Computational Combinatorics

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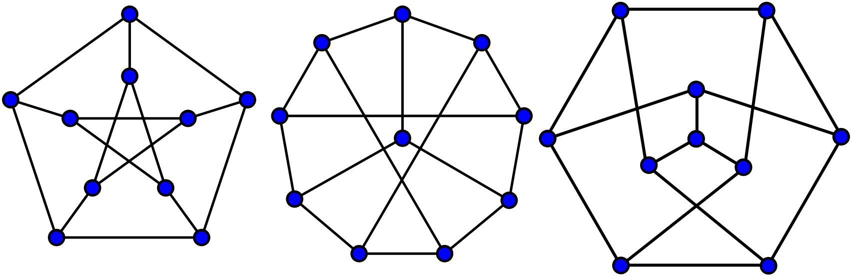
Math 101

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.



Two Flavors of Graph Theory

Structural Graph Theory:

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What conditions guarantee that certain **substructures** exist?

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Extremal Graph Theory:

Two Flavors of Graph Theory

Structural Graph Theory:

What conditions guarantee that certain **substructures** exist?

Extremal Graph Theory:

Given some structure, what **size restrictions** are guaranteed?

TONCAS Theorems

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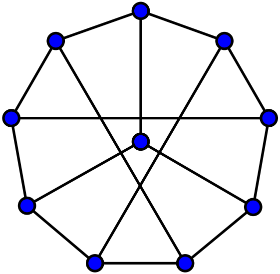

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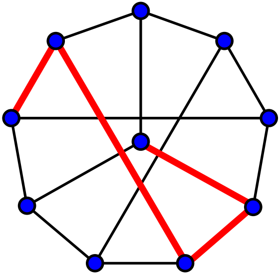

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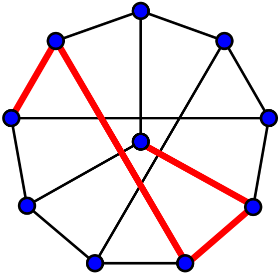

Think of the "6-Degrees of Kevin Bacon" game, played on the IMDB graph.

Connectedness : A TONCAS Theorem

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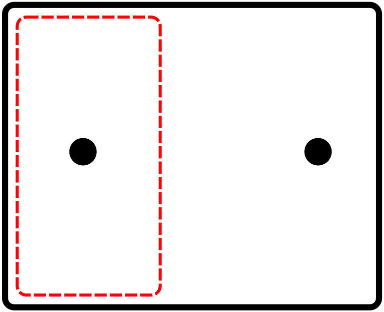
Theorem A graph G is connected **if and only if** for every set $S \subseteq V(G)$ where $S \neq \varnothing$ and $S \neq V(G)$ there exists at least one edge $uv \in E(G)$ where $u \in S$ and $v \notin S$.



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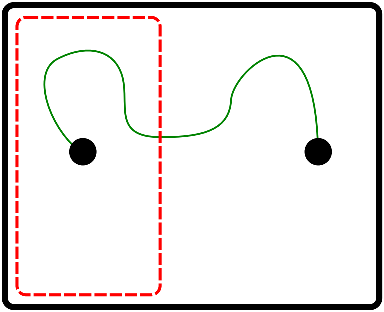

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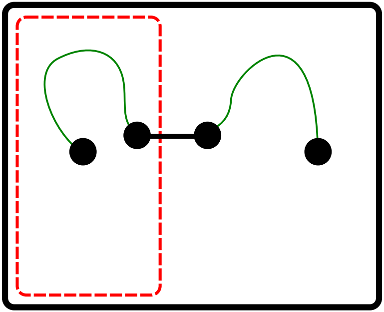
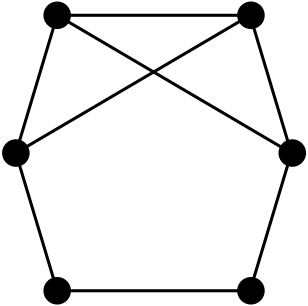


Perfect Matchings

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



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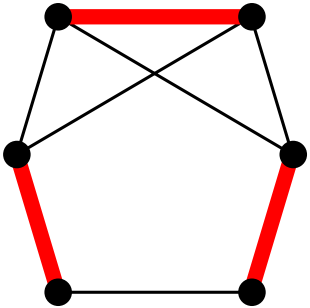

TONCAS for Perfect Matchings

Theorem (Tutte's Theorem) A graph has a perfect matching if and only if there is no set $S \subseteq V(G)$ so that the number of odd components in $G - S$ is greater than $|S|$.

