

Listing All Maximal Cliques in Sparse Graphs in Near-Optimal Time

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UC Irvine

Joint work with David Eppstein and Maarten Löffler

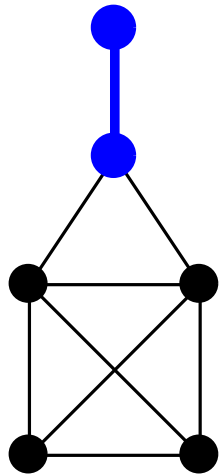
What is a Maximal Clique?

A clique that cannot be extended by adding more vertices

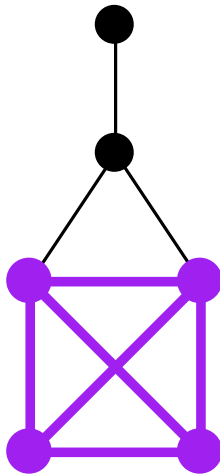
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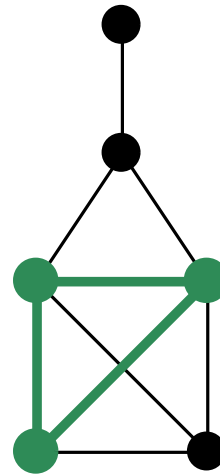
Maximal



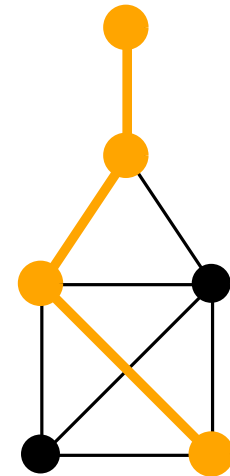
Maximal,
Maximum



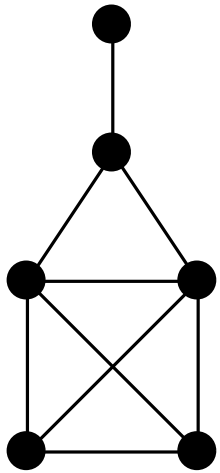
Not Maximal



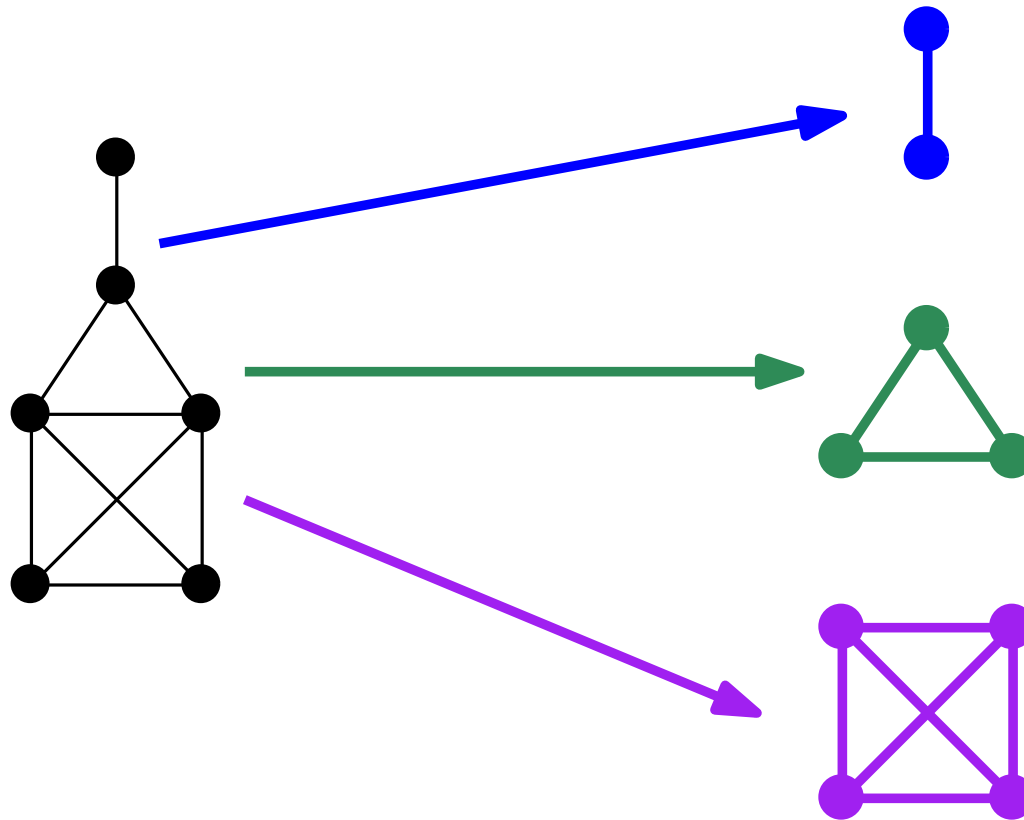
Not Clique



Goal: Design an algorithm to list all maximal cliques



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Motivation

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Features in ERGM

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Detect structural motifs from similarities between proteins

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Detect structural motifs from similarities between proteins

Determine the docking regions between biomolecules

Motivation

Features in ERGM

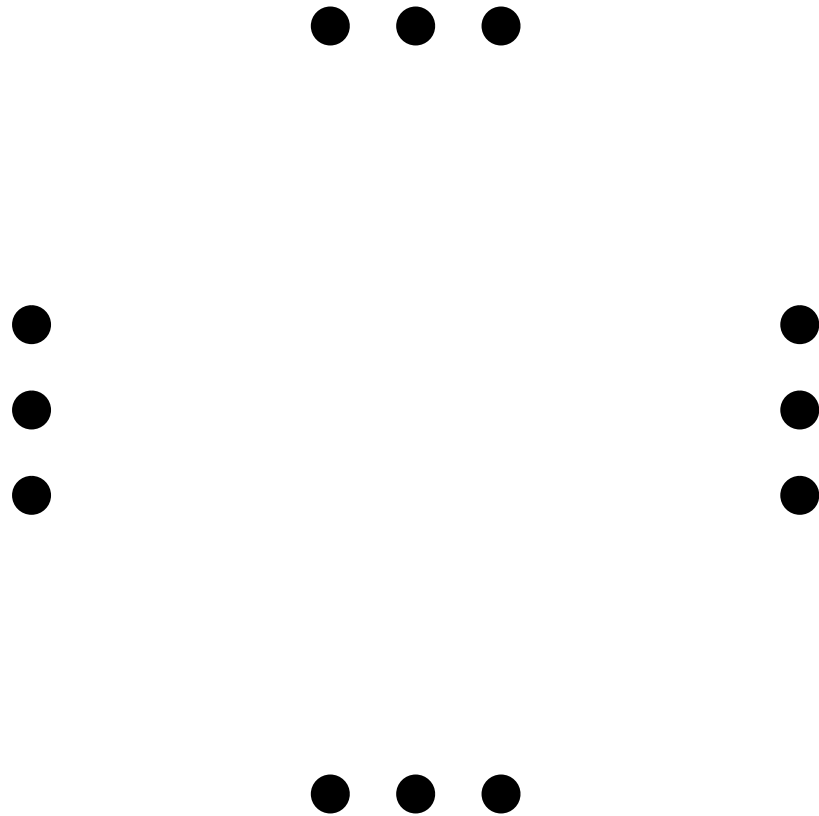
Detect structural motifs from similarities between proteins

Determine the docking regions between biomolecules

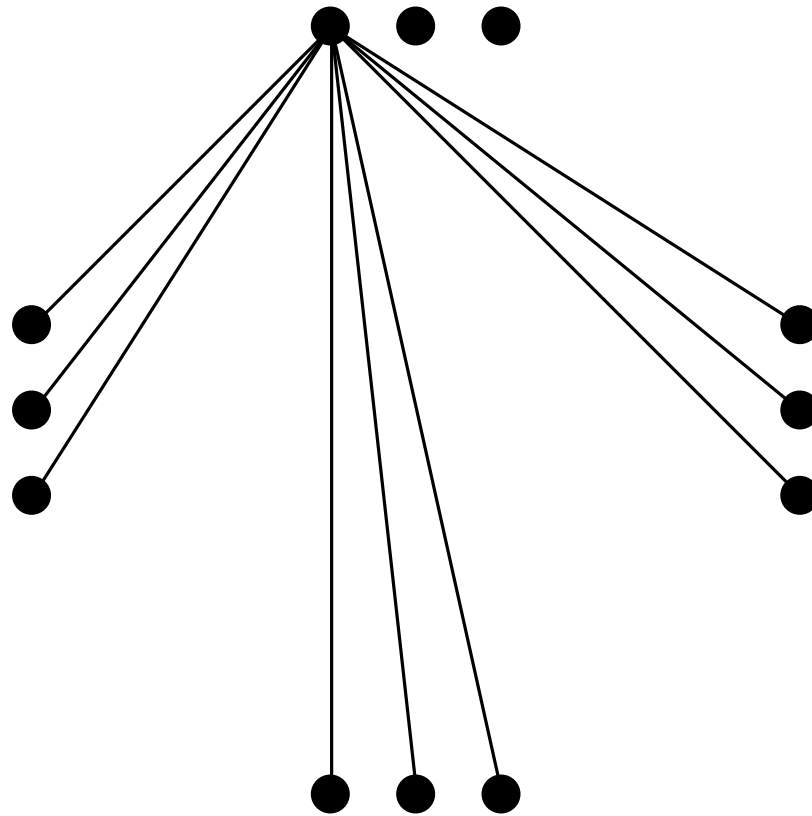
Document clustering for information retrieval

There may be many maximal cliques.

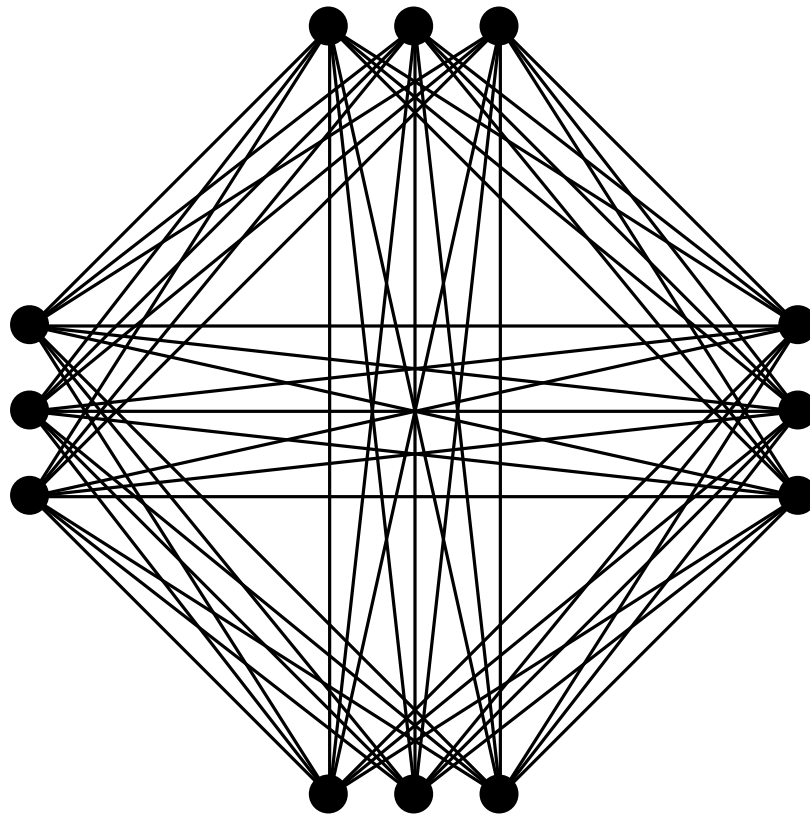
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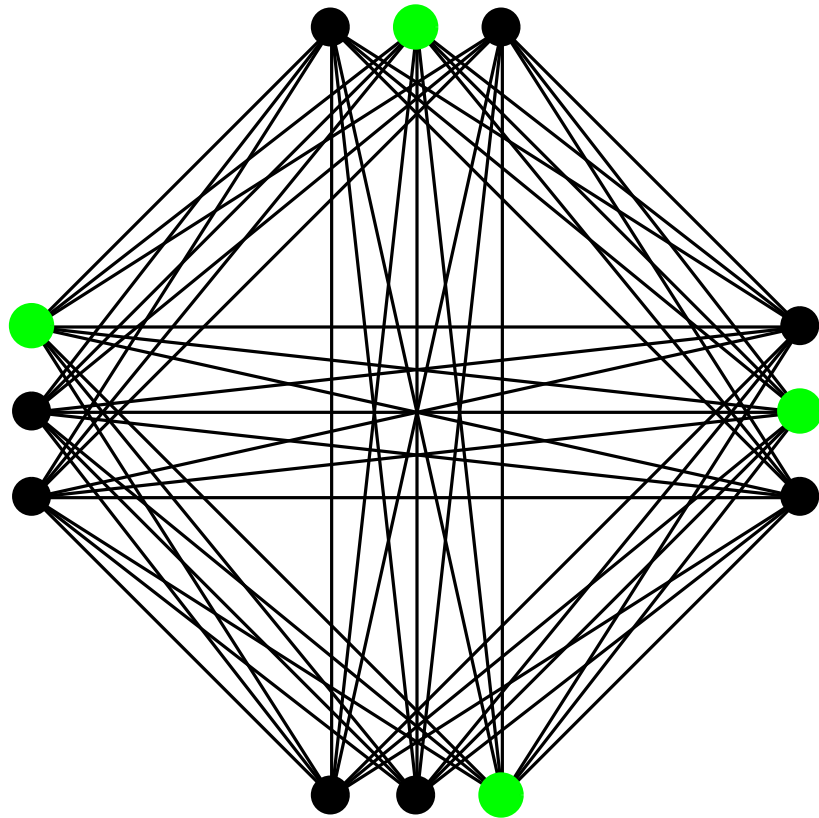
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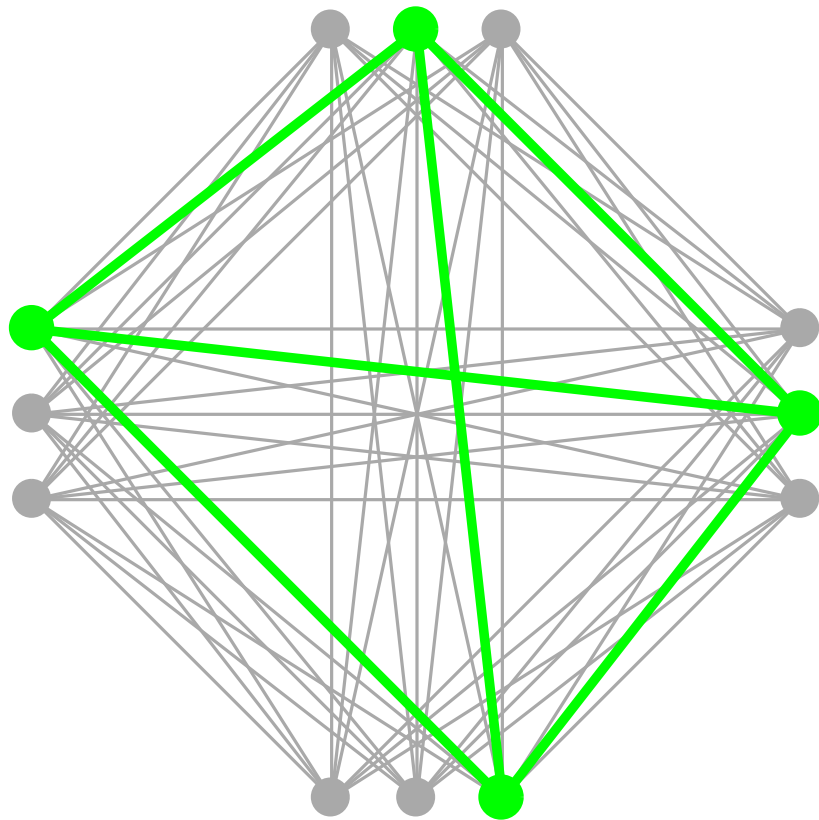
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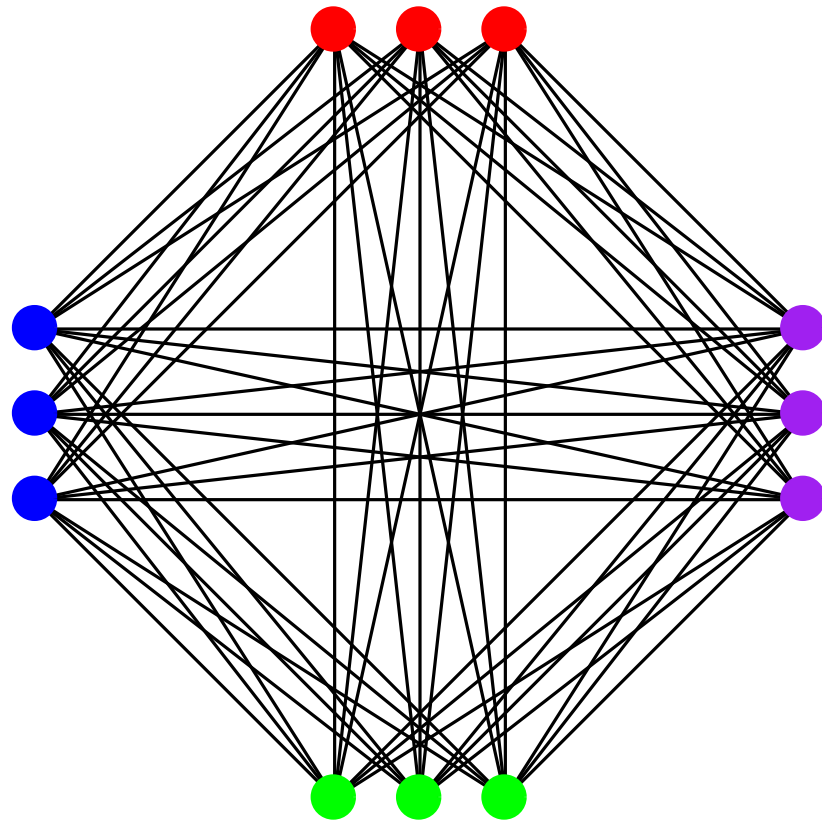
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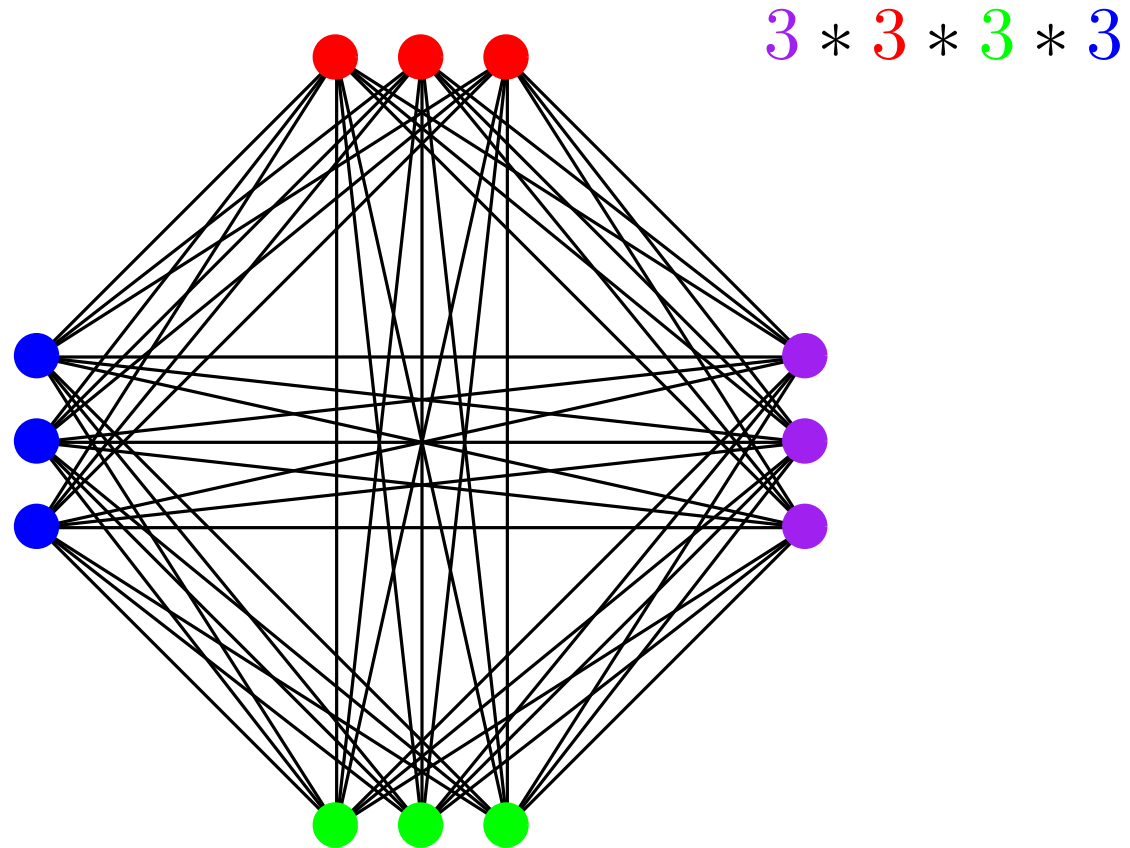
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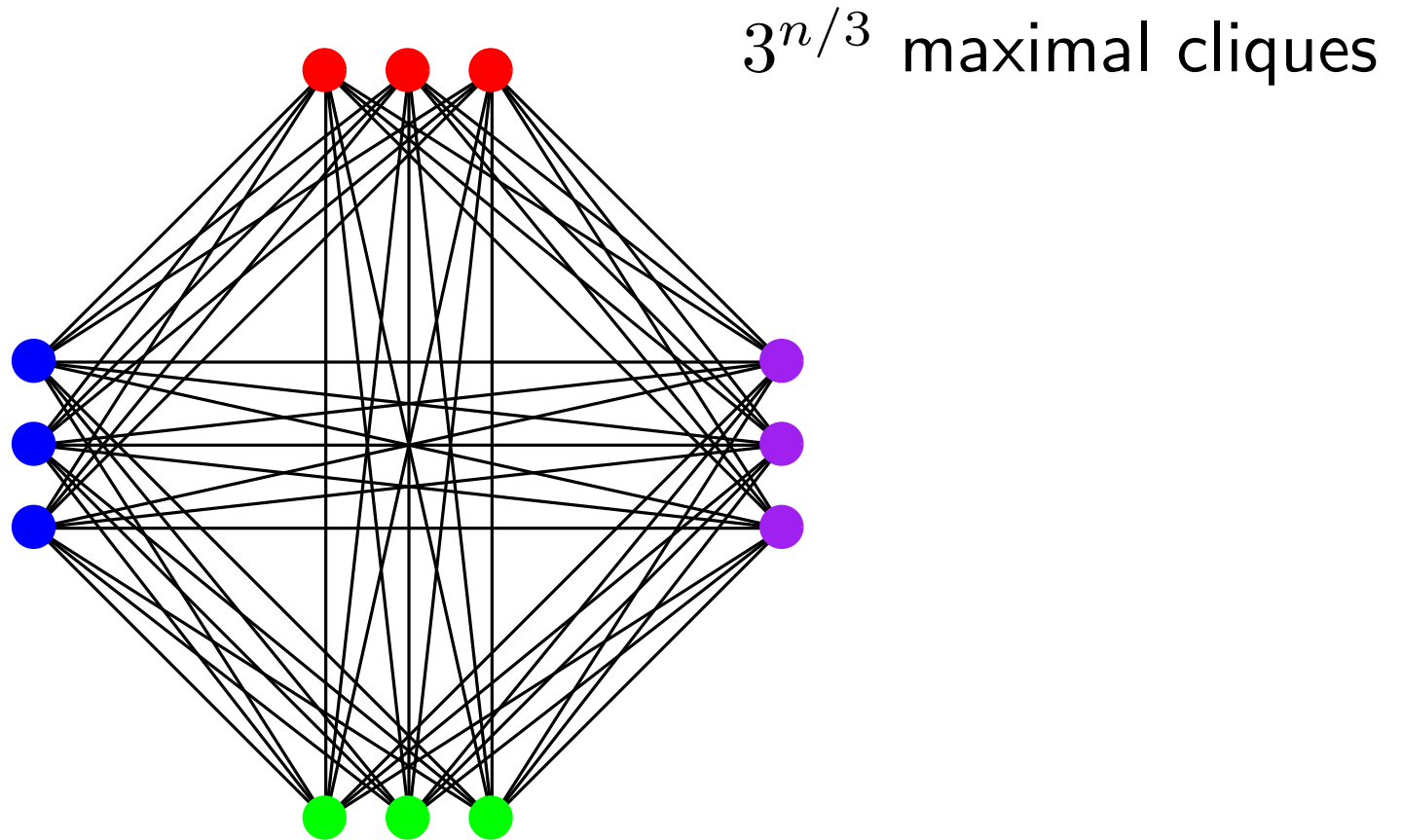
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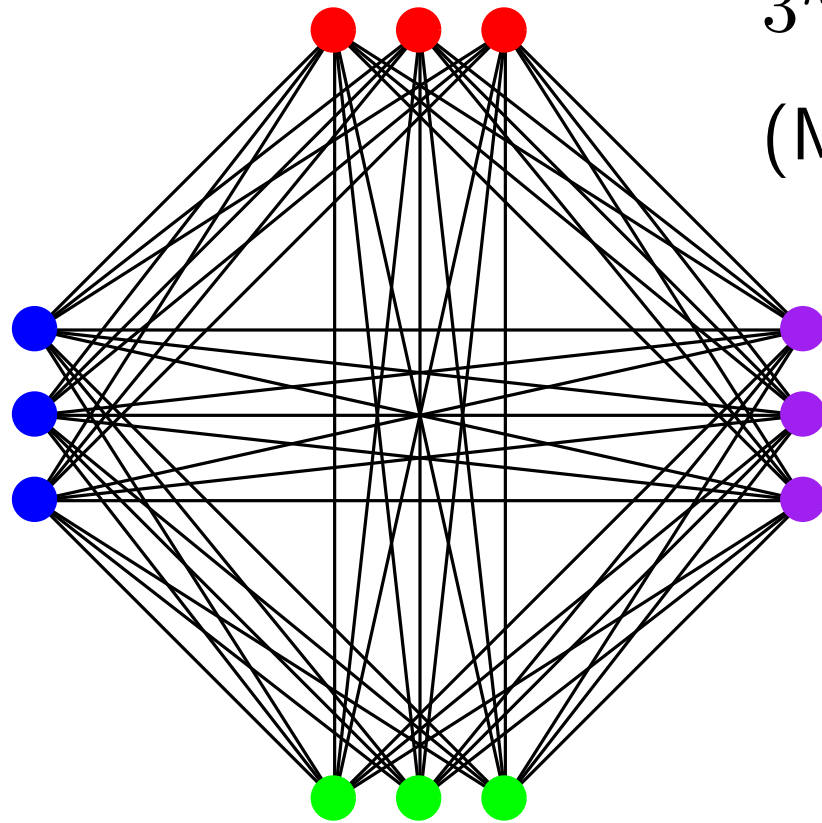
There may be many maximal cliques.



