Combinatorial Generation in the Presence of Symmetry

Derrick Stolee

Iowa State University
dstolee@iastate.edu
http://www.math.iastate.edu/dstolee/

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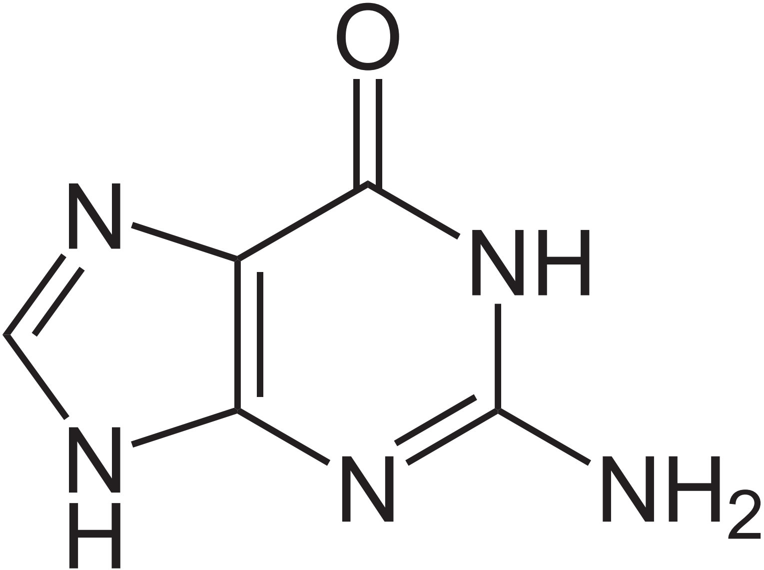
Application: Generating Chemical Molecules



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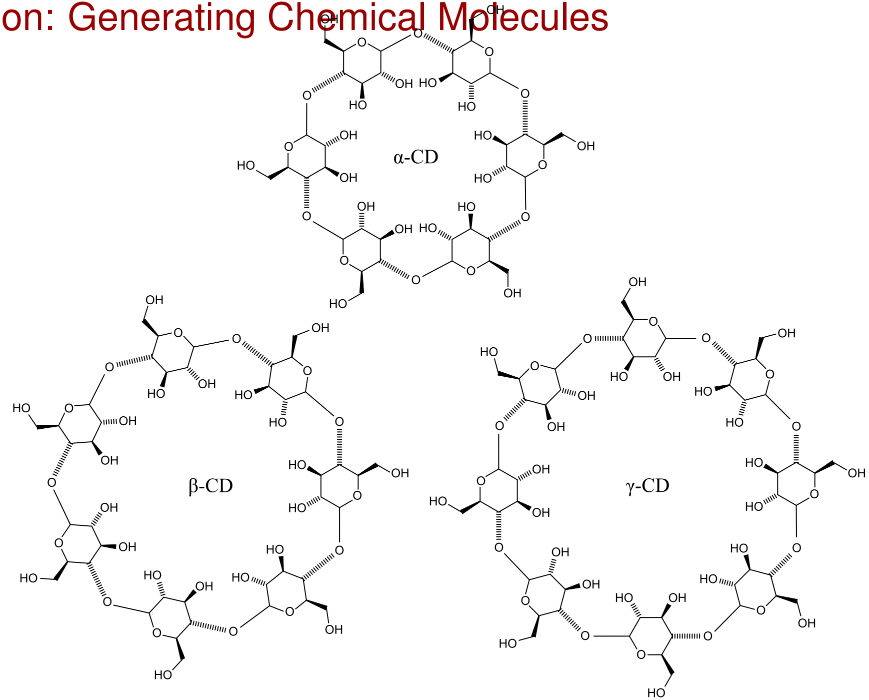
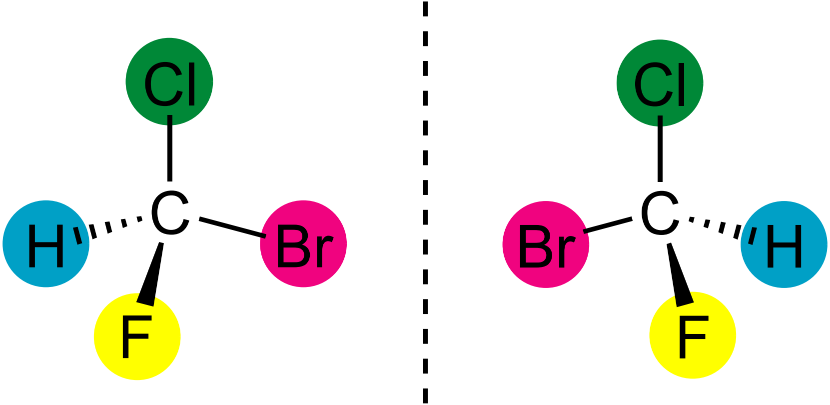
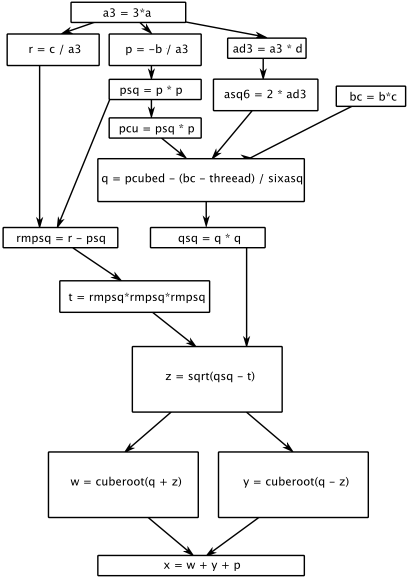


Application: Generating Chemical Molecules

Chirality?



Application: Compiling Software



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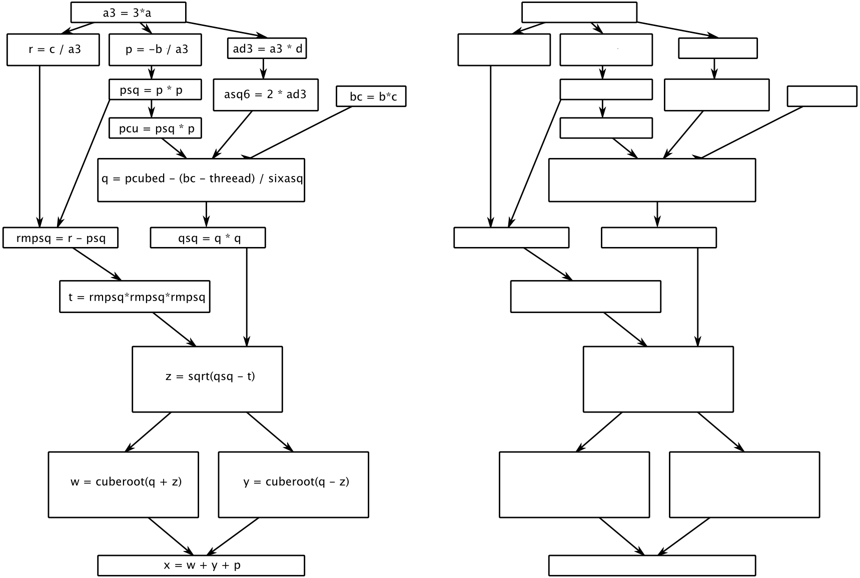

Exponential Behavior is Unavoidable

When dealing with NP-hard problems (or **worse!**), exponential behavior is unavoidable.

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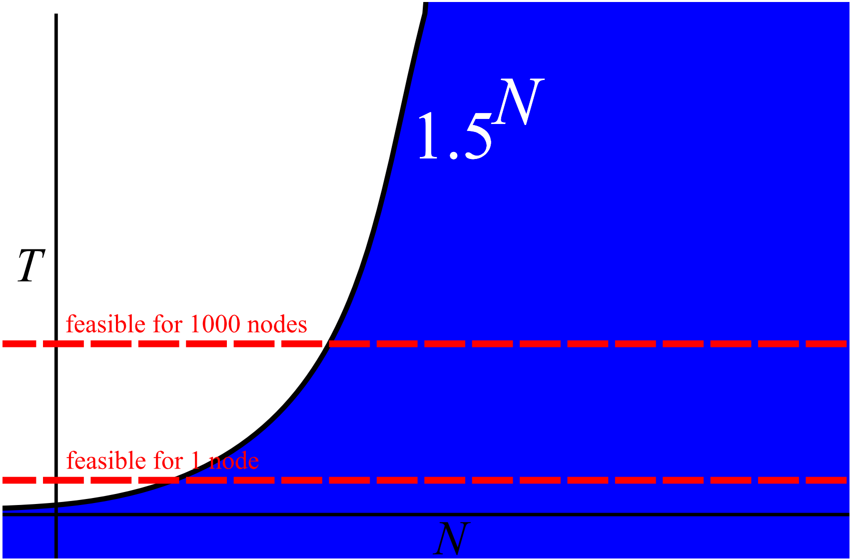
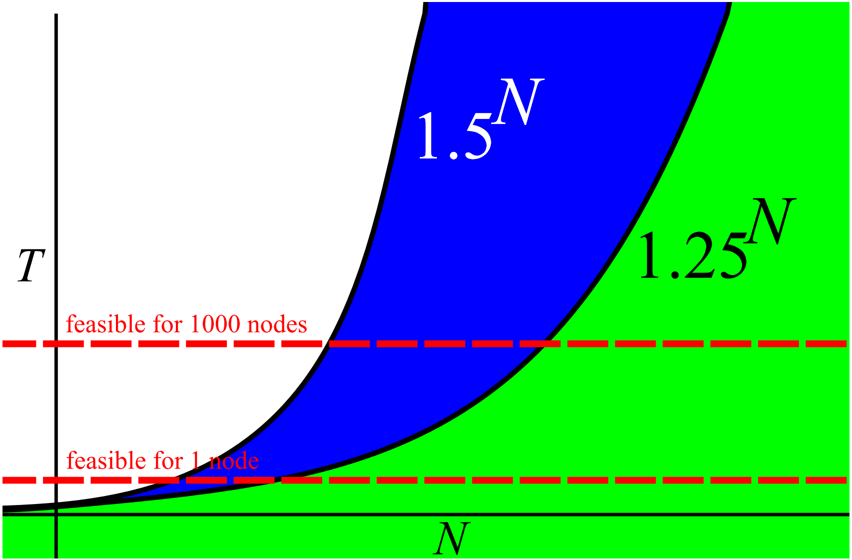
All we can do is **delay** or **diminish** that exponential behavior.

