Modularity Graph Clustering on the GPU

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Introduction

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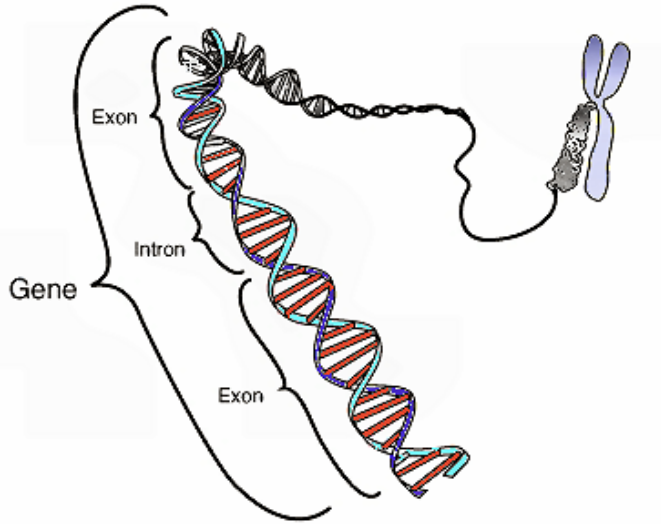
- Clustering $\approx$ isolating 'related' groups of vertices in a graph.
- Our primary interests are speed and parallelisation.

Applications of Clustering

- Bioinformatics: group genes with similar expressions.



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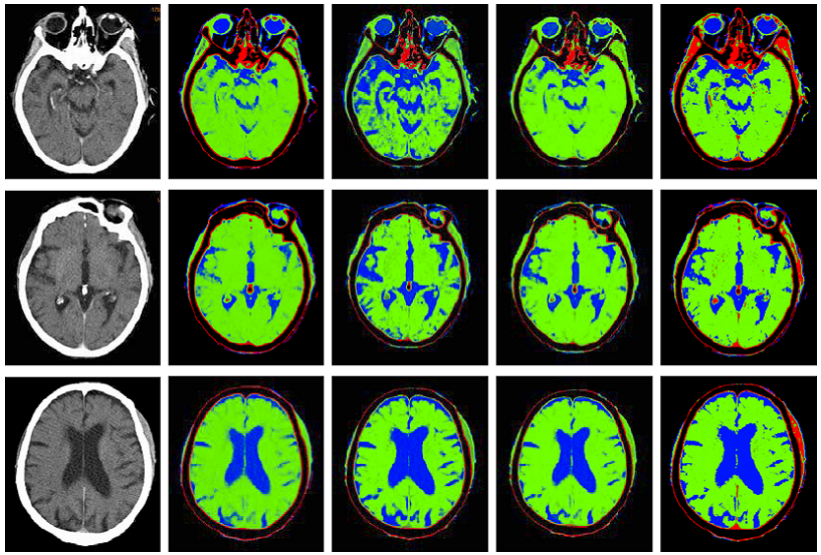
- Medical imaging: image segmentation in CT/MRI.



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- Market research: consumer grouping.

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Applications of Clustering

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- Medical imaging: image segmentation in CT/MRI.
- Market research: consumer grouping.
- Social networks: community detection.

Social Media Landscape

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Modularity

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$$V = \bigcup_{C \in \mathcal{C}} C \qquad \text{as a disjoint union.}$$

- Quality of a clustering is measured by its modularity $\mathrm{mod}(\mathcal{C})$, introduced in 2004 by Newman and Girvan.

Modularity clustering

- Clustering modularity is defined as

$$\mathrm{mod}(\mathcal{C}) := \frac{\sum_{C \in \mathcal{C}} \sum_{\substack{\{u,v\} \in E \\ u,v \in C}} \omega(\{u,v\})}{\sum_{e \in E} \omega(e)} - \frac{\sum_{C \in \mathcal{C}} \left(\sum_{v \in C} \zeta(v) \right)^2}{4 \left(\sum_{e \in E} \omega(e) \right)^2}.$$

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- We have $-\frac{1}{2} \leq \mathrm{mod}(\mathcal{C}) \leq 1$.

Modularity clustering

- $\mathrm{mod}(\mathcal{C})$ can be rewritten to

$$\frac{1}{4\,\Omega^2} \sum_{C \in \mathcal{C}} \left[\zeta(C)\,(2\,\Omega - \zeta(C)) - 2\,\Omega \left(\sum_{\substack{C' \in \mathcal{C} \\ C' \neq C}} \omega(\mathrm{cut}(C, C')) \right) \right].$$

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- To calculate modularity, we only need to keep track of summed vertex weights of clusters and summed edge weights between clusters.

Merging clusters

- Merge two clusters $C, C' \in \mathcal{C}$ to a single larger cluster $C \cup C'$.

