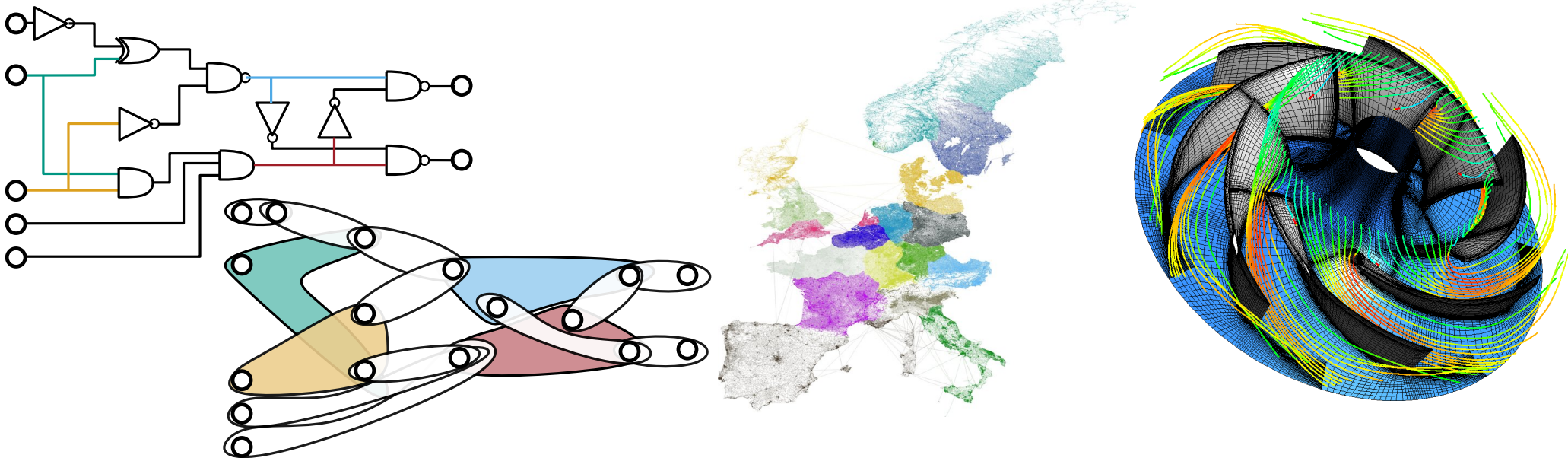


Brief Introduction to Hypergraph Partitioning

Bioinformatics Programming Practical Kickoff Meeting · April 19, 2018
Sebastian Schlag

INSTITUTE OF THEORETICAL INFORMATICS · ALGORITHMICS GROUP

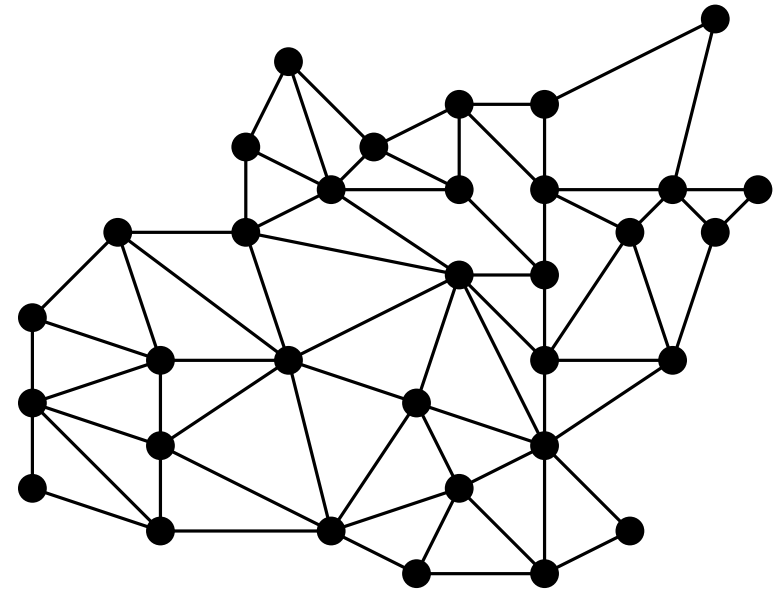


Graphs and Hypergraphs

Graph $G = (V, E)$

vertices   edges

- models **relationships** between **objects**
- dyadic (**2-ary**) relationships

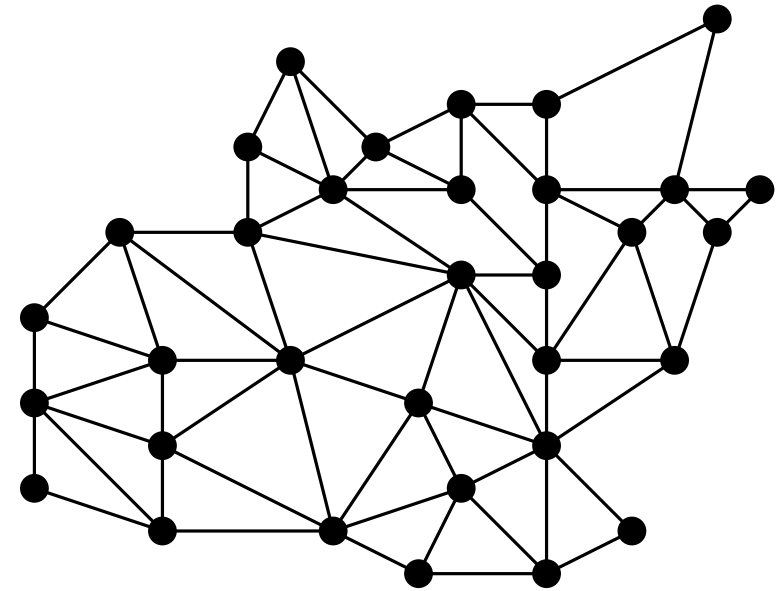


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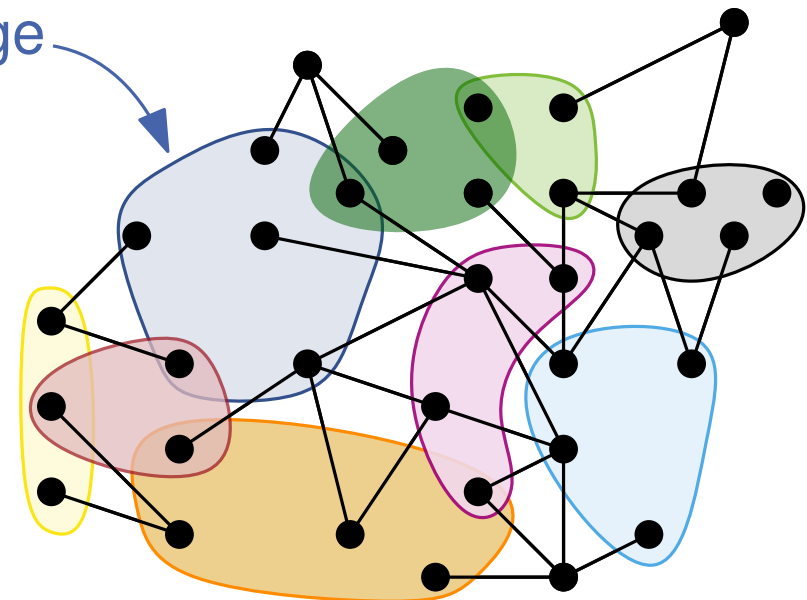
- models **relationships** between **objects**
- dyadic (**2-ary**) relationships



Hypergraph $H = (V, E)$

- generalization of a graph
 \Rightarrow hyperedges connect ≥ 2 nodes
- arbitrary (**d-ary**) relationships
- edge set $E \subseteq \mathcal{P}(V) \setminus \emptyset$

hyperedge 



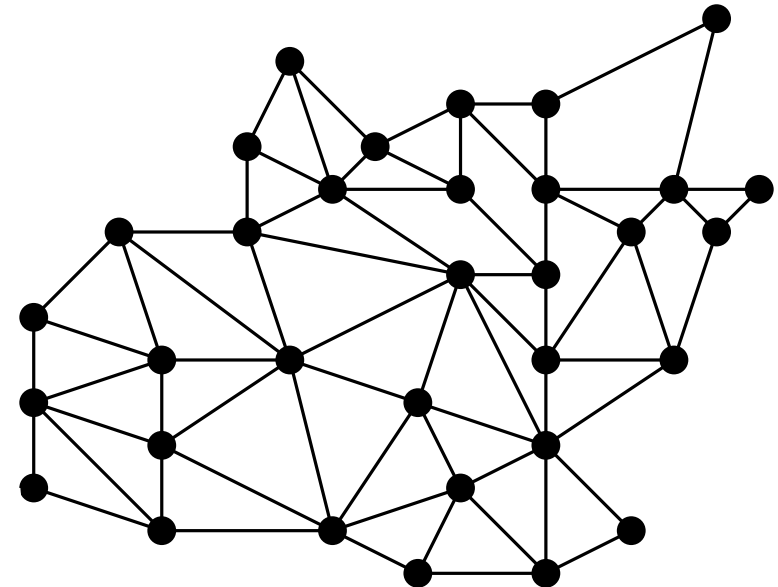
ε -Balanced Graph and Hypergraph Partitioning

Partition (hyper)graph $G = (V, E, c : V \rightarrow \mathbb{R}_{>0}, \omega : E \rightarrow \mathbb{R}_{>0})$
into k disjoint blocks V_1, \dots, V_k s.t.

- blocks V_i are **roughly equal-sized**:

$$c(V_i) \leq (1 + \varepsilon) \left\lceil \frac{c(V)}{k} \right\rceil$$

- **objective** function on edges is **minimized**



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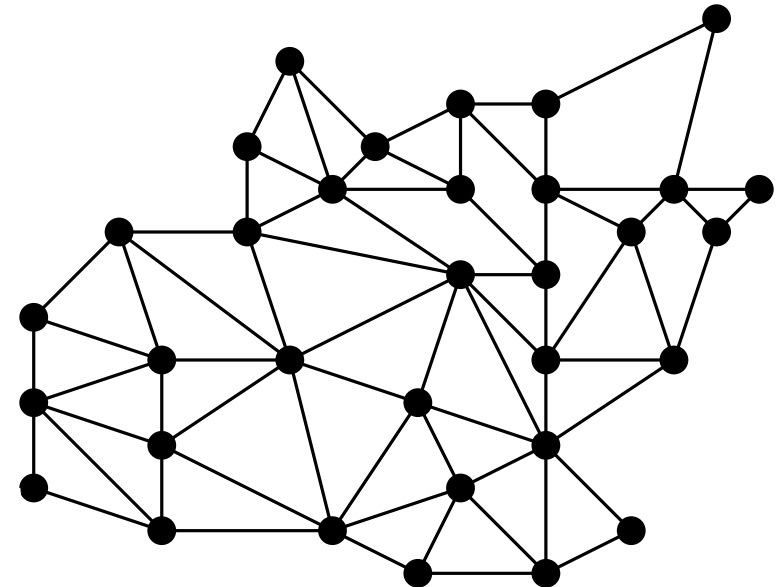
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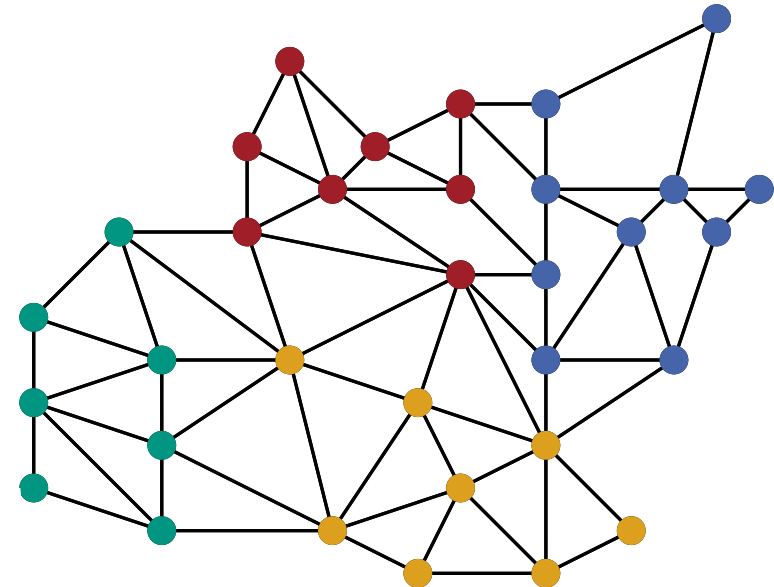
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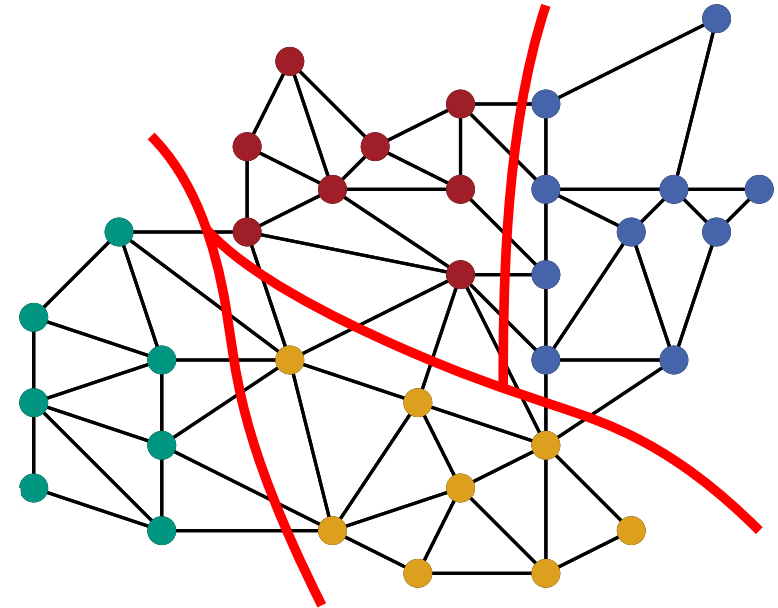
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Common Objectives:

- Graphs:

- **cut**: $\sum_{e \in \text{cut}} \omega(e)$



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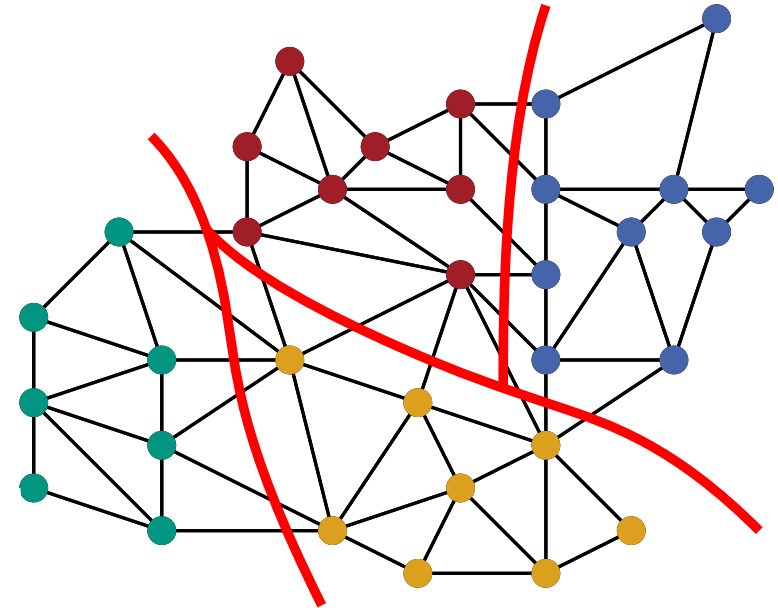
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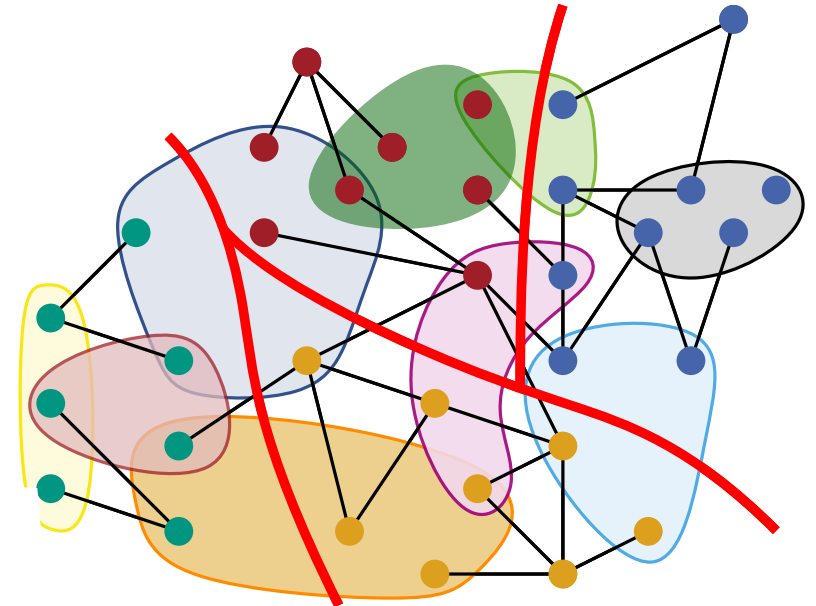
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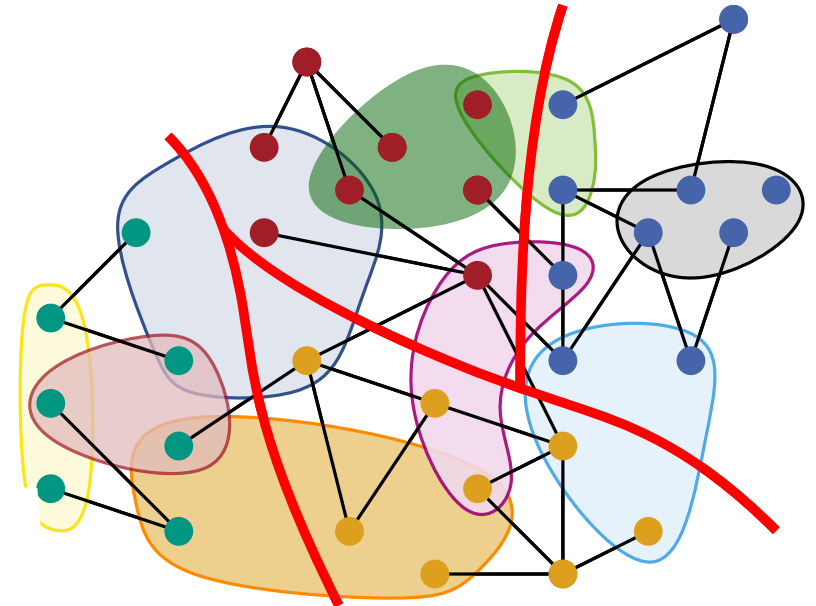
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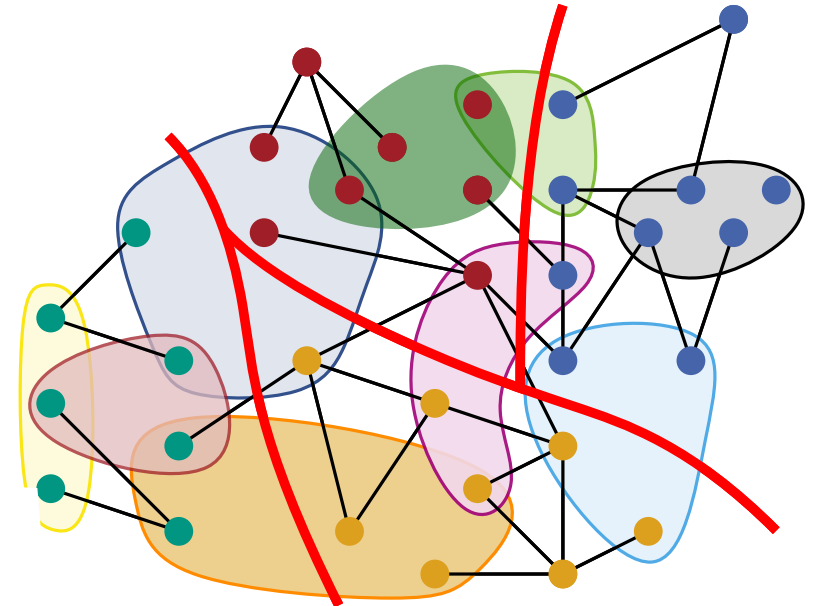
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- **cut**: $\sum_{e \in \text{cut}} \omega(e) = 10$



