Isomorph-free generation of 2-connected graphs with applications

Derrick Stolee University of Nebraska-Lincoln s-dstolee1@math.unl.edu

March 19, 2011

#### **Computer Search**

Computers are extremely useful to graph theorists:



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

#### **Computer Search**

Computers are extremely useful to graph theorists:

• Find examples/counterexamples.

▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

#### **Computer Search**

Computers are extremely useful to graph theorists:

- Find examples/counterexamples.
- Verify conjectures (on small examples).

◆□▶ ◆□▶ ◆□▶ ◆□▶ → □ ・ つくぐ

#### **Computer Search**

Computers are extremely useful to graph theorists:

- Find examples/counterexamples.
- Verify conjectures (on small examples).
- Generate theorems.

Generation ••••••

▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

#### 2-connected graphs

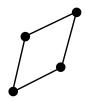
#### A graph is 2-connected if there are no cut vertices.

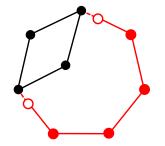
▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

#### 2-connected graphs

A graph is 2-connected if there are no cut vertices.

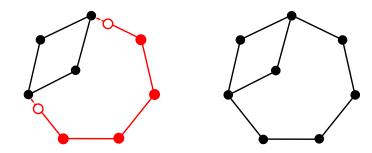
2-connected graphs are exactly the graphs with ear decompositions.



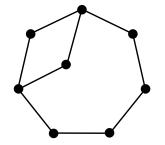


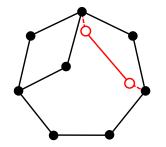


▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ



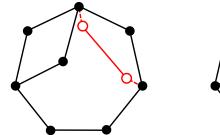
▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

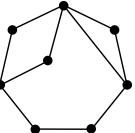






#### 2-connected graphs and ear augmentations





▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

# Generating by Ear Augmentations

# Starting at each cycle, adding all possible ear augmentations will generate all 2-connected graphs.

# Generating by Ear Augmentations

# Starting at each cycle, adding all possible ear augmentations will generate all 2-connected graphs.

LOTS of redundancy!





#### Brendan McKay

#### "Isomorph-free Exhaustive Generation"

イロト イヨト イヨト イヨト

æ

# Isomorph-free Exhaustive Generation

#### The goal:

Generate all graphs of a given type with each isomorphism class represented exactly once.



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

# Isomorph-free Exhaustive Generation

#### The goal:

Generate all graphs of a given type with each isomorphism class represented exactly once.

The recipe:

# Isomorph-free Exhaustive Generation

#### The goal:

Generate all graphs of a given type with each isomorphism class represented exactly once.

The recipe:



An augmentation (vertex, edge, leaf, ear).



◆□▶ ◆□▶ ◆□▶ ◆□▶ → □ ・ つくぐ

# Isomorph-free Exhaustive Generation

#### The goal:

Generate all graphs of a given type with each isomorphism class represented exactly once.

The recipe:

- An augmentation (vertex, edge, leaf, ear).
- A canonical deletion.

イロト イ理ト イヨト イヨト ヨー のくぐ

# Isomorph-free Exhaustive Generation

#### The goal:

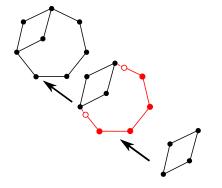
Generate all graphs of a given type with each isomorphism class represented exactly once.

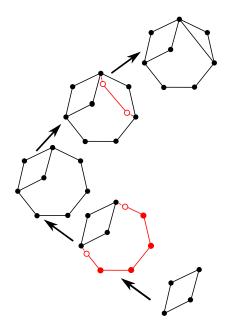
The recipe:

- An augmentation (vertex, edge, leaf, ear).
- A canonical deletion.
- A pruning procedure.

