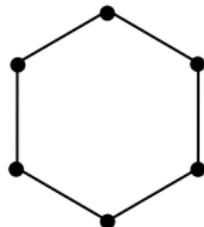
Combinatorial Object: Graphs

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.



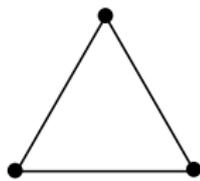
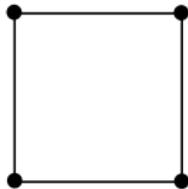
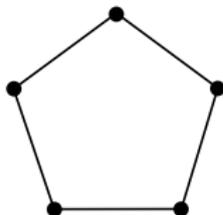
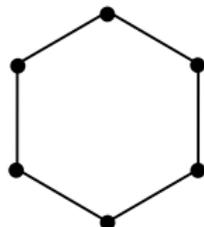
Combinatorial Object: Graphs

Cycles C_k

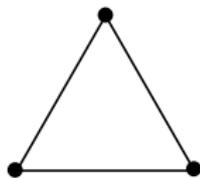
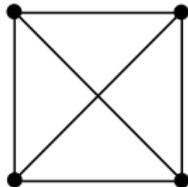
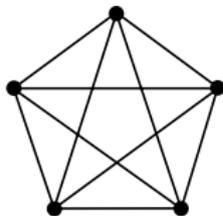
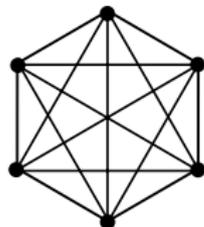
 C_3  C_4  C_5  C_6

Combinatorial Object: Graphs

Cycles C_k

 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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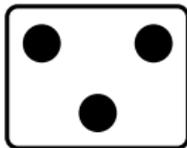
The computer performs a long, detailed case analysis.

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

- Combinatorial Generation
- Combinatorial Optimization
- Graph Algorithms

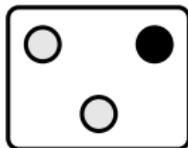
Example: Generating Graphs by Edges

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



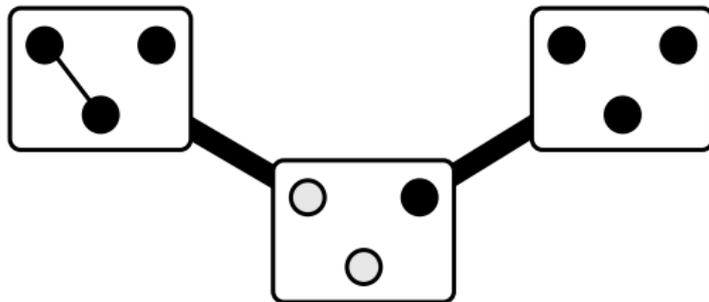
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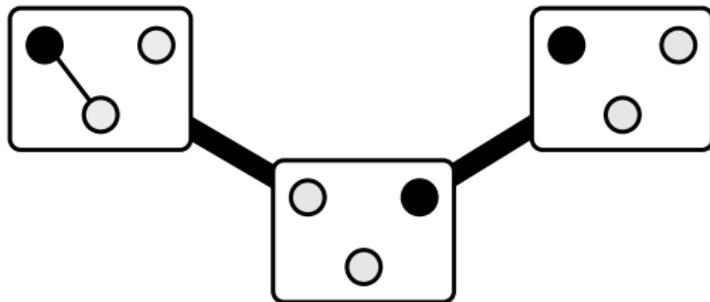
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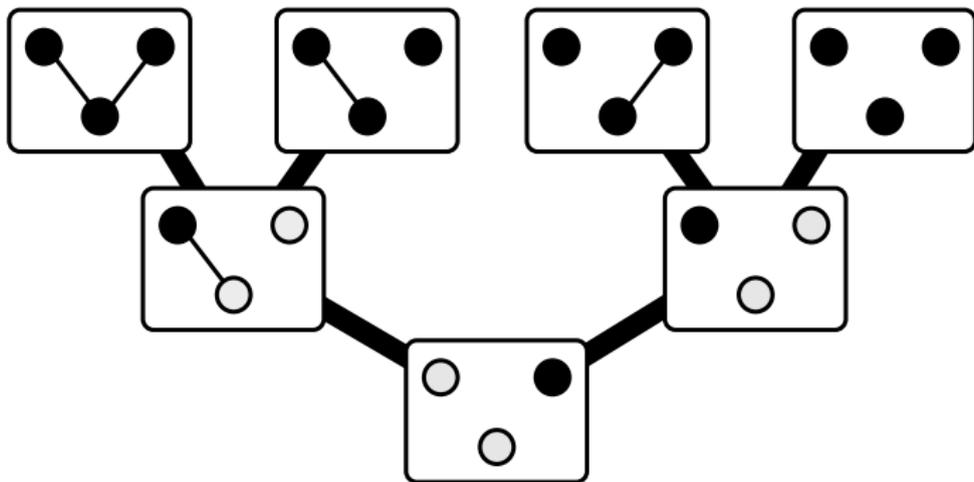
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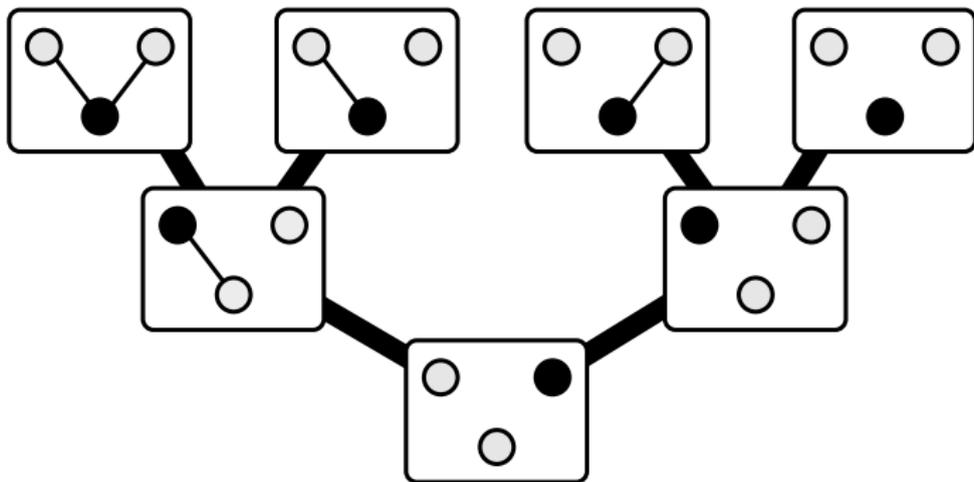
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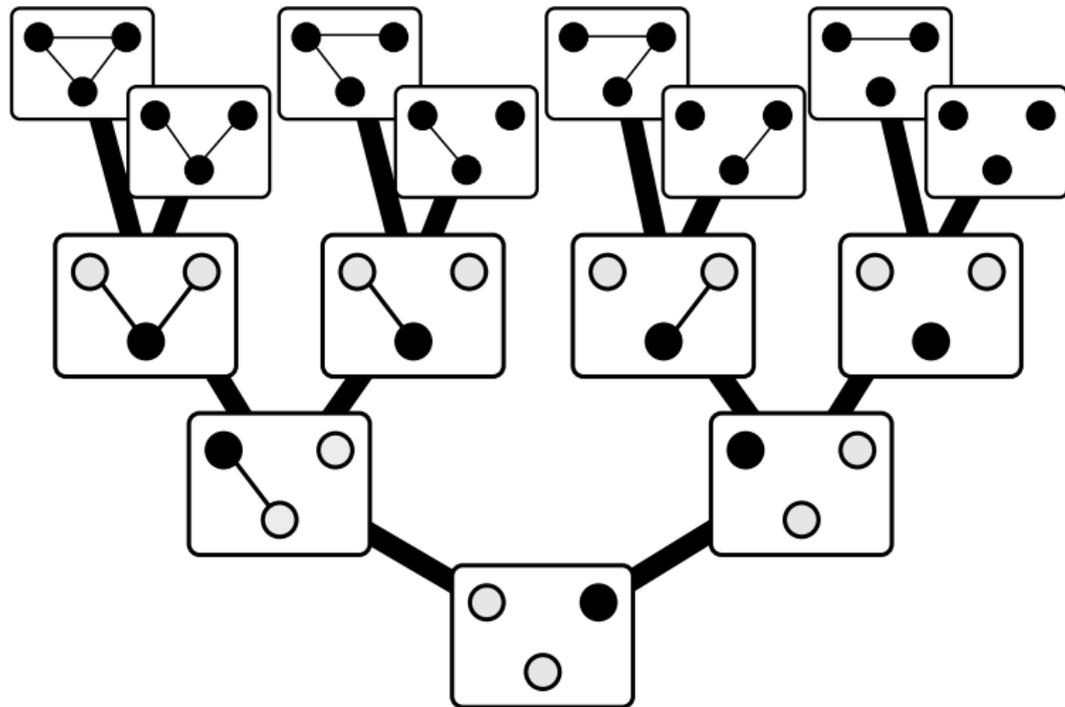
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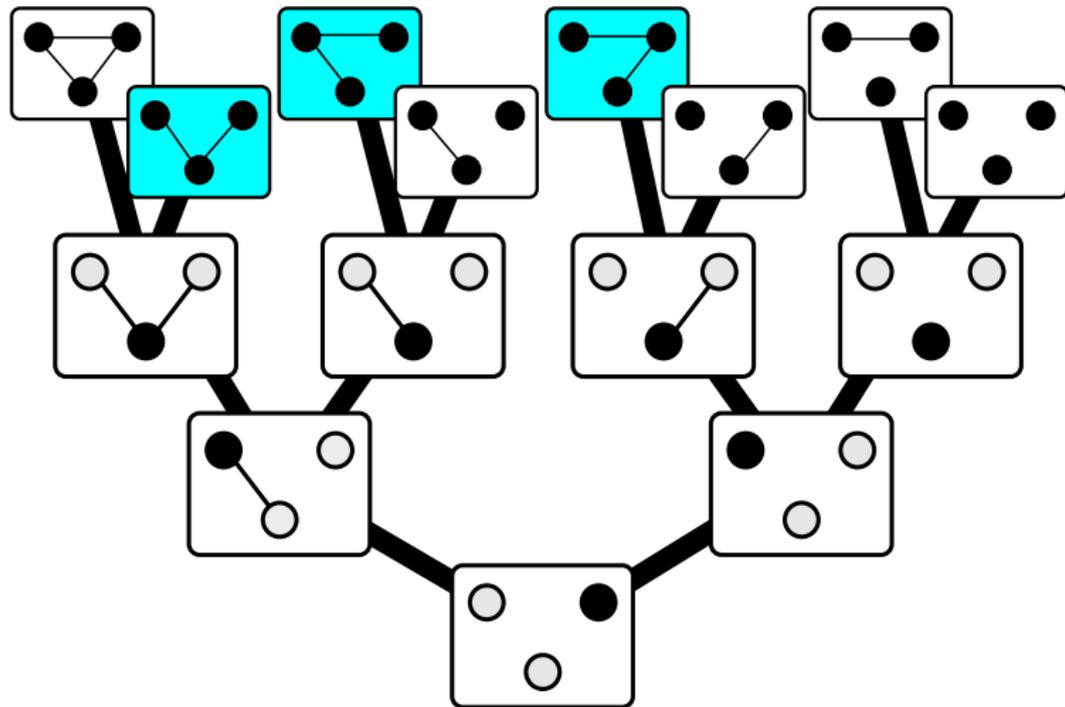
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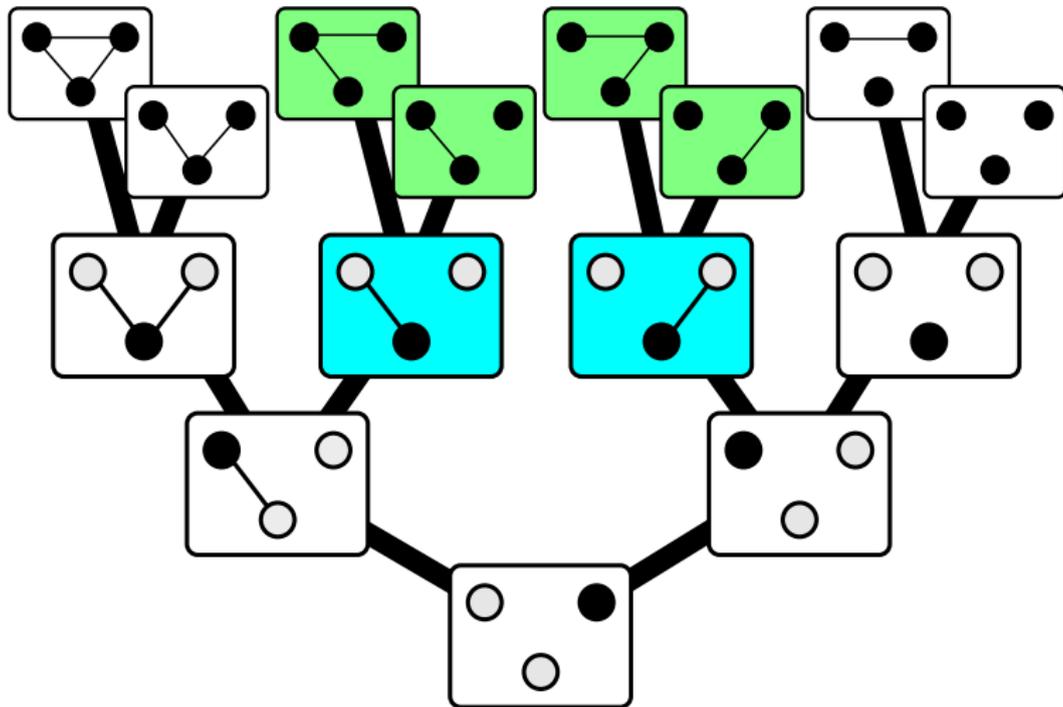
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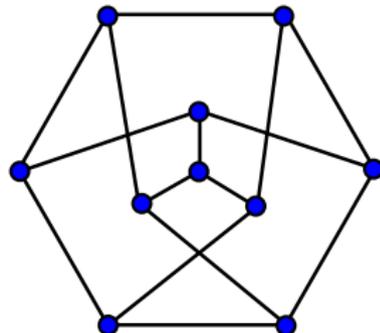
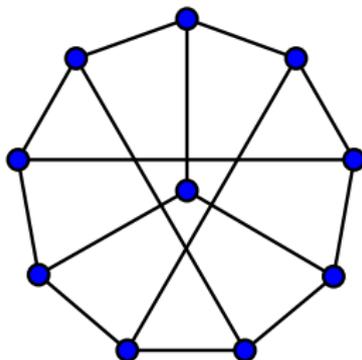
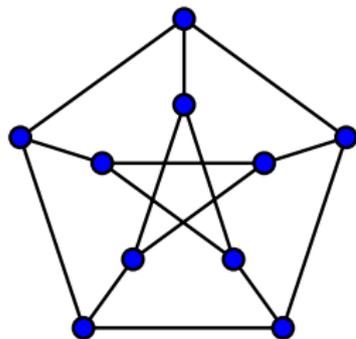


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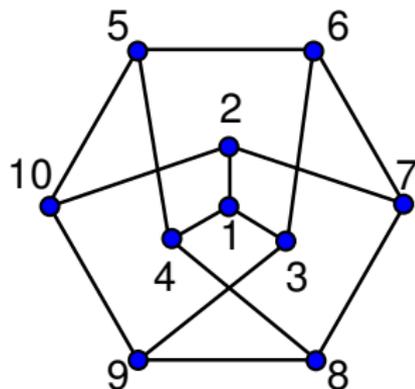
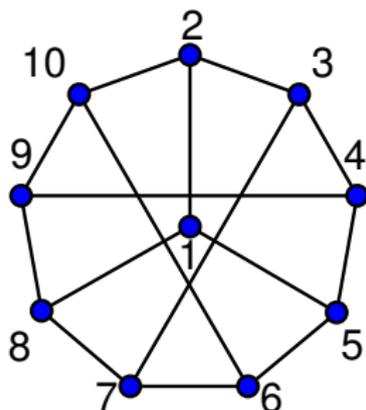
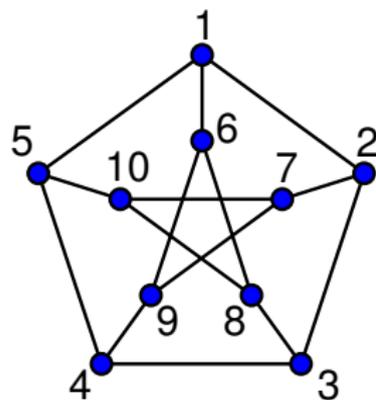
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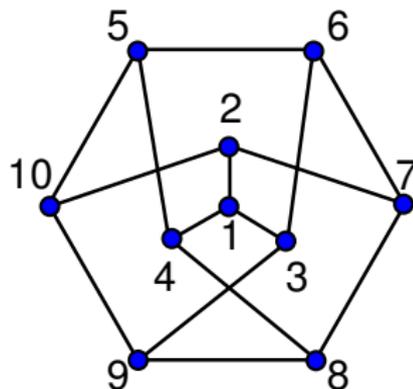
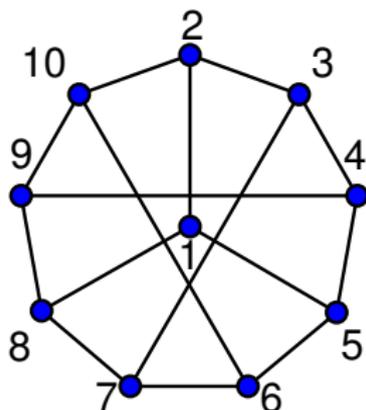
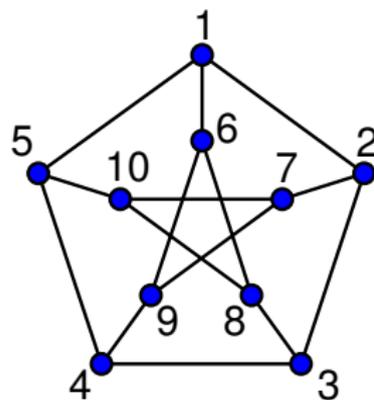


Example: Generating Graphs by Edges



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 $2^{\Omega(n^2)}$.

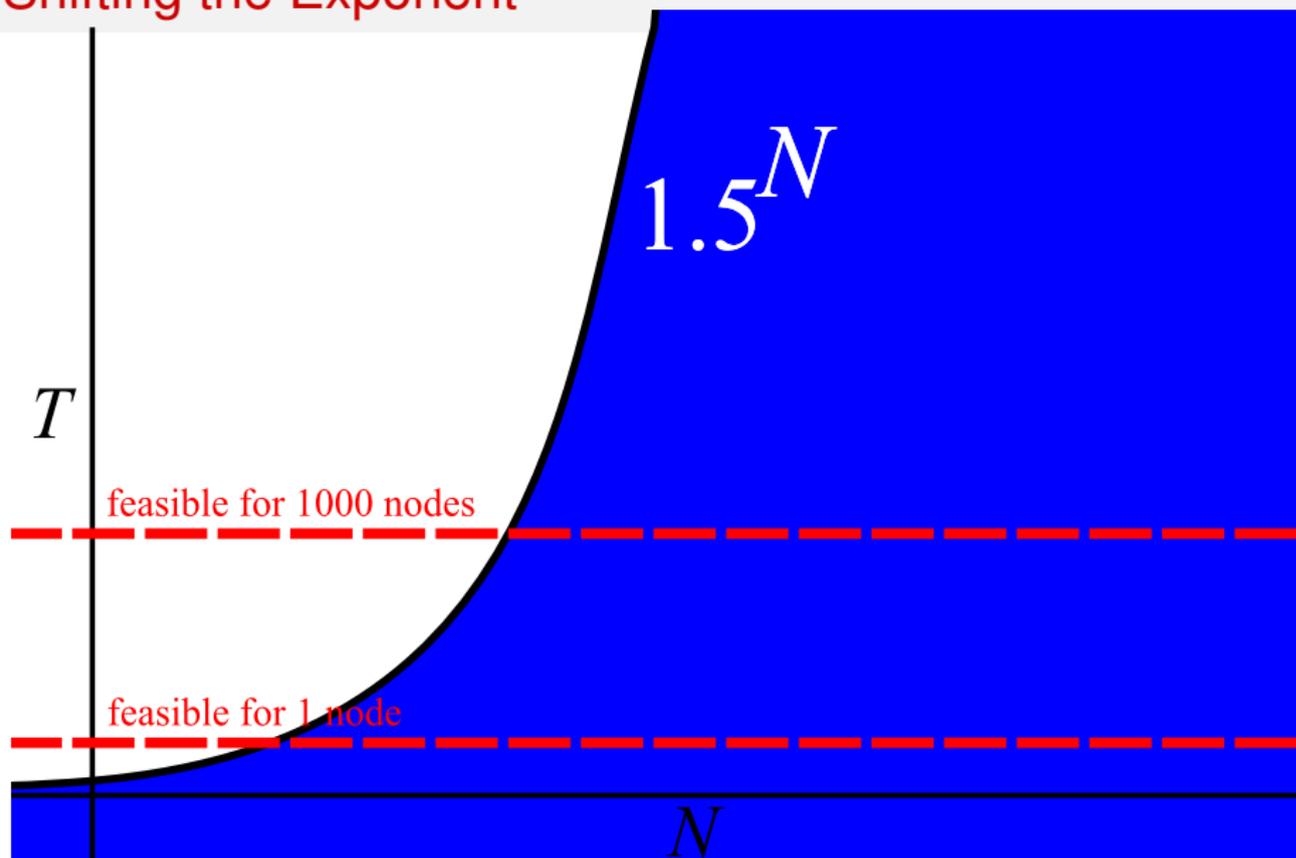
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Requires about **1 day** of CPU Time.

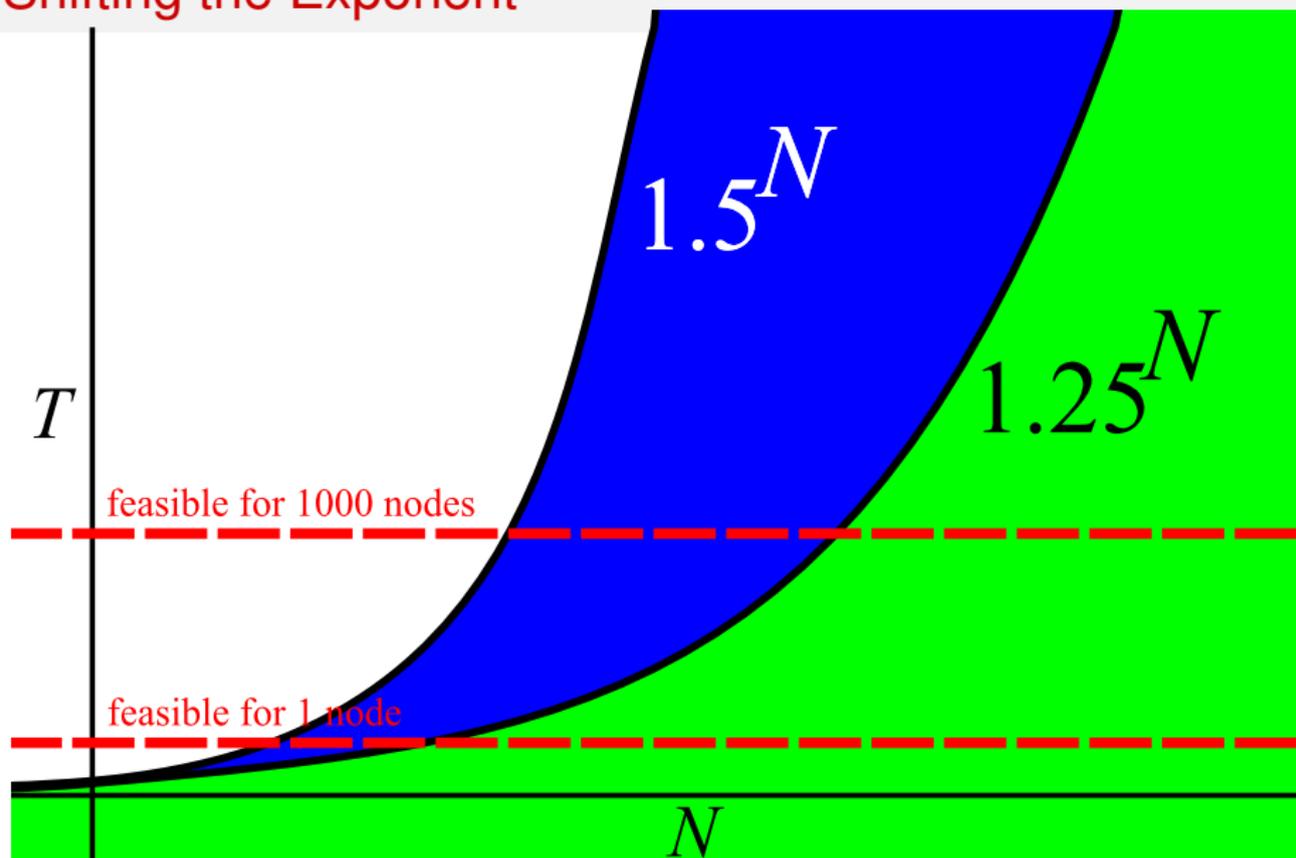
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Requires over **1 year** of CPU Time.