There may be many maximal cliques.



There may be many maximal cliques.



$3^{n/3}$ maximal cliques
(Moon–Moser bound)

Maximal Clique Listing Algorithms

Author	Year	Running Time
Bron and Kerbosch	1973	???
Tsukiyama et al.	1977	$O(nm\mu)$
Chiba and Nishizeki	1985	$O(\alpha m\mu)$
Makino and Uno	2004	$O(\Delta^4\mu)$

n = number of vertices

m = number of edges

μ = number of maximal cliques

α = arboricity

Δ = maximum degree of the graph

Tomita et al. (2006)

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Worst-case optimal running time $O(3^{n/3})$

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Computational experiments:

AMC	AMC*	CLIQUES
[14]	[14]	
261.27	9.51	10.49
952.25	49.45	10.20
3,601.09	130.76	9.90
14,448.21	431.20	10.95
35,866.69	530.53	12.97
> 24 h	1,066.62	16.85
> 24 h	4,350.94	33.75
> 24 h	15,655.05	65.06
> 24 h	> 24 h	293.97

Tomita et al. (2006)

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Computational experiments:

slow

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fast!

The Bron–Kerbosch Algorithm

Easy to understand

Easy to implement

There are many heuristics, which make it faster

Its variations work well in practice.

Confirmed through computational experiments
[Johnston \(1976\)](#), [Koch \(2001\)](#), [Baum \(2003\)](#)

One variation is worst-case optimal ($O(3^{n/3})$ time)
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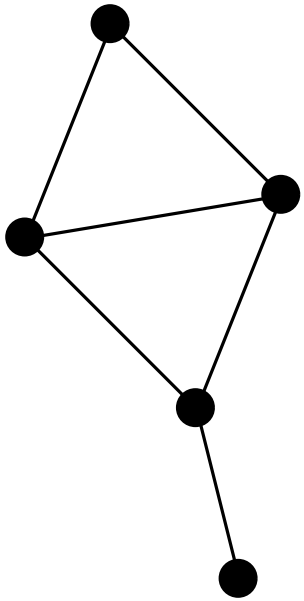
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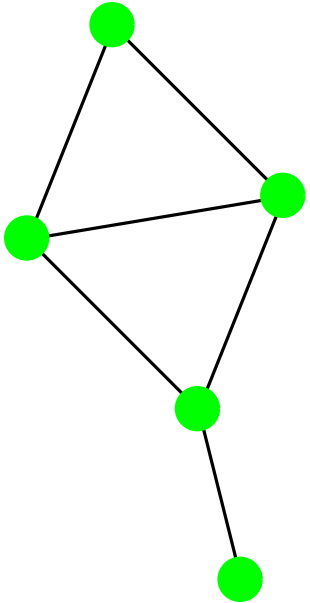
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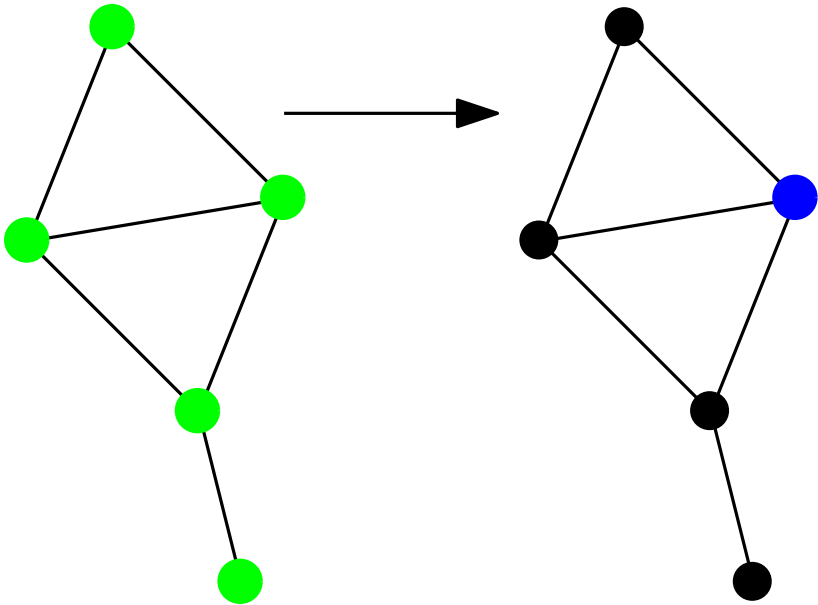
Finding one maximal clique



