NOCS 2016

Average Shortest Path Length of Graphs of Diameter 3

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0. Introduction

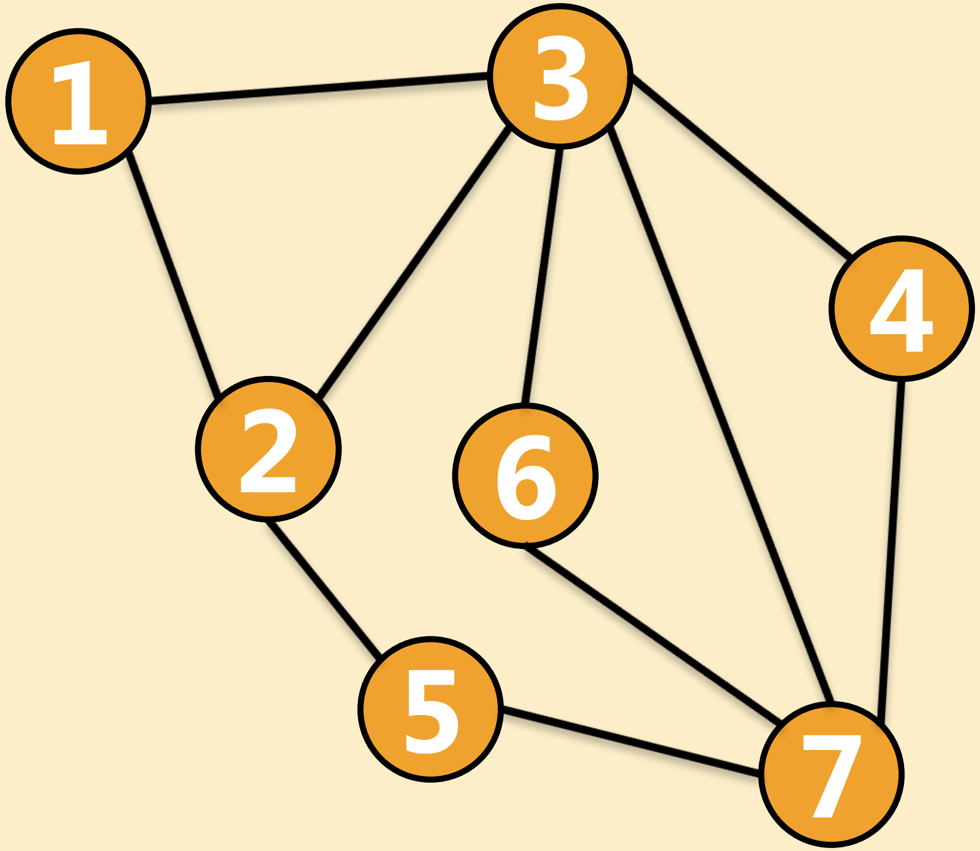
Average Shortest Path Length (ASPL)

Definition

- $G = (V, E)$: undirected graph
- $\mathrm{dist}(i, j)$: length of shortest i-j path
- $\mathrm{ASPL} = \mathrm{ASPL}(G) := \sum_{i \neq j \in V} \mathrm{dist}(i, j) \Big/ \binom{n}{2}$
- $\mathrm{diam}(G) := \max_{i \neq j \in V} \mathrm{dist}(i, j)$: diameter

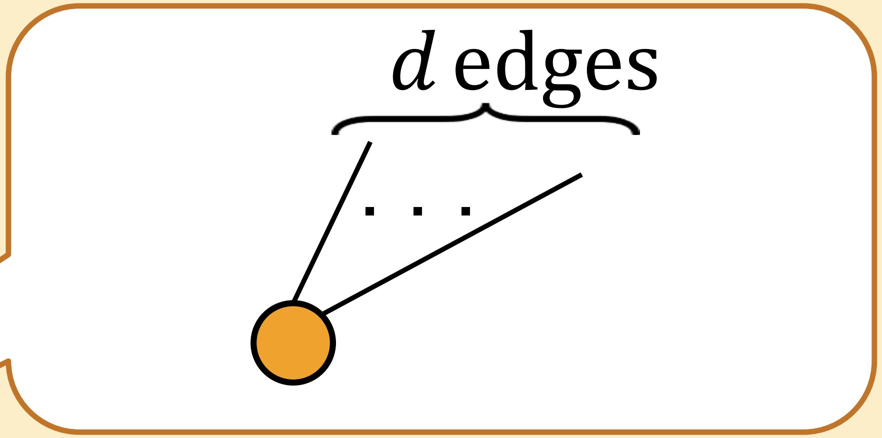
Average Shortest Path Length (ASPL)

	1	2	3	4	5	6	7
1	0	1	1	2	2	2	2
2		0	1	2	1	2	2
3			0	1	2	1	1
4				0	2	2	1
5					0	2	1
6						0	1
7							0



$$\text{ASPL} = \frac{1 \times 10 + 2 \times 11}{21} = 1.523\ldots \qquad \text{diam}(G) = 2$$

Our Problem



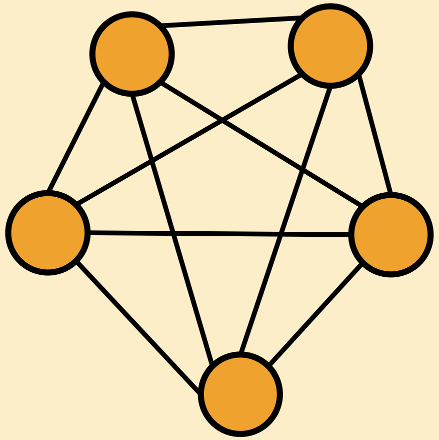
Problem

- Given n and d
- Find a d-regular graph of n nodes with minimum ASPL.

(d-regular graph : all degrees = d)

Background

- lower ASPL → less hops → better performance
- complete graphs → minimum ASPL
- In practice, degree (# of links) is limited
  - ➢ low ASPL graphs with limited degree


Complete Graph

Related Problems

- Order / Degree Problem
  - Given n and d
  - Find a d-regular graph of n vertices with minimum diameter.

unexplored

- Degree / Diameter Problem
  - Given D and d
  - Find a d-regular graph of diameter D with maximum number of nodes.

explored (graph theory)