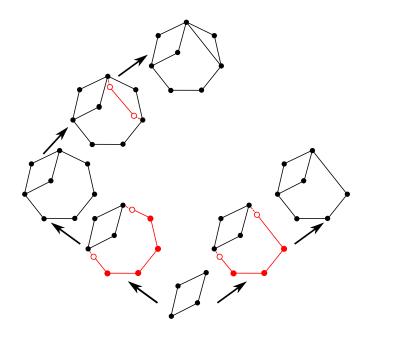


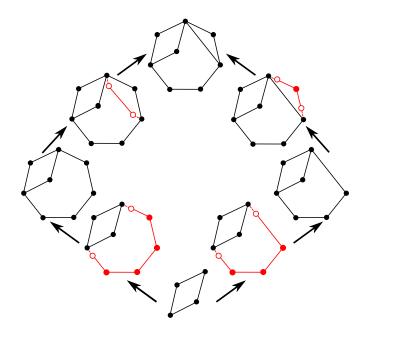
◆□▶ ◆□▶ ◆臣▶ ◆臣▶ 臣 のへで

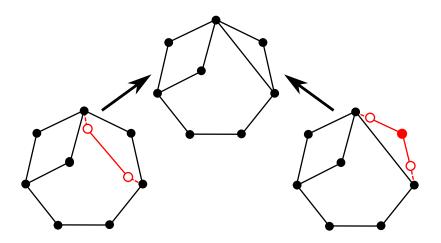




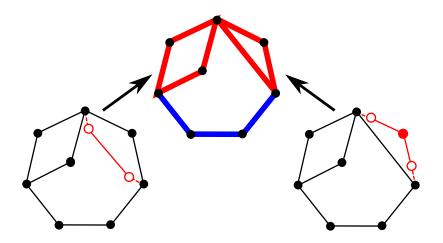
◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 - のへで



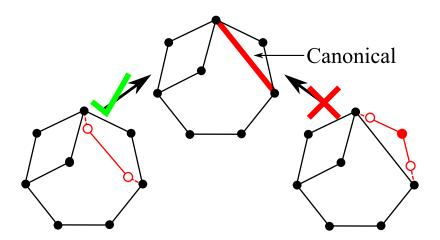




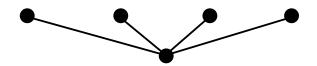
◆□▶ ◆□▶ ◆臣▶ ◆臣▶ 臣 のへで

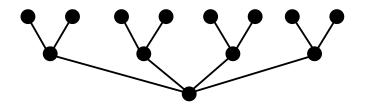


◆□▶ ◆□▶ ◆臣▶ ◆臣▶ 臣 のへで

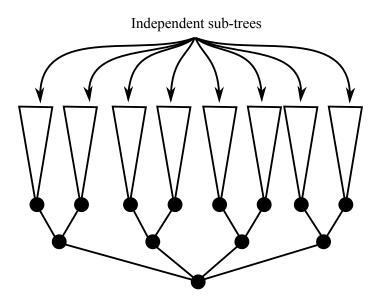


#### ・ロト ・雪 ・ ・ヨ ・ ヨ ・ シュの





- イロト イヨト イヨト イヨト ヨー のへで



| ◆ □ ▶ | ◆ □ ▶ | ◆ □ ▶ | ● | ● ○ ○ ○ ○

# Implementation

Implemented in the TreeSearch library for parallelization in the Condor scheduler.

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





▲□▶ ▲□▶ ▲ □▶ ▲ □▶ ▲ □ ● ● ● ●

#### Generating 2-connected Graphs

Ν	$C_N$	CPU time
5	10	0.01s
6	56	0.11s
7	468	0.26s
8	7123	10.15s
9	194066	5m 17.27s
10	9743542	7h 39m 28.47s
11	900969091	71d 22h 22m 49.12s

▲□▶ ▲□▶ ▲ □▶ ▲ □▶ ▲ □ ● ● ● ●

#### Generating 2-connected Graphs

	Ν	$C_N$	CPU time
_	5	10	0.01s
	6	56	0.11s
	7	468	0.26s
	8	7123	10.15s
	9	194066	5m 17.27s
	10	9743542	7h 39m 28.47s
	11	900969091	71d 22h 22m 49.12s

Slower than vertex-augmentations, faster than edge-augmentations.

Future Work

#### Three Applications

## Three Applications



Uniquely K<sub>r</sub>-Saturated Graphs

Strength: ear-monotone constraints and sparse family.