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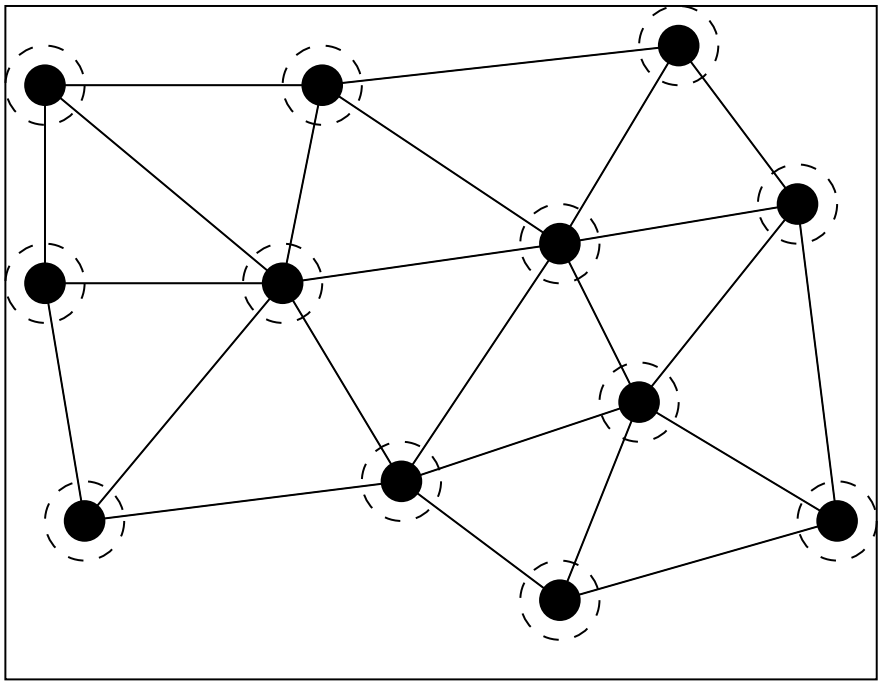
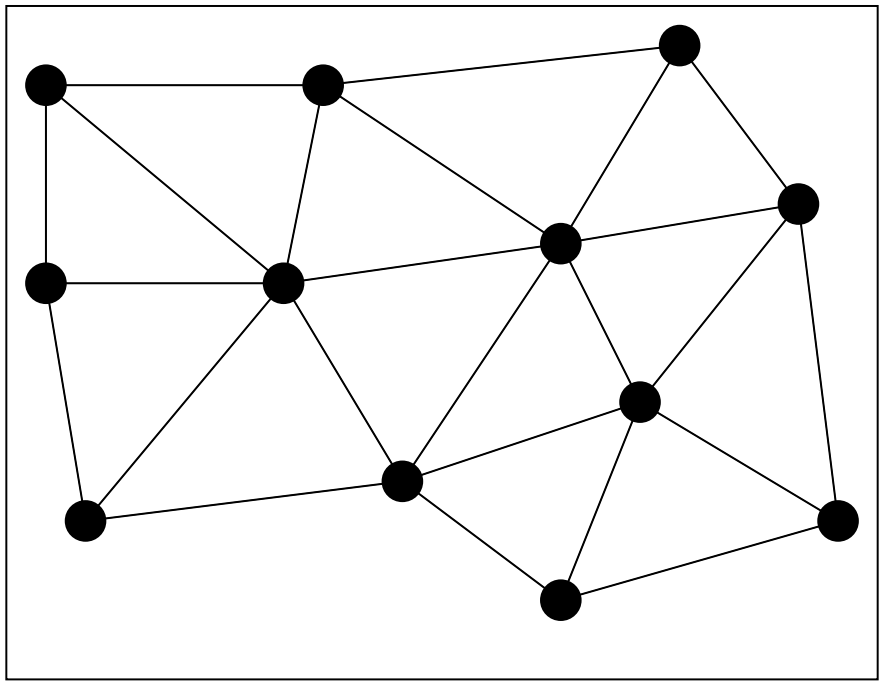
$$\frac{1}{2\,\Omega^2}\left(2\,\Omega\,\omega(\mathrm{cut}(C, C')) - \zeta(C)\,\zeta(C')\right).$$

- This suggests a greedy agglomerative strategy (e.g. Zhu et al., 2008).