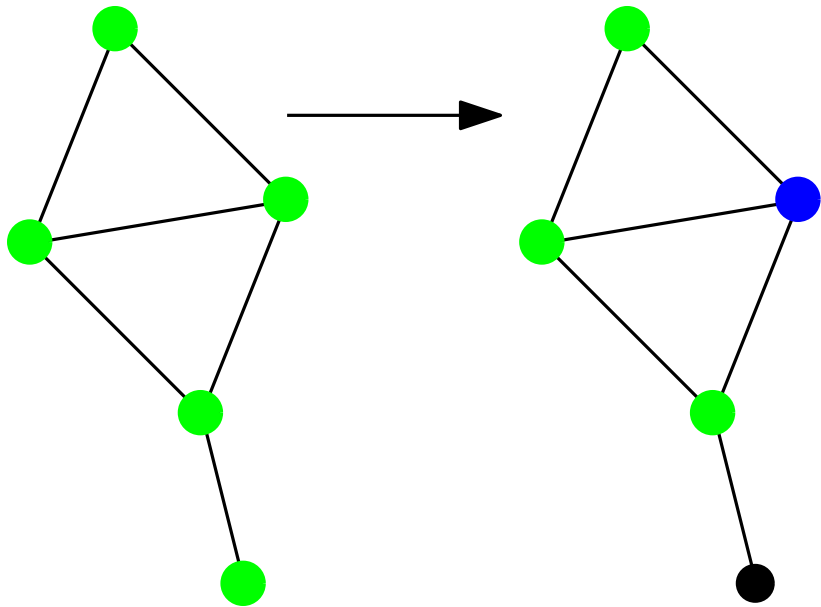
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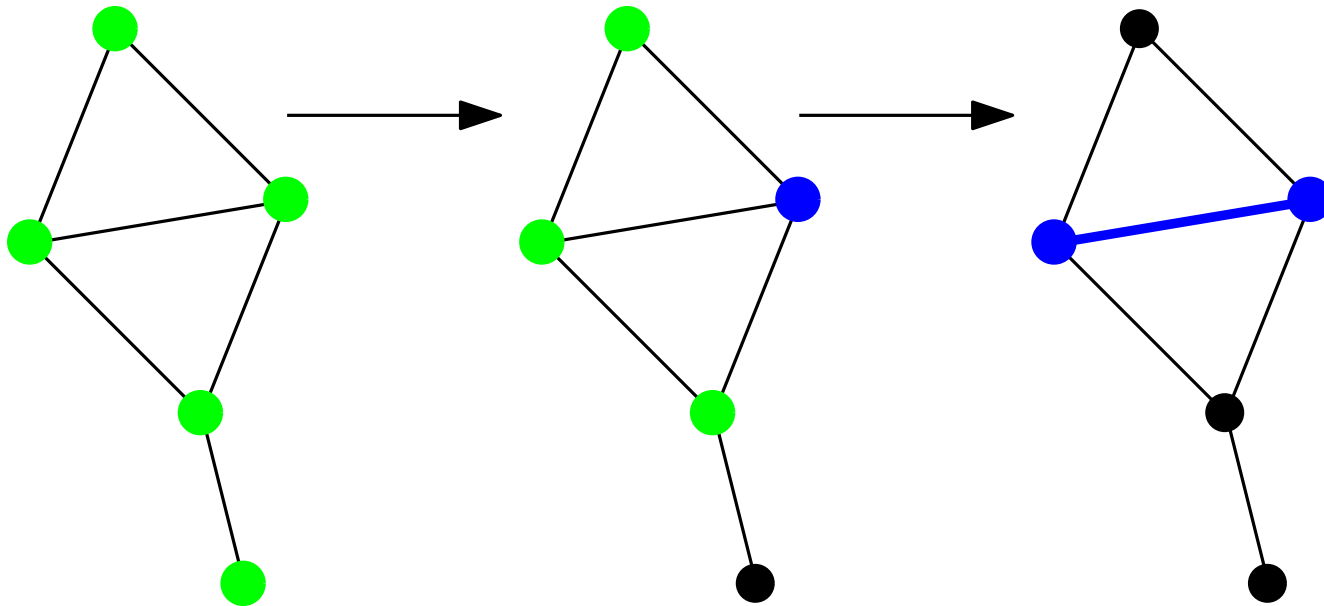
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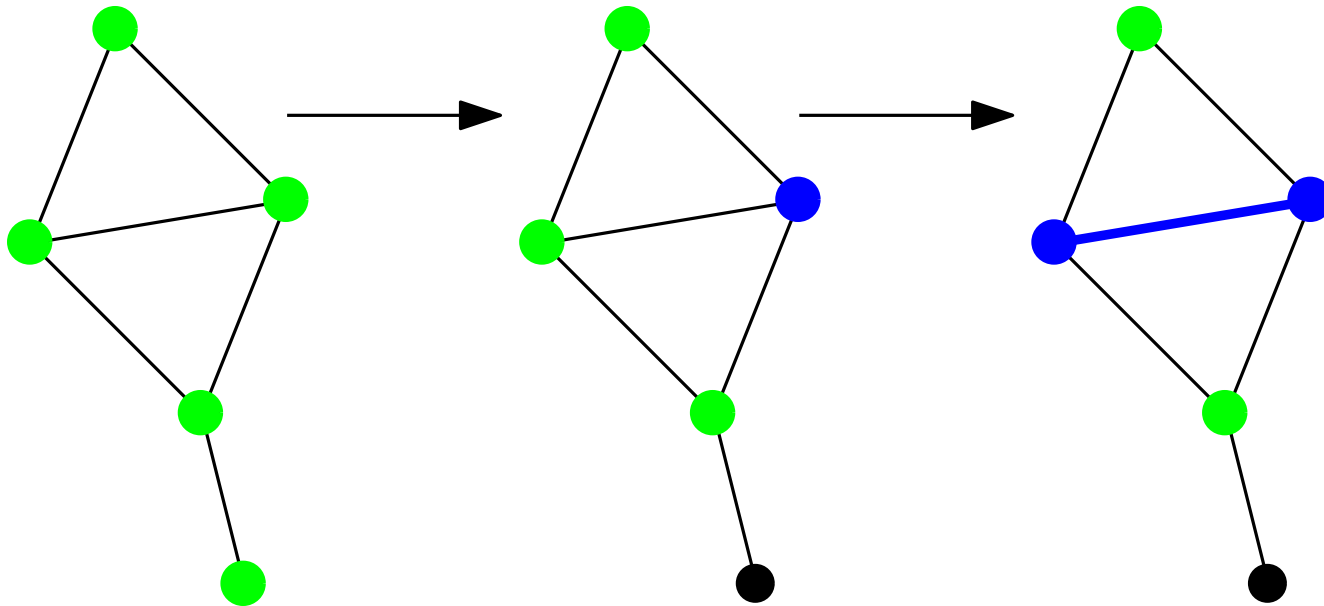
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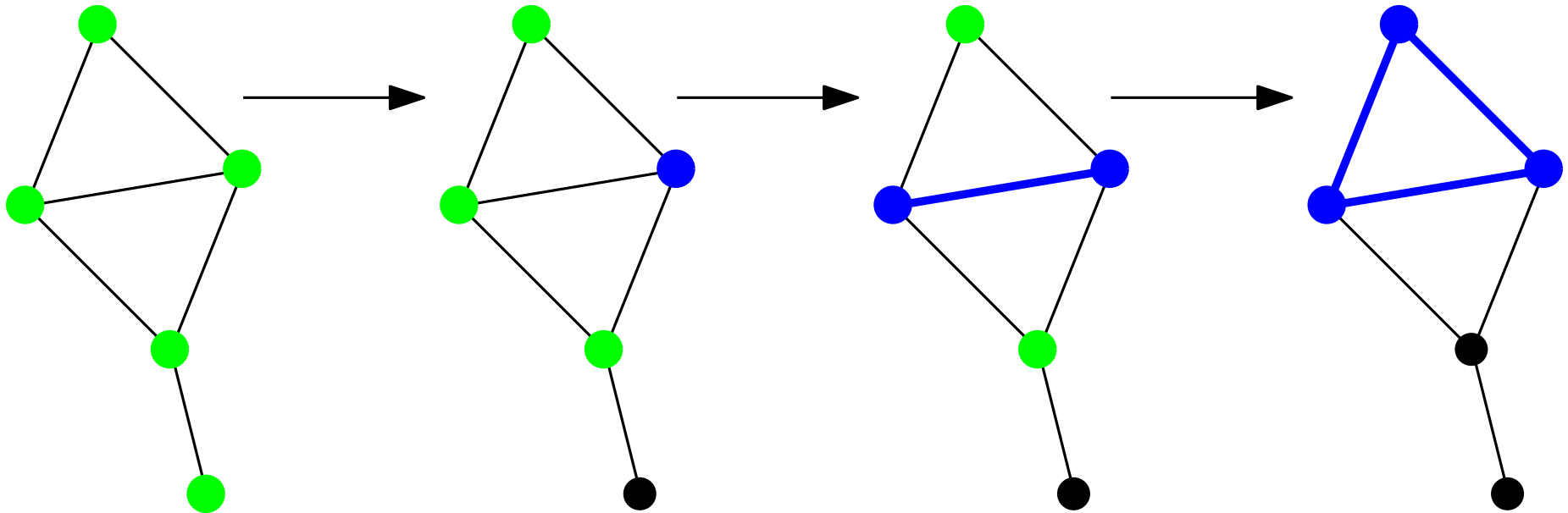
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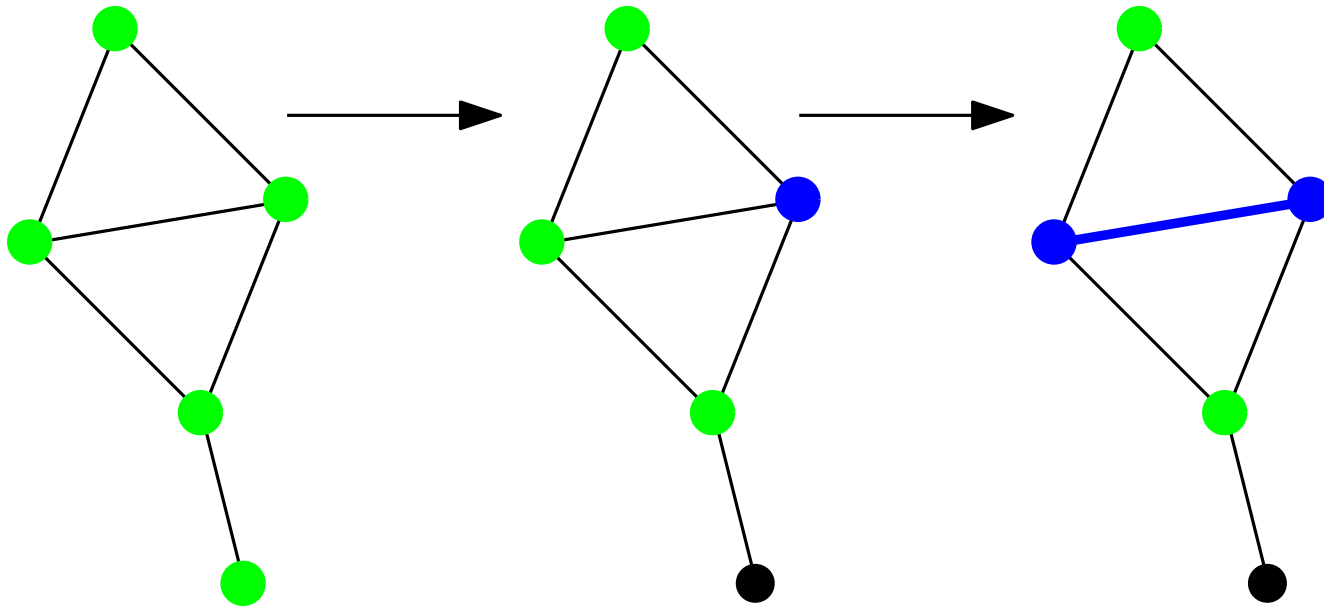
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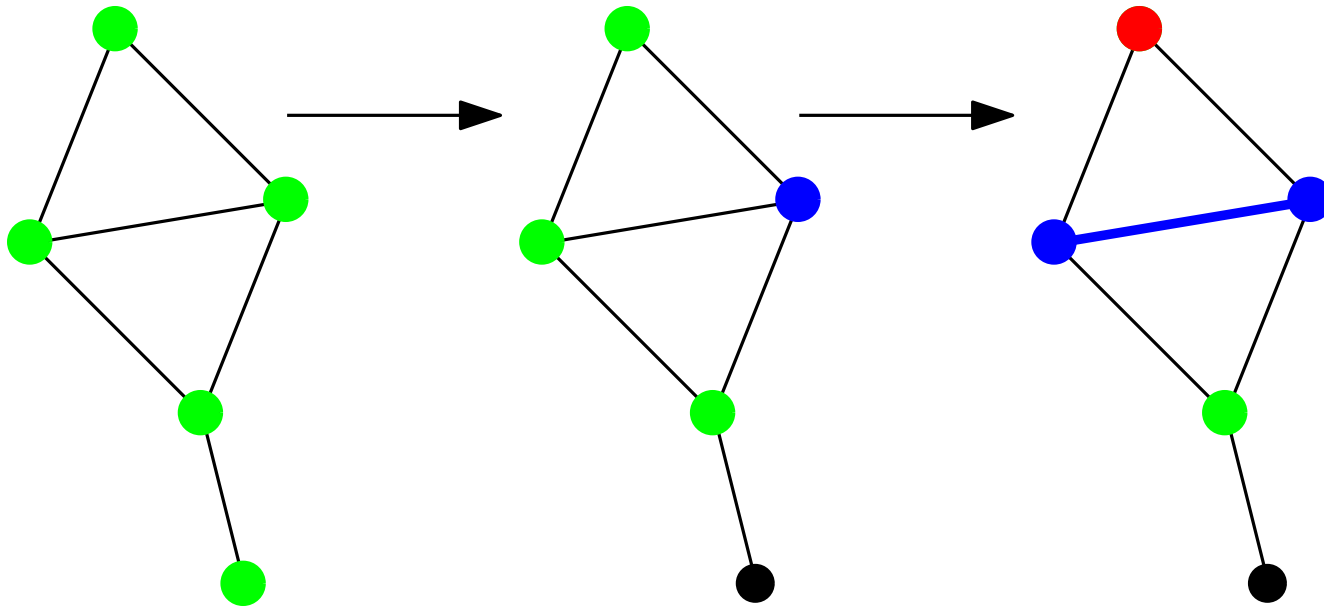
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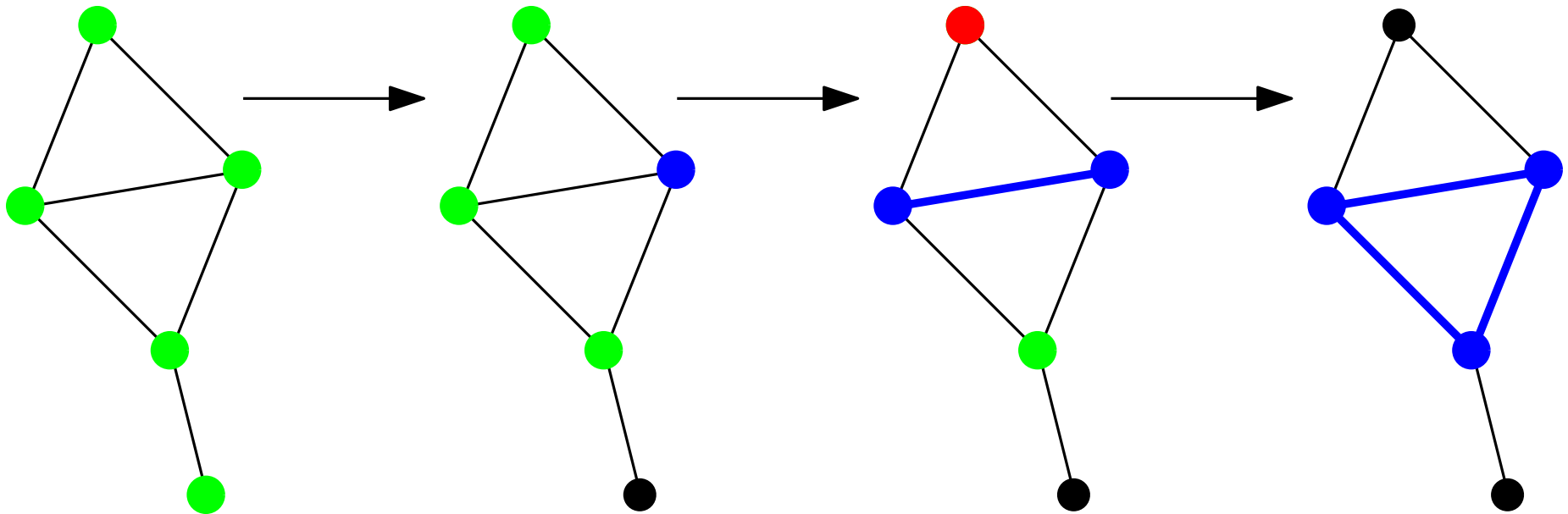
The Bron-Kerbosch Algorithm