イロト イ理ト イヨト イヨト ヨー のくぐ

## **Three Applications**

- Uniquely K<sub>r</sub>-Saturated Graphs
  - Strength: ear-monotone constraints and sparse family.
- 2 Edge Reconstruction Conjecture
  - Strength: sparse family and structure of search.

イロト イ理ト イヨト イヨト ヨー のくぐ

# **Three Applications**

#### Uniquely K<sub>r</sub>-Saturated Graphs

Strength: ear-monotone constraints and sparse family.

- 2 Edge Reconstruction Conjecture
  - Strength: sparse family and structure of search.
- *p*-Extremal Graphs
  - Sparse family.
  - ② Ear-monotone constraints.
  - Structure of search.

▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

#### Application 3: *p*-Extremal Graphs

A *perfect matching* (or *1-factor*) is a set of edges which cover each vertex exactly once.

▲□▶▲□▶▲□▶▲□▶ □ のQで

#### Application 3: *p*-Extremal Graphs

A *perfect matching* (or *1-factor*) is a set of edges which cover each vertex exactly once.

Let  $\Phi(G)$  denote the number of perfect matchings in a graph *G*.

イロト イ理ト イヨト イヨト ヨー のくぐ

# Application 3: *p*-Extremal Graphs

#### Definition

Let *n* and *p* be integers. f(n, p) is the maximum number of edges in a graph with *n* vertices and exactly *p* perfect matchings.

# Application 3: *p*-Extremal Graphs

#### Definition

Let *n* and *p* be integers. f(n, p) is the maximum number of edges in a graph with *n* vertices and exactly *p* perfect matchings.

#### Definition

A graph on *n* vertices is *p*-extremal if it has *p* perfect matchings and f(n, p) edges.

# Application 3: *p*-Extremal Graphs

#### Definition

Let *n* and *p* be integers. f(n, p) is the maximum number of edges in a graph with *n* vertices and exactly *p* perfect matchings.

#### Definition

A graph on *n* vertices is *p*-extremal if it has *p* perfect matchings and f(n, p) edges.

#### Question

How does f(n, p) behave, and which graphs are *p*-extremal?





(日) (四) (王) (王) (王)

1

#### Andrzej Dudek John Schmitt

#### "On the Size and Structure of Graphs with a Constant Number of 1-Factors"

## Dudek & Schmitt

#### Dudek & Schmitt

• If *G* has *p* perfect matchings,  $n_0$  vertices and  $\frac{n_0^2}{4} + c$  edges, then for all  $n \ge n_0$ ,  $f(n, p) \ge \frac{n^2}{4} + c$ .

## **Dudek & Schmitt**

• If *G* has *p* perfect matchings,  $n_0$  vertices and  $\frac{n_0^2}{4} + c$  edges, then for all  $n \ge n_0$ ,  $f(n, p) \ge \frac{n^2}{4} + c$ .

#### Definition

The *excess* of a graph is the value  $c(G) = |E(G)| - \frac{n(G)^2}{4}$ .



うして 山田 マイボマ エリア しょうくしゃ

## **Dudek & Schmitt**

• If *G* has *p* perfect matchings,  $n_0$  vertices and  $\frac{n_0^2}{4} + c$  edges, then for all  $n \ge n_0$ ,  $f(n, p) \ge \frac{n^2}{4} + c$ .

#### Definition

The excess of a graph is the value  $c(G) = |E(G)| - \frac{n(G)^2}{4}$ .

**2** For each *p*, there exist constants  $n_p$ ,  $c_p$  so that for all even  $n \ge n_p$ ,

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

## **Dudek & Schmitt**

• If *G* has *p* perfect matchings,  $n_0$  vertices and  $\frac{n_0^2}{4} + c$  edges, then for all  $n \ge n_0$ ,  $f(n, p) \ge \frac{n^2}{4} + c$ .

#### Definition

The *excess* of a graph is the value  $c(G) = |E(G)| - \frac{n(G)^2}{4}$ .

**2** For each *p*, there exist constants  $n_p$ ,  $c_p$  so that for all even  $n \ge n_p$ ,

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

Somputed  $c_p$  for  $p \in \{1, \ldots, 6\}$ .