Contributions

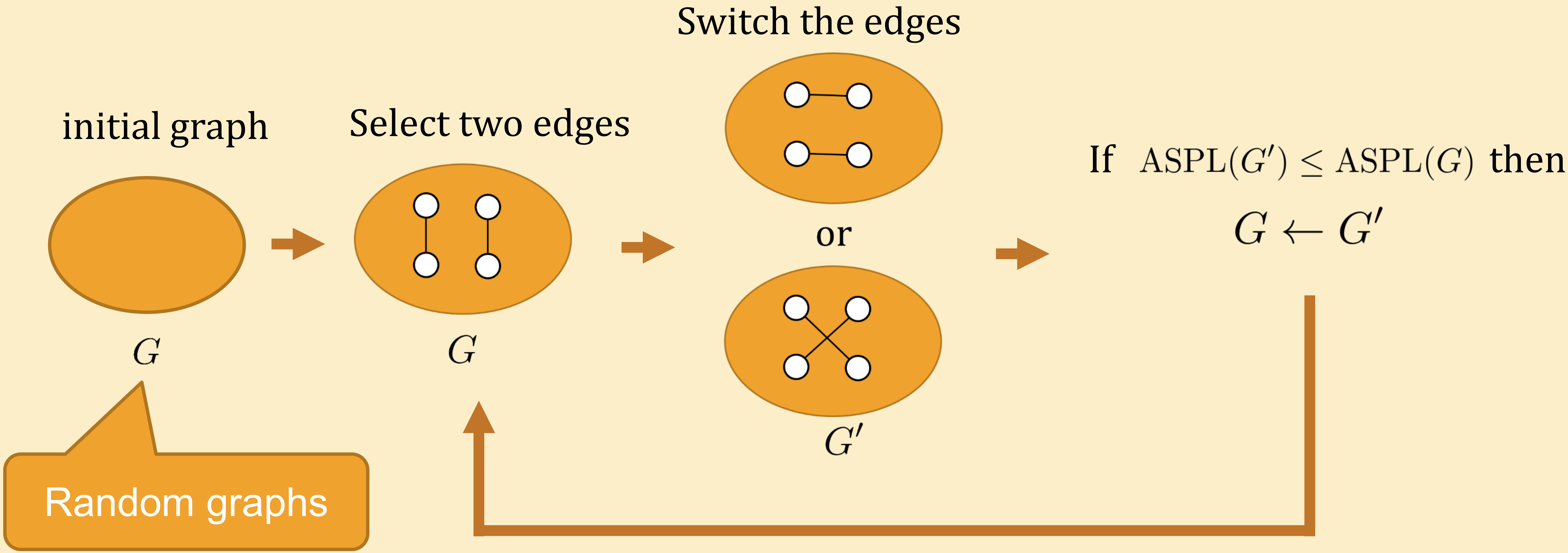
- Derive an equality and inequalities of the ASPL of graphs of diameter 3.
- Propose an efficient algorithm for our problem.

1. Naïve Algorithm

Local Search

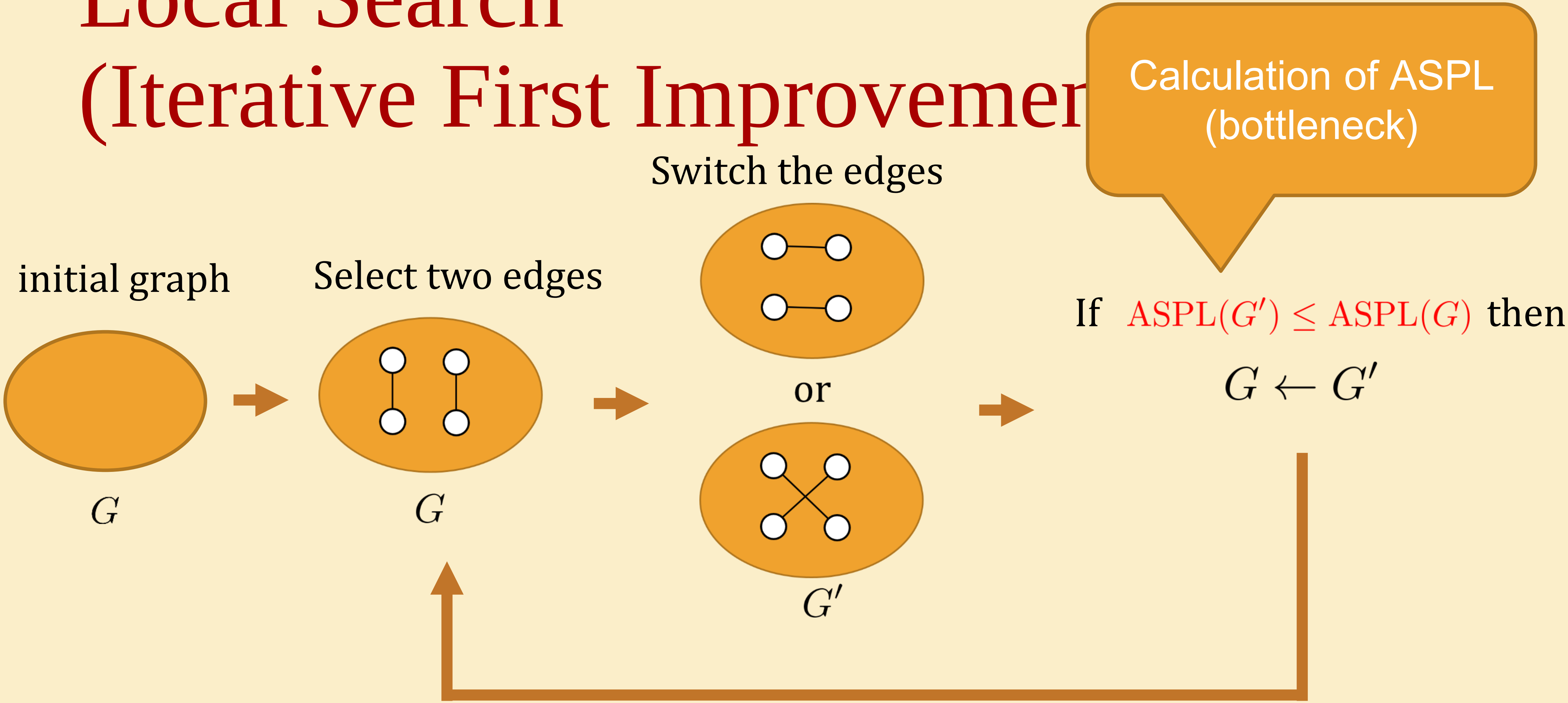
- Construct a d-regular graph (initial graph).
- Repeat improving the graph.
- Terminate when some condition is satisfied.

Local Search (Iterative First Improvement)



- If G cannot be improved for any edge pairs, terminate

Local Search (Iterative First Improvemen



- If G cannot be improved for any edge pairs, terminate

Time Complexity

n = # of nodes
d = degree

- Calculating $\mathrm{ASPL}(G) \cdots O(VE) = O(n^2 d)$ → too slow
- For G of diameter 3 $\cdots O(d)$ ($\mathrm{ASPL}(G') - \mathrm{ASPL}(G)$) → still slow

Time Complexity

n = # of nodes
d = degree

Does not work well!!!

- For

Our Target

n = # of nodes
d = degree

- The input (n, d) for which a.e. graphs are diameter 3
- More precisely, $n \approx d^2$ (n is near to d^2)

From numerical experiments

2. Observation & Main Theorem

Observation

distance table of graphs of diameter 3:

	1	2	3	4	5	6	7
1	0	*	*	*	*	*	*
2		0	*	*	*	*	*
3			0	*	*	*	*
4				0	*	*	*
5					0	*	*
6						0	*
7							0

each nonzero value = 1,2 or 3

# of cells of 1 = # of edges = nd/2

- $\mathrm{ASPL}(G) \propto 1 \times \#1 + 2 \times \#2 + 3 \times \#3$
- $\#1 + \#2 + \#3 = \binom{n}{2}$

Observation

distance table of graphs of diameter 3:

	1	2	3	4	5	6	7
1	0	*	*	*	*	*	*
2		0	*	*	*	*	*
3			0	*	*	*	*
4				0	*	*	*
5					0	*	*
6						0	*
7							0

each nonzero value = 1,2 or 3

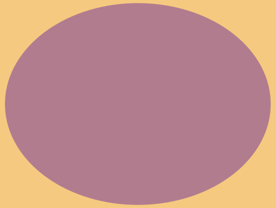
We want to increase them!!