Shifting the Exponent



Shifting the Exponent



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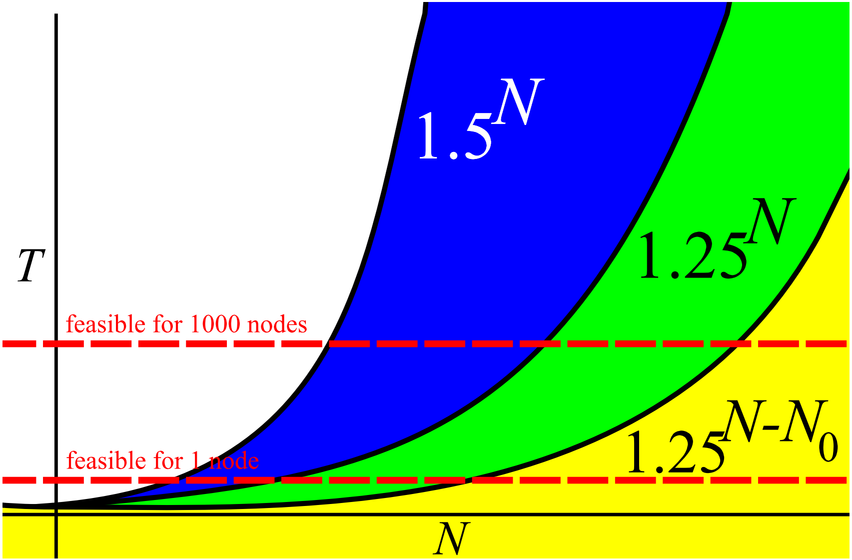
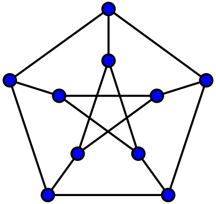
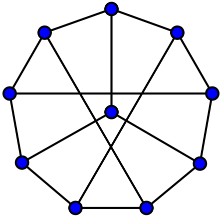
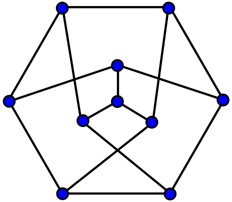


Graphs







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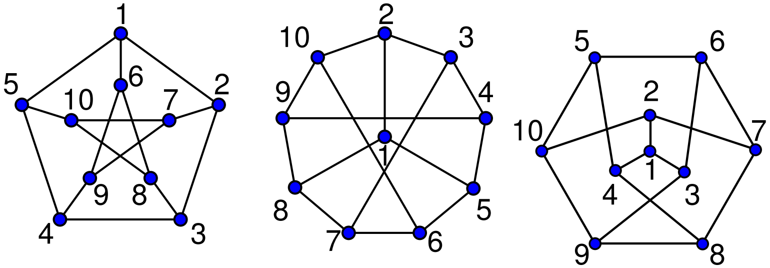

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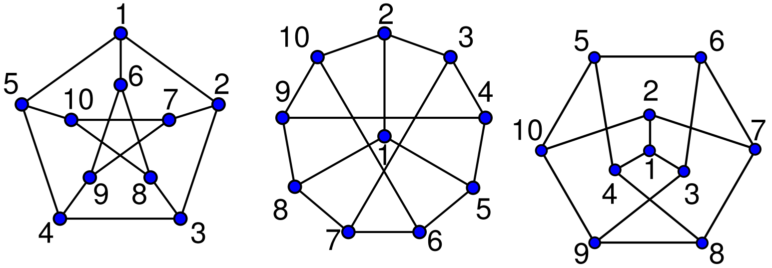

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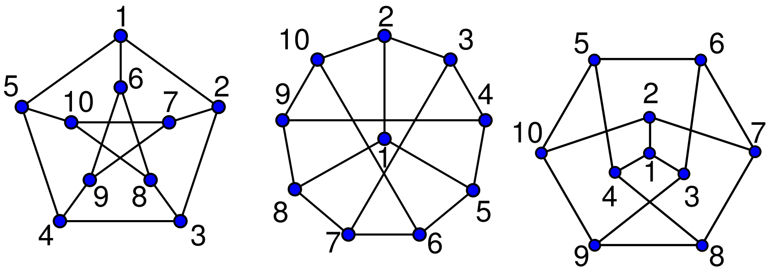

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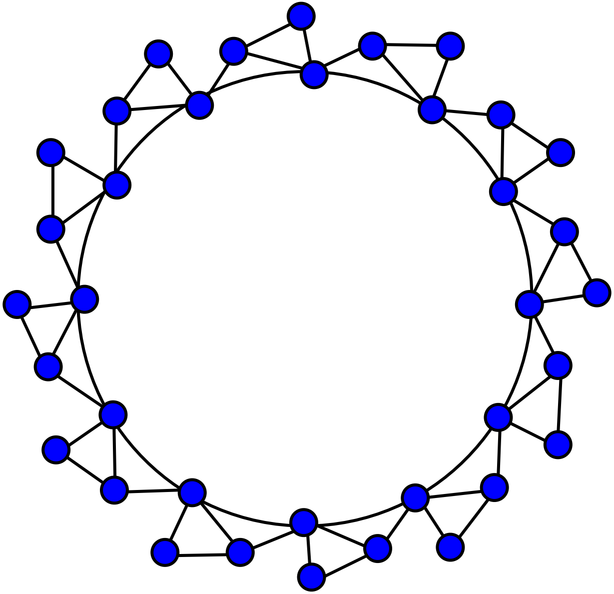
An **automorphism** of G is a bijection from $V(G)$ to $V(G)$ that induces a bijection from $E(G)$ to $E(G)$.

Graphs: Automorphisms

The set of **automorphisms** form a **group**.



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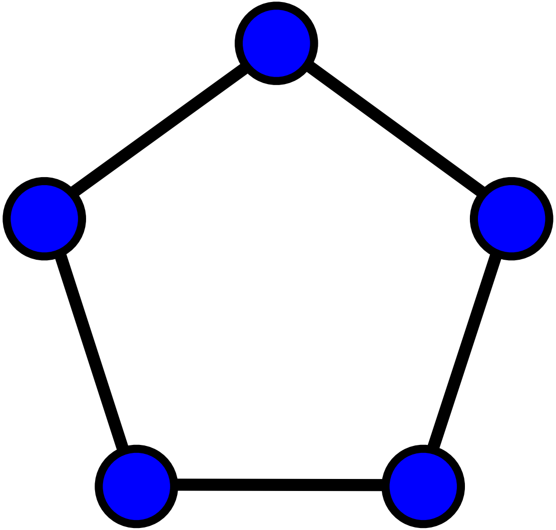