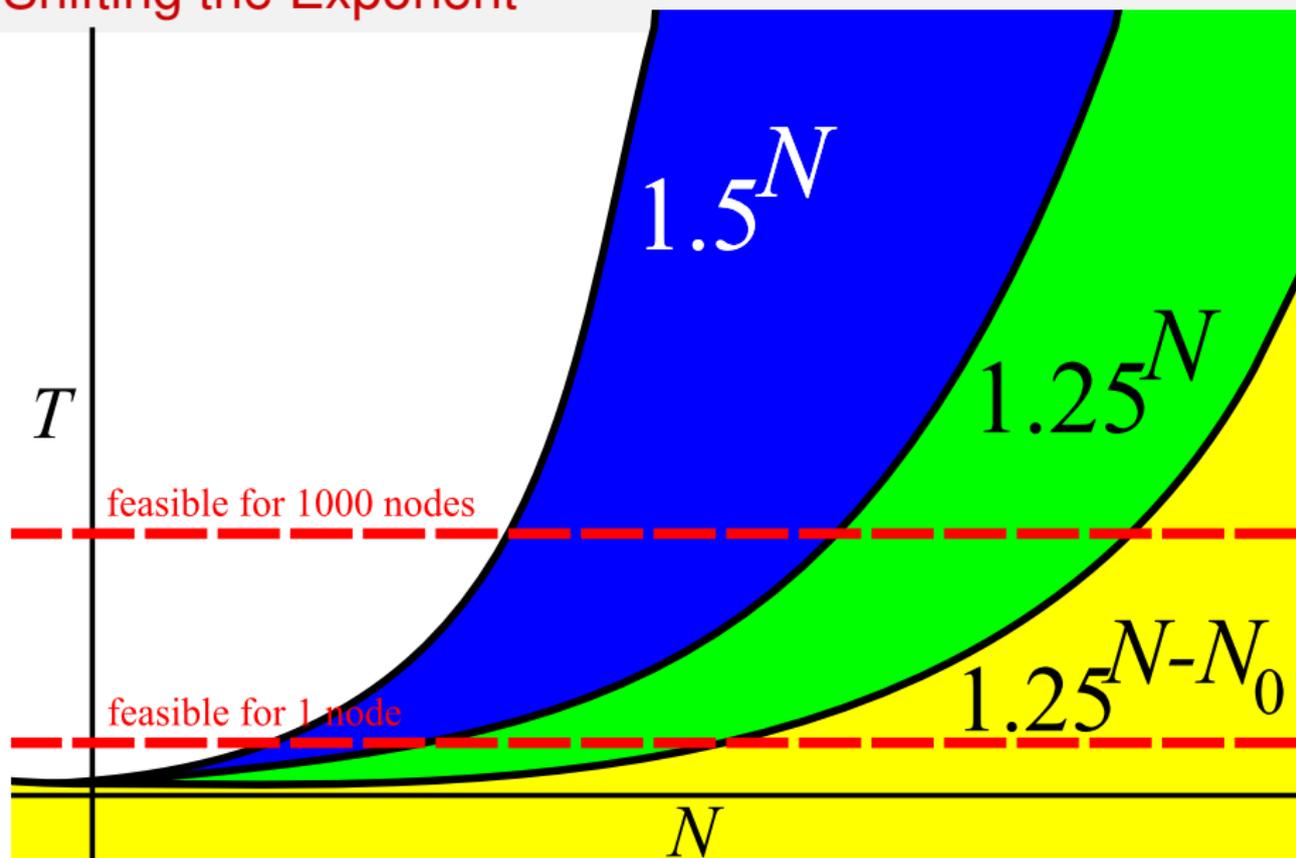
Shifting the Exponent



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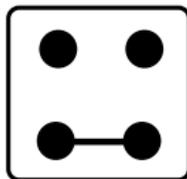


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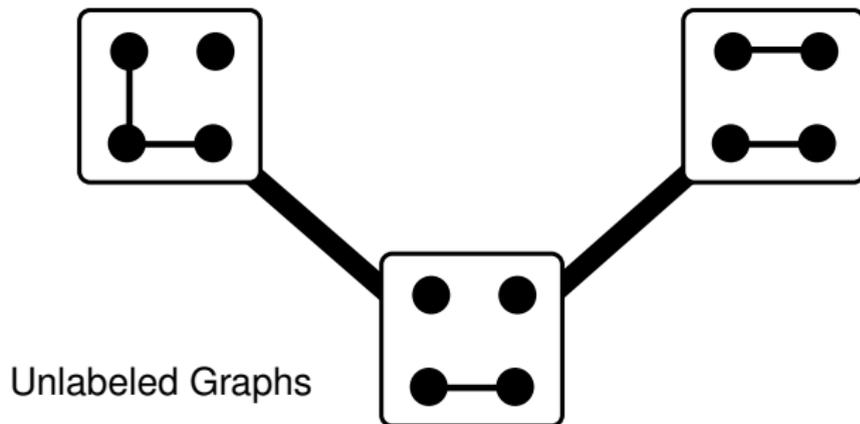


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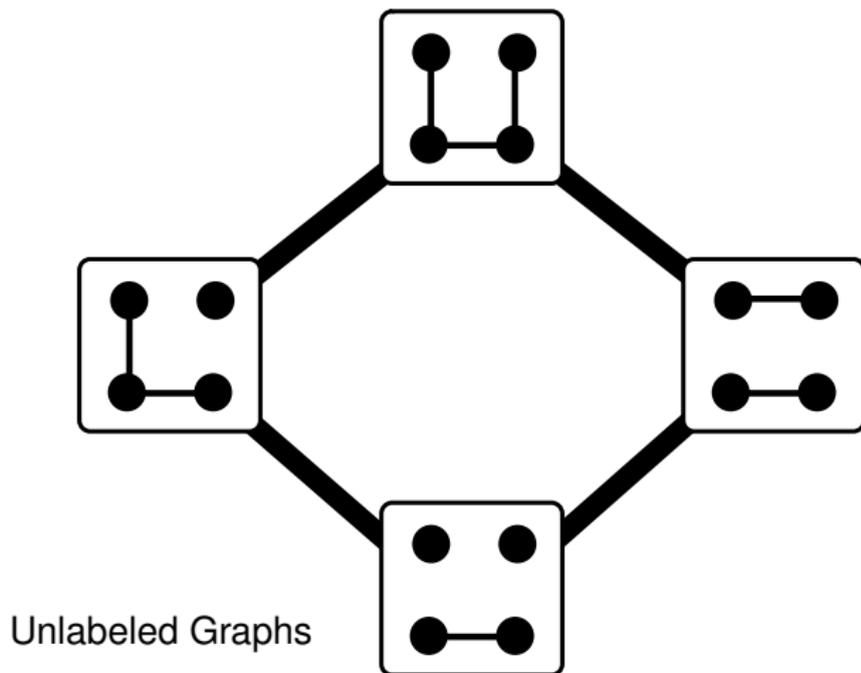
Unlabeled Graphs



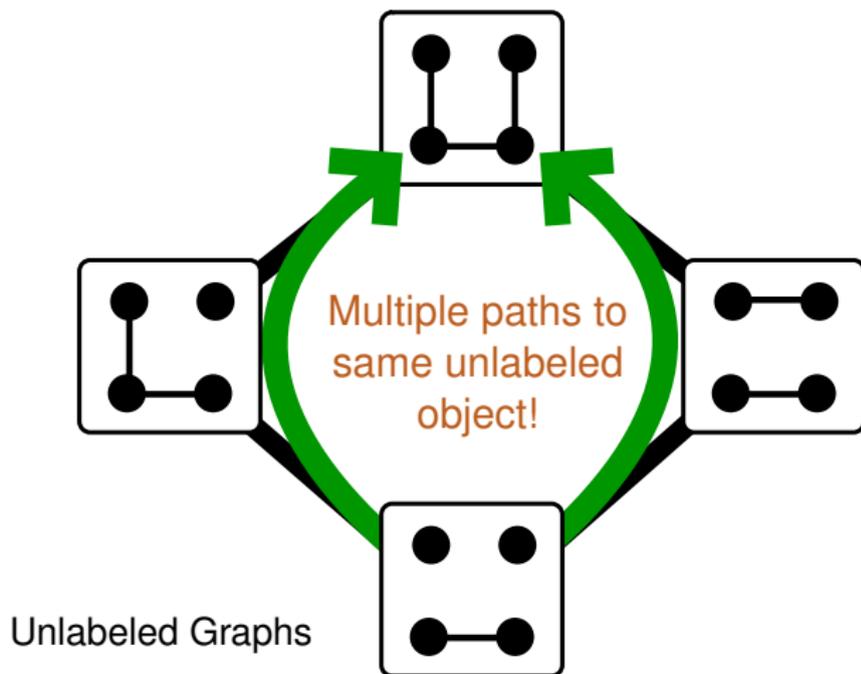
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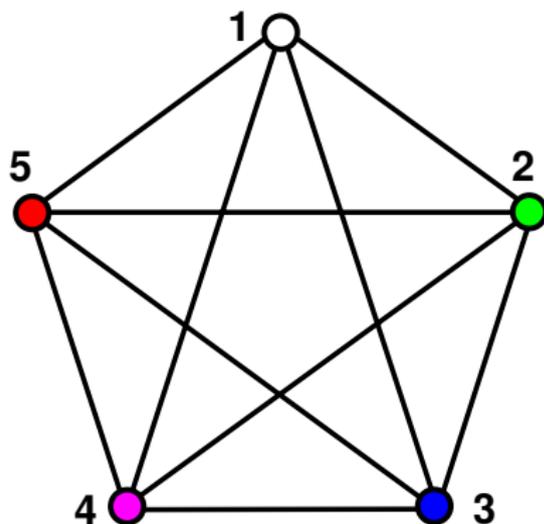
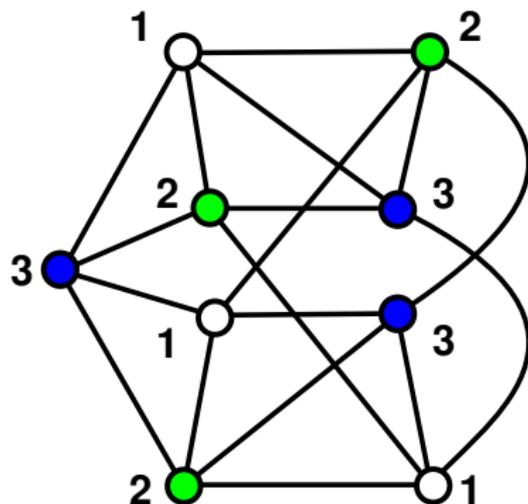
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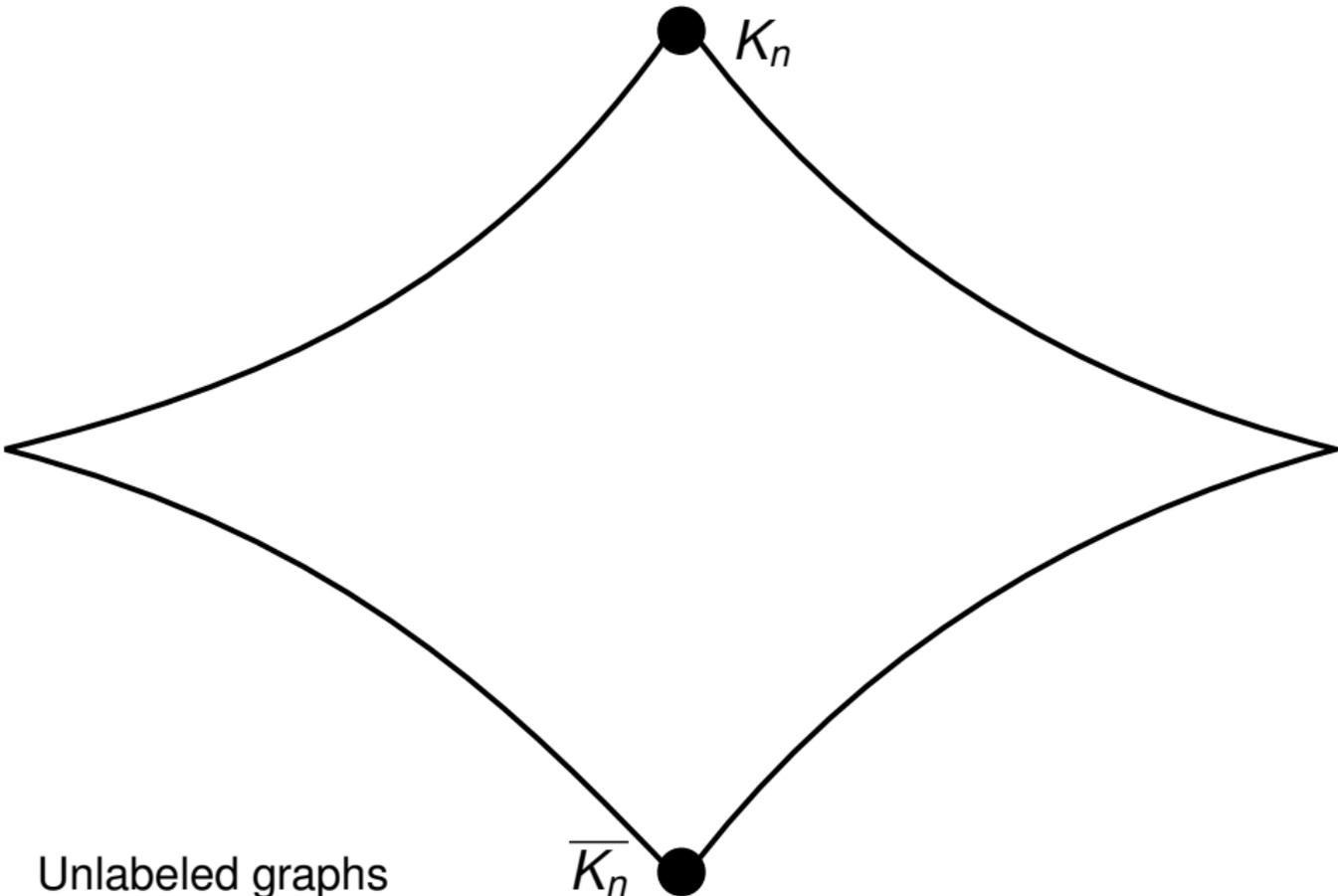


Toy Example

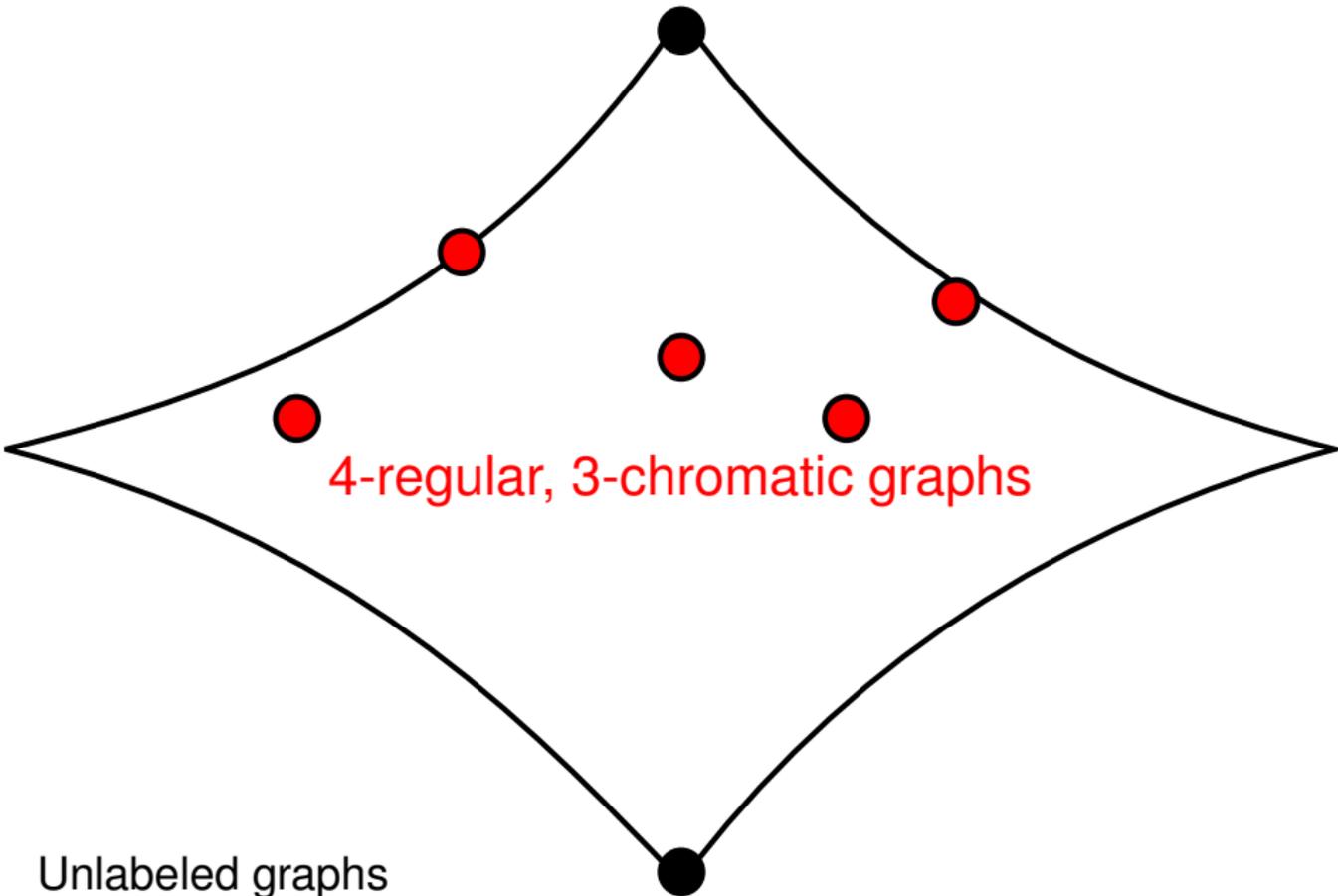
Suppose we are searching for graphs which are:

- 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.