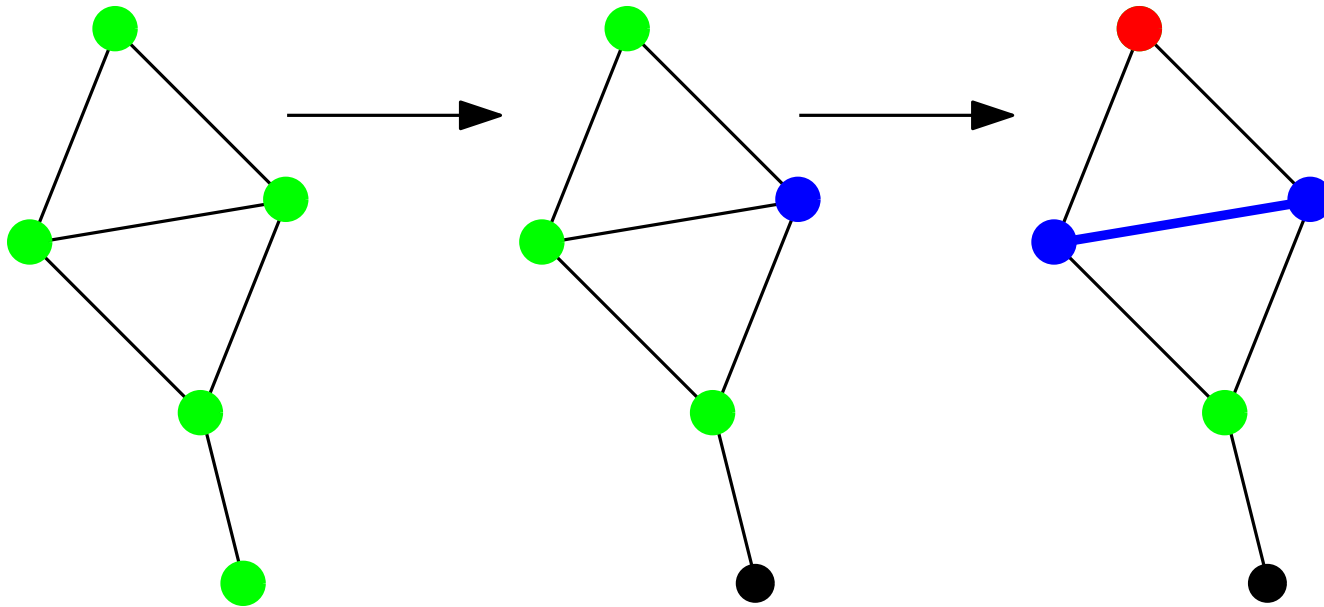
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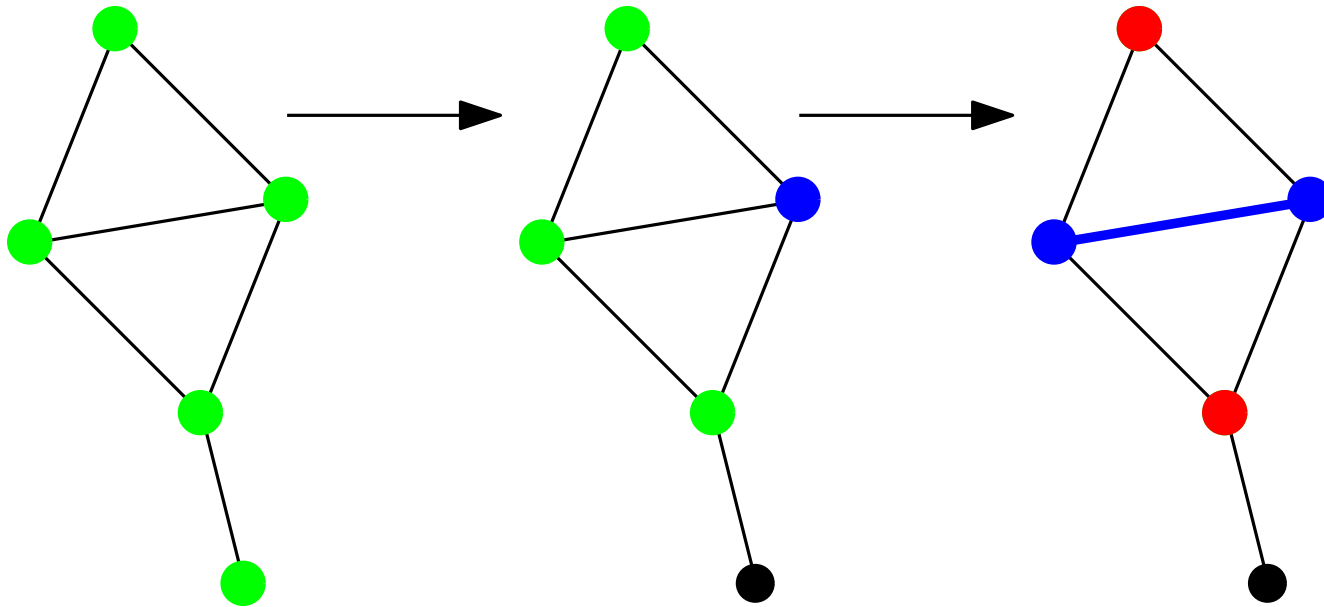
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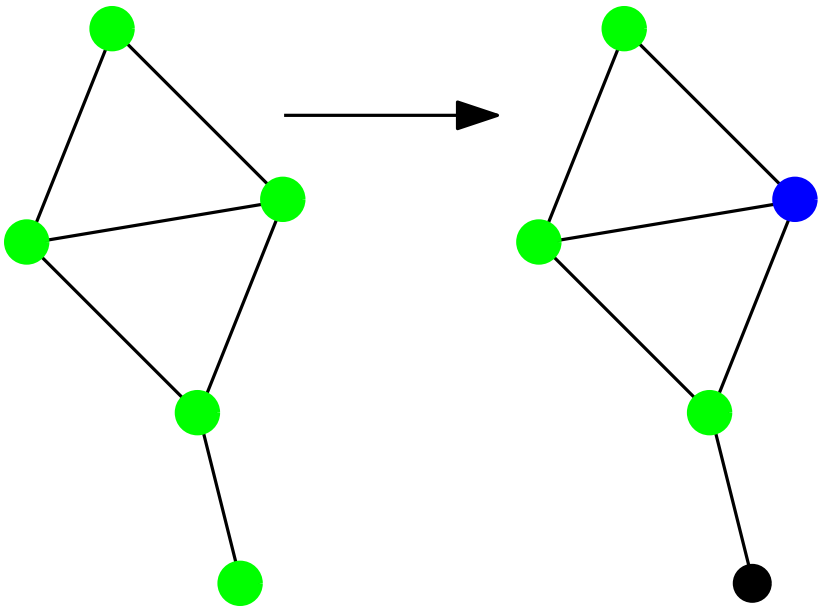
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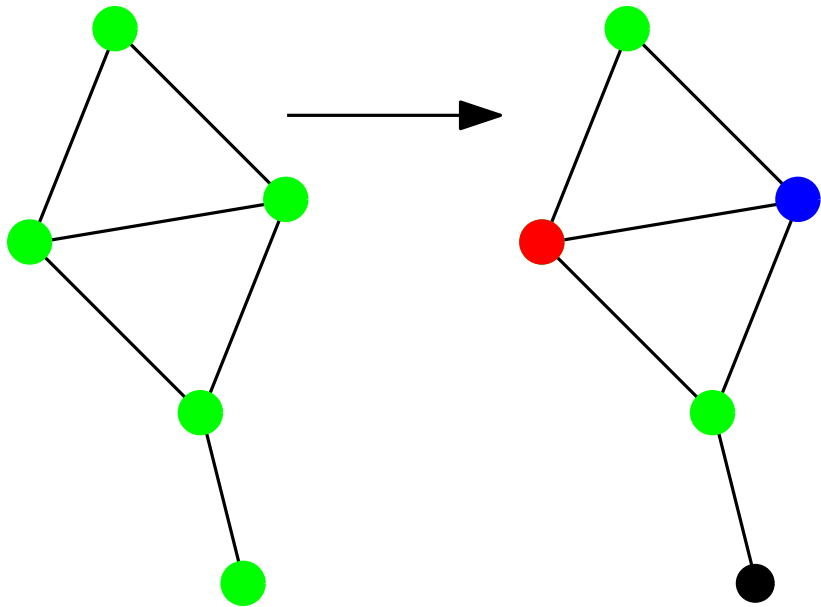
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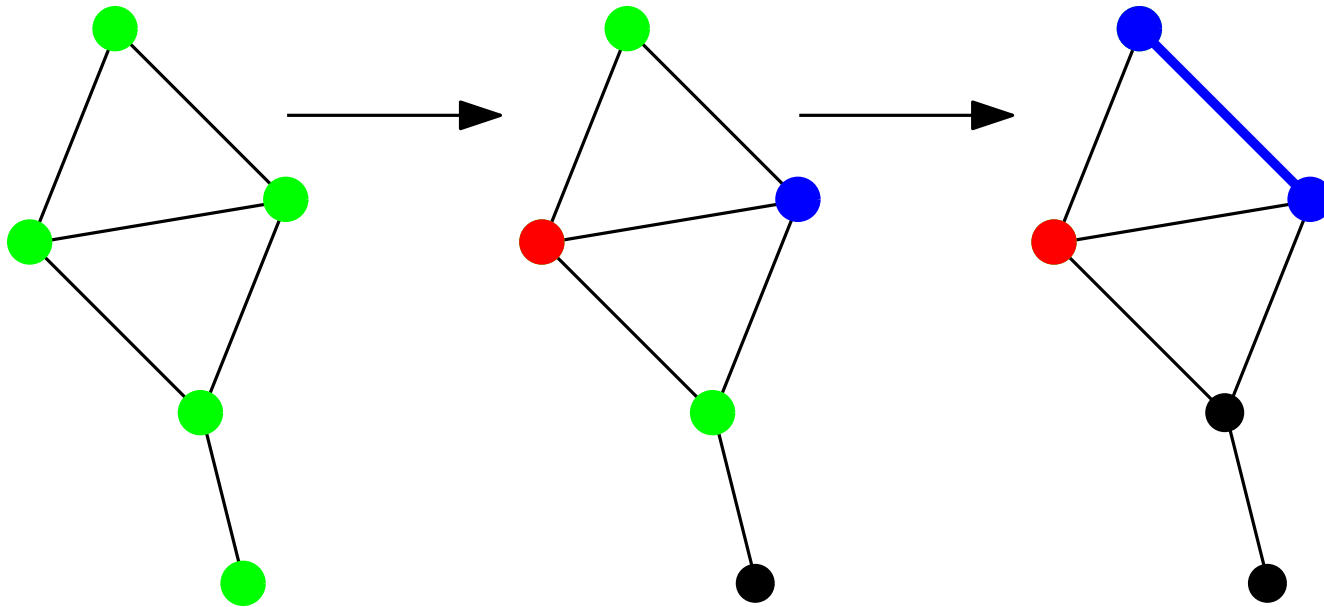
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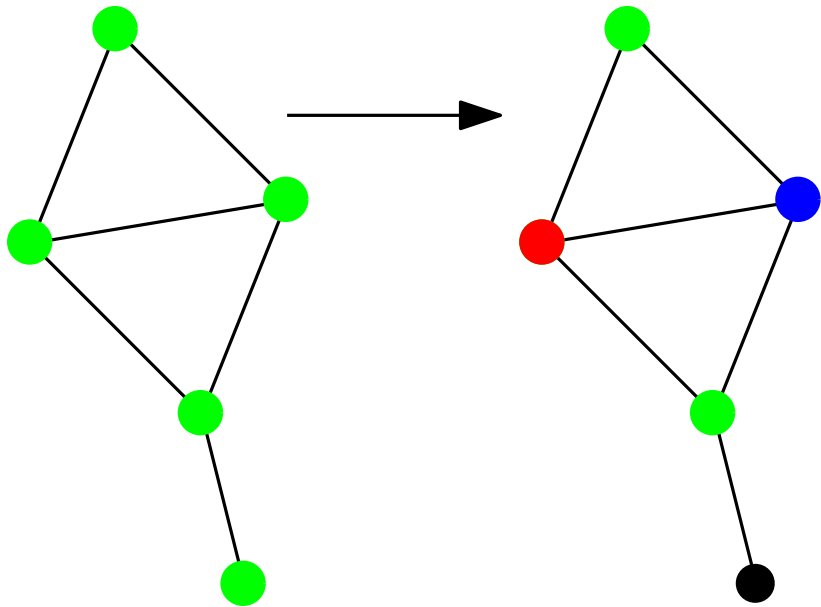
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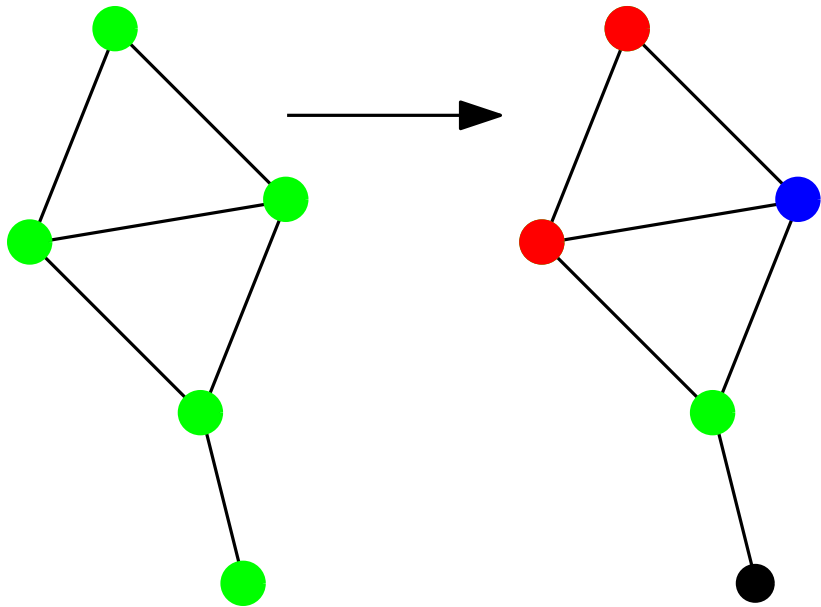
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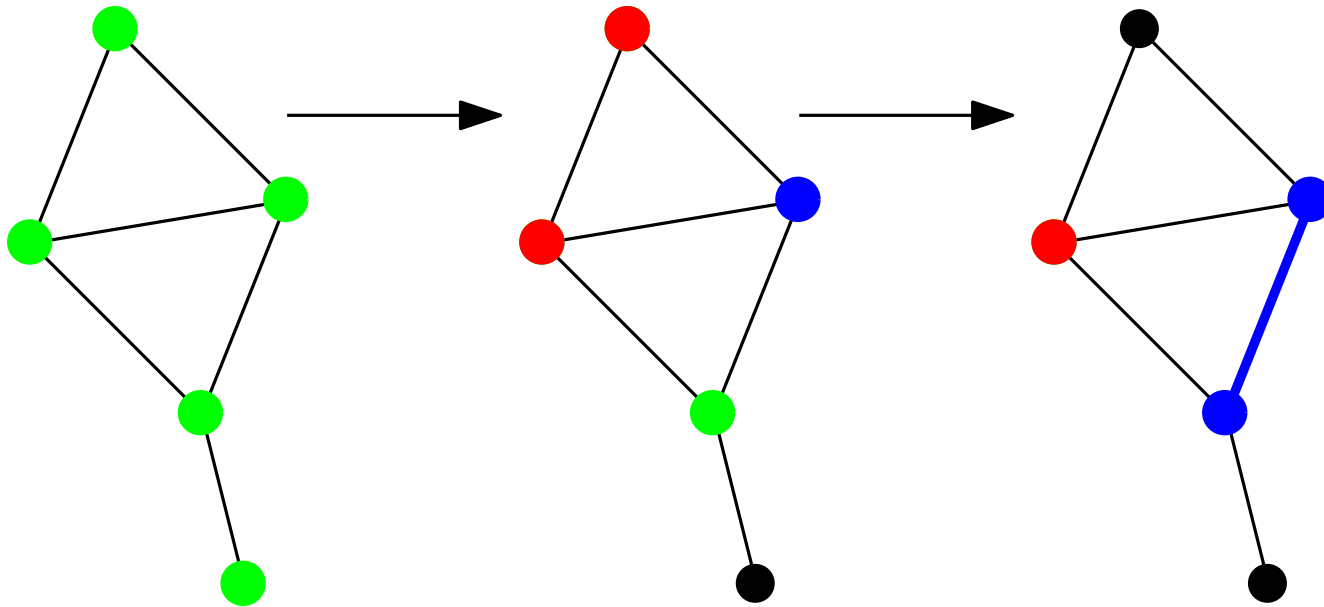
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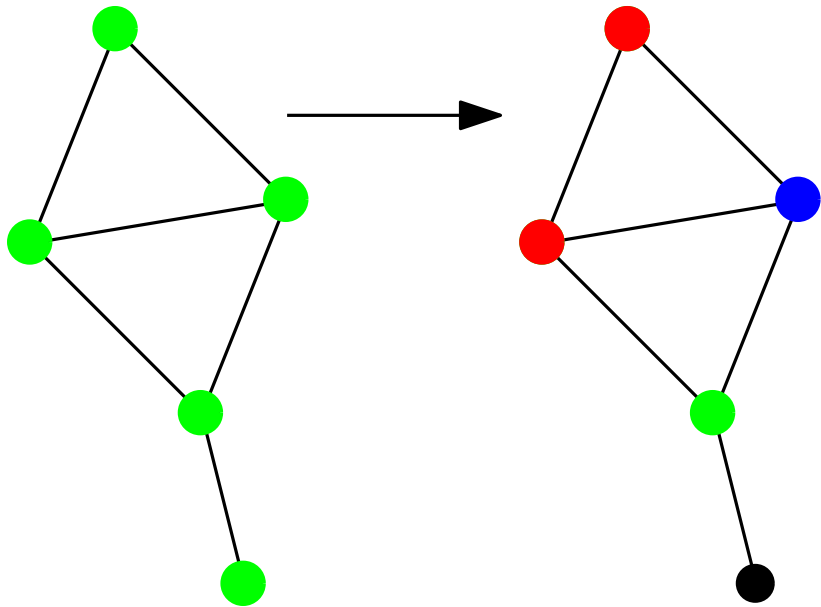
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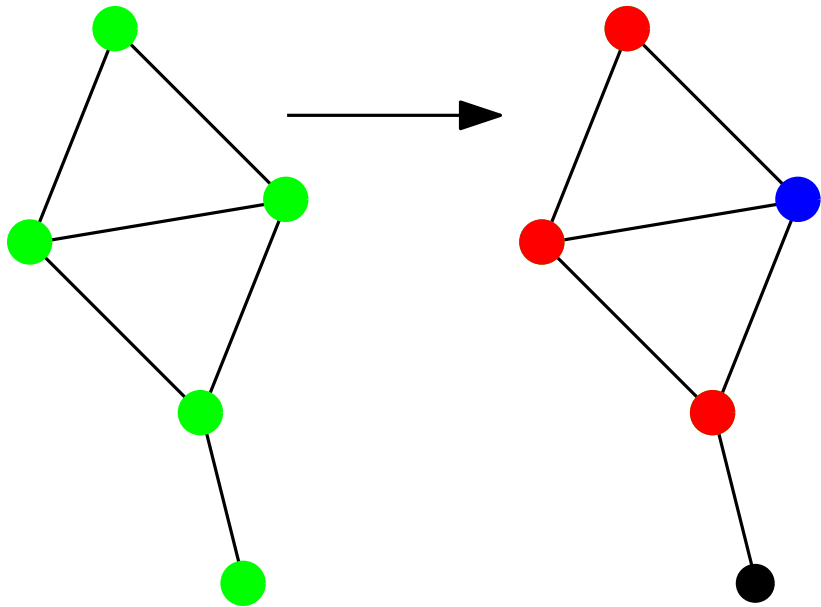
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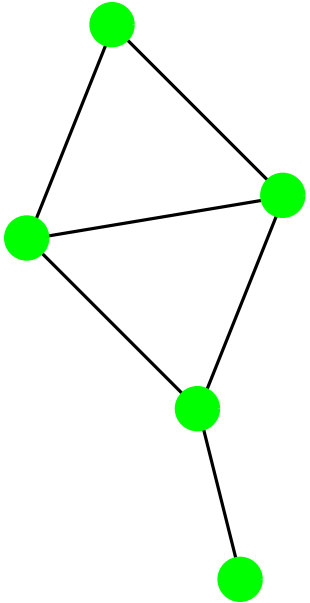
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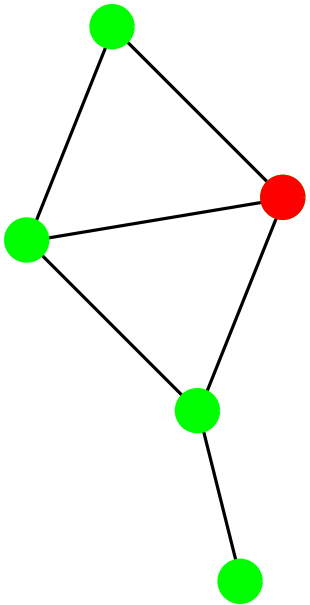
The Bron-Kerbosch Algorithm



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The Bron–Kerbosch Algorithm

proc BronKerbosch(P , R , X)

1: **if** $P \cup X = \emptyset$ **then**

2: report R as a maximal clique

3: **end if**

4: **for each** vertex $v \in P$ **do**

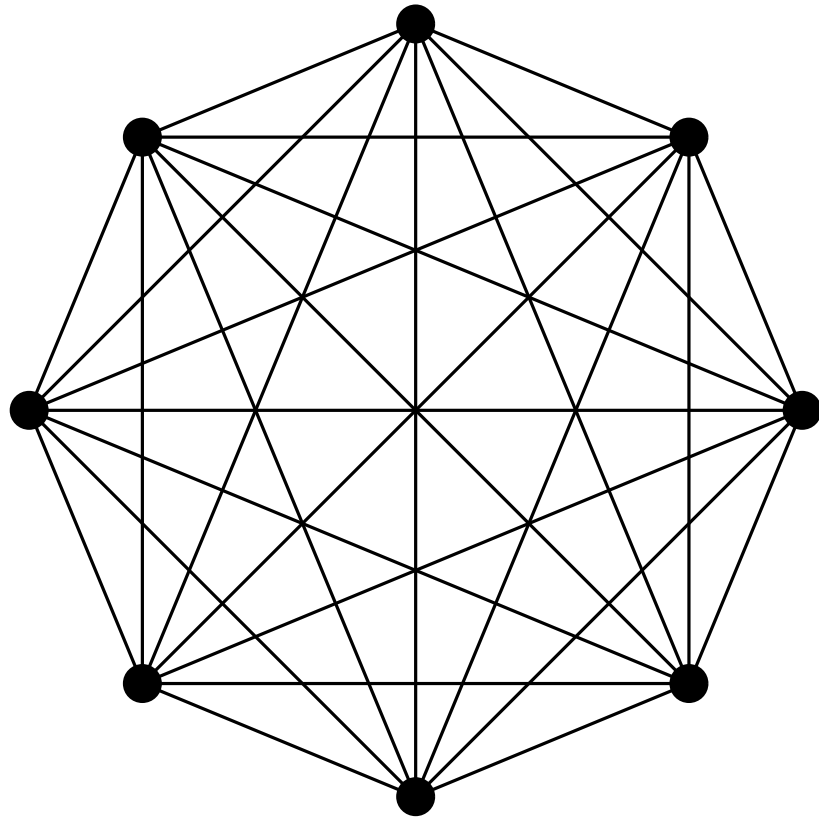
5: BronKerbosch($P \cap \Gamma(v)$, $R \cup \{v\}$, $X \cap \Gamma(v)$)