うして 山田 マイボマ エリア しょうくしゃ

## **Dudek & Schmitt**

• If *G* has *p* perfect matchings,  $n_0$  vertices and  $\frac{n_0^2}{4} + c$  edges, then for all  $n \ge n_0$ ,  $f(n, p) \ge \frac{n^2}{4} + c$ .

#### Definition

The *excess* of a graph is the value  $c(G) = |E(G)| - \frac{n(G)^2}{4}$ .

Por each *p*, there exist constants *n<sub>p</sub>*, *c<sub>p</sub>* so that for all even *n* ≥ *n<sub>p</sub>*,

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

- Somputed  $c_p$  for  $p \in \{1, \ldots, 6\}$ .
- Sound structure for *p*-extremal graphs with  $p \in \{1, 2, 3\}$ .



Stephen G. Hartke



Douglas B. West



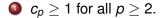
**Derrick Stolee** 



Matthew Yancey

# "On extremal graphs with a given number of perfect matchings"

▲□▶ ▲□▶ ▲ □▶ ▲ □▶ ▲ □ ● ● ● ●





▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ ○ ヘ

- $c_p \geq 1$  for all  $p \geq 2$ .
- **2** Bounded  $n_p = O(\sqrt{p})$ .

▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

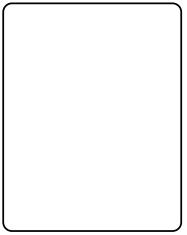
- $c_p \geq 1$  for all  $p \geq 2$ .
- **2** Bounded  $n_p = O(\sqrt{p})$ .
- Used naive search to find  $c_p$  and structure of *p*-extremal graphs for  $p \le 10$ .

▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

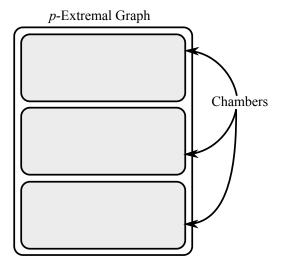
- $c_p \geq 1$  for all  $p \geq 2$ .
- **2** Bounded  $n_p = O(\sqrt{p})$ .
- Used naive search to find  $c_p$  and structure of *p*-extremal graphs for  $p \le 10$ .

p	1	2	3	4	5	6	7	8	9	10
Cp	0	1	2	2	2	3	3	3	4	4
$n_p$	2	4	4	6	6	6	6	6	6	6
	[DS10]						[HSWY11+]			

p-Extremal Graph



◆ロト ◆聞 ト ◆ 臣 ト ◆ 臣 ト ○臣 - のへで



・ロト ・ 理 ・ モ ト ・ モ ・ う へ の・

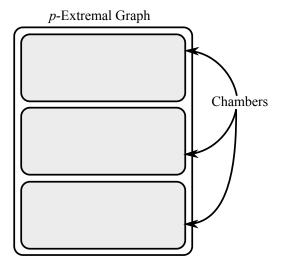
◆□▶ ◆□▶ ◆□▶ ◆□▶ → □ ・ つくぐ

## The Structure of *p*-Extremal Graphs

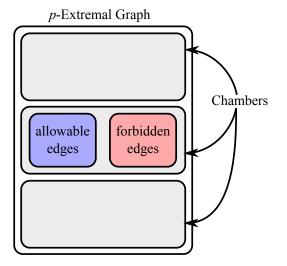
Chambers are the connected components in the subgraph of edges appearing in perfect matchings (*allowable* edges).

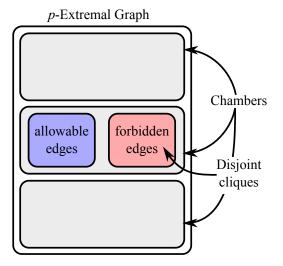
For *G* a graph with chambers  $G_1, \ldots, G_k$ ,