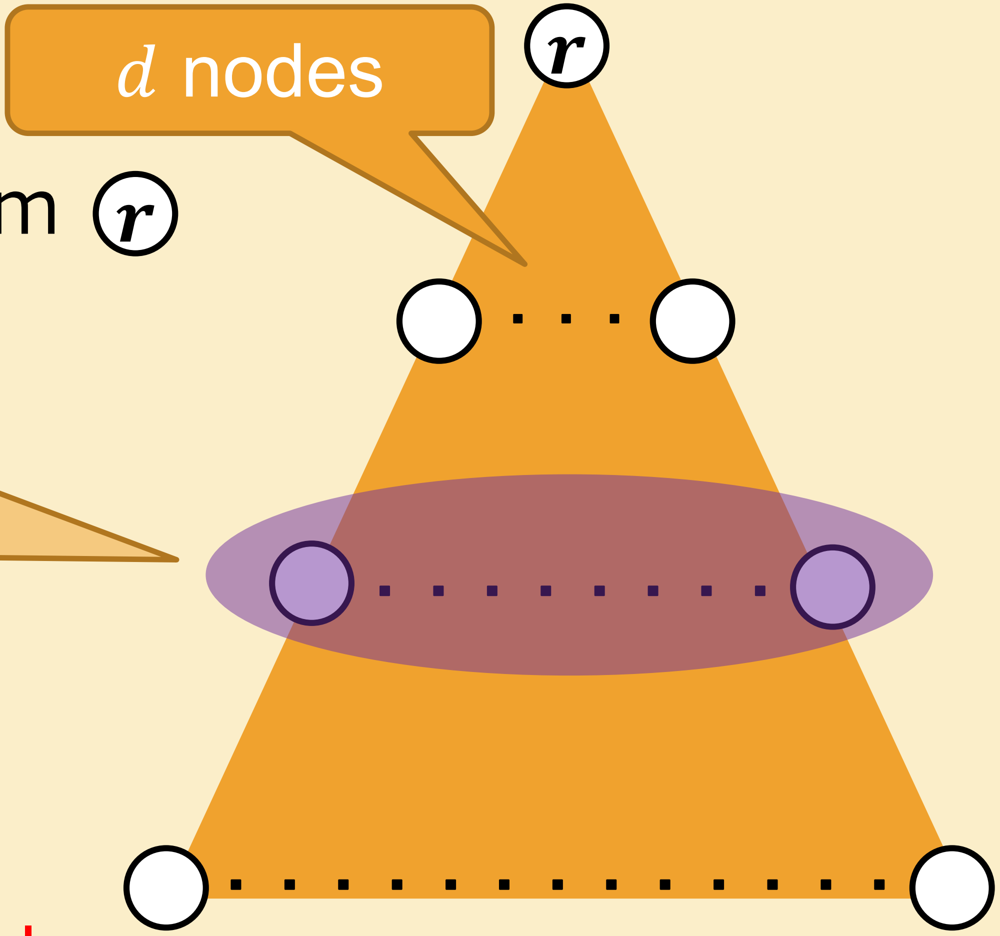
- $\mathrm{ASPL}(G) \propto 1 \times \#1 + 2 \times \#2 + 3 \times \#3$
- $\#1 + \#2 + \#3 = \binom{n}{2}$

Observation

Assume $\mathrm{diameter} = 3$

Consider "Breadth First Search" from $\boldsymbol{r}$

- many nodes → low ASPL
- We want to increase them
- # of  $\leq d(d-1)$



equality holds → graph is optimal

Moore Bound

Fact (the Moore Bound)

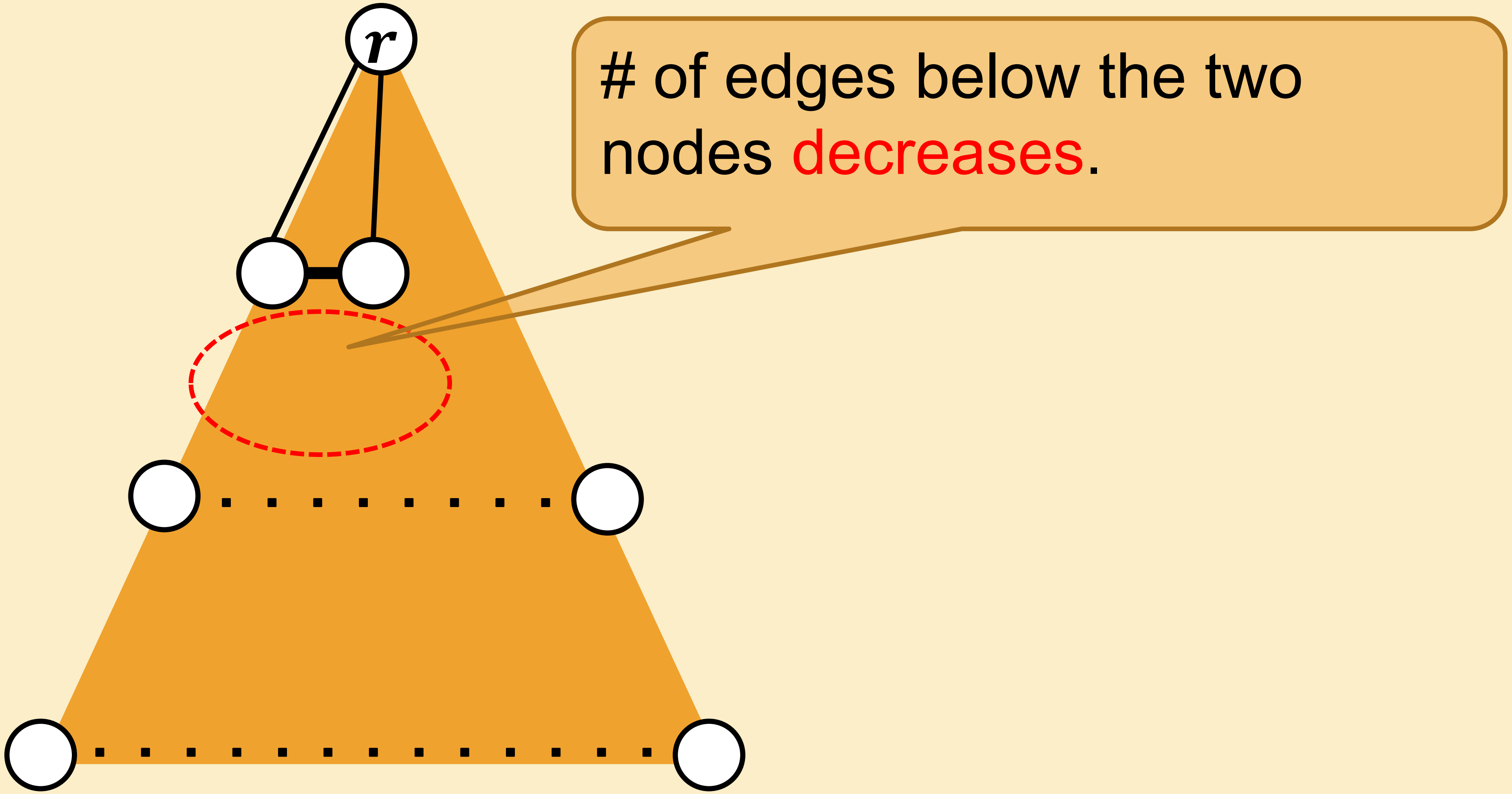
$G=(V,E)$: d-regular, n nodes, diameter $=3$