Agglomerative clustering





Start with vertices in a separate cluster: $\mathcal{C} = \{\{v\} \mid v \in V\}$.

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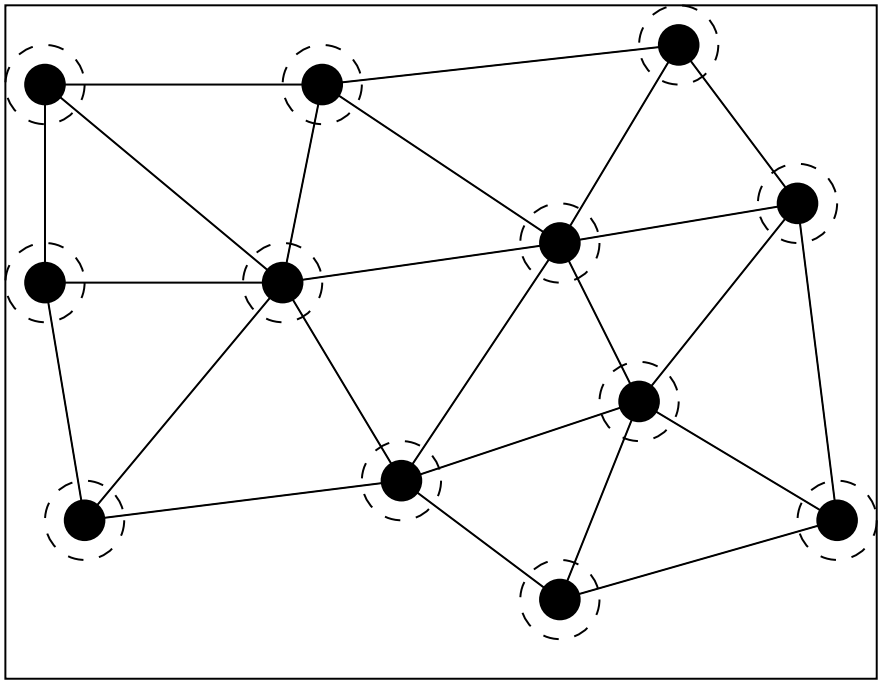
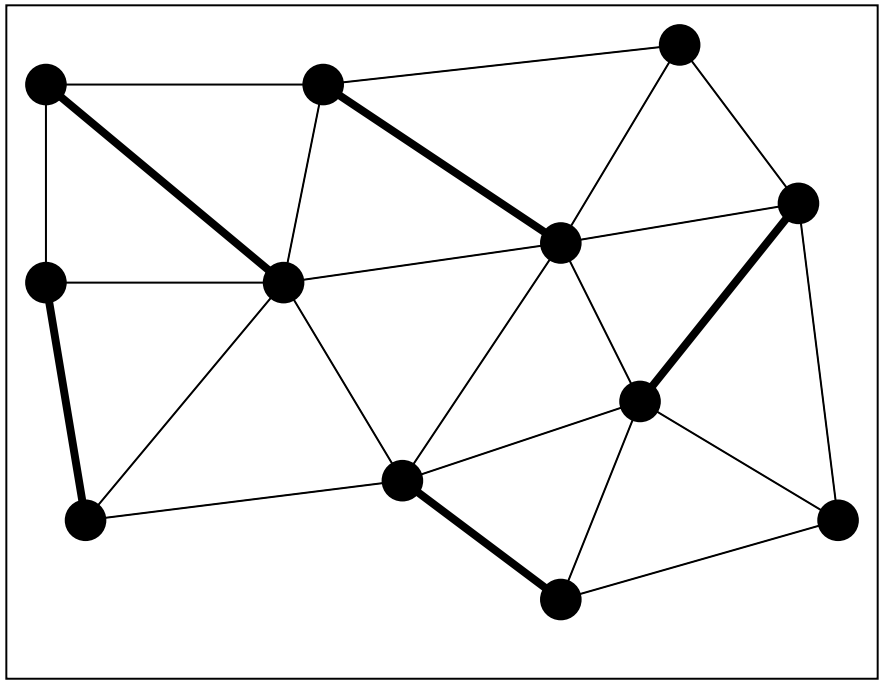
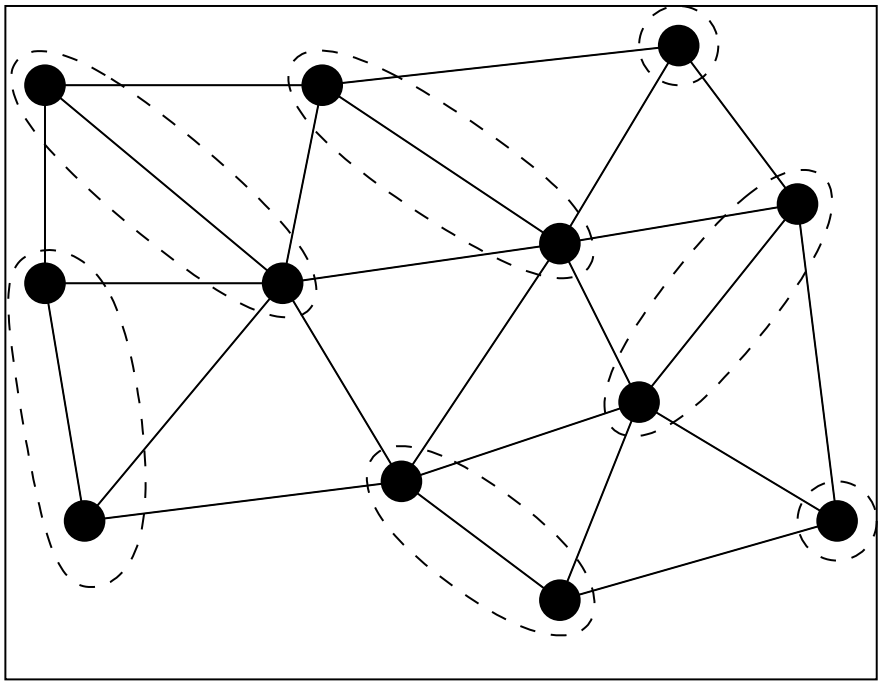
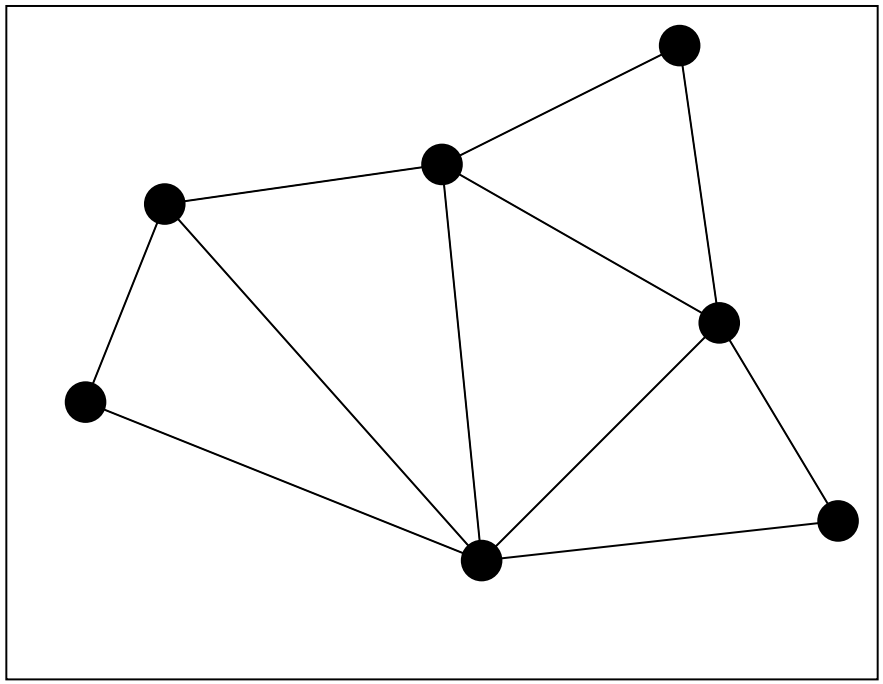