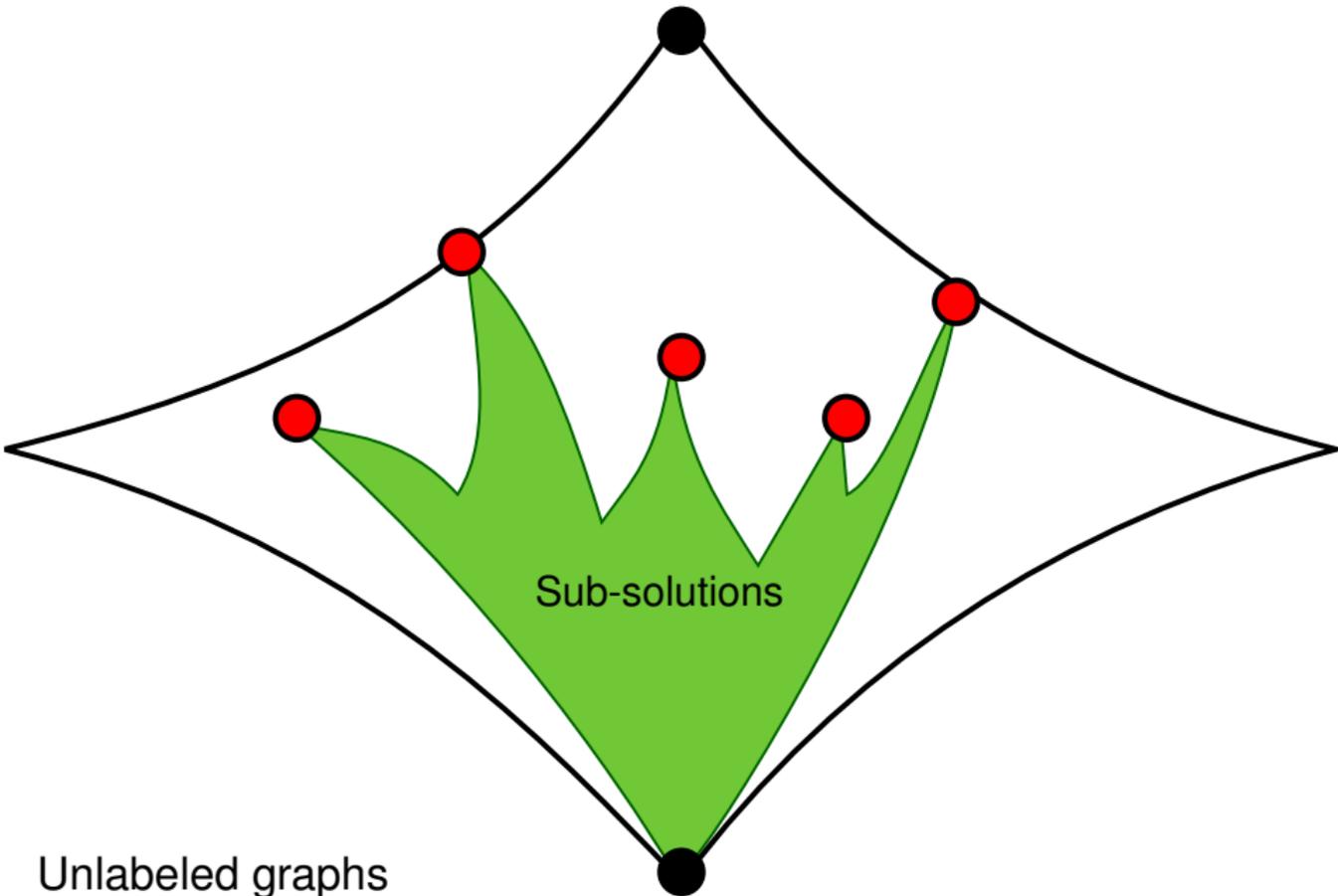


Unlabeled graphs



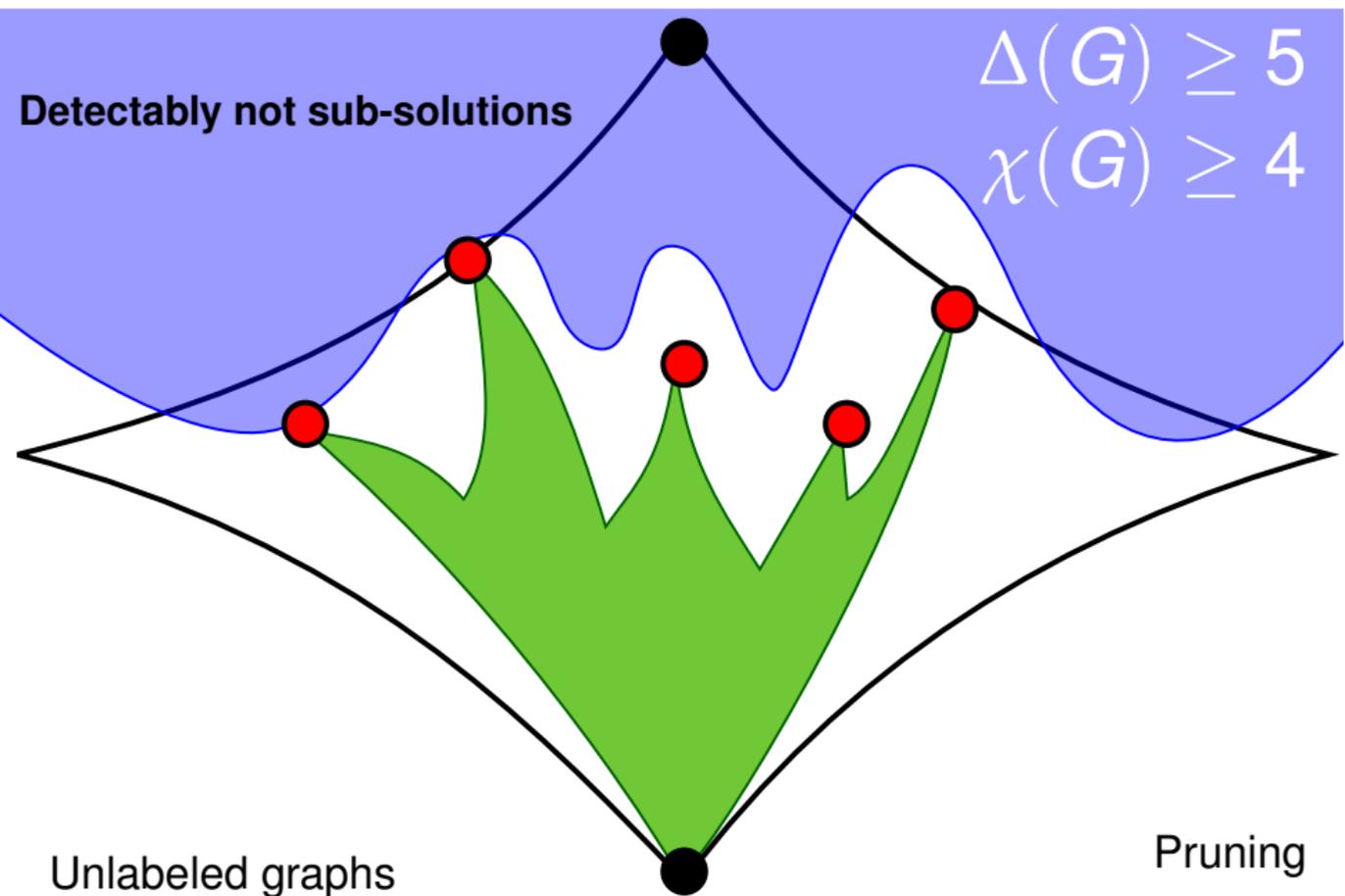
4-regular, 3-chromatic graphs

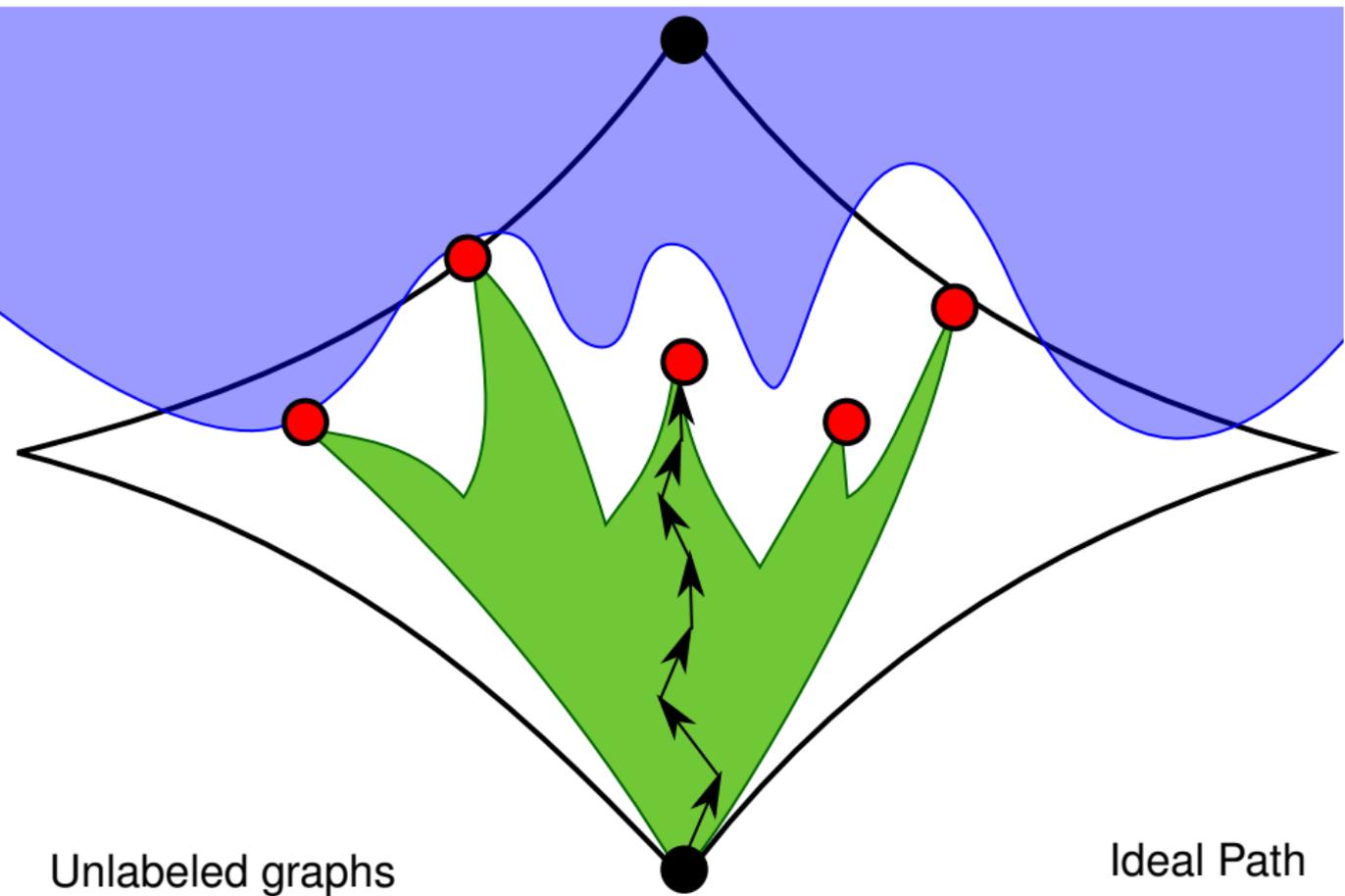
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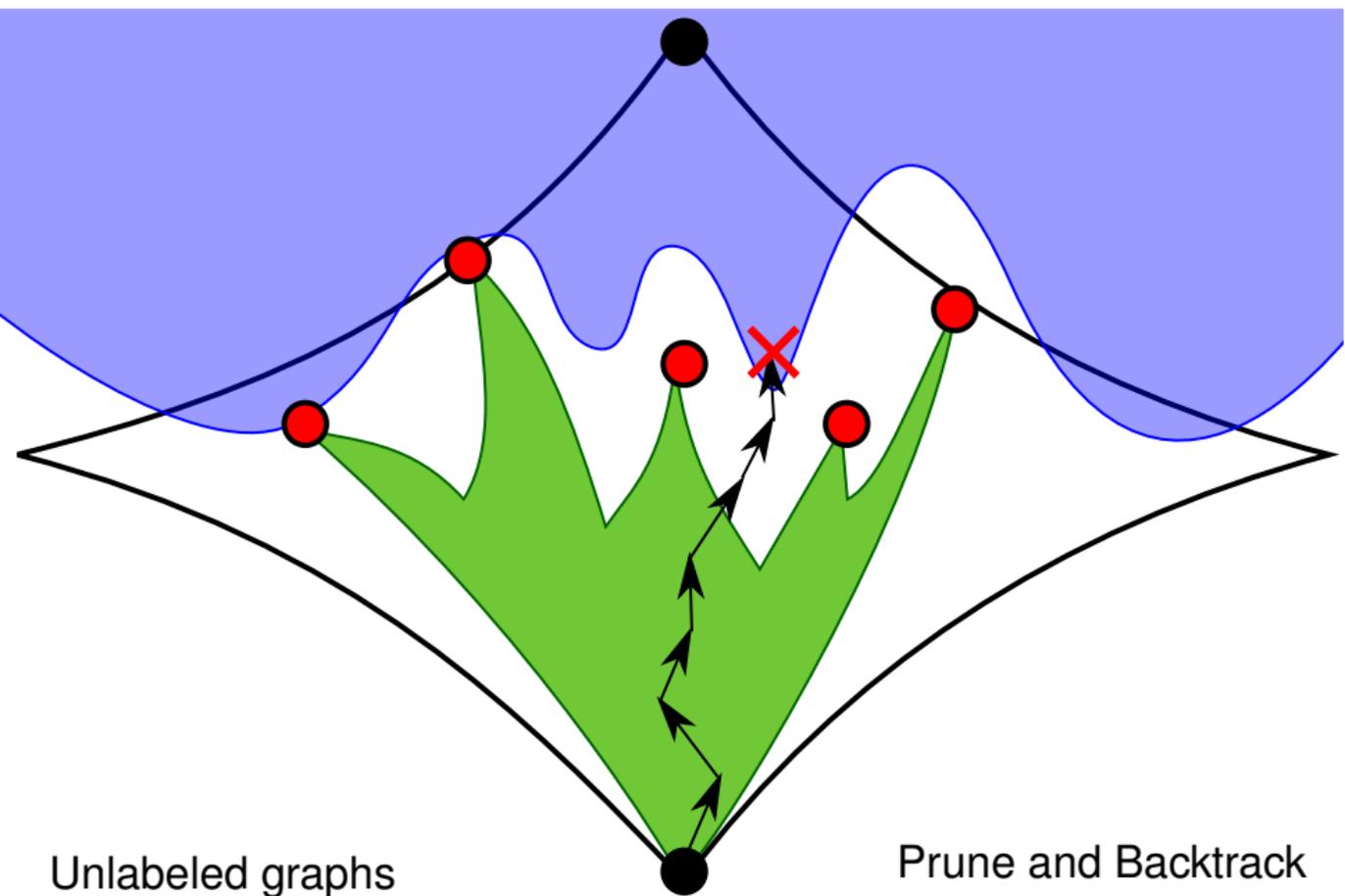
Sub-solutions

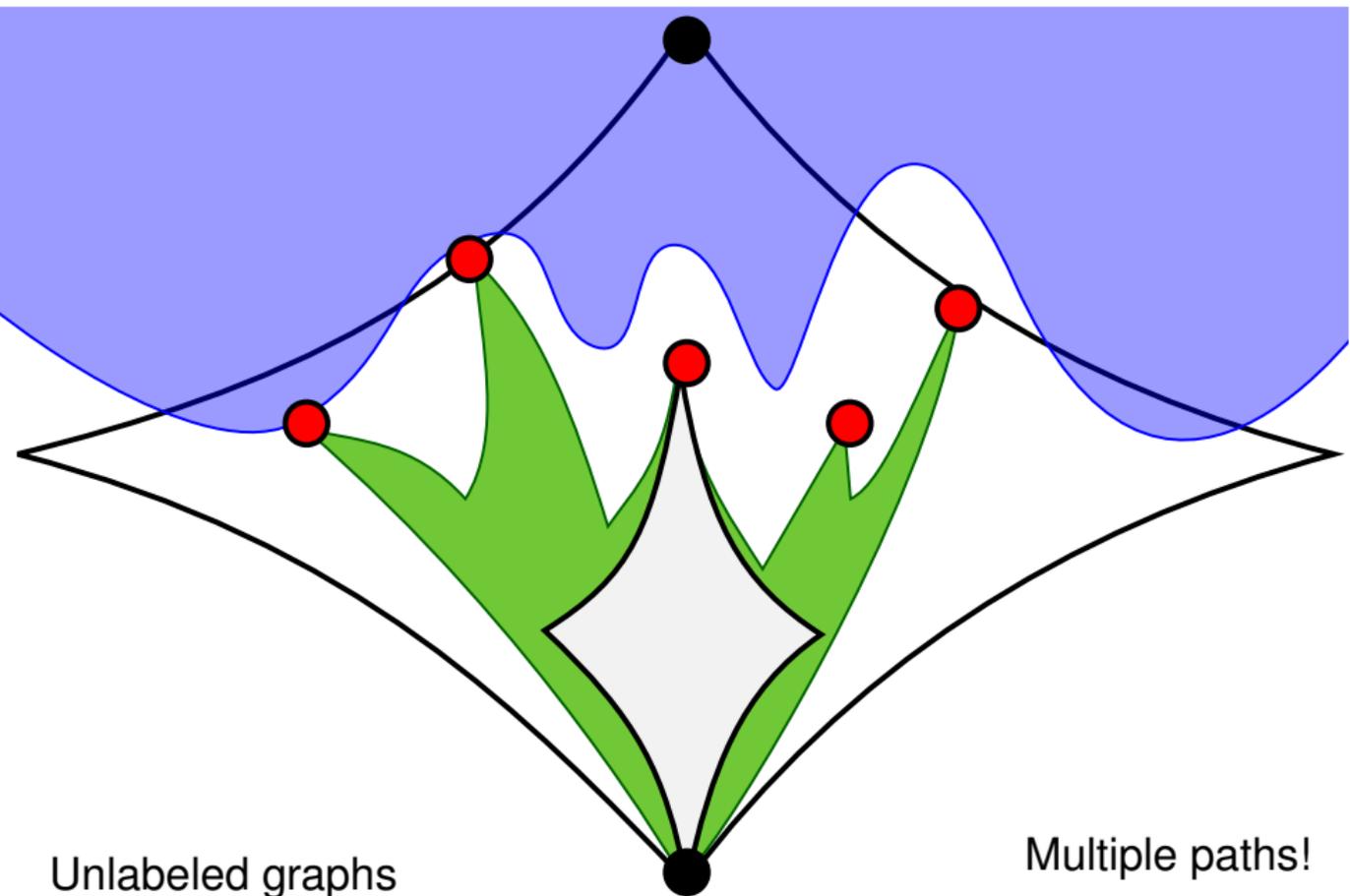




Unlabeled graphs

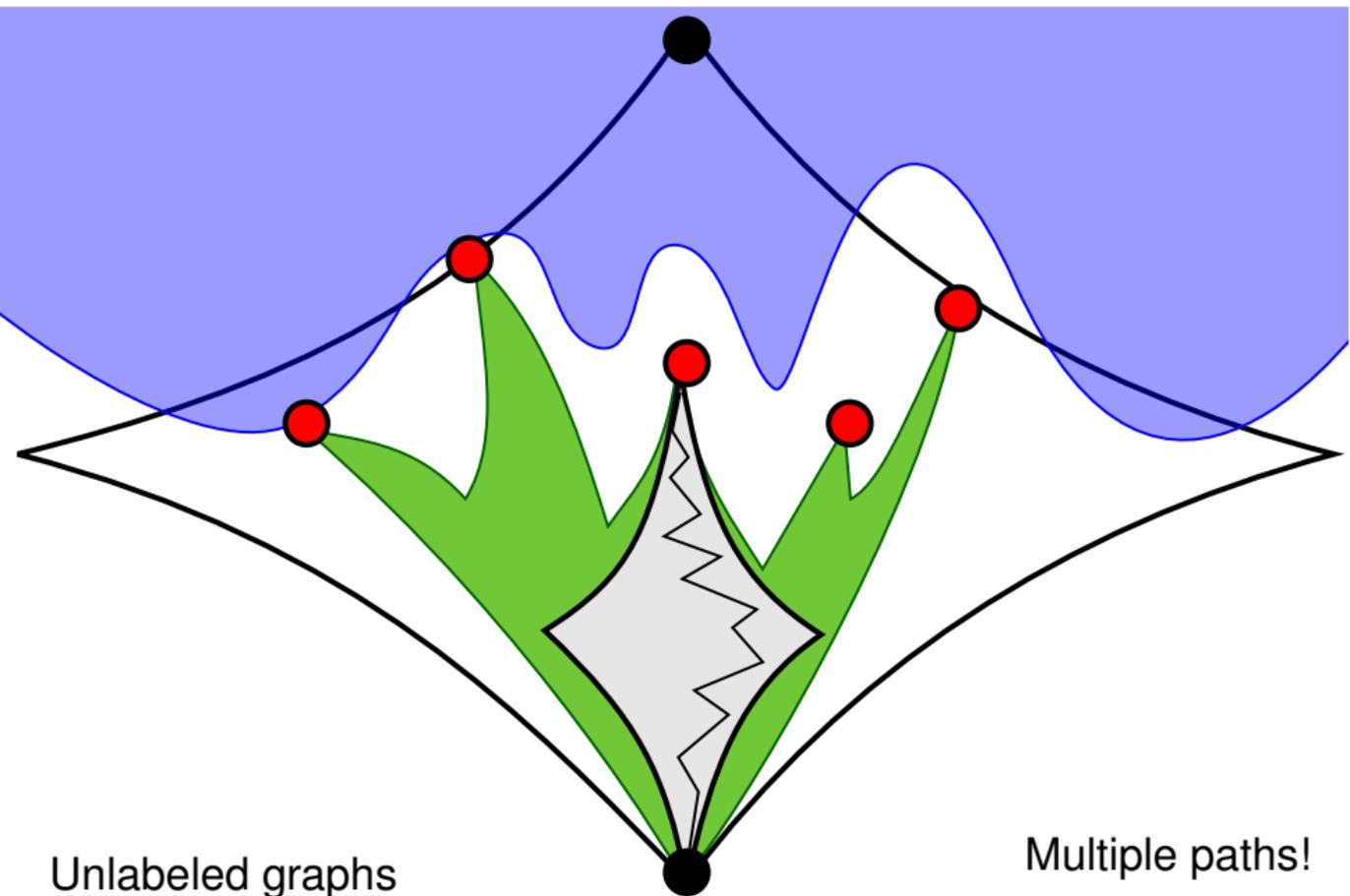
Ideal Path





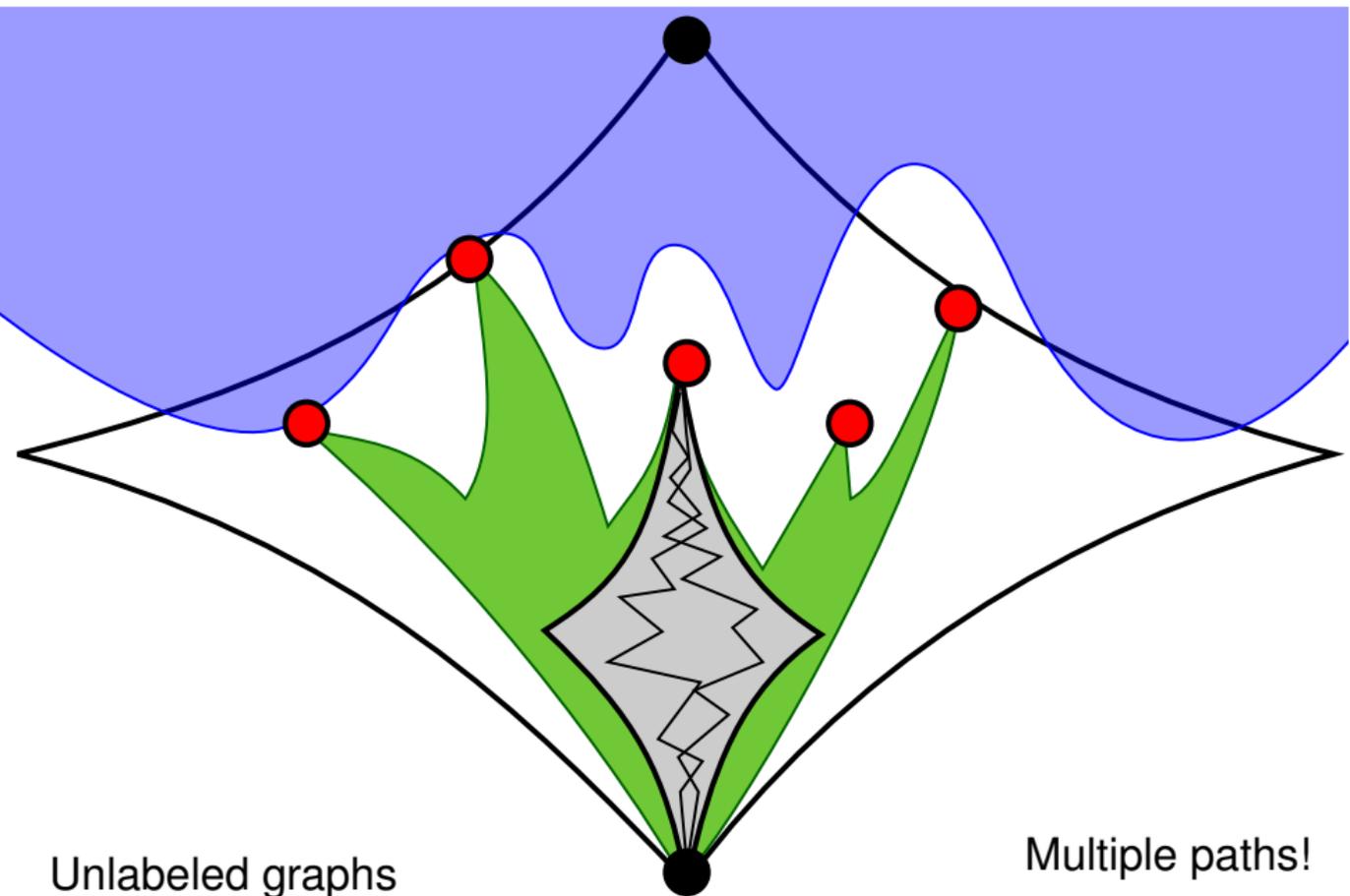
Unlabeled graphs

Multiple paths!