$$\binom{n}{2}\cdot \mathrm{ASPL}(G) \geq 3\binom{n}{2} - \frac{nd}{2} - nd^2$$

the ASPL when # of is maximum

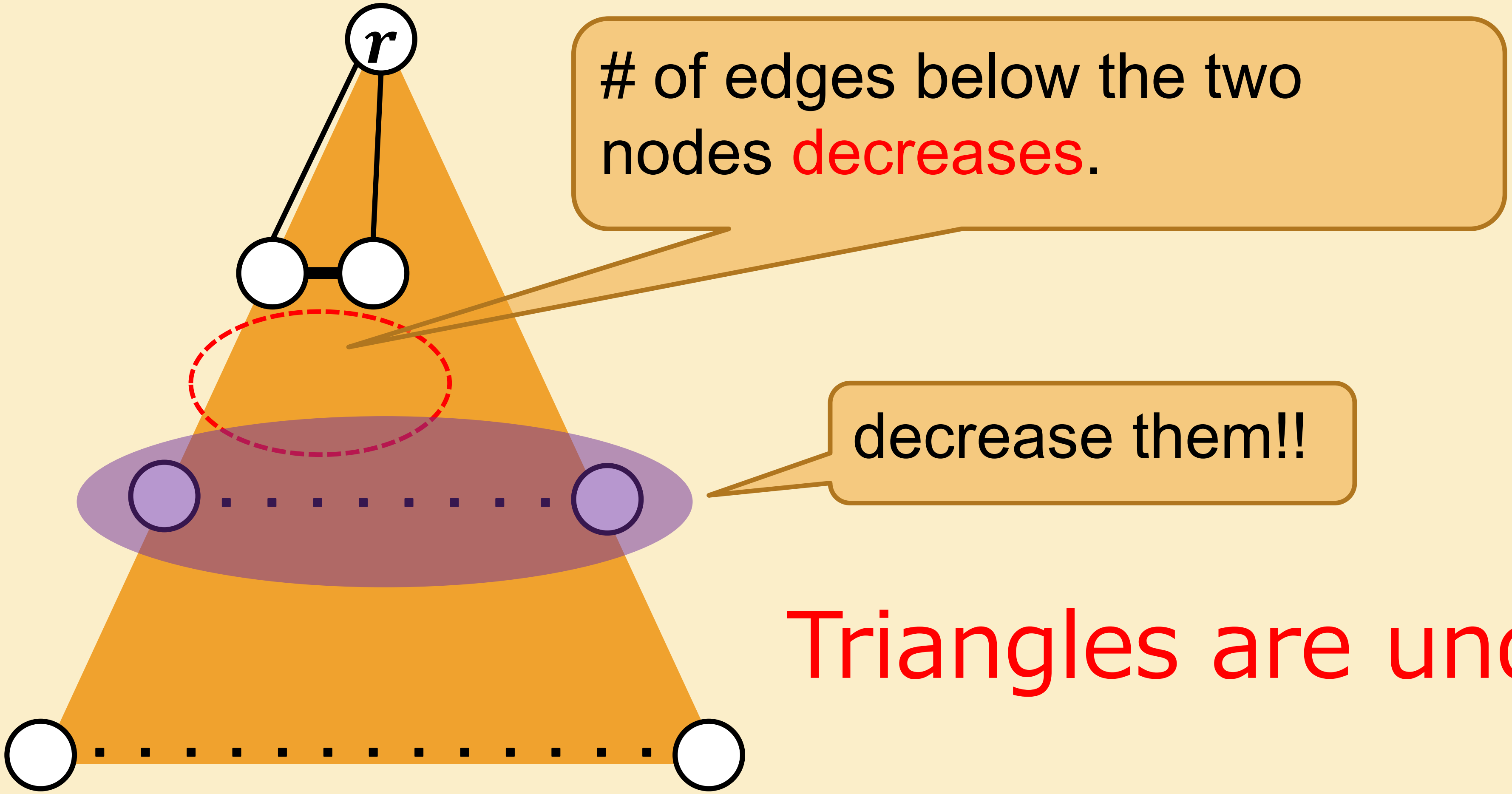
Observation

Here is a triangle...



Observation

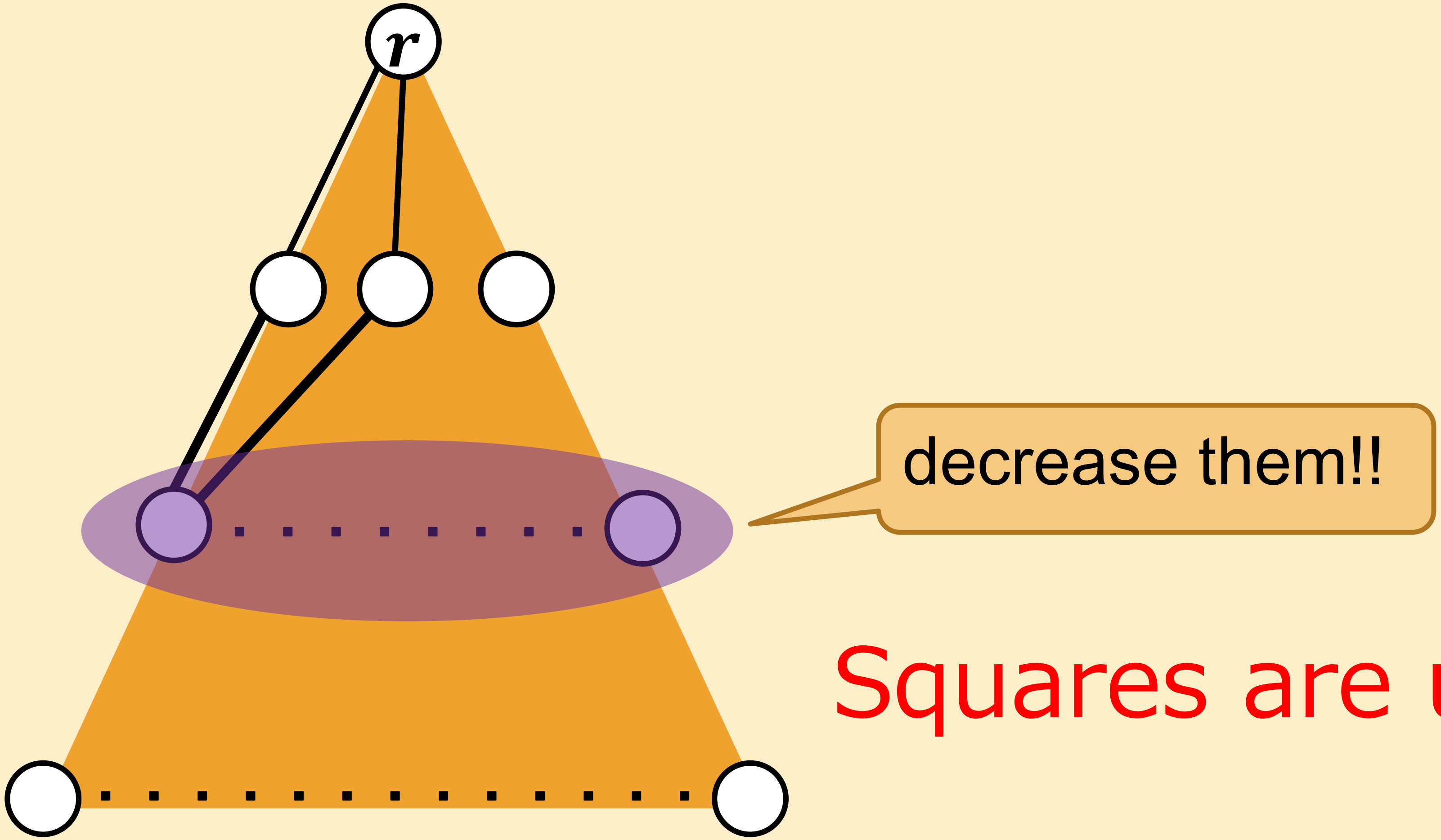
Here is a triangle...



