

# Fast Algorithms for the Maximum Clique Problem on Massive Sparse Graphs

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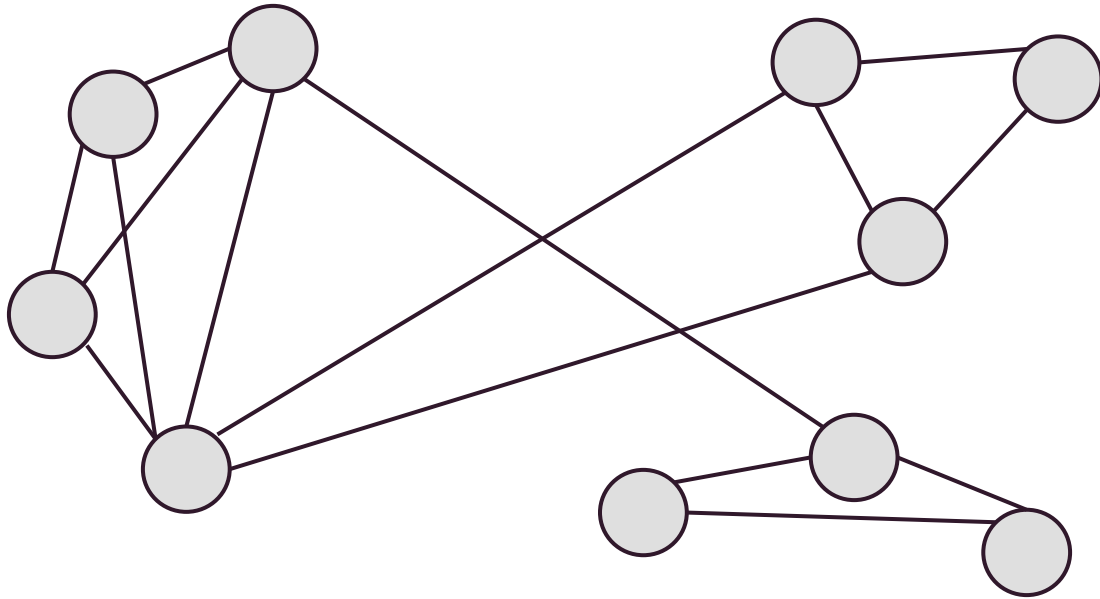
# Outline

- Introduction
- Motivation
- Existing Algorithms
- New Algorithm
- Performance Comparison
- Future Work

# Clique Problem

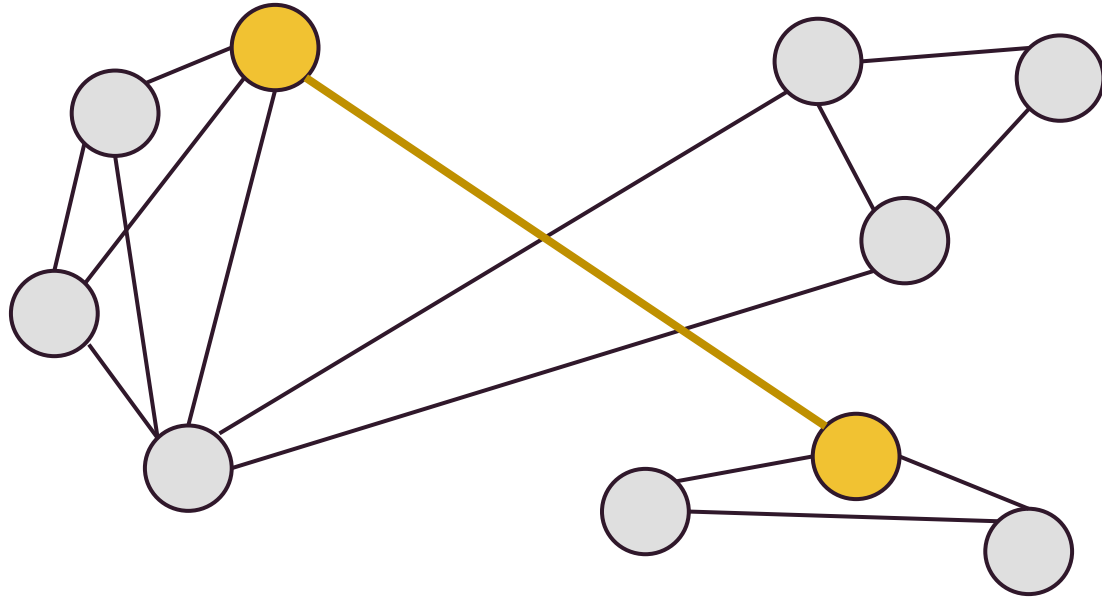
- $G = (V, E)$  is an undirected graph
- **Clique** - a subset of  $V$  such that every node is connected to every other in the subset
- **Maximal Clique** - a clique that cannot be enlarged by adding more vertices i.e. one that is not a subset of a larger clique
- **Maximum Clique** - the (maximal) clique with largest number of vertices

# Clique Problem



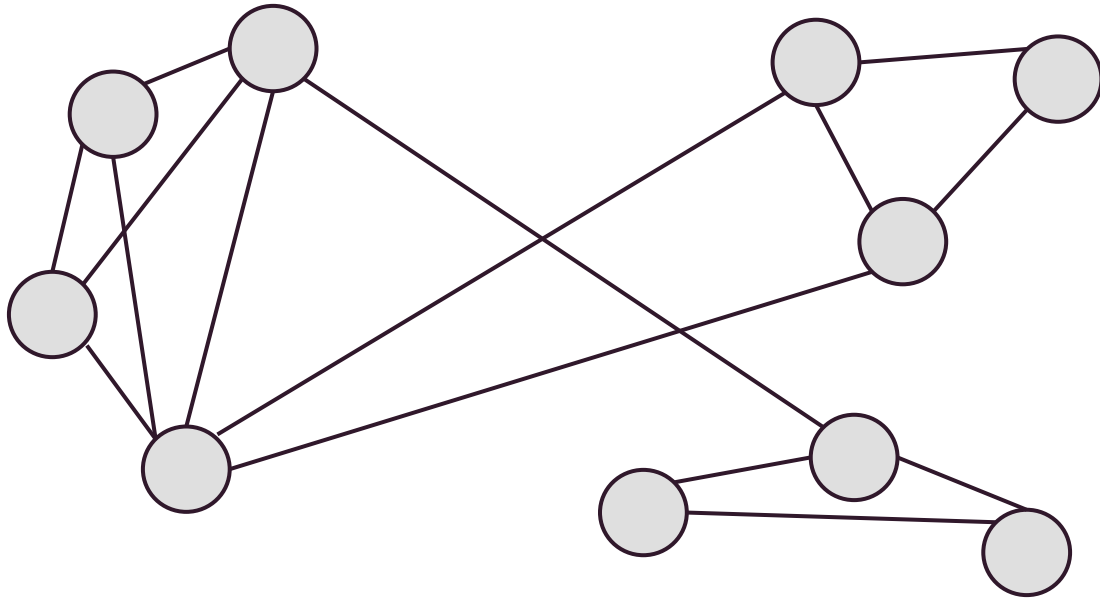
- Cliques of size 2 ?
  - every connected pair of vertices
- Maximal cliques of size 2 ?

# Clique Problem



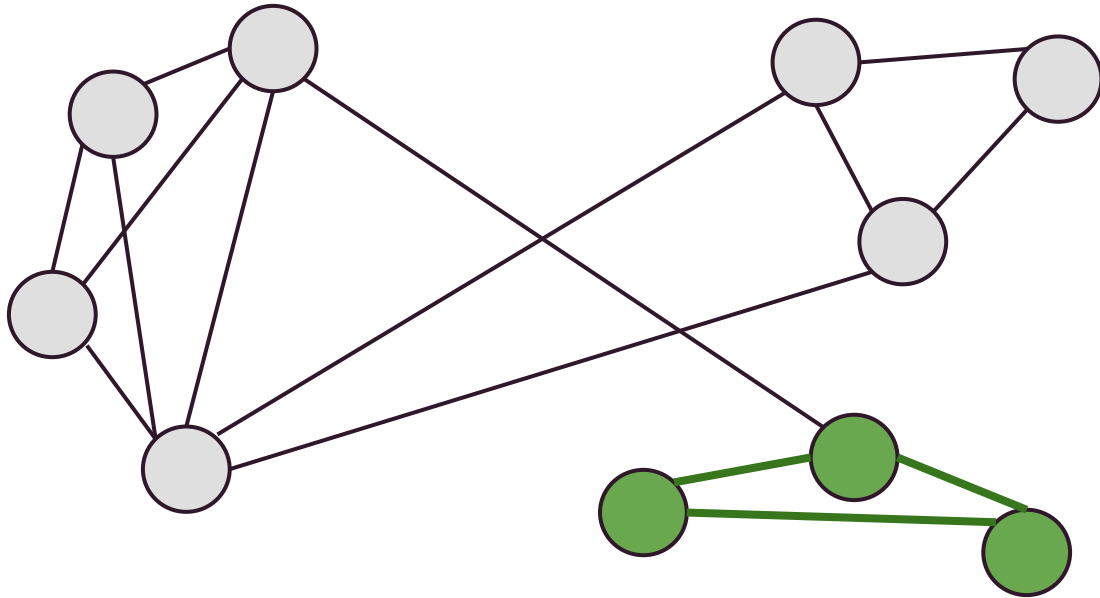
- Cliques of size 2 ?
  - every connected pair of vertices
- Maximal cliques of size 2 ?

# Clique Problem



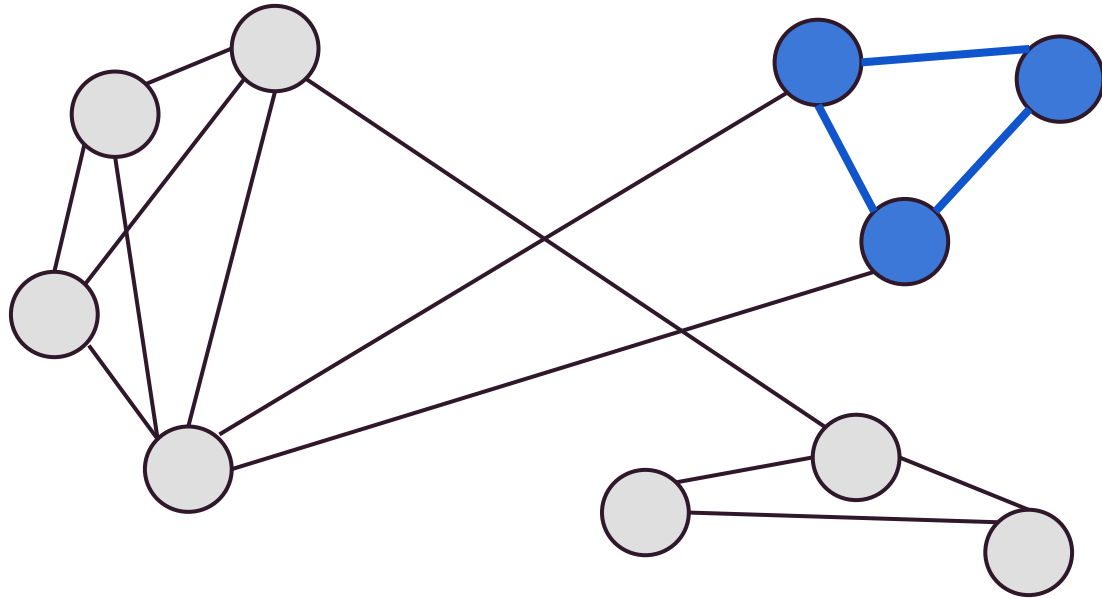
- Maximal cliques of size 3 ?

# Clique Problem



- Maximal cliques of size 3 ?

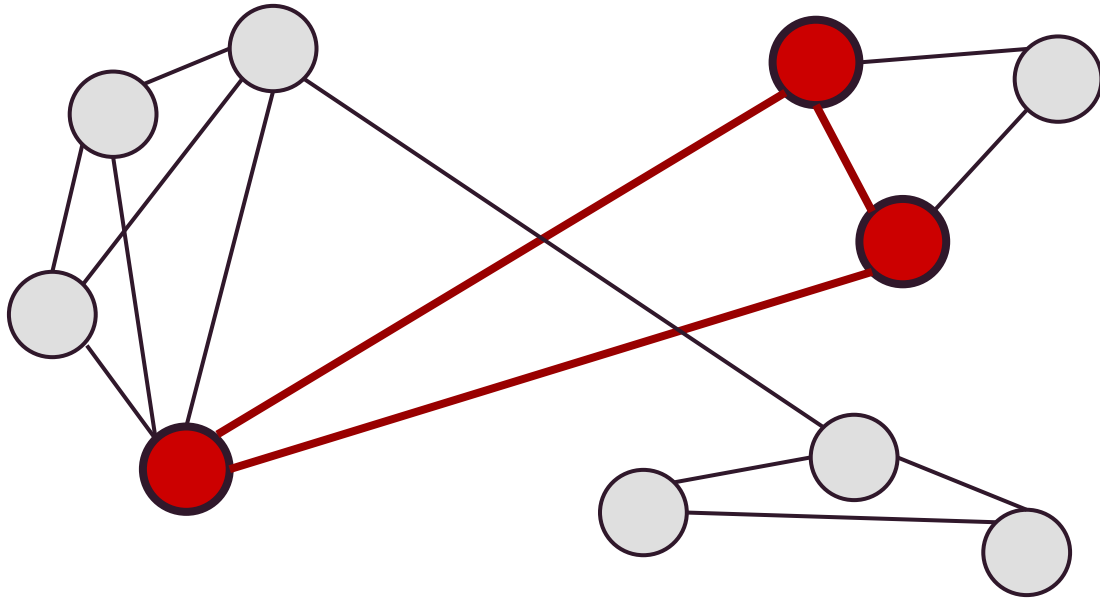
# Clique Problem



- Maximal cliques of size 3 ?