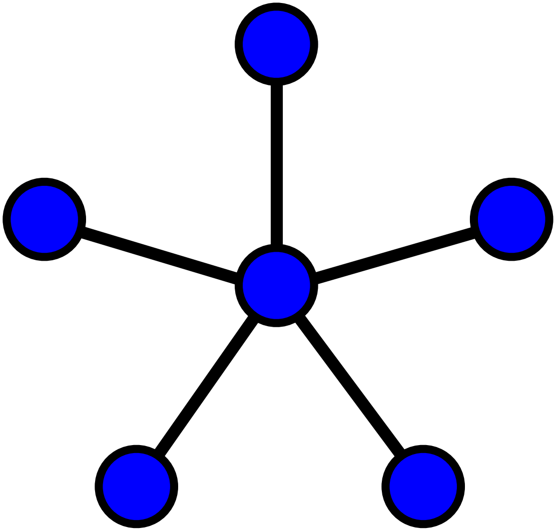

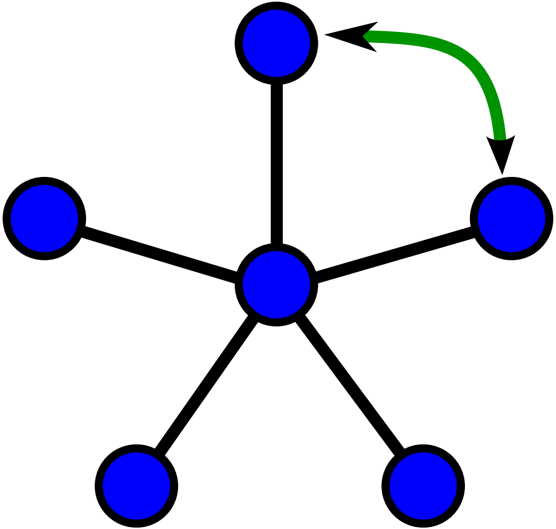

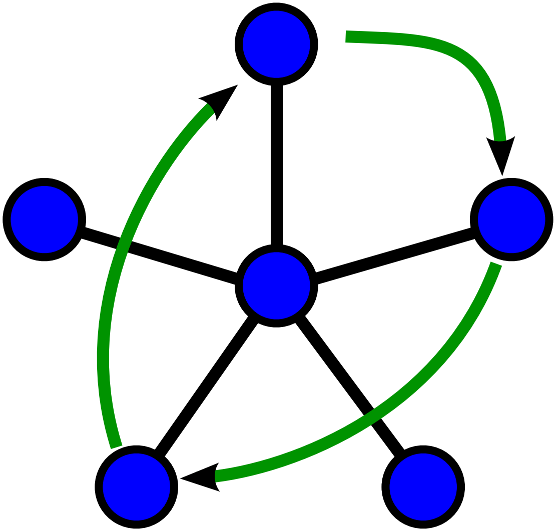

Permutations

1	2	3	4	5
5	3	4	1	2

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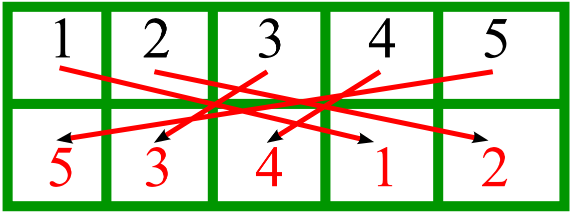

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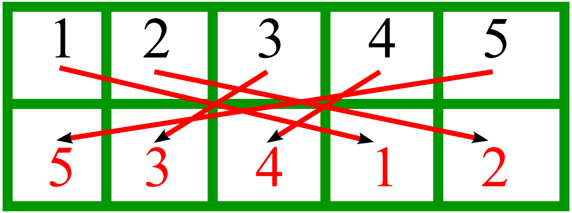

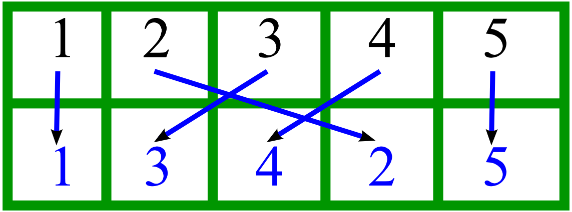

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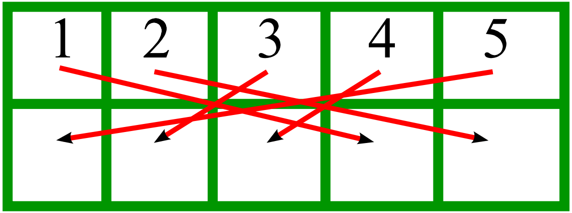

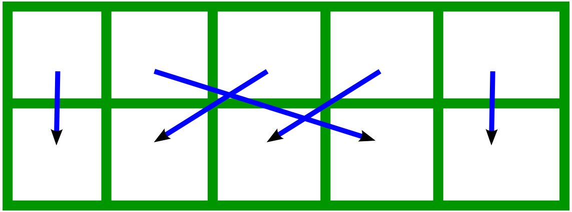

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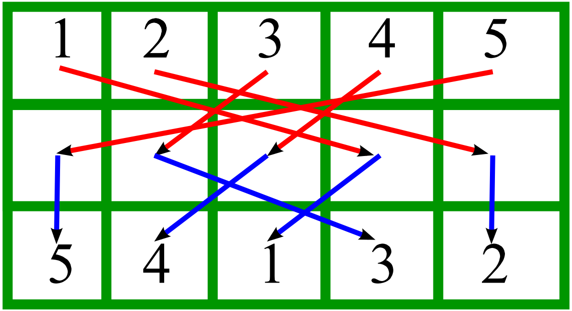
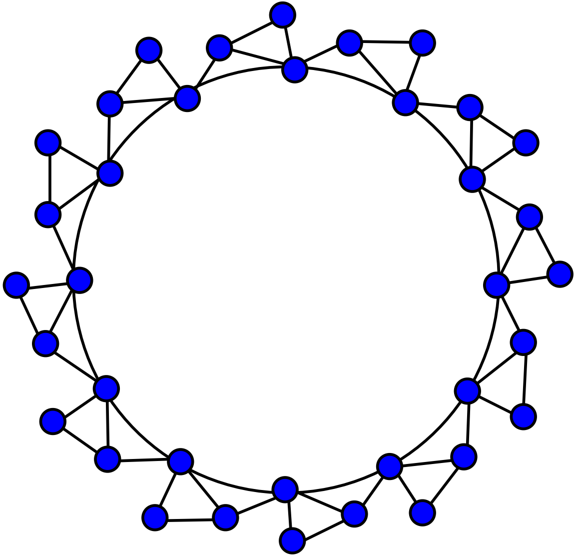


Graphs: Orbits

An **orbit** is a maximal set of objects such that every object is sent to every other object by some automorphism.



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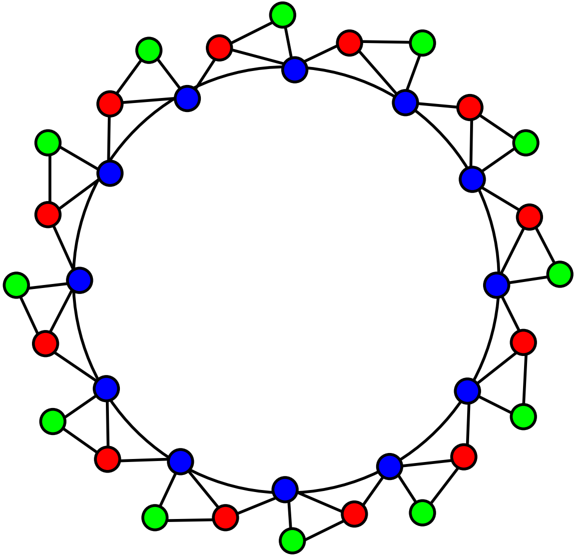

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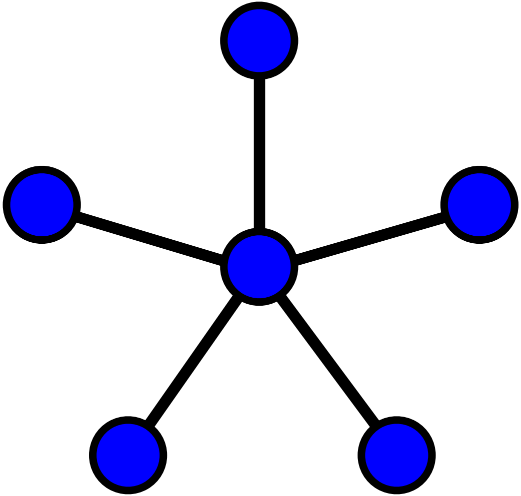

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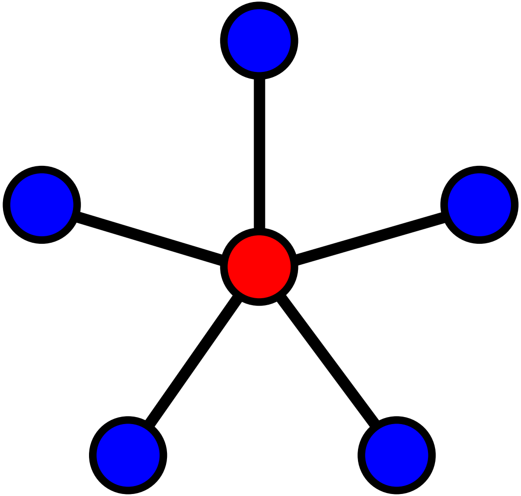
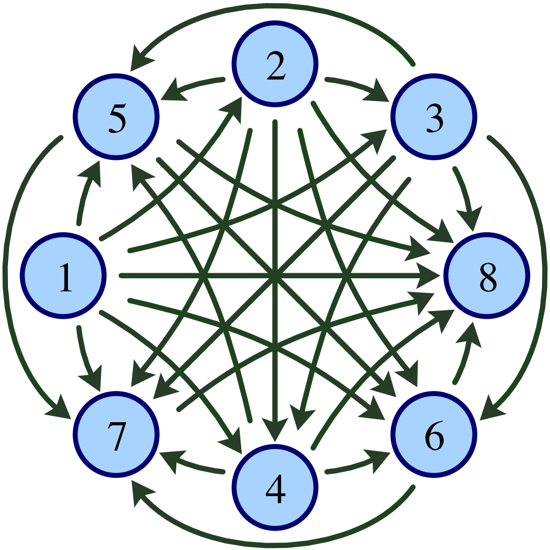