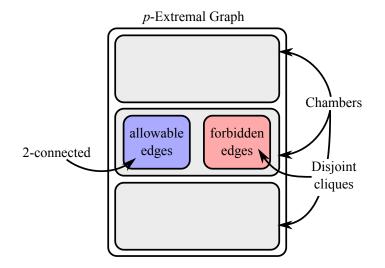
$$\Phi(G) = \prod_{i=1}^{k} \Phi(G_i).$$
  
$$c(G) \leq \sum_{i=1}^{k} c(G_i).$$



・ロト ・ 理 ・ モ ト ・ モ ・ う へ の・







## The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.



# The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.

#### Theorem (Lovász Two-Ears Theorem)

If H is a 1-extendable graph, there is a graded ear decomposition  $H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_k$  So that

# The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.

#### Theorem (Lovász Two-Ears Theorem)

If H is a 1-extendable graph, there is a graded ear decomposition  $H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_k$  So that

• 
$$H_0 \cong C_{2\ell}$$
 for some  $\ell$  and  $H_k = H$ .

# The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.

#### Theorem (Lovász Two-Ears Theorem)

If H is a 1-extendable graph, there is a graded ear decomposition  $H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_k$  So that

• 
$$H_0 \cong C_{2\ell}$$
 for some  $\ell$  and  $H_k = H$ .

# The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.

#### Theorem (Lovász Two-Ears Theorem)

If H is a 1-extendable graph, there is a graded ear decomposition  $H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_k$  So that

**()** 
$$H_0 \cong C_{2\ell}$$
 for some  $\ell$  and  $H_k = H$ .

Solution  $H_i \subset H_{i+1}$  uses one or two ears.

# The Structure of Allowable Edges

A connected graph with all edges allowable is 1-extendable.

#### Theorem (Lovász Two-Ears Theorem)

If H is a 1-extendable graph, there is a graded ear decomposition  $H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_k$  So that

**1** 
$$H_0 \cong C_{2\ell}$$
 for some  $\ell$  and  $H_k = H$ .

2 Each 
$$H_i$$
 is 1-extendable.

Solution  $H_i \subset H_{i+1}$  uses one or two ears.

Graphs which appear "between" two 1-extendable graphs in a two-ear augmentation are *almost 1-extendable* graphs.

Generation

#### The Search Space

**Input:** *p*, *N*, *c*.

### The Search Space

**Input:** *p*, *N*, *c*.

Graphs: 1-extendable and almost 1-extendable graphs H with

### The Search Space

**Input:** *p*, *N*, *c*.

Graphs: 1-extendable and almost 1-extendable graphs H with

• At most N vertices.



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ ○ ヘ

### The Search Space

**Input:** *p*, *N*, *c*.

Graphs: 1-extendable and almost 1-extendable graphs H with

- At most N vertices.
- At most *p* perfect matchings.

▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ ○ ヘ

### The Search Space

**Input:** *p*, *N*, *c*.

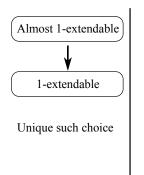
Graphs: 1-extendable and almost 1-extendable graphs H with

- At most N vertices.
- At most *p* perfect matchings.

**Solutions:** Chambers *G* with *p* perfect matchings and  $c(G) \ge c$ .

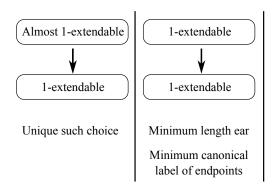
### **Canonical Deletion**

### **Canonical Deletion**

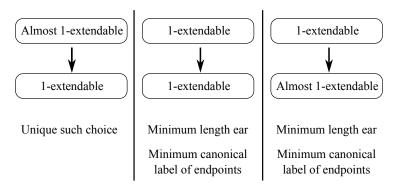


▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

## **Canonical Deletion**



## **Canonical Deletion**



## **Finding Solutions**

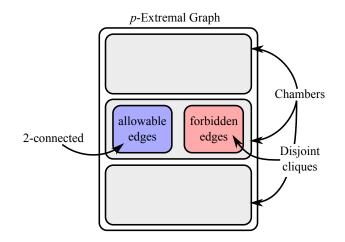
### Question

How do we transition from 1-extendable graphs to extremal chambers?