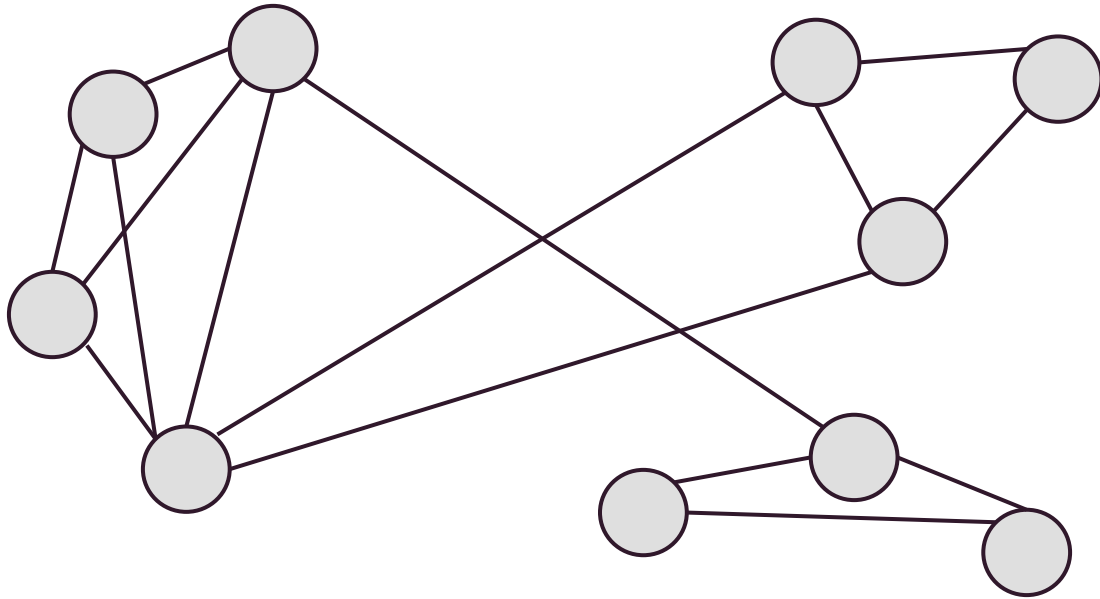


# Clique Problem



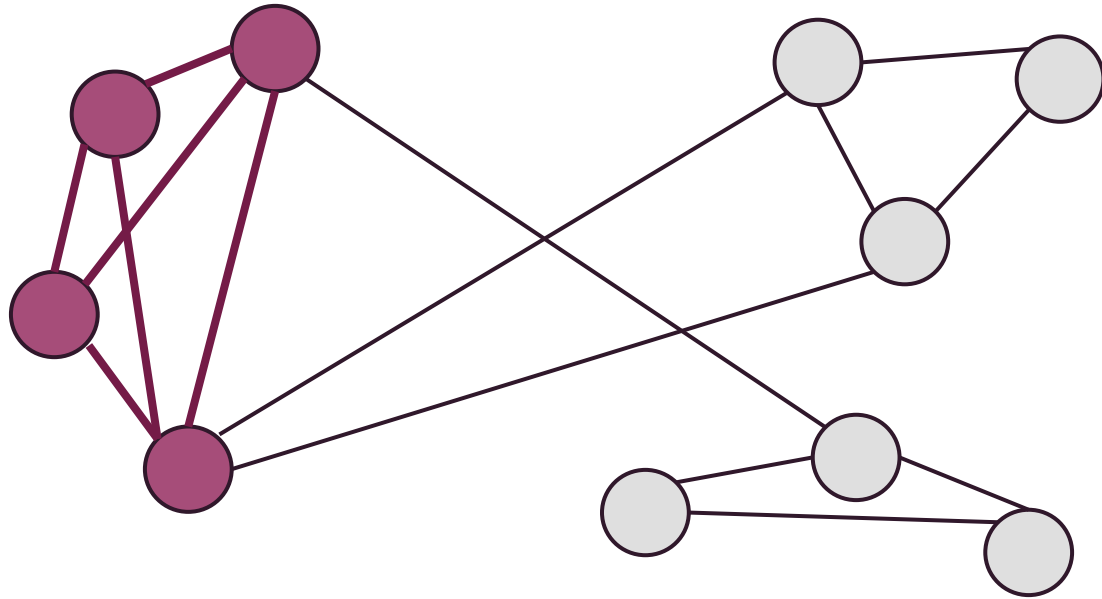
- Maximal cliques of size 3 ?

# Clique Problem



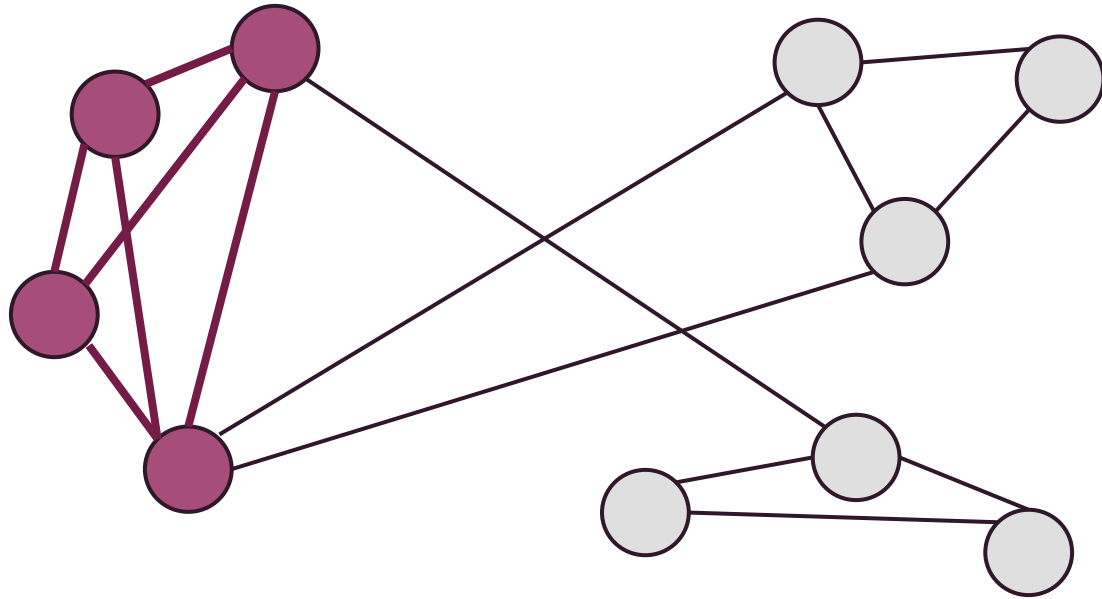
- Maximal cliques of size 4 ?

# Clique Problem



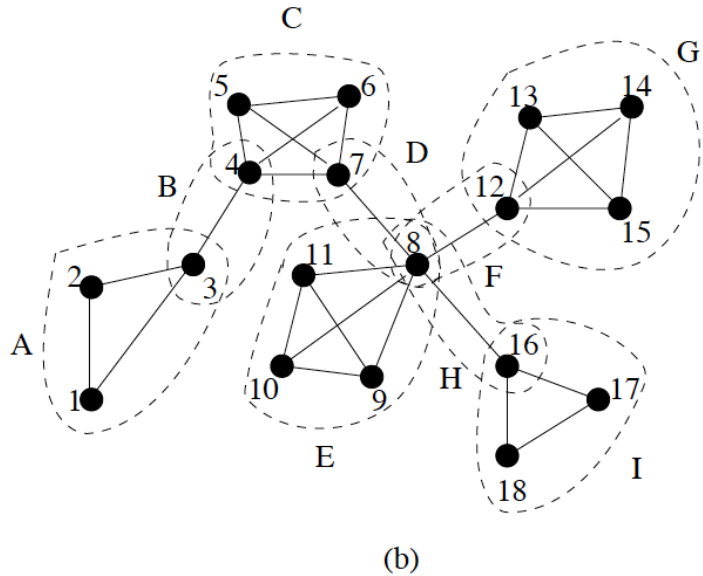
- Maximal cliques of size 4 ?

# Clique Problem



- Maximal cliques of size 4 ?
- Also the **maximum** clique

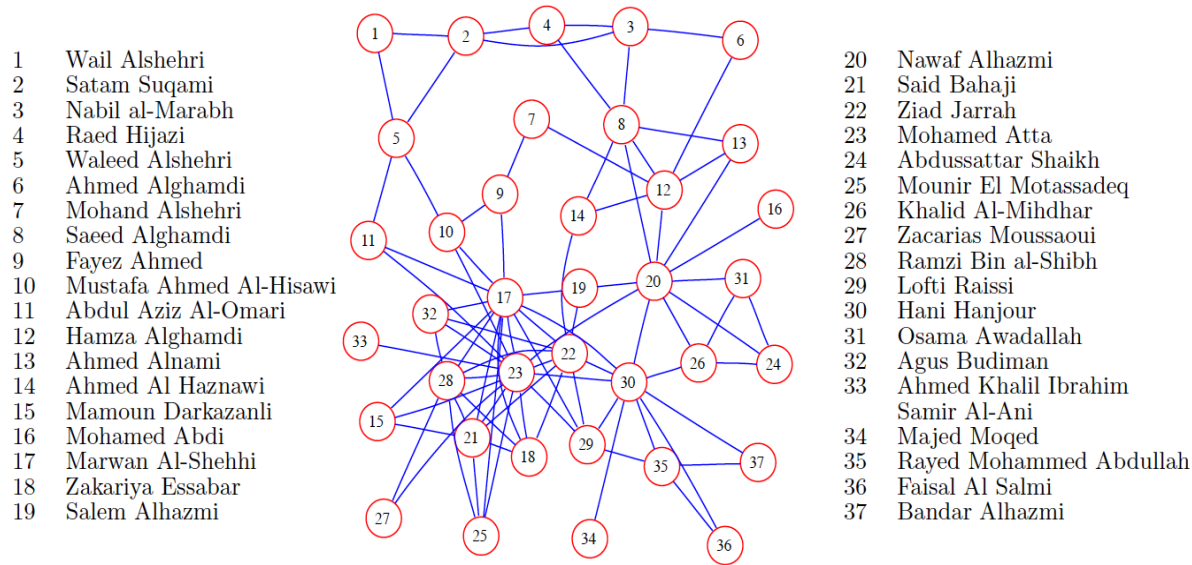
# Applications



- Clustering

Figure 1: An Example of Clusters

# Applications

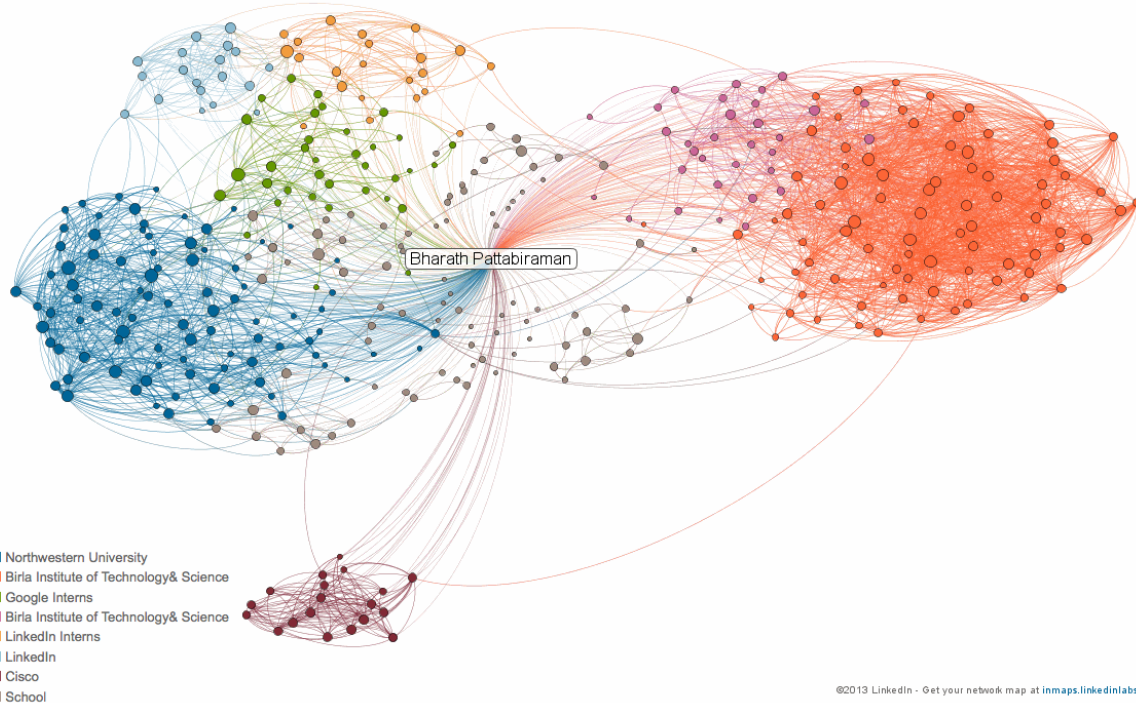


- Clustering
- Social Network Analysis

**Fig. 1** The network surrounding the tragic events of September 11, 2001.

# Applications

LinkedIn Maps Bharath Pattabiraman's Professional Network  
as of December 13, 2013



- Clustering
- Social Network Analysis

# Applications

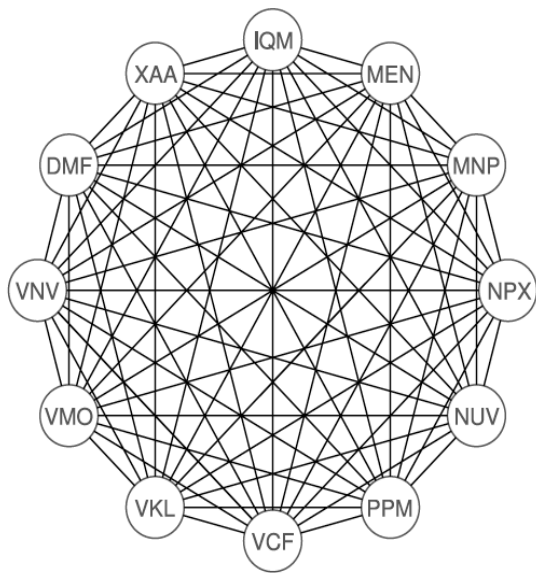
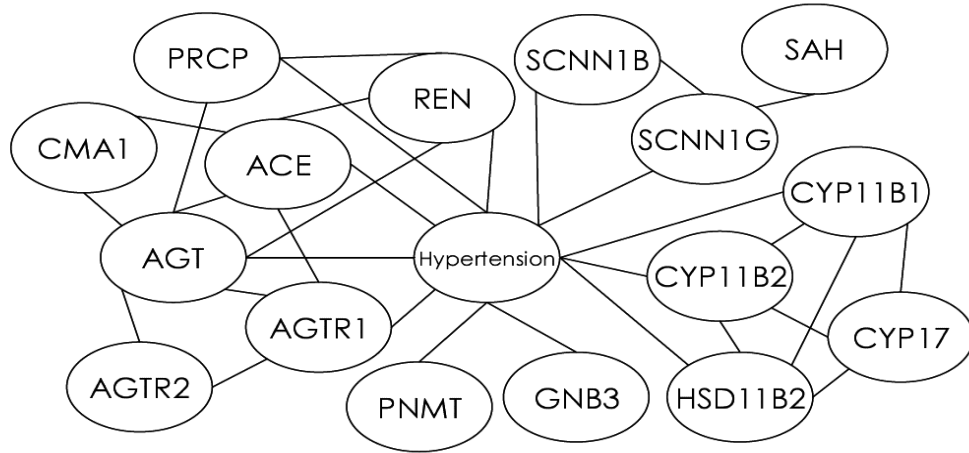


Fig. 1. The maximum closed clique in the stock market database with correlation coefficient threshold 0.90 and minimum relative support threshold 100%.