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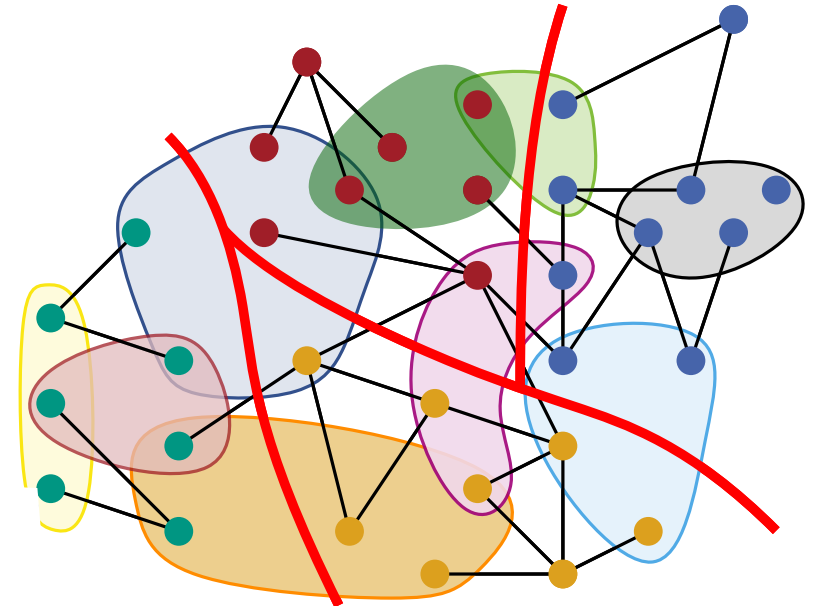
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- **connectivity**: $\sum_{e \in \text{cut}} (\lambda - 1) \omega(e)$



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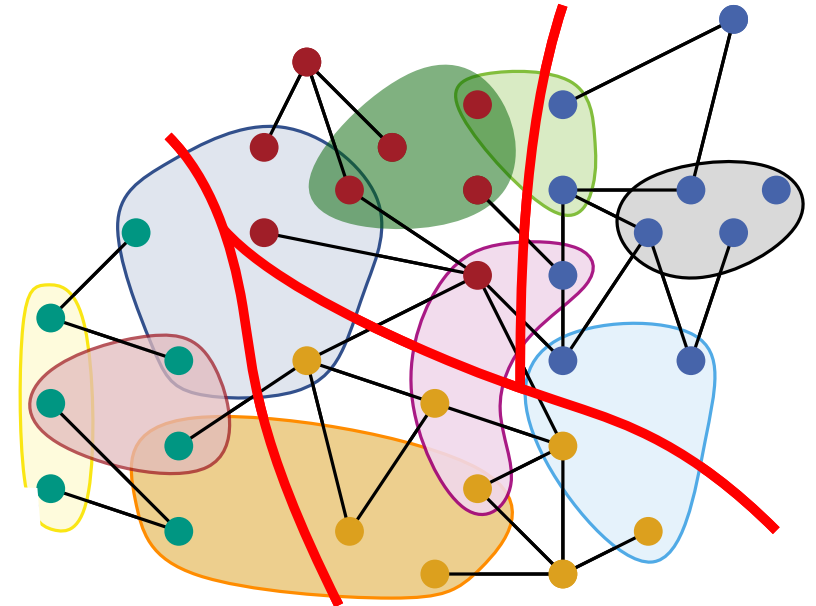
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blocks connected by e



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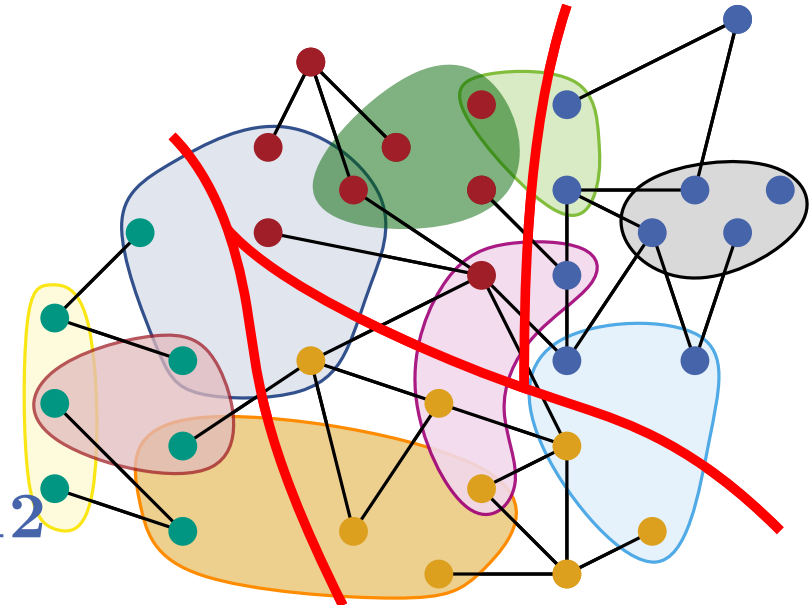
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- Hypergraphs:

- **cut**: $\sum_{e \in \text{cut}} \omega(e) = 10$

- **connectivity**: $\sum_{e \in \text{cut}} (\lambda - 1) \omega(e) = 12$

blocks connected by e

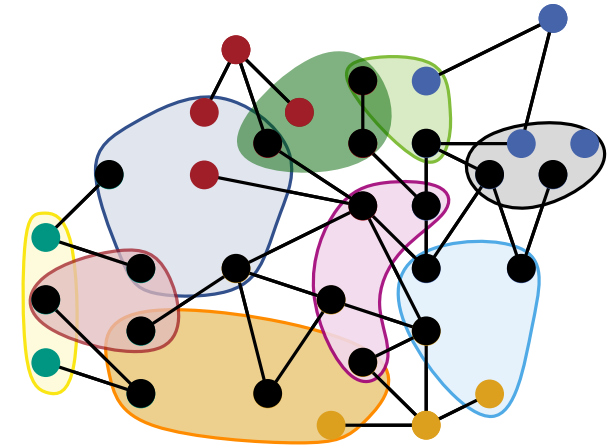


Variants of Standard Hypergraph Partitioning

Possibly relevant/interesting variants:

Partitioning with Fixed Vertices:

- some vertices are preassigned to blocks
- fixed vertices must remain in their block



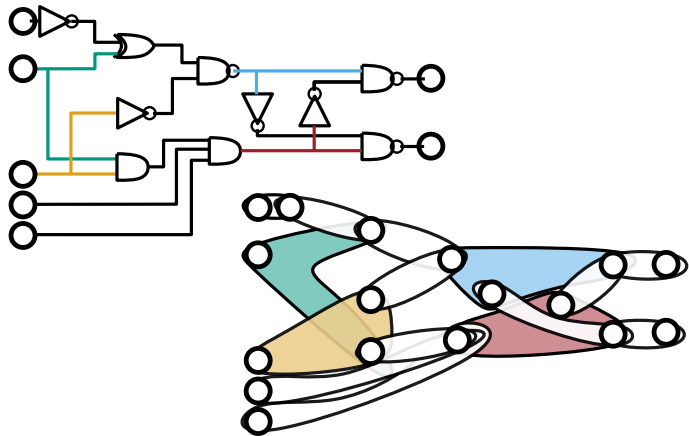
Partitioning with Variable Block Weights:

- individual block weights $U := \{U_1, \dots, U_k\}$
- $\forall V_i : c(V_i) \leq U_i$



$$U := \{12, 8, 11, 6\}$$

Applications



VLSI Design



Warehouse Optimization

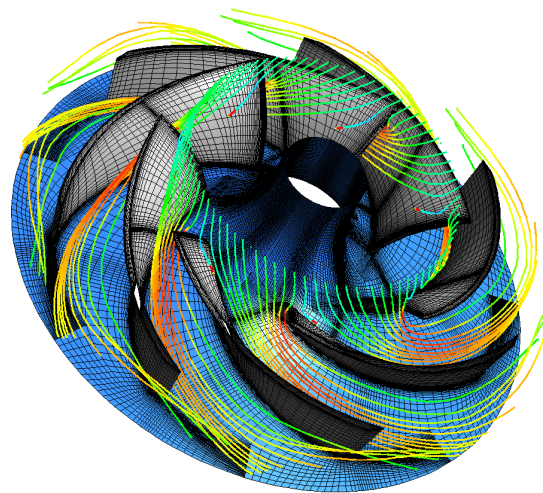
[Martin Grandjean, via Wikimedia Commons]



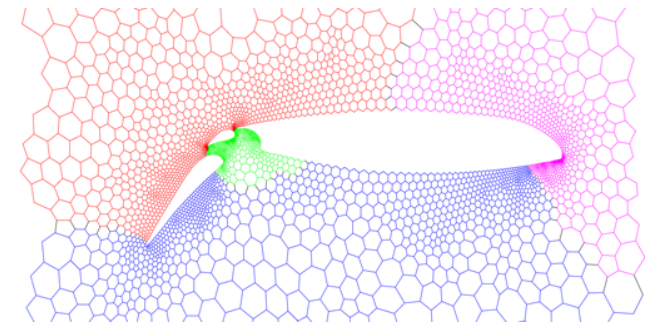
Complex Networks



Route Planning



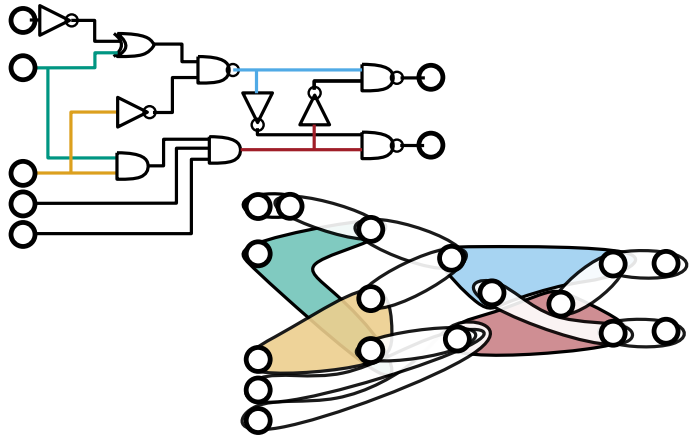
Simulation



$$\mathbb{R}^{n \times n} \ni Ax = b \in \mathbb{R}^n$$

Scientific Computing

Applications



VLSI Design



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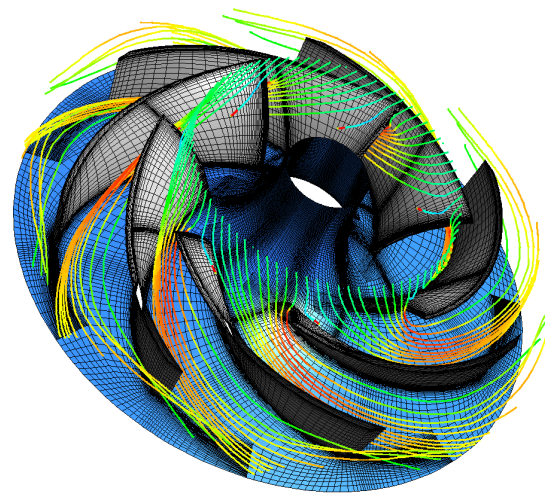
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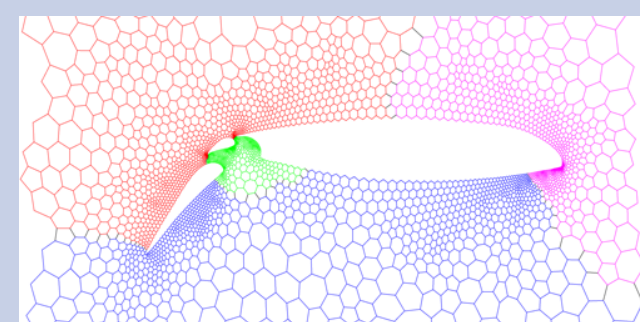
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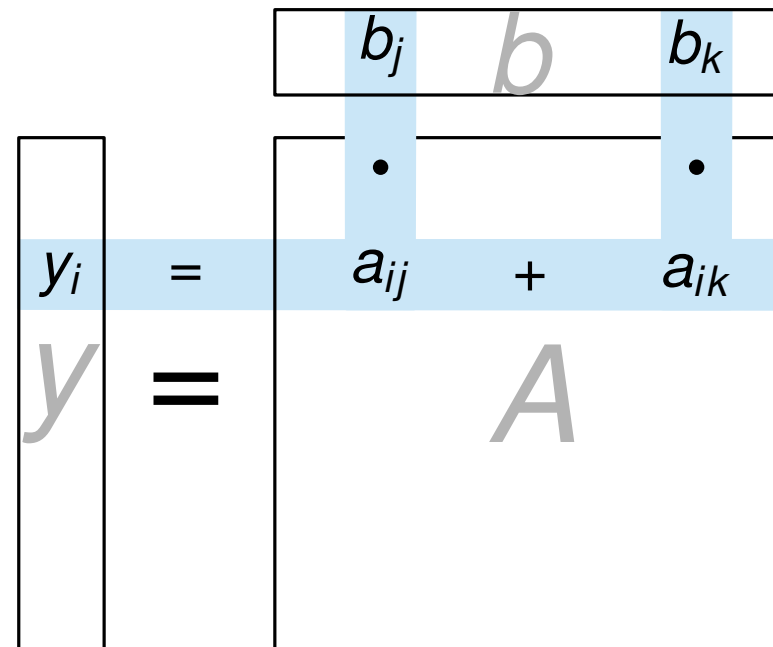
A visualization of a scientific computing problem. It shows a grid of points (hexagons) with a central region where the points are colored in a gradient from red to blue. The grid is surrounded by a blue border.

$$\mathbb{R}^{n \times n} \ni Ax = b \in \mathbb{R}^n$$

Scientific Computing

Parallel Sparse-Matrix Vector Product ($\text{SpM} \times \text{V}$)

$$y = A b$$

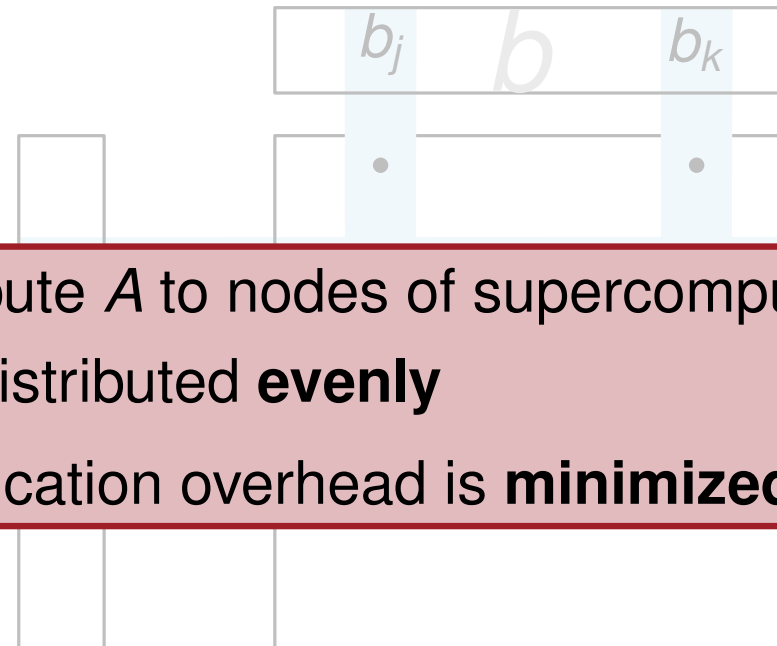


Setting:

- repeated $\text{SpM} \times \text{V}$ on supercomputer
- A is large \Rightarrow distribute on multiple nodes
- symmetric partitioning $\Rightarrow y$ & b divided conformally with A

Parallel Sparse-Matrix Vector Product ($\text{SpM} \times \text{V}$)

$$y = A b$$



Task: distribute A to nodes of supercomputer such that

- work is distributed **evenly**
- communication overhead is **minimized**

Setting:

- repeated $\text{SpM} \times \text{V}$ on supercomputer
- A is large \Rightarrow distribute on multiple nodes
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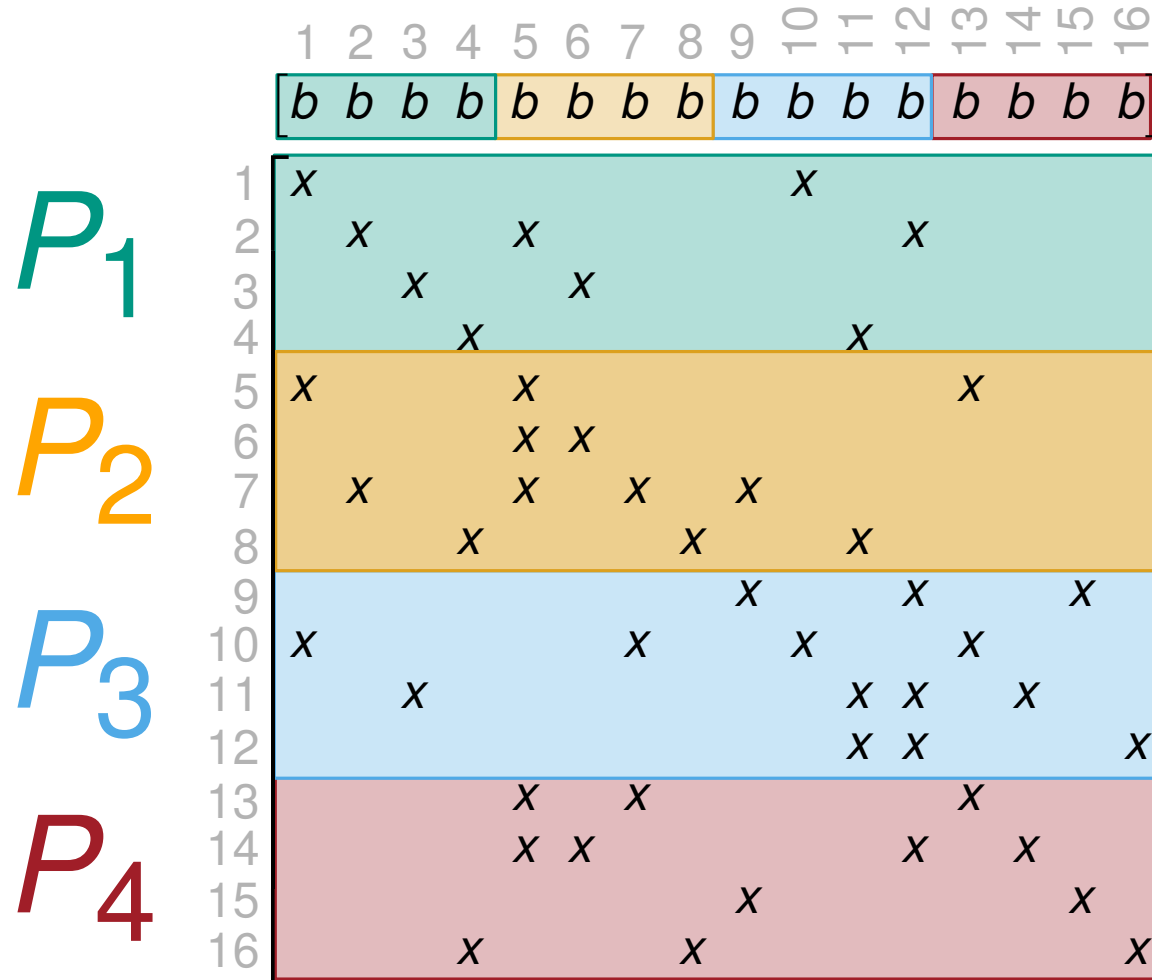
Naive Approach: Rowwise Decomposition

$$A \in \mathbb{R}^{16 \times 16}$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	[b b b b b b b b b b b b b b b b]															
1	x									x						
2		x			x							x				
3			x			x										
4				x							x					
5	x				x								x			
6					x	x										
7		x			x		x		x							
8				x				x			x					
9									x			x			x	
10	x						x			x			x			
11			x								x	x		x		
12											x	x				x
13					x		x						x			
14					x	x						x		x		
15									x						x	
16				x				x								x