Triangles are undesirable

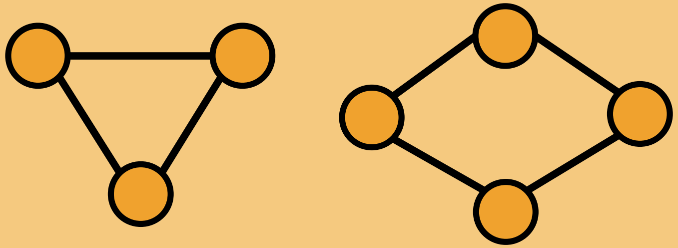
Observation

Here is a Square...



Squares are undesirable

Observation

- no triangles, no squares
  - ➢ ASPL is minimum (i.e. the Moore Bound)
-  are undesirable
  - ➢ we want to decrease triangles and squares

Moore Bound (again)

Fact (the Moore Bound)

$G = (V, E)$: d-regular, n nodes, diameter $= 3$

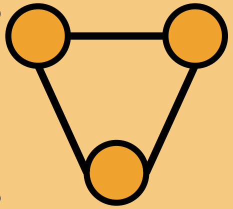
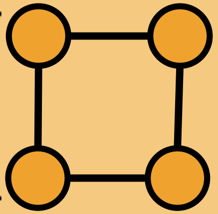
$$\binom{n}{2} \cdot \mathrm{ASPL}(G) \geq 3\binom{n}{2} - \frac{nd}{2} - nd^2$$

the ASPL when # of is maximum

ASPL Upper Bound

Theorem

$G = (V, E)$: d-regular, n nodes, diameter $= 3$

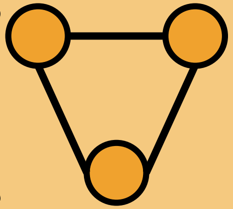
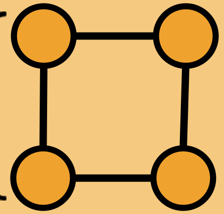
$$\binom{n}{2} \cdot \mathrm{ASPL}(G) \leq 3\binom{n}{2} - \frac{nd}{2} - nd^2 + 3\#\Bigg\{$$  $$\Bigg\} + 2\#\Bigg\{$$  $$\Bigg\}$$

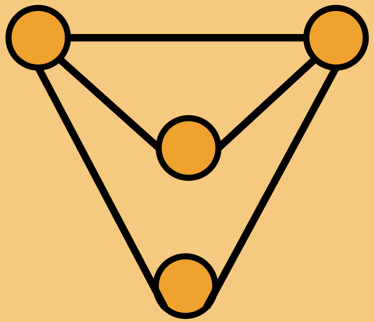
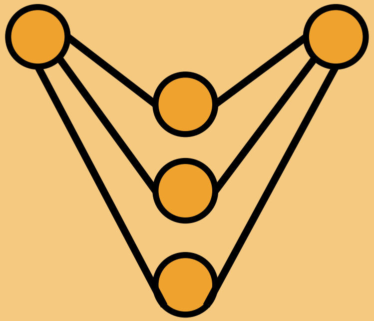
(This bound can be seen as an approximation.)

ASPL Lower Bound

Theorem

$G = (V, E)$: d-regular, n nodes, diameter $= 3$

$\binom{n}{2} \cdot \mathrm{ASPL}(G) \geq 3\binom{n}{2} - \frac{nd}{2} - nd^2 + 3\#\{$  $\}$ $+2\#\{$  $\}$

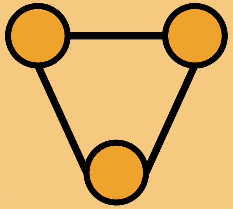
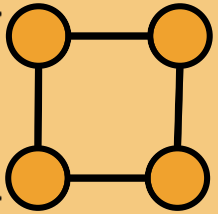
$-\#\{$  $\}$ $-\#\{$  $\}$

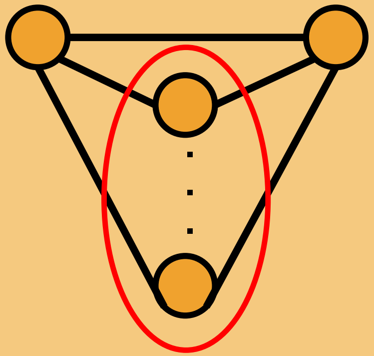
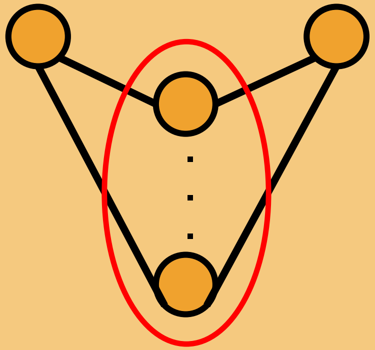
(This bound can be seen as an approximation.)

ASPL Characterization

Theorem

$G = (V, E)$: d-regular, n nodes, diameter $= 3$

$\binom{n}{2} \cdot \mathrm{ASPL}(G) = 3\binom{n}{2} - \frac{nd}{2} - nd^2 + 3\#\{$  $\} + 2\#\{$  $\}$

$+ \sum_{m=3}^{n-1} (-1)^m \Big[\#\{$  $\}$ $\#\{$  $\} \Big]$

$m-1$ nodes $\qquad$ m nodes

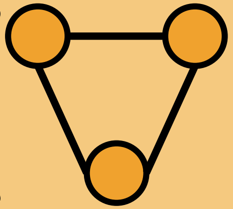
3. Proposed Algorithm

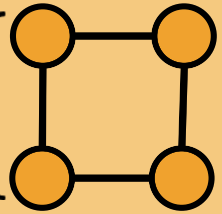
Proposed Algorithm

Evaluate graphs by

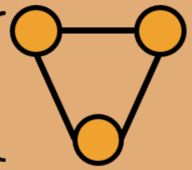
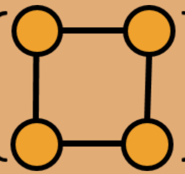
$$f(G) = 3\triangle + 2\square$$

where

$\triangle$ = # {  }

$\square$ = # {  }

Proposed Algorithm

$\binom{n}{2} \cdot ASPL(G) \leq 3 - \frac{nd}{2} - nd^2 + 3\#\{$  $\} + 2\#\{$  $\}$

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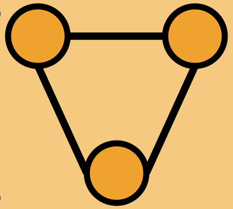
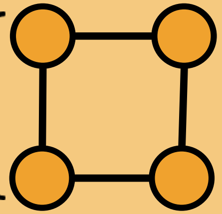
$\triangle = \#\{$  $\}$