Match clusters to increase modularity.

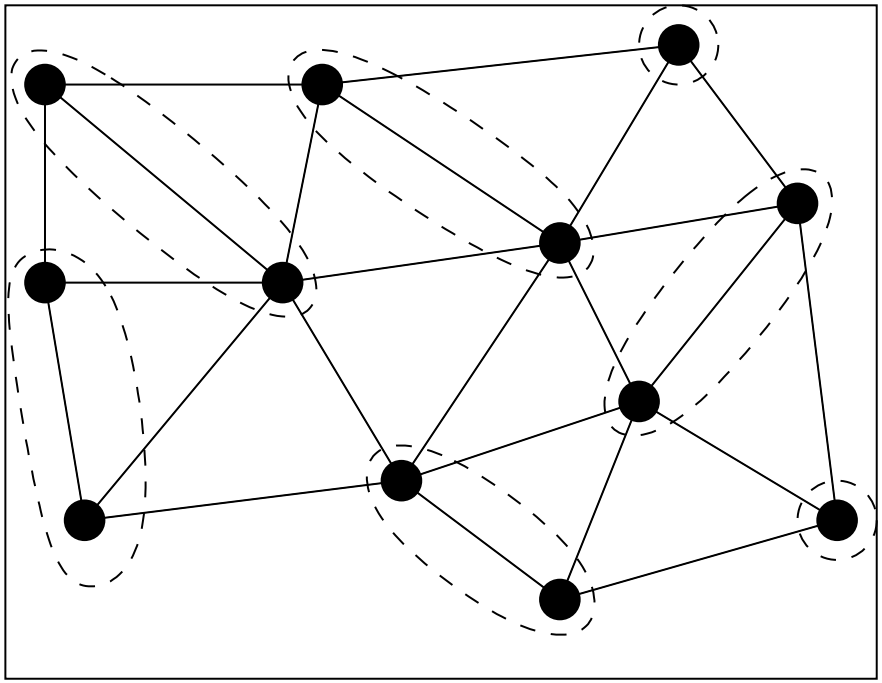
Agglomerative clustering

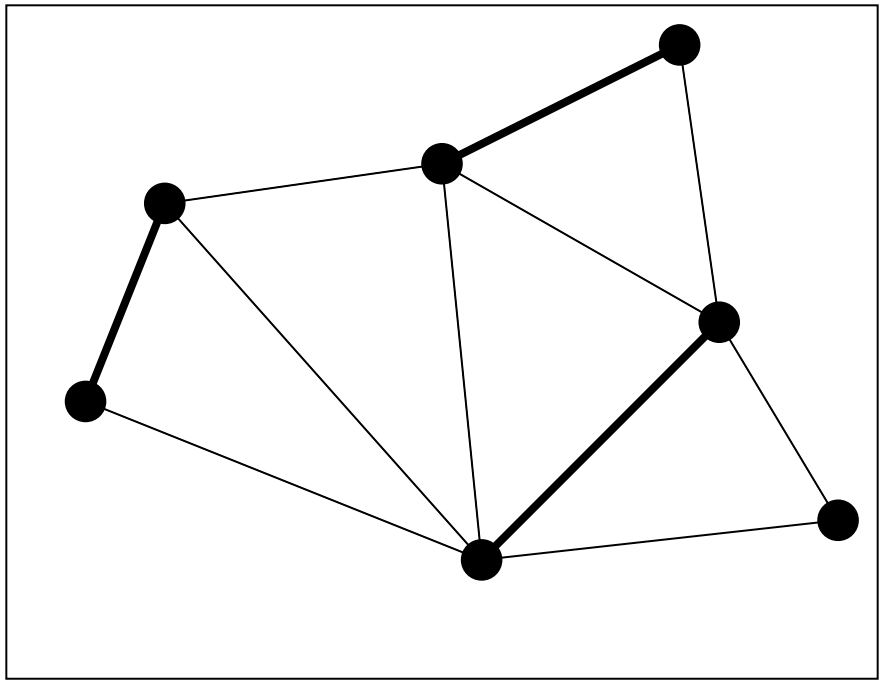




Merge matched clusters (sum ω and ζ).

Agglomerative clustering





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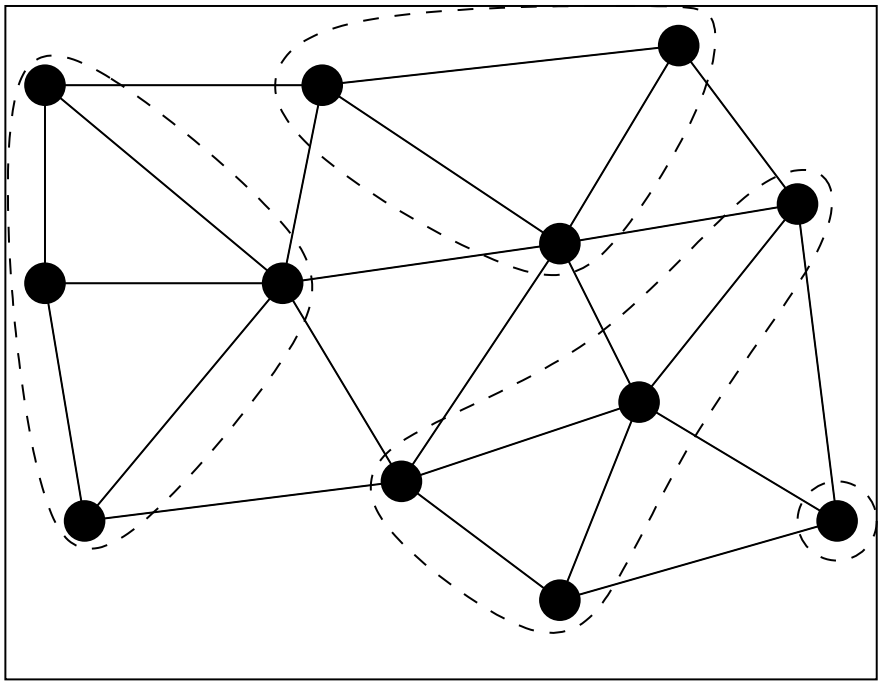

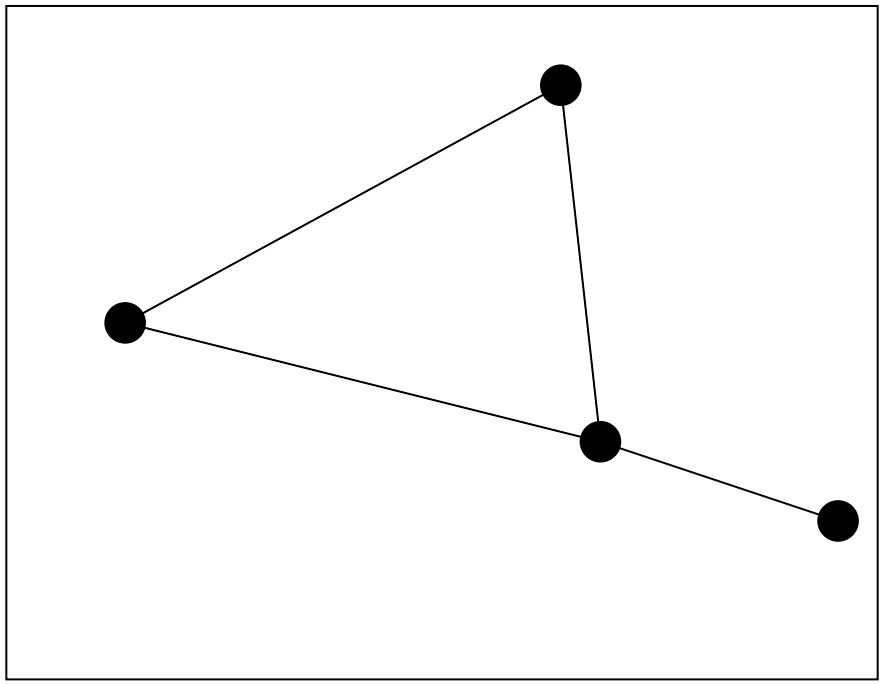

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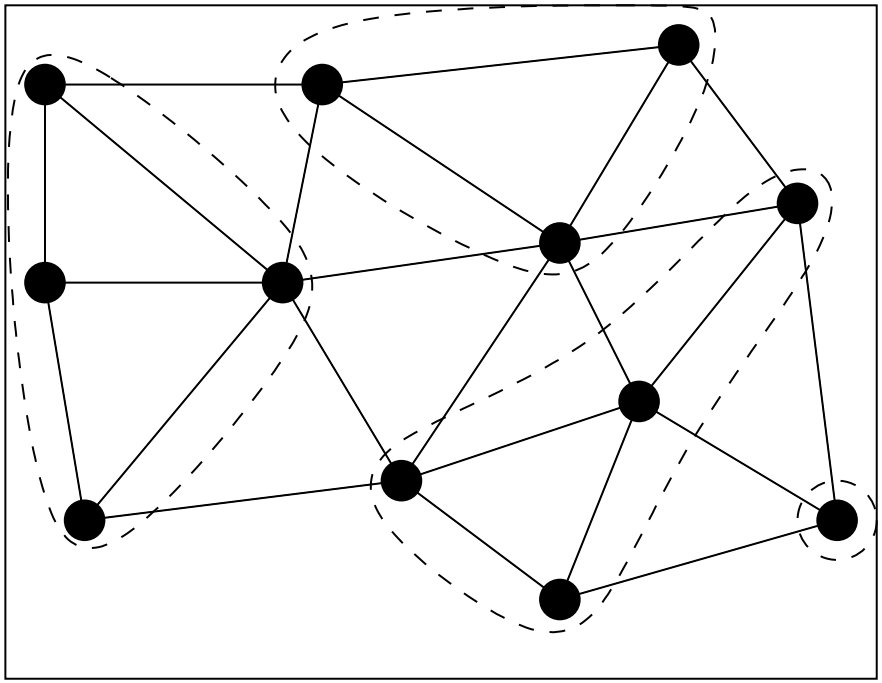