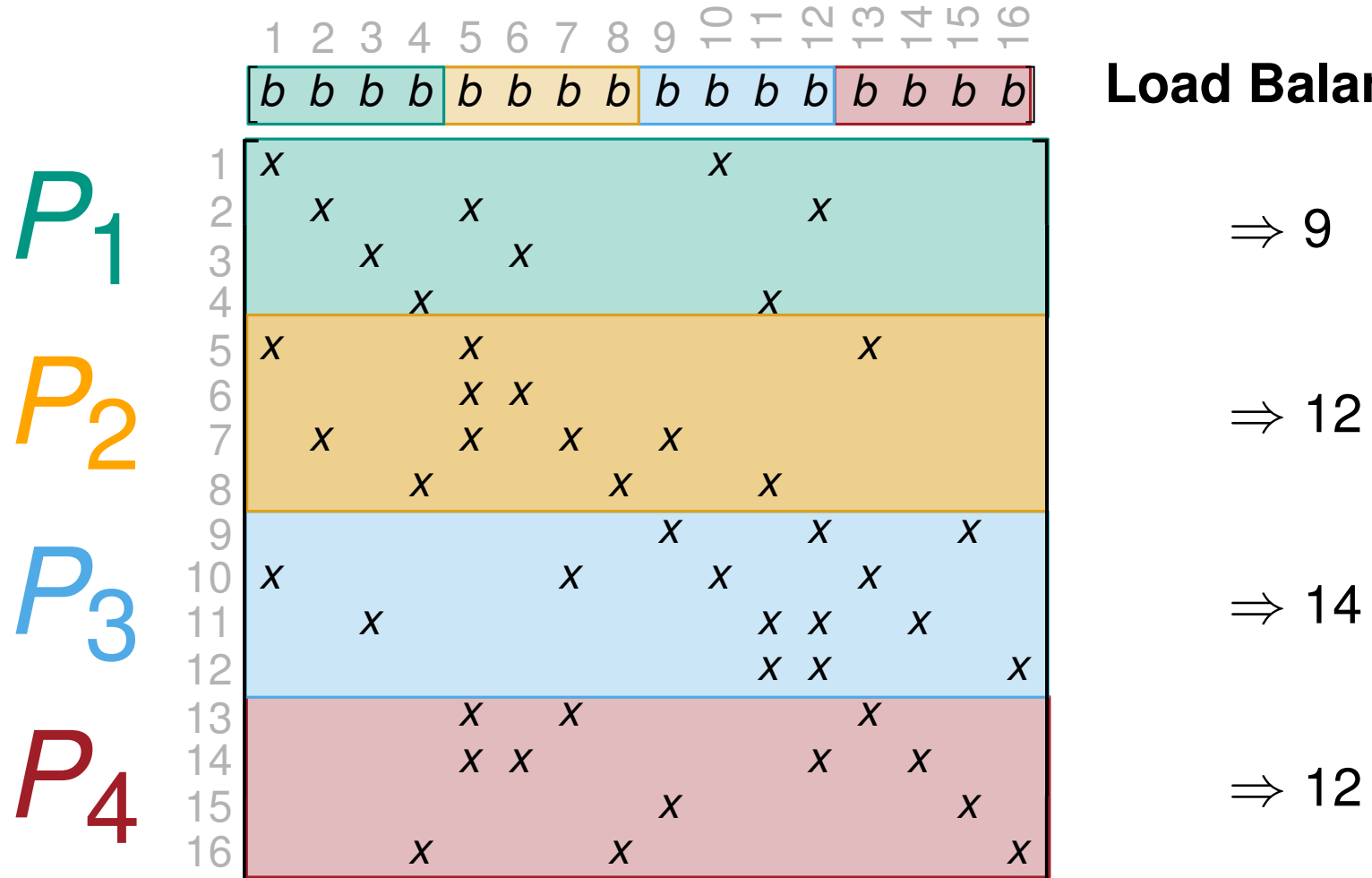
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Load Balancing?

⇒ 9

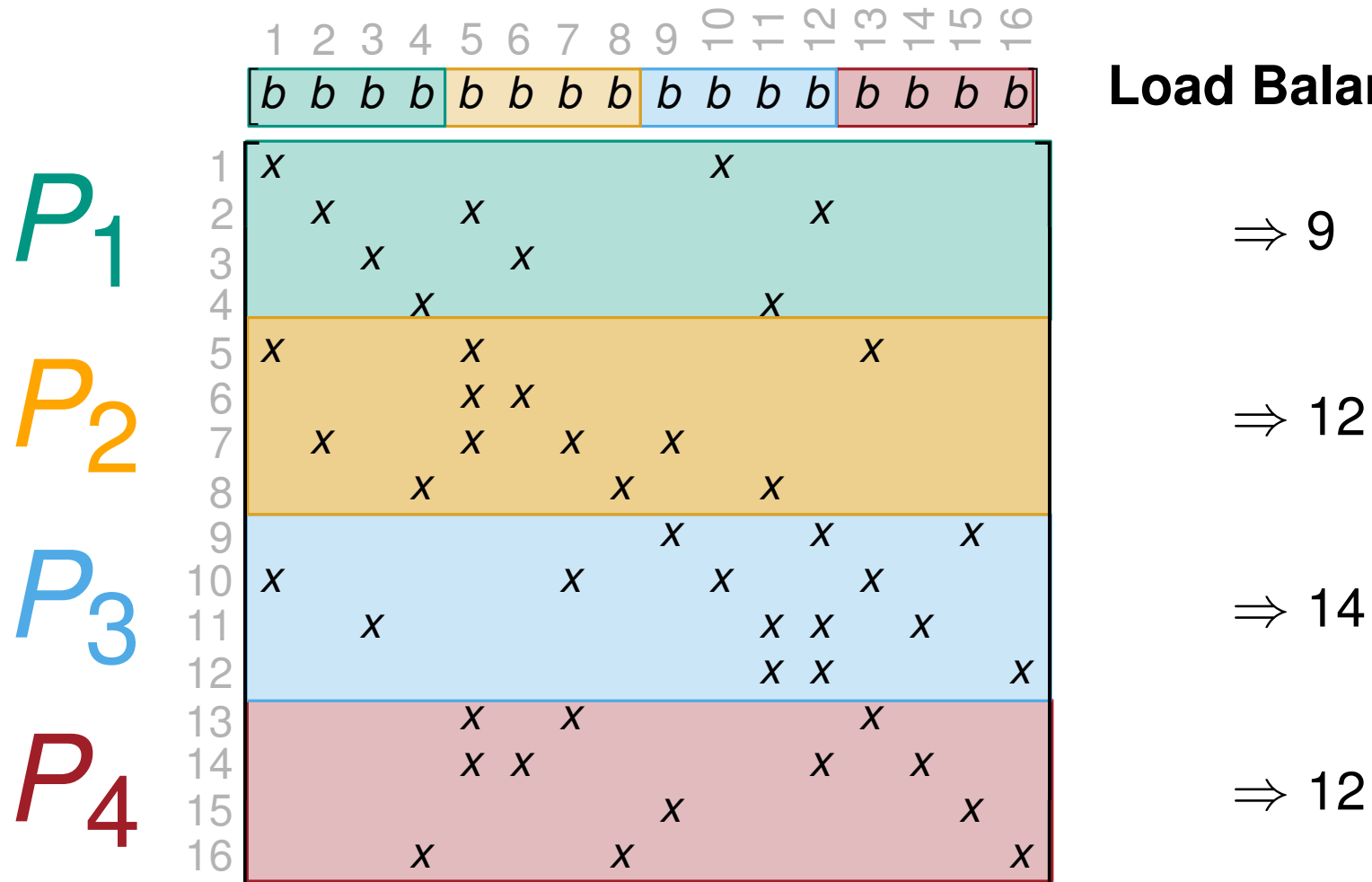
⇒ 12

⇒ 14

⇒ 12

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Load Balancing?

$\Rightarrow 9$

$\Rightarrow 12$

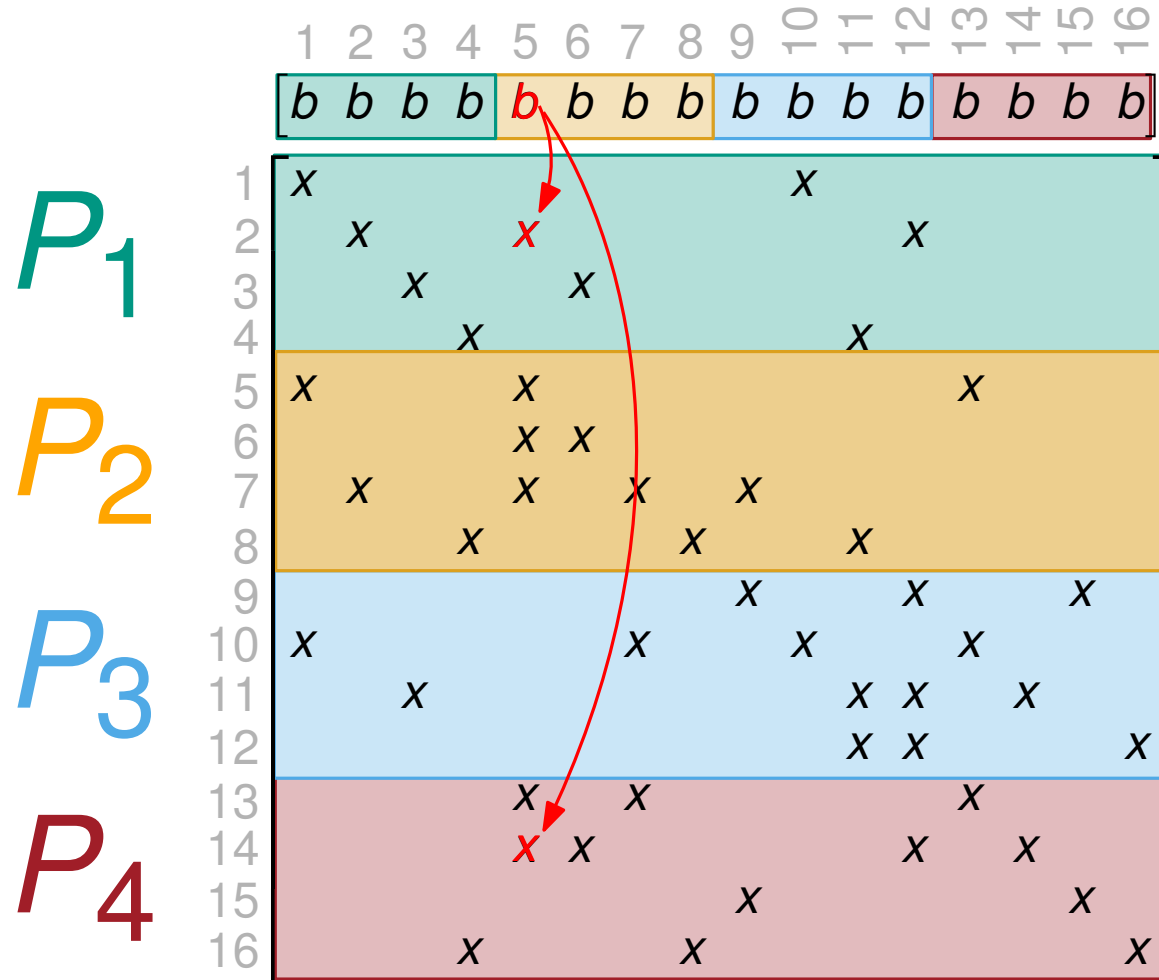
$\Rightarrow 14$

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Communication Volume?

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Load Balancing?

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⇒ 12

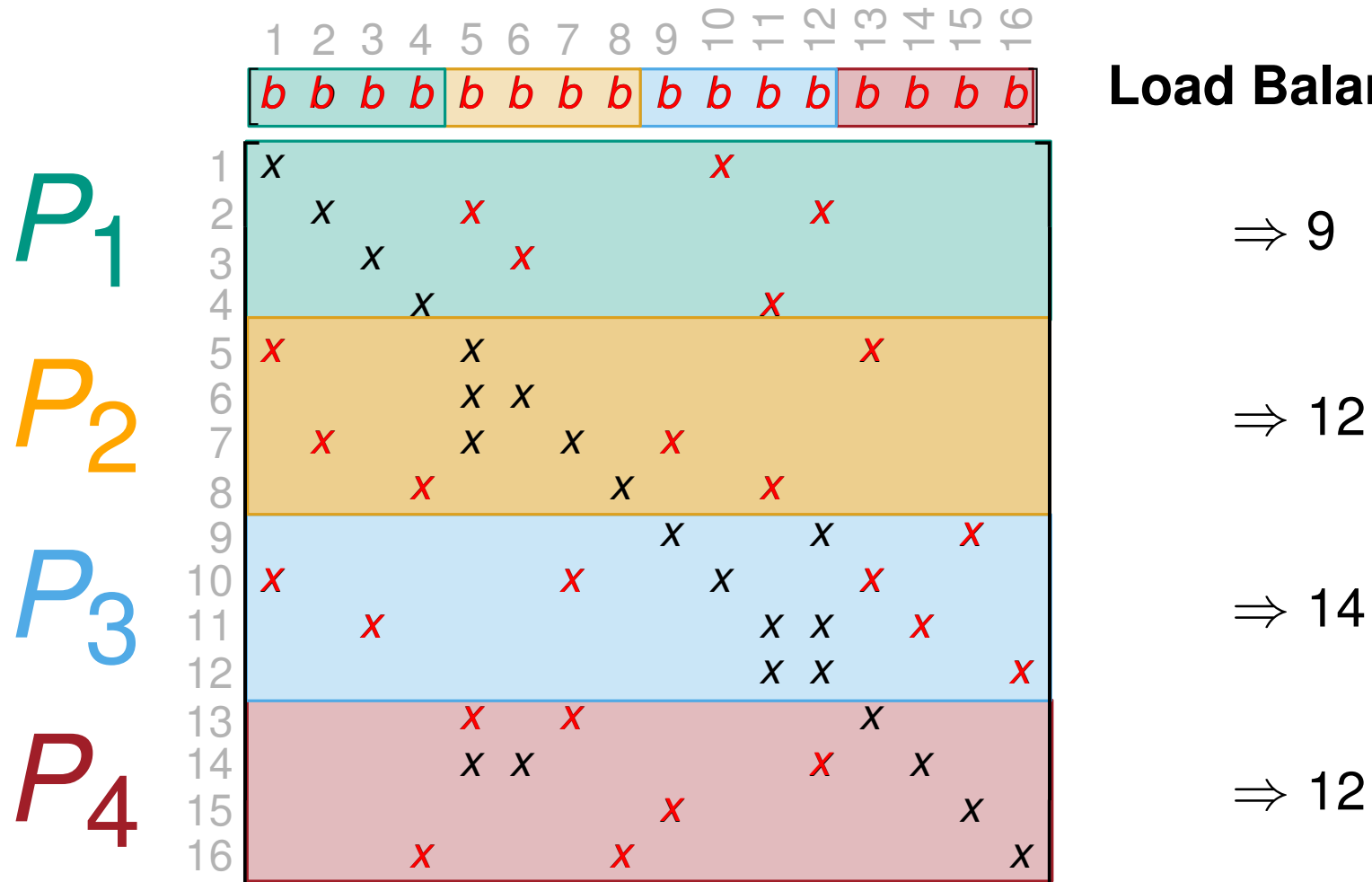
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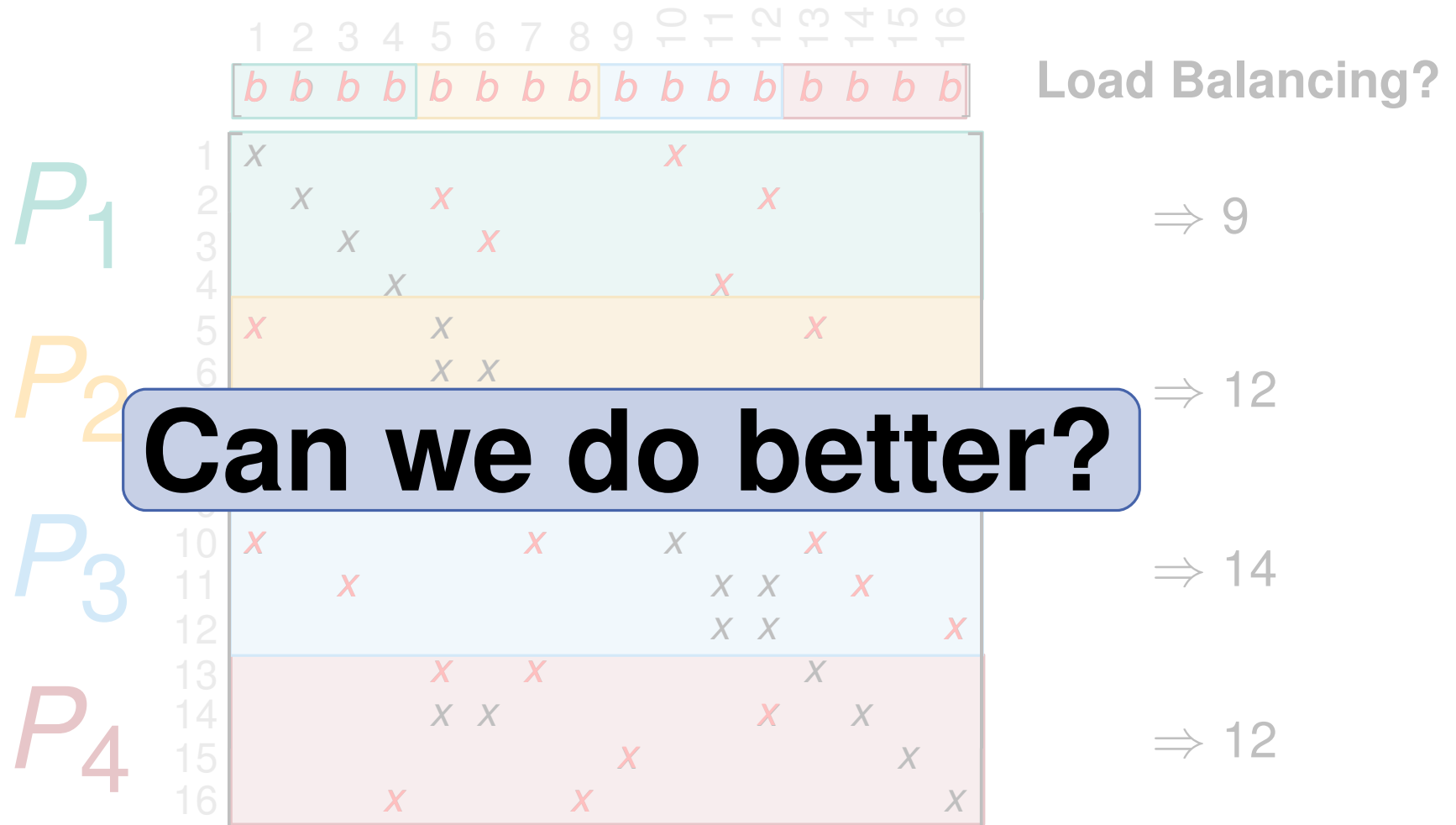
⇒ 14

⇒ 12

Communication Volume? ⇒ 24 entries!