- Clustering
- Social Network Analysis
- Financial Network Analysis



# Applications



**Figure 1**  
**Example of a biomedical relational graph.** Hypertension and hypertension-related genes are represented by nodes, and the associations between them are represented by edges.

**Clique-based data mining for related genes in a biomedical database**

Tsutomu Matsunaga<sup>\*1</sup>, Chikara Yonemori<sup>1</sup>, Etsuji Tomita<sup>2,3</sup> and Masaaki Muramatsu<sup>4,5</sup>

- Clustering
- Social Network Analysis
- Financial Network Analysis
- Biomedical data analysis and Bioinformatics

# Algorithms

- Maximum clique problem
  - NP-complete
  - Still infeasible for large instances
  - Practical tricks to obtain acceptable runtimes
  - Heuristic approaches

# Related Work

- Branch and bound algorithms
  - enumerate all candidate solutions, discard fruitless candidates (a.k.a **pruning**) using estimated upper bounds of the max clique size
  - Carraghan and Pardalos 1990
  - Ostergard 2002
  - Tomita and Seki 2003 - MCQ (vertex coloring as upper bound)
  - Konc and Janezic 2007 - MCQD (improved MCQ)

# Related Work

- Base Algorithm of most published work
  - Carraghan and Pardalos 1990
  - Branch and Bound algorithm
  - Variant of depth first search on each vertex
  - Store the size of largest clique encountered, and use for pruning fruitless candidates

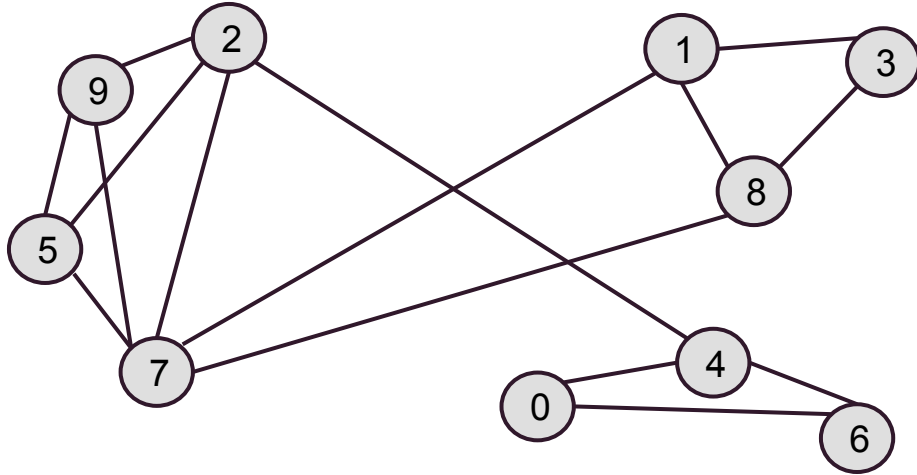
# Pardalos Algorithm

```
function clique(U, size)
  if  $|U| = 0$  then
    if  $size > max$  then
       $max := size$ 
      New record; save it.
    end if
    return
  end if
  while  $U \neq \emptyset$  do
     $i := \min\{j \mid v_j \in U\}$ 
     $U := U \setminus \{v_i\}$ 
    clique( $U \cap N(v_i)$ ,  $size + 1$ )
  end while
  return
function old
   $max := 0$ 
  clique( $V$ , 0)
  return
```

- pick a vertex from the candidate list
- add it to current clique
- updated candidate list = intersection of current candidate list and neighbors of added vertex
- recurse until all cliques are examined

# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 0  
Max clique set =  $\{\}$

Current clique size = 0  
Current clique set =  $\{\}$   
Current Node = ---  
Current Neighbors = ---  
Candidate set =  $\{0, 1, \dots, 9\}$

Recursion Tree



Current Step:

---

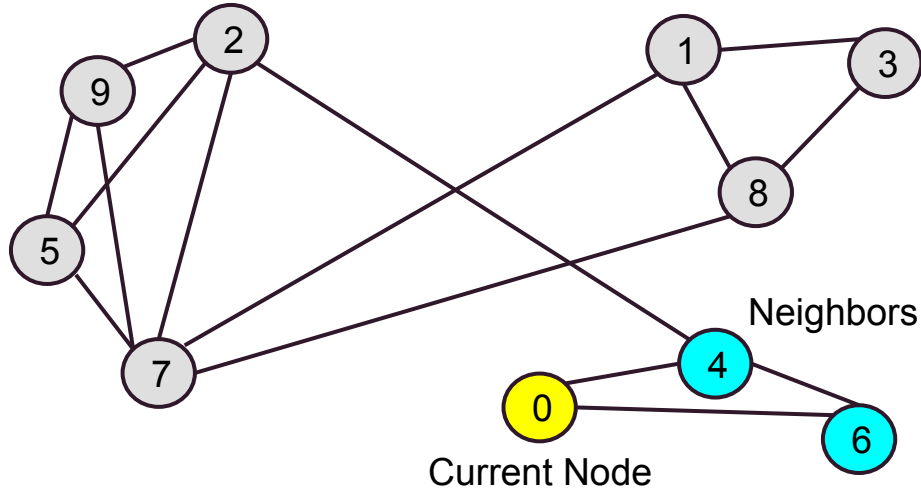
Next Step:

Pick Current Node  
Update Current Neighbors

Current Clique

# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 0  
Max clique set =  $\{\}$

Current clique size = 0  
Current clique set =  $\{\}$   
Current Node = **Node 0**  
Current Neighbors =  $\{4, 6\}$   
Candidate set =  $\{0, 1, \dots, 9\}$

Recursion Tree



Current Step:

Pick Current Node  
Update Current Neighbors

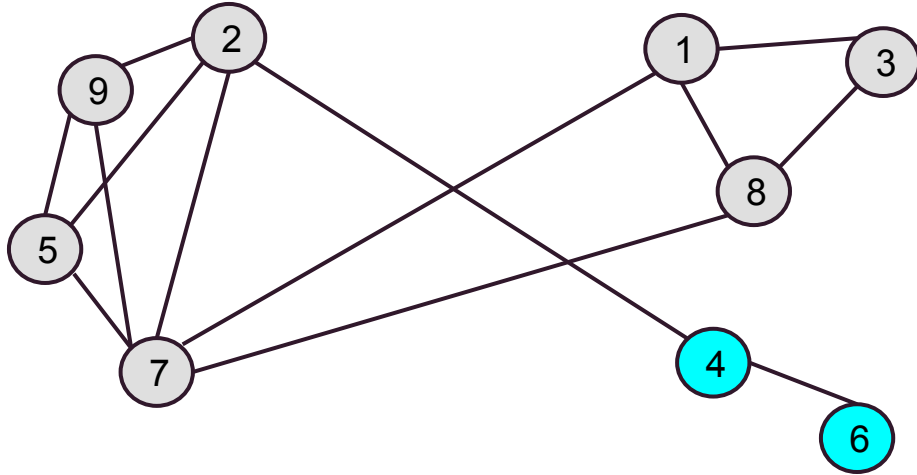
Next Step:

Update clique set and size  
Update Candidate set

Current Clique

# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 0  
Max clique set =  $\{\}$

Current clique size = 1  
Current clique set =  $\{0\}$   
Current Node = ---  
Current Neighbors = ---  
Candidate set =  $\{4,6\}$

Recursion Tree



Current Step:

Update clique set and size  
Update Candidate set

Next Step:

Pick Current Node  
Update Current Neighbors

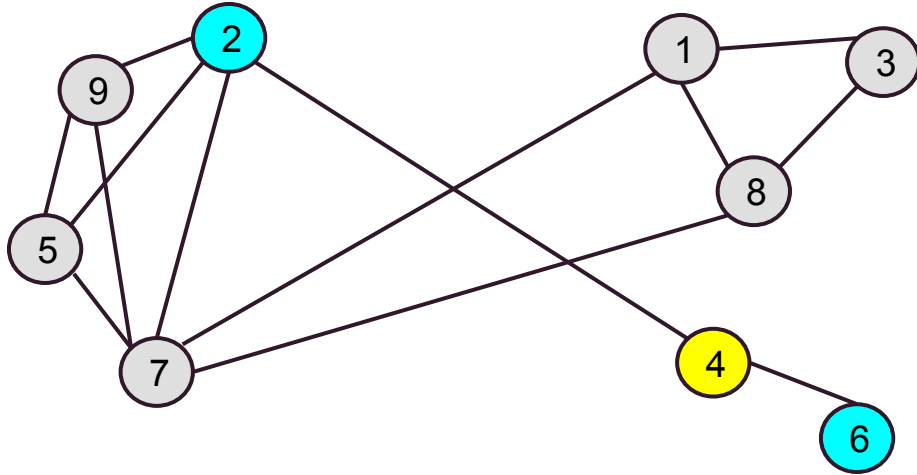
Current Clique

0



# Pardalos Algorithm

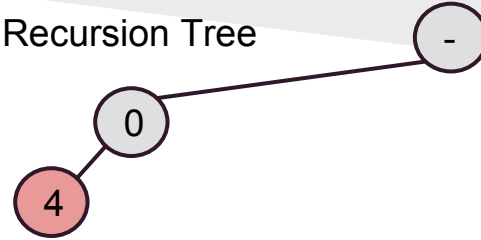
$|V| = 10, |E| = 15$



Max clique size = 0  
Max clique set =  $\{\}$

Current clique size = 1  
Current clique set =  $\{0\}$   
Current Node = **Node 4**  
Current Neighbors =  $\{2,6\}$   
Candidate set =  $\{4,6\}$

Recursion Tree



Current Step:

Pick Current Node  
Update Current Neighbors

Next Step:

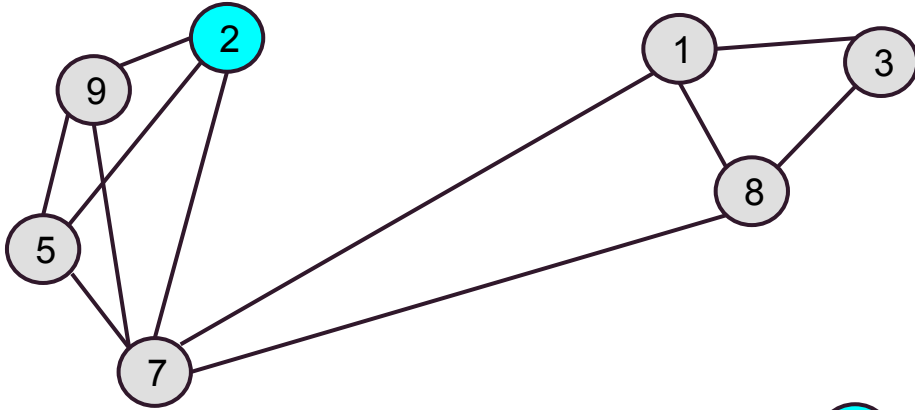
Update clique set and size  
Update Candidate set

Current Clique

0

# Pardalos Algorithm

$|V| = 10, |E| = 15$

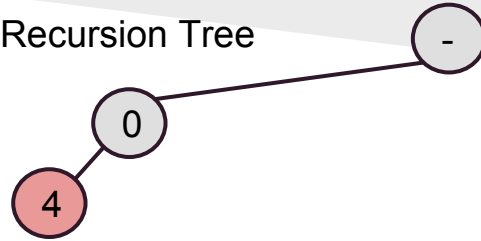


6

Max clique size = 0  
Max clique set = {}

Current clique size = 2  
Current clique set = {0,4}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {6}

Recursion Tree



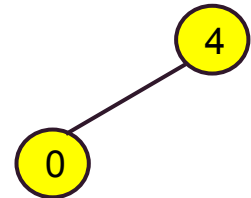
Current Step:

Update clique set and size  
Update Candidate set

Next Step:

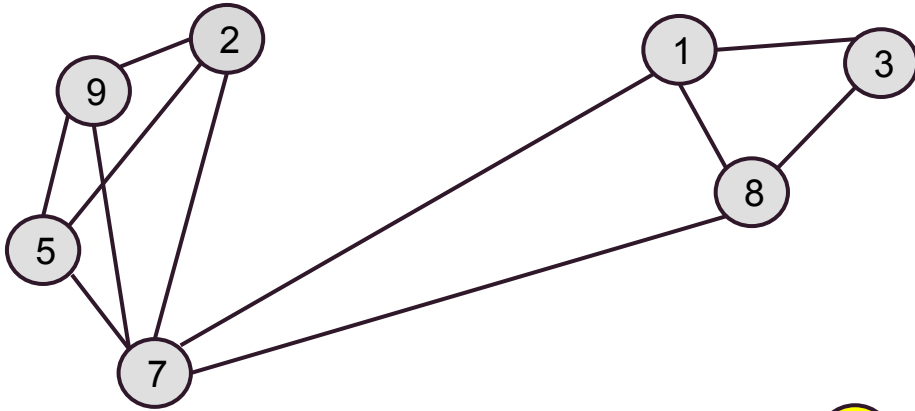
Pick Current Node  
Update Current Neighbors

Current Clique



# Pardalos Algorithm

$|V| = 10, |E| = 15$

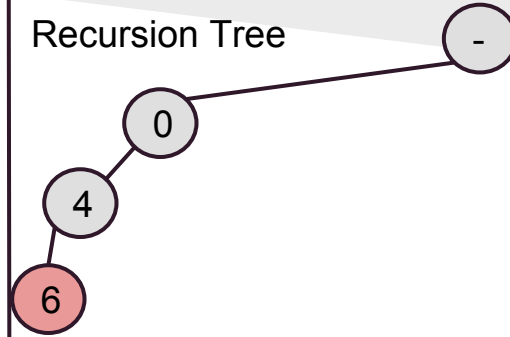


6

Current clique size = 2  
Current clique set = {0,4}  
Current Node = **Node 6**  
Current Neighbors = {}  
Candidate set = {6}

Max clique size = 0  
Max clique set = {}

Recursion Tree



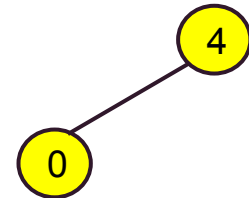
Current Step:

Pick Current Node  
Update Current Neighbors

Next Step:

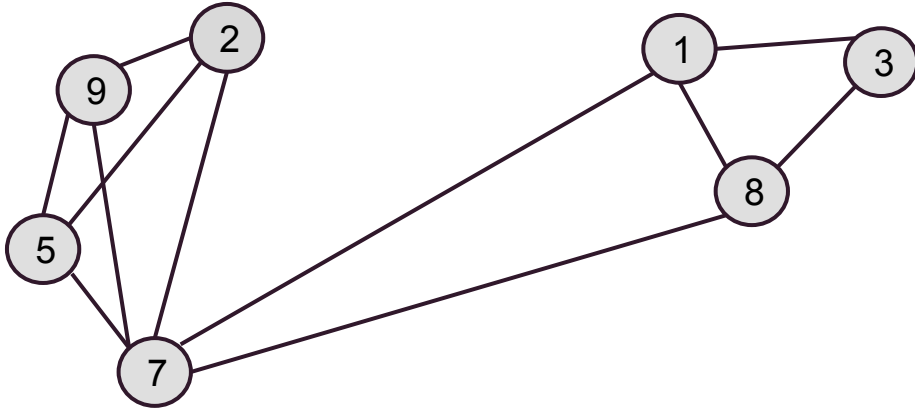
Update clique set and size  
Update Candidate set

Current Clique

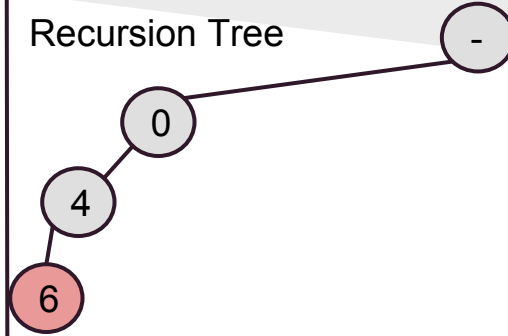


# Pardalos Algorithm

$|V| = 10, |E| = 15$



Recursion Tree



Max clique size = 0  
Max clique set = {}

Current clique size = 3  
Current clique set = {0,4,6}  
Current Node = ---  
Current Neighbors = {}  
Candidate set = {}

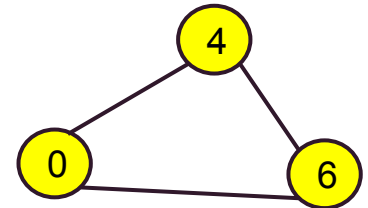
Current Step:

Update clique set and size  
Update Candidate set

Next Step:

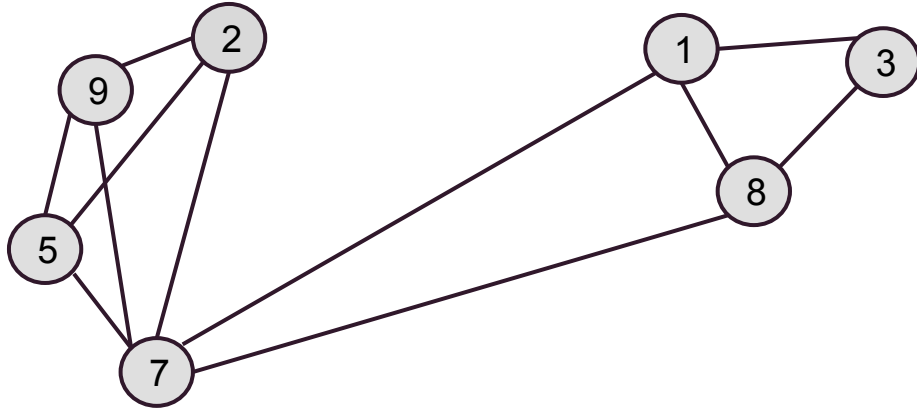
Update Max Clique

Current Clique



# Pardalos Algorithm

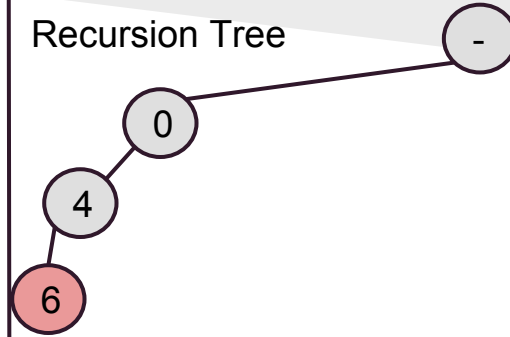
$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

Current clique size = 3  
Current clique set = {0,4,6}  
Current Node = ---  
Current Neighbors = {}  
Candidate set = {}

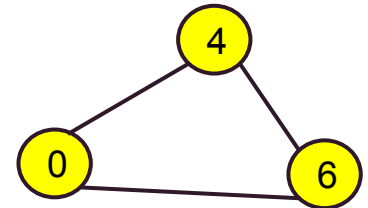
Recursion Tree



Current Step:  
Update Max Clique

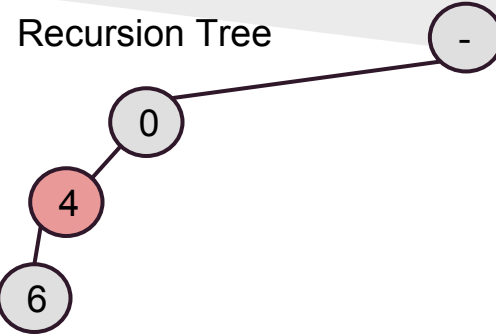
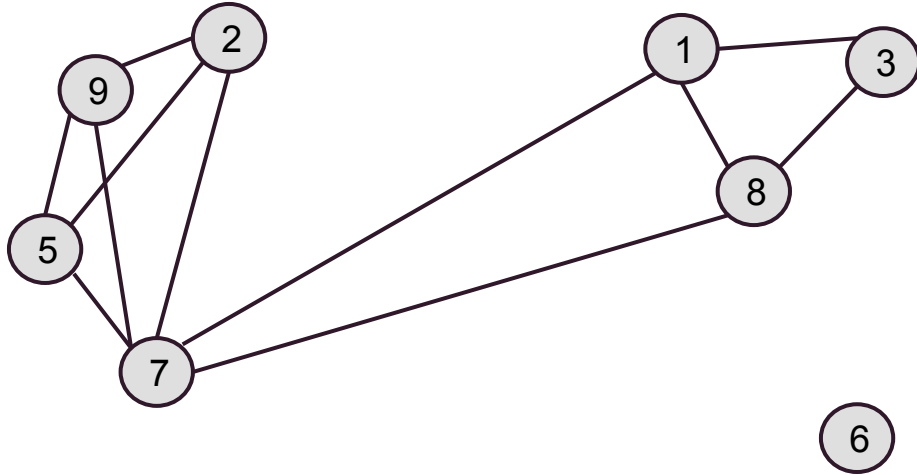
Next Step:  
---

Current Clique



# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

Current clique size = 0  
Current clique set = {}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {6}

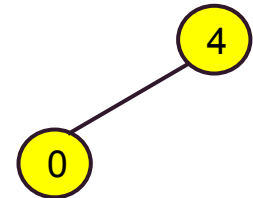
Current Step:

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Next Step:

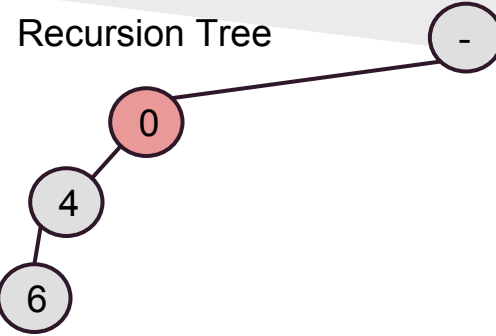
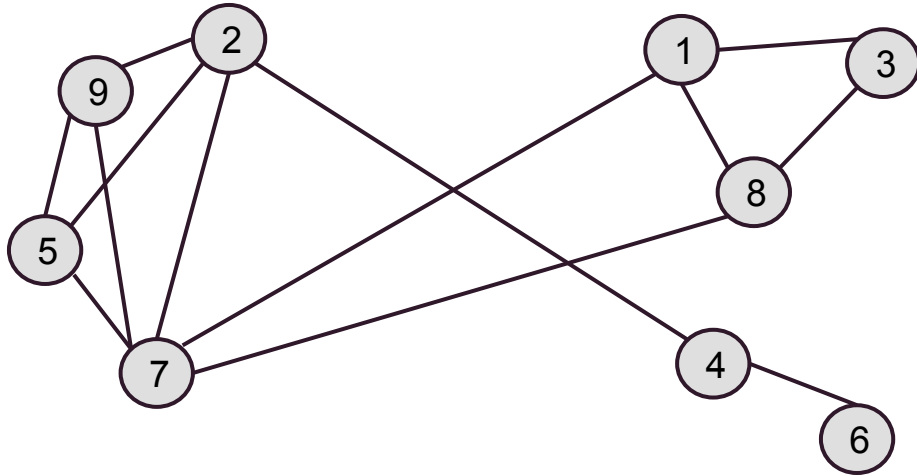
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Current Clique



# Pardalos Algorithm

$|V| = 10, |E| = 15$



Current clique size = 0  
 Current clique set =  $\{\}$   
 Current Node = ---  
 Current Neighbors = ---  
 Candidate set =  $\{4,6\}$

Current Step:

---

Next Step:

---

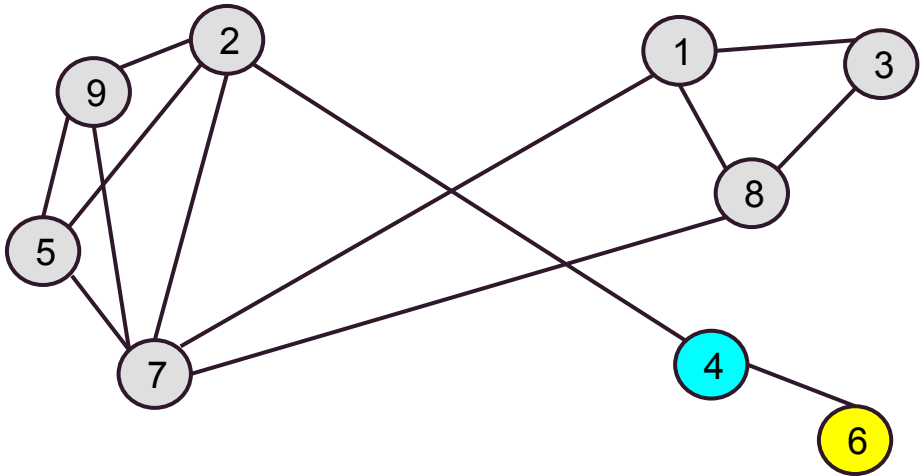
Current Clique

0

Max clique size = 3  
 Max clique set =  $\{0,4,6\}$

# Pardalos Algorithm

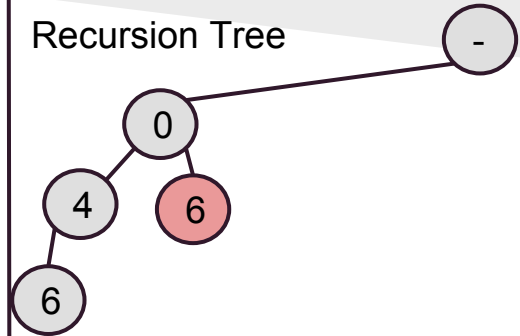
$|V| = 10, |E| = 15$



Max clique size = 3  
 Max clique set = {0,4,6}

Current clique size = 1  
 Current clique set = {0}  
 Current Node = **Node 6**  
 Current Neighbors = {4}  
 Candidate set = {4,6}

Recursion Tree



Current Step:

Pick Current Node  
 Update Current Neighbors

Next Step:

Update clique set and size  
 Update Candidate set

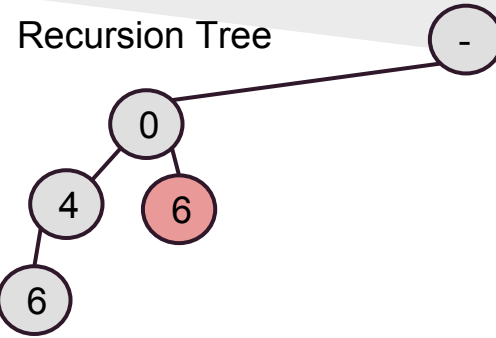
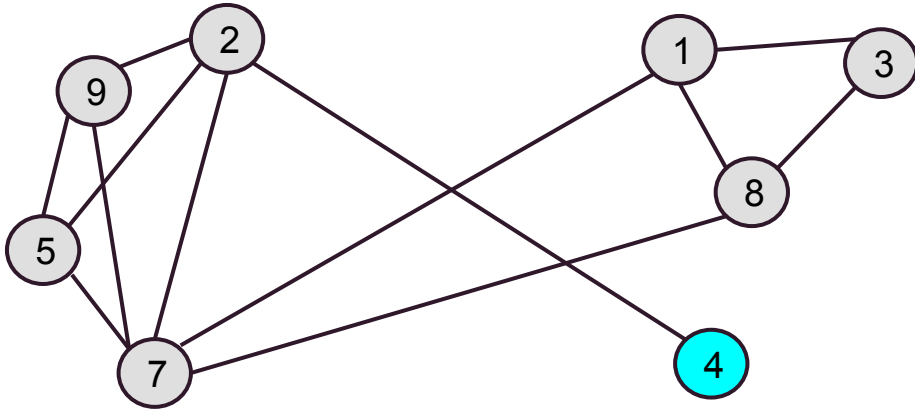
Current Clique





# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

Current clique size = 2  
Current clique set = {0,6}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {4}

Current Step:

Update clique set and size  
Update Candidate set

Next Step:

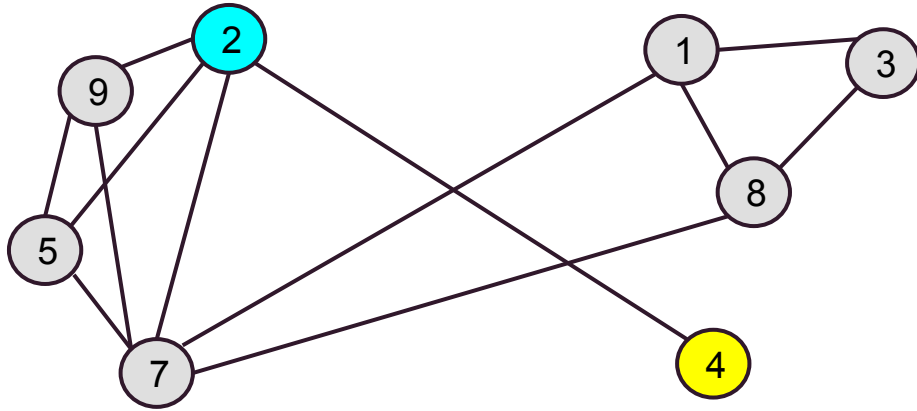
Pick Current Node  
Update Current Neighbors

Current Clique



# Pardalos Algorithm

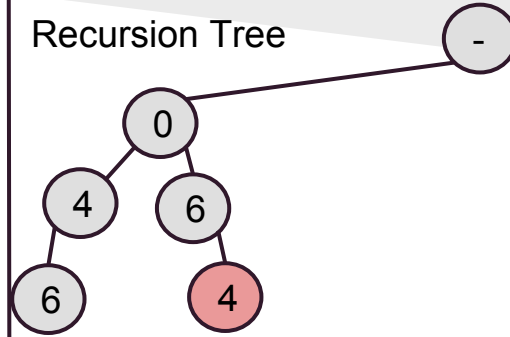
$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

Current clique size = 2  
Current clique set = {0,6}  
Current Node = **Node 4**  
Current Neighbors = {2}  
Candidate set = {4}

Recursion Tree



Current Step:

Pick Current Node  
Update Current Neighbors

Next Step:

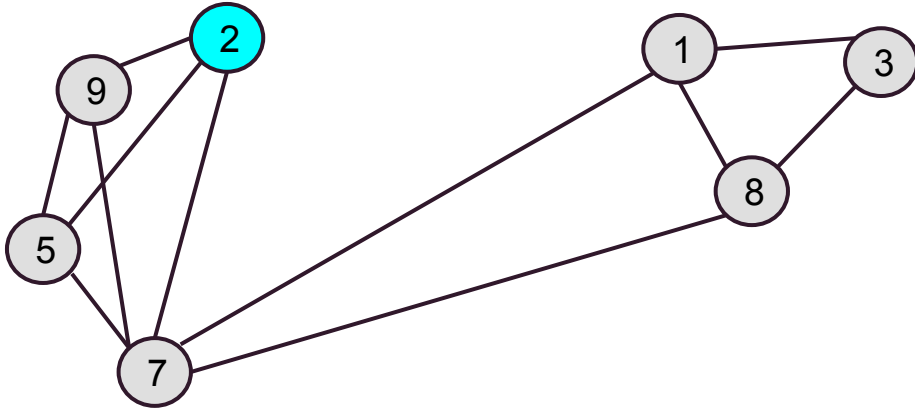
Update clique set and size  
Update Candidate set

Current Clique



# Pardalos Algorithm

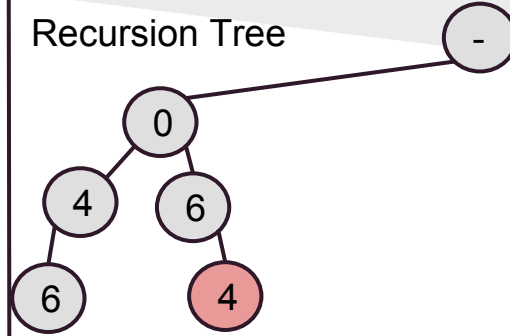
$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

Current clique size = 3  
Current clique set = {0,6,4}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {}

Recursion Tree



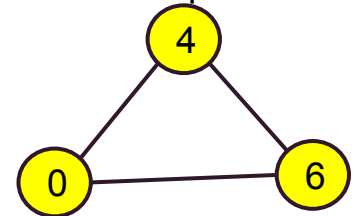
Current Step:

Pick Current Node  
Update Current Neighbors

Next Step:

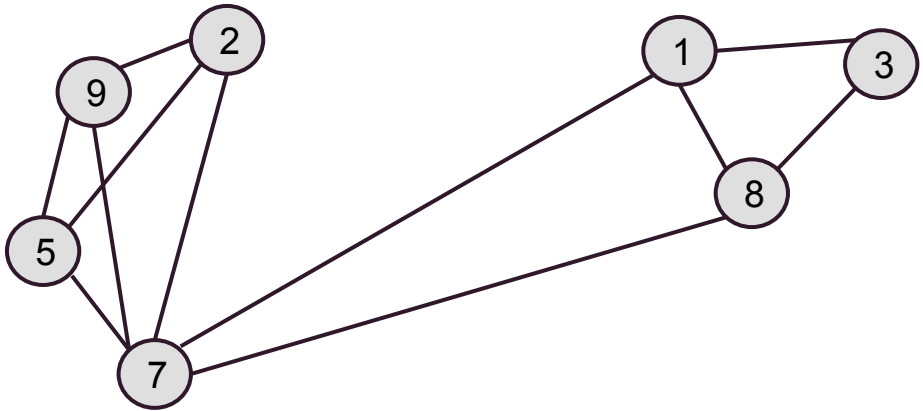
Update Max Clique

Current Clique



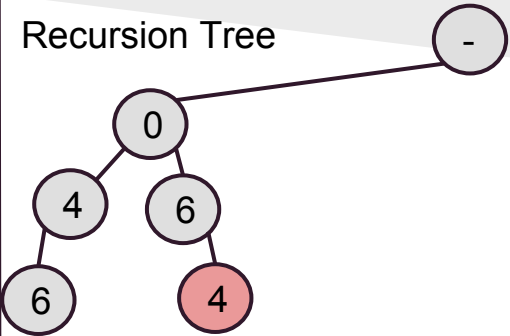
# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 3  
Max clique set = {0,4,6}

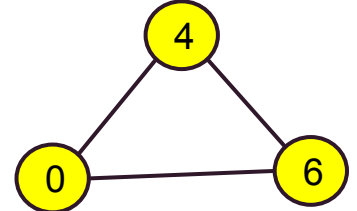
Current clique size = 3  
Current clique set = {0,6,4}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {}



Current Step:  
Update Max Clique

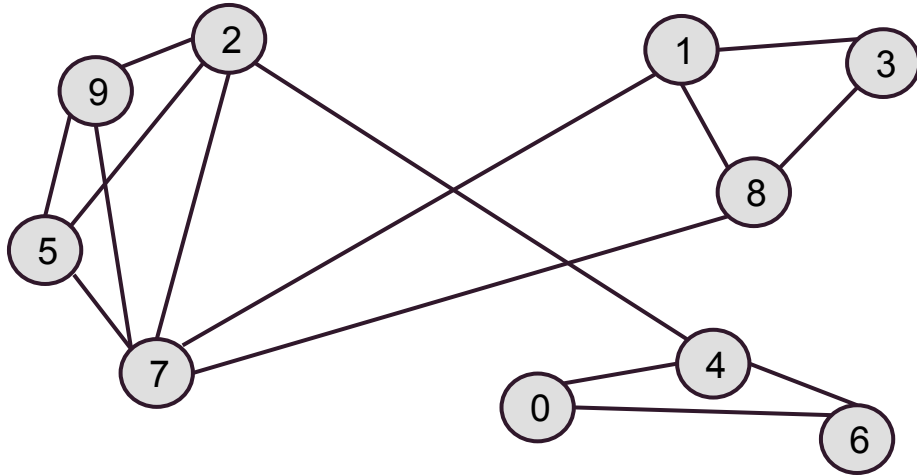
Next Step:  
---

Current Clique



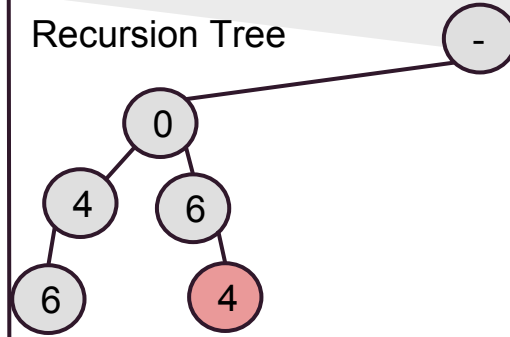
# Pardalos Algorithm

$|V| = 10, |E| = 15$



Skipping...

Recursion Tree



Current Step:

---

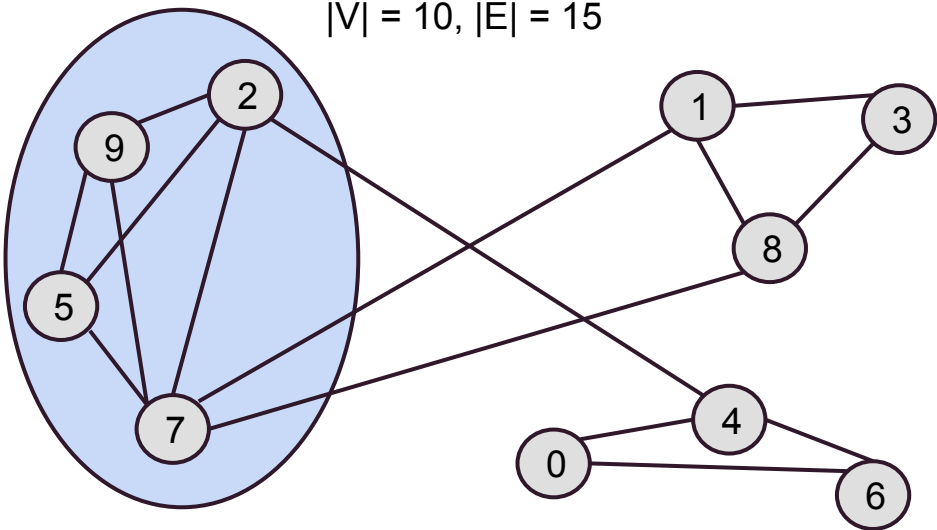
Next Step:

---

Current Clique

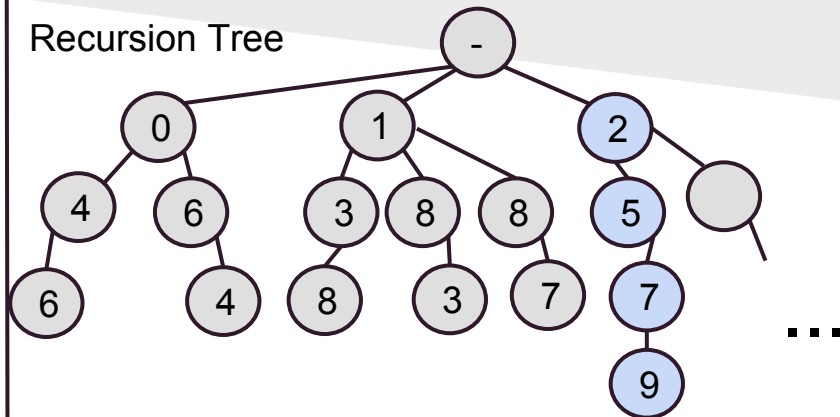
# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 4  
 Max clique set = {2,5,7,9}

Recursion Tree



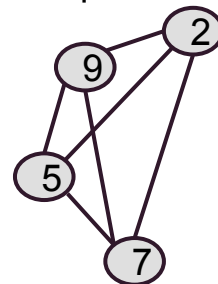
Current Step:

---

Next Step:

---

Current Clique



# Modified Pardalos Algorithm

**procedure** MAXCLIQUE( $G = (V, E), lb$ )

$max \leftarrow lb$

**for**  $i : 1$  to  $n$  **do**

$U \leftarrow \emptyset$

**for each**  $v_j \in N(v_i)$  **do**

$U \leftarrow U \cup \{v_j\}$

CLIQUE( $G, U, 1$ )

**procedure** CLIQUE( $G = (V, E), U, size$ )

**if**  $U = \emptyset$  **then**

**if**  $size > max$  **then**

$max \leftarrow size$

**return**

**while**  $|U| > 0$  **do**

Select any vertex  $u$  from  $U$

$U \leftarrow U \setminus \{u\}$

CLIQUE( $G, U \cap N'(u), size + 1$ )