6: $P \leftarrow P \setminus \{v\}$

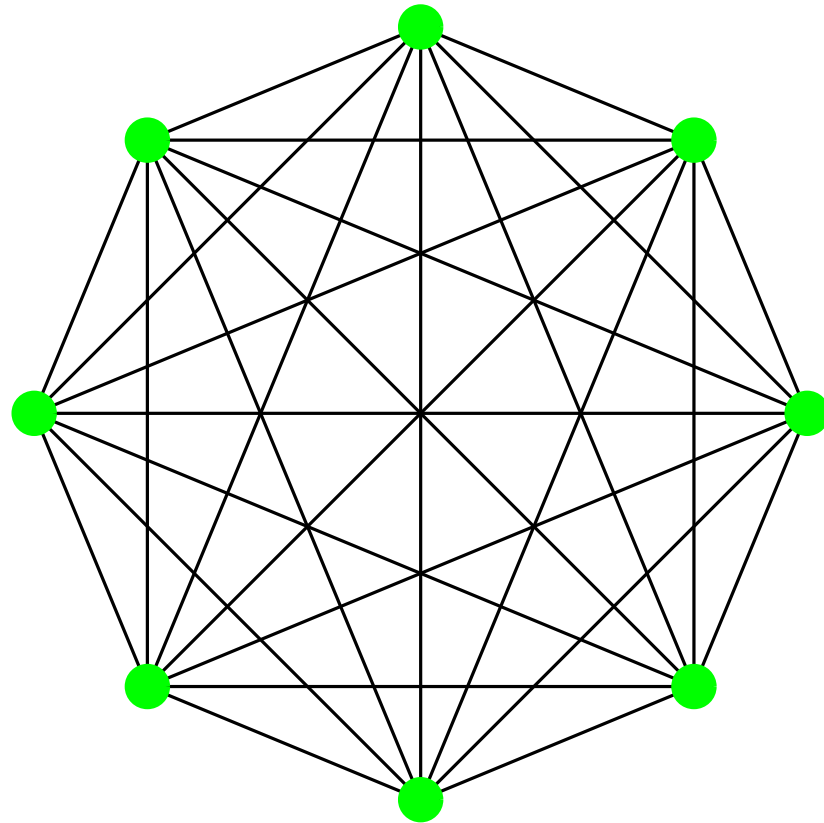
7: $X \leftarrow X \cup \{v\}$

8: **end for**

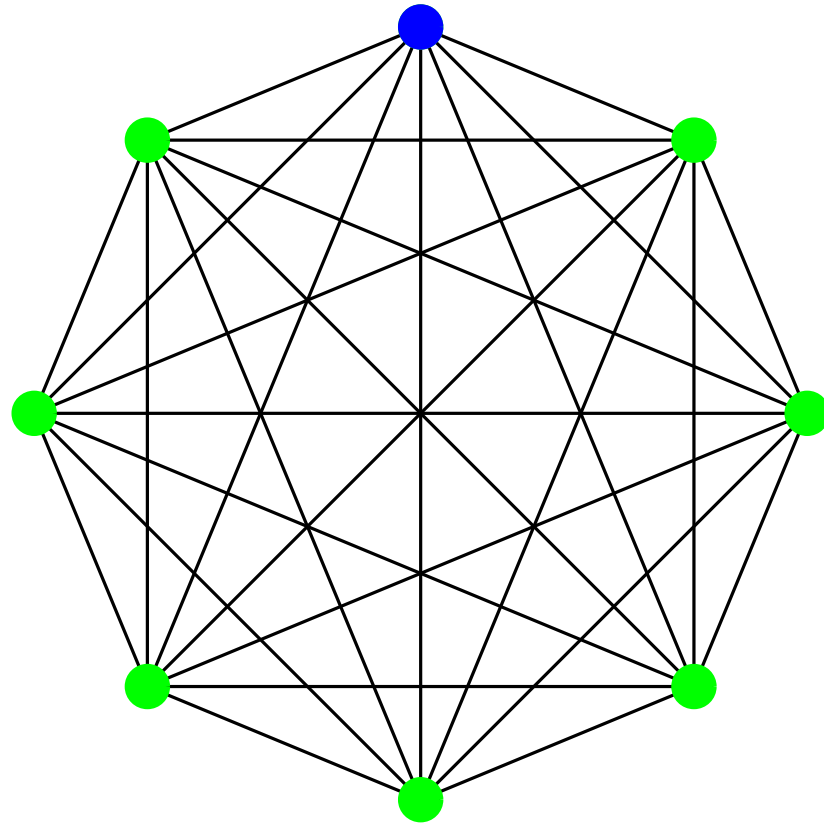
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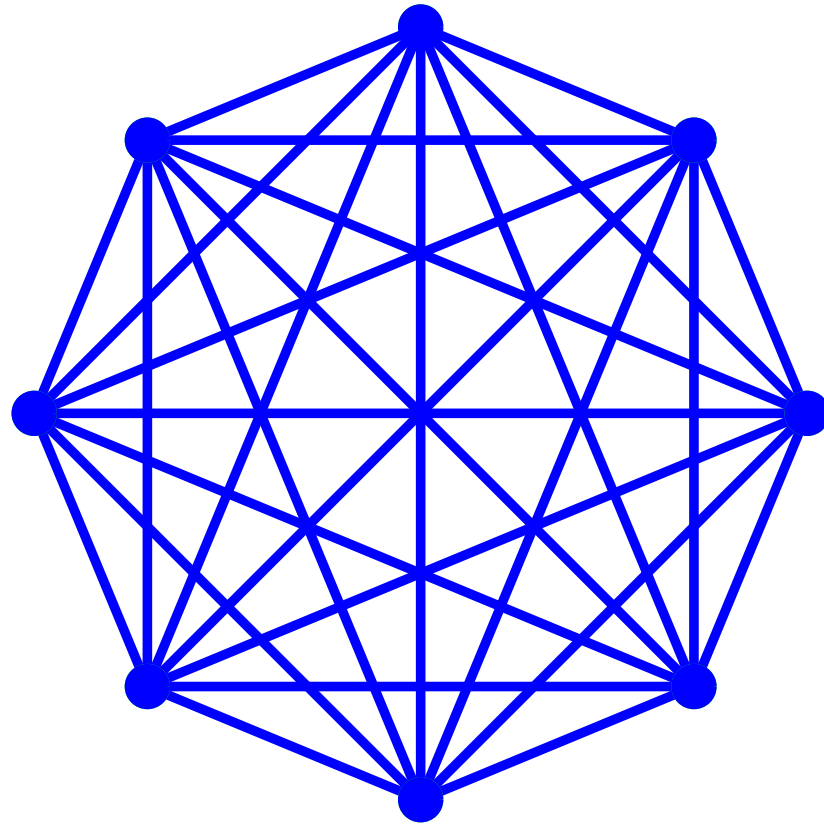
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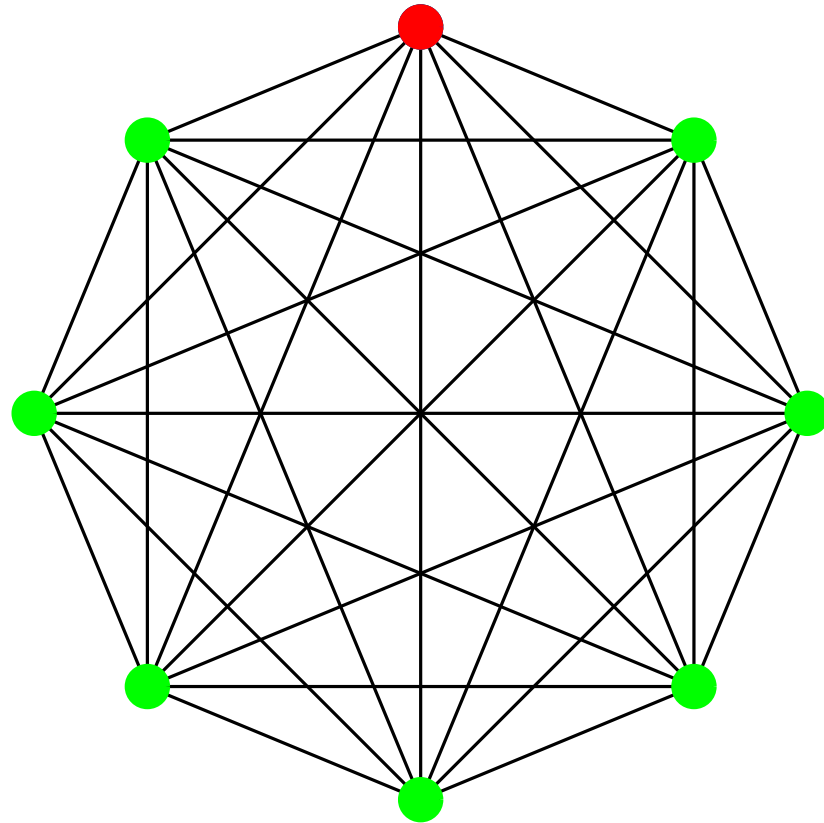
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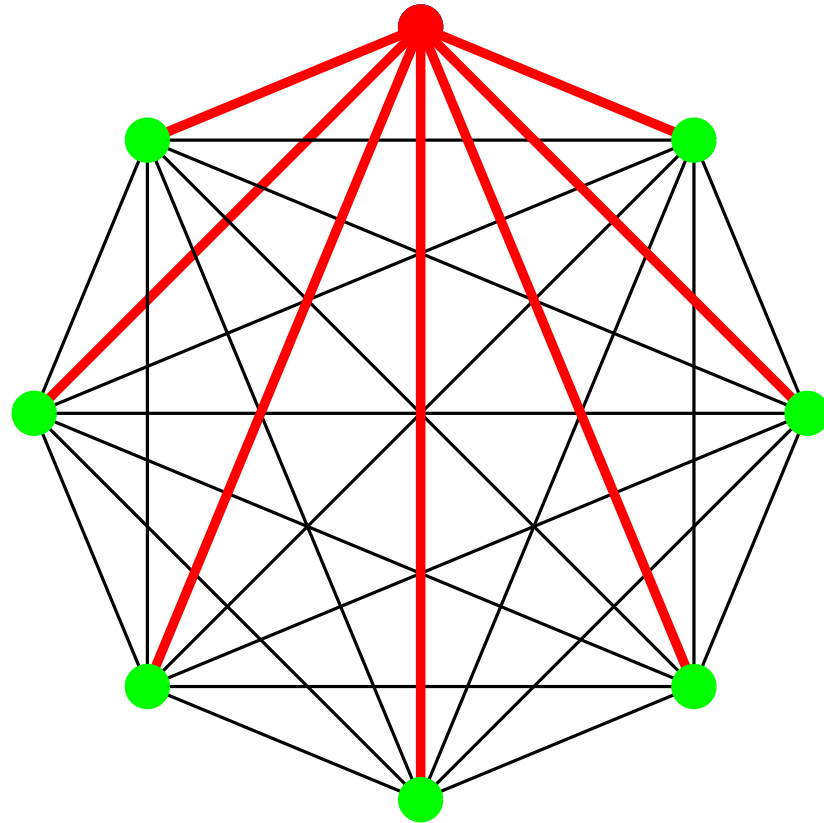
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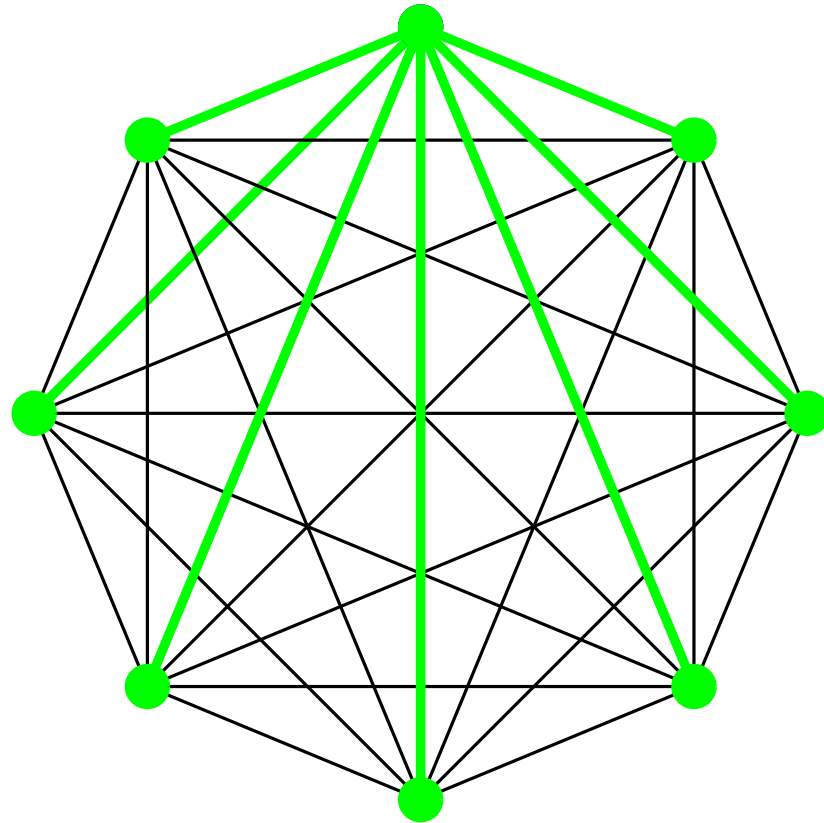
The Bron-Kerbosch Algorithm



The Bron–Kerbosch Algorithm



The Bron–Kerbosch Algorithm



The Bron–Kerbosch Algorithm with Pivoting

proc BronKerboschPivot(P, R, X)

- 1: **if** $P \cup X = \emptyset$ **then**
- 2: report R as a maximal clique
- 3: **end if**
- 4: choose a pivot $u \in P \cup X$
- 5: **for each** vertex $v \in P \setminus \Gamma(u)$ **do**
- 6: BronKerboschPivot($P \cap \Gamma(v), R \cup \{v\}, X \cap \Gamma(v)$)
- 7: $P \leftarrow P \setminus \{v\}$
- 8: $X \leftarrow X \cup \{v\}$
- 9: **end for**

The Bron–Kerbosch Algorithm with Pivoting

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- 1: **if** $P \cup X = \emptyset$ **then**
- 2: report R as a maximal clique
- 3: **end if**
- 4: choose a pivot $u \in P \cup X$ to minimize $|P \setminus \Gamma(u)|$
- 5: **for each** vertex $v \in P \setminus \Gamma(u)$ **do**
- 6: BronKerboschPivot($P \cap \Gamma(v), R \cup \{v\}, X \cap \Gamma(v)$)
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The Bron–Kerbosch Algorithm with Pivoting

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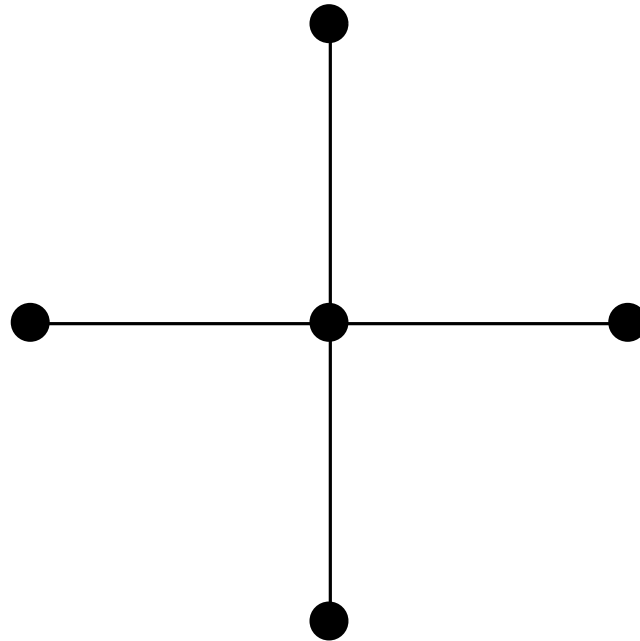
$$T(n) \leq \max_k \{kT(n - k)\} + O(n^2)$$

The Bron–Kerbosch Algorithm with Pivoting

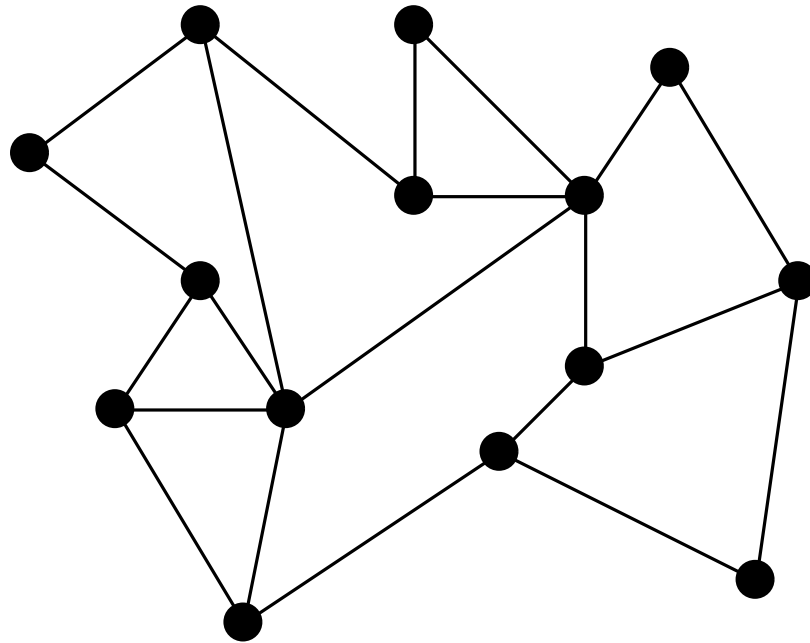
$$T(n) \leq \max_k \{kT(n - k)\} + O(n^2)$$

$$T(n) = O(3^{n/3})$$

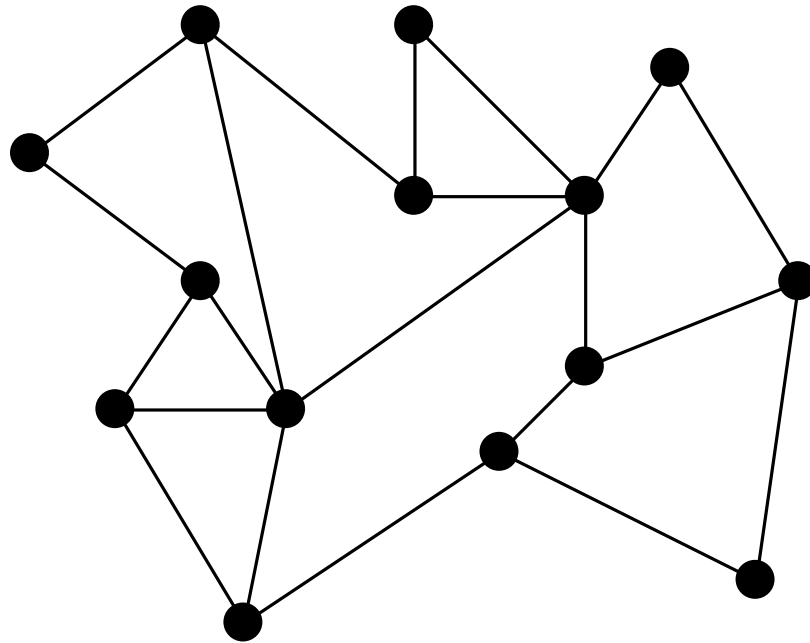
The Bron–Kerbosch Algorithm



The Bron-Kerbosch Algorithm



The Bron–Kerbosch Algorithm



All cliques in planar graphs may be listed in time $O(n)$
Chiba and Nishizeki (1985), Chrobak and Eppstein (1991)

The Bron–Kerbosch Algorithm

Want to characterize the running time with a parameter.

Let p be our parameter of choice.

An algorithm is *fixed-parameter tractable* with parameter p if it has running time

$$f(p)n^{O(1)}$$

The key is to avoid things like n^p .

Parameterize on Sparsity

Parameterize on Sparsity

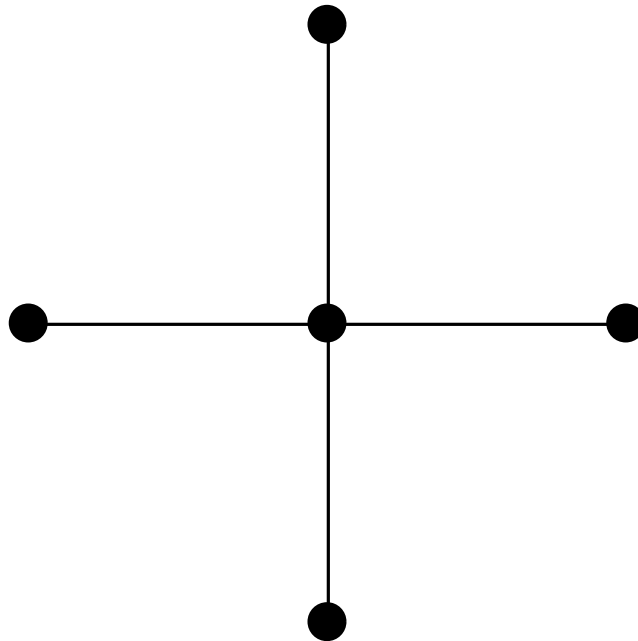
degeneracy:

Parameterize on Sparsity

degeneracy:

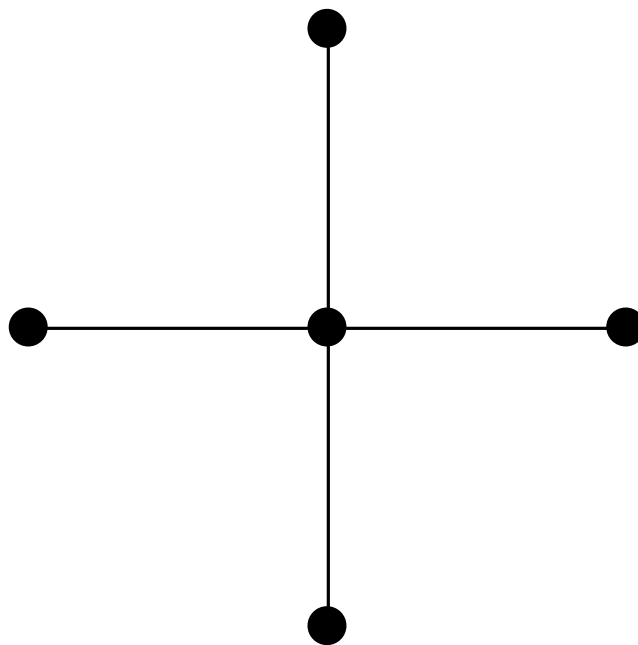
The minimum integer d such that every subgraph of G has a vertex of degree d or less.