Naive Approach: Rowwise Decomposition

$$A \in \mathbb{R}^{16 \times 16}$$



Communication Volume? $\Rightarrow 24$ entries!

From $\text{SpM} \times V$ to Hypergraph Partitioning

$$A \in \mathbb{R}^{16 \times 16} \Rightarrow H = (V_R, E_C)$$

- one vertex per row:

$$\Rightarrow V_R = \{v_1, v_2, \dots, v_{16}\}$$

- one hyperedge per column:

$$\Rightarrow E_C = \{e_1, e_2, \dots, e_{16}\}$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
1	x									x						
2		x			x							x				
3			x			x										
4				x							x					
5	x				x								x			
6					x	x										
7		x			x		x		x							
8				x				x			x					
9									x			x				x
10	x						x			x			x			
11			x								x	x		x		
12											x	x				x
13					x		x						x			
14					x	x						x		x		
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16				x				x								x

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$v_i \in V_R$:

- task to compute inner product of row i with b
- $\Rightarrow c(v_i) := \# \text{ nonzeros}$

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1	x				x					x						
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3			x			x										
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6					x	x										
7		x			x		x		x							
8				x				x			x					
9									x			x			x	
10	x						x			x			x			
11			x								x	x		x		
12											x	x				x
13					x		x						x			
14					x	x						x		x		
15									x						x	
16				x				x								x

$e_j \in E_C$: set of vertices that need b_j

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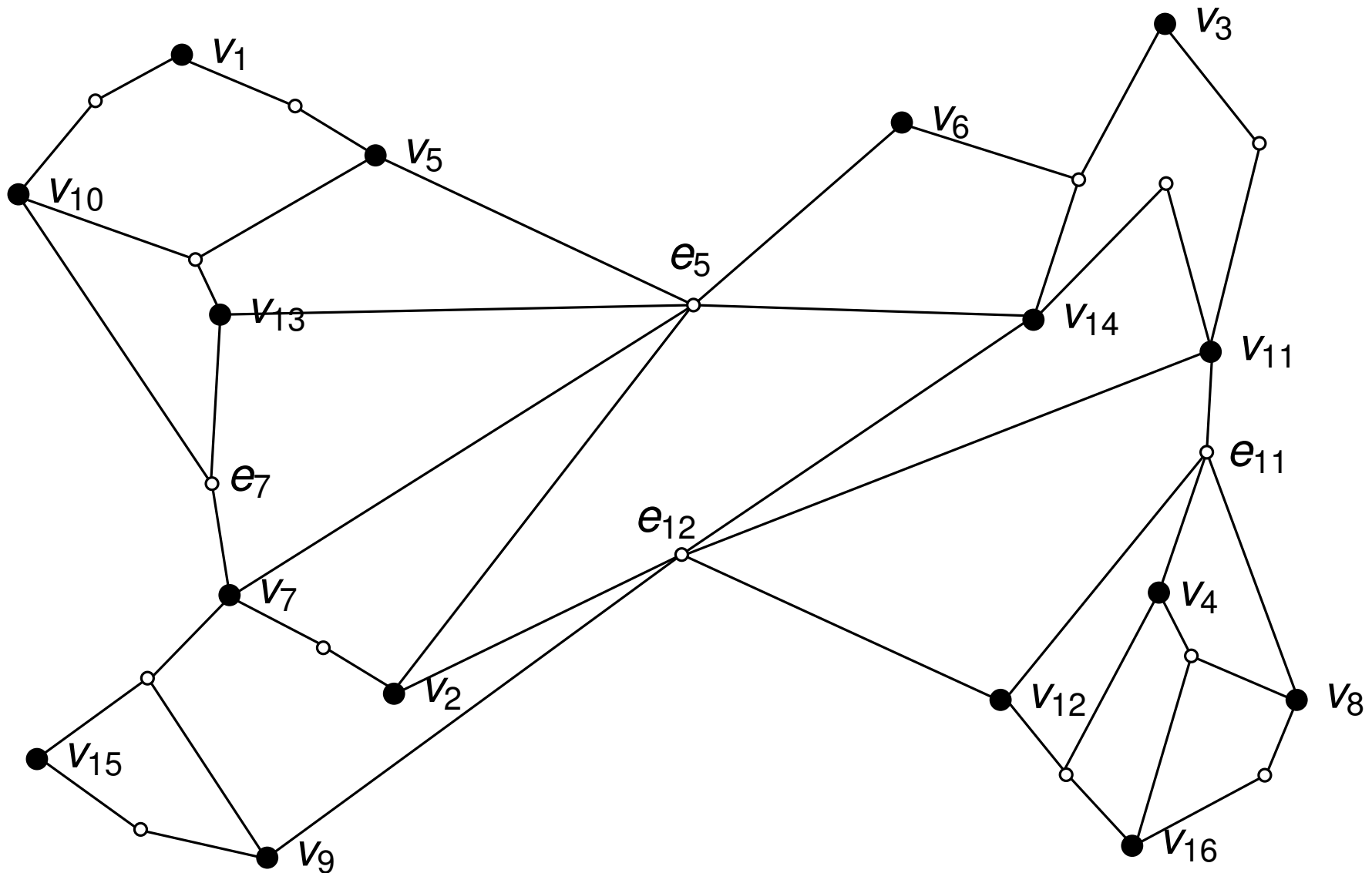
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2		x			x							x				
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11																
12										x	x					x
13					x		x						x			
14					x	x					x			x		
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16				x				x								x

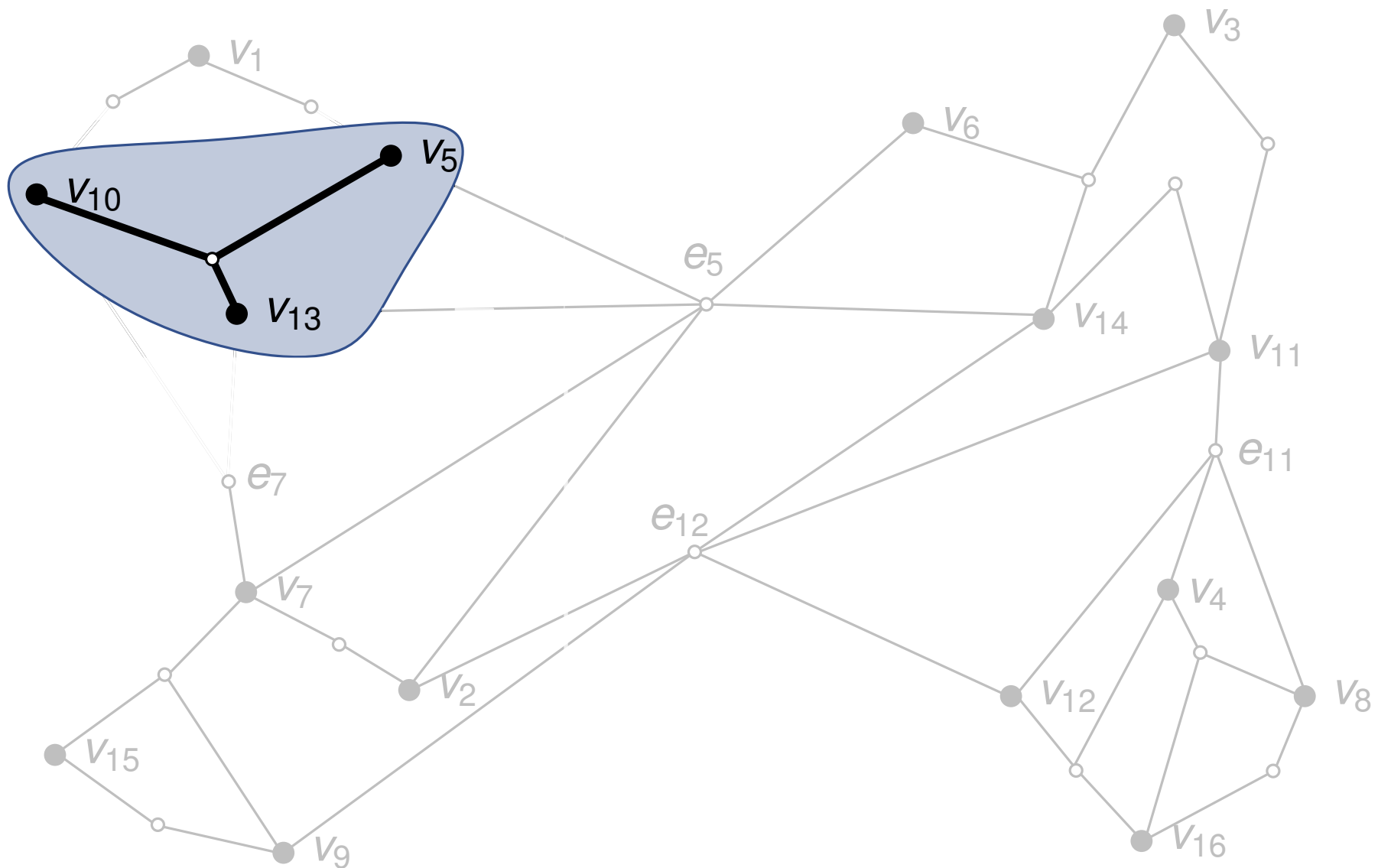
Solution: ε -balanced partition of H

- balanced partition \rightsquigarrow computational load balance
- small $(\lambda - 1)$ -cutsizes \rightsquigarrow minimizing communication volume

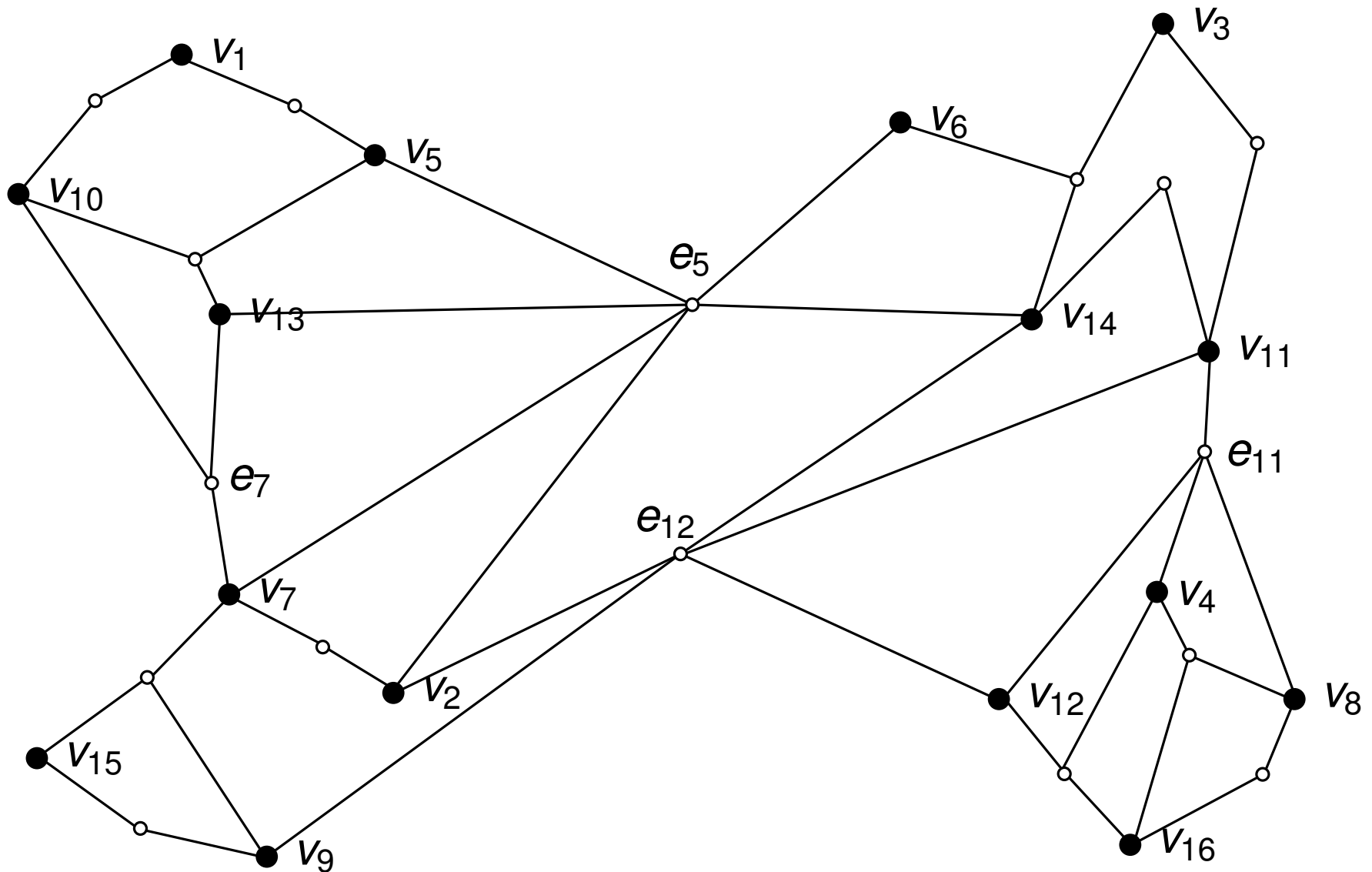
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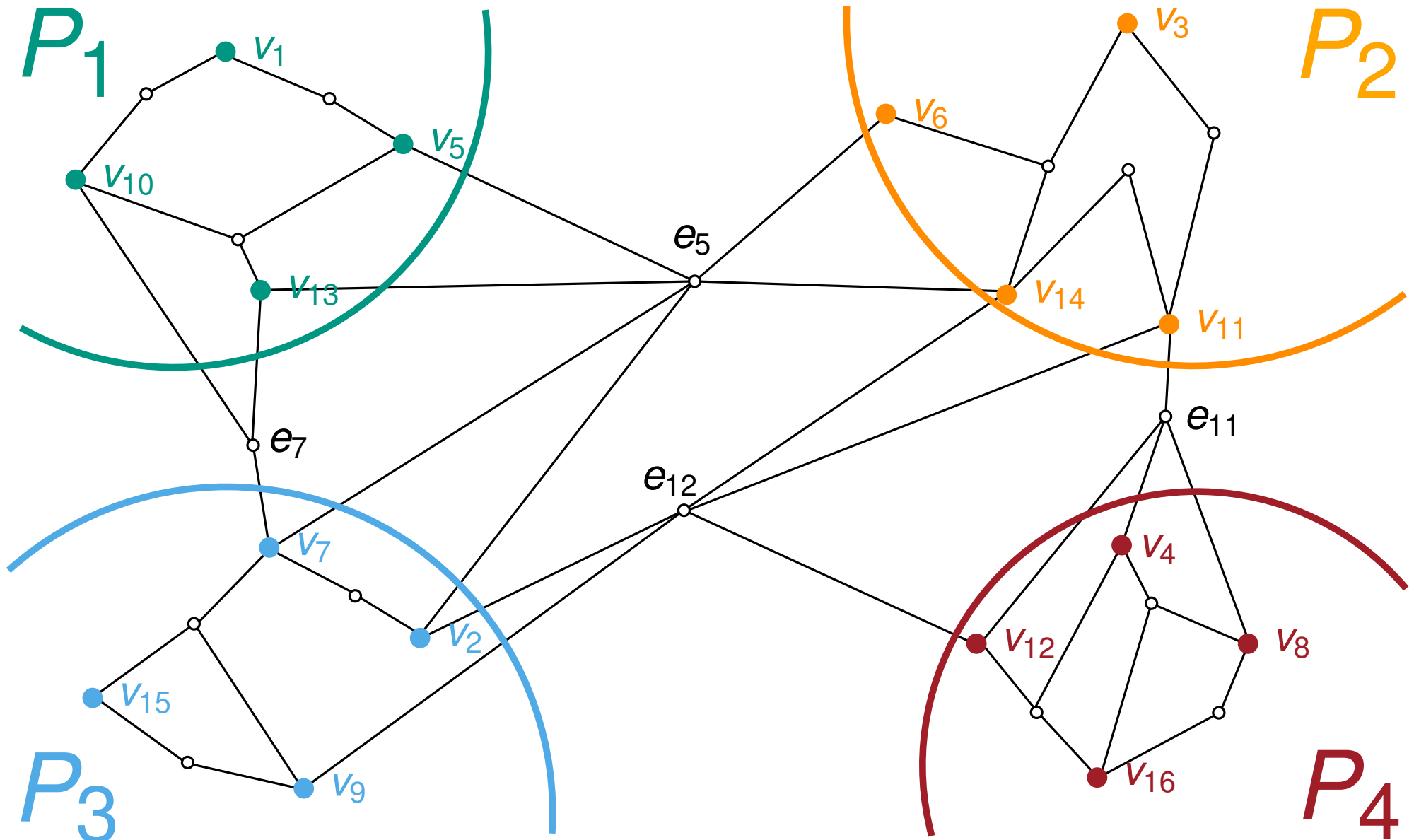
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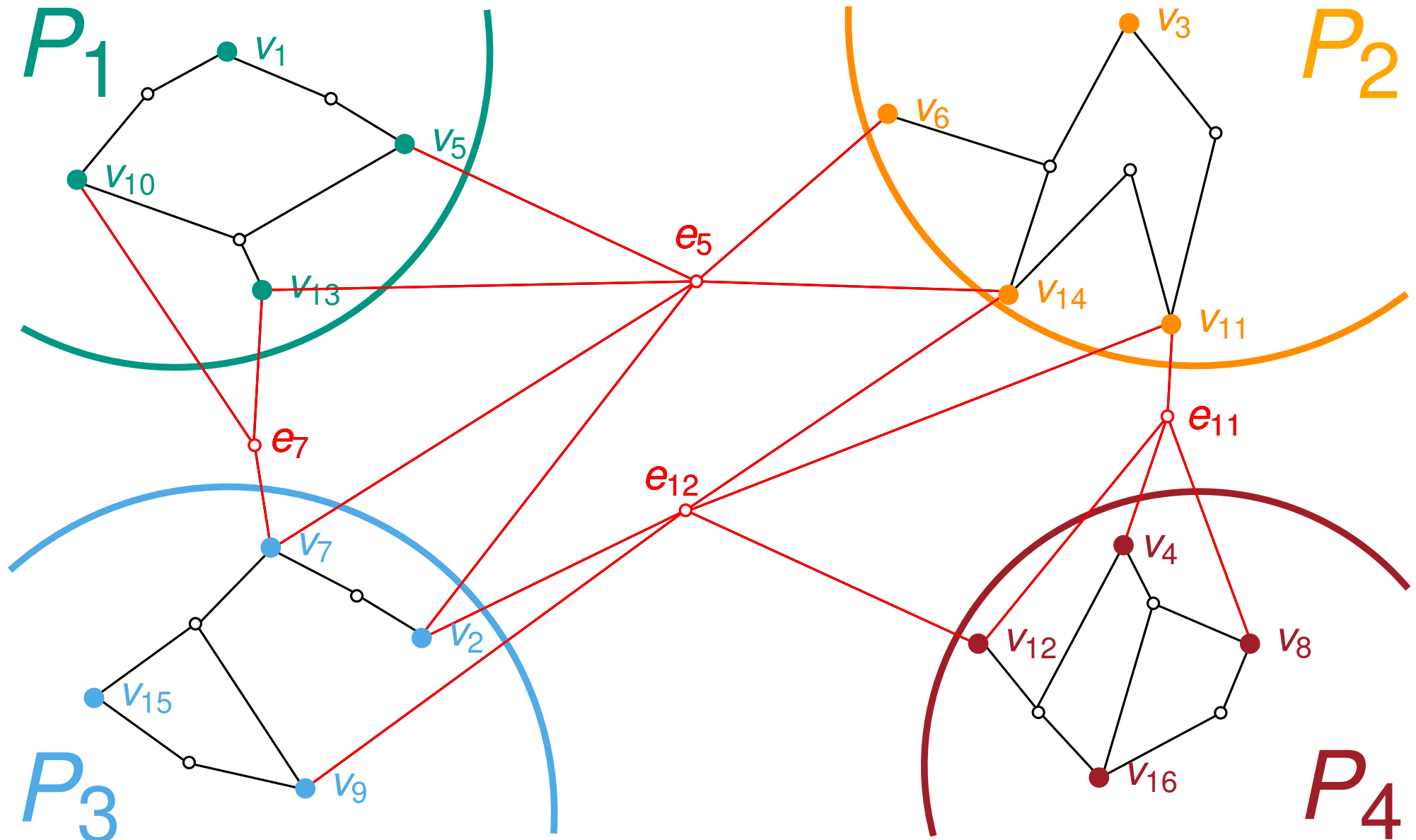
From $\text{SpM} \times V$ to Hypergraph Partitioning