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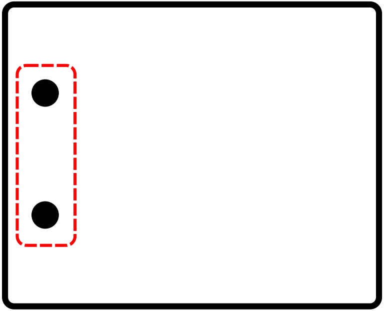

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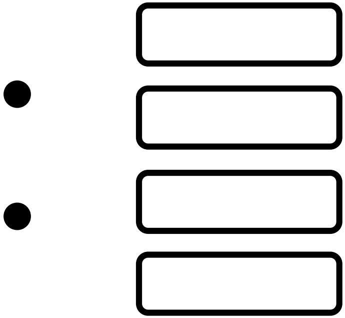

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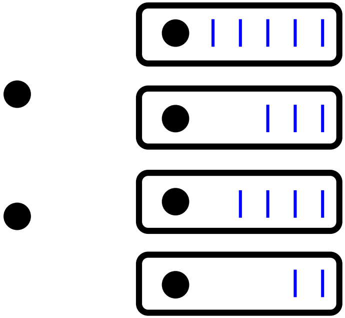

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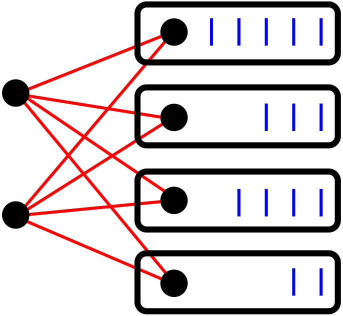

Extremal Graph Theory

Given specified **structure**, determine bounds on **size**.

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Another perspective: Specific values of one parameter influence the value of another.

Turán's Theorem

An ***r*-clique** is a set of r vertices that are pairwise adjacent.

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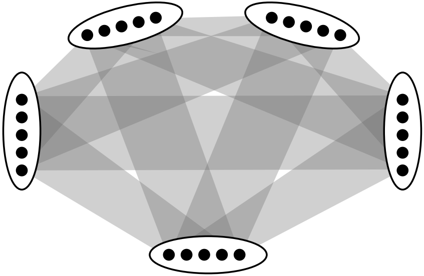

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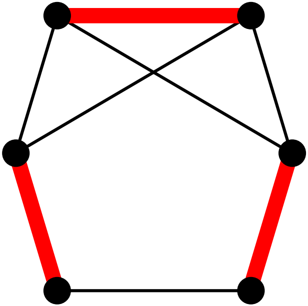

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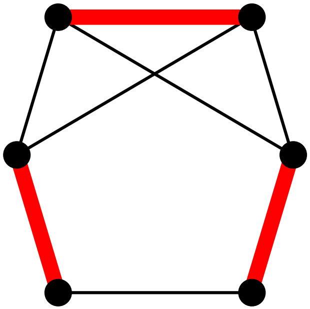
$\Phi(G)$ is the number of perfect matchings in the graph G.



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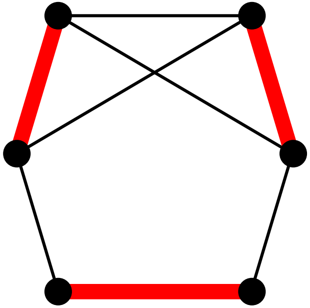

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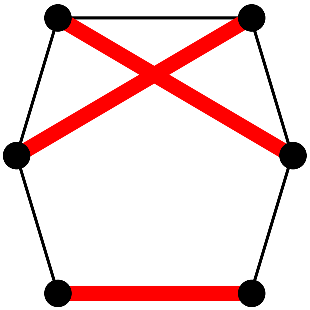