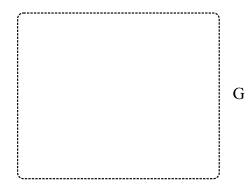
▲□▶ ▲□▶ ▲ □▶ ▲ □▶ ▲ □ ● ● ● ●

## **Finding Solutions**



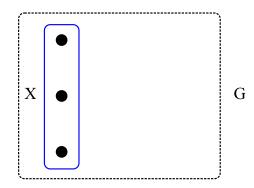
## **Finding Solutions**

### Use barriers:



## **Finding Solutions**

### Use barriers:

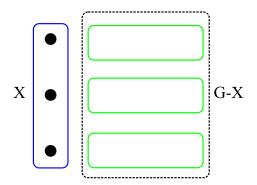


▲ロト ▲園 ト ▲臣 ト ▲臣 ト → 臣 → の々で

▲□▶▲圖▶▲≧▶▲≧▶ 差 うくぐ

## **Finding Solutions**

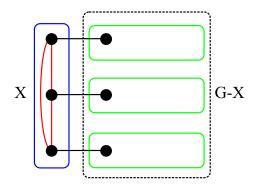
### Use barriers:



▲□▶▲圖▶▲≧▶▲≧▶ 差 うくぐ

## **Finding Solutions**

### Use barriers:



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

## **Finding Solutions**

### Definition

A *barrier* in a graph G with  $\Phi(G) > 0$  is a set  $X \subset V(G)$  so that  $c_o(G - X) = |X|$ .

In a *p*-extremal chamber, every barrier is a clique of forbidden edges.

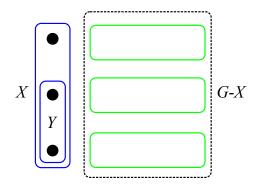
### **Conflicting Barriers**

Two barriers X, Y conflict if:



## **Conflicting Barriers**

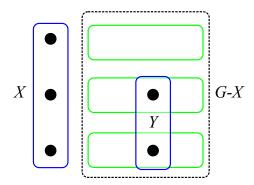
Two barriers X, Y conflict if:



◆□> ◆□> ◆豆> ◆豆> ・豆 ・ ��や

## **Conflicting Barriers**

Two barriers X, Y conflict if:



## **Finding Solutions**

# {Maximal chamber supergraphs of H}

### {Maximal sets of non-conflicting barriers in *H*}



### Pruning

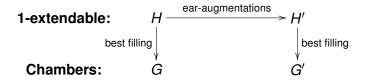
We want to prune when the excess can never reach *c*, no matter what augmentations we use.



◆□▶ ◆□▶ ◆□▶ ◆□▶ → □ ・ つくぐ

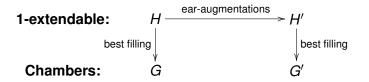
## Pruning

We want to prune when the excess can never reach *c*, no matter what augmentations we use.



### Pruning

We want to prune when the excess can never reach *c*, no matter what augmentations we use.



$$c(G') \le c(G) + 2(\Phi(H') - \Phi(H)) - \frac{1}{4}(n(H') - n(H))(n(H) - 2)$$

◆□▶ ◆□▶ ◆臣▶ ◆臣▶ ─臣 ─の�?

▲□▶ ▲□▶ ▲目▶ ▲目▶ 三目 - のへぐ

### Pruning and Optimizations

### Let H be the current 1-extendable graph and G a best filling.

### Pruning and Optimizations

Let H be the current 1-extendable graph and G a best filling.

**1** If 
$$c(G) + 2(p - \Phi(H)) < c$$
, then prune.



▲□▶▲□▶▲□▶▲□▶ □ のQで

## Pruning and Optimizations

Let H be the current 1-extendable graph and G a best filling.

**1** If 
$$c(G) + 2(p - \Phi(H)) < c$$
, then prune.

2 Let N be the maximum so that

$$c(G) + 2(p - \Phi(H)) - \frac{1}{4}(N - n(H))(n(H) - 2) \ge c.$$

We do not need to augment beyond N vertices.

## Pruning and Optimizations

Let H be the current 1-extendable graph and G a best filling.

**1** If 
$$c(G) + 2(p - \Phi(H)) < c$$
, then prune.

2 Let N be the maximum so that

$$c(G) + 2(p - \Phi(H)) - \frac{1}{4}(N - n(H))(n(H) - 2) \ge c.$$

We do not need to augment beyond N vertices.