$\square = \#\{$  $\}$

Time Complexity

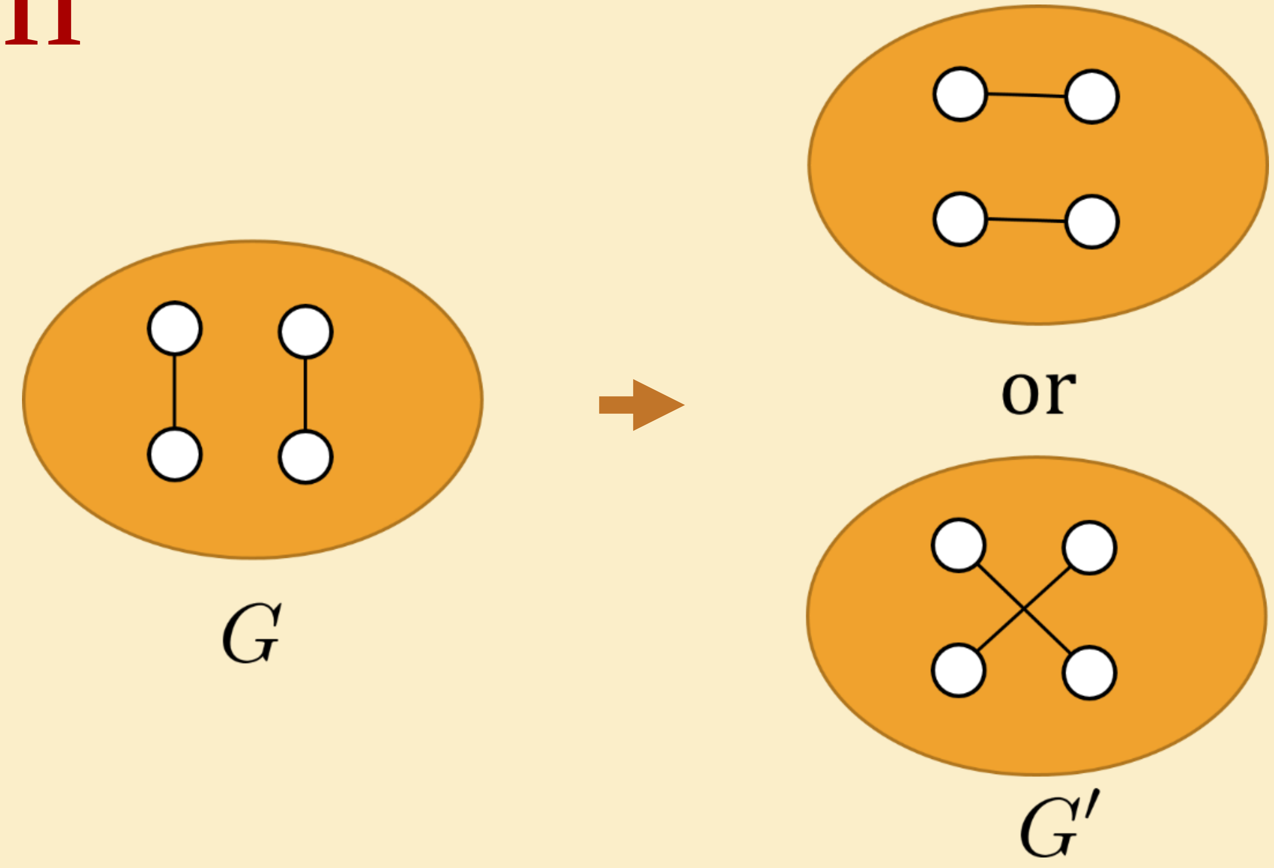
- $f(G') - f(G)$: can be calculated in $O(1)$ time

Obtained by switching two edges of G

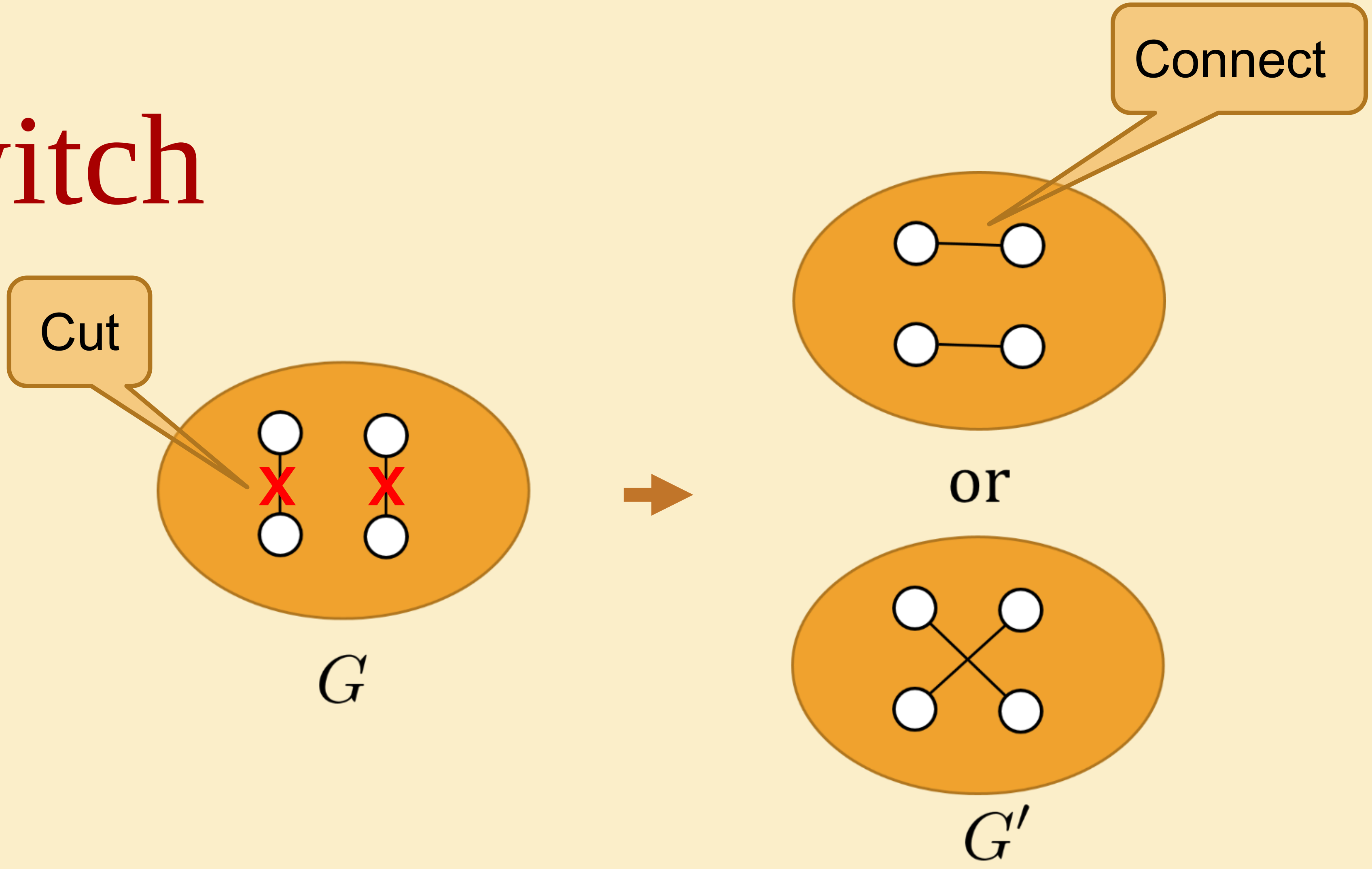
We use

- $\mathrm{T2}[i][j]$:= # of i-j paths of length 2
- $\mathrm{T3}[i][j]$:= # of non-backtracking i-j paths of length 3

Switch



Switch



How many triangles/squares appear & disappear ?