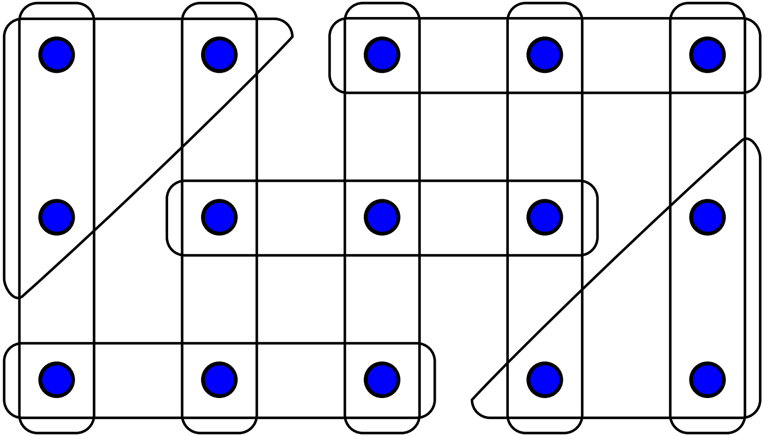
Other Objects

Directed Graphs



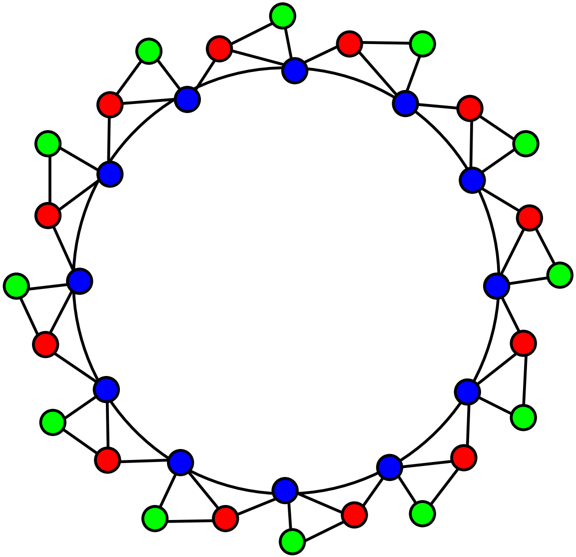
Other Objects

Hypergraphs



Other Objects

Colored (Partitioned) Graphs



Other Objects

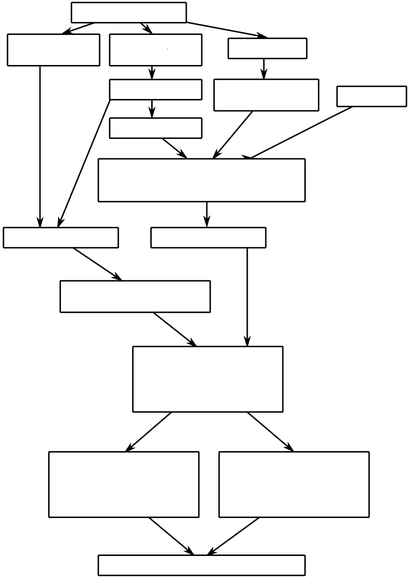
Latin Squares

A	B	P	C	O	D	N	E	M	F	L	G	K	H	J	I
B	C	A	D	P	E	O	F	N	G	M	H	L	I	K	J
C	D	B	E	A	F	P	G	O	H	N	I	M	J	L	K
D	E	C	F	B	G	A	H	P	I	O	J	N	K	M	L
E	F	D	G	C	H	B	I	A	J	P	K	O	L	N	M
F	G	E	H	D	I	C	J	B	K	A	L	P	M	O	N
G	H	F	I	E	J	D	K	C	L	B	M	A	N	P	O
H	I	G	J	F	K	E	L	D	M	C	N	B	O	A	P
I	J	H	K	G	L	F	M	E	N	D	O	C	P	B	A
J	K	I	L	H	M	G	N	F	O	E	P	D	A	C	B
K	L	J	M	I	N	H	O	G	P	F	A	E	B	D	C
L	M	K	N	J	O	I	P	H	A	G	B	F	C	E	D
M	N	L	O	K	P	J	A	I	B	H	C	G	D	F	E
N	O	M	P	L	A	K	B	J	C	I	D	H	E	G	F
O	P	N	A	M	B	L	C	K	D	J	E	I	F	H	G
P	A	O	B	N	C	M	D	L	E	K	F	J	G	I	H

This 16×16 *latin square assists in the construction of a Williams Design.*

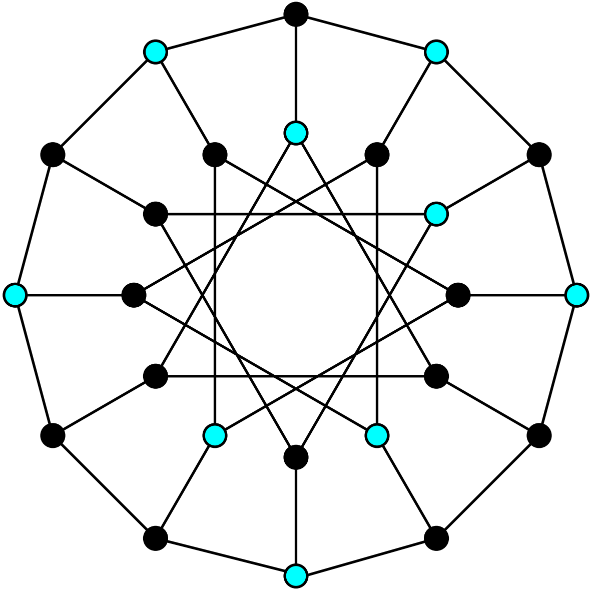
Other Objects

Partially-Ordered Sets



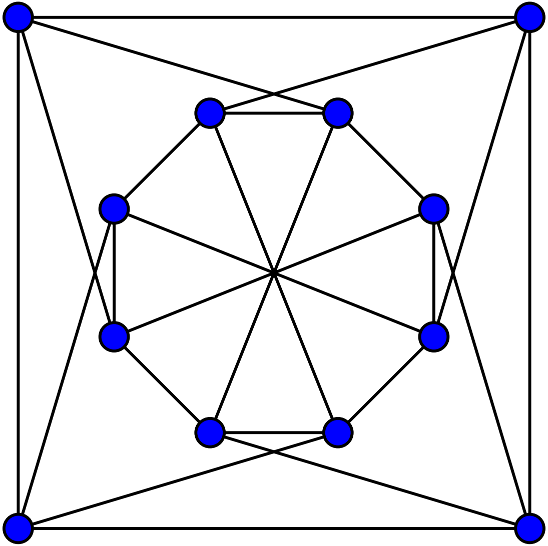
Subobjects

Independent Sets



Subobjects

(Induced) Subgraphs



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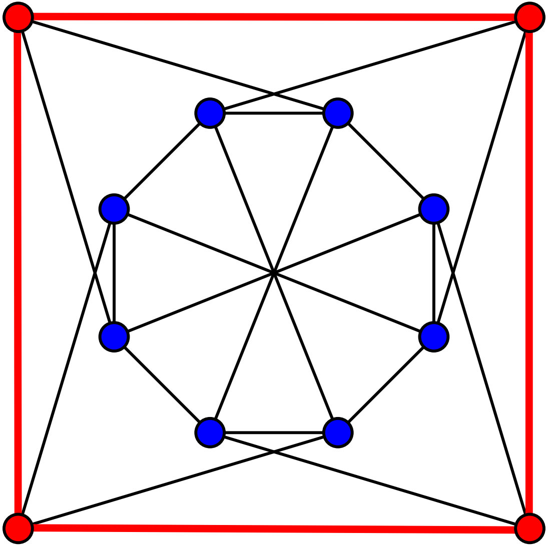

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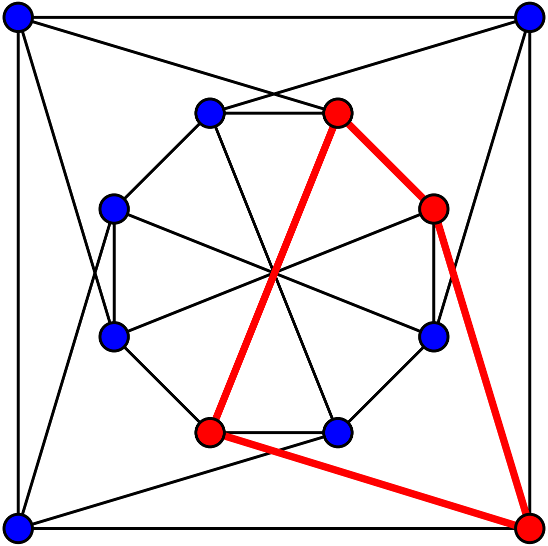