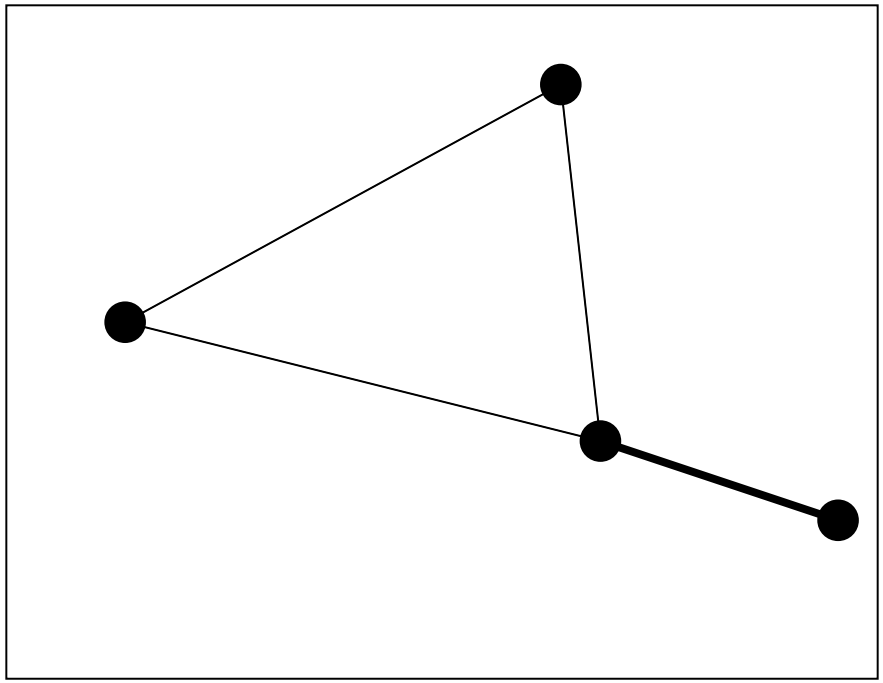

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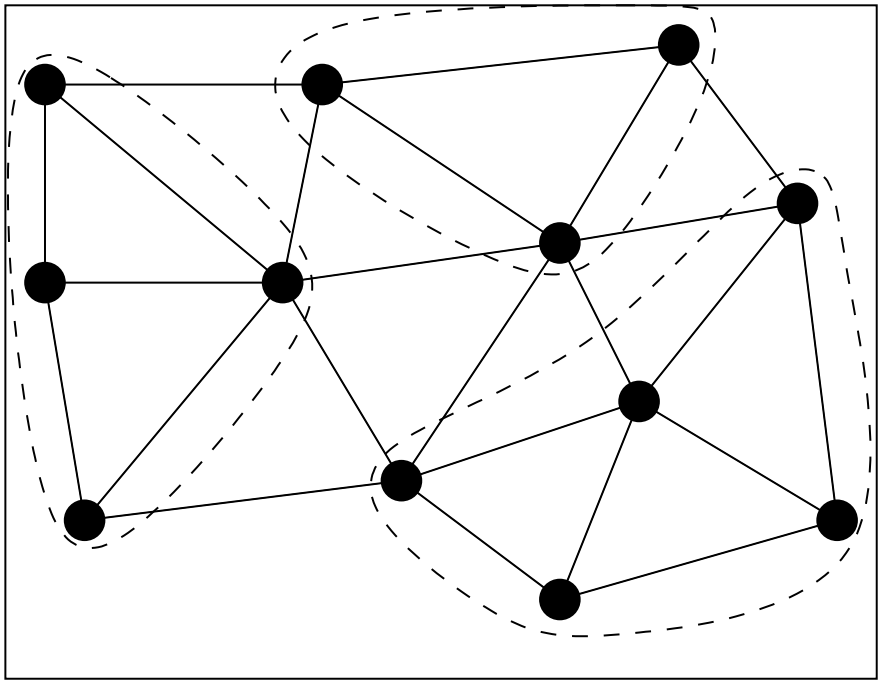
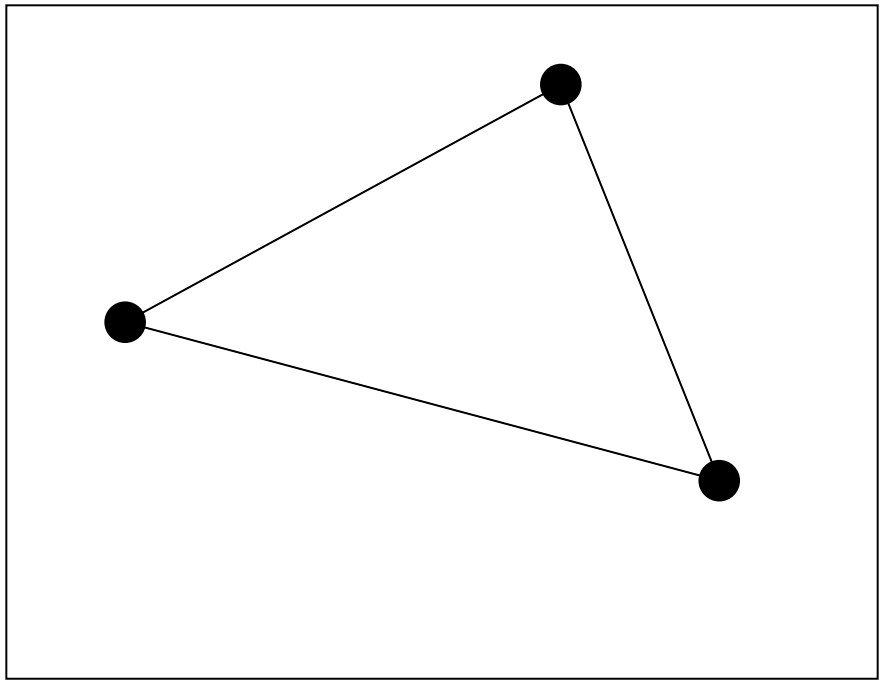
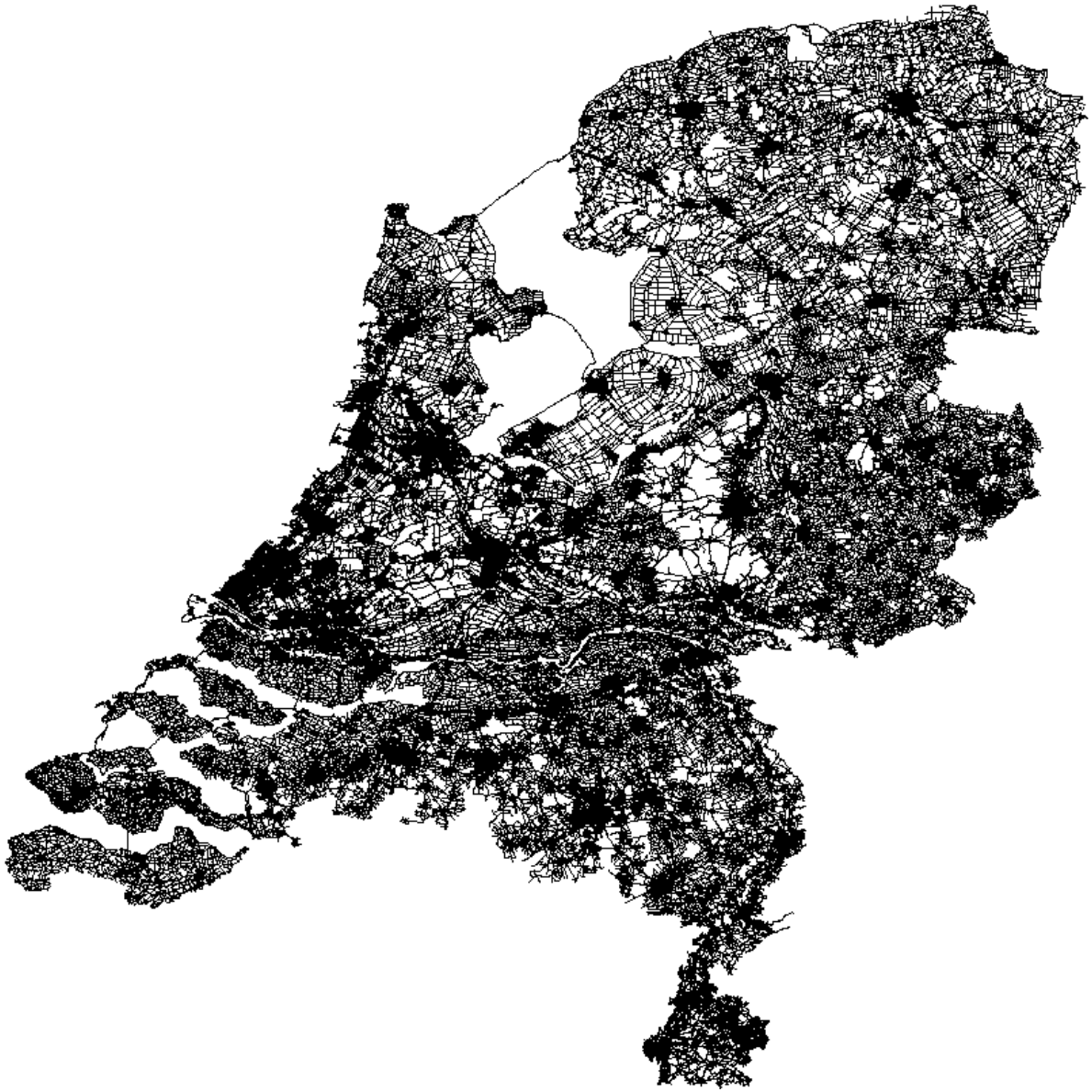