Evaluation Algorithm

Let G' be a graph obtained by switching

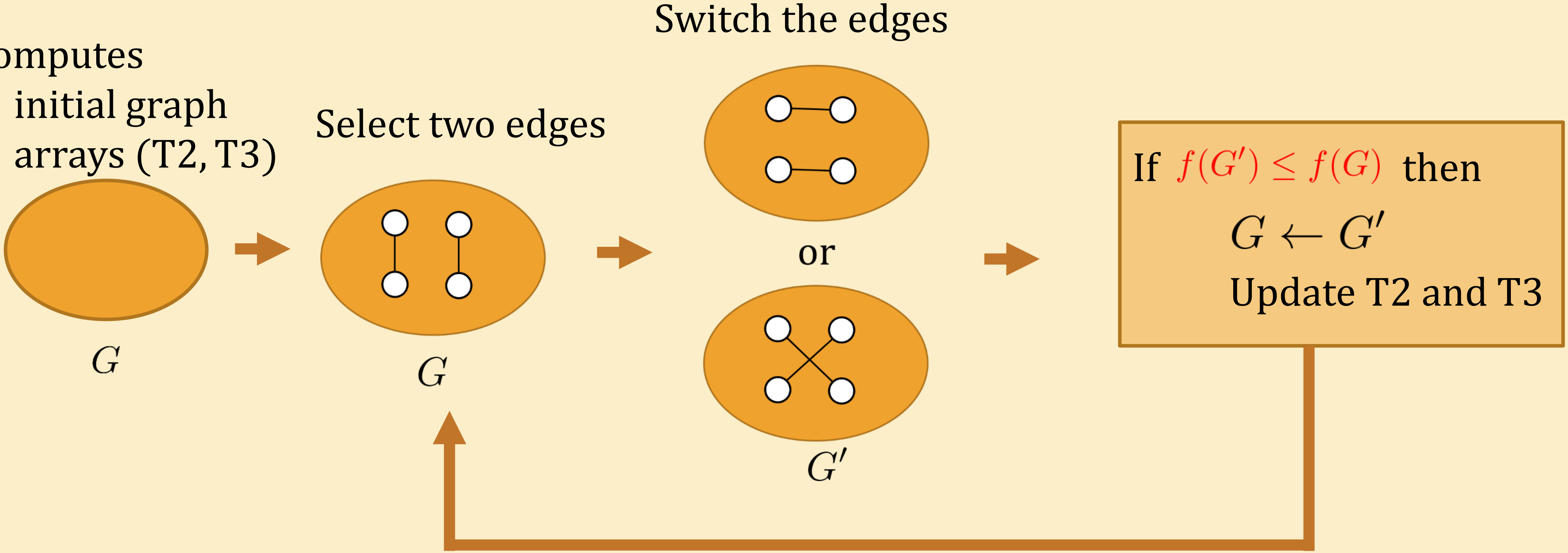
Then

$$f(G') - f(G) = 3\big(- \mathrm{T2}[a][b] - \mathrm{T2}[c][d] + \mathrm{T2}[a][c] + \mathrm{T2}[b][d] \\ - 2(\mathrm{T1}[a][d] + \mathrm{T1}[b][c])\big) \\ +2\big(- \mathrm{T3}[a][b] - \mathrm{T3}[c][d] + \mathrm{T3}[a][c] + \mathrm{T3}[b][d] \\ - 2(\mathrm{T2}[a][d] + \mathrm{T2}[b][c] - \mathrm{T1}[a][d]\mathrm{T1}[b][c])\big)$$

$f(G) = 3\triangle + 2\square$

Proposed Local Search (Iterative First Improvement)

computes
- initial graph
- arrays (T2, T3)

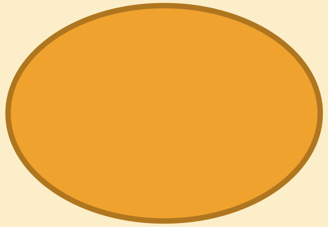


- If G cannot be improved for any edge pairs, terminate

Proposed Local Search (Iterative First Improvement)

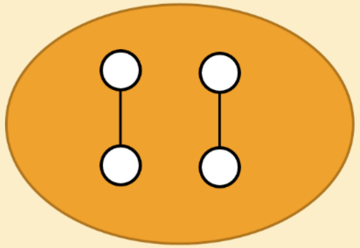
$O(nd^3)$ time

computes
- initial graph
- arrays (T2, T3)



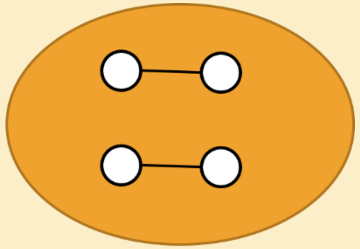
G

Select two edges

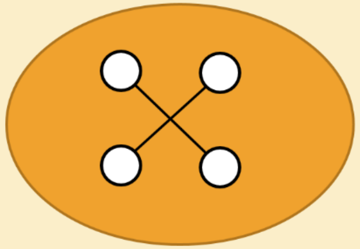


G

Switch the edges



or



G'

calculation : $O(1)$ time
with arrays T2 and T3

If $f(G') \leq f(G)$ then
$G \leftarrow G'$
Update T2 and T3

update : $O(d^2)$ time
(occurs rarely)

- If G cannot be improved for any edge pairs, terminate

$f(G) = 3\triangle + 2\square$

Proposed Local Search (Iterative First Improvement)

computes

- initial graph

We could obtain the local optimal solution!!

then

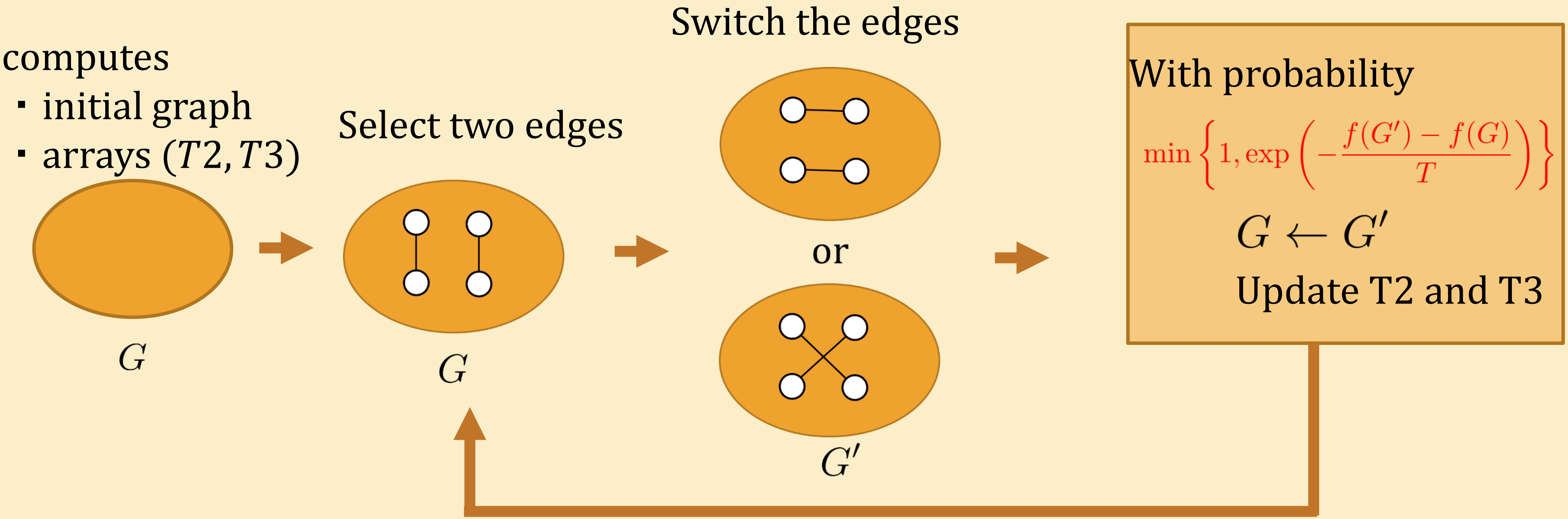
G'