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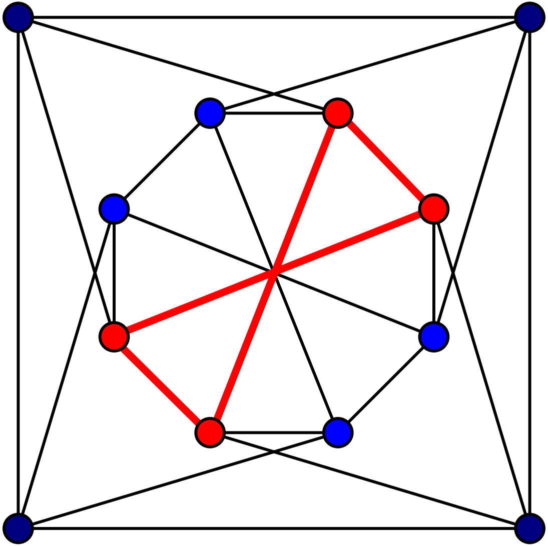
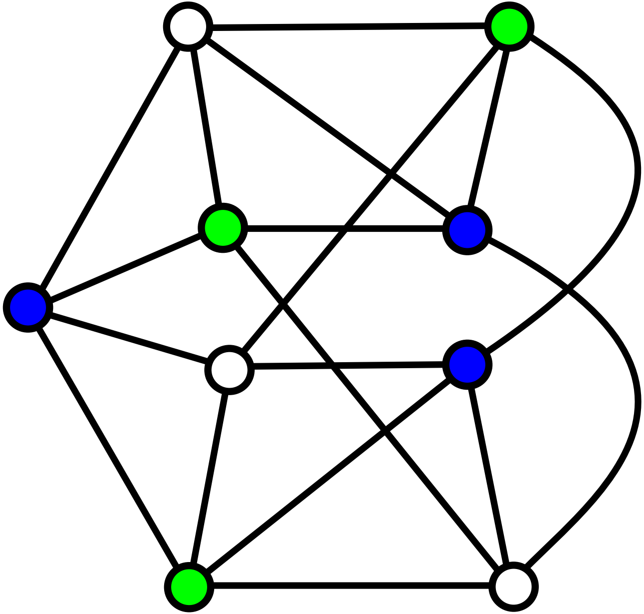


Subobjects

(Proper) Colorings



Generation Algorithms

Goal: Generate all *unlabeled* objects that satisfy the constraints.

Symmetry Breaking

1. Reduces isomorphic duplicates.
2. Does not allow for dynamic symmetry updates.
3. Removes symmetry, then uses standard symmetry-unaware algorithms.

Orbital Branching

1. Reduces isomorphic duplicates.
2. Allows for dynamic symmetry updates.
3. Branching method can be customized to the given problem.
4. Integrates well with branch-and-bound methods and constraint propagation.

(Ostrowski talked about this, also my CS Colloquium)

Canonical Deletion

1. Eliminates isomorphic duplicates*.
2. Allows for dynamic symmetry updates.
3. Augmentation method can be customized to the given problem.
4. Does not integrate well with branch-and-bound methods or constraint propagation.

Brendan McKay, Isomorph-free exhaustive generation, *J. of Algorithms* (1997).

Canonical Deletion

1. Build objects piece-by-piece.
2. Define a *canonical construction path* to every unlabeled object.
3. Only follow paths that agree with the canonical construction path.

Example: Generating Graphs by Vertex Additions

Let's generate all graphs of order n by adding vertices one-by-one.

Augmentation: Add a vertex adjacent to a set $S \subset V(G)$.

Deletion: Select a vertex $v \in V(G)$ to delete, $G' = G - v$.

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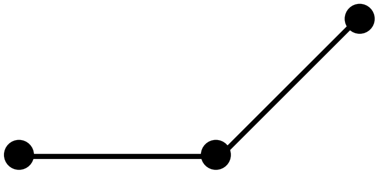

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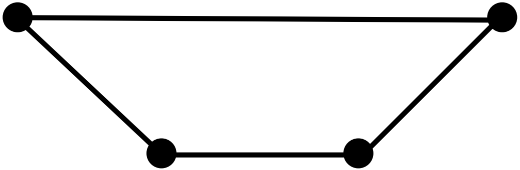

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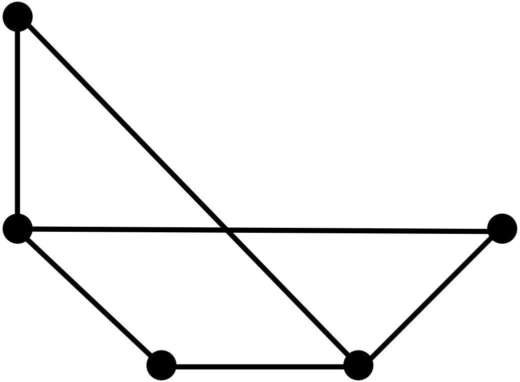

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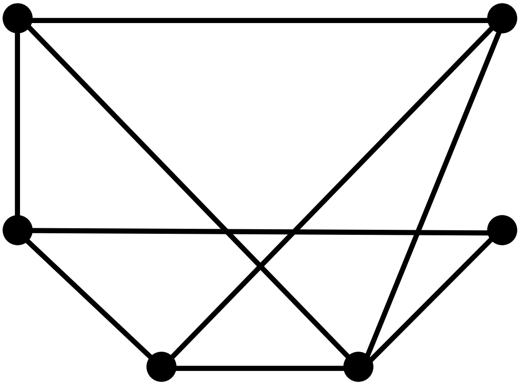

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IMPORTANT: Only one augmentation per orbit!

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Canonical Labeling

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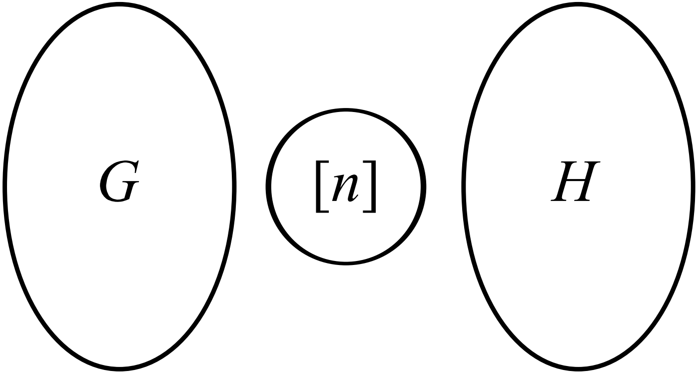

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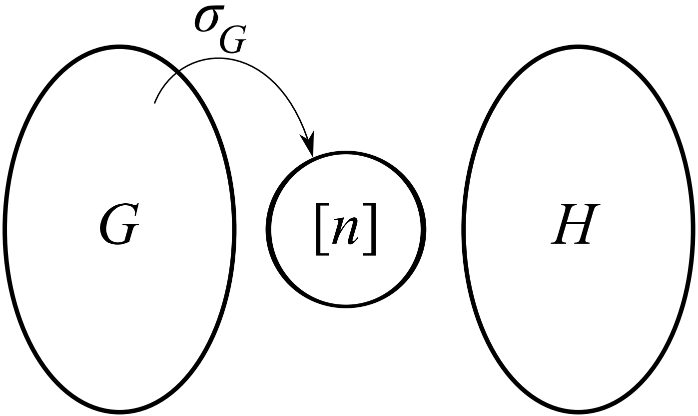

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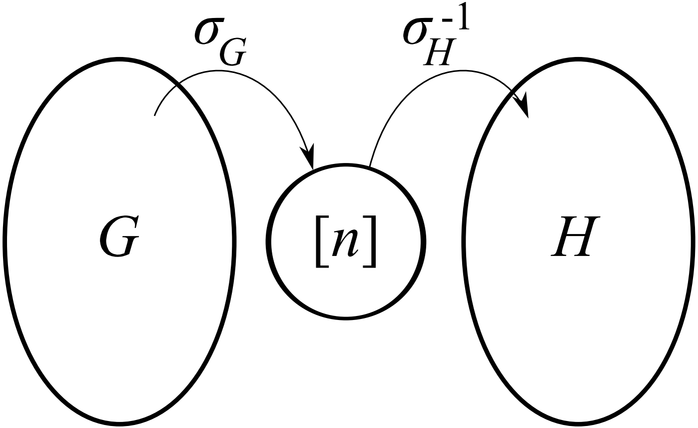

Canonical labels can be computed by McKay's `nauty` software.

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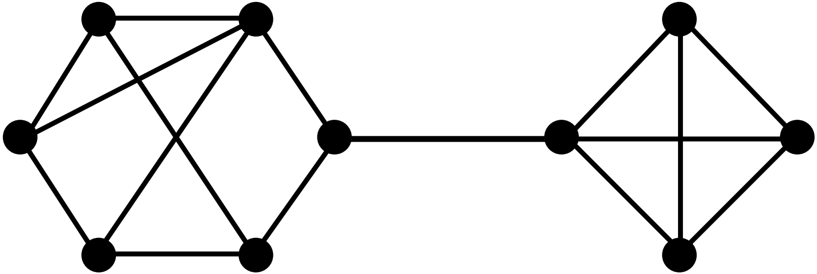
The vertex v is the canonical deletion.