From $\text{SpM} \times V$ to Hypergraph Partitioning



From $\text{SpM} \times V$ to Hypergraph Partitioning



From Hypergraph Partitioning to $\text{SpM} \times \text{V}$

	0	3	5	1	6	14	11	3	2	15	7	9	8	16	12	4
	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>
P_1	10	x	x		x							x				
	13		x	x								x				
	5		x	x	x											
	1	x			x											
P_2	6			x		x										
	14		x		x	x										x
	11					x	x	x								x
	3				x			x								
P_3	2		x						x							x
	15									x		x				
	7		x						x		x	x				
	9									x		x				x
P_4	8						x						x			x
	16												x	x		x
	12						x							x	x	
	4						x							x		x

From Hypergraph Partitioning to $\text{SpM} \times \text{V}$

	0	3	5	1	6	14	11	3	2	15	7	9	8	16	12	4
	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>	<i>b</i>
P_1	x	x		x							x					
		x	x								x					
			x	x	x											
	x				x											
P_2			x		x											
			x		x	x										x
						x	x	x								x
					x			x								
P_3			x						x							x
										x		x				
			x						x		x	x				
										x		x				x
P_4							x						x			x
													x	x		x
							x							x	x	
							x							x		x

Load Balancing?

From Hypergraph Partitioning to $\text{SpM} \times \text{V}$

	0	3	5	1	6	14	11	3	2	15	7	9	8	16	12	4
	b				b				b				b			
P_1	x	x		x							x					
		x	x								x					
		x	x	x												
	x			x												
P_2			x		x											
		x			x	x									x	
						x	x	x							x	
				x				x								
P_3			x						x							x
										x		x				
		x							x		x	x				
										x		x				x
P_4							x						x			x
													x	x		x
							x							x	x	
							x							x		x

Load Balancing?

$\Rightarrow 12$

$\Rightarrow 12$

$\Rightarrow 12$

$\Rightarrow 12$

From Hypergraph Partitioning to $\text{SpM} \times \text{V}$

Where are the cut-hyperedges?

	0	3	5	1	6	4	7	3	2	5	7	9	8	6	2	4
	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
P_1	10	x	x		x							x				
	13		x	x								x				
	5		x	x	x											
	1	x			x											
P_2	6			x		x										
	14		x		x	x										x
	11					x	x	x								x
	3				x			x								
P_3	2		x						x							x
	15									x		x				
	7		x						x		x	x				
	9									x		x				x
P_4	8							x					x			x
	16												x	x		x
	12							x						x	x	
	4							x						x		x

Load Balancing?

$\Rightarrow 12$

$\Rightarrow 12$

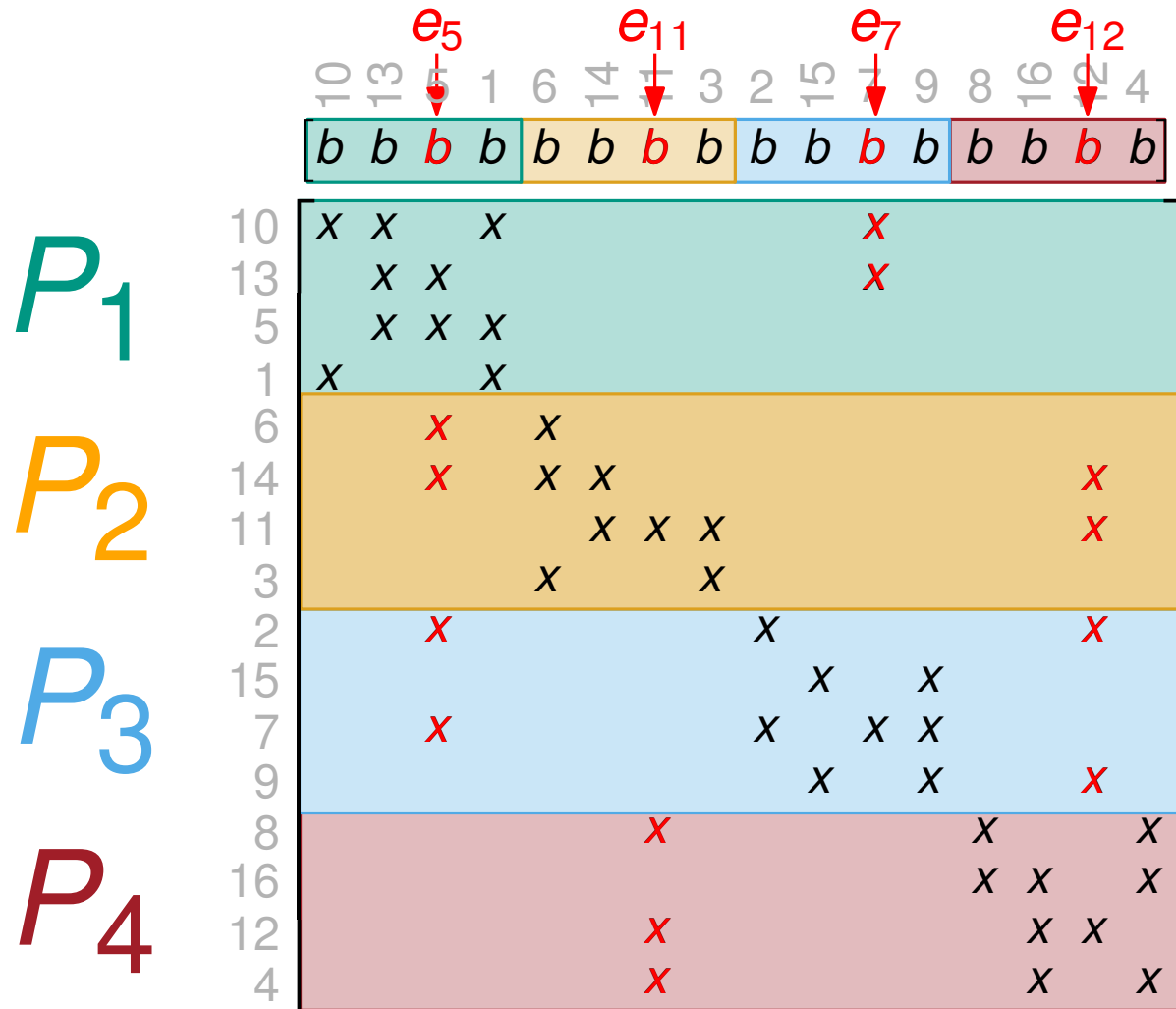
$\Rightarrow 12$

$\Rightarrow 12$

Communication Volume?

From Hypergraph Partitioning to $\text{SpM} \times \text{V}$

Where are the cut-hyperedges?



Load Balancing?

$\Rightarrow 12$

$\Rightarrow 12$

$\Rightarrow 12$

$\Rightarrow 12$

Communication Volume? $\Rightarrow 6$ entries!

How does Hypergraph Partitioning work?

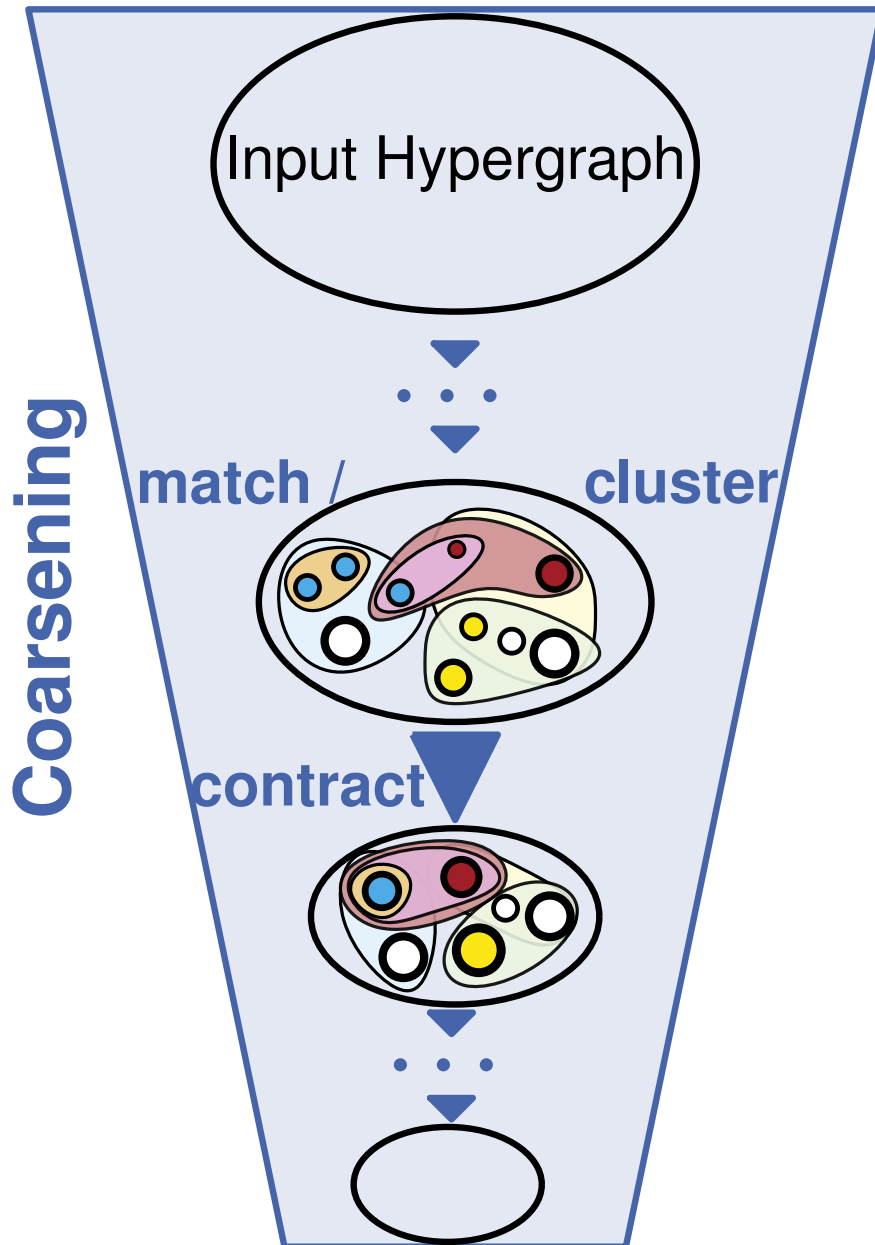
How does

Bad News:

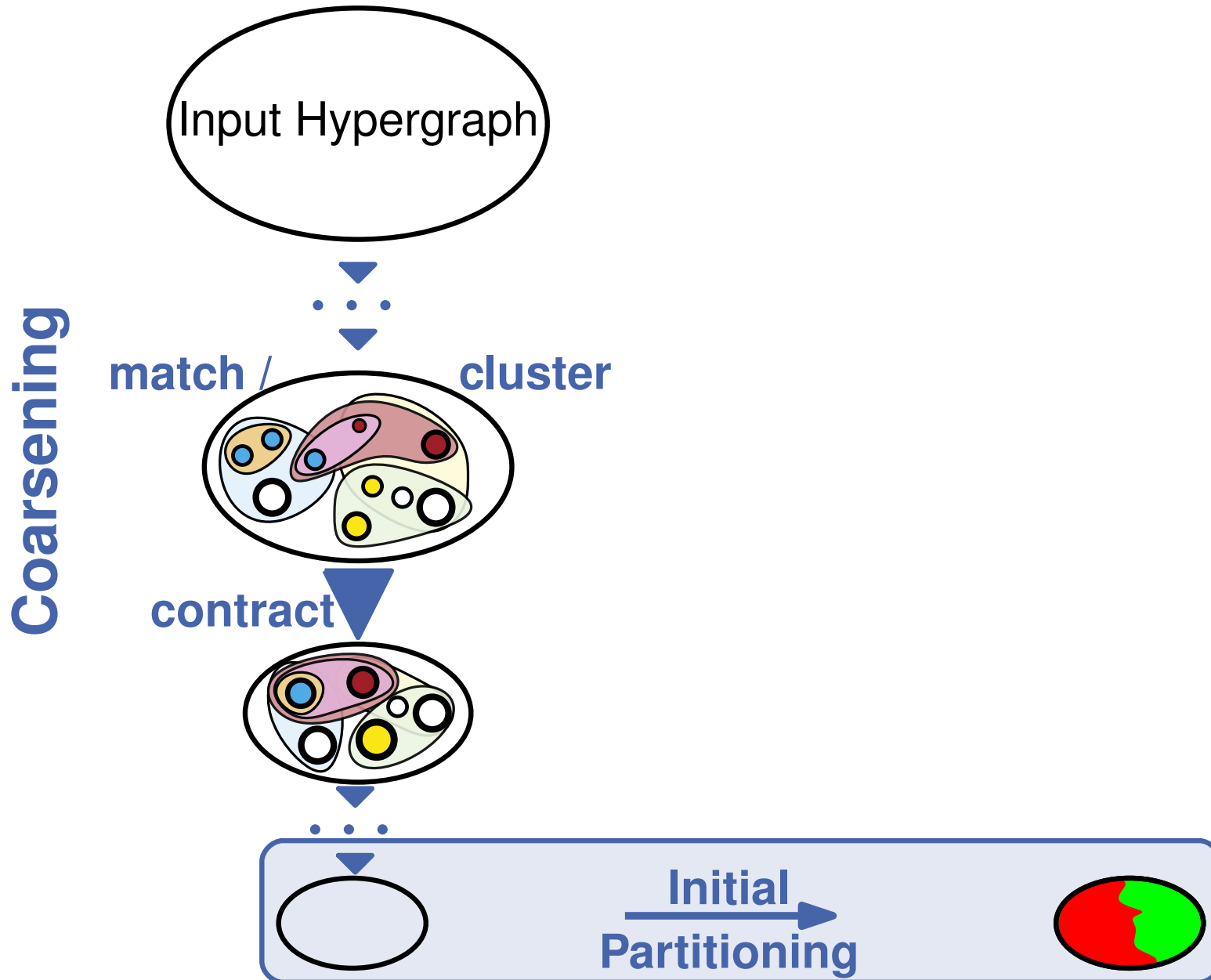
- hypergraph partitioning is **NP**-hard
- even finding **good approximate** solutions for graphs is **NP**-hard

work?

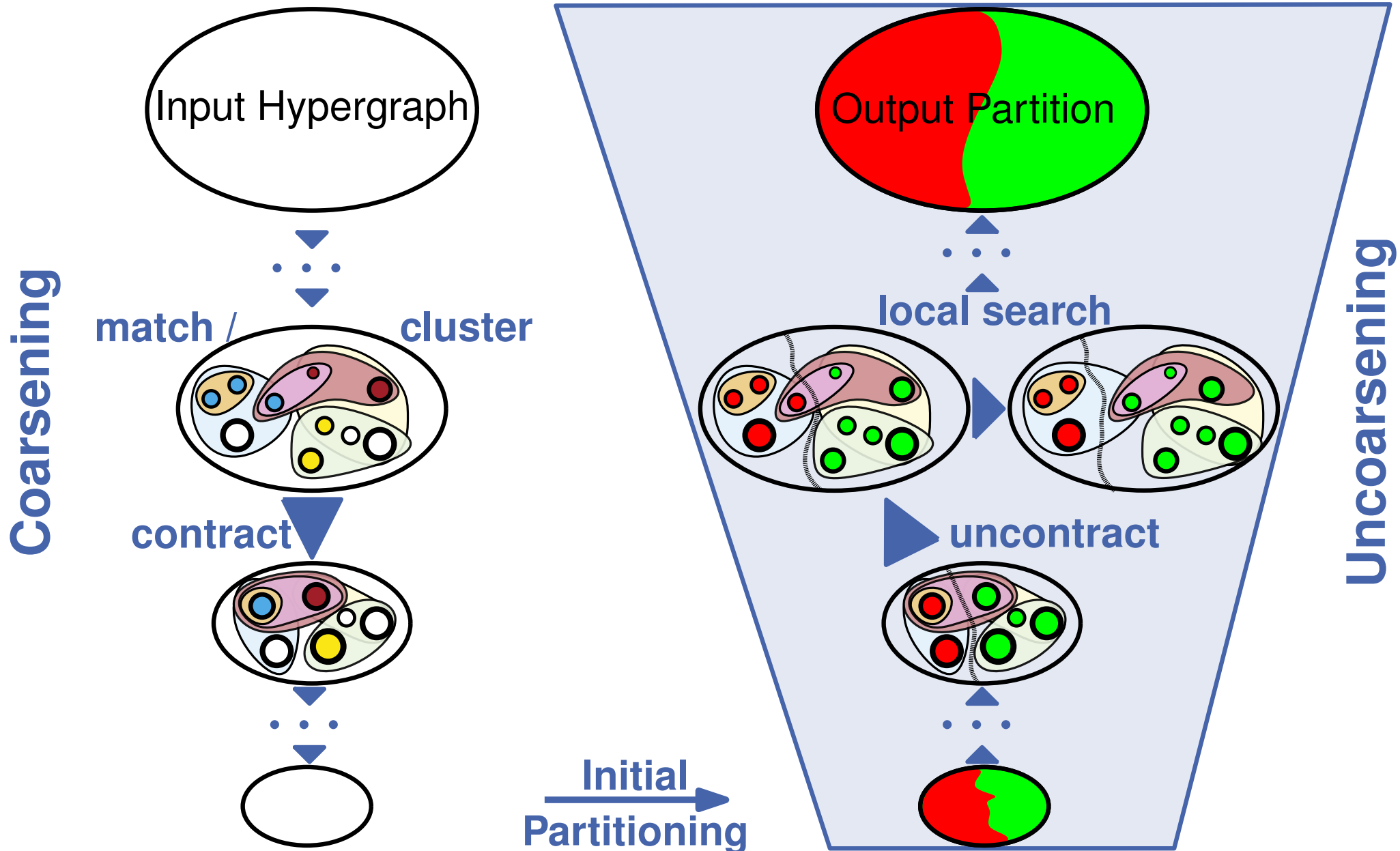
Successful Heuristic: Multilevel Paradigm