If adding an ear at endpoints x, y increases  $\Phi(H)$  beyond p, never augment on that pair again.

### **Results**

		1				6				
Cp	0	1	2	2	2	3	3	3	4	4
n <sub>p</sub>	2	4	4	6	6	6	6	6	6	6

	р	11	12	13	14	15	16	17	18	19	20
C	р	3	5	3	4	6	4	4	5	4	5
n	l <sub>p</sub>	8	6	8	8	6	8	8	8	8	8

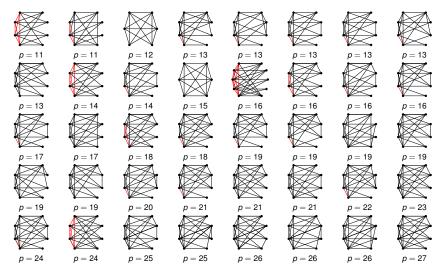
p	21	22	23	24	25	26	27		
Cp	5	5	5	6	5	5	6		
n <sub>p</sub>	8	8	8	8	8	8	8		

# Timing

-

р	Nρ	c <sub>p</sub>	Total CPU Time							
11	14	3					43.29s			
12	14	5					44.01s			
13	14	3				6m	39.80s			
14	16	4				12m	10.40s			
15	16	6				12m	42.72s			
16	16	4			2h	07m	58.60s			
17	16	4			6h	46m	07.72s			
18	18	5			11h	45m	01.95s			
19	18	4		2d	17h	12m	31.85s			
20	18	5		4d	05h	28m	11.79s			
21	18	5		13d	17h	29m	12.45s			
22	20	5		42d	20h	40m	30.41s			
23	20	5		118d	07h	38m	36.84s			
24	20	6		209d	10h	09m	54.98s			
25	20	5	2y	187d	21h	48m	46.31s			
26	20	5	7y	75d	13h	55m	10.27s			
27	22	6	10y	247d	21h	03m	13.94s			

### p-Extremal Chambers



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

### **Future Work**

### For *p*-extremal graphs:

- Find a "strong" upper bound on c<sub>p</sub> for an infinite family of values of p.
- A start: prove the complete graphs on 2*t* vertices are *p*-extremal for p = (2t 1)!!.
- **(a)** A lower bound on  $c_p$  which grows in the limit.

## **Future Work**

### For the technique:

- More applications!
- Ø More optimizations?



▲ロト ▲周 ト ▲ ヨ ト ▲ ヨ ト ・ シ へ つ ヘ

## **Future Work**

### For the tools:

- Implement vertex/edge/leaf augmentations.
- Apply to new problems.
- Ompare to current applications.

Isomorph-free generation of 2-connected graphs with applications

Derrick Stolee<sup>1</sup> University of Nebraska-Lincoln s-dstolee1@math.unl.edu

March 19, 2011

<sup>1</sup>Supported by NSF grants CCF-0916525 and DMS-0914815

3

## Application 1: Uniquely $K_r$ -Saturated Graphs

#### Definition

A graph *G* is *uniquely*  $K_r$ -saturated if *G* contains no  $K_r$  and for every edge  $e \in \overline{G}$  admits exactly one copy of  $K_r$  in G + e.



(a) 1-book

(b) 2-book

(c) 3-book

Figure: The (r - 2)-books are uniquely  $K_r$  saturated.





Joshua Cooper Paul Wenger

Two Conjectures:

1. For each r, there are a finite number of uniquely  $K_r$ -saturated graphs with no dominating vertex.

2. For each r, every uniquely  $K_r$ -saturated graph with no dominating vertex is regular.

Previously verified to 9 vertices.

### Application 1: Uniquely $K_r$ -Saturated Graphs

- Uniquely K<sub>r</sub>-saturated graphs have diameter 2 (and are 2-connected).
- **2** Strength:  $K_4$ -free is a sparse, monotone property.
- Solution Verified for r = 4 and  $n \le 12$ .
- Verified for  $r \in \{5, 6\}$  and  $n \le 11$ .