Return clustering with highest modularity.

Agglomerative clustering (netherlands)

0 iterations.



Agglomerative clustering (netherlands)

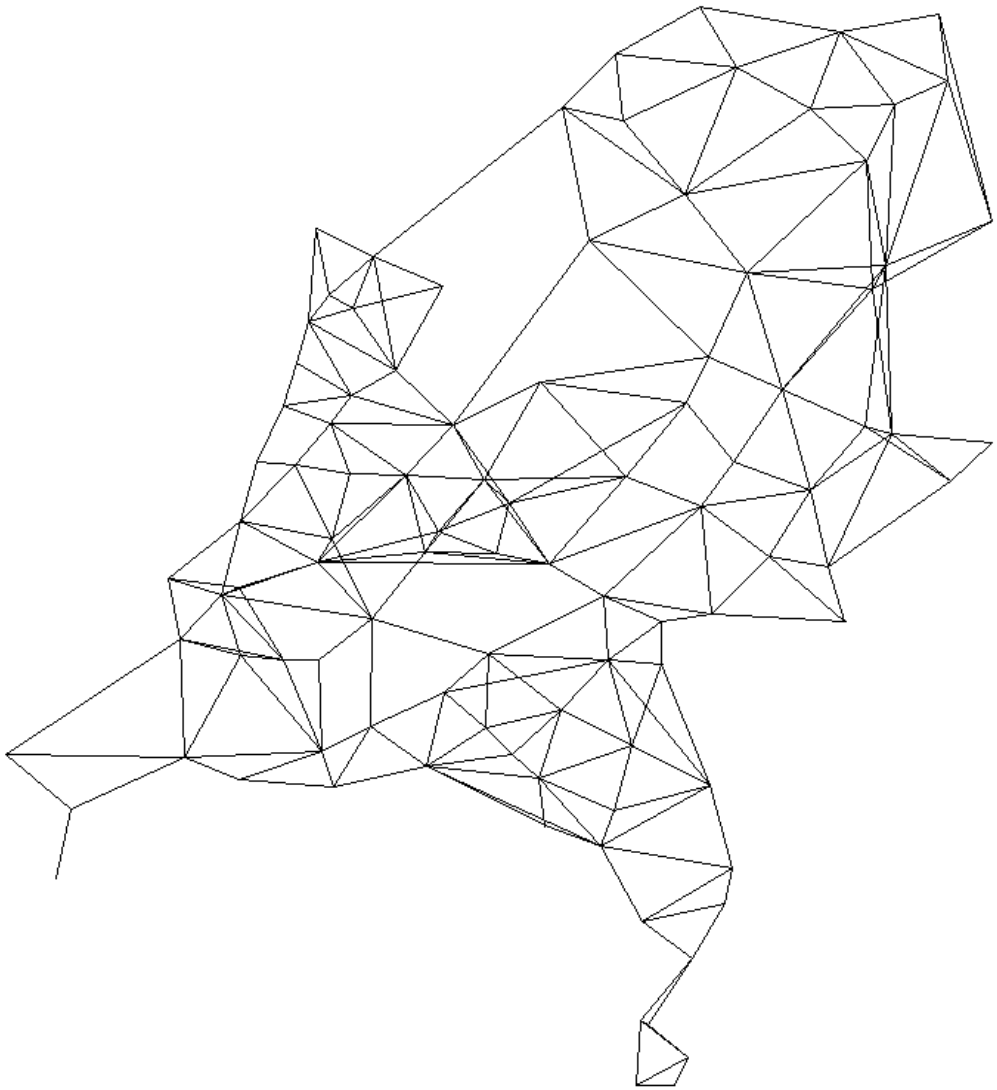
11 iterations.