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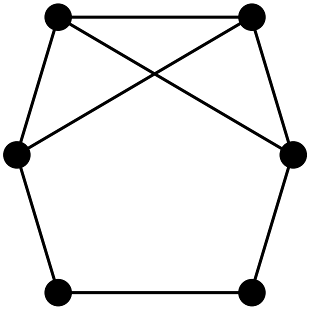

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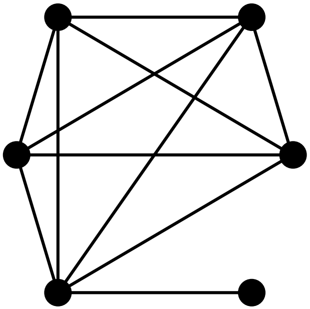

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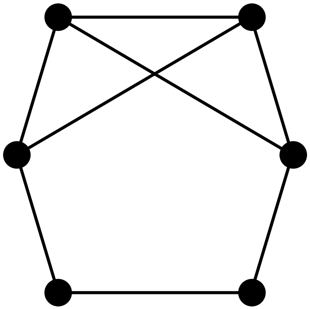

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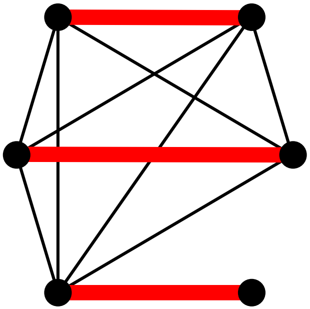

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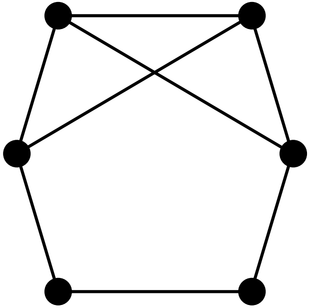

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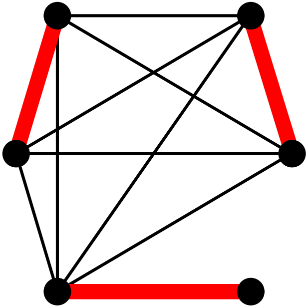

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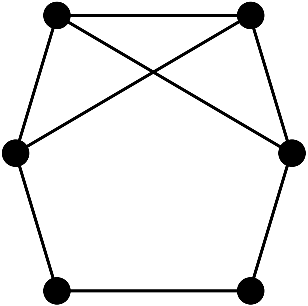

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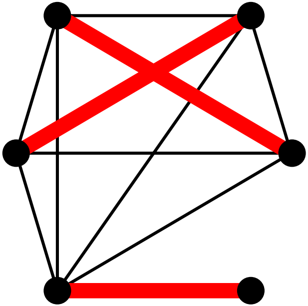

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Question (Dudek, Schmitt, 2010) What is the maximum number of edges in a graph with exactly n vertices and p perfect matchings?

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

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

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

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Theorem (Hetyei's Theorem, 1986) For all even $n \geq 2$,

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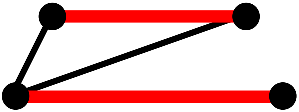

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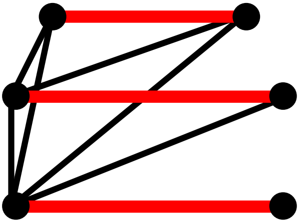

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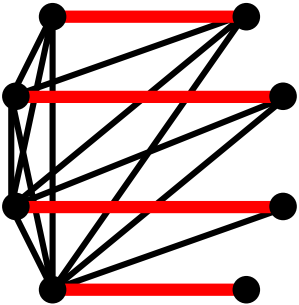

The Form of $f(n, p)$

Theorem (Dudek, Schmitt, 2010) For each p, there exist constants n_p, c_p so that for all $n \geq n_p$,

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p	1	2	3	4	5	6
c_p	0	1	2	2	2	3
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Structure Theorem

Theorem (Hartke, Stolee, West, Yancey, 2013) For a fixed p, every graph G with n vertices, p perfect matchings, and $f(n,p) = \frac{n^2}{4} + c_p$ edges is composed of a finite list of **fundamental graphs** combined in specified ways.