Successful Heuristic: Multilevel Paradigm



Successful Heuristic: Multilevel Paradigm



Coarsening

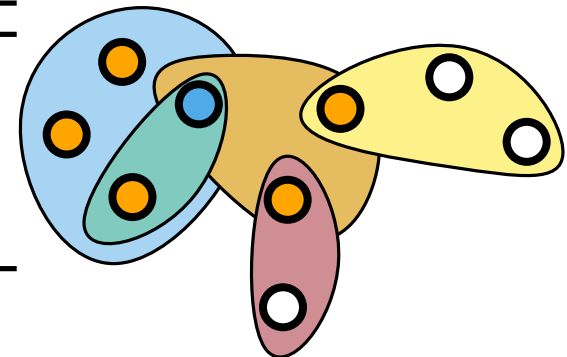
Clustering-based Coarsening

Common Strategy: **avoid** global decisions \rightsquigarrow **local**, greedy algorithms

Objective: identify highly connected vertices

using...

```
foreach vertex  $v$  do
  cluster[ $v$ ] := argmaxneighbor  $u$  rating( $v, u$ )
```



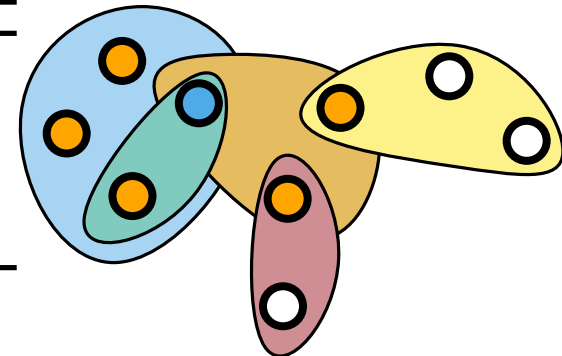
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Main Design Goals:^[Karypis, Kumar 99]

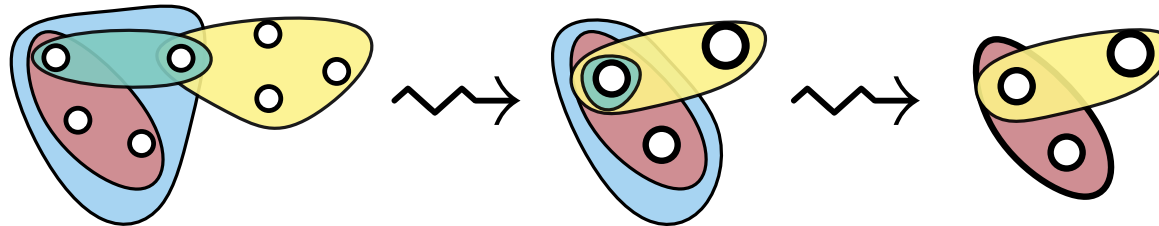
- 1: reduce **size** of nets \rightsquigarrow easier local search
- 2: reduce **number** of nets \rightsquigarrow easier initial partitioning
- 3: maintain **structural similarity** \rightsquigarrow good coarse solutions

Clustering-based Coarsening

Main Design Goals:

1: reduce **size** of nets \rightsquigarrow easier local search

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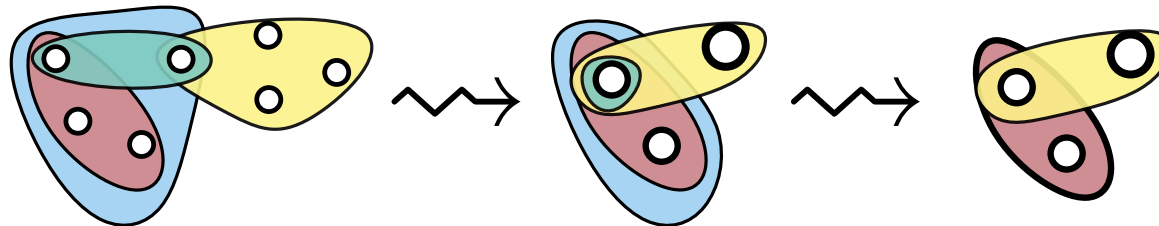


Clustering-based Coarsening

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\Rightarrow hypergraph-tailored rating functions:

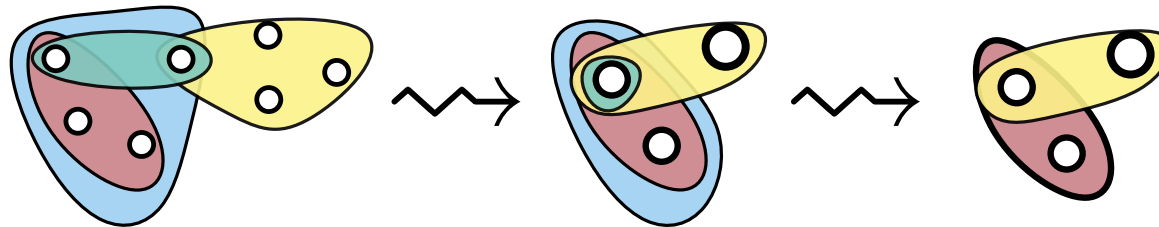
$$r(u, v) := \sum_{\substack{\text{net } e \\ \text{containing } u, v}} \frac{\omega(e)}{|e|-1}$$

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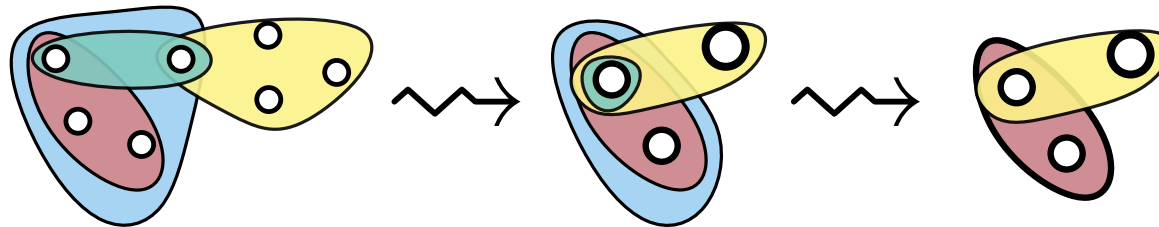
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large number ... \rightarrow containing u, v

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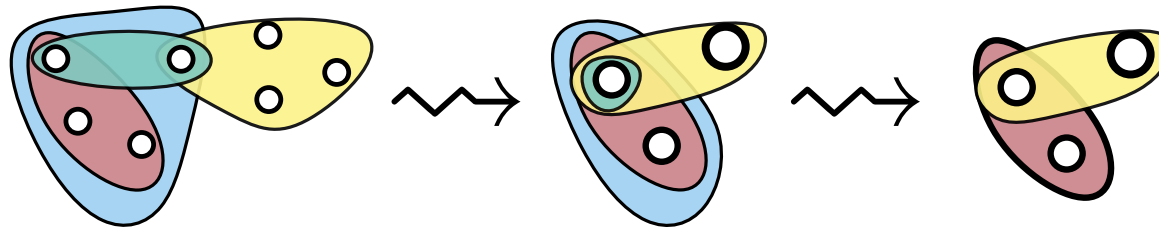
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large number ... \rightarrow containing u, v \leftarrow of heavy nets ...

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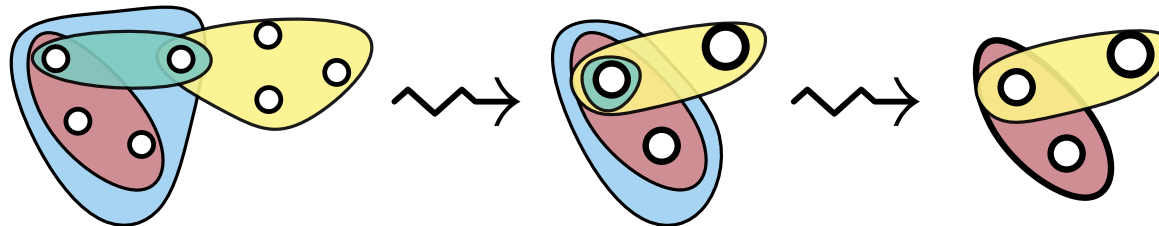
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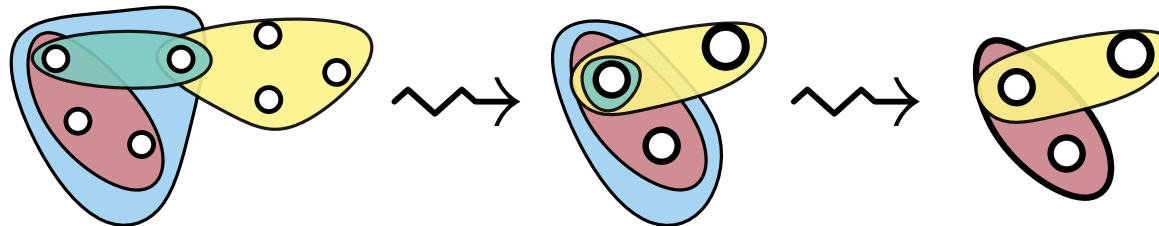
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3: maintain **structural similarity** \rightsquigarrow good coarse solutions

\Rightarrow prefer clustering over matching

\Rightarrow ensure \sim balanced vertex weights

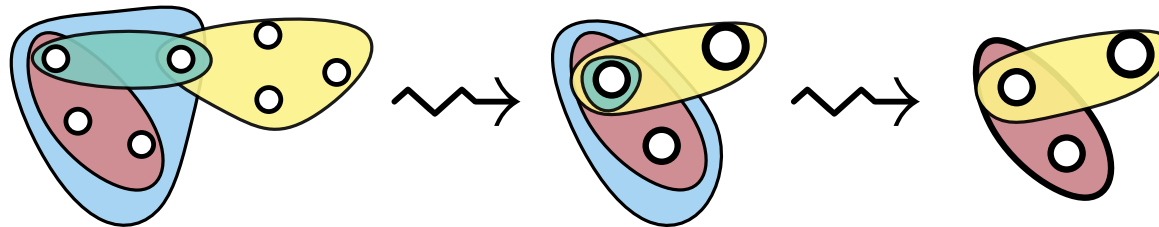
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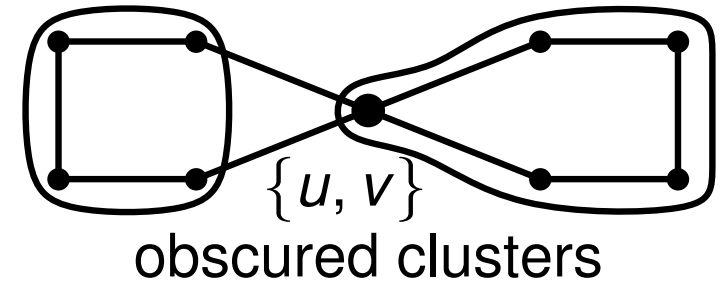
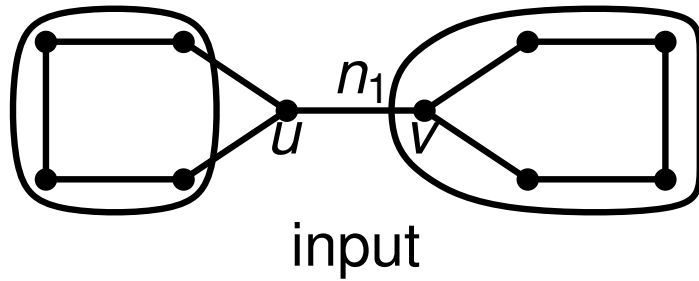
\Rightarrow prefer clustering over matching

\Rightarrow ensure \sim balanced vertex weights

enough?

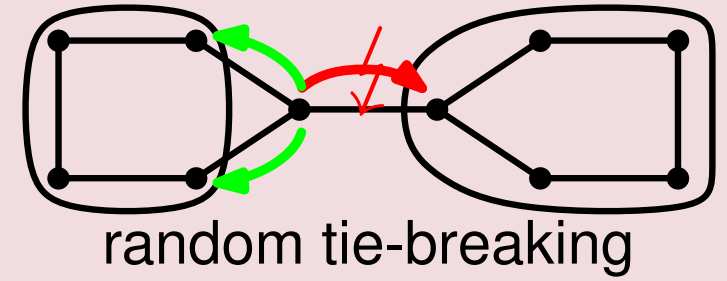
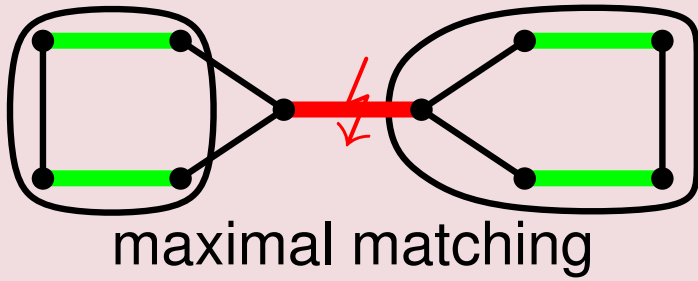
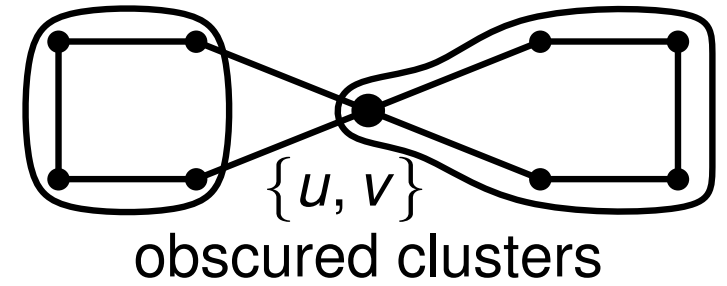
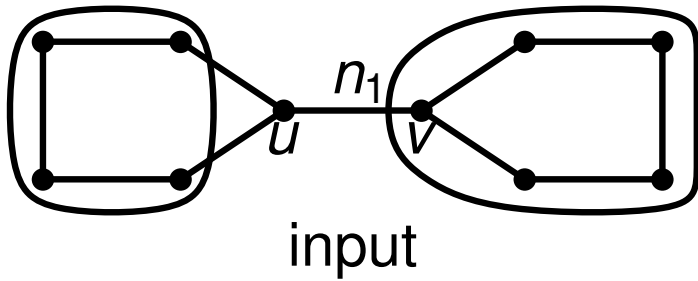
What could possibly go wrong?

... a lot:

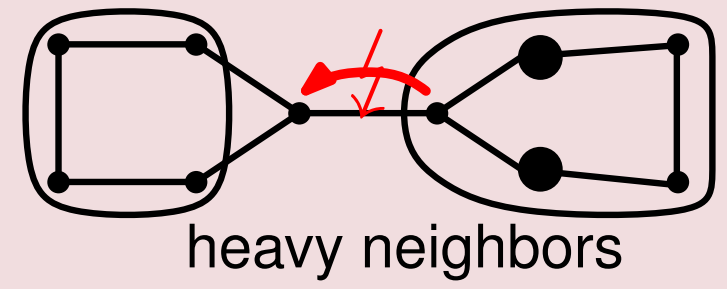
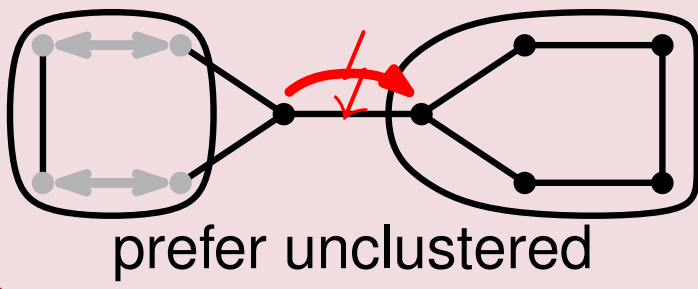


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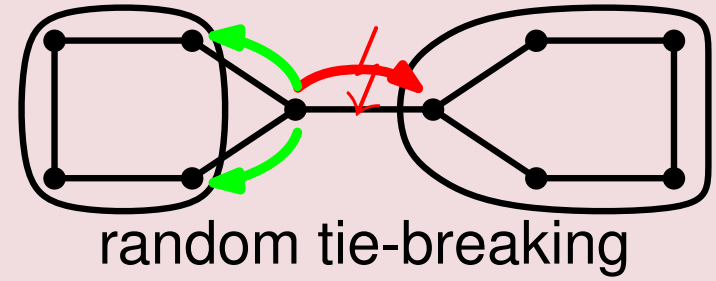
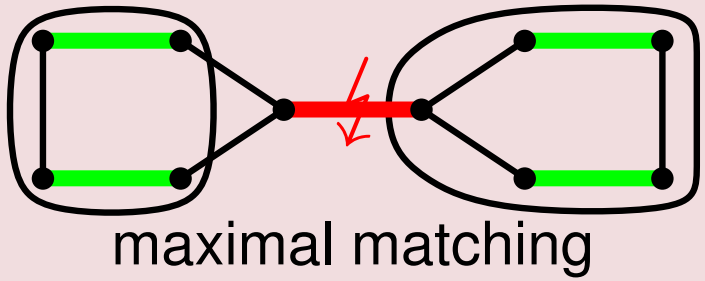
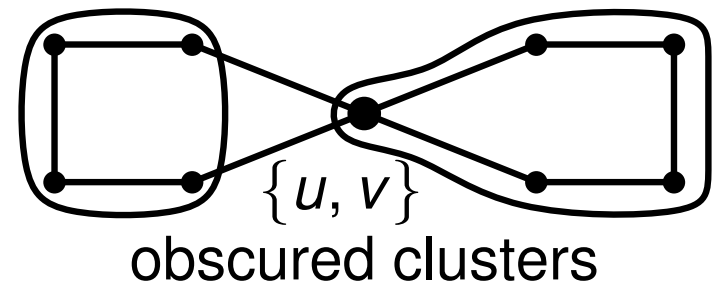
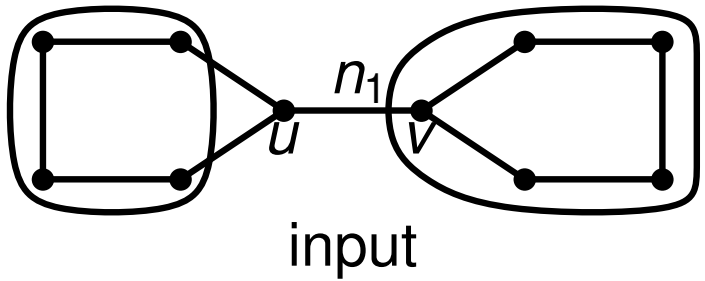