Canonical Vertex Deletions



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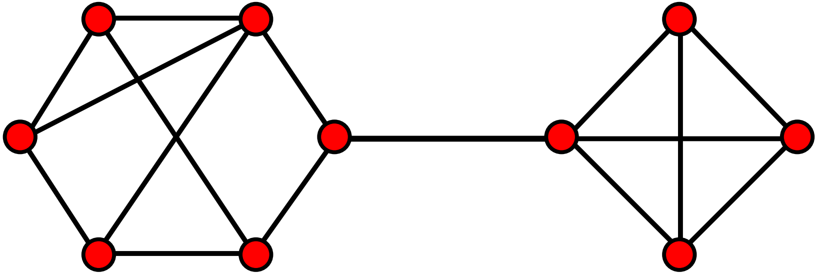

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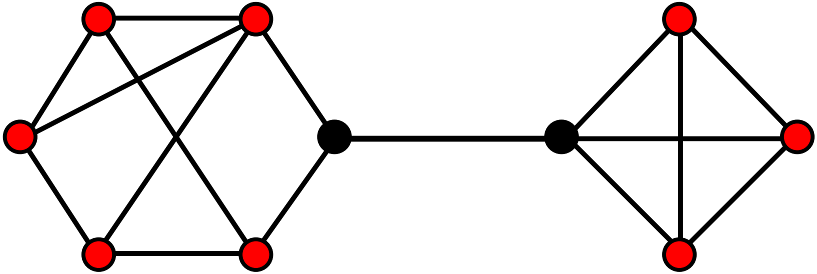

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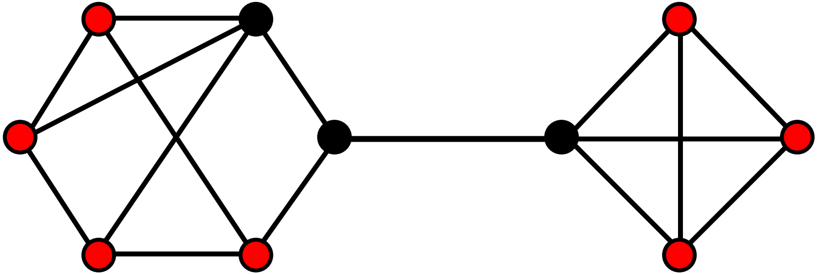

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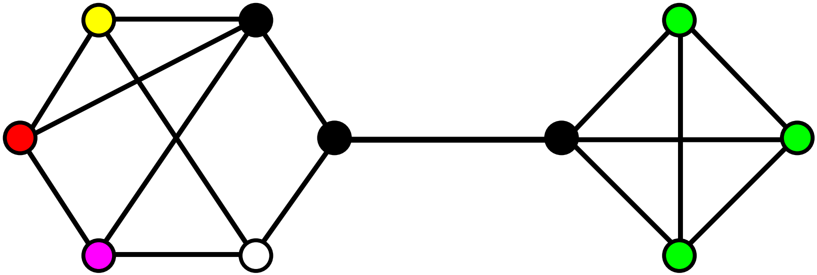
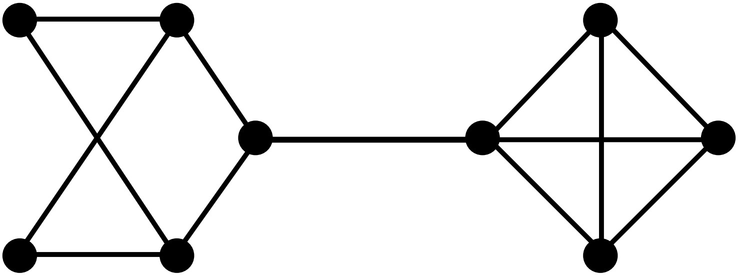


Canonical Vertex Deletions



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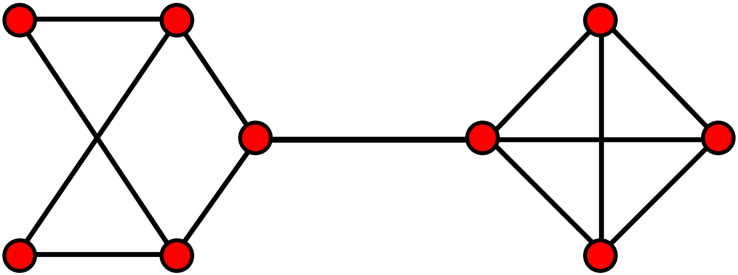

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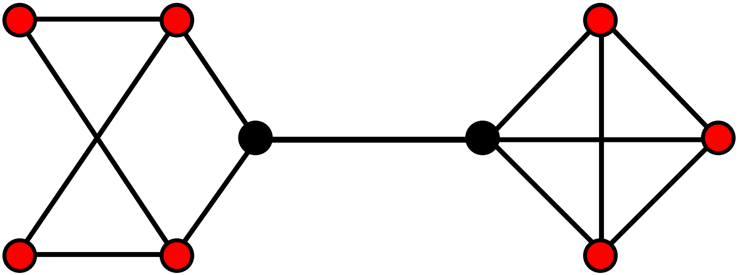

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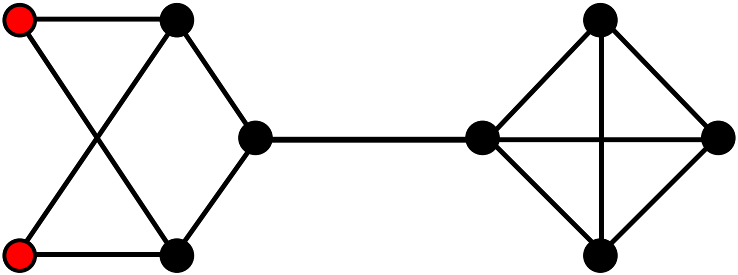

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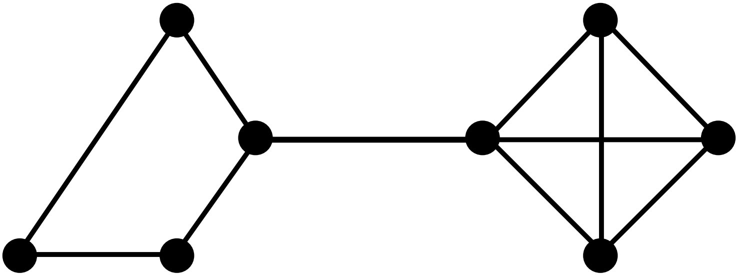

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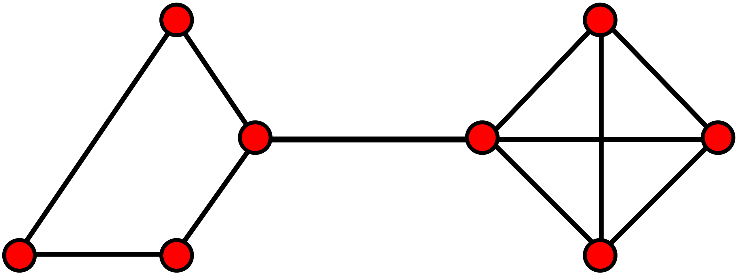

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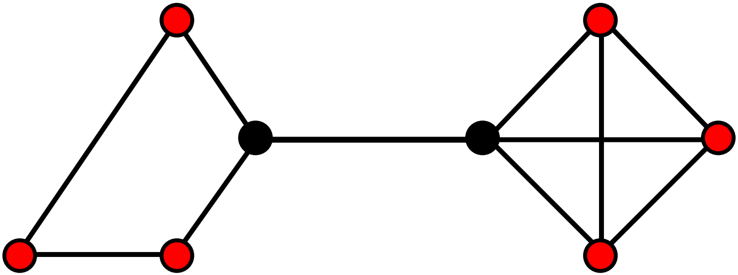

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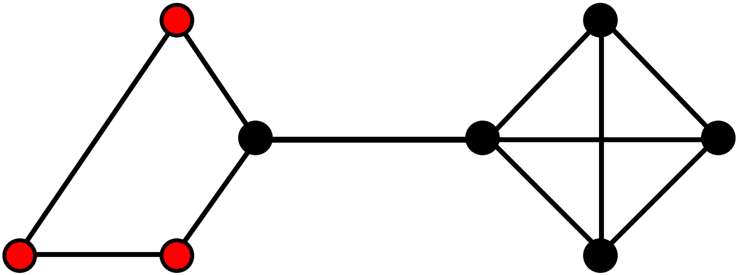

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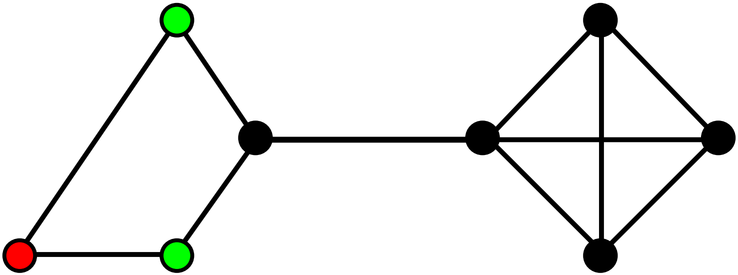

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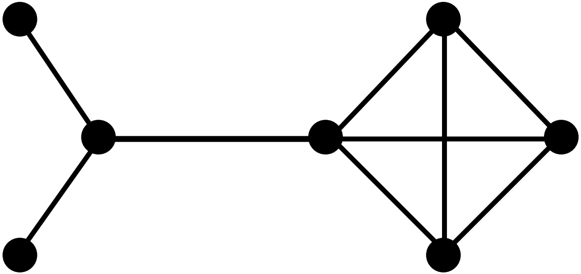