Agglomerative clustering (netherlands)

21 iterations.

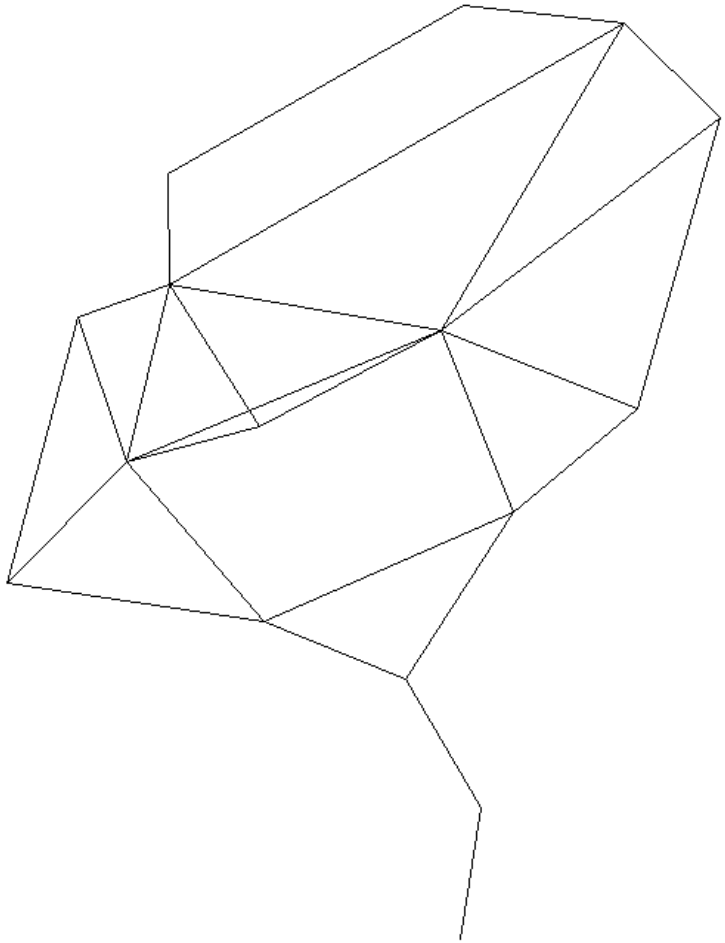
Agglomerative clustering (netherlands)

26 iterations.



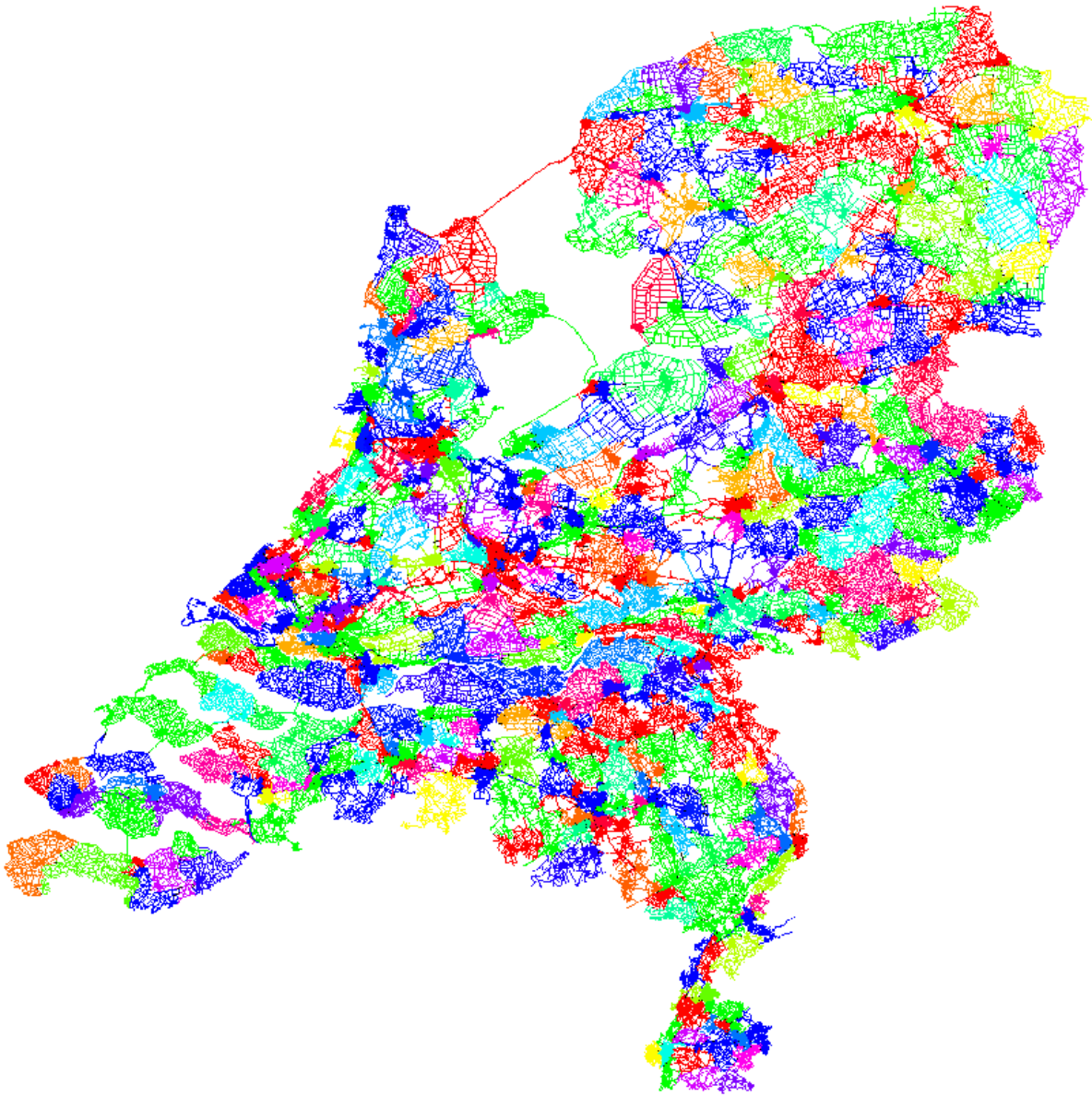
Agglomerative clustering (netherlands)

33 iterations.