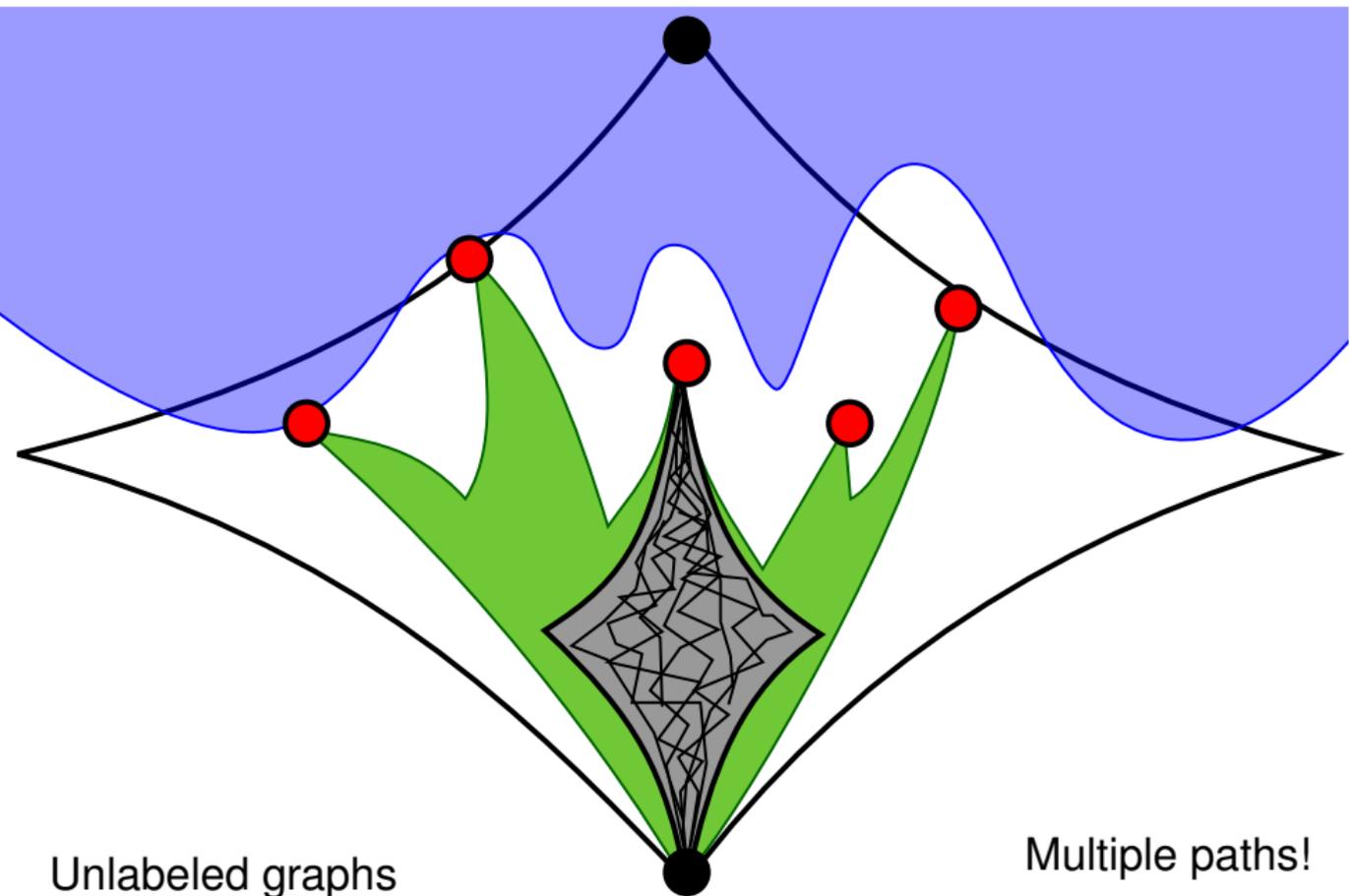
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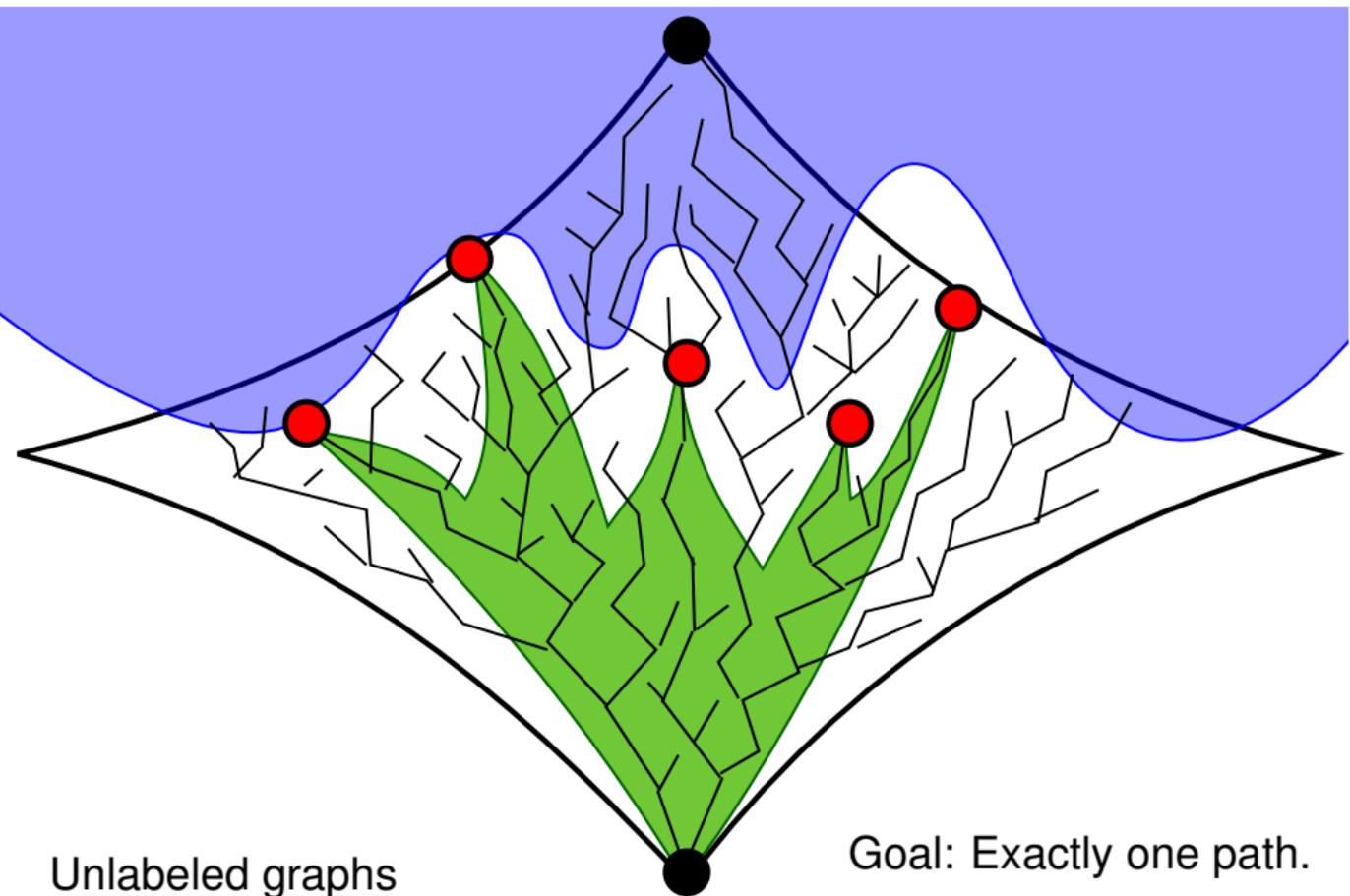
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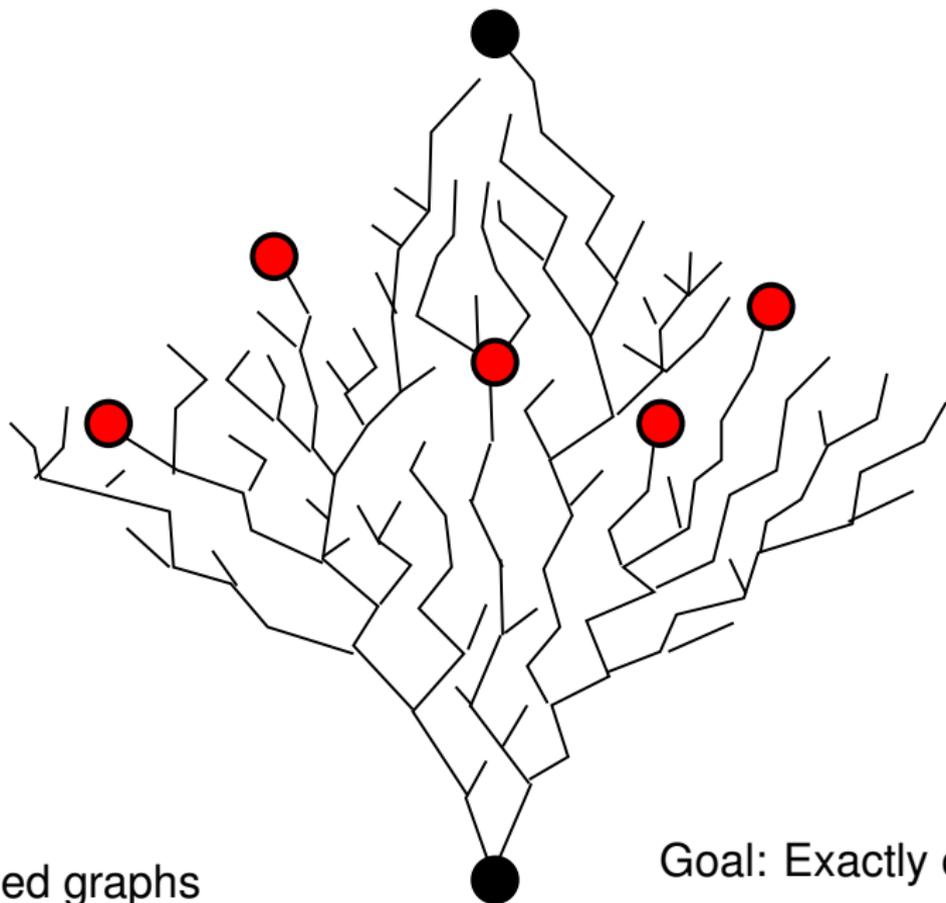
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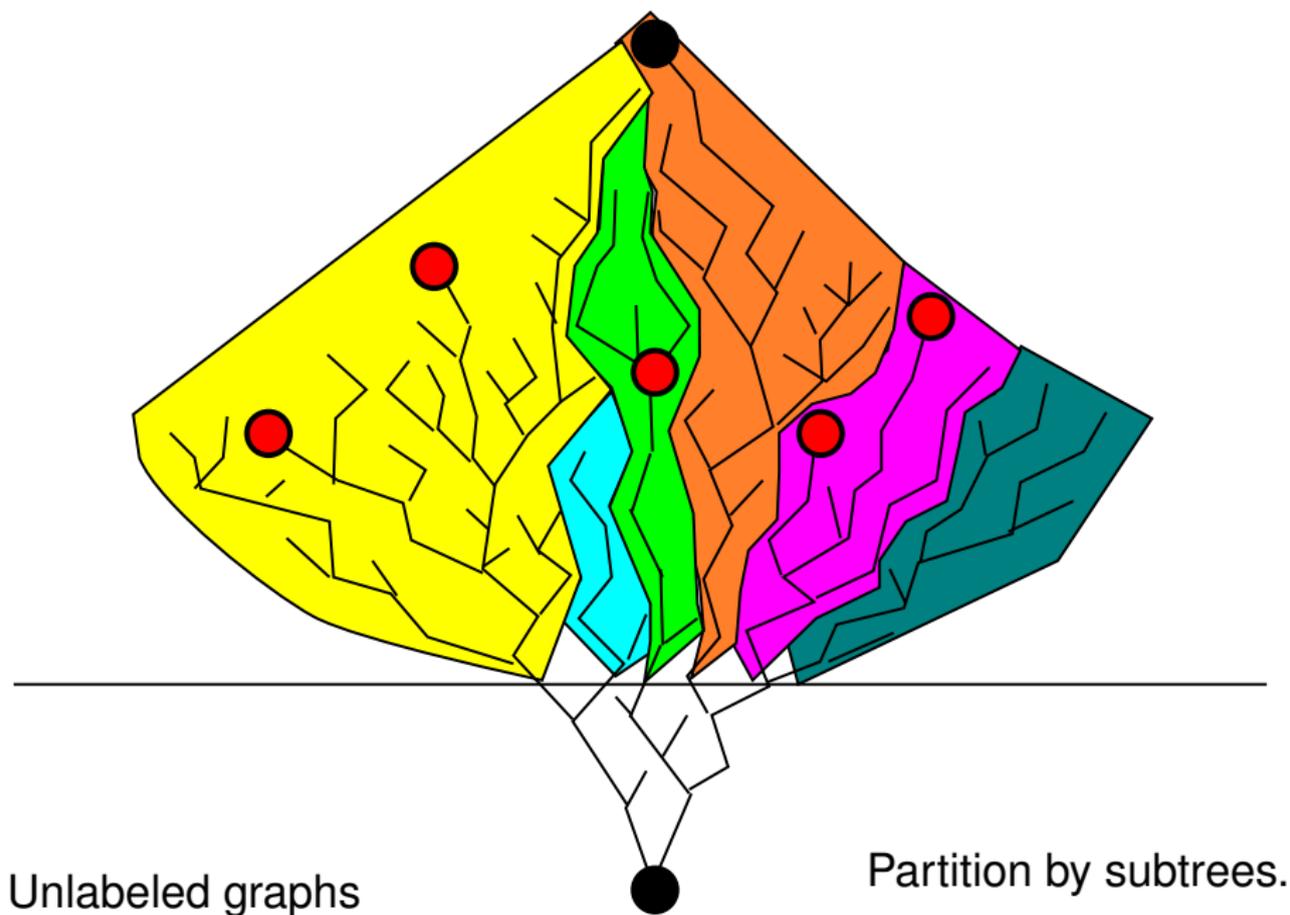
Unlabeled graphs

Goal: Exactly one path.



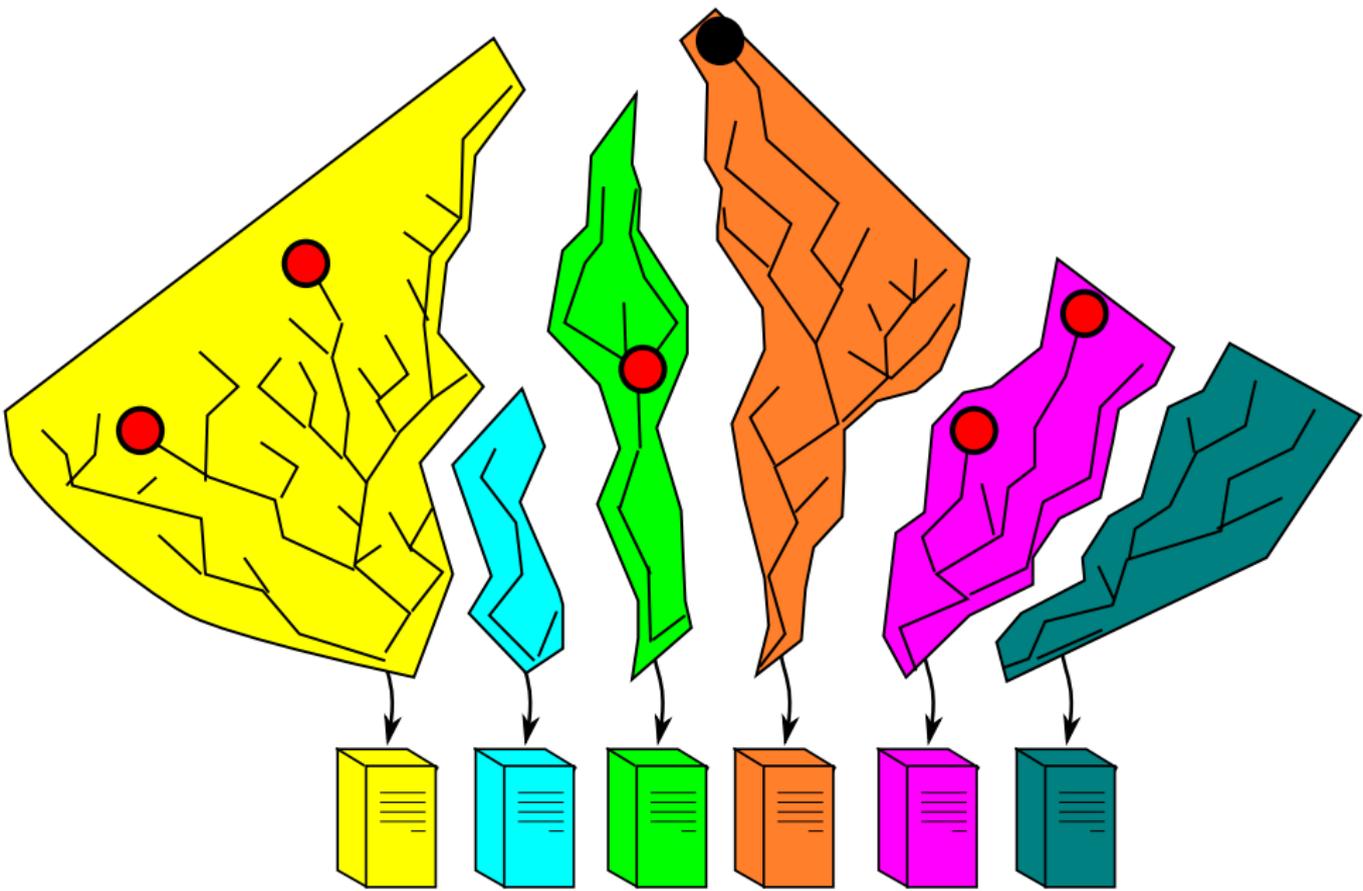
Unlabeled graphs

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Unlabeled graphs

Partition by subtrees.



Parallelize!

Implementation

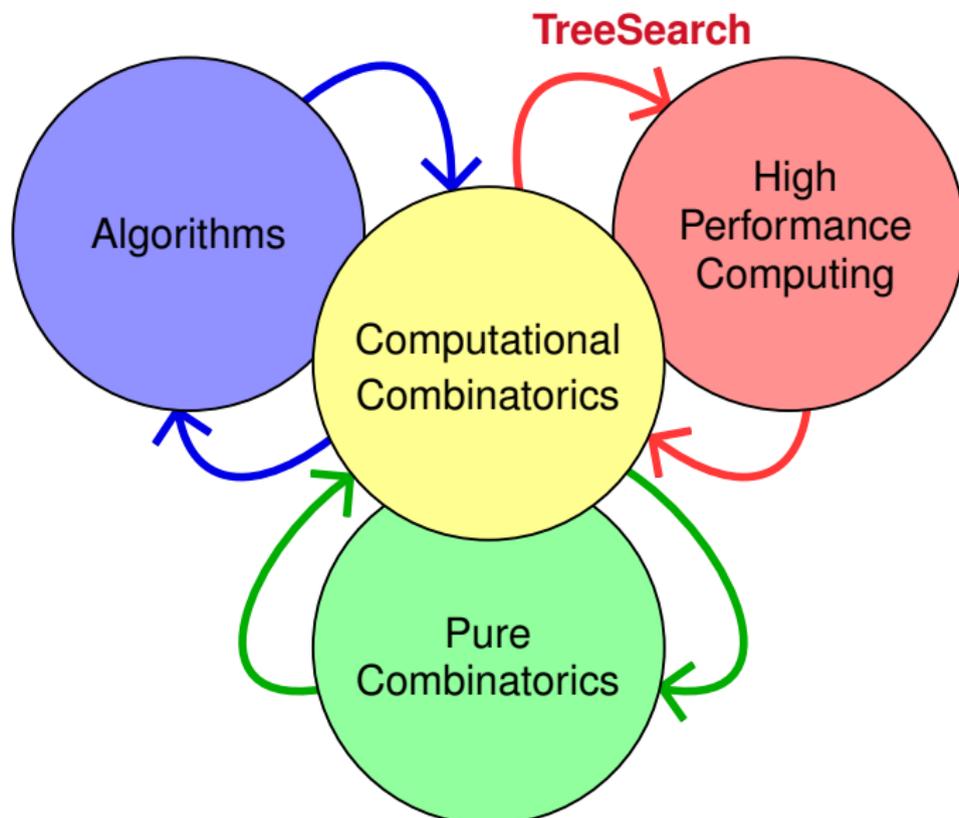
The **TreeSearch** library enables parallelization in the Condor scheduler.

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



Open Science Grid

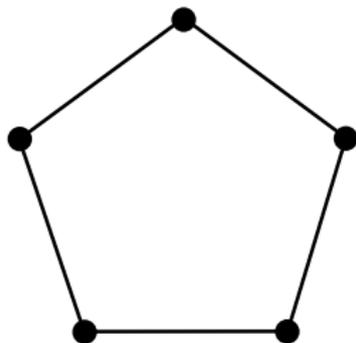
Computational Combinatorics



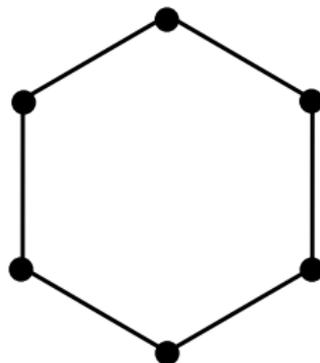
H -Saturated Graphs

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



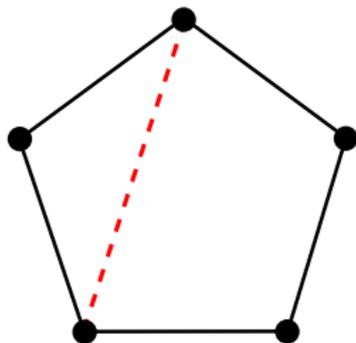
6-cycle

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

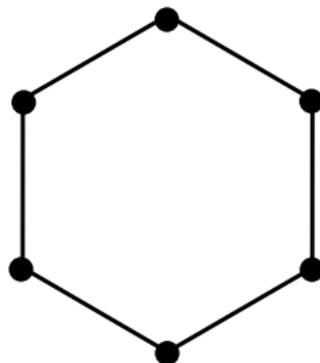
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5-cycle
is K_3 -saturated



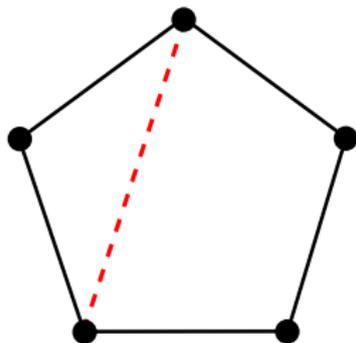
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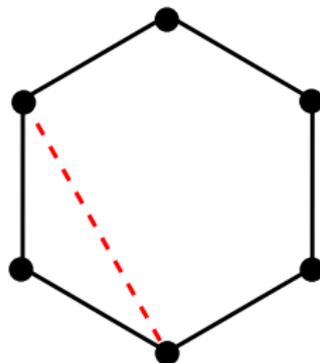
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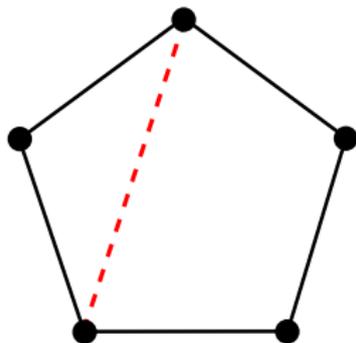
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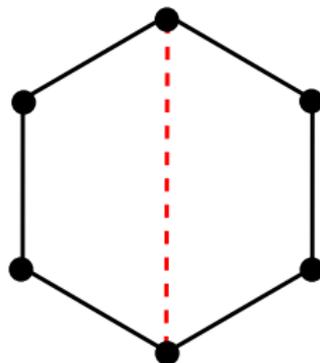
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5-cycle
is K_3 -saturated



6-cycle
is **not** K_3 -saturated

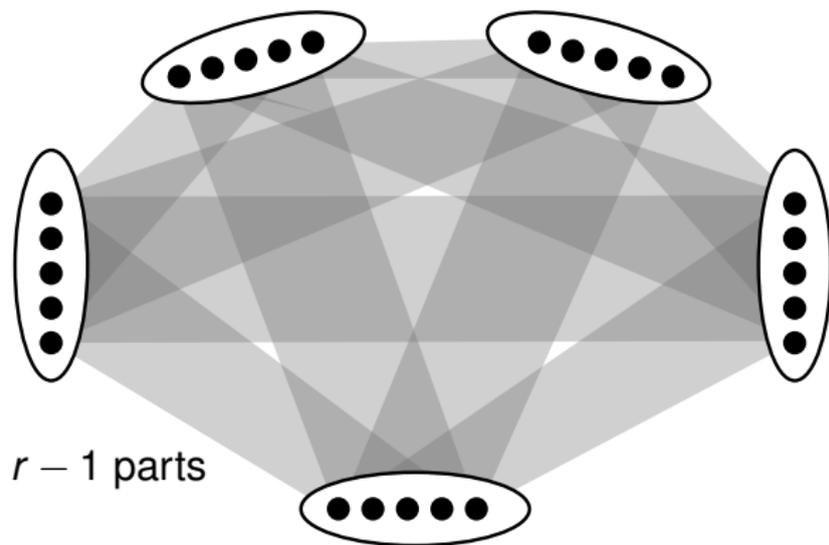
Example: $H = K_3$ where K_r is the **complete graph** on r vertices.

Turán's Theorem

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

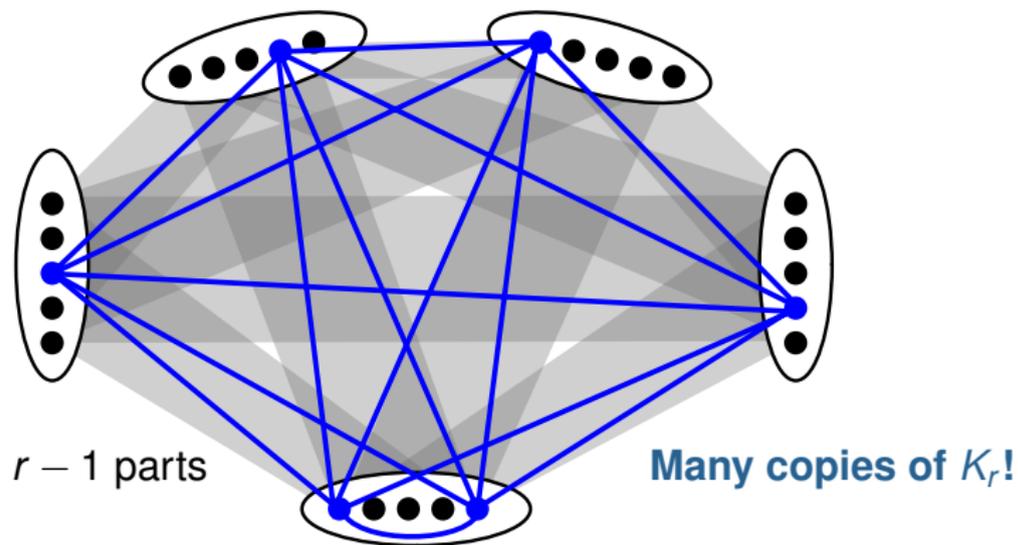
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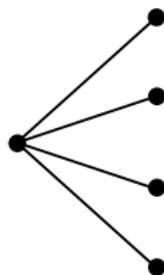


Erdős, Hajnal, and Moon

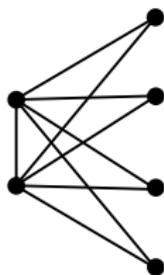
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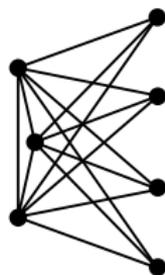
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1-book



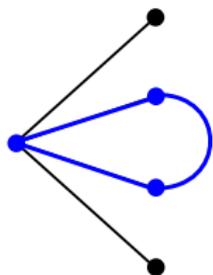
2-book



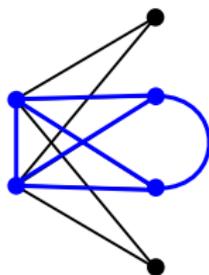
3-book

Erdős, Hajnal, and Moon

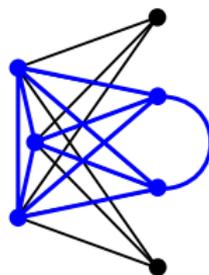
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1-book



2-book



3-book

Exactly one copy of K_r !

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 $G + e$.

Uniquely C_k -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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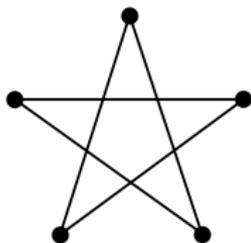
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Uniquely C_k -Saturated Graphs

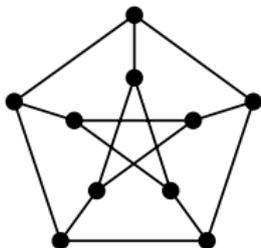
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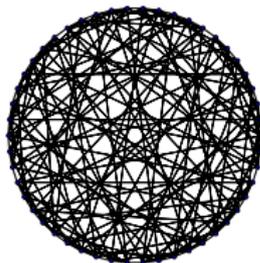
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C_5



Petersen



Hoffman–
Singleton

?

57-Regular
Order 3250

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The only uniquely C_5 -saturated graphs are **friendship graphs**.

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Theorem (Wenger, 2010)

For $k \in \{6, 7, 8\}$, no uniquely C_k -saturated graph exists.

Conjecture (Wenger, 2010)

For $k \geq 9$, no uniquely C_k -saturated graph exists.

Uniquely K_r -Saturated Graphs

We consider the case where $H = K_r$ (an r -**clique**) for $r \geq 4$.