FindMaximumClique( $G$ )

$max\_clq = lower\_bound;$

For each vertex  $v_i$

Remove  $v_i$  from  $G$

FindMaximalCliqueOfV(Neighbors( $v_i$ ), 1)

FindMaximalCliqueOfV( $U, size$ )

if  $U$  is empty then

if  $size > max\_clq$

$max\_clq = size$

return

For each vertex  $v_j$  in  $U$

Remove  $v_j$  from  $U$

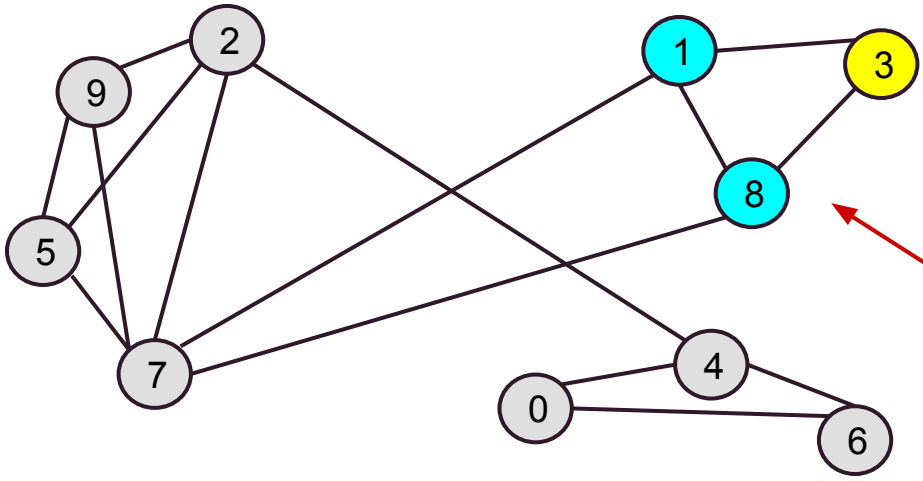
$U_{new} = Neighbors(v_j) \cap U$

FindMaximalCliqueOfV( $U_{new}, size+1$ )

ignore for now

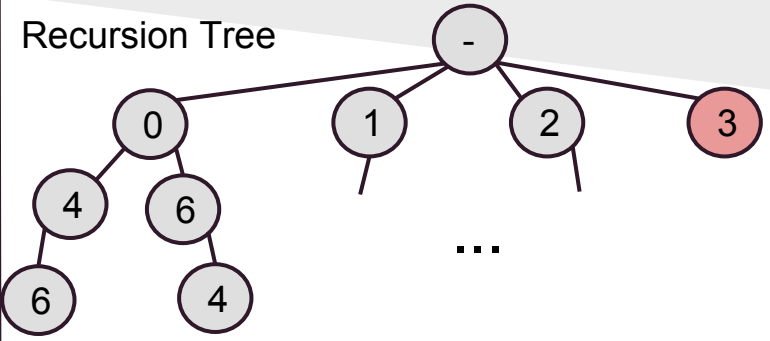
# Pardalos Algorithm

$|V| = 10, |E| = 15$



Max clique size = 4  
 Max clique set = {2,5,7,9}

Current clique size = 0  
 Current clique set = {}  
 Current Node = **Node 3**  
 Current Neighbors = {1,8}  
 Candidate set = {3,...,9}



Current Step:

---

Next Step:

---

Has only 2 neighbors.  
 Even if all neighbors were included, only a size 3 clique can be formed ( $\leq 4$ )



# Modified Pardalos Algorithm

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
```

```
   $max \leftarrow lb$ 
```

```
  for  $i : 1$  to  $n$  do
```

```
     $U \leftarrow \emptyset$ 
```

```
    for each  $v_j \in N(v_i)$  do
```

```
       $\bar{U} \leftarrow U \cup \{v_j\}$ 
```

```
    CLIQUE( $G, U, 1$ )
```

```
procedure CLIQUE( $G = (V, E), U, size$ )
```

```
  if  $U = \emptyset$  then
```

```
    if  $size > max$  then
```

```
       $max \leftarrow size$ 
```

```
    return
```

```
  while  $|U| > 0$  do
```

```
    Select any vertex  $u$  from  $U$ 
```

```
     $U \leftarrow U \setminus \{u\}$ 
```

```
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
```

```
   $max \leftarrow lb$ 
```

```
  for  $i : 1$  to  $n$  do
```

```
    if  $d(v_i) \geq max$  then ▷ Pruning 1
```

```
       $U \leftarrow \emptyset$ 
```

```
      for each  $v_j \in N(v_i)$  do
```

```
         $\bar{U} \leftarrow U \cup \{v_j\}$ 
```

```
      CLIQUE( $G, U, 1$ )
```

```
procedure CLIQUE( $G = (V, E), U, size$ )
```

```
  if  $U = \emptyset$  then
```

```
    if  $size > max$  then
```

```
       $max \leftarrow size$ 
```

```
    return
```

```
  while  $|U| > 0$  do
```

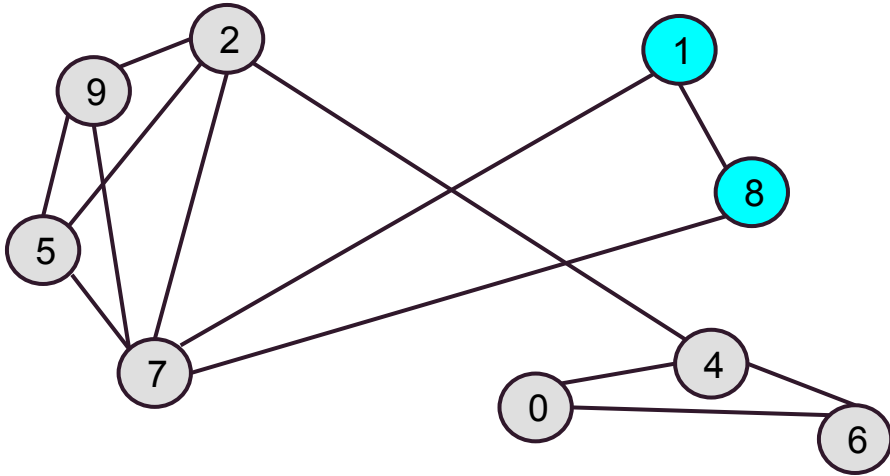
```
    Select any vertex  $u$  from  $U$ 
```

```
     $U \leftarrow U \setminus \{u\}$ 
```

```
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

# Pardalos Algorithm

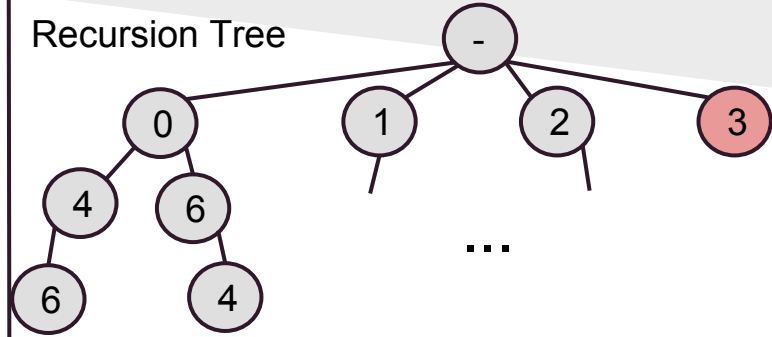
$|V| = 10, |E| = 15$



Current clique size = 1  
Current clique set = {3}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {1,8}

Max clique size = 4  
Max clique set = {2,5,7,9}

Recursion Tree



All cliques containing  
Node 3 already  
examined. Can discard  
this node and edges from  
any future computation.



# Modified Pardalos Algorithm

```
procedure MAXCLIQUE( $G = (V, E), lb$ )  
   $max \leftarrow lb$   
  for  $i : 1$  to  $n$  do  
    if  $d(v_i) \geq max$  then ▷ Pruning 1  
       $U \leftarrow \emptyset$   
      for each  $v_j \in N(v_i)$  do  
         $U \leftarrow U \cup \{v_j\}$   
      CLIQUE( $G, U, 1$ )
```

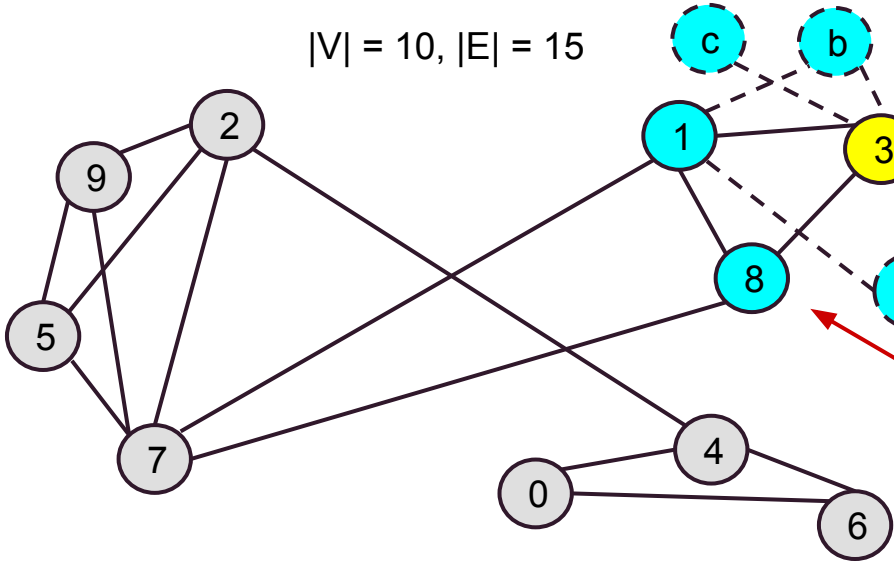
```
procedure CLIQUE( $G = (V, E), U, size$ )  
  if  $U = \emptyset$  then  
    if  $size > max$  then  
       $max \leftarrow size$   
    return  
  while  $|U| > 0$  do  
    Select any vertex  $u$  from  $U$   
     $U \leftarrow U \setminus \{u\}$   
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

```
procedure MAXCLIQUE( $G = (V, E), lb$ )  
   $max \leftarrow lb$   
  for  $i : 1$  to  $n$  do  
    if  $d(v_i) \geq max$  then ▷ Pruning 1  
       $U \leftarrow \emptyset$   
      for each  $v_j \in N(v_i)$  do  
        if  $j > i$  then ▷ Pruning 2  
           $U \leftarrow U \cup \{v_j\}$   
      CLIQUE( $G, U, 1$ )
```

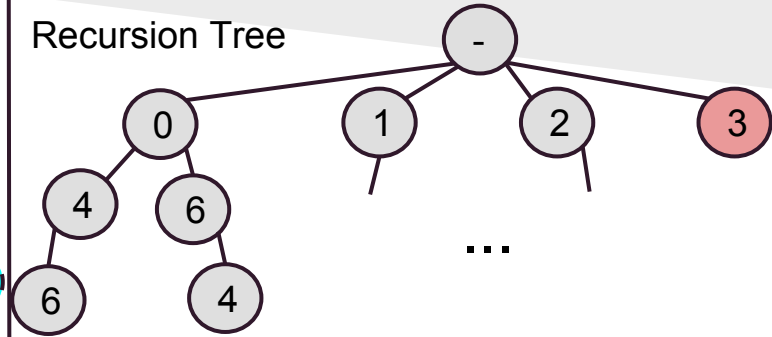
```
procedure CLIQUE( $G = (V, E), U, size$ )  
  if  $U = \emptyset$  then  
    if  $size > max$  then  
       $max \leftarrow size$   
    return  
  while  $|U| > 0$  do  
    Select any vertex  $u$  from  $U$   
     $U \leftarrow U \setminus \{u\}$   
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

# Pardalos Algorithm

$|V| = 10, |E| = 15$



Recursion Tree



Max clique size = 4  
Max clique set = {2,5,7,9}

Current clique size = 0  
Current clique set = {}  
Current Node = **Node 3**  
Current Neighbors = {1,8}  
Candidate set = {3,...,9}

Current Step:

---

Next Step:

---

Each neighbor also should also have  $\geq 4$  neighbors to be a part of a clique of larger than 4 nodes. In this case only Node 1 can possibly form a clique of size  $\geq 4$ .