G

G

- If G cannot be improved for any edge pairs, terminate

Simulated Annealing



- T is a parameter called *temperature*
- Algorithm terminates when T is sufficiently small.

Simulated Annealing

computes
- initial graph
- arrays (T…

Select two edges

Switch the edges

With probability

$$\min\left\{1, \exp\left(-\frac{f(G') - f(G)}{T}\right)\right\}$$

$G \leftarrow G'$

Update T2 and T3

- High T → random search
- Low T → Similar to Iterative First Improvement

We decrease T gradually.

G

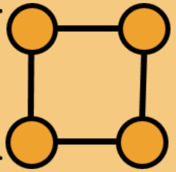
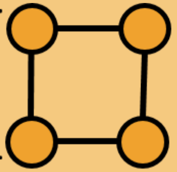
G'

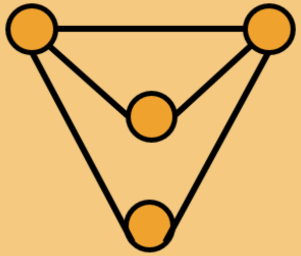
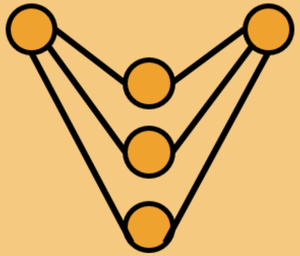
- T is a parameter called *temperature*
- Algorithm terminates when T is sufficiently small.

4. Numerical Experiments

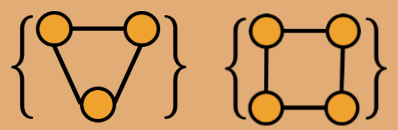
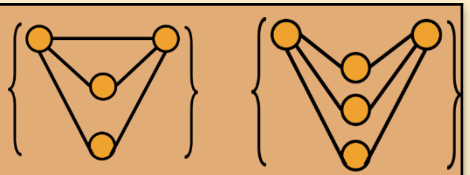
Numerical Experiments (1/2)

Check the accuracy of approximations of the ASPL :

- $\binom{n}{2} \cdot ASPL(G) \geq 3 - \frac{nd}{2} - nd^2$ (the Moore Bound)
- $\binom{n}{2} \cdot ASPL(G) \leq 3 - \frac{nd}{2} - nd^2 + 3\#\{$  $\}$ $+2\#\{$  $\}$
- $\binom{n}{2} \cdot ASPL(G) \geq 3 - \frac{nd}{2} - nd^2 + 3\#\{$  $\}$ $+2\#\{$  $\}$

  $-\#\{$  $\}$ $-\#\{$  $\}$

Numerical Experiments (1/2)

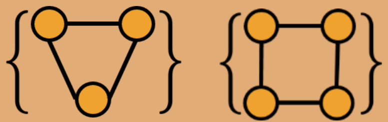
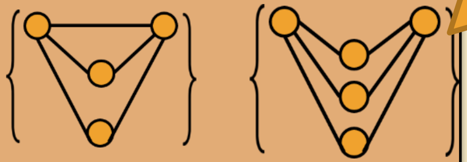
$(\boldsymbol{n}, \boldsymbol{d})$	**Moore**		
$(4096, 60)$	-0.1206	0.0355	-0.0074
$(4096, 64)$	-0.1544	0.0523	-0.0124
$(10000, 60)$	-0.0209	0.0024	-0.0002
$(10000, 64)$	-0.0270	0.0036	-0.0003

relative error:
(approx. val – ASPL) / ASPL

Numerical Experiments

Better than 

But difficult to calculation

$(\boldsymbol{n}, \boldsymbol{d})$	**Moore**		
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$(10000, 60)$	-0.0209	0.0024	-0.0002
$(10000, 64)$	-0.0270	0.0036	-0.0003

Graph is sparse
→ higher accuracy

Numerical Experiments (2/2)

- Apply the proposed algorithm.
- (n, d) for which $\mathrm{diameter} = 3$ and sparse
  - $(n, d) = (10000, 60), (10000, 64)$
- Start with random regular graphs.
- Compare the Iterative First Improvement (IFI) and the Simulated Annealing (SA). (After the SA, do IFI)

Numerical Experiments (2/2)

- Apply the proposed algorithm.
- (n, d) for which diameter $= 3$ and sparse
  - ➢ $(n, d) = (10000, 60), (10000, 64)$

Some speed-up techniques (omit in this presentation)

- Start with random regu… …hs.
- Compare the Iterative First Improvement (IFI) and the Simulated Annealing (SA). (After the SA, do IFI)

Numerical Experiments (2/2)

initial temperature $T_0 = 11$
k-th temperature $T_k = T_0 / \log k$

	Random	**IFI**		**SA**	
(n, d)	ASPL gap	ASPL gap	Time	ASPL gap	Time
$(10000, 60)$	21.3×10^{-3}	6.8×10^{-3}	40h 30m	6.2×10^{-3}	60 days
$(10000, 64)$	27.7×10^{-3}	10.8×10^{-3}	37h 00m	10.0×10^{-3}	60 days

ASPL gap = (solution ASPL – Moore Bound) / solution ASPL

Numerical Experiments (2)

The best graphs in Graph Golf!!

	Random	**IFI**			
(n, d)	ASPL gap	ASPL gap	Time	ASPL gap	Time
$(10000, 60)$	21.3×10^{-3}	6.8×10^{-3}	40h 30m	6.2×10^{-3}	60 days
$(10000, 64)$	27.7×10^{-3}	10.8×10^{-3}	37h 00m	10.0×10^{-3}	60 days

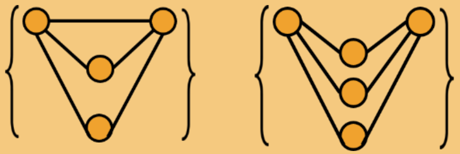
ASPL gap = (solution ASPL – Moore Bound) / solution ASPL

5. Conclusion

Conclusion

For graphs of diameter 3

- Characterize the ASPL by # of specific structures in the graph.
- Propose an efficient algorithm calculating one of the upper bounds.
- We found low ASPL graphs by the proposed algorithm.

Future Work 1: Evaluation algorithm of 

Future Work 2: Graphs of diameter 4 or more...