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

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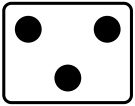
We should “simply” list all graphs of this size and pick the best ones!

Example: Generating Graphs by Edges

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



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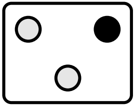

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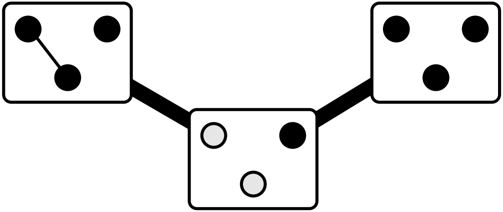

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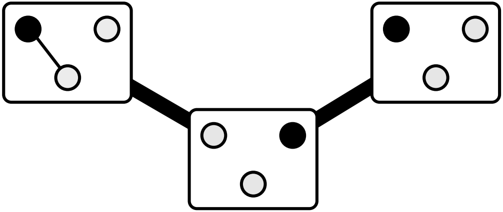

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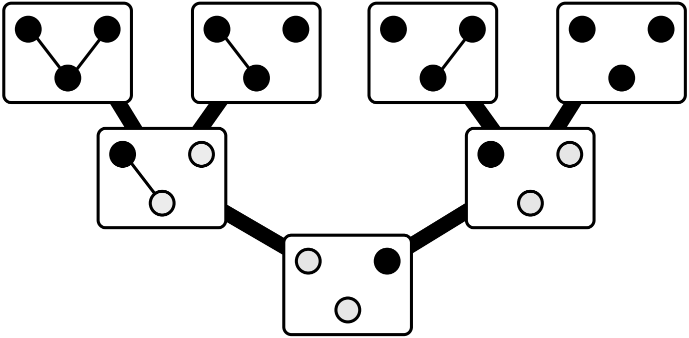

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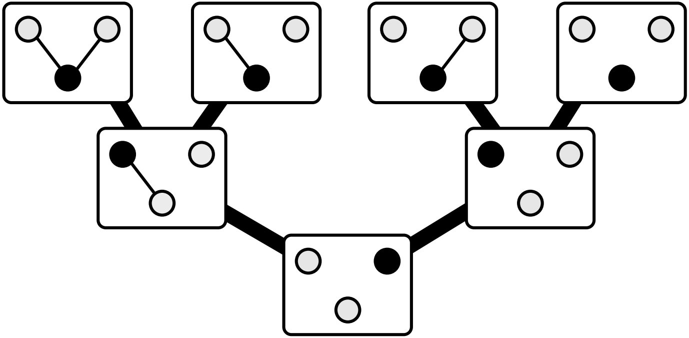

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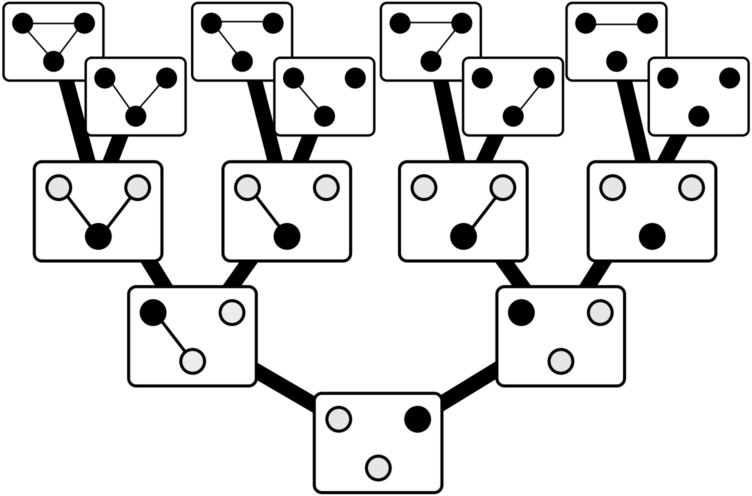