# Modified Pardalos Algorithm

**procedure** MAXCLIQUE( $G = (V, E), lb$ )

$max \leftarrow lb$

**for**  $i : 1$  to  $n$  **do**

**if**  $d(v_i) \geq max$  **then** ▷ Pruning 1

$U \leftarrow \emptyset$

**for each**  $v_j \in N(v_i)$  **do**

**if**  $j > i$  **then** ▷ Pruning 2

$U \leftarrow U \cup \{v_j\}$

CLIQUE( $G, U, 1$ )

**procedure** CLIQUE( $G = (V, E), U, size$ )

**if**  $U = \emptyset$  **then**

**if**  $size > max$  **then**

$max \leftarrow size$

**return**

**while**  $|U| > 0$  **do**

Select any vertex  $u$  from  $U$

$U \leftarrow U \setminus \{u\}$

CLIQUE( $G, U \cap N'(u), size + 1$ )

**procedure** MAXCLIQUE( $G = (V, E), lb$ )

$max \leftarrow lb$

**for**  $i : 1$  to  $n$  **do**

**if**  $d(v_i) \geq max$  **then** ▷ Pruning 1

$U \leftarrow \emptyset$

**for each**  $v_j \in N(v_i)$  **do**

**if**  $j > i$  **then** ▷ Pruning 2

**if**  $d(v_j) \geq max$  **then** ▷ Pruning 3

$U \leftarrow U \cup \{v_j\}$

CLIQUE( $G, U, 1$ )

**procedure** CLIQUE( $G = (V, E), U, size$ )

**if**  $U = \emptyset$  **then**

**if**  $size > max$  **then**

$max \leftarrow size$

**return**

**while**  $|U| > 0$  **do**

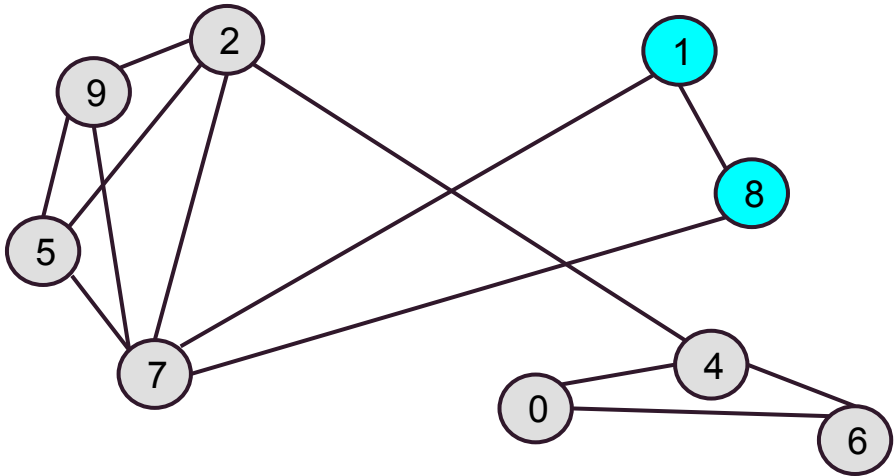
Select any vertex  $u$  from  $U$

$U \leftarrow U \setminus \{u\}$

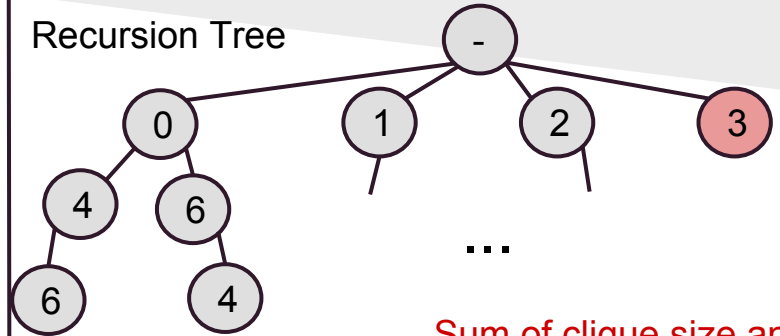
CLIQUE( $G, U \cap N'(u), size + 1$ )

# Pardalos Algorithm

$|V| = 10, |E| = 15$



Recursion Tree



Sum of clique size and size of candidate set must be larger than max clique

Max clique size = 4  
Max clique set = {2,5,7,9}

Current clique size = 1  
Current clique set = {3}  
Current Node = ---  
Current Neighbors = ---  
Candidate set = {1,8}

3

# Modified Pardalos Algorithm

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
```

```
   $max \leftarrow lb$ 
```

```
  for  $i : 1$  to  $n$  do
```

```
    if  $d(v_i) \geq max$  then ▷ Pruning 1
```

```
       $U \leftarrow \emptyset$ 
```

```
      for each  $v_j \in N(v_i)$  do
```

```
        if  $j > i$  then ▷ Pruning 2
```

```
          if  $d(v_j) \geq max$  then ▷ Pruning 3
```

```
             $U \leftarrow U \cup \{v_j\}$ 
```

```
      CLIQUE( $G, U, 1$ )
```

```
procedure CLIQUE( $G = (V, E), U, size$ )
```

```
  if  $U = \emptyset$  then
```

```
    if  $size > max$  then
```

```
       $max \leftarrow size$ 
```

```
    return
```

```
  while  $|U| > 0$  do
```

```
    Select any vertex  $u$  from  $U$ 
```

```
     $U \leftarrow U \setminus \{u\}$ 
```

```
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
```

```
   $max \leftarrow lb$ 
```

```
  for  $i : 1$  to  $n$  do
```

```
    if  $d(v_i) \geq max$  then ▷ Pruning 1
```

```
       $U \leftarrow \emptyset$ 
```

```
      for each  $v_j \in N(v_i)$  do
```

```
        if  $j > i$  then ▷ Pruning 2
```

```
          if  $d(v_j) \geq max$  then ▷ Pruning 3
```

```
             $U \leftarrow U \cup \{v_j\}$ 
```

```
      CLIQUE( $G, U, 1$ )
```

```
procedure CLIQUE( $G = (V, E), U, size$ )
```

```
  if  $U = \emptyset$  then
```

```
    if  $size > max$  then
```

```
       $max \leftarrow size$ 
```

```
    return
```

```
  while  $|U| > 0$  do
```

```
    if  $size + |U| \leq max$  then ▷ Pruning 4
```

```
      return
```

```
      Select any vertex  $u$  from  $U$ 
```

```
       $U \leftarrow U \setminus \{u\}$ 
```

```
      CLIQUE( $G, U \cap N'(u), size + 1$ )
```

# Modified Pardalos Algorithm

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
   $max \leftarrow lb$ 
  for  $i : 1$  to  $n$  do
    if  $d(v_i) \geq max$  then           ▷ Pruning 1
       $U \leftarrow \emptyset$ 
      for each  $v_j \in N(v_i)$  do
        if  $j > i$  then             ▷ Pruning 2
          if  $d(v_j) \geq max$  then ▷ Pruning 3
             $U \leftarrow U \cup \{v_j\}$ 
      CLIQUE( $G, U, 1$ )
  procedure CLIQUE( $G = (V, E), U, size$ )
    if  $U = \emptyset$  then
      if  $size > max$  then
         $max \leftarrow size$ 
      return
    while  $|U| > 0$  do
      if  $size + |U| \leq max$  then   ▷ Pruning 4
        return
      Select any vertex  $u$  from  $U$ 
       $U \leftarrow U \setminus \{u\}$ 
      CLIQUE( $G, U \cap N'(u), size + 1$ )
```

```
procedure MAXCLIQUE( $G = (V, E), lb$ )
   $max \leftarrow lb$ 
  for  $i : 1$  to  $n$  do
    if  $d(v_i) \geq max$  then       ▷ Pruning 1
       $U \leftarrow \emptyset$ 
      for each  $v_j \in N(v_i)$  do
        if  $j > i$  then           ▷ Pruning 2
          if  $d(v_j) \geq max$  then ▷ Pruning 3
             $U \leftarrow U \cup \{v_j\}$ 
      CLIQUE( $G, U, 1$ )
  procedure CLIQUE( $G = (V, E), U, size$ )
    if  $U = \emptyset$  then
      if  $size > max$  then
         $max \leftarrow size$ 
      return
    while  $|U| > 0$  do
      if  $size + |U| \leq max$  then ▷ Pruning 4
        return
      Select any vertex  $u$  from  $U$ 
       $U \leftarrow U \setminus \{u\}$ 
       $N'(u) := \{w | w \in N(u) \wedge d(w) \geq max\}$  ▷
      Pruning 5
      CLIQUE( $G, U \cap N'(u), size + 1$ )
```



# Modified Pardalos Algorithm

```
procedure MAXCLIQUE( $G = (V, E), lb$ )  
   $max \leftarrow lb$   
  for  $i : 1$  to  $n$  do  
    if  $d(v_i) \geq max$  then ▷ Pruning 1  
       $U \leftarrow \emptyset$   
      for each  $v_j \in N(v_i)$  do  
        if  $j > i$  then ▷ Pruning 2  
          if  $d(v_j) \geq max$  then ▷ Pruning 3  
             $U \leftarrow U \cup \{v_j\}$   
  
      CLIQUE( $G, U, 1$ )  
procedure CLIQUE( $G = (V, E), U, size$ )  
  if  $U = \emptyset$  then  
    if  $size > max$  then  
       $max \leftarrow size$   
    return  
  while  $|U| > 0$  do  
    if  $size + |U| \leq max$  then ▷ Pruning 4  
      return  
    Select any vertex  $u$  from  $U$   
     $U \leftarrow U \setminus \{u\}$   
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

```
procedure MAXCLIQUE( $G = (V, E), lb$ )  
   $max \leftarrow lb$   
  for  $i : 1$  to  $n$  do  
    if  $d(v_i) \geq max$  then ▷ Pruning 1  
       $U \leftarrow \emptyset$   
      for each  $v_j \in N(v_i)$  do  
        if  $j > i$  then ▷ Pruning 2  
          if  $d(v_j) \geq max$  then ▷ Pruning 3  
             $U \leftarrow U \cup \{v_j\}$   
  
      CLIQUE( $G, U, 1$ )  
procedure CLIQUE( $G = (V, E), U, size$ )  
  if  $U = \emptyset$  then  
    if  $size > max$  then  
       $max \leftarrow size$   
    return  
  while  $|U| > 0$  do  
    if  $size + |U| \leq max$  then ▷ Pruning 4  
      return  
    Select any vertex  $u$  from  $U$   
     $U \leftarrow U \setminus \{u\}$   
     $N'(u) := \{w | w \in N(u) \wedge d(w) \geq max\}$  ▷  
    Pruning 5  
    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

# New Algorithms

**Algorithm 1** Algorithm for finding the maximum clique of a given graph. *Input:* Graph  $G = (V, E)$ , lower bound on clique  $lb$  (default, 0). *Output:* Size of maximum clique.

```
1: procedure MAXCLIQUE( $G = (V, E), lb$ )
2:    $max \leftarrow lb$ 
3:   for  $i : 1$  to  $n$  do
4:     if  $d(v_i) \geq max$  then           ▷ Pruning 1
5:        $U \leftarrow \emptyset$ 
6:       for each  $v_j \in N(v_i)$  do
7:         if  $j > i$  then             ▷ Pruning 2
8:           if  $d(v_j) \geq max$  then ▷ Pruning 3
9:              $U \leftarrow U \cup \{v_j\}$ 
10:      CLIQUE( $G, U, 1$ )
```

– *Subroutine*

```
1: procedure CLIQUE( $G = (V, E), U, size$ )
2:   if  $U = \emptyset$  then
3:     if  $size > max$  then
4:        $max \leftarrow size$ 
5:     return
6:   while  $|U| > 0$  do
7:     if  $size + |U| \leq max$  then     ▷ Pruning 4
8:       return
9:     Select any vertex  $u$  from  $U$ 
10:     $U \leftarrow U \setminus \{u\}$ 
11:     $N'(u) := \{w | w \in N(u) \wedge d(w) \geq max\}$  ▷
    Pruning 5
12:    CLIQUE( $G, U \cap N'(u), size + 1$ )
```

**Algorithm 2** Heuristic for finding the maximum clique in a graph. *Input:* Graph  $G = (V, E)$ . *Output:* Approximate size of maximum clique.

```
1: procedure MAXCLIQUEHEU( $G = (V, E)$ )
2:   for  $i : 1$  to  $n$  do
3:     if  $d(v_i) \geq max$  then
4:        $U \leftarrow \emptyset$ 
5:       for each  $v_j \in N(v_i)$  do
6:         if  $d(v_j) \geq max$  then
7:            $U \leftarrow U \cup \{v_j\}$ 
8:       CLIQUEHEU( $G, U, 1$ )
```

– *Subroutine*

```
1: procedure CLIQUEHEU( $G = (V, E), U, size$ )
2:   if  $U = \emptyset$  then
3:     if  $size > max$  then
4:        $max \leftarrow size$ 
5:     return
6:   Select a vertex  $u \in U$  of maximum degree in  $G$ 
7:    $U \leftarrow U \setminus \{u\}$ 
8:    $N'(u) := \{w | w \in N(u) \wedge d(w) \geq max\}$ 
9:   CLIQUEHEU( $G, U \cap N'(u), size + 1$ )
```

# Experiments

- Testbed
  - Real world graphs
  - Synthetic graphs
  - DIMACS graphs

# Testbed

- Real world graphs
  - Obtained from Florida Matrix Collection\* - a large and actively growing set of sparse matrices that arise in real applications

Graph	Description
<i>cond-mat-2003</i> [26]	A collaboration network of scientists posting preprints on the condensed matter archive at <a href="http://www.arxiv.org">www.arxiv.org</a> in the period
<i>email-Enron</i> [23]	A communication network representing email exchanges.
<i>dictionary28</i> [4]	Pajek network of words.
<i>Fault_639</i> [14]	A structural problem discretizing a faulted gas reservoir with tetrahedral Finite Elements and triangular Interface Elements.
<i>audikw_1</i> [11]	An automotive crankshaft model of TETRA elements.
<i>bone010</i> [39]	A detailed micro-finite element model of bones representing the porous bone micro-architecture.
<i>af_shell</i> [11]	A sheet metal forming simulation network.
<i>as-Skitter</i> [23]	An Internet topology graph from trace routes run daily in 2005.
<i>roadNet-CA</i> [23]	A road network of California. Nodes represent intersections and endpoints and edges represent the roads connecting them.
<i>kkt_power</i> [11]	An Optimal Power Flow (nonlinear optimization) network.

\* <http://www.cise.ufl.edu/research/sparse/matrices/>

# Testbed

- Synthetic graphs

- Generated using the RMAT algorithm\*

**A. Random graphs (5 graphs)** – Erdős-Rényi random graphs generated using R-MAT with the parameters (0.25, 0.25, 0.25, 0.25). Denoted with prefix *rmat\_er*.

**B. Skewed Degree, Type 1 graphs (5 graphs)** – graphs generated using R-MAT with the parameters (0.45, 0.15, 0.15, 0.25). Denoted with prefix *rmat\_sd1*.

**C. Skewed Degree, Type 2 graphs (5 graphs)** – graphs generated using R-MAT with the parameters (0.55, 0.15, 0.15, 0.15). Denoted with prefix *rmat\_sd2*.

- DIMACS graphs

- From the Second DIMACS Implementation Challenge
- Established benchmark for the maximum clique problem

\* D. Chakrabarti and C. Faloutsos, *Graph mining: Laws, generators, and algorithms*, ACM Comput. Surv. 38 (2006).

# Testbed

**Table 2.** Structural properties (the number of vertices,  $|V|$ ; edges,  $|E|$ ; and the maximum degree,  $\Delta$ ) of the graphs,  $G$  in the testbed: DIMACS Challenge graphs (upper left); UF Collection (lower and middle left); RMAT graphs (right).