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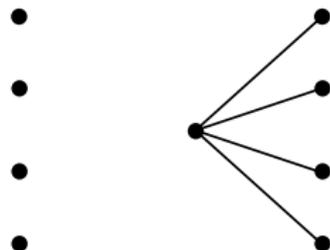
Dominating Vertices

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

-
-
-
-

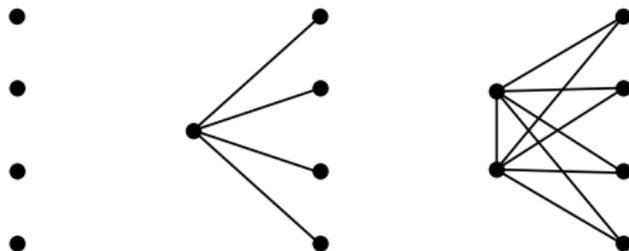
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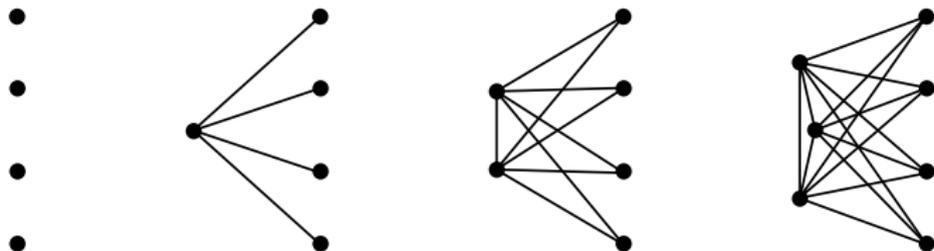
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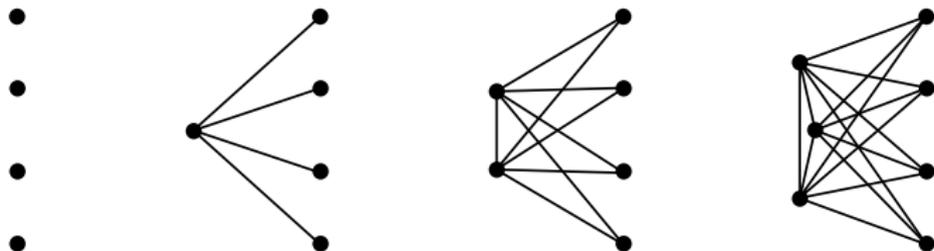
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Dominating Vertices

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Call uniquely K_r -saturated graphs without a dominating vertex

r -primitive.

r -Primitive Graphs

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

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

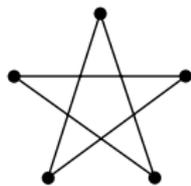
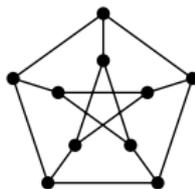
2-primitive graphs are **empty graphs**.

r -Primitive Graphs

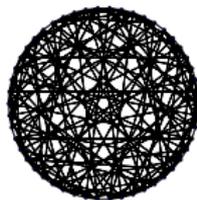
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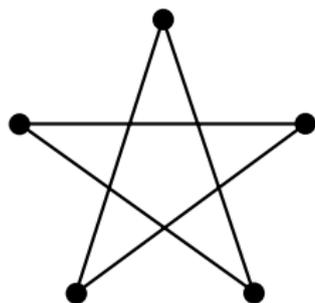
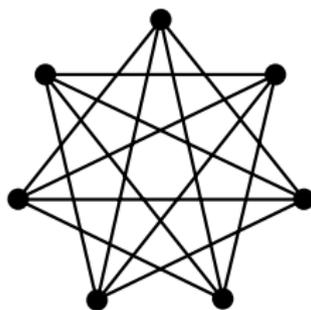
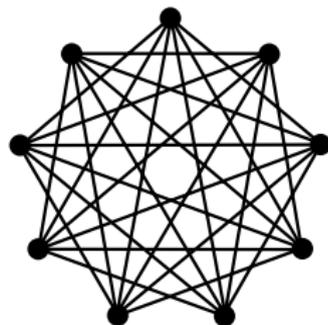
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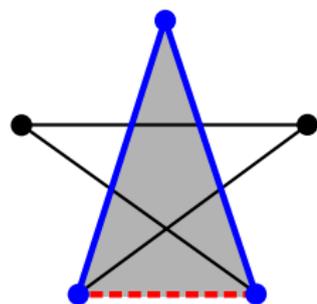
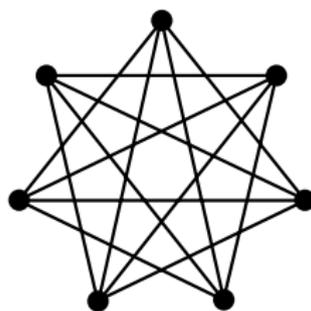
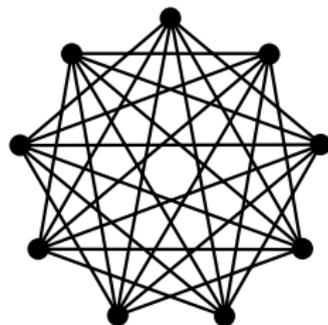

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 $\overline{C_7}$

 $\overline{C_9}$

(Collins, Cooper, Kay, Wenger, 2010)

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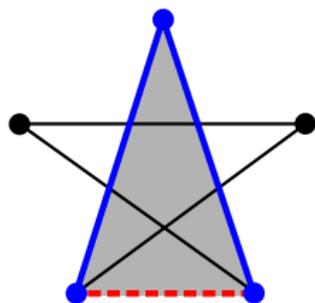
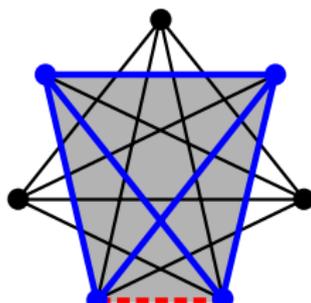
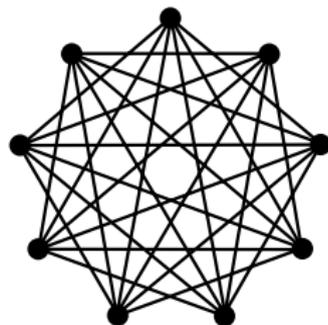

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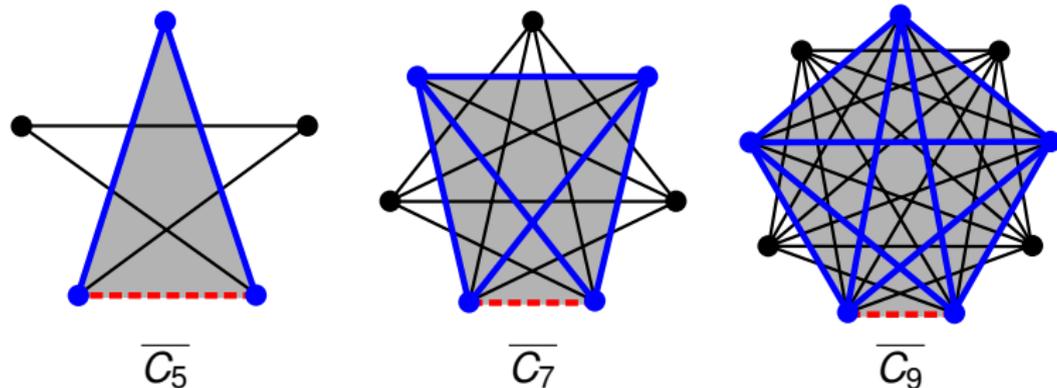

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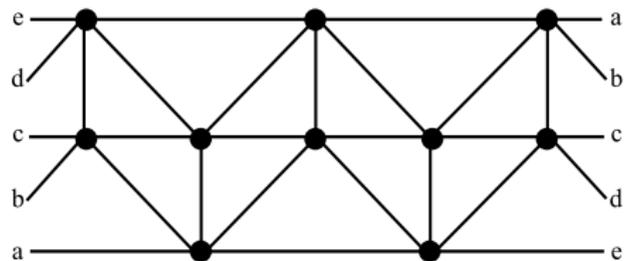
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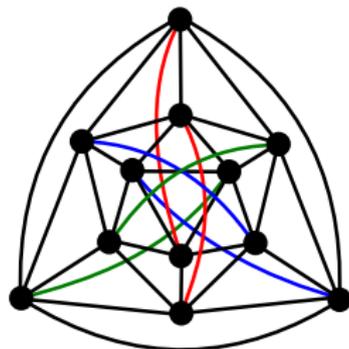


(Collins, Cooper, Kay, Wenger, 2010)

Uniquely K_4 -Saturated Graphs



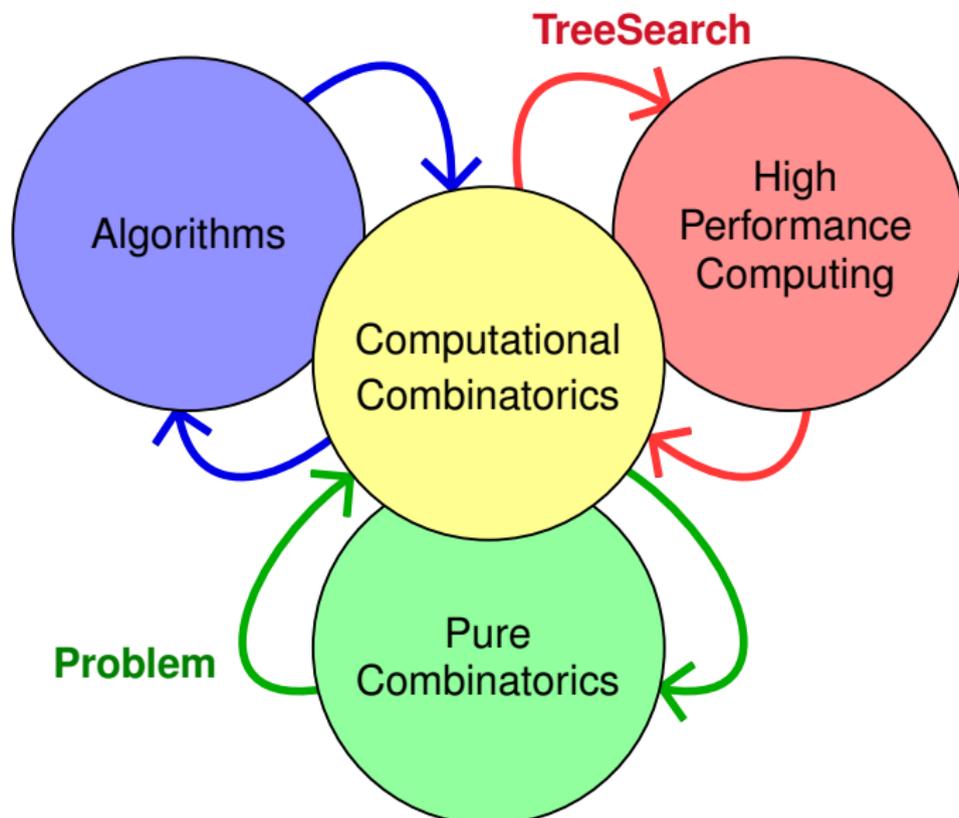
10 vertices



12 vertices

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

Computational Combinatorics



The Problem

Goal: Characterize uniquely K_r -saturated graphs.

First Step: Reduce to r -primitive graphs.

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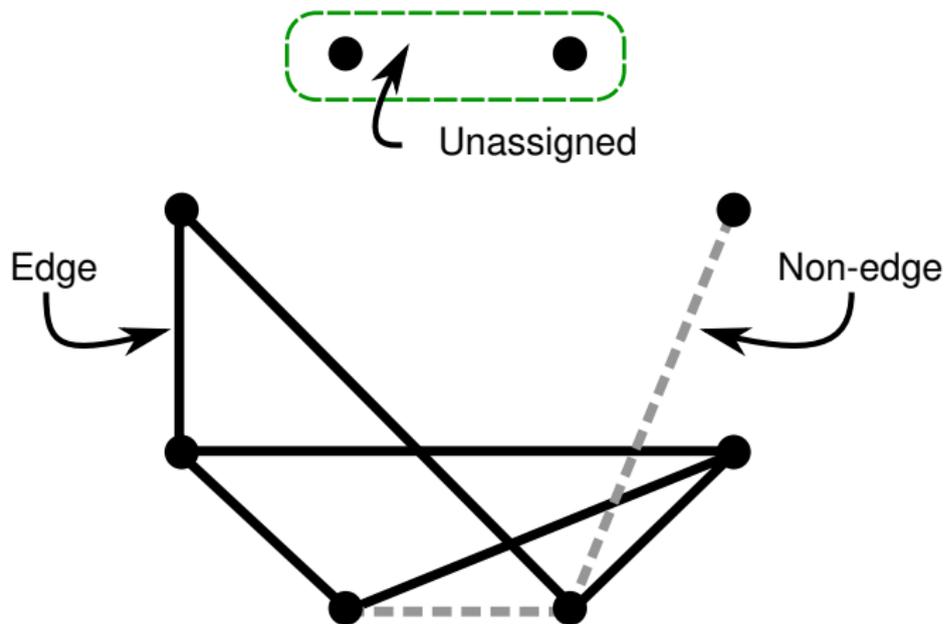
1. Fix $r \geq 3$. Are there a **finite number** of r -primitive graphs?
2. Is every r -primitive graph **regular**?

Edges and Non-Edges

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

Edges and Non-Edges

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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

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

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

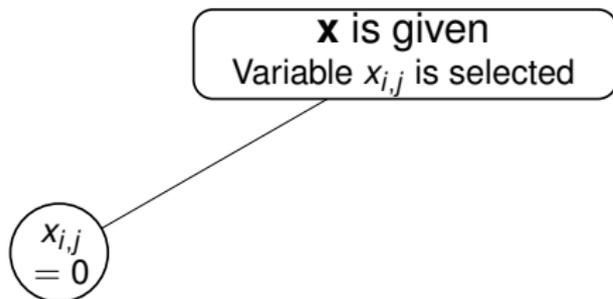
Orbital branching reduces the number of isomorphic duplicates.
(Ostrowski, Linderoth, Rossi, Smriglio, 2007)

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

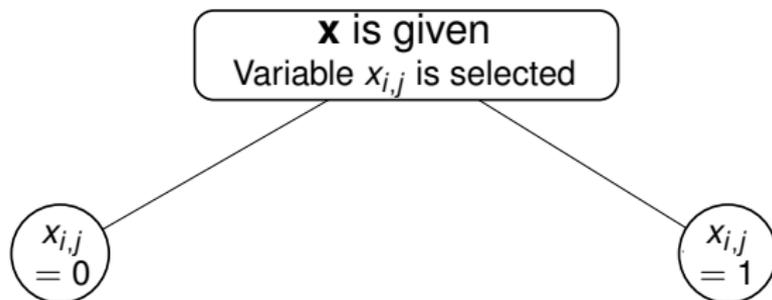
Branch-and-Bound

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

Branch-and-Bound



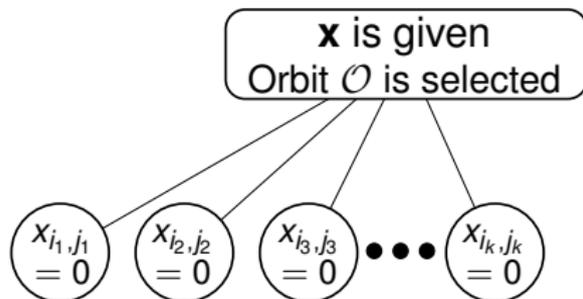
Branch-and-Bound



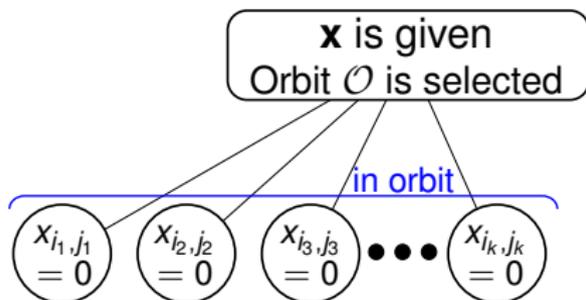
Orbital Branching

x is given
Orbit \mathcal{O} is selected

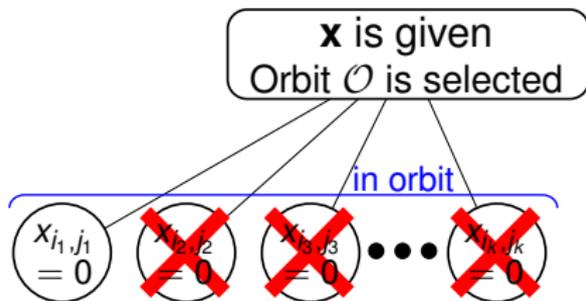
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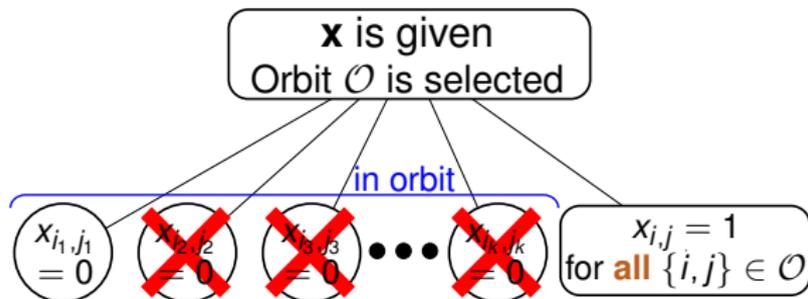
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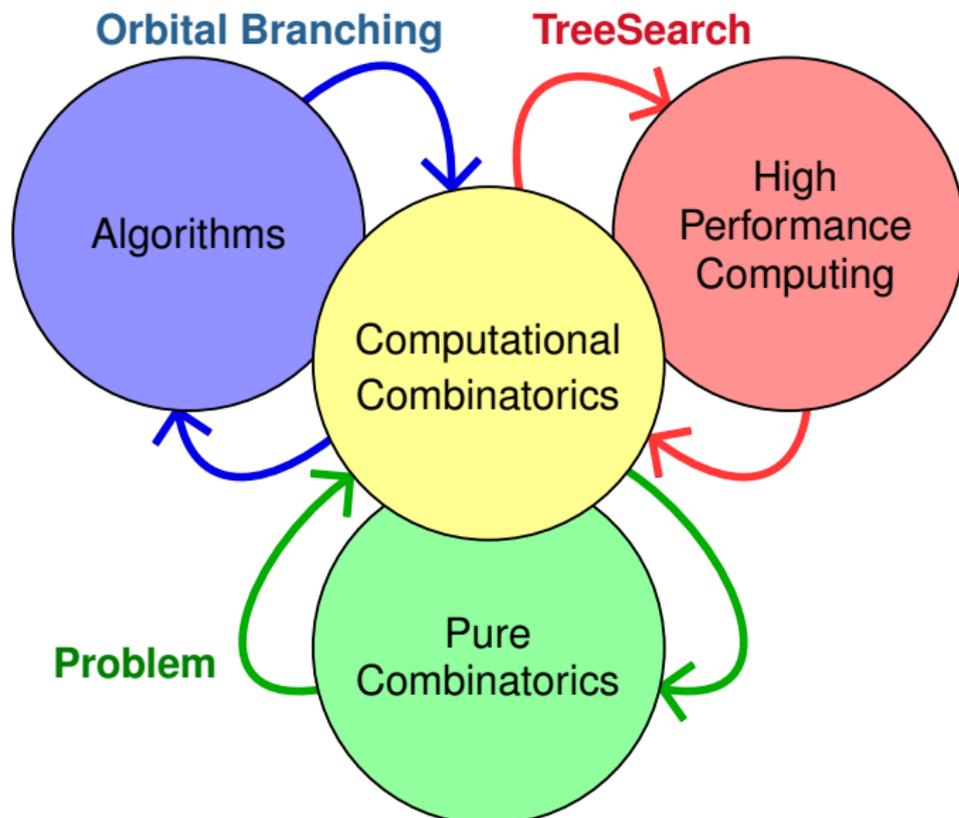
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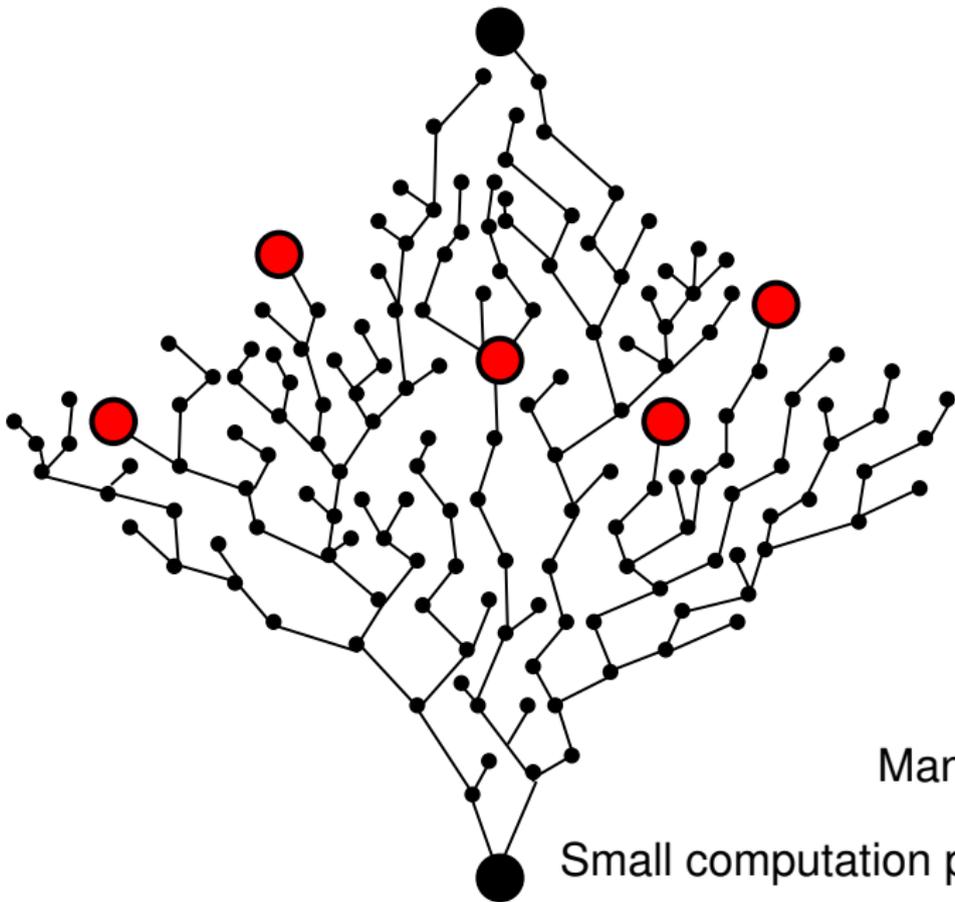


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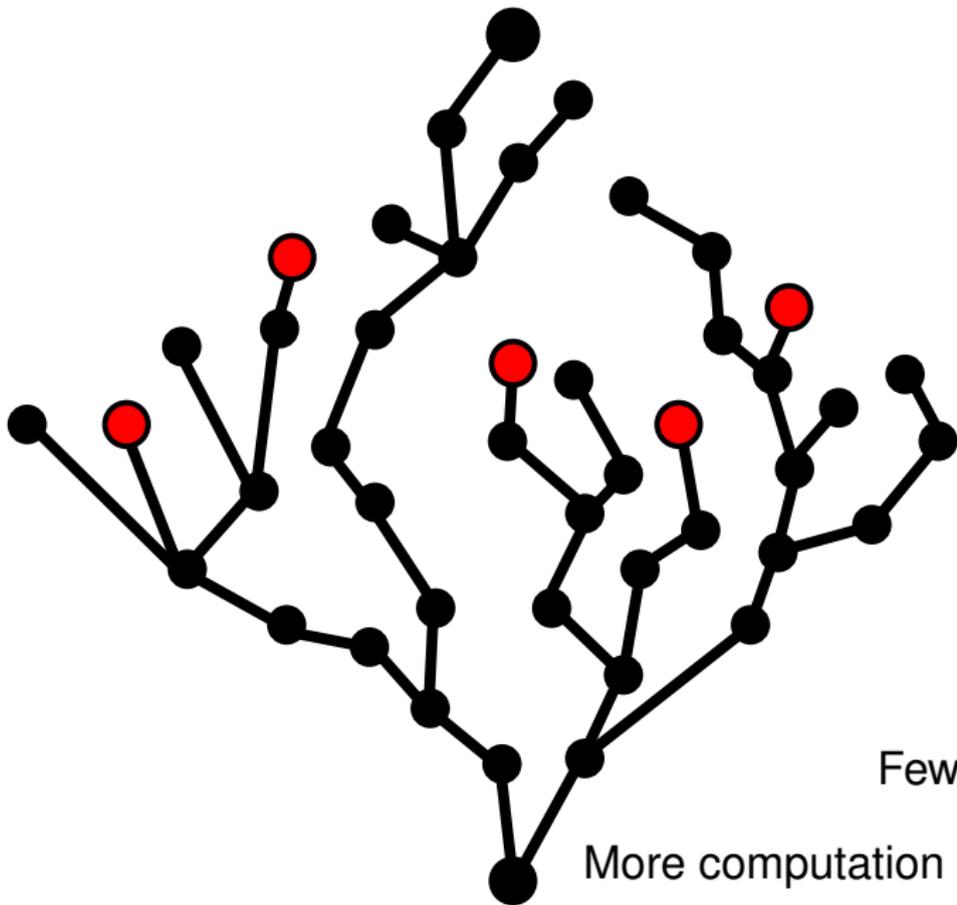
Computational Combinatorics





Many nodes.

Small computation per node.



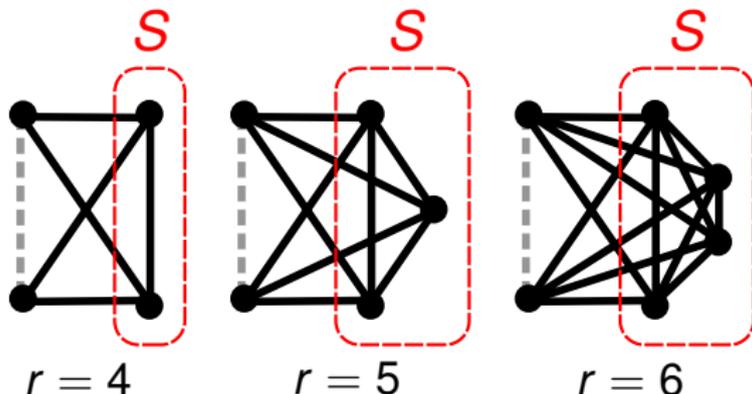
Fewer nodes.

More computation per node.