Degeneracy



Degeneracy

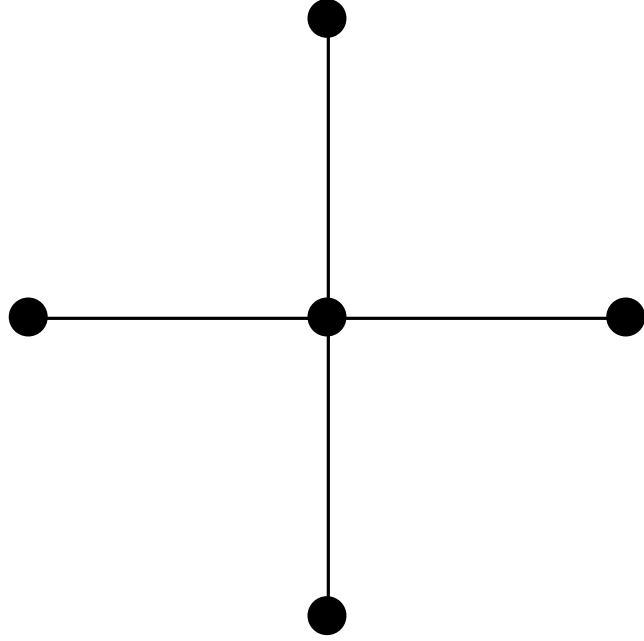
$$d = 1$$

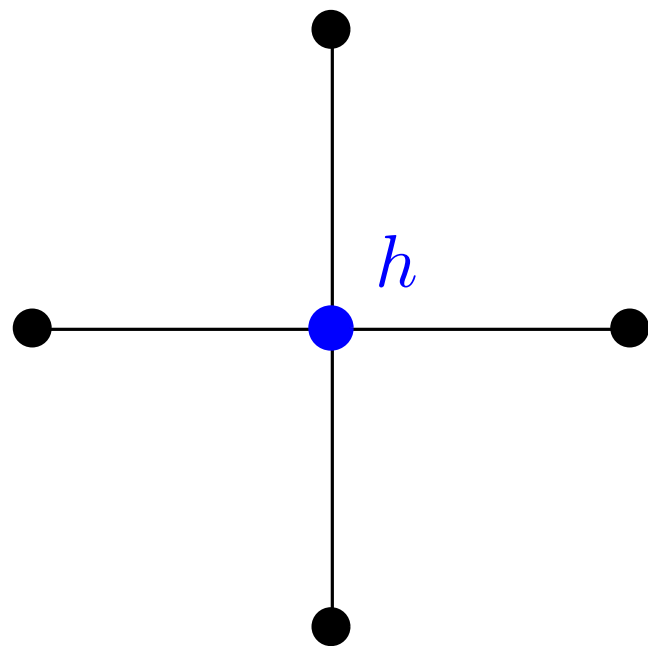


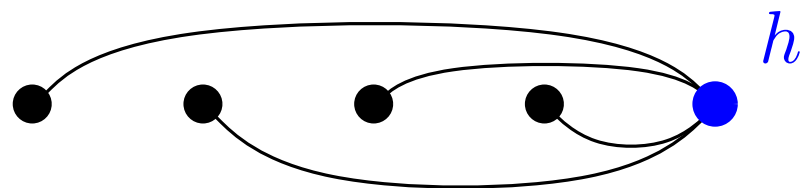
Degeneracy

degeneracy:

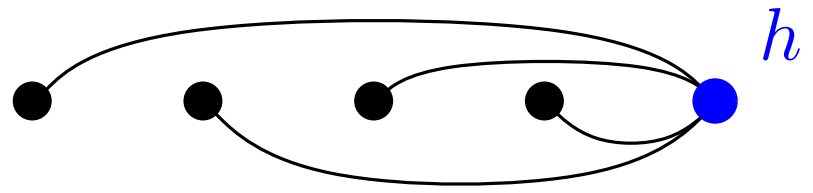
The minimum integer d such that there is an ordering of the vertices where each vertex has at most d neighbors later in the ordering.



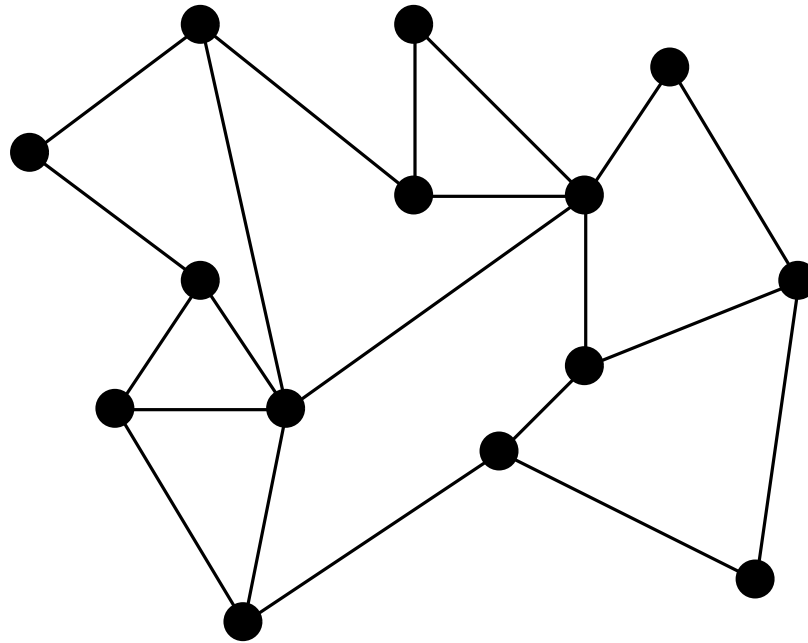




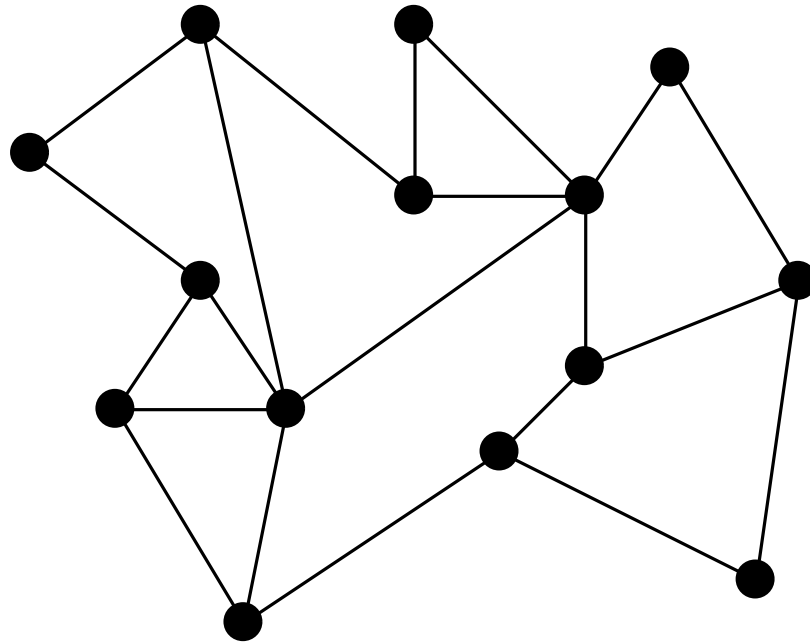
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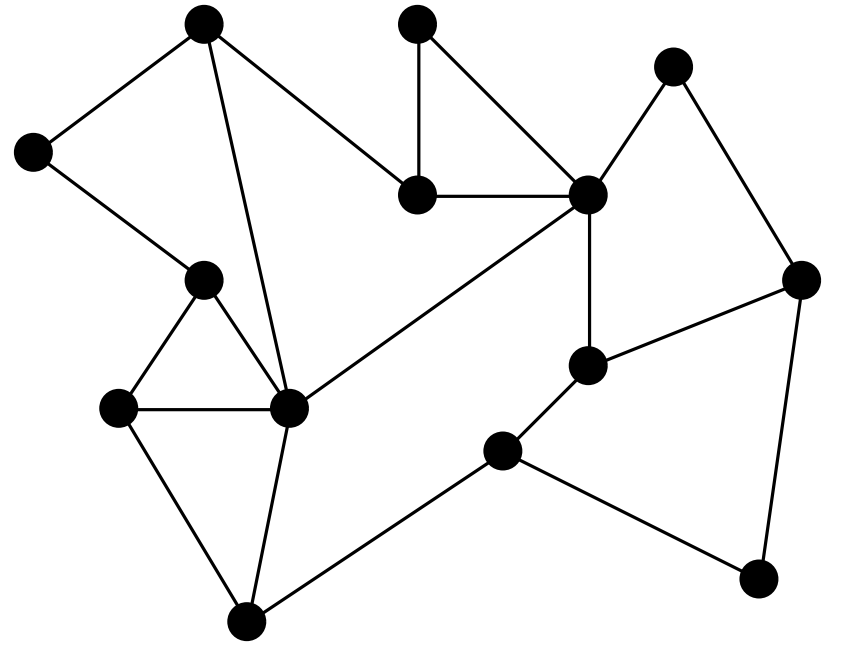


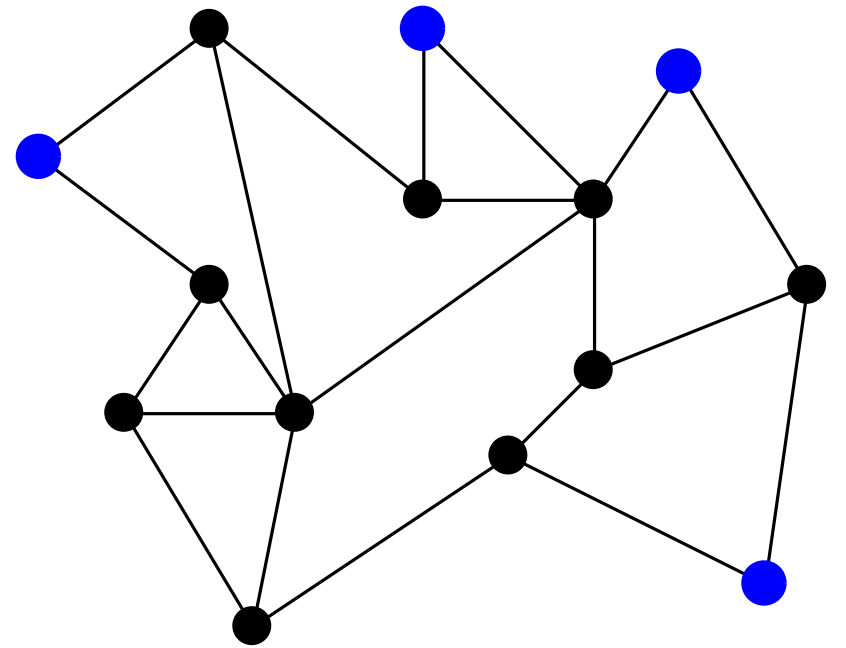
Planar graphs have degeneracy at most 5

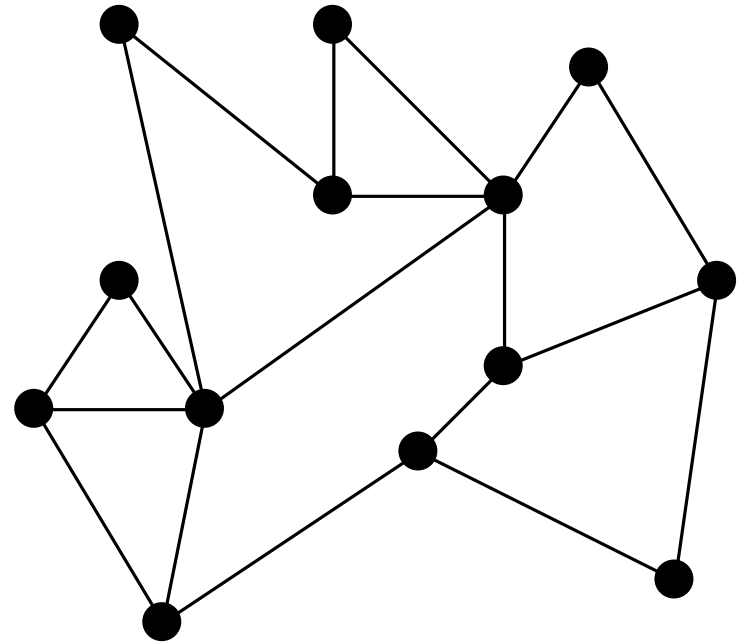


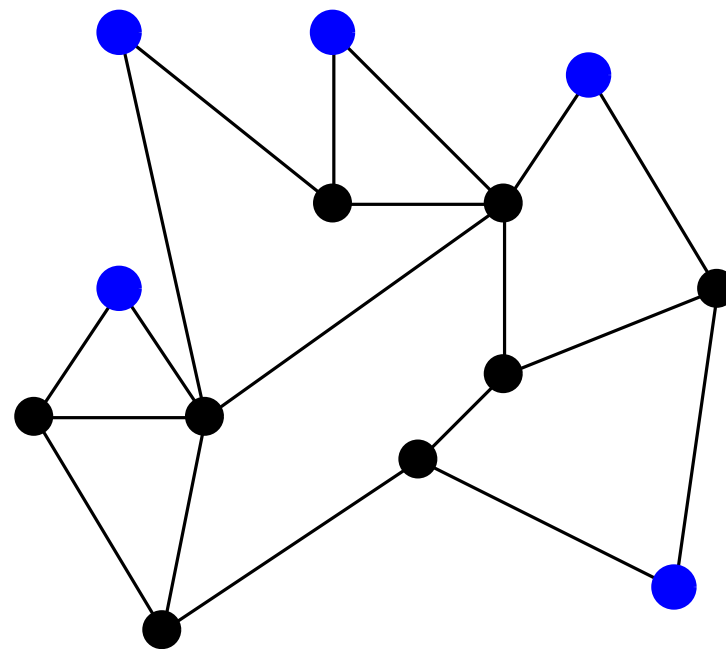
Degeneracy is easy to compute

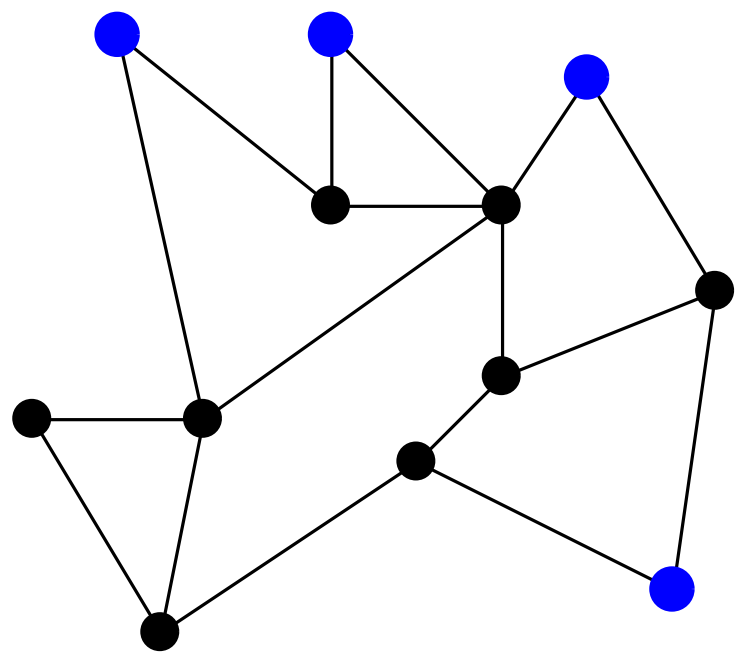


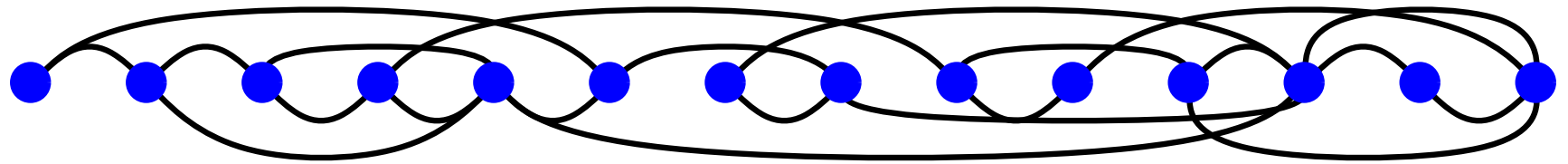












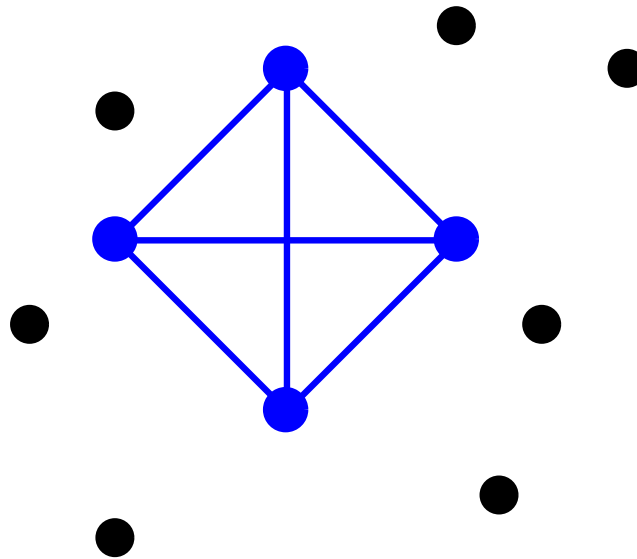
d -degenerate graphs...

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cannot contain cliques with more than $d + 1$ vertices

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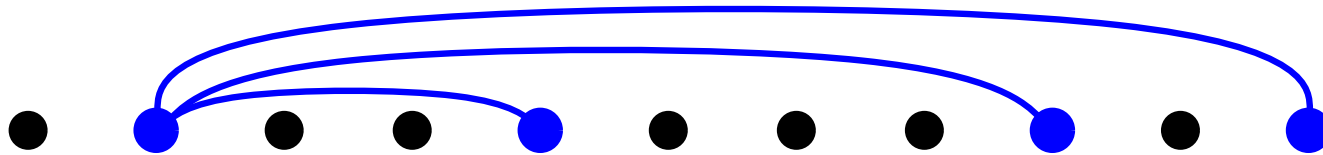
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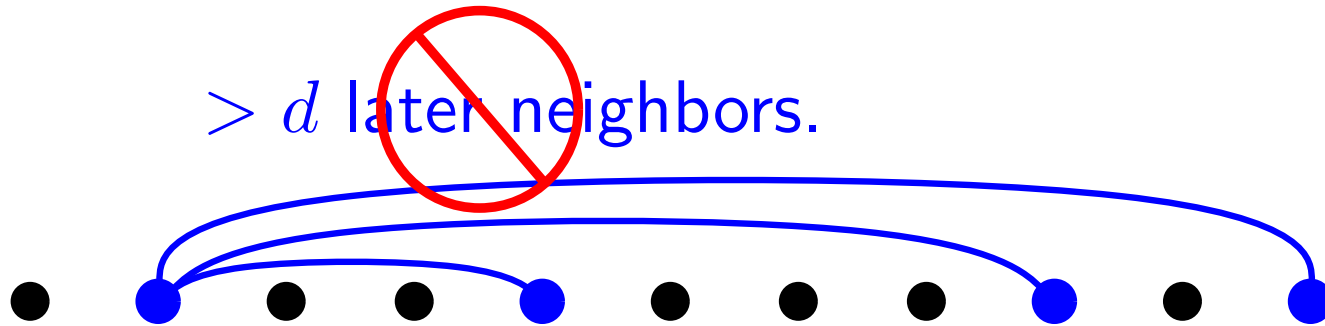
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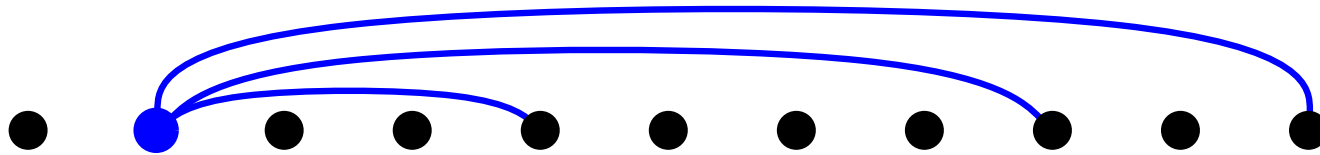
d -degenerate graphs...

have fewer than dn edges.

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have fewer than dn edges.

$\leq d$ later neighbors.



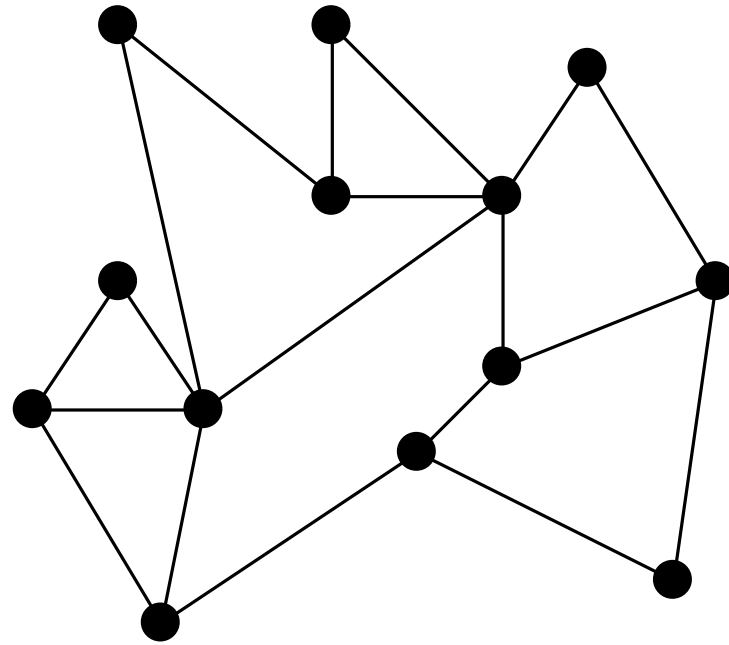
A few more facts about degeneracy...