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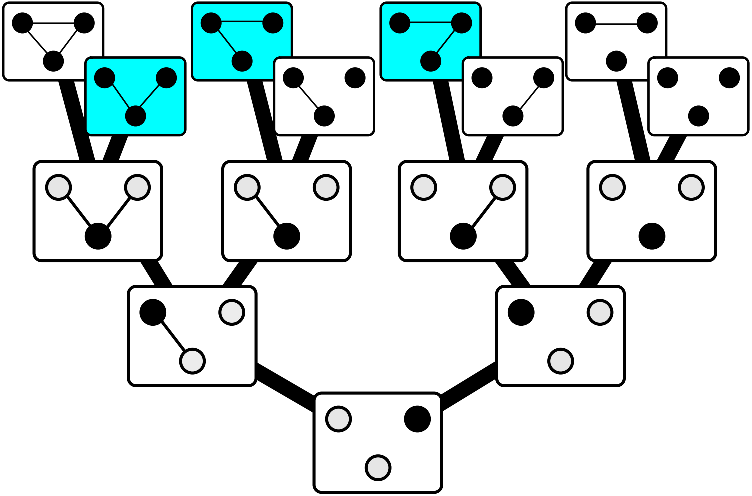

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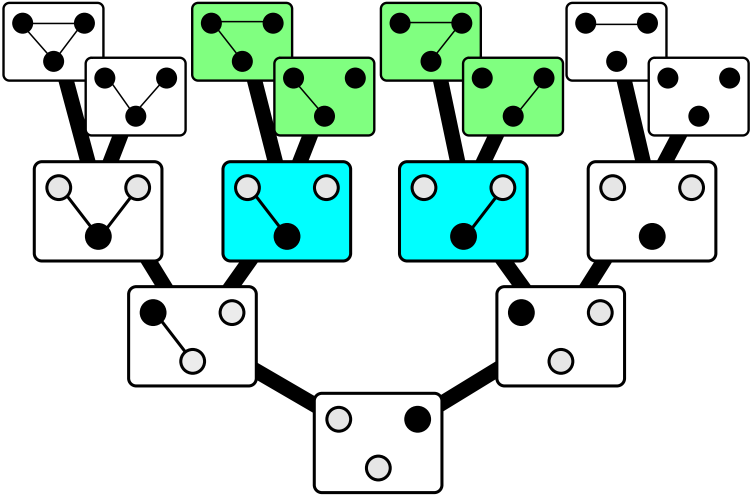

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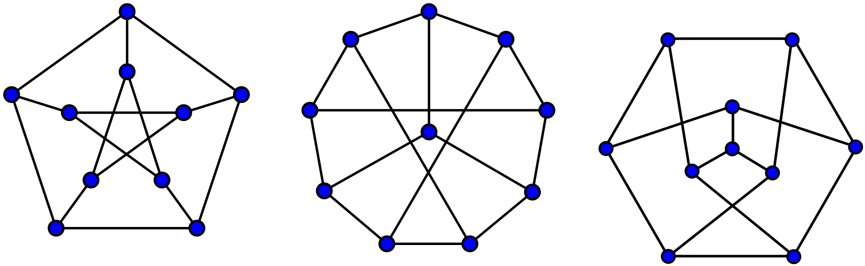

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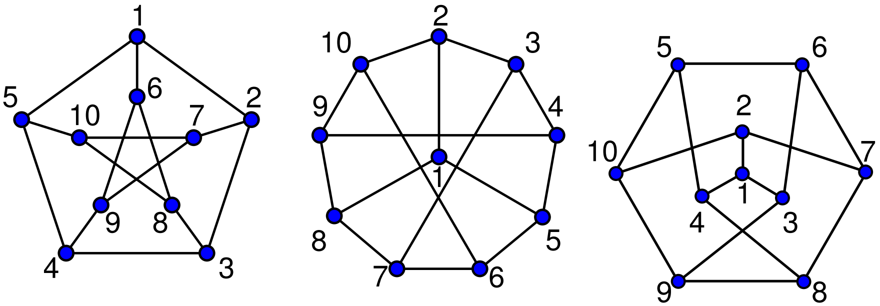
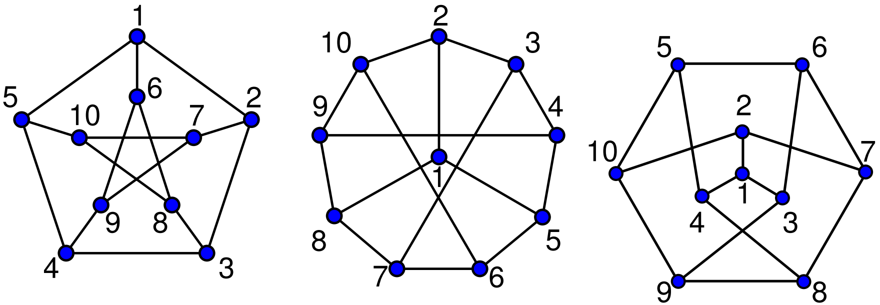