ISSUES

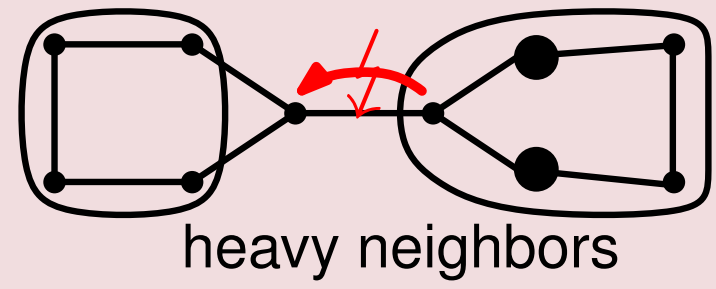
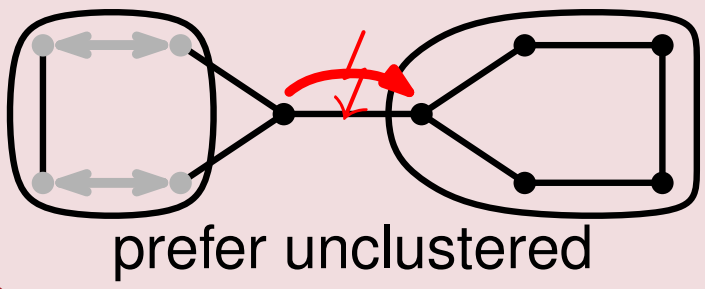


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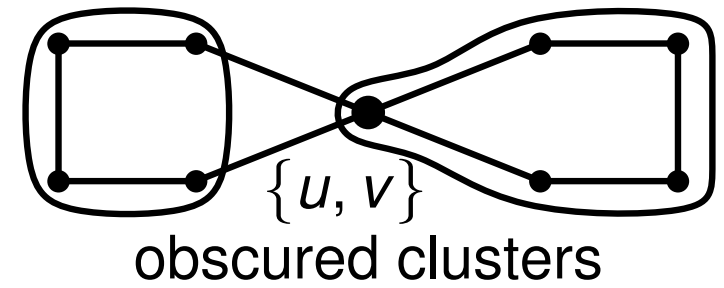
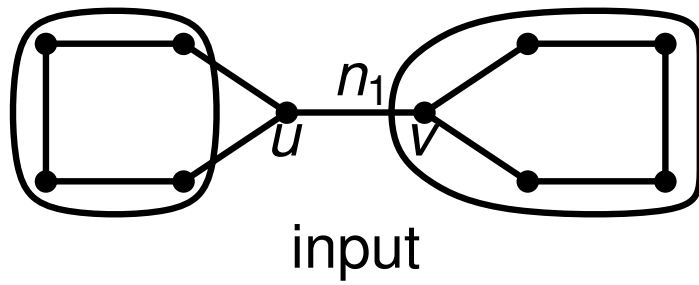


ISSUES

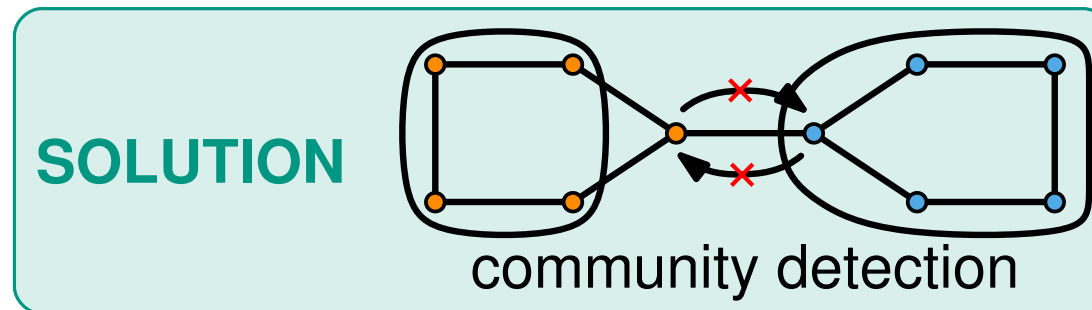
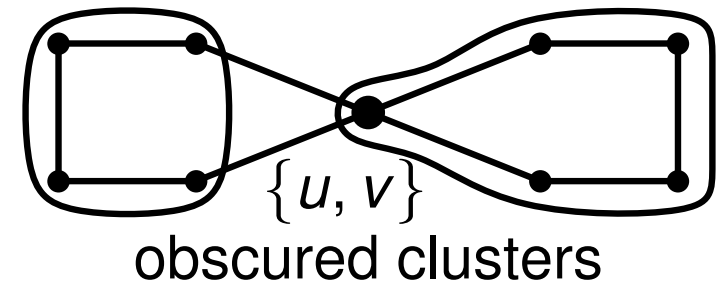
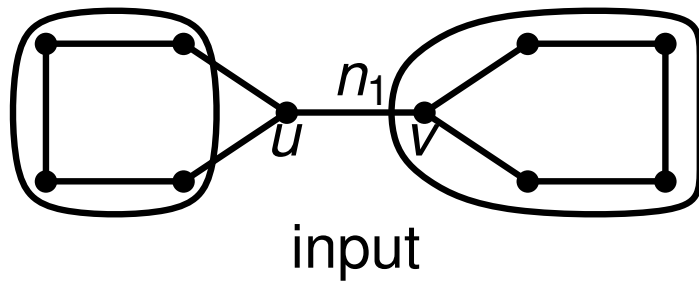


⇒ **Problem:** relying **only** on **local** information!

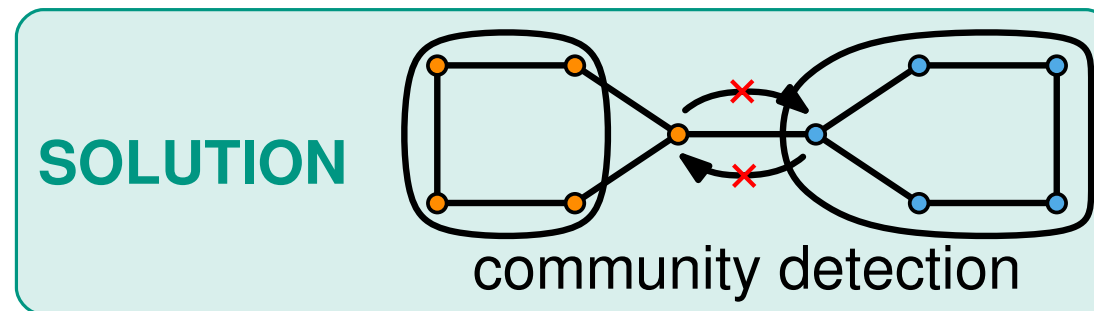
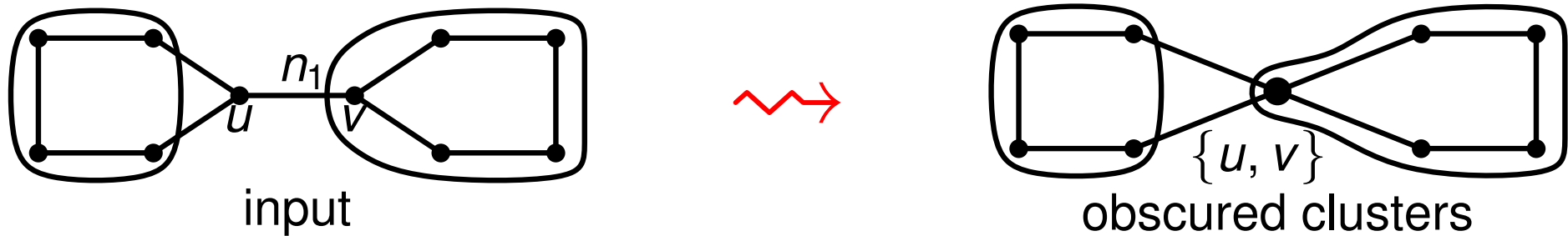
Community-aware Coarsening



Community-aware Coarsening



Community-aware Coarsening



Framework:

- preprocessing: determine **community structure**
- only allow **intra-community** contractions

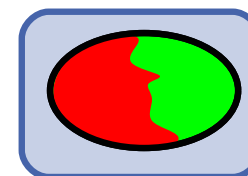
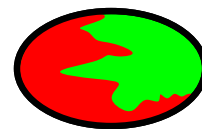
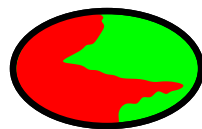
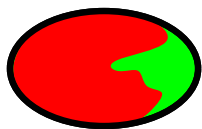
Initial Partitioning

Initial Partitioning

- use **portfolio** of algorithms \rightsquigarrow diversification
 - random partitioning
 - breadth-first search
 - greedy hypergraph growing
 - size-constrained label propagation

⇒ try all algorithms multiple times

⇒ select partition with **best** cut & **lowest** imbalance as initial partition



initial partition

Local Search

Fiduccia-Mattheyses Algorithm

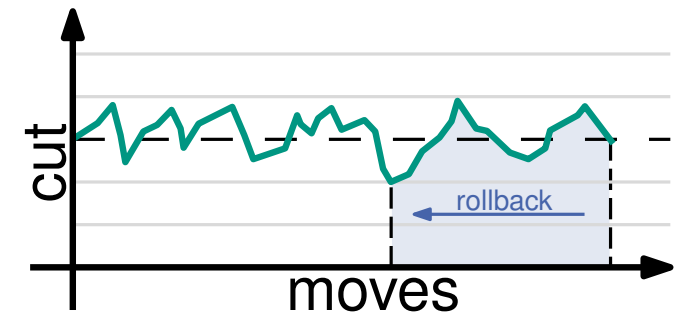
Algorithm 1: FM Local Search

while \neg *done* **do**

 find best move

 perform best move

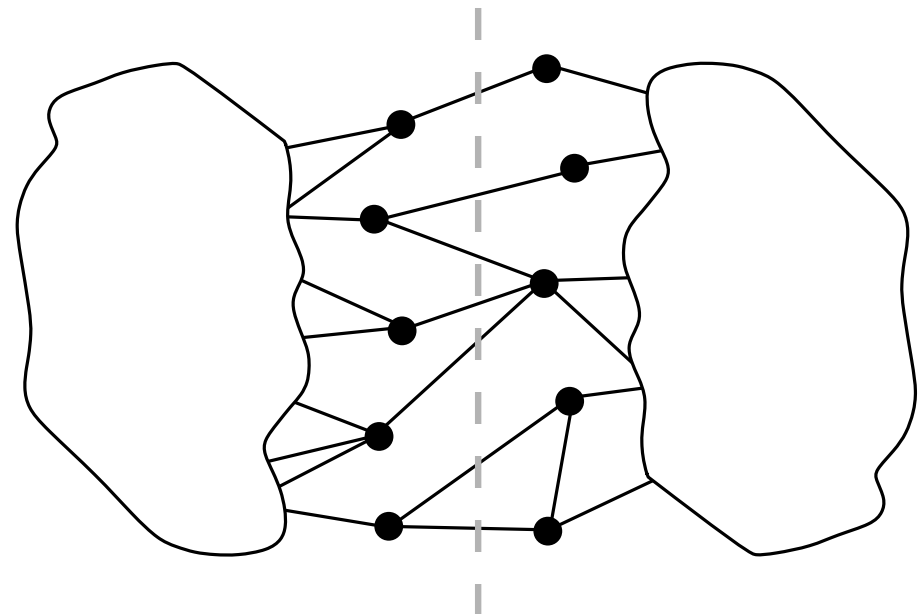
rollback to best solution



can worsen solution

Example for Graphs:

- compute gain $g(v) = d_{\text{ext}}(v) - d_{\text{int}}(v)$
- alternate between blocks
- edge-cut: 7



Fiduccia-Mattheyses Algorithm

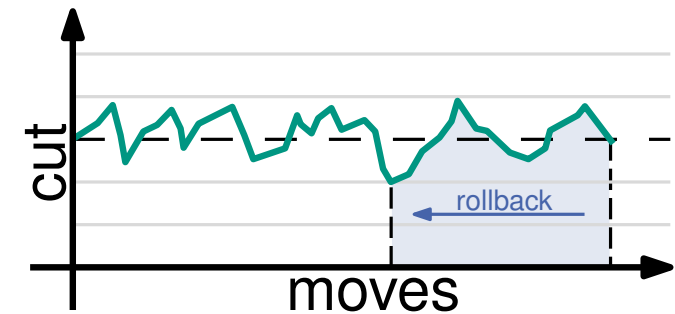
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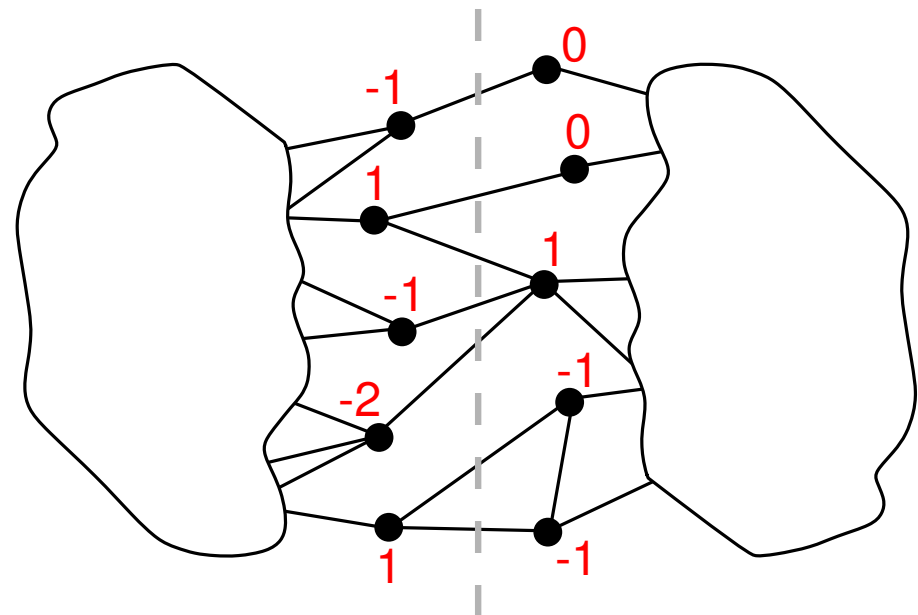
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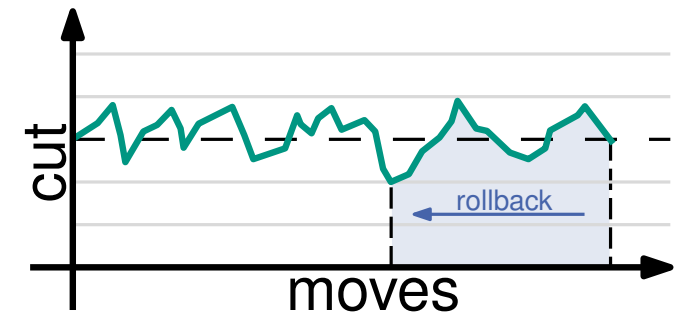
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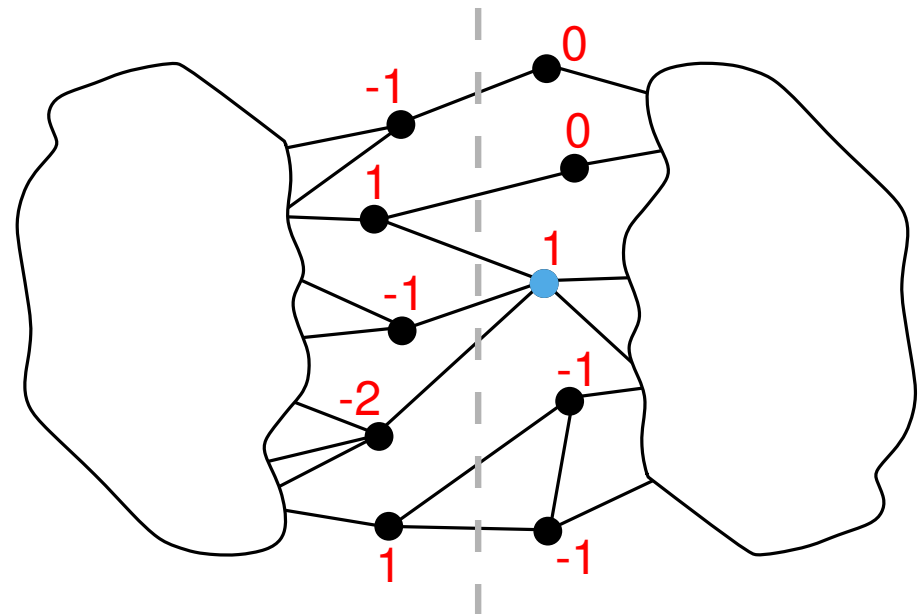
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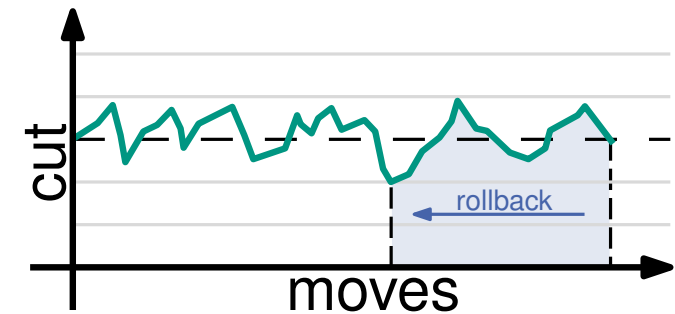
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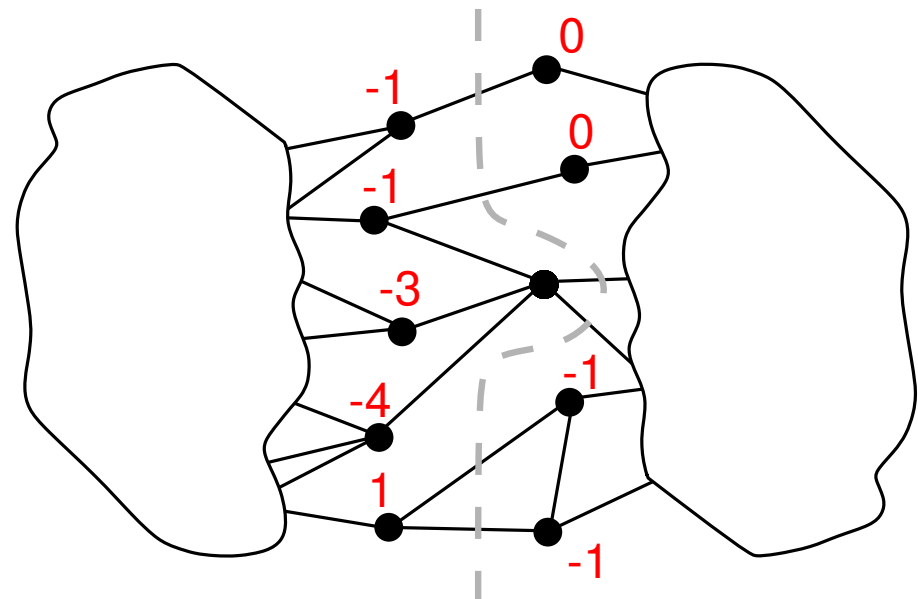
rollback to best solution



can worsen solution

Example for Graphs:

- **recalculate** gain $g(v)$ of neighbors
- move each node at most once
- edge-cut: 7, 6