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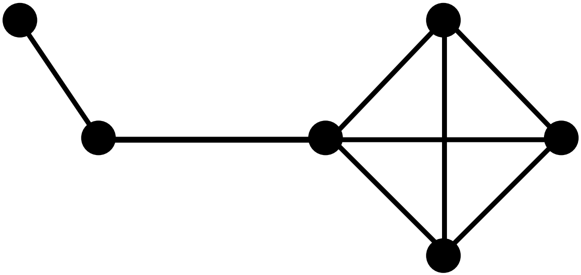

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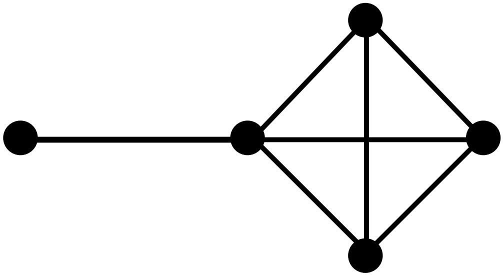

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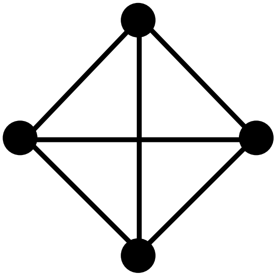

Using Deletion To Minimize Augmentations

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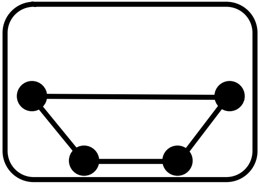
1. If minimizing degree, do not add anything of degree more than $\delta(G) + 1$.
2. If not deleting cut-vertices, everything has degree at least one.

Canonical Vertex Deletions



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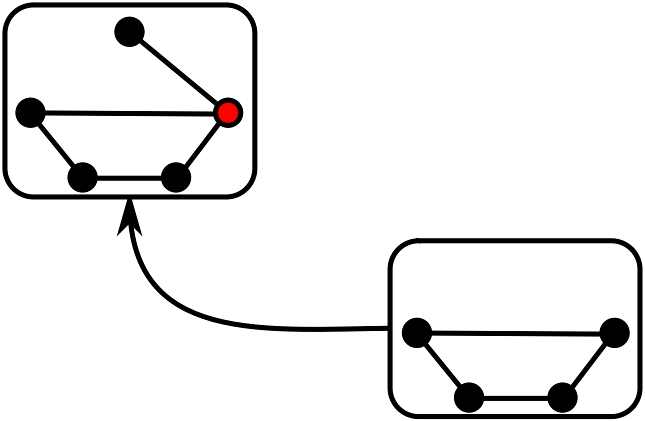

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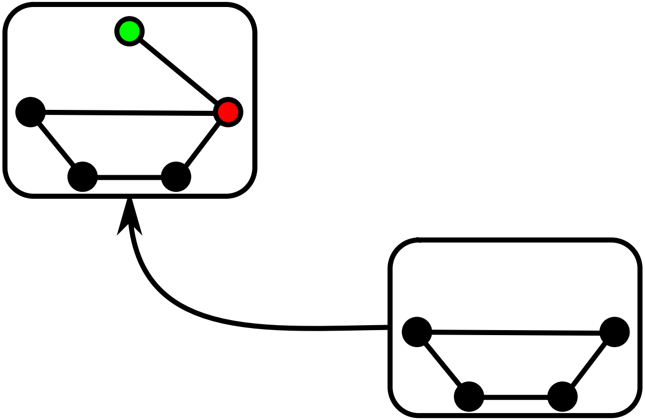

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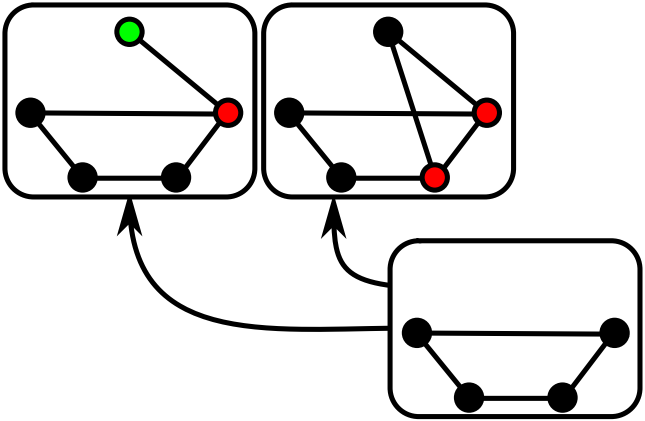

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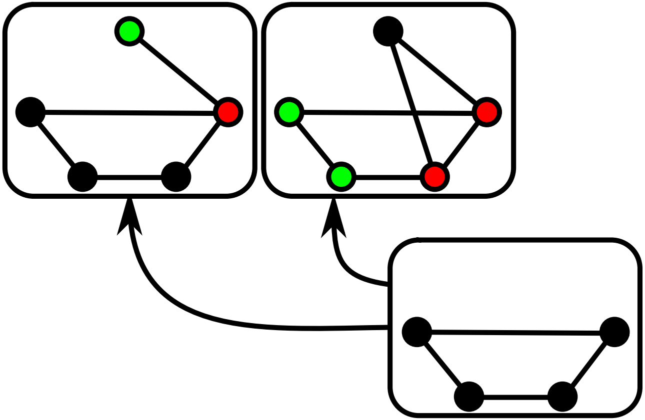

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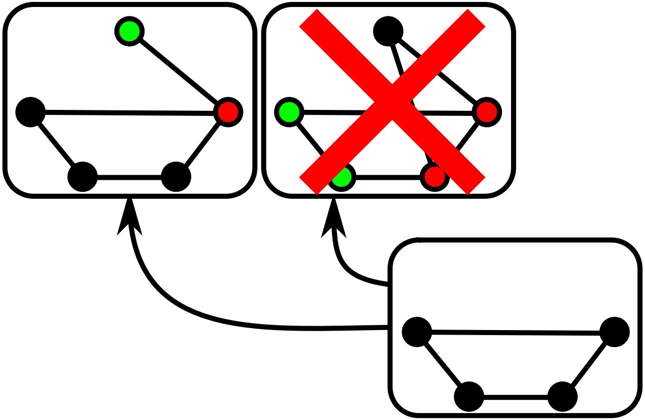

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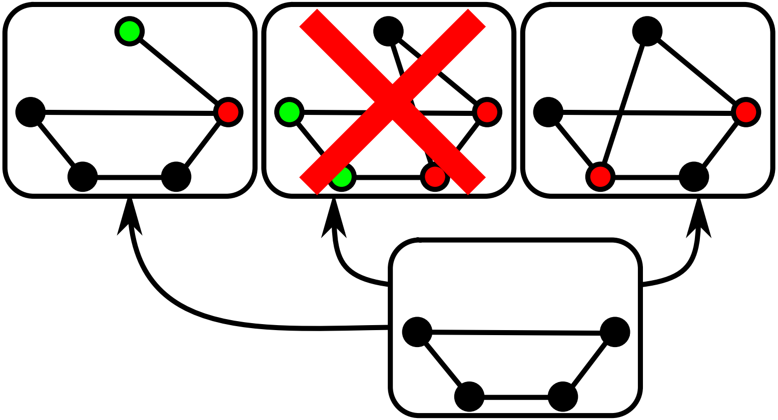

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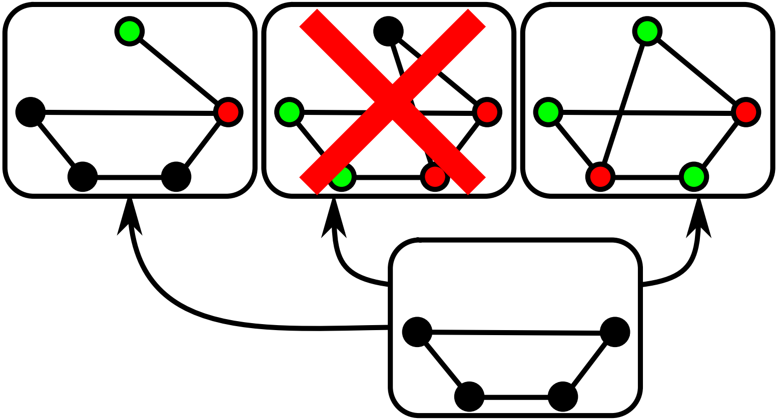

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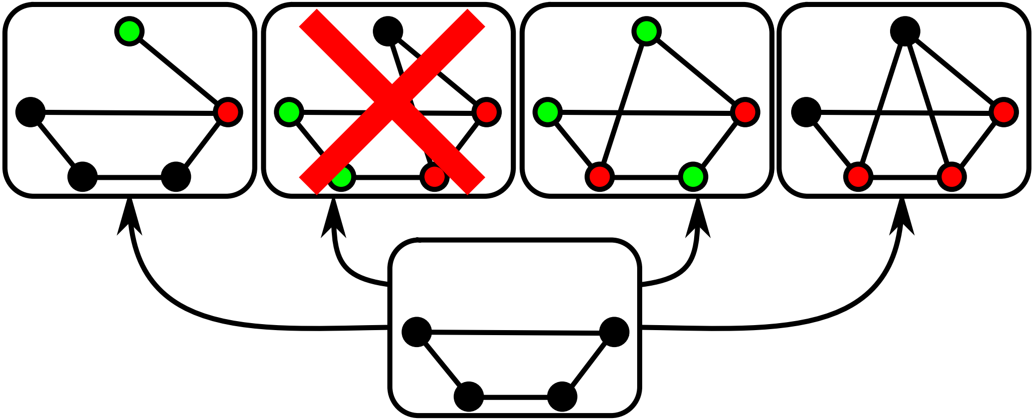

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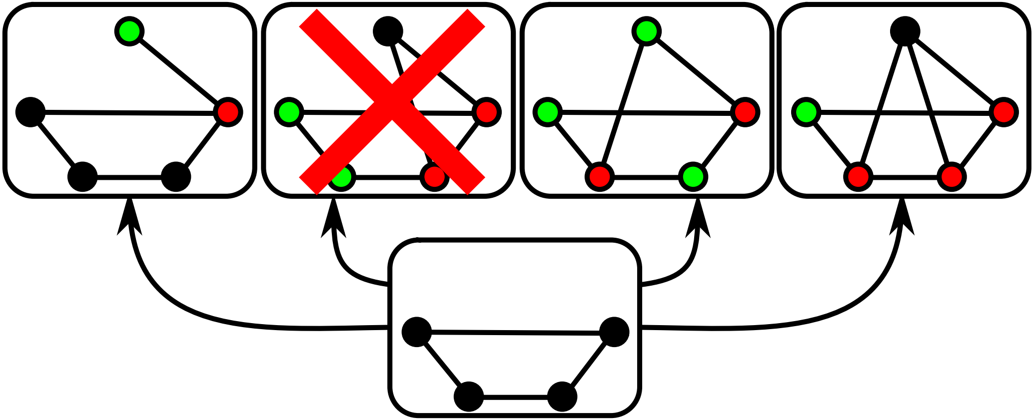

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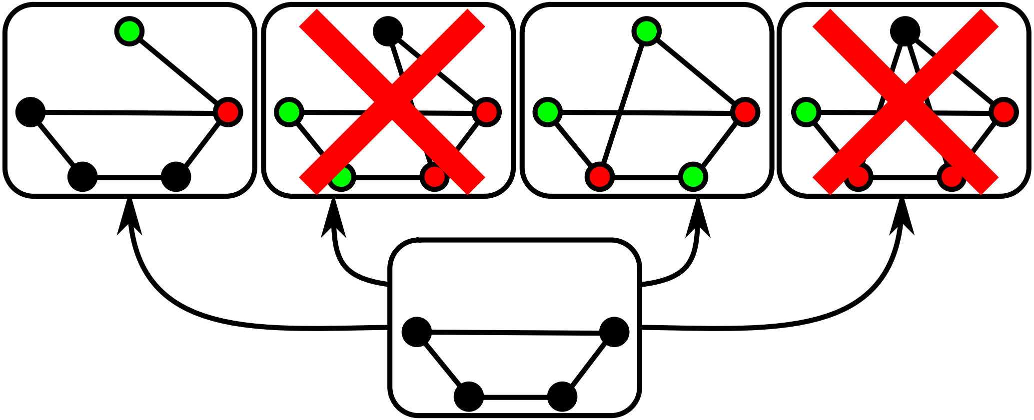

Effectiveness of Canonical Deletion

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Most unlabeled graphs have $n!$ different labelings.

So the resulting computation time is about

$$\sum_{n=1}^{N} 2^{\binom{n}{2}} \cdot \frac{nf(n)}{n!} \approx 2^{N^2 - N \log N}$$

where $f(n)$ is the average time to compute canonical labels and automorphisms.

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

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

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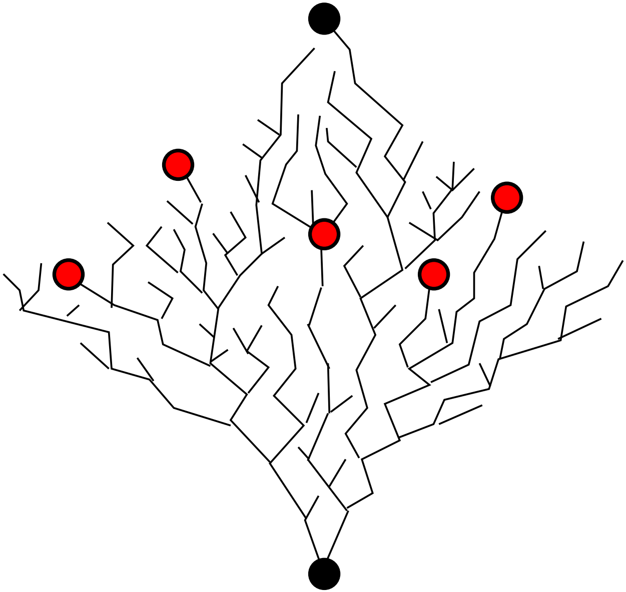
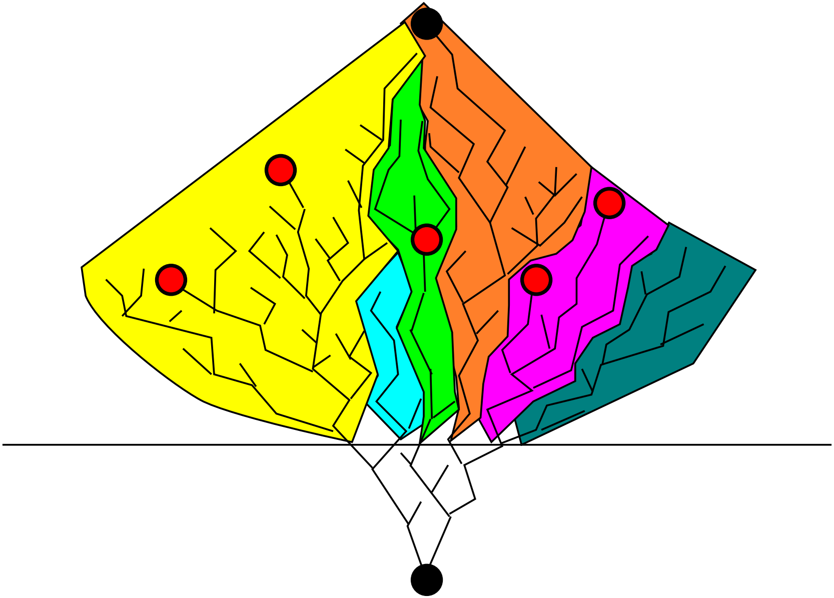
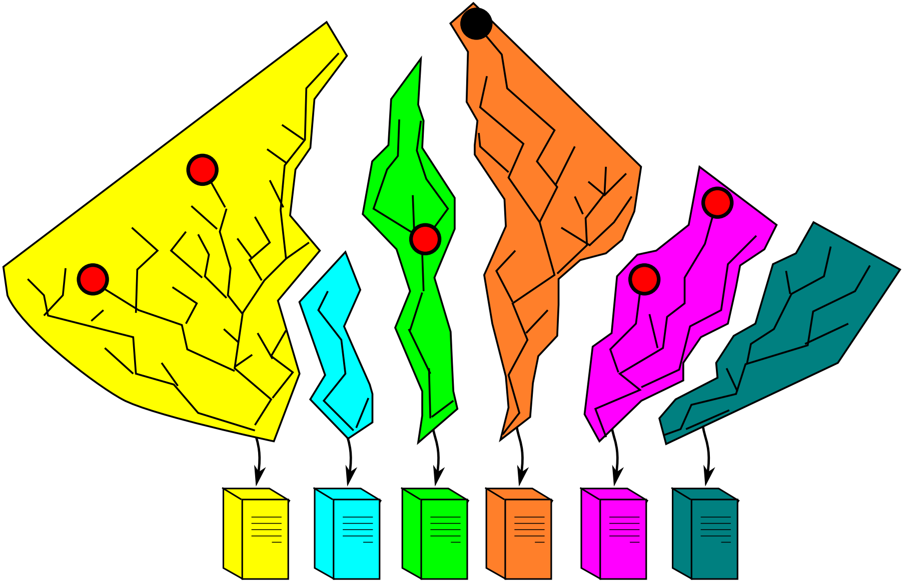
Requires over **1 year** of CPU Time.







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

Research Problem

Q: How can we integrate **constraint propagation** with canonical deletion?

Next Week: Generating Graphs with p Perfect Matchings

Let $f(n, p)$ be the **maximum number of edges** in a graph of order n with **exactly p perfect matchings**.

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We determine this value and characterize all graphs achieving this bound for all n (for small p).

Requires building a canonical deletion that has the number of perfect matchings be **monotonic!**

To learn more...

- B. D. McKay. Isomorph-free exhaustive generation.
- B. D. McKay. Small graphs are reconstructible.
- F. Margot. Pruning by isomorphism in branch-and-cut.
- B. D. McKay, A. Meynert. Small latin squares, quasigroups, and loops.
- G. Brinkmann, B. D. McKay. Posets on up to 16 points.
- P. Kaski, P. R. J. Östergard. The Steiner triple systems of order 19.
- D. Stolee. Isomorph-free generation of 2-connected graphs with applications.
- D. Stolee. Generating p-extremal graphs.

Combinatorial Generation in the Presence of Symmetry

Derrick Stolee

Iowa State University
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http://www.math.iastate.edu/dstolee/

December 2, 2013
ISU MECS Seminar