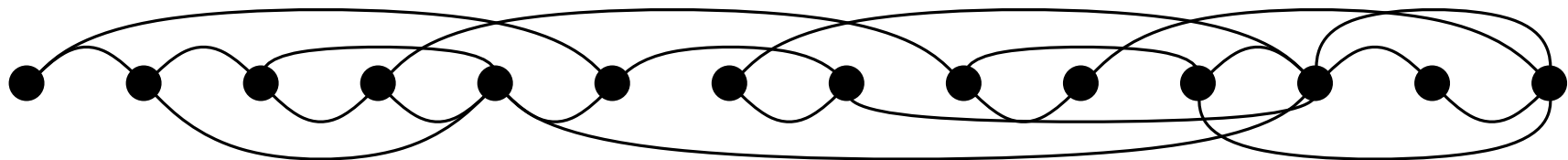
Degeneracy is within a constant factor of other popular sparsity measures.

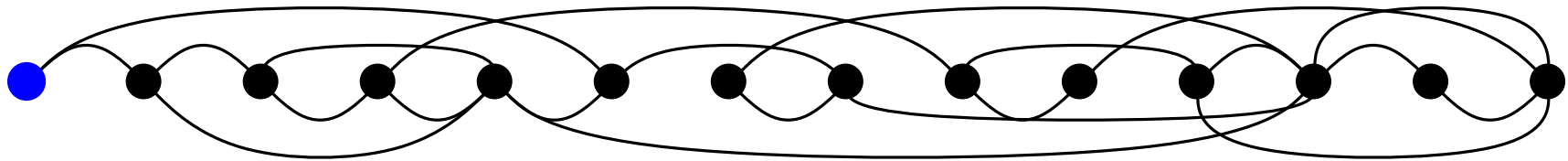
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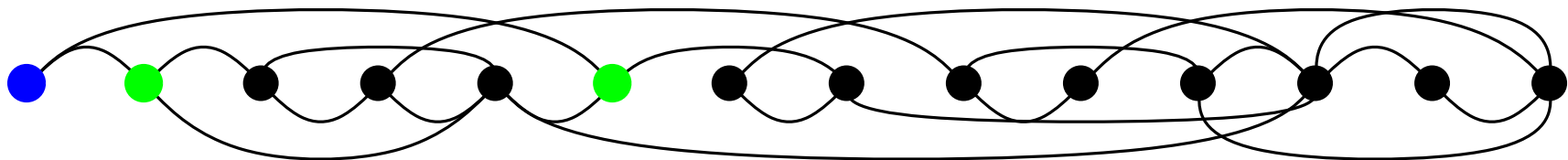
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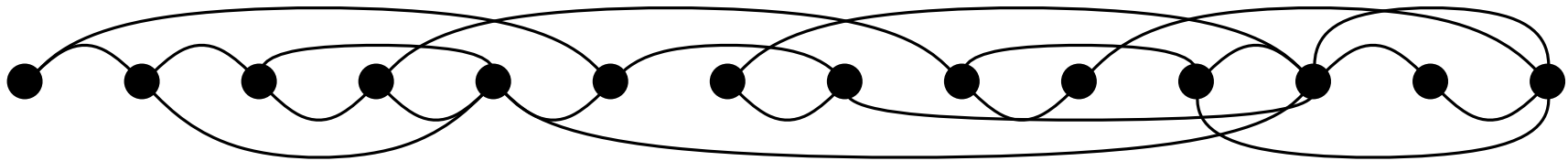
Graphs generated by the preferential attachment mechanism of Barabási and Albert have low degeneracy.

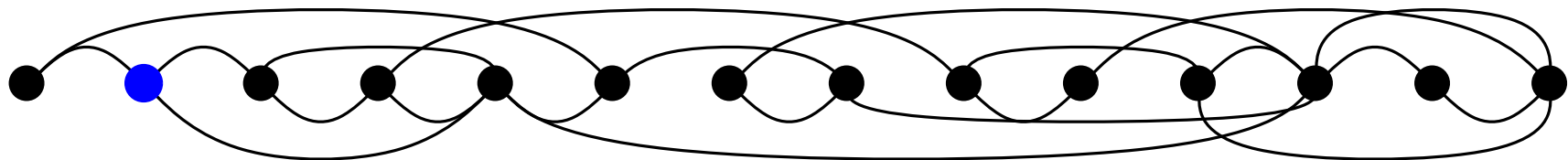


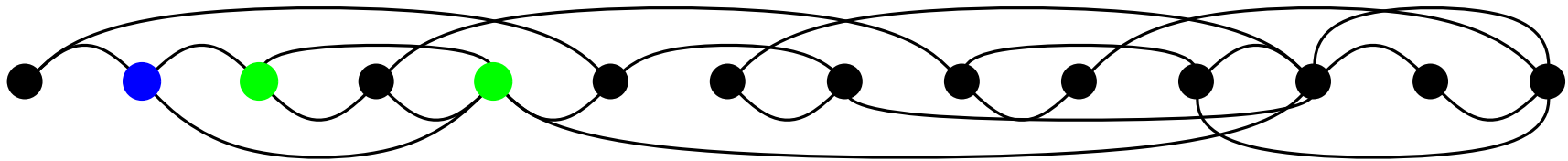


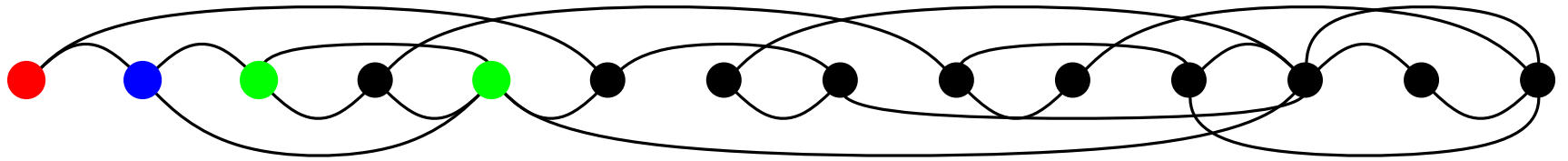










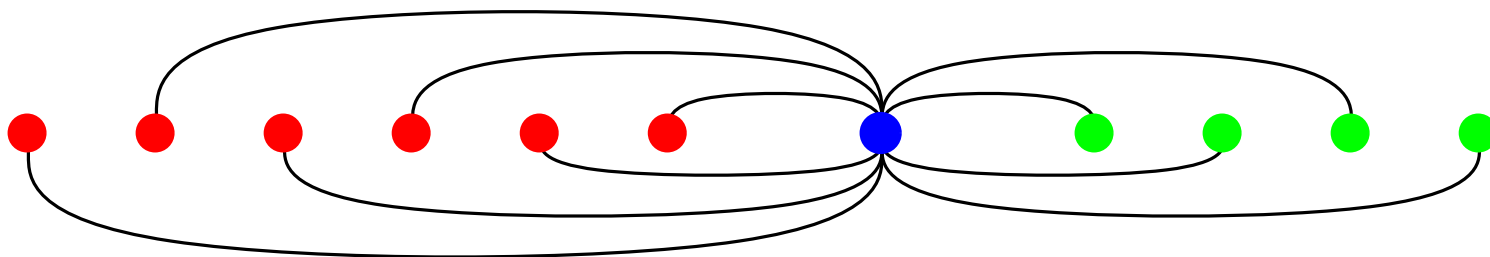


proc BronKerboschDegeneracy(V, E)

- 1: **for** each vertex v_i in a degeneracy ordering v_0, v_1, v_2, \dots of (V, E)
do
- 2: $P \leftarrow v_i$'s later neighbors
- 3: $X \leftarrow v_i$'s earlier neighbors
- 4: BronKerboschPivot($P, \{v_i\}, X$)
- 5: **end for**

X

$|P| \leq d$



Computing the pivot

Pick $u \in X \cup P$ that maximizes $|P \cap \Gamma(u)|$.

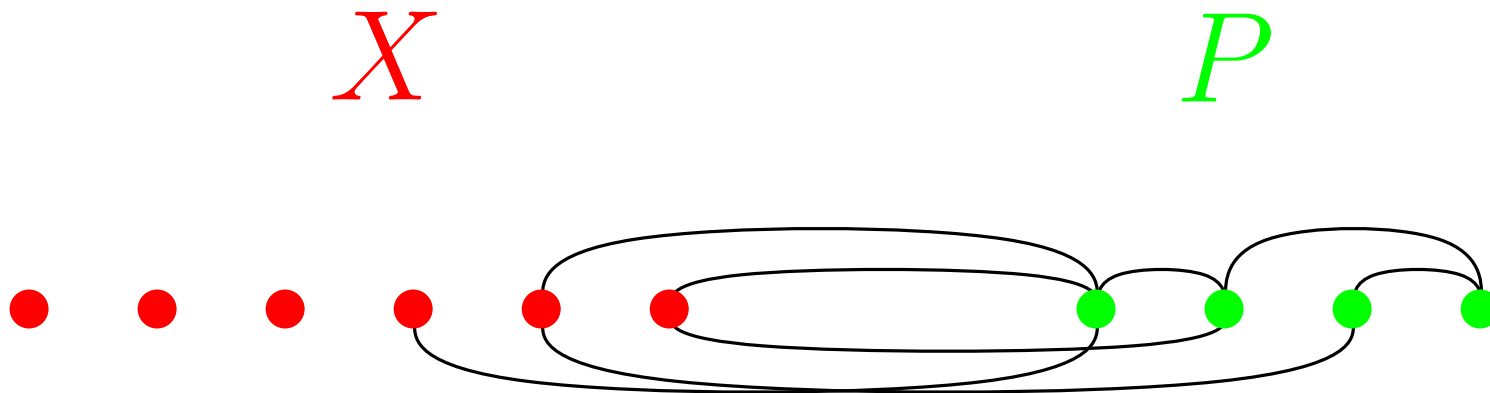
X

P



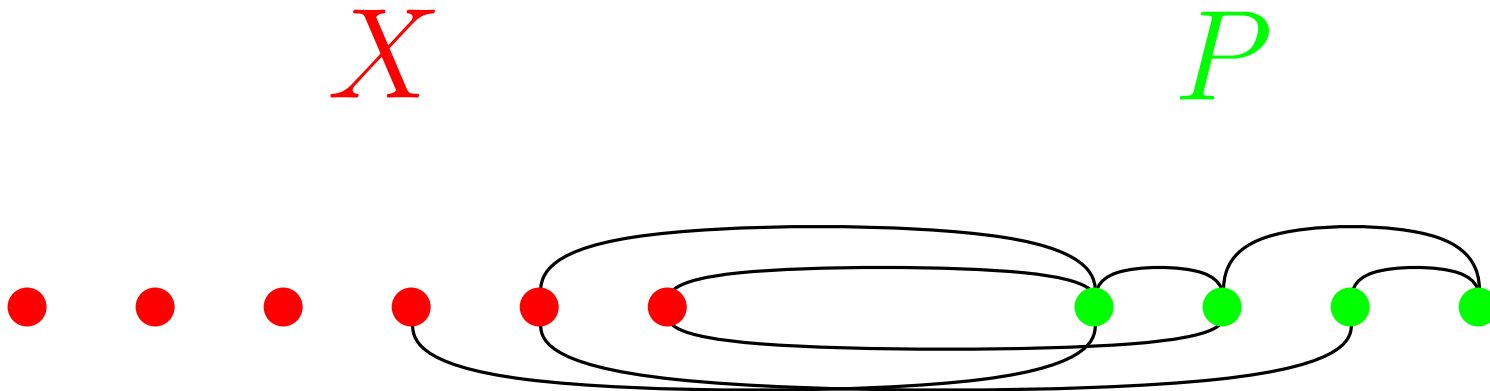
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$$O(|P|(|X| + |P|))$$

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6: BronKerboschPivot($P \cap \Gamma(v), R \cup \{v\}, X \cap \Gamma(v)$)

7: $P \leftarrow P \setminus \{v\}$

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9: **end for**

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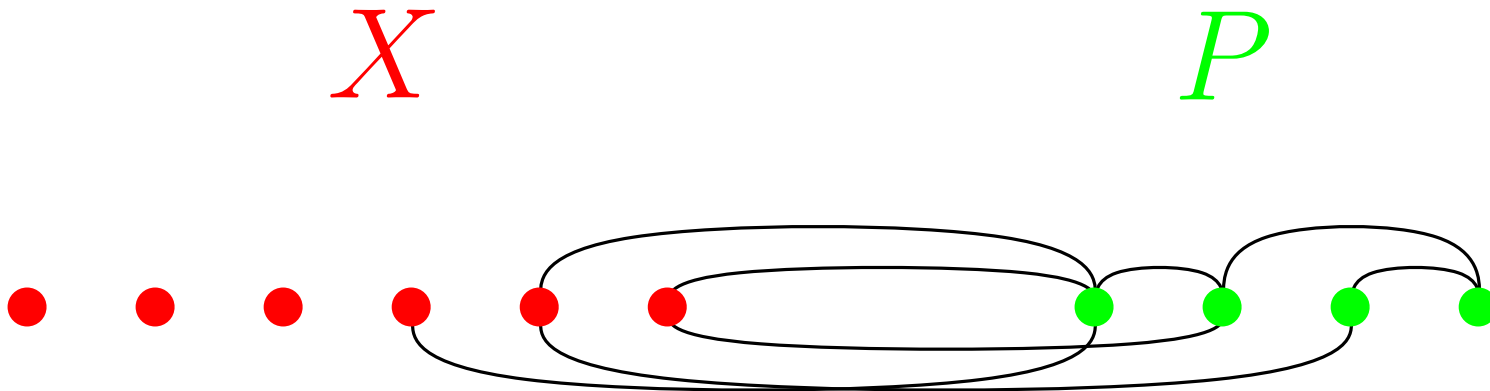
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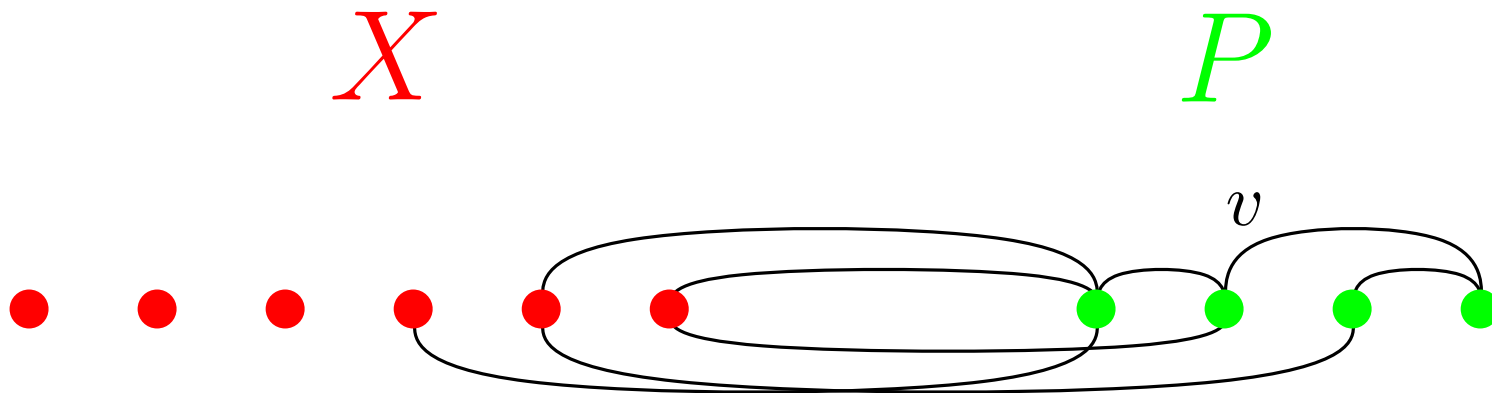
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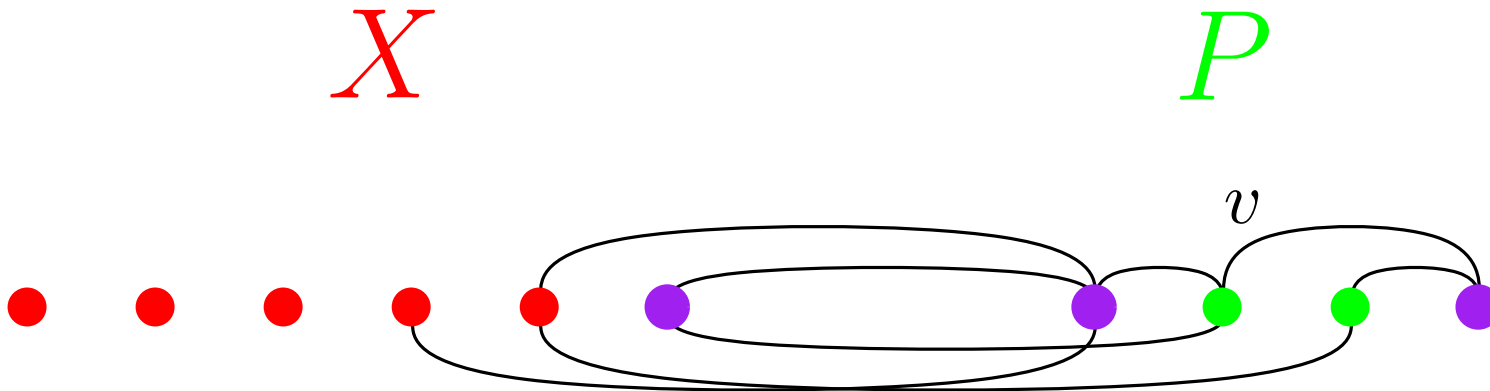
Find subgraph induced by v 's neighbors.