Example: Generating Graphs by Edges

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	Number of unlabeled connected graphs of order n
2	1
3	2
4	5
5	19
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
16	1,894,152,284,590
17	453,090,162,062,723
18	11,523,392,072,541,432
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20	8,832,736,318,937,756,165

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

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

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19	310,467,244,165,539,782
20	8,832,736,318,937,756,165

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

Structure Theorem

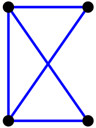
Theorem (Hartke, Stolee, West, Yancey, 2013) For a fixed p, every graph G with n vertices, p perfect matchings, and $f(n, p) = \frac{n^2}{4} + c_p$ edges is composed of a finite list of **fundamental graphs** combined in specified ways.

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

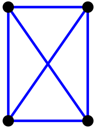
For $p \leq 10$, the graphs have order at most 12.

We should “simply” list all graphs of this size and pick the best ones!

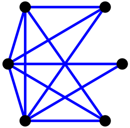
Fundamental Graphs for $2 \leq p \leq 10$



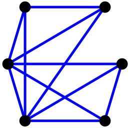
$p = 2$



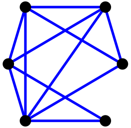
$p = 3$



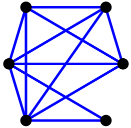
$p = 4$



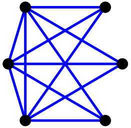
$p = 5$



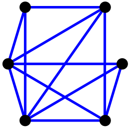
$p = 5$



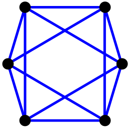
$p = 6$



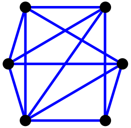
$p = 6$



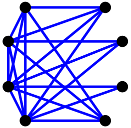
$p = 7$



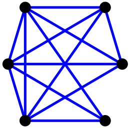
$p = 8$



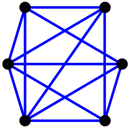
$p = 8$



$p = 8$



$p = 9$



$p = 10$

c_p for small p

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

c_p for small p

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

Structural Theorem, Redux

Without more involved computational methods, brute force methods cannot go farther.

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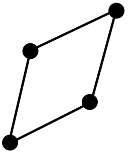

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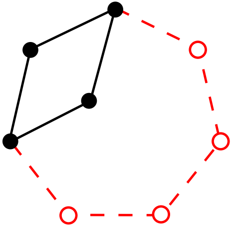

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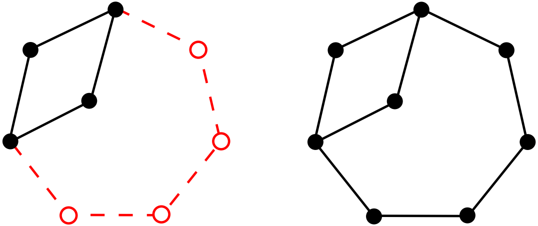

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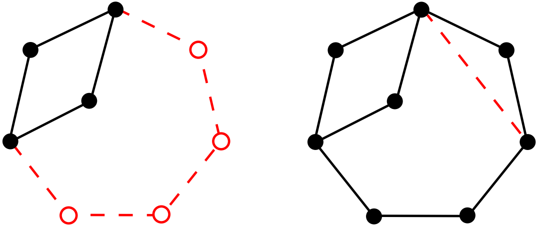