$G$	$ V $	$ E $	$\Delta$	$G$	$ V $	$ E $	$\Delta$
<i>cond-mat-2003</i>	31,163	120,029	202	<i>rmat_sd1_1</i>	131,072	1,046,384	407
<i>email-Enron</i>	36,692	183,831	1,383	<i>rmat_sd1_2</i>	262,144	2,093,552	558
<i>dictionary28</i>	52,652	89,038	38	<i>rmat_sd1_3</i>	524,288	4,190,376	618
<i>Fault_639</i>	638,802	13,987,881	317	<i>rmat_sd1_4</i>	1,048,576	8,382,821	802
<i>audikw_1</i>	943,695	38,354,076	344	<i>rmat_sd1_5</i>	2,097,152	16,767,728	1,069
<i>bone010</i>	986,703	35,339,811	80	<i>rmat_sd2_1</i>	131,072	1,032,634	2,980
<i>af_shell10</i>	1,508,065	25,582,130	34	<i>rmat_sd2_2</i>	262,144	2,067,860	4,493
<i>as-Skitter</i>	1,696,415	11,095,298	35,455	<i>rmat_sd2_3</i>	524,288	4,153,043	6,342
<i>roadNet-CA</i>	1,971,281	2,766,607	12	<i>rmat_sd2_4</i>	1,048,576	8,318,004	9,453
<i>kkt_power</i>	2,063,494	6,482,320	95	<i>rmat_sd2_5</i>	2,097,152	16,645,183	14,066
<i>rmat_er_1</i>	131,072	1,048,515	82	<i>hamming6-4</i>	64	704	22
<i>rmat_er_2</i>	262,144	2,097,104	98	<i>johnson8-4-4</i>	70	1,855	53
<i>rmat_er_3</i>	524,288	4,194,254	94	<i>keller4</i>	171	9,435	124
<i>rmat_er_4</i>	1,048,576	8,388,540	97	<i>c-fat200-5</i>	200	8,473	86
<i>rmat_er_5</i>	2,097,152	16,777,139	102	<i>brock200_2</i>	200	9,876	114

# Algorithms - Comparison

- Carraghan and Pardalos 1990 - Self-implemented
- Ostergard 2002 - *cliquer* software package
  - <http://users.tkk.fi/pat/cliquer.html>
- MCQD+CS 2007 - *MaxCliqueDyn* software package
  - <http://www.sicmm.org/~konc/maxclique/>

# Experiments

- Setup

- Linux workstation (64-bit Red Hat Enterprise Server release)
- 6.22 GHz Intel Xeon E7540 processor
- Implemented in C++
- gcc version 4.4.6 with -O3 optimization.
- Single threaded



# Results - real-world graphs

Graph	$\omega$	$\tau_{MCQD}$				$\tau_{A1}$	P1	P2	P3	P5	$\omega_{A2}$	$\tau_{A2}$
		$\tau_{CP}$	$\tau_{cliquer}$	+CS								
<i>cond-mat-2003</i>	25	4.875	11.17	2.41	<b>0.011</b>	29K	48K	6,527	17K	25	<0.01	
<i>email-Enron</i>	20	7.005	15.08	3.70	<b>0.998</b>	32K	155K	4,060	8M	18	0.261	
<i>dictionary28</i>	26	7.700	32.74	7.69	<b>&lt;0.01</b>	52K	4,353	2,114	107	26	<0.01	
<i>Fault_639</i>	18	14571.20	4437.14	-	<b>20.03</b>	36	13M	126	1,116	18	5.80	
<i>audikw_1</i>	36	*	9282.49	-	<b>190.17</b>	4,101	38M	59K	721K	36	58.38	
<i>bone010</i>	24	*	10002.67	-	<b>393.11</b>	37K	34M	361K	44M	24	24.39	
<i>af_shell10</i>	15	*	21669.96	-	<b>50.99</b>	19	25M	75	2,105	15	10.67	
<i>as-Skitter</i>	67	24385.73	*	-	<b>3838.36</b>	1M	6M	981K	737M	66	27.08	
<i>roadNet-CA</i>	4	*	*	-	<b>0.44</b>	1M	1M	370K	4,302	4	0.08	
<i>kkt_power</i>	11	*	*	-	<b>2.26</b>	1M	4M	401K	2M	11	1.83	

LEGEND:	<i>CP</i>	-	Pardalos 1990	<i>P1, P2, P3, P5</i>	-	Nodes/Computation Pruned
	<i>cliquer</i>	-	Ostergard 2001	$\omega_{A2}$	-	Max clique by Heuristic
	<i>MCQD+CS</i>	-	Konc & Janezic 2007	$\tau_{A2}$	-	Time taken by Heuristic
	<i>A1</i>	-	Our new algorithm	$\omega$	-	Actual max clique
	*	-	More than 25,000 sec	-	-	Implementation couldn't handle

# Results - real-world graphs

Graph	$\omega$	$\tau_{MCQD}$				$\tau_{A1}$	$P1$	$P2$	$P3$	$P5$	$\omega_{A2}$	$\tau_{A2}$
		$\tau_{CP}$	$\tau_{cliquer}$	$+CS$								
<i>rmat_er_1</i>	3	256.37	215.18	49.79	<b>0.38</b>	780	1M	915	8,722	3	0.12	
<i>rmat_er_2</i>	3	1016.70	865.18	-	<b>0.78</b>	2,019	2M	2,351	23K	3	0.24	
<i>rmat_er_3</i>	3	4117.35	3456.39	-	<b>1.87</b>	4,349	4M	4,960	50K	3	0.49	
<i>rmat_er_4</i>	3	16419.80	13894.52	-	<b>4.16</b>	9,032	8M	10K	106K	3	1.44	
<i>rmat_er_5</i>	3	*	*	-	<b>9.87</b>	18K	16M	20K	212K	3	2.57	
<i>rmat_sd1_1</i>	6	225.93	214.99	50.08	<b>1.39</b>	39K	1M	23K	542K	6	0.45	
<i>rmat_sd1_2</i>	6	912.44	858.80	-	<b>3.79</b>	90K	2M	56K	1M	6	0.98	
<i>rmat_sd1_3</i>	6	3676.14	3446.02	-	<b>8.17</b>	176K	4M	106K	2M	6	1.78	
<i>rmat_sd1_4</i>	6	14650.40	13923.93	-	<b>25.61</b>	369K	8M	214K	5M	6	4.05	
<i>rmat_sd1_5</i>	6	*	*	-	<b>46.89</b>	777K	16M	455K	12M	6	9.39	
<i>rmat_sd2_1</i>	26	427.41	213.23	<b>48.17</b>	242.20	110K	853K	88K	614M	26	32.83	
<i>rmat_sd2_2</i>	35	4663.62	<b>851.84</b>	-	3936.55	232K	1M	195K	1B	35	95.89	
<i>rmat_sd2_3</i>	39	13626.23	<b>3411.14</b>	-	10647.84	470K	3M	405K	1B	37	245.51	
<i>rmat_sd2_4</i>	43	*	<b>13709.52</b>	-	*	*	*	*	*	42	700.05	
<i>rmat_sd2_5</i>	N	*	*	-	*	*	*	*	*	51	1983.21	

LEGEND:

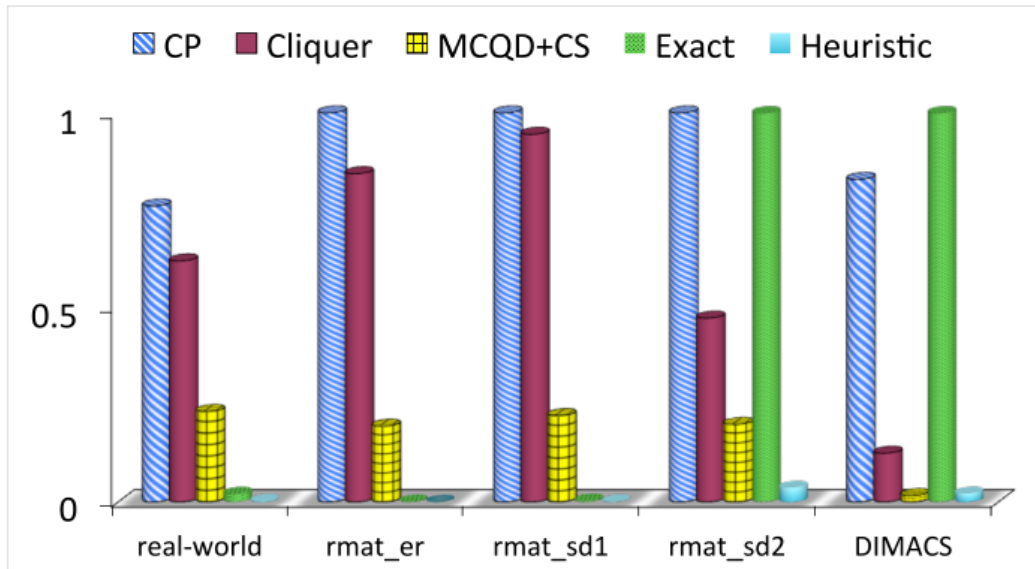
<i>CP</i>	-	Pardalos 1990	$P1, P2, P3, P5$	-	Nodes/Computation Pruned
<i>cliquer</i>	-	Ostergard 2001	$\omega_{A2}$	-	Max clique by Heuristic
<i>MCQD+CS</i>	-	Konc & Janezic 2007	$\tau_{A2}$	-	Time taken by Heuristic
<i>A1</i>	-	Our new algorithm	$\omega$	-	Actual max clique
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# Results - real-world graphs

Graph	$\omega$	$\tau_{MCQD}$				$\tau_{A1}$	$P1$	$P2$	$P3$	$P5$	$\omega_{A2}$	$\tau_{A2}$
		$\tau_{CP}$	$\tau_{cliquer}$	$+CS$								
<i>hamming6-4</i>	4	<0.01	<0.01	<0.01	<0.01	0	704	0	0	4	<0.01	
<i>johnson8-4-4</i>	14	0.19	<0.01	<0.01	0.23	0	1,855	0	0	14	<0.01	
<i>keller4</i>	11	22.19	0.15	0.02	23.35	0	9,435	0	0	11	<0.01	
<i>c-fat200-5</i>	58	0.60	0.33	0.01	0.93	0	8,473	0	0	58	0.04	
<i>brock200-2</i>	12	0.98	0.02	<0.01	1.10	0	9,876	0	0	10	<0.01	

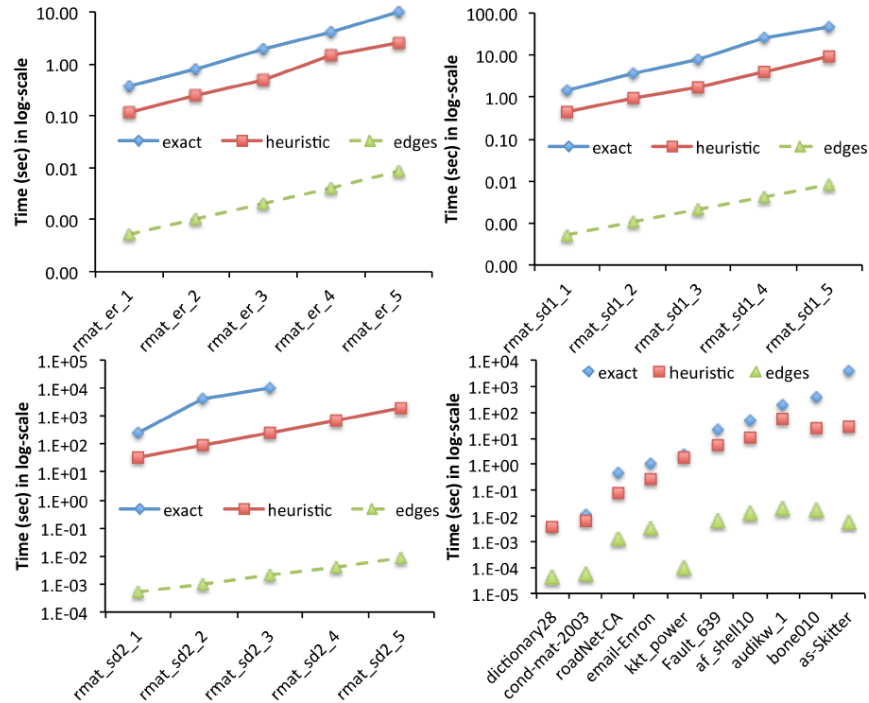
LEGEND:	<i>CP</i>	-	Pardalos 1990	$P1, P2, P3, P5$	-	Nodes/Computation Pruned
	<i>cliquer</i>	-	Ostergard 2001	$\omega_{A2}$	-	Max clique by Heuristic
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	<i>A1</i>	-	Our new algorithm	$\omega$	-	Actual max clique
	*	-	More than 25,000 sec	-	-	Implementation couldn't handle

# Results - summary



**Fig. 1.** Runtime (normalized, mean) comparison between various algorithms. For each category of graph, first, all runtimes for each graph were normalized by the runtime of the slowest algorithm for that graph, and then the mean was calculated for each algorithm. Graphs were considered only if the runtimes for at least three algorithms was less than the 25,000 seconds limit set.

# Results - summary



**Fig. 2.** Run time plots of the new exact and heuristic algorithms. The third curve, labeled *edges*, shows the quantity, number of edges in the graph divided by the clock frequency of the computing platform used in the experiment.

# Summary

- New algorithm
  - Very effective and orders of magnitude times faster on large sparse graphs compared to existing algorithms
  - For certain synthetic graphs and DIMACS graphs, slower than existing algorithms
- Heuristic
  - Delivers optimal solution for 83% of graphs in testbed
  - When sub-optimal, accuracy ranges between 0.83 - 0.99

# Future Work

- Thorough analysis on effect of pruning steps
- Effect of vertex ordering
- Use heuristic-based approximate lower bound to improve pruning
- Compare with more recent algorithms (implementation not publicly available)
- Compare heuristic with others