K_r -Completions

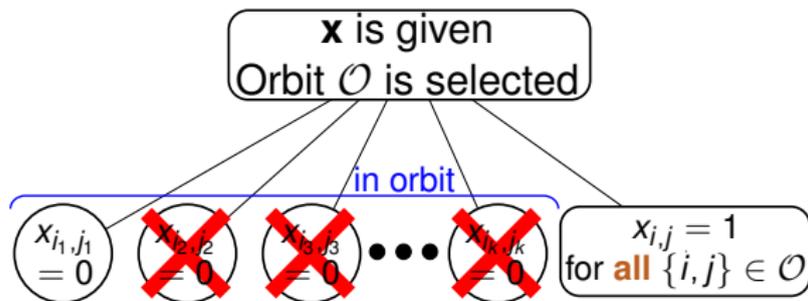
For every non-edge we add, we add a K_r -**completion**:

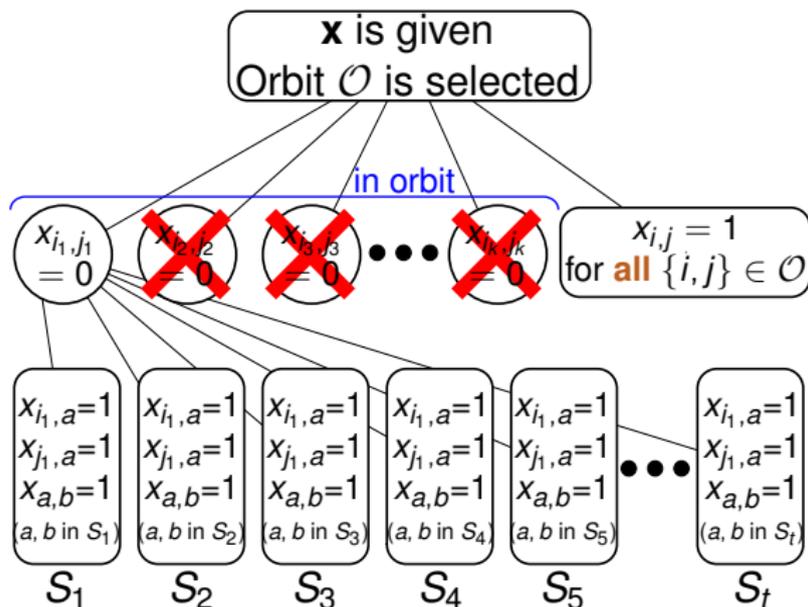
$x_{i,j} = 0$ **if and only if** there exists a set $S \subset [n]$, $|S| = r - 2$,
so that $x_{i,a} = x_{j,a} = x_{a,b} = 1$ for all $a, b \in S$.

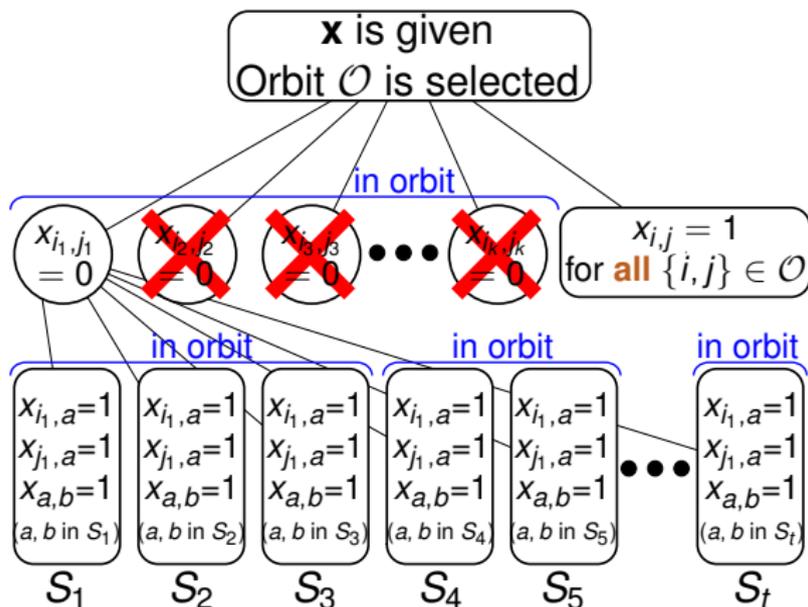


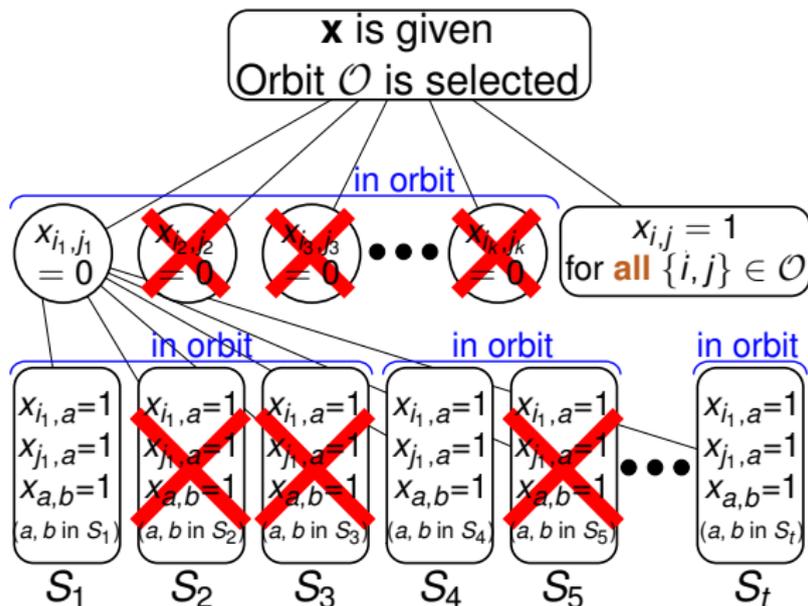
Orbital Branching with K_r -Completions

x is given
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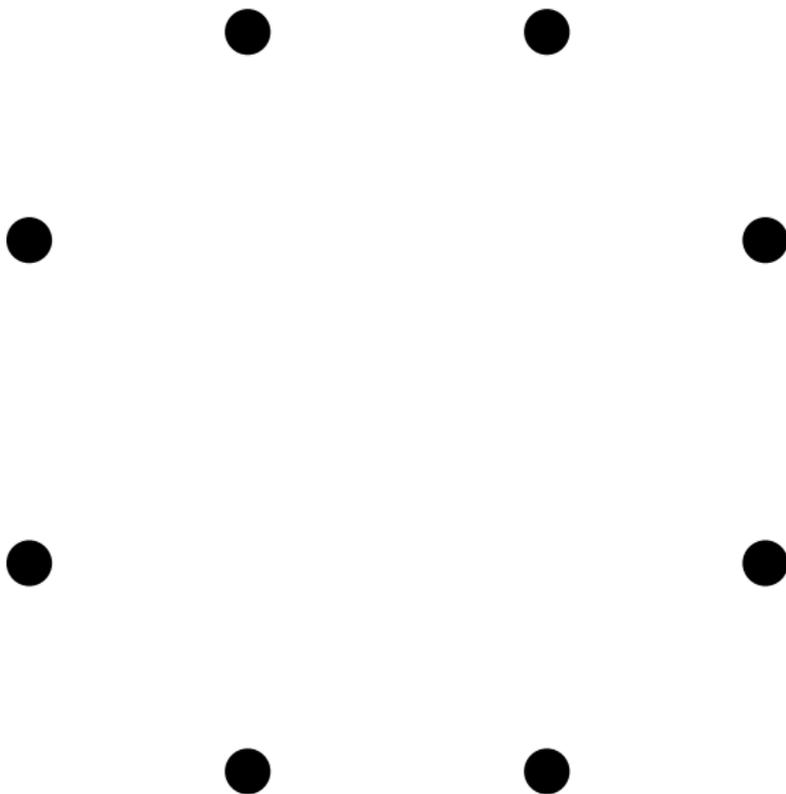
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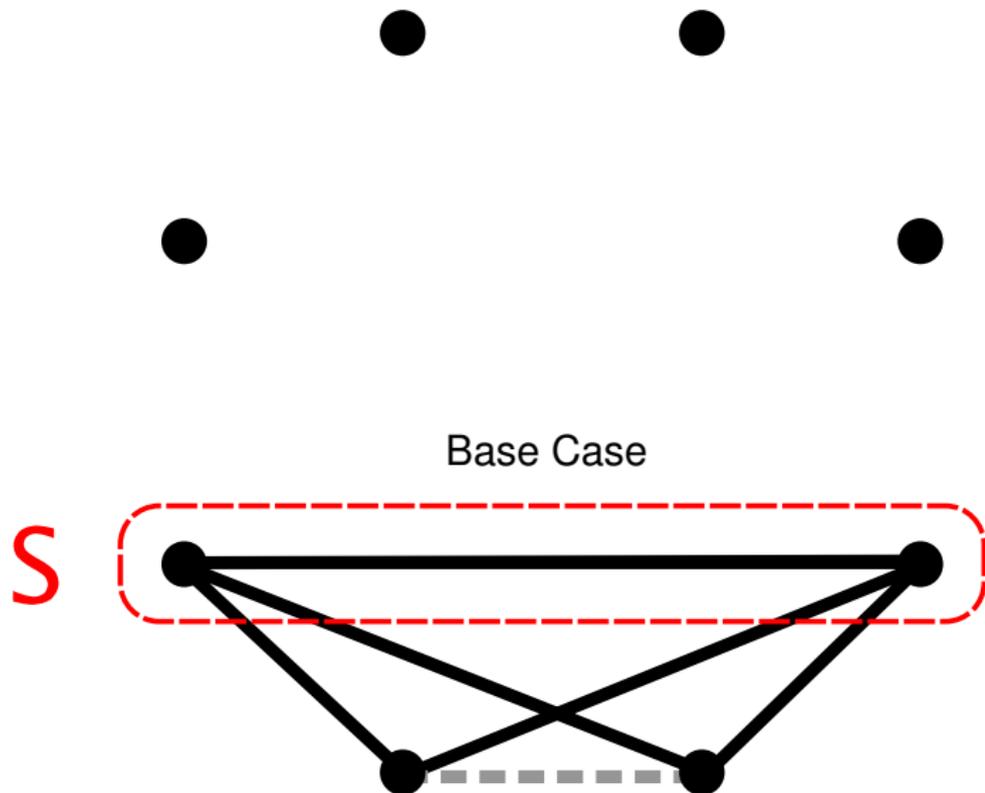
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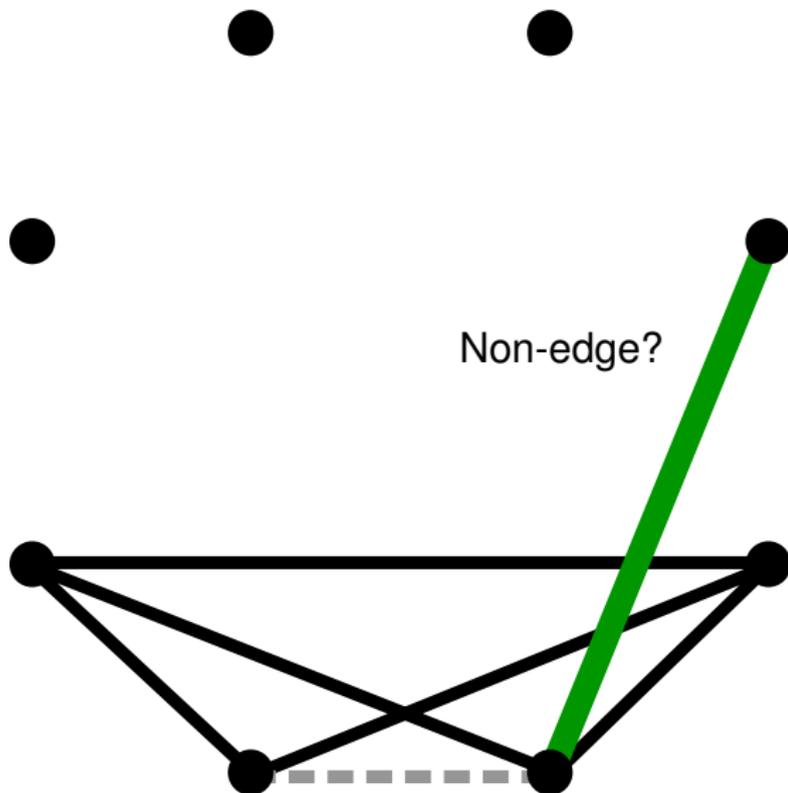
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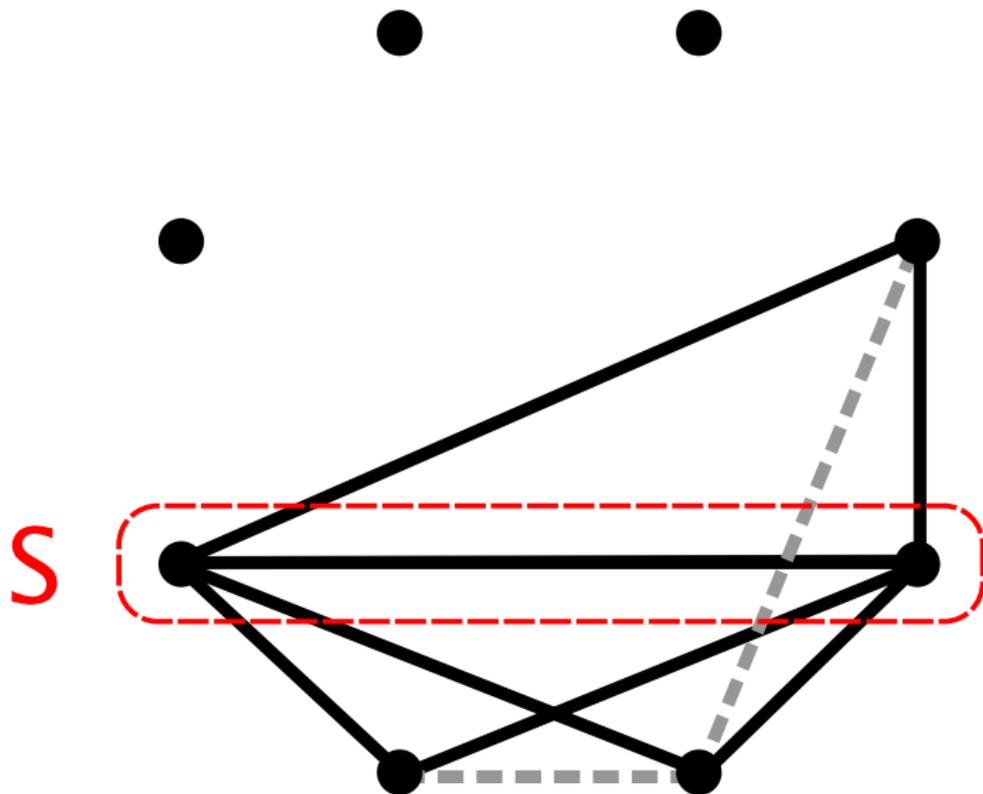


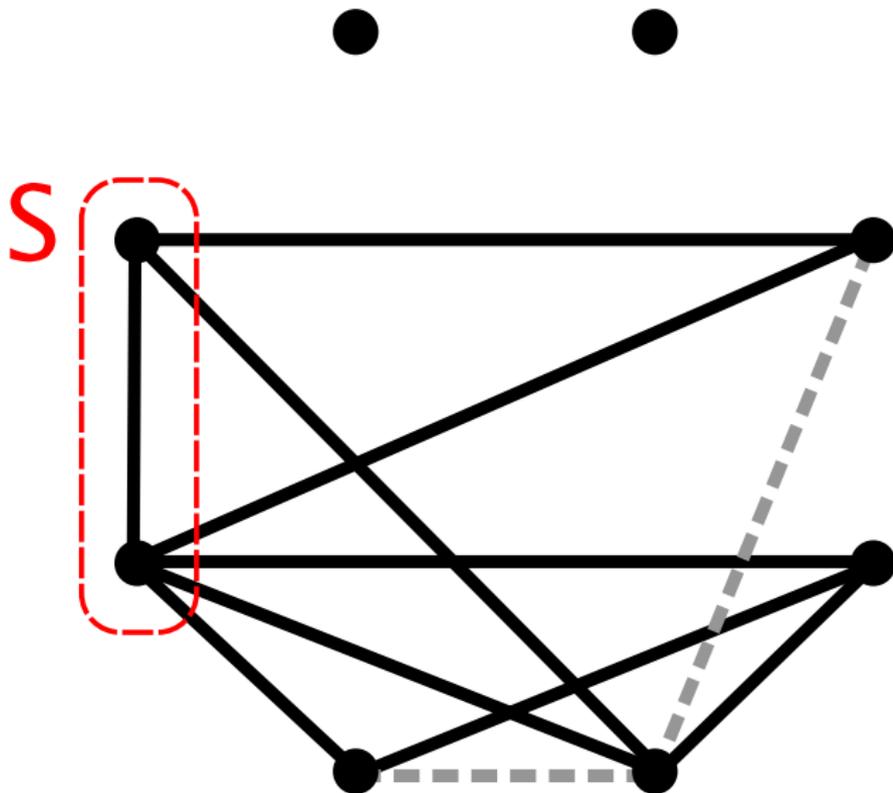
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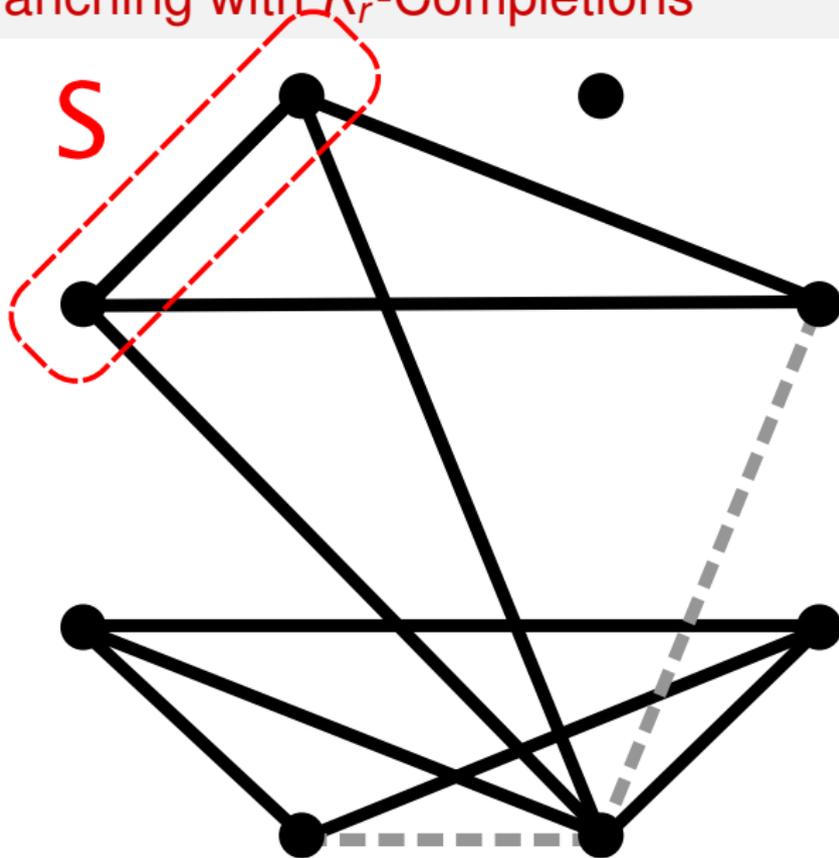


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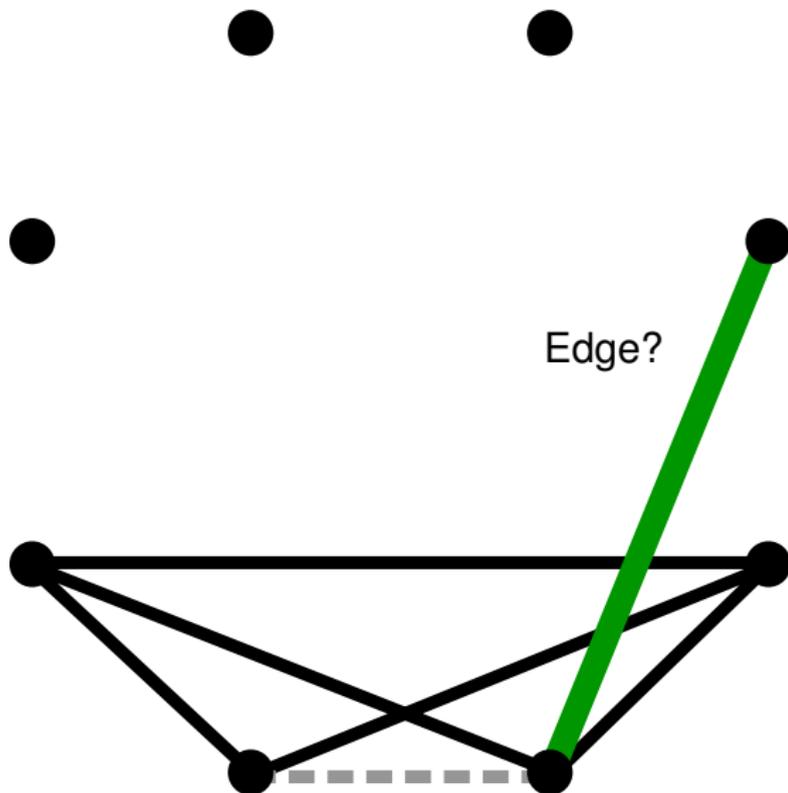


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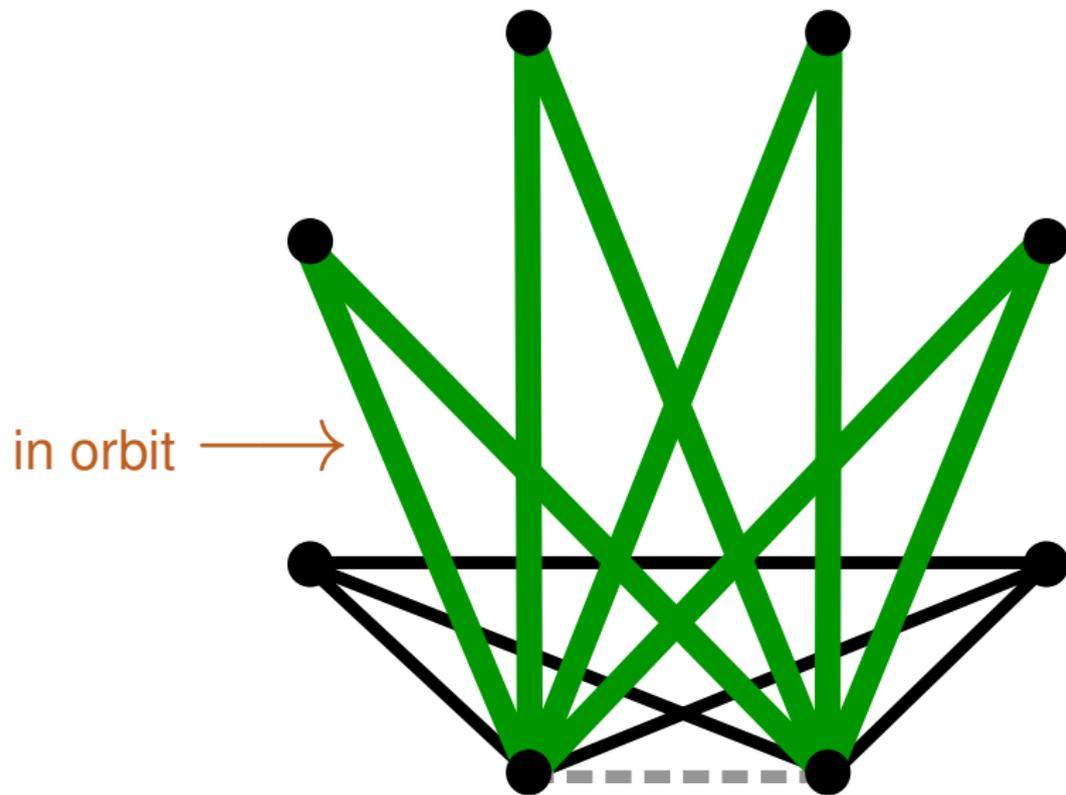
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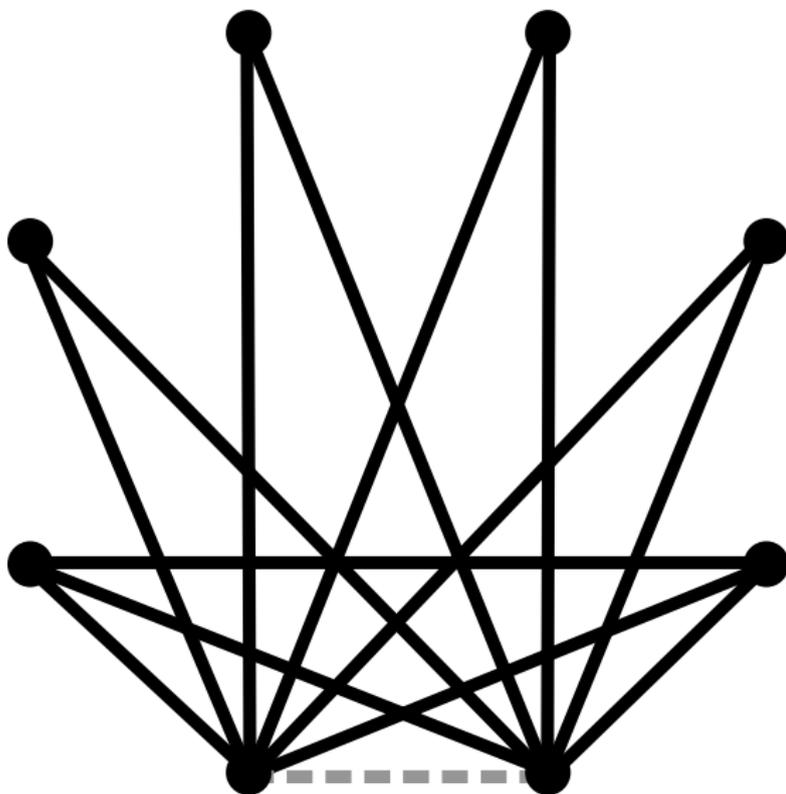
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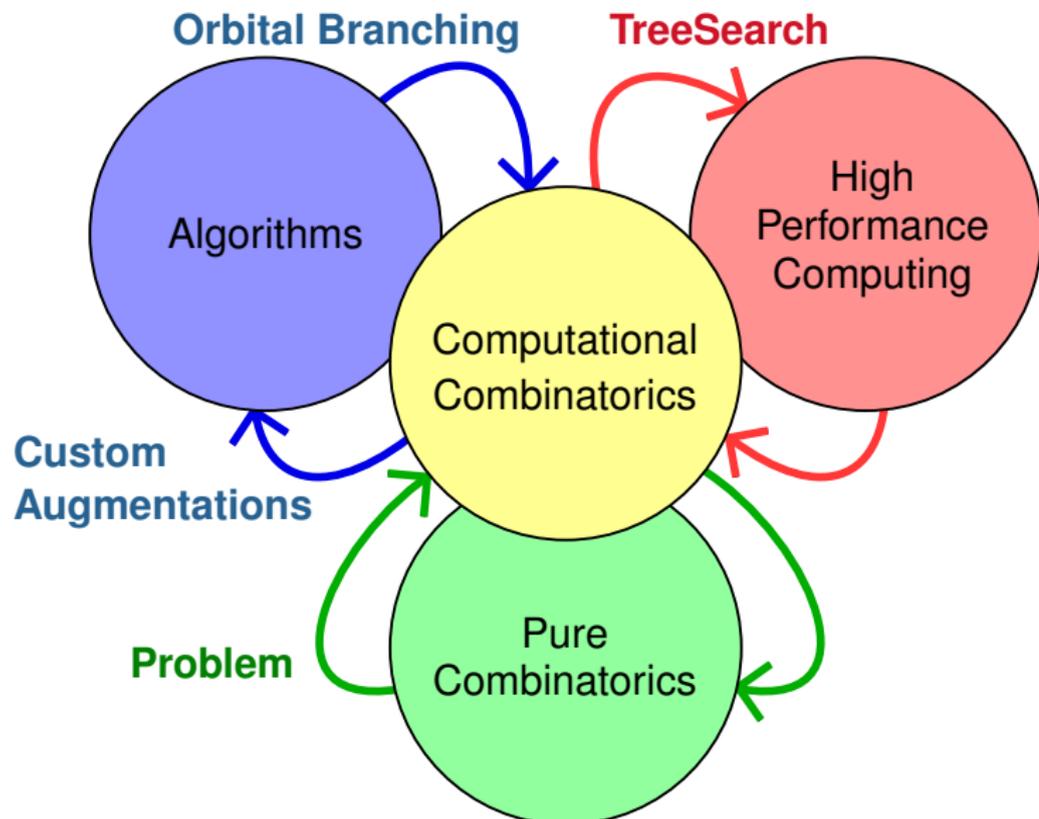
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Computational Combinatorics



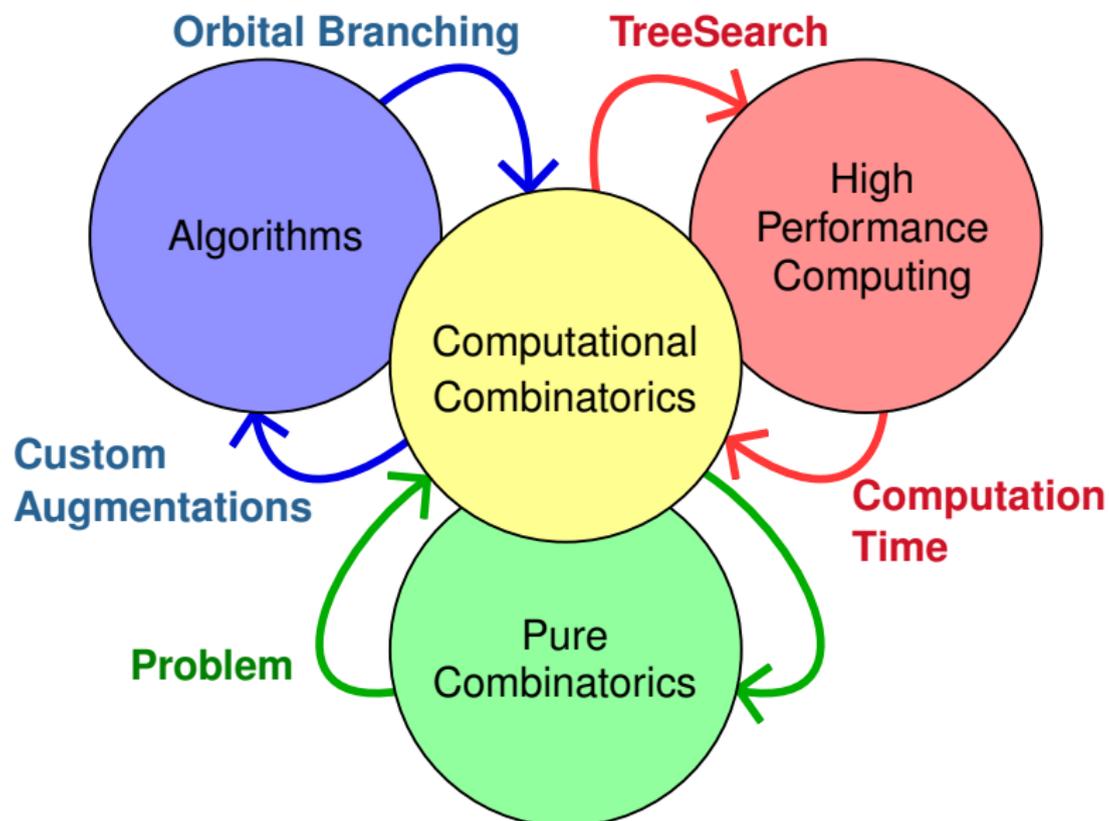
Exhaustive Search Times

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 →

$n \setminus r$	2	3	4	5	6	7	8	
2								
3								
4								
5								
6								
7								
8								
9								
10								
11								
12								
13								
14								
15								
16								
17								
18								
19								

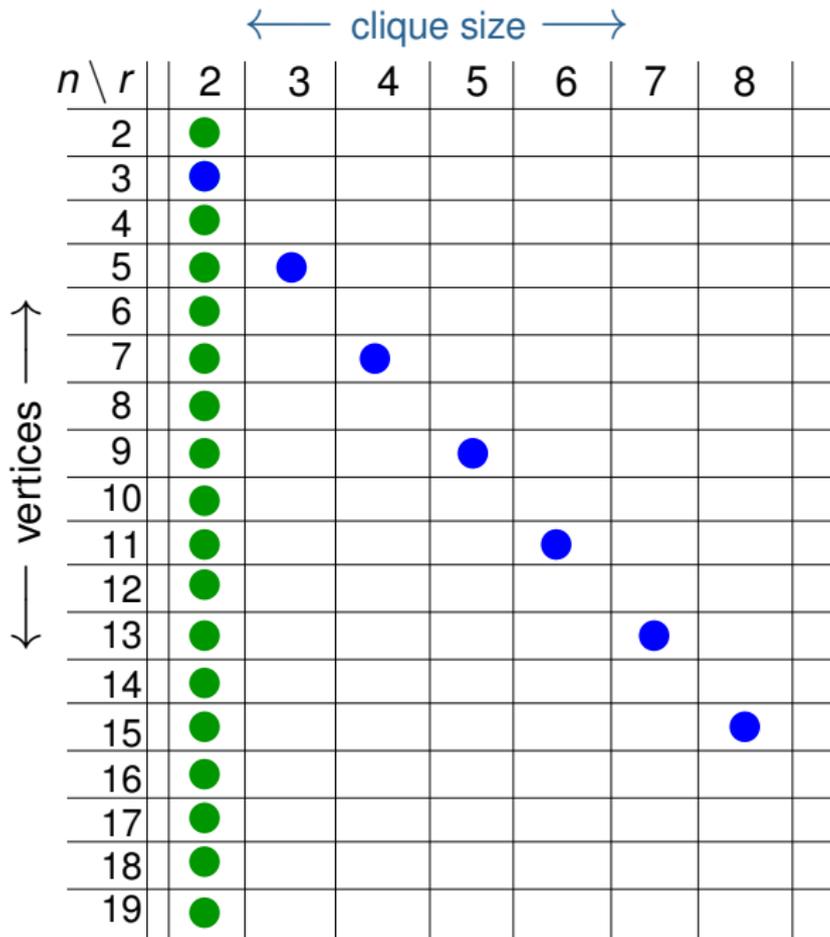
↑ vertices
↓

← clique size →

$n \setminus r$	2	3	4	5	6	7	8	
2	●							
3	●							
4	●							
5	●							
6	●							
7	●							
8	●							
9	●							
10	●							
11	●							
12	●							
13	●							
14	●							
15	●							
16	●							
17	●							
18	●							
19	●							

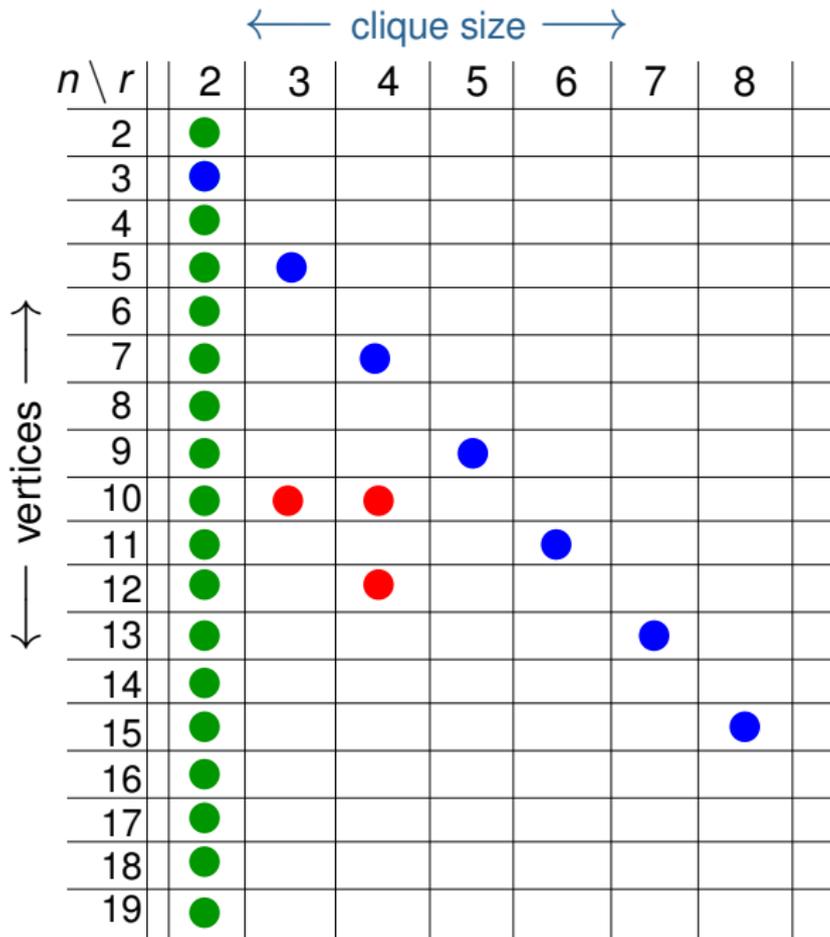
↑ vertices
↓

Empty graphs



Empty graphs

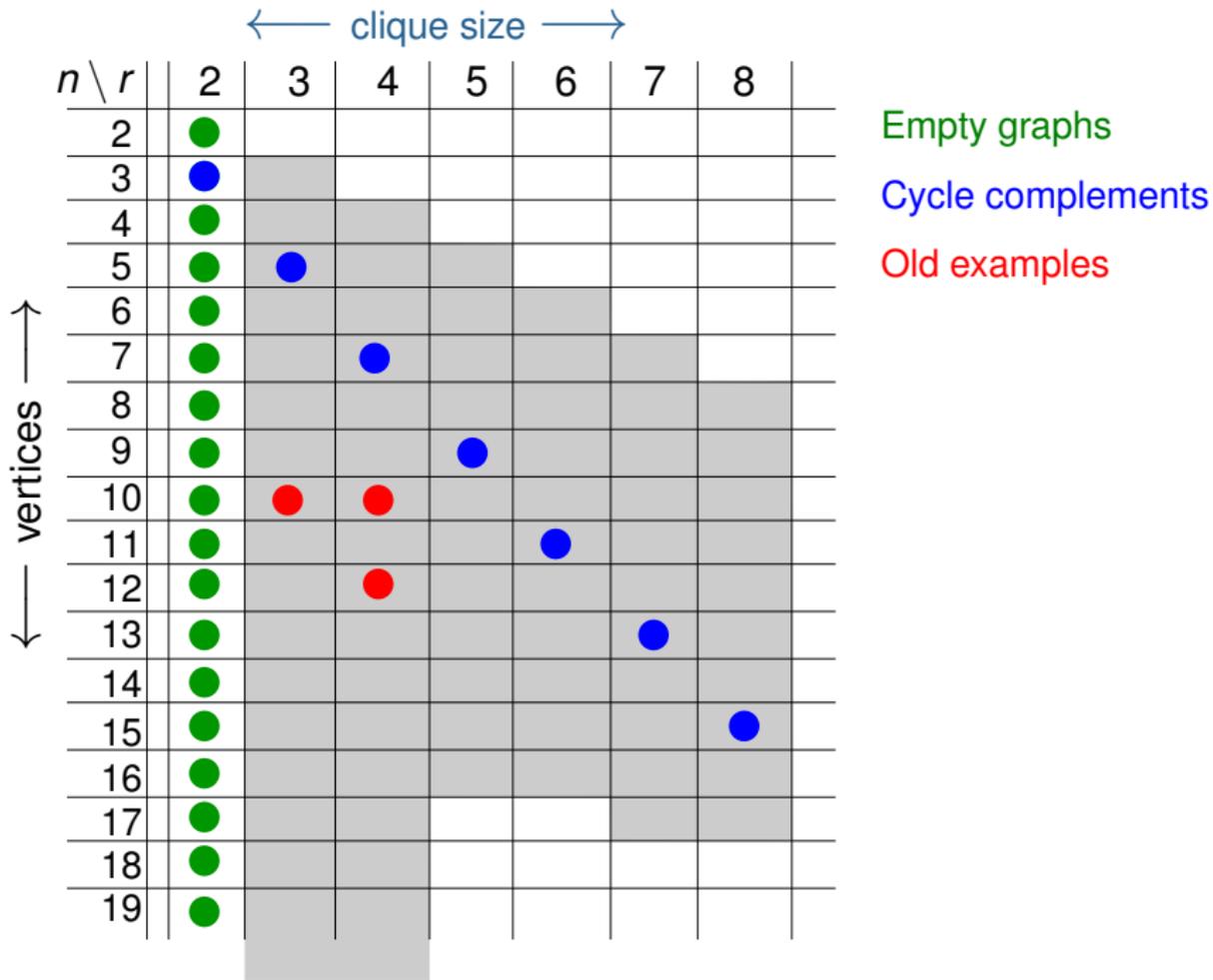
Cycle complements

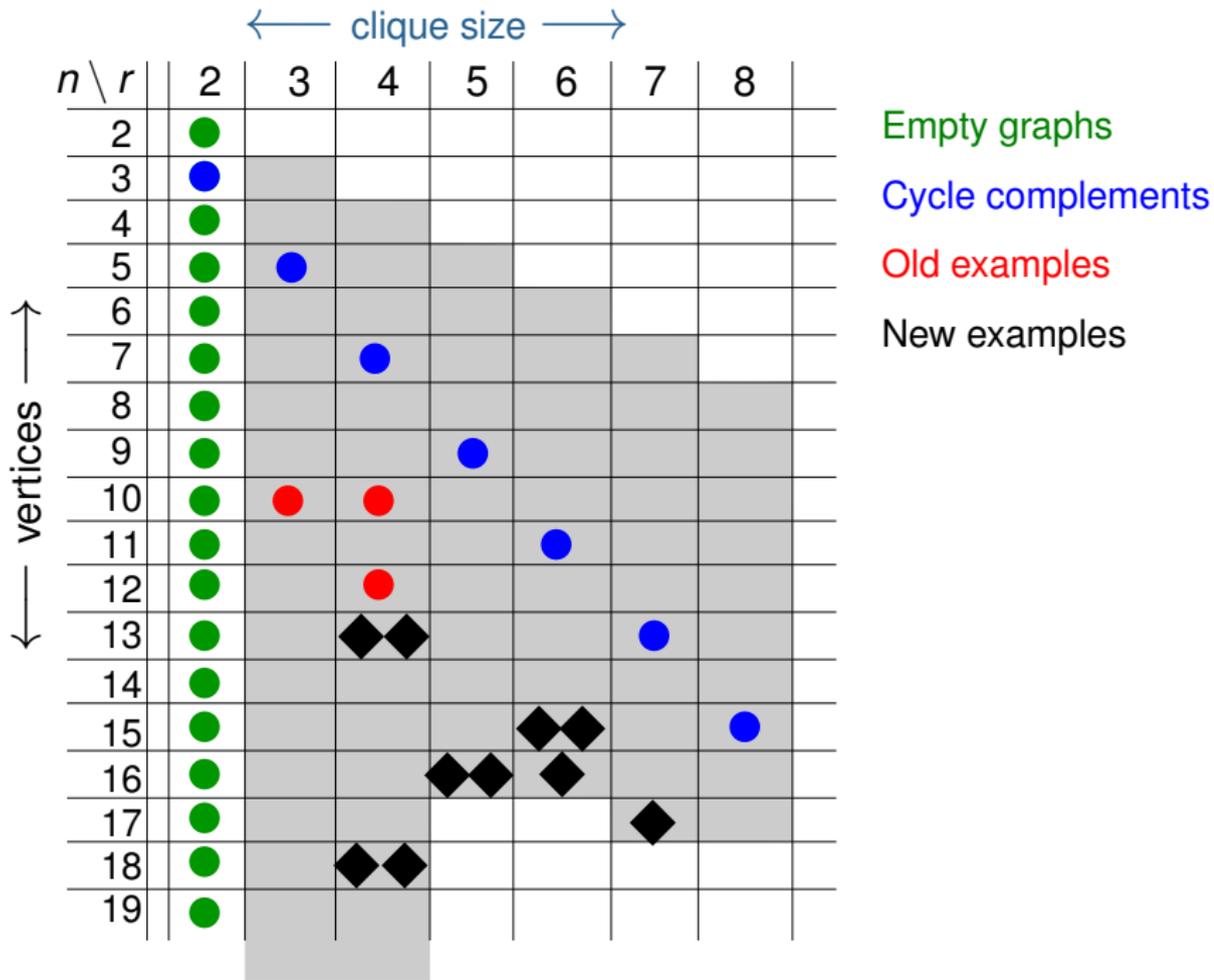


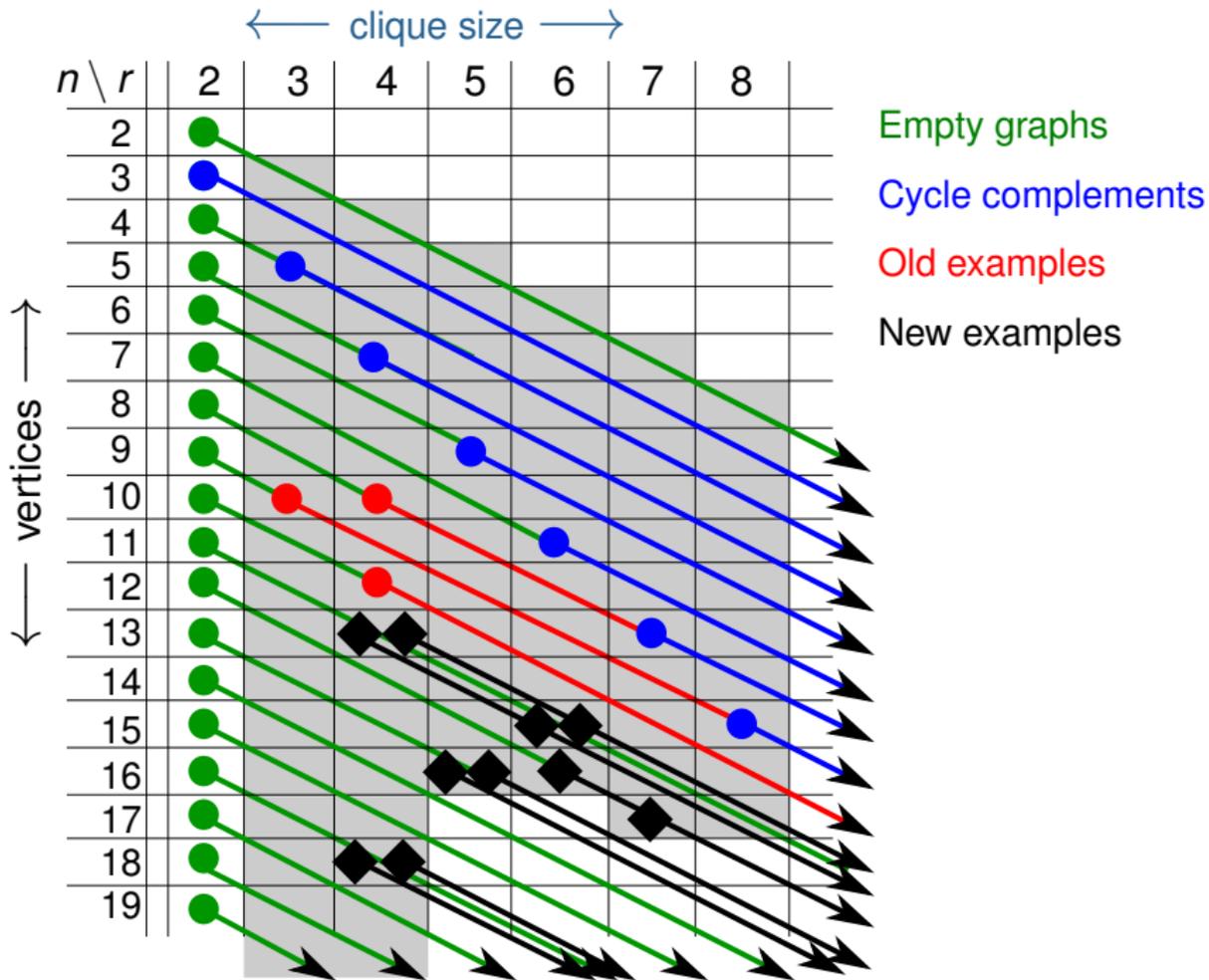
Empty graphs

Cycle complements

Old examples

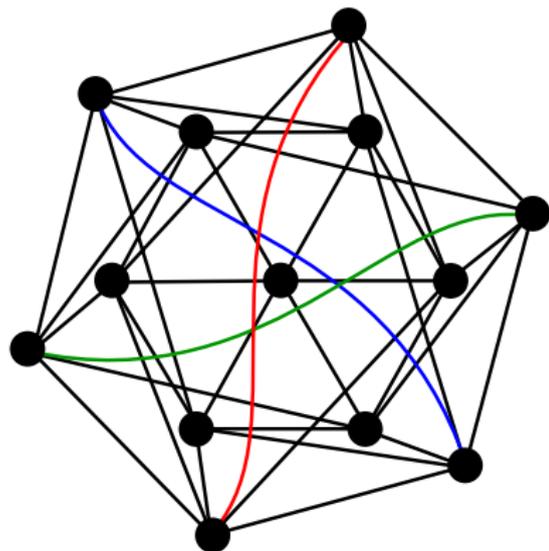




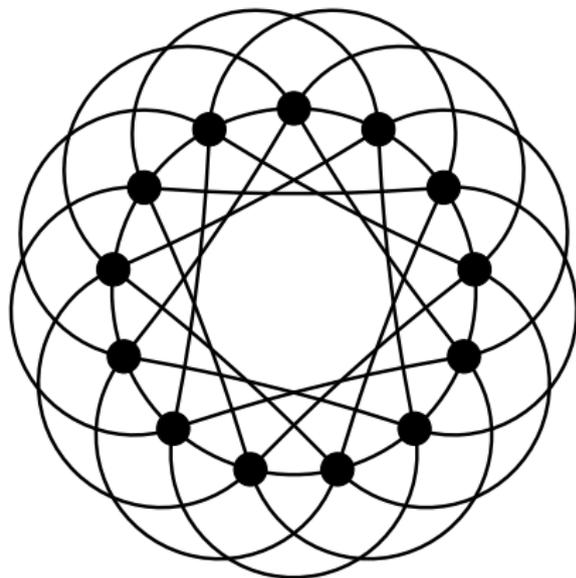


4-Primitive Graphs

$n = 13$



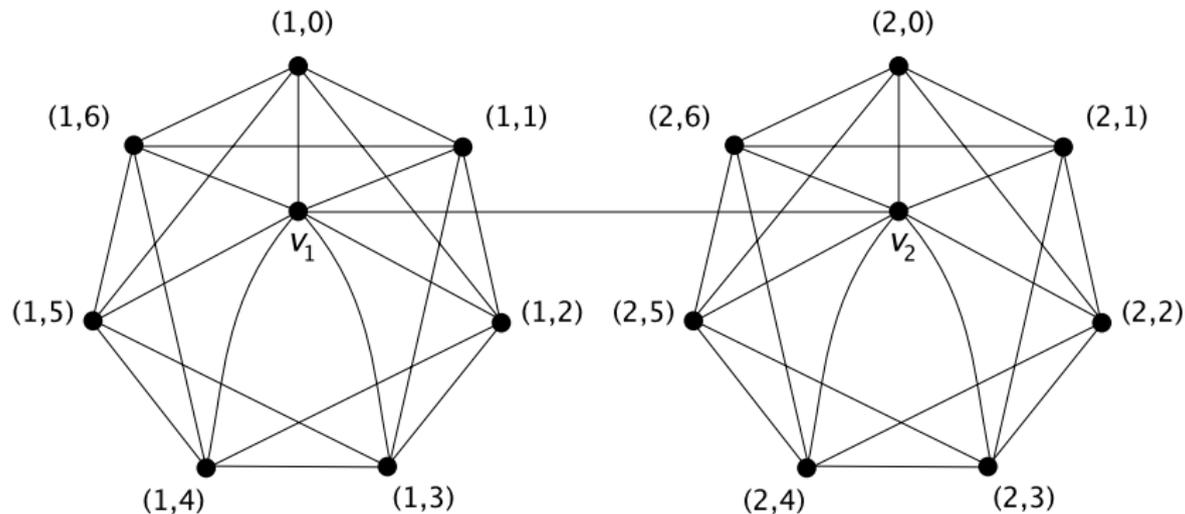
$G_{13}^{(A)}$



Paley(13)

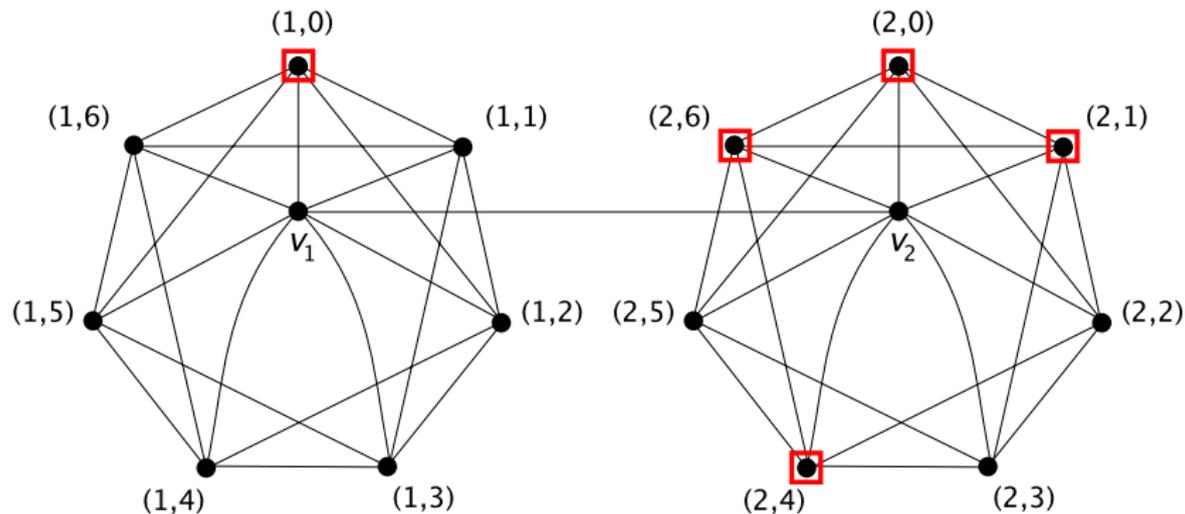
5-Primitive Graph

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



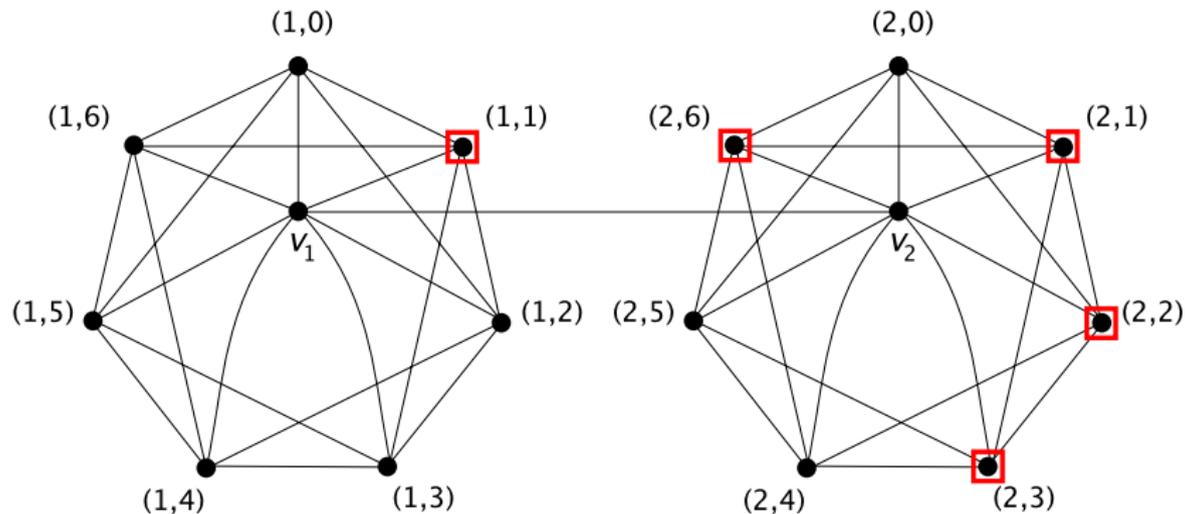
5-Primitive Graph

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



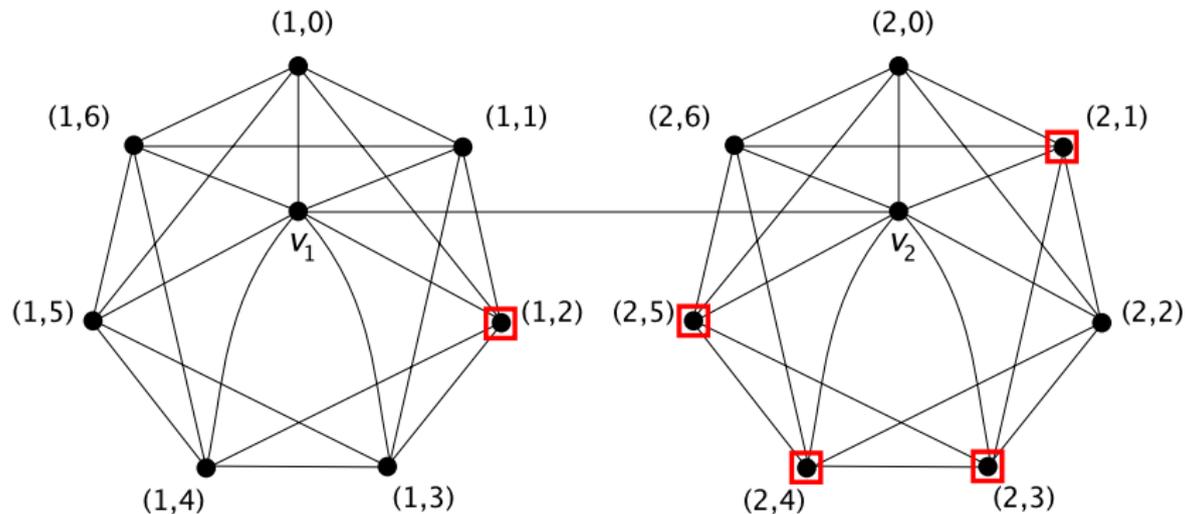
5-Primitive Graph

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



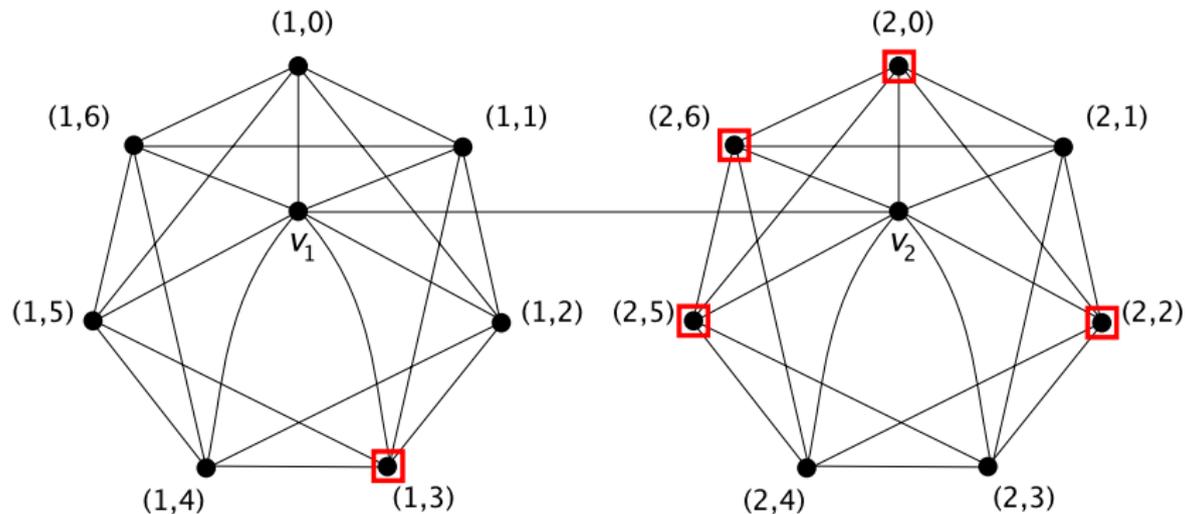
5-Primitive Graph

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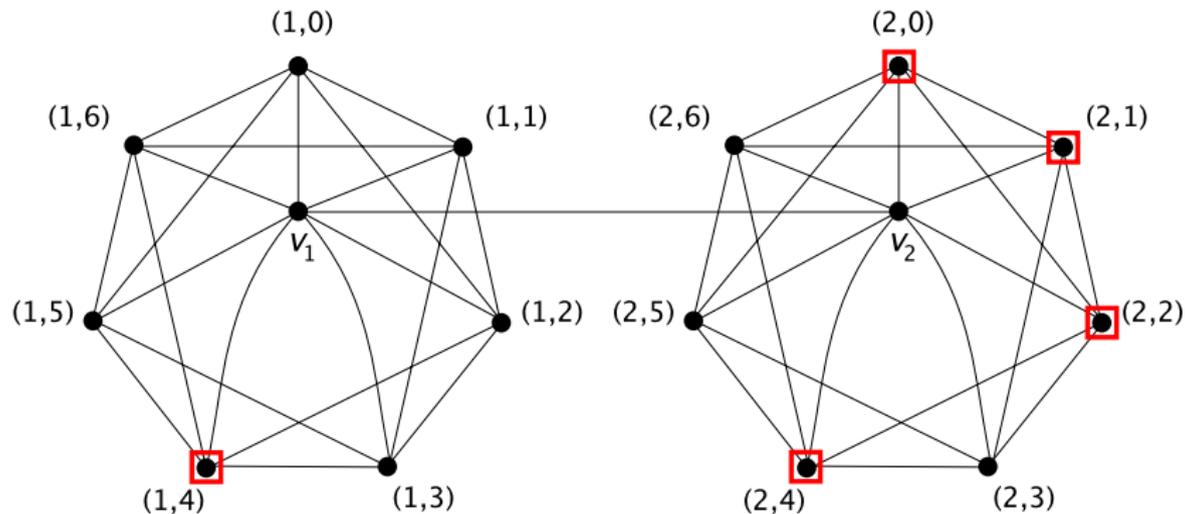
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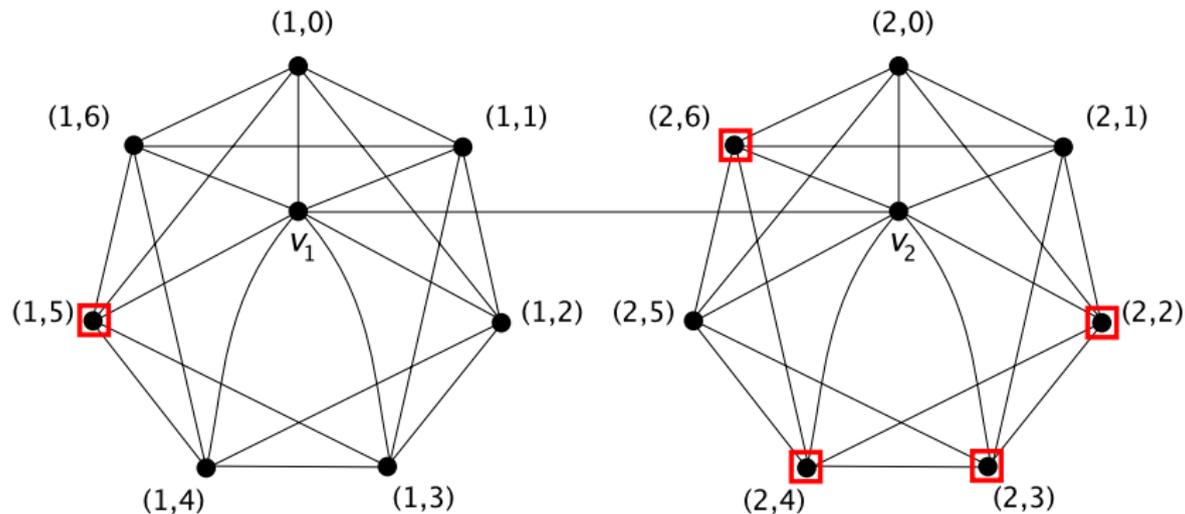
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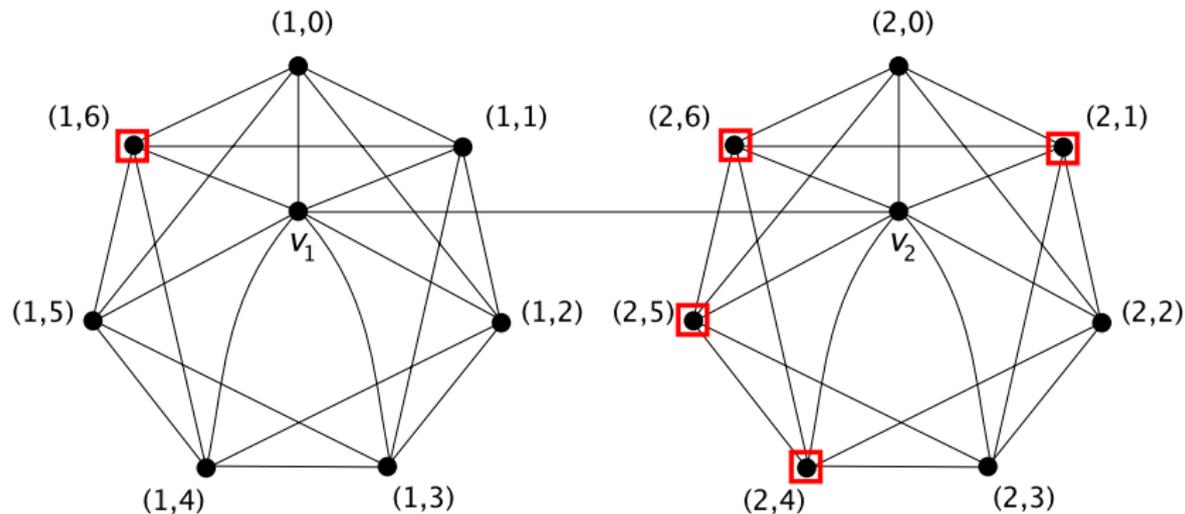
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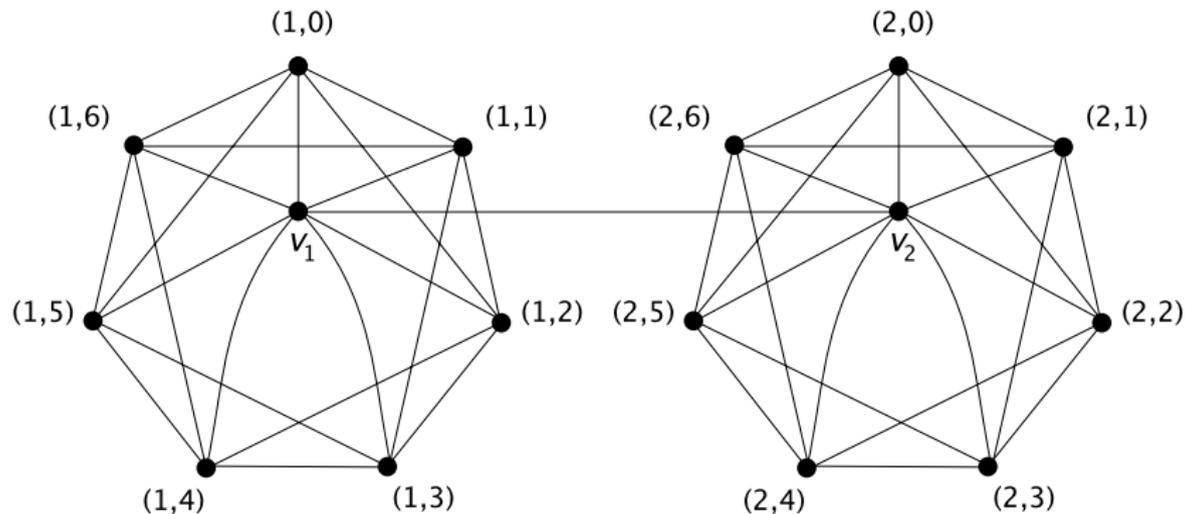
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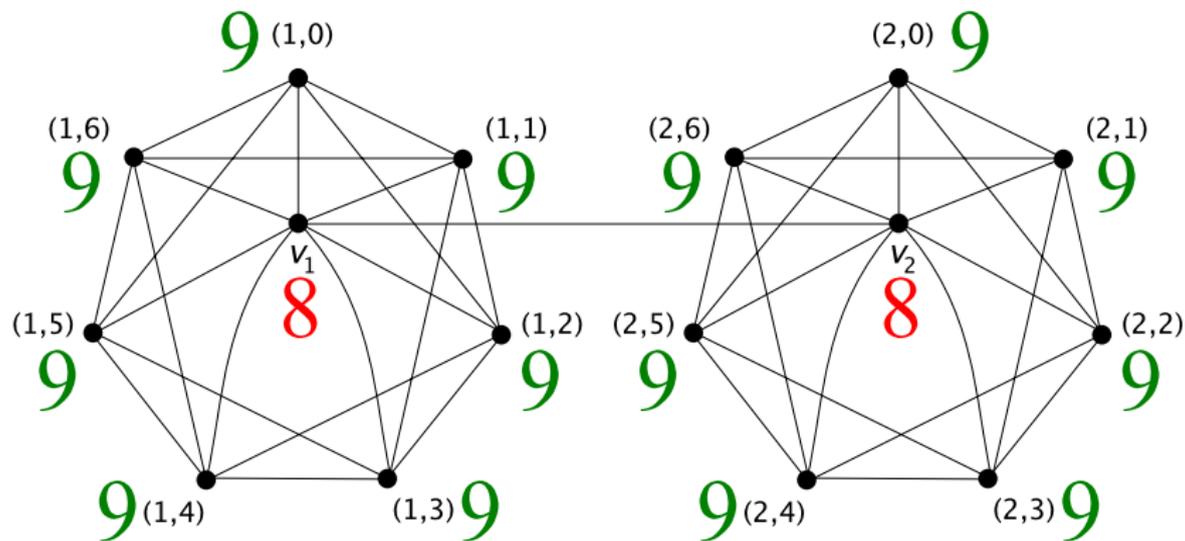
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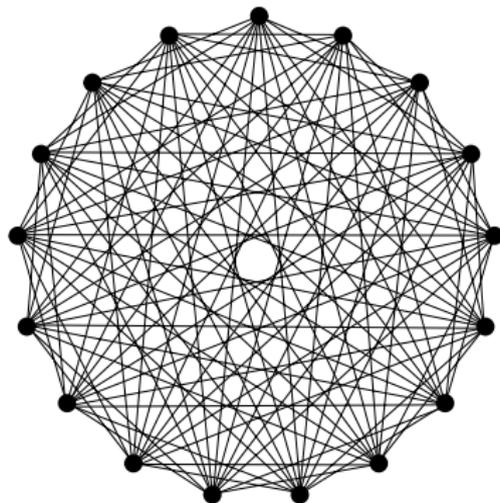
$$n = 16 : G_{16}^{(A)}$$



Not all r -primitive graphs are regular!

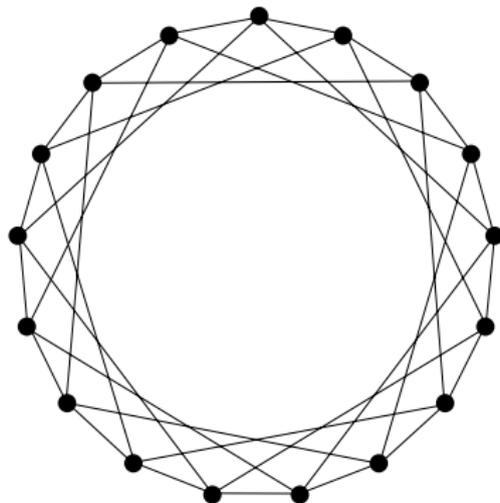
7-Primitive Graph

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



7-Primitive Graph

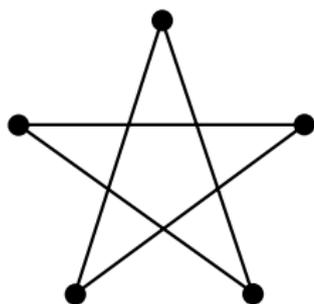
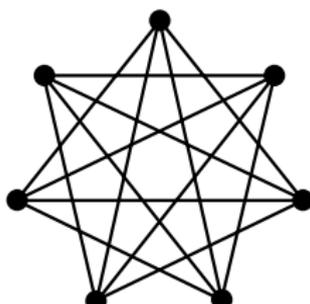
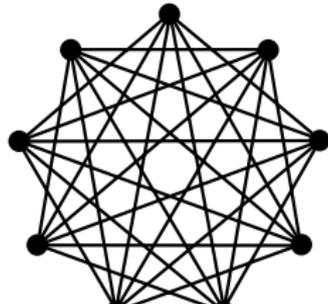
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The **Cayley complement** $\overline{C}(\mathbb{Z}_n, S)$ has vertex set $\{0, 1, \dots, n-1\}$ and an edge ij if and only if $|i-j| \pmod{n} \notin S$.

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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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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 $t \geq 1$,

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

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

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

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

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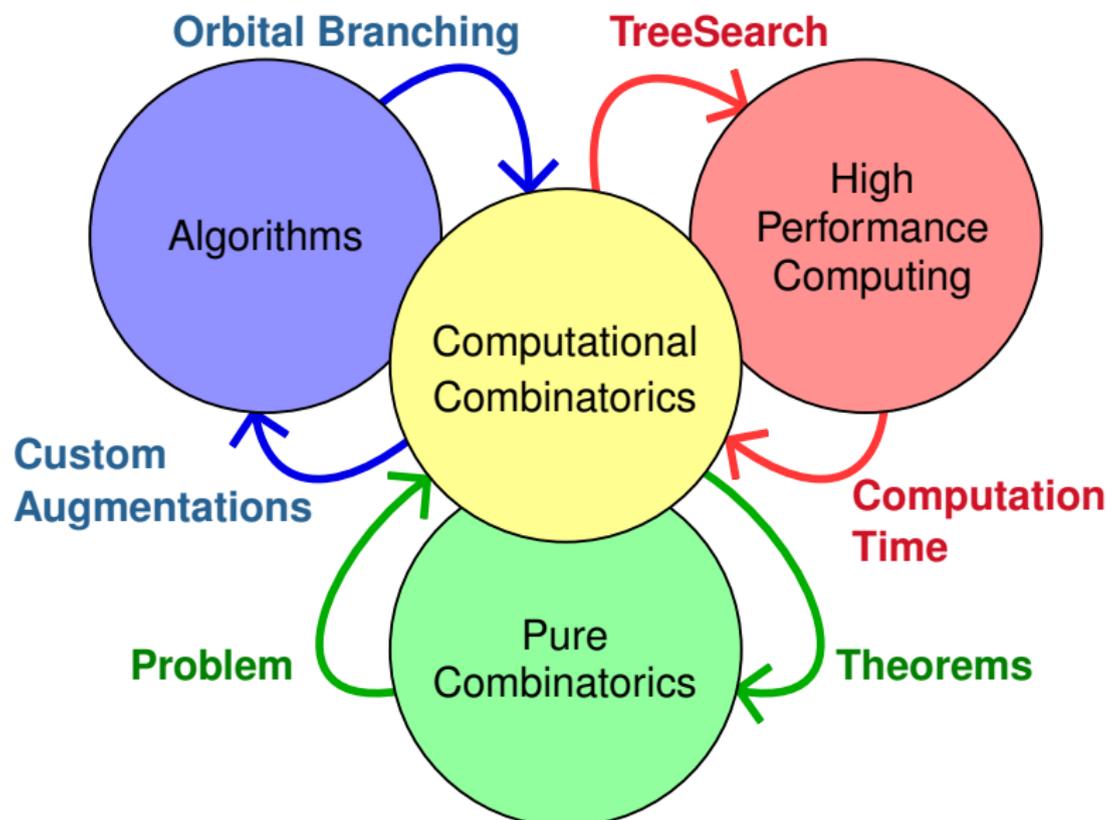
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Proof uses **discharging** method.

Computational Combinatorics



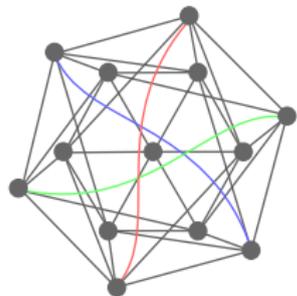
What Next?

Technique-specific

1. **Orbital Branching:** Formalize custom augmentations for arbitrary constraint systems. Apply to problems like strongly regular graphs.
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

Stephen G. Hartke



University of Nebraska–Lincoln, USA
hartke@math.unl.edu
<http://www.math.unl.edu/~shartke2/>