Fiduccia-Mattheyses Algorithm

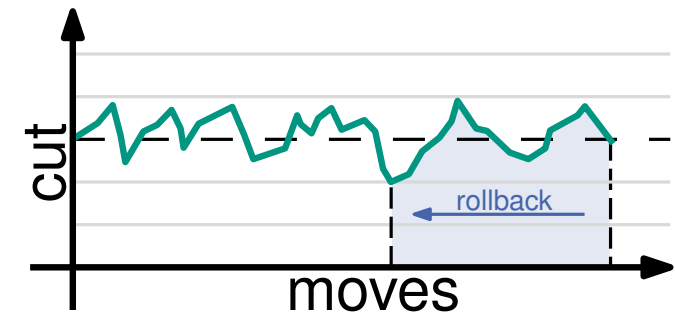
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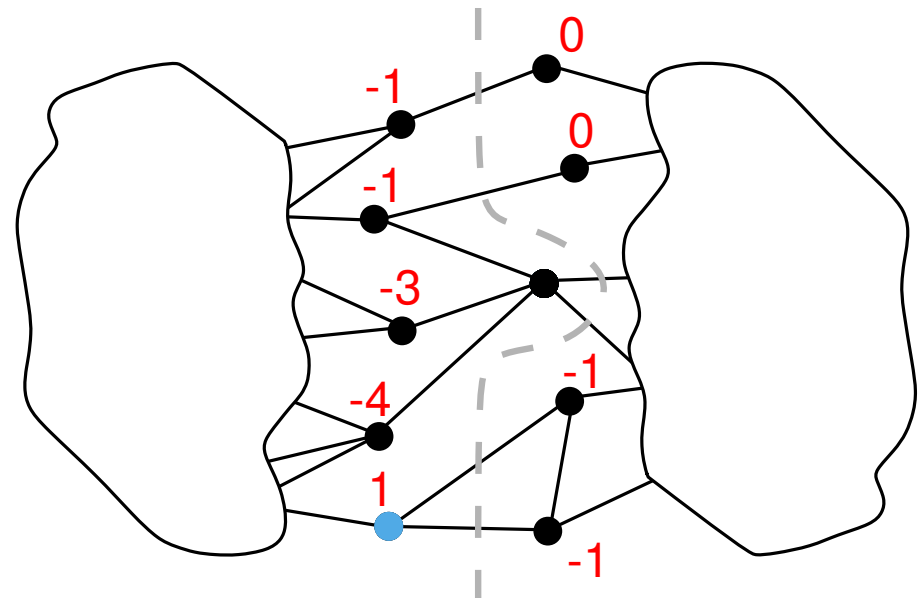
rollback to best solution



can worsen solution

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Fiduccia-Mattheyses Algorithm

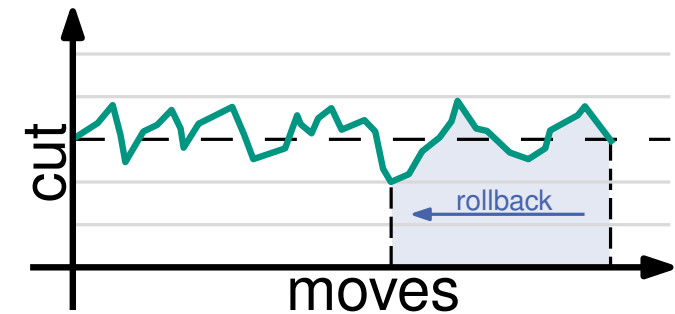
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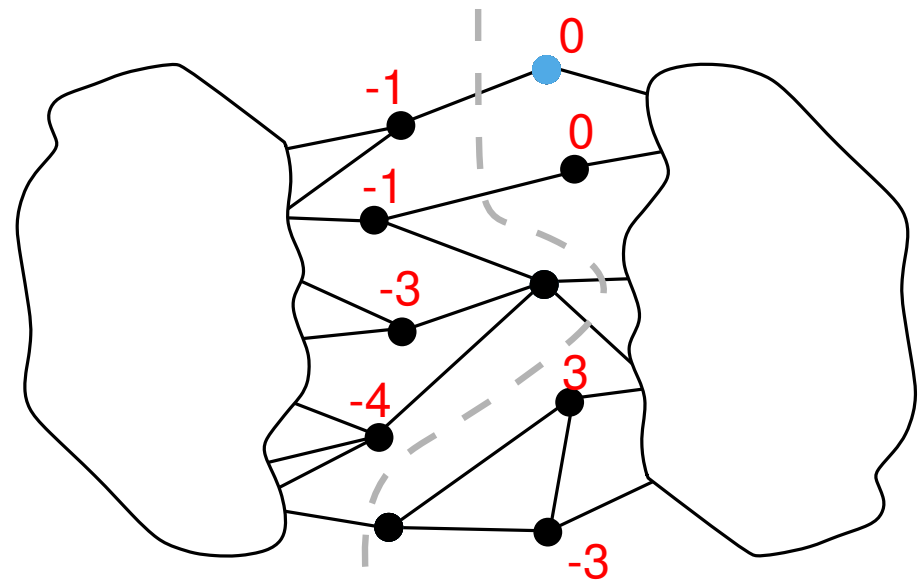
rollback to best solution



can worsen solution

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- edge-cut: 7, 6,5



Fiduccia-Mattheyses Algorithm

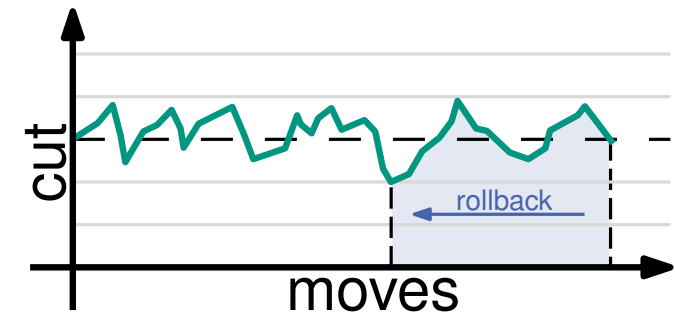
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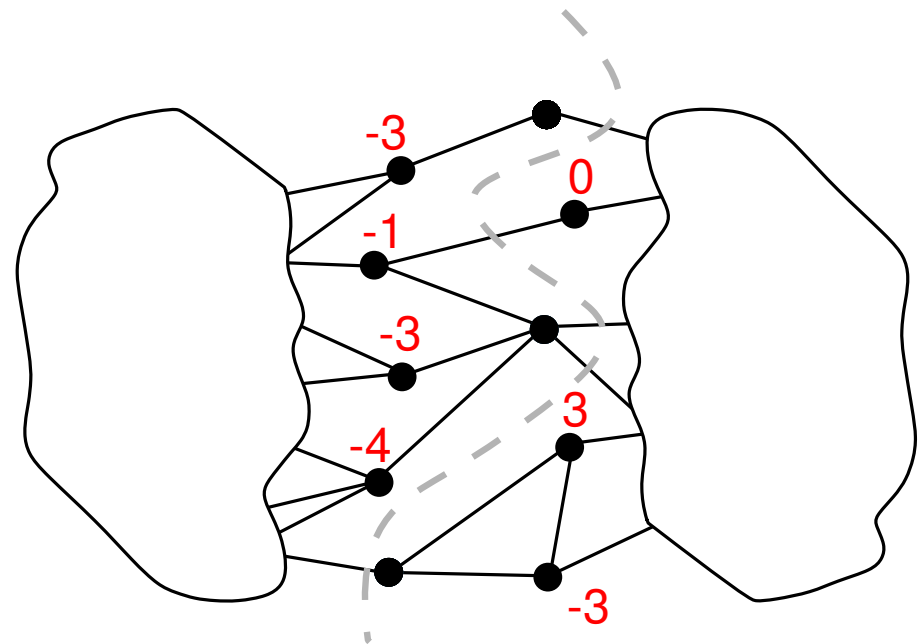
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can worsen solution

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Fiduccia-Mattheyses Algorithm

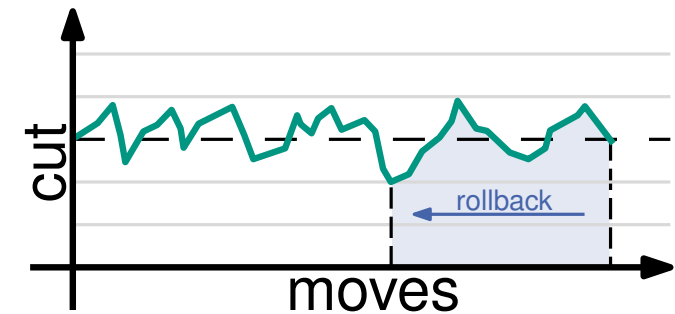
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 find best move

 perform best move

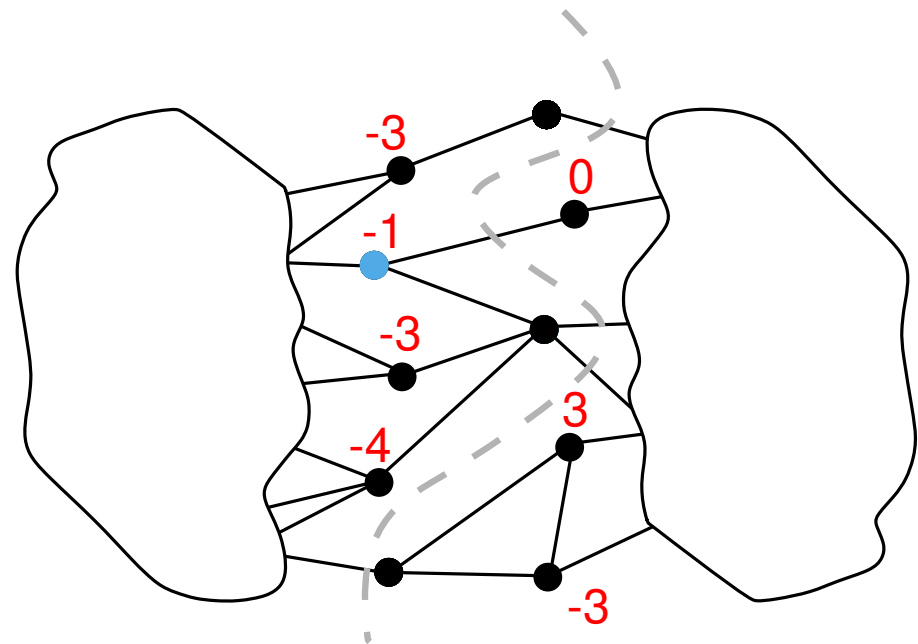
rollback to best solution



can worsen solution

Example for Graphs:

- **recalculate** gain $g(v)$ of neighbors
- move each node at most once
- edge-cut: 7, 6, 5, 5



Fiduccia-Mattheyses Algorithm

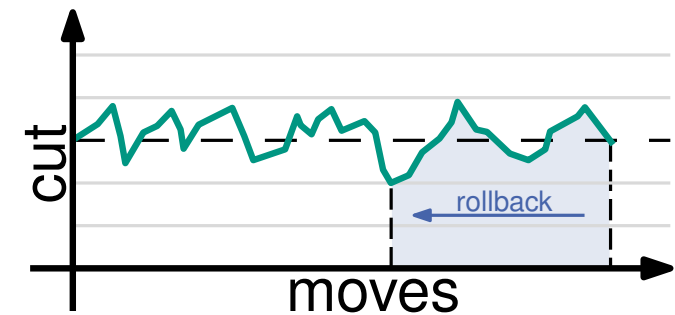
Algorithm 1: FM Local Search

while \neg *done* **do**

 find best move

 perform best move

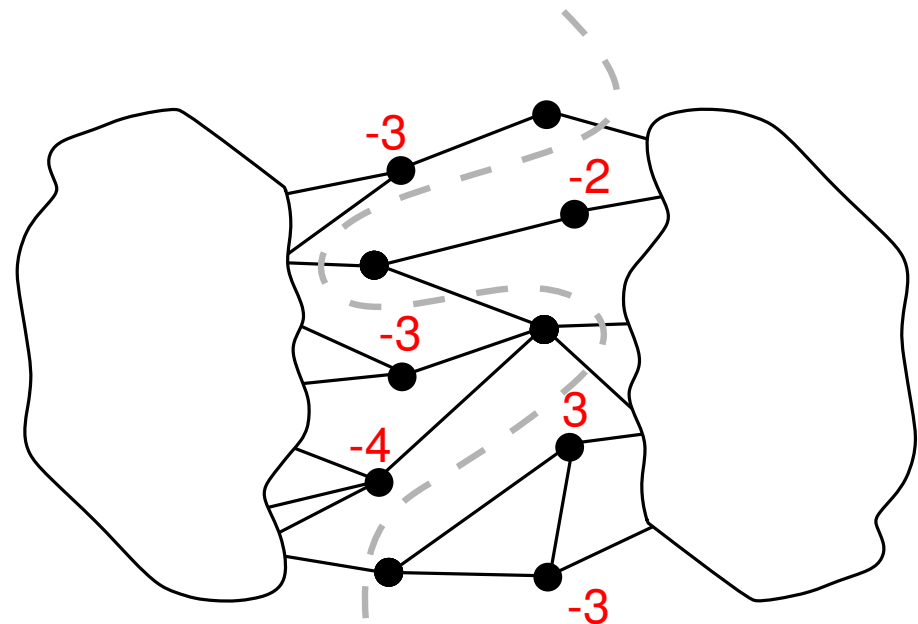
rollback to best solution



can worsen solution

Example for Graphs:

- **recalculate** gain $g(v)$ of neighbors
- move each node at most once
- edge-cut: **7, 6, 5, 5, 6**



Fiduccia-Mattheyses Algorithm

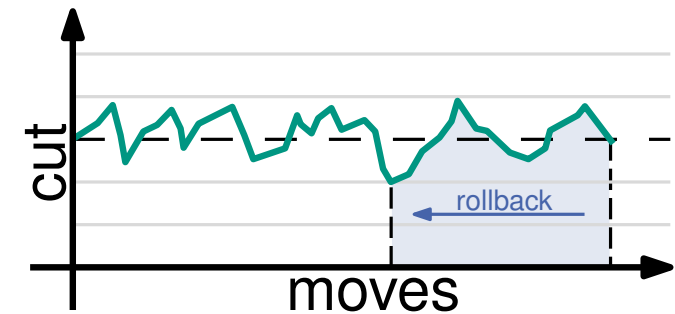
Algorithm 1: FM Local Search

while \neg *done* **do**

 find best move

 perform best move

rollback to best solution

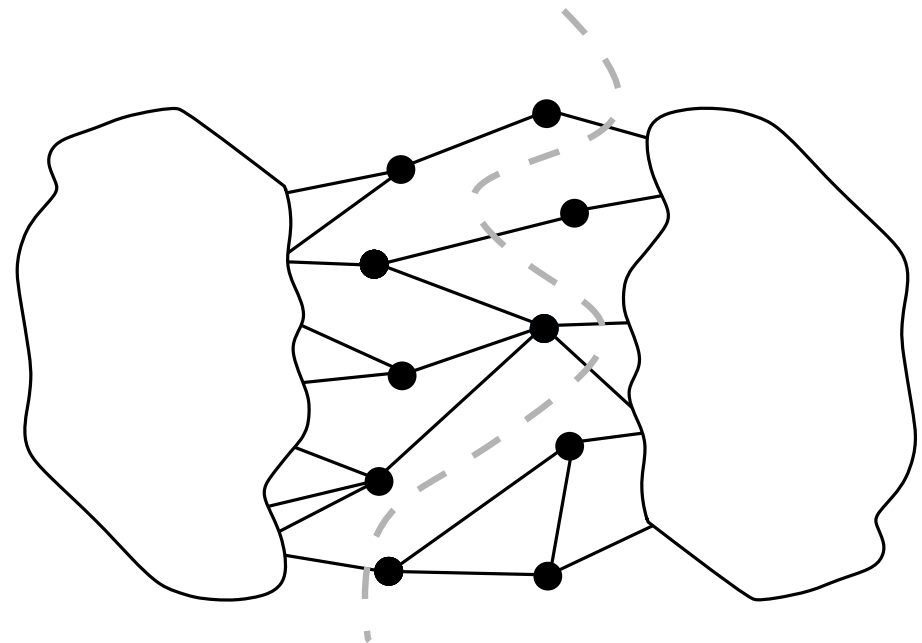



can worsen solution

Example for Graphs:

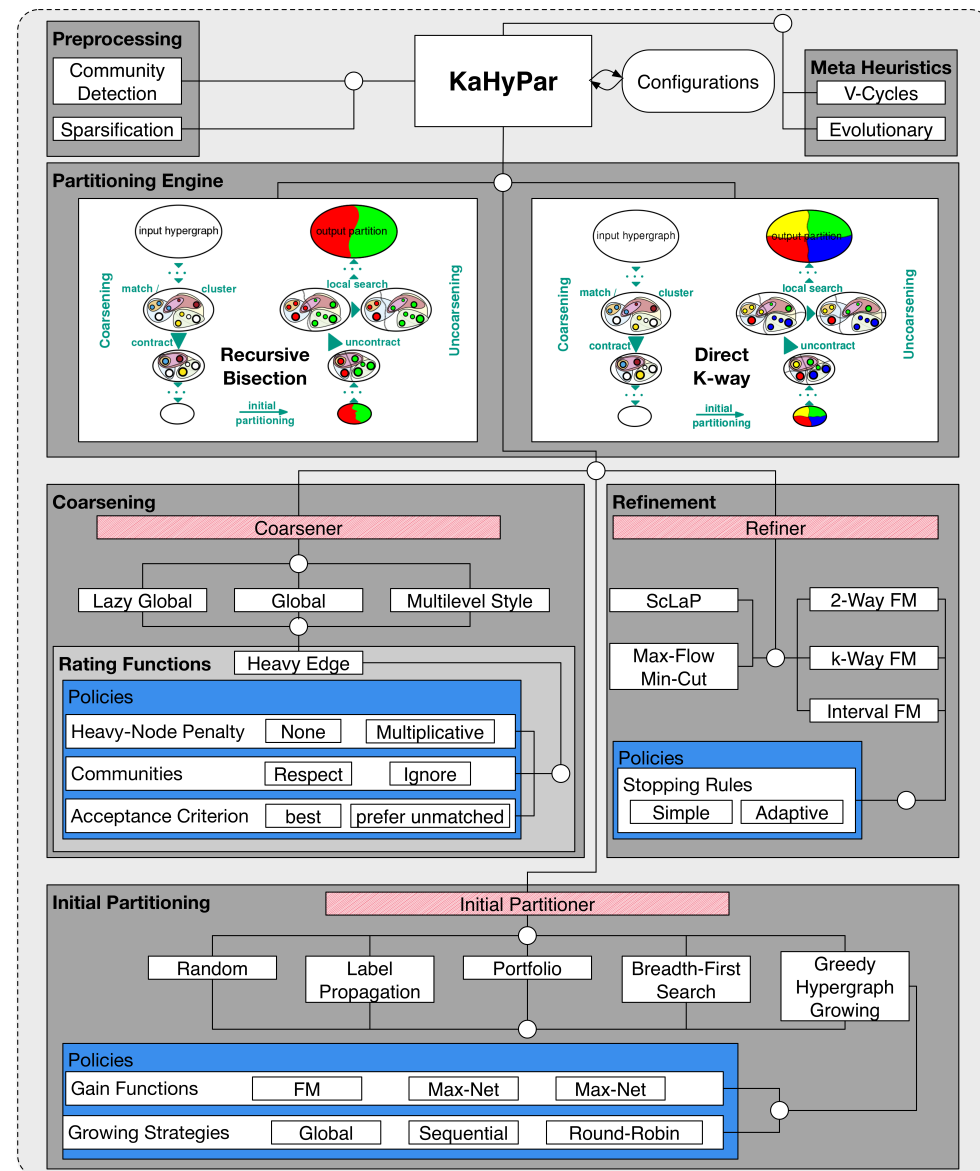
- **recalculate** gain $g(v)$ of neighbors
- move each node at most once
- edge-cut: 7, 6, 5, 5, 6

rollback



KaHyPar - Karlsruhe Hypergraph Partitioning

- *n*-Level Partitioning Framework
- Objectives:
 - hyperedge cut
 - connectivity ($\lambda - 1$)
- Partitioning Modes:
 - recursive bisection
 - direct *k*-way
- Additional Features:
 - evolutionary algorithm
 - flow-based refinement
 - fixed vertices
 - variable block weights
- <http://www.kahypar.org>



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