Agglomerative clustering (netherlands)

Final clustering.



Parallel agglomerative clustering

1. Start with all vertices being a separate cluster: $\mathcal{C} = \{\{v\} \mid v \in V\}$.
2. Find a heavy matching of clusters with edge weights

$$\frac{1}{2\,\Omega^2}\left(2\,\Omega\,\omega(\mathrm{cut}(C, C')) - \zeta(C)\,\zeta(C')\right).$$

3. Extend matching to avoid getting stuck.
4. Merge all matched clusters, summing ζ and ω.
5. Go to step 2 until only a single cluster remains.
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We make use of parallelism in steps 2, 3, and 4.

GPU matching problems

- For a graph $G = (V, E)$, a matching is a collection $M \subseteq E$ of edges that are disjoint.

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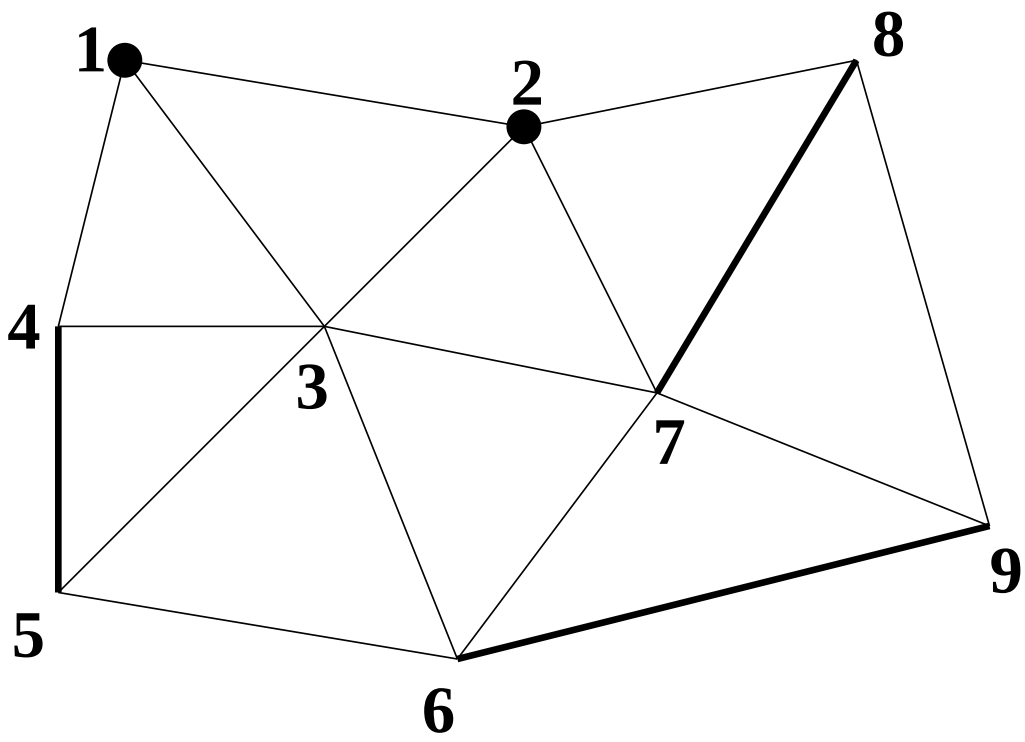
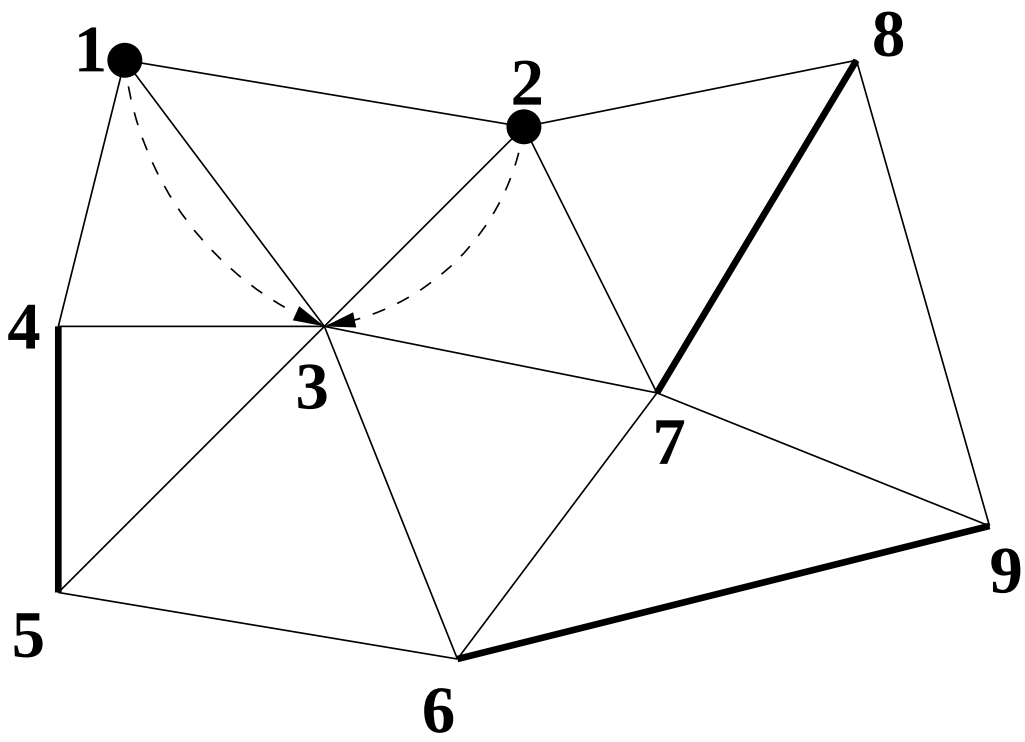
- Performing matching in parallel is problematic.
- Disjoint edges requirement leads to serialisation.

GPU matching problems