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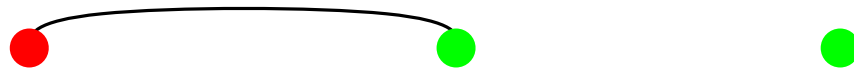
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$X \cap \Gamma(v)$

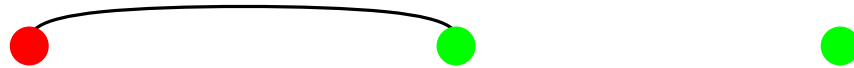
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$X \cap \Gamma(v)$

$P \cap \Gamma(v)$



$$O(|P|(|X| + |P|))$$

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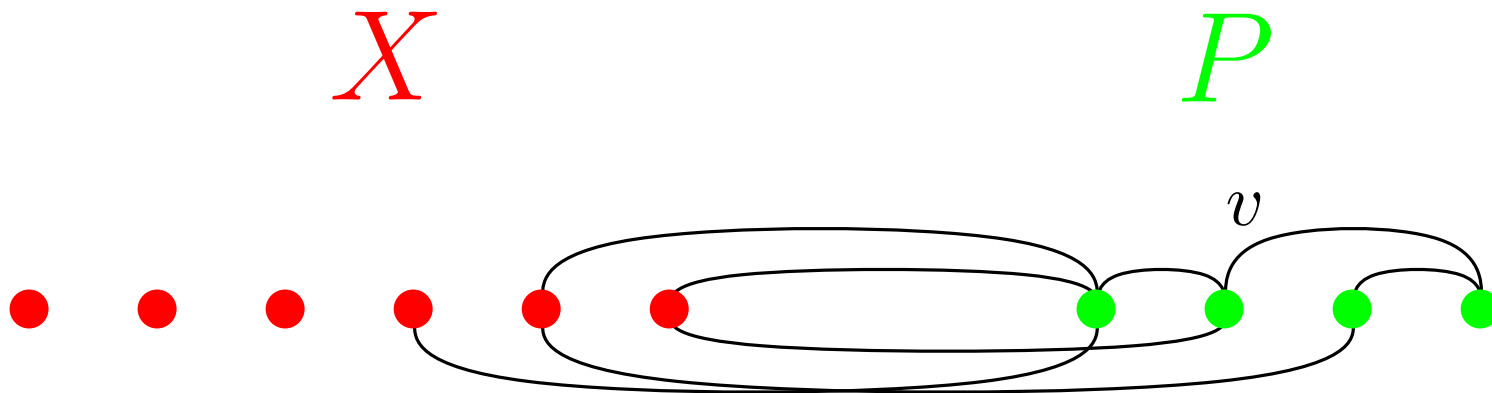
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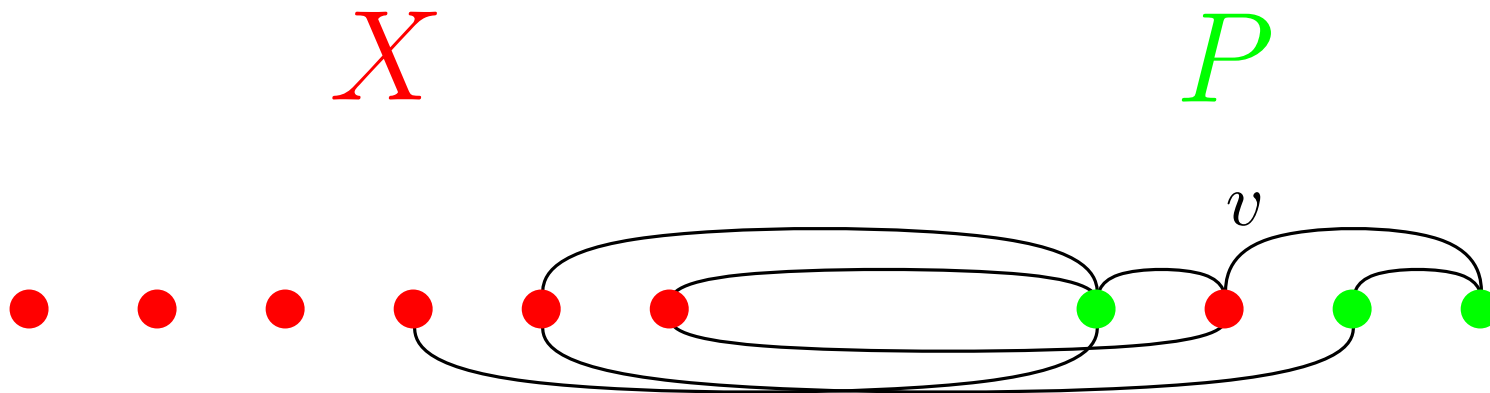
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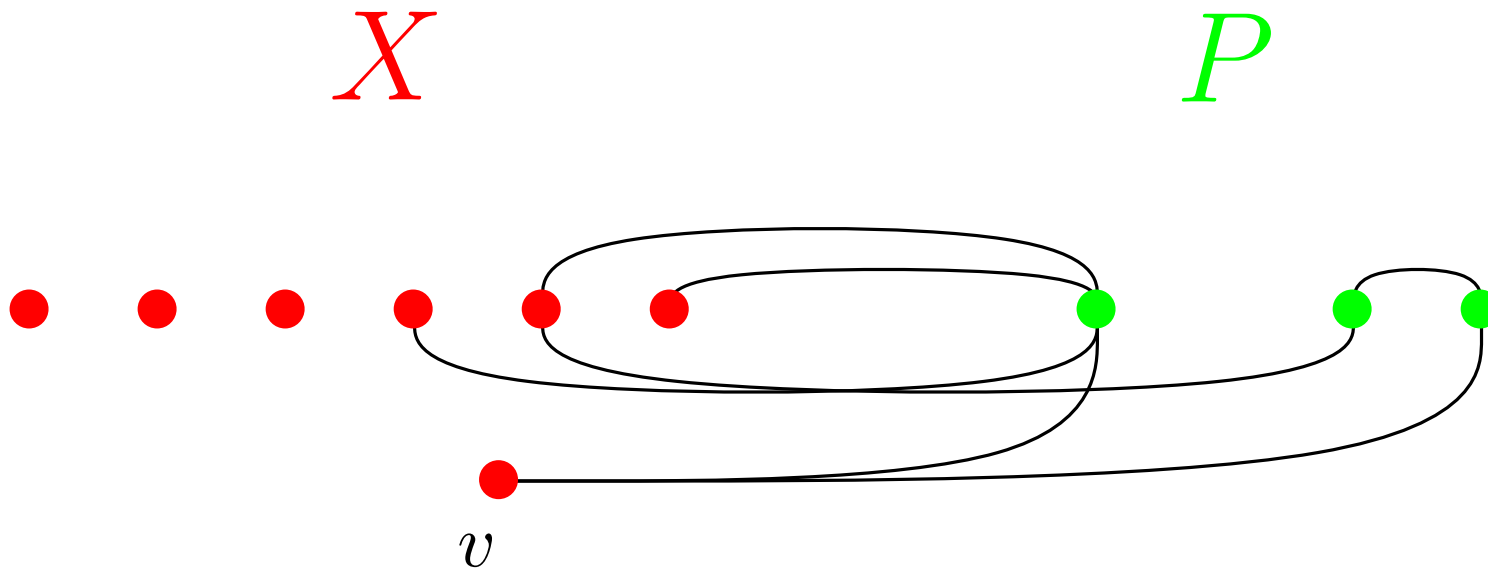
Remove v from P and add it to X .



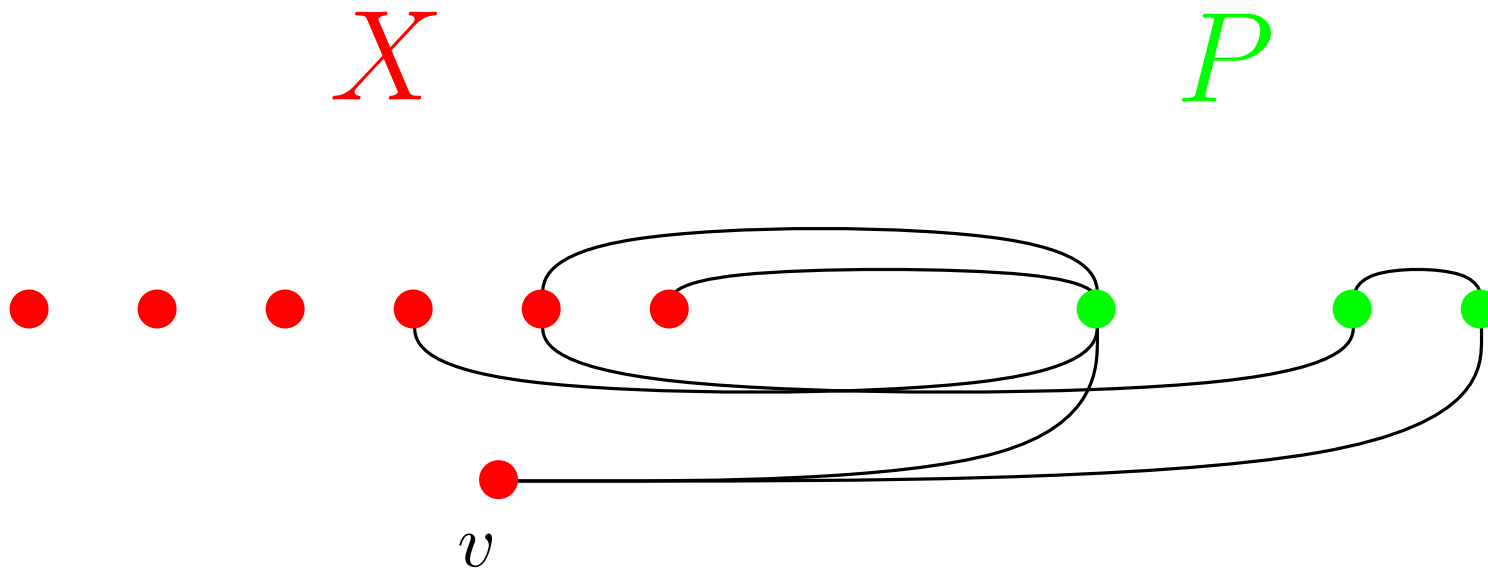
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9: **end for**

$$O(|P|^2(|X| + |P|))$$

$$\begin{aligned} T(n) &\leq \max_k \{kT(n-k)\} + O(n^2) \\ &= O(3^{n/3}) \end{aligned}$$

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$$\sum_{v \in V} O(d + |X_v|) 3^{d/3}$$

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$$= O(f(d)n) \quad \text{where } f(d) = d 3^{d/3}$$

Our running time: $O(dn3^{d/3})$

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Worst-case output size: $O(d(n - d)3^{d/3})$

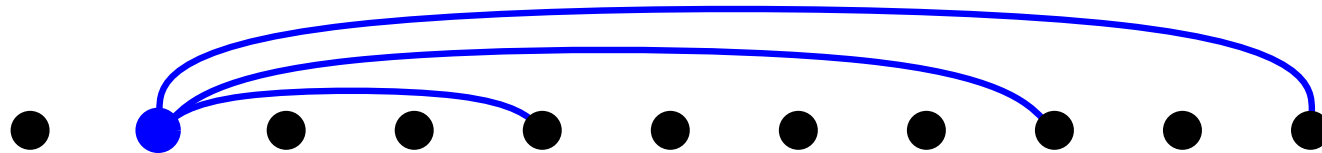
Our running time: $O(dn3^{d/3})$

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When $n - d = \Omega(n)$, our algorithm is worst-case optimal.

An upper bound

$\leq d$ later neighbors.



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at most $O(3^{d/3})$ maximal cliques

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at most $O(3^{d/3})$ maximal cliques

An upper bound

$n - d - 3$ vertices

$d + 3$ vertices



An upper bound

$$(n - d - 3)3^{d/3}$$

$n - d - 3$ vertices

$$3^{\frac{d+3}{3}}$$

$d + 3$ vertices



An upper bound

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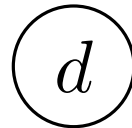
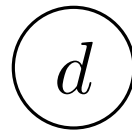
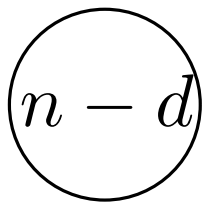


A lower bound

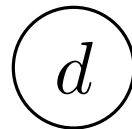
$$K_{n-d,3,3,3,\dots}$$

A lower bound

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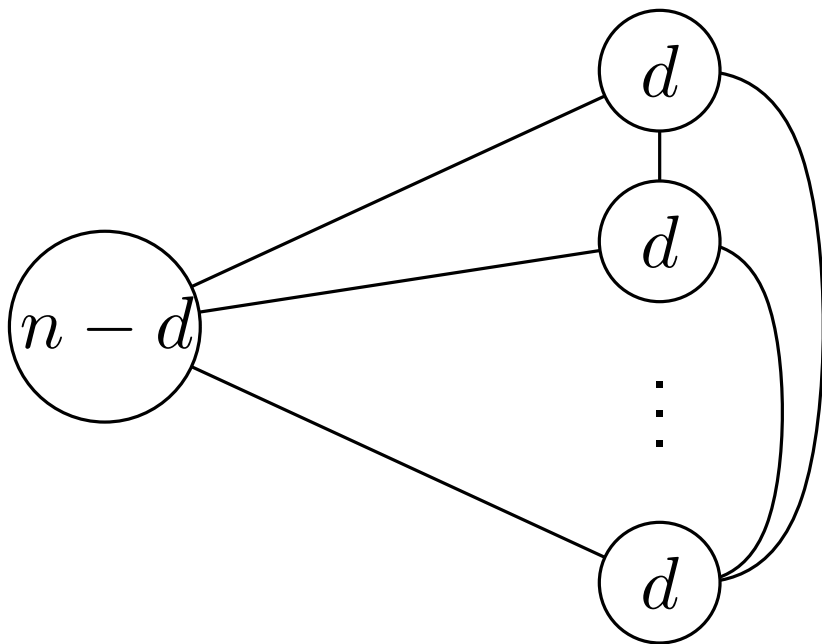


⋮



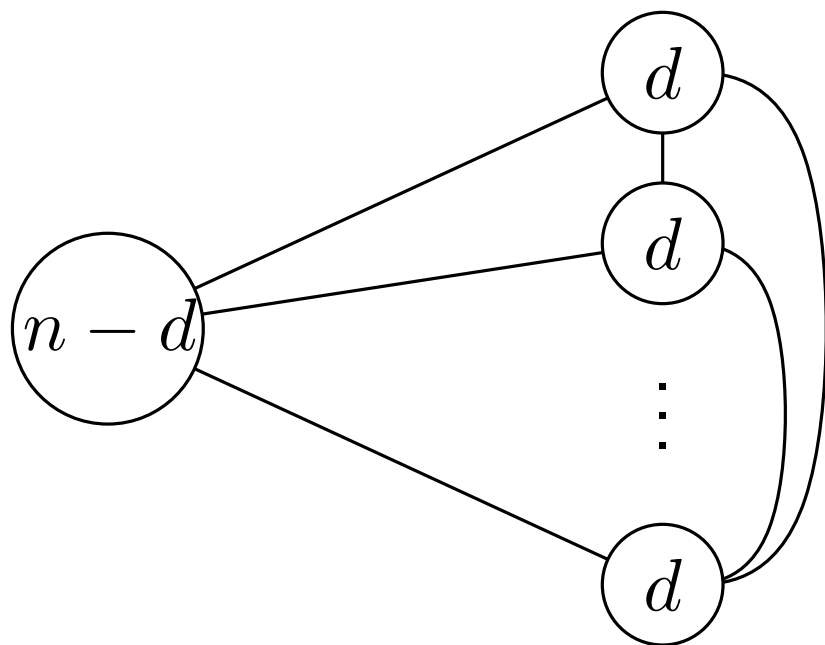
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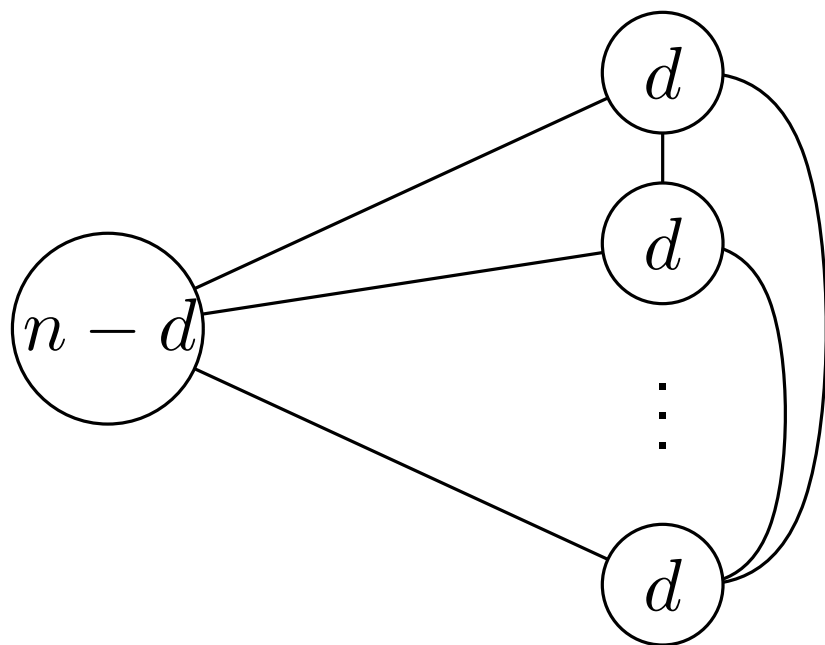
$$K_{n-d,3,3,3,\dots}$$



$(n-d)3^{d/3}$
maximal cliques

A lower bound

$$K_{n-d,3,3,3,\dots}$$



$(n - d)3^{d/3}$
maximal cliques

has degeneracy d
when $(n - d) \geq 3$

at most $(n - d)3^{d/3}$ maximal cliques

each clique is of size at most $d + 1$

$O(d(n - d)3^{d/3})$ worst-case output size.

The Bron–Kerbosch Algorithm

```
proc BronKerbosch( $P$ ,  $R$ ,  $X$ )  
1: if  $P \cup X = \emptyset$  then  
2:   report  $R$  as a maximal clique  
3: end if  
4: for each vertex  $v \in P$  do  
5:   BronKerbosch( $P \cap \Gamma(v)$ ,  $R \cup \{v\}$ ,  $X \cap \Gamma(v)$ )  
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Experiments

Linux Workstation: 3.00Ghz Pentium 4, 1GB RAM

Experimental results for UCI data sets

graph	d	BK	BK-pivot	BK-hybrid	BK-degen	Uno
karate	4	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec*
dolphins	4	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
power	5	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
polbooks	6	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
adjnoun	6	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
football	8	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
lesmis	9	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
celegens	9	< 1sec	< 1sec	< 1sec	< 1sec	seg. fault*
netscience	19	2.8sec	< 1sec	< 1sec	< 1sec	< 1sec
internet	25	19.4sec	10.3sec	< 1sec	< 1 sec	< 1sec*
condmat	29	> 3min	65sec	1.6sec	2.61sec	< 1sec
polblogs	36	> 3min	2sec	1.5sec	1.2sec	1.8sec
astro	56	> 3min	12.3sec	1.4sec	3.14sec	< 1sec

Experimental results for BIOGRID data sets (PPI Networks)

graph	d	BK	BK-pivot	BK-hybrid	BK-degen	Uno
mouse	6	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
worm	10	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
plant	12	< 1sec	< 1sec	< 1sec	< 1sec	< 1sec
fruitfly	12	< 1sec	2.2sec	< 1sec	< 1sec	< 1sec
human	12	1.4sec	3.3sec	< 1sec	< 1sec	< 1sec
fission-yeast	34	2.8sec	1.1sec	< 1sec	< 1sec	< 1sec
yeast	64	> 3min	81sec	44.3sec	20.5sec	121.1sec*

Experimental results for Pajek data sets

graph	d	BK	BK-pivot	BK-hybrid	BK-degen	Uno
foldoc	12	4.2sec	9sec	< 1sec	1sec	< 1sec
patents	24	> 5min	> 5min	4.3sec	5.3sec	2.2sec
eatRS	34	19.8sec	53sec	12.3sec	9.12sec	14.9sec
hep-th	37	> 5min	69.6sec	22.6sec	17.2sec	41.5sec*
days-all	73	> 5min	379.1sec	206.5sec	51.4sec	10min 25sec
ND-www	155	> 5min	> 5min	27.8sec	41.11sec	9.7sec*

Thank you!