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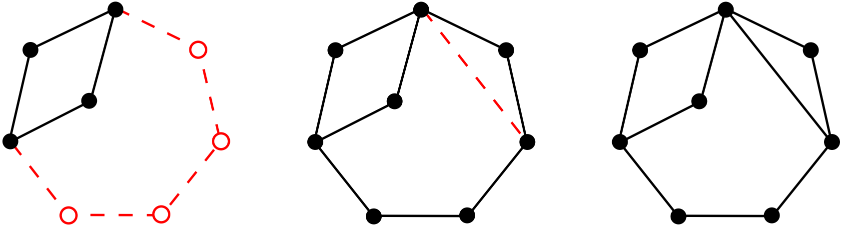

Computational Method

Developed a computational method from:

1. **Augmentations:** Lovász Two Ear Theorem.
2. **Isomorphs:** McKay's Isomorph-Free Generation Method.
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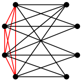
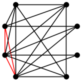
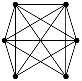
Before: Stuck at $p \leq 10$ when searching on most 12 vertices.

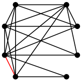
Now: Found graphs for all $p \leq 27$ on up to 22 vertices.

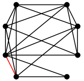
Fundamental Graphs for 11 $\leq p \leq$ 27

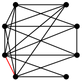

$p = 11$

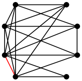

$p = 11$

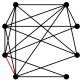

$p = 12$

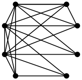

$p = 13$

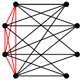

$p = 13$

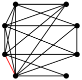

$p = 13$

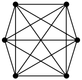

$p = 13$

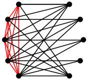

$p = 13$

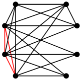

$p = 13$

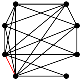

$p = 14$

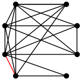

$p = 14$

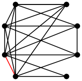

$p = 15$

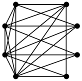

$p = 16$

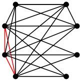

$p = 16$


$p = 16$


$p = 16$


$p = 17$


$p = 17$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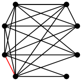
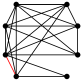
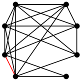
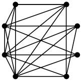
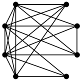
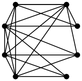

$p = 18$

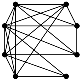

$p = 19$

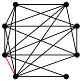

$p = 19$


$p = 19$


$p = 19$


$p = 19$


$p = 19$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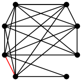
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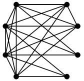
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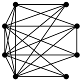
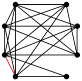
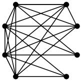
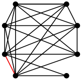
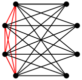

$p = 21$


$p = 22$


$p = 23$


$p = 24$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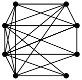
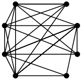

$p = 25$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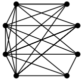
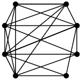
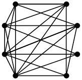
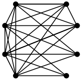

$p = 26$


$p = 26$


$p = 26$


$p = 27$

c_p for small p

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

p	11	12	13	14	15	16	17	18	19	20
c_p	3	5	3	4	6	4	4	5	4	5
	Stolee									

p	21	22	23	24	25	26	27
c_p	5	5	5	6	5	5	6
	Stolee						

c_p for small p

p	1	2	3	4	5	6	7	8	9	10
c_p	**0**	**1**	**2**	**2**	**2**	**3**	**3**	**3**	**4**	**4**
	H	Dudek, Schmitt					HSWY			

p	11	12	13	14	15	16	17	18	19	20
c_p	3	**5**	3	4	**6**	4	4	5	4	5
	Stolee									

p	21	22	23	24	25	26	27
c_p	5	5	5	**6**	5	5	**6**
	Stolee						

c_p not monotonic in p !

Blue numbers match conjectured upper bound.

What can you do?

Does this sound interesting? Here are some things **you** can do:

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1. Take MATH 304 (Combinatorics) and/or 314 (Graph Theory)

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3. Participate in the Discrete Mathematics Seminar:
   `http://orion.math.iastate.edu/dept/seminar/dmseminar.htm`

Computational Combinatorics

Derrick Stolee

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

November 3 & 5, 2014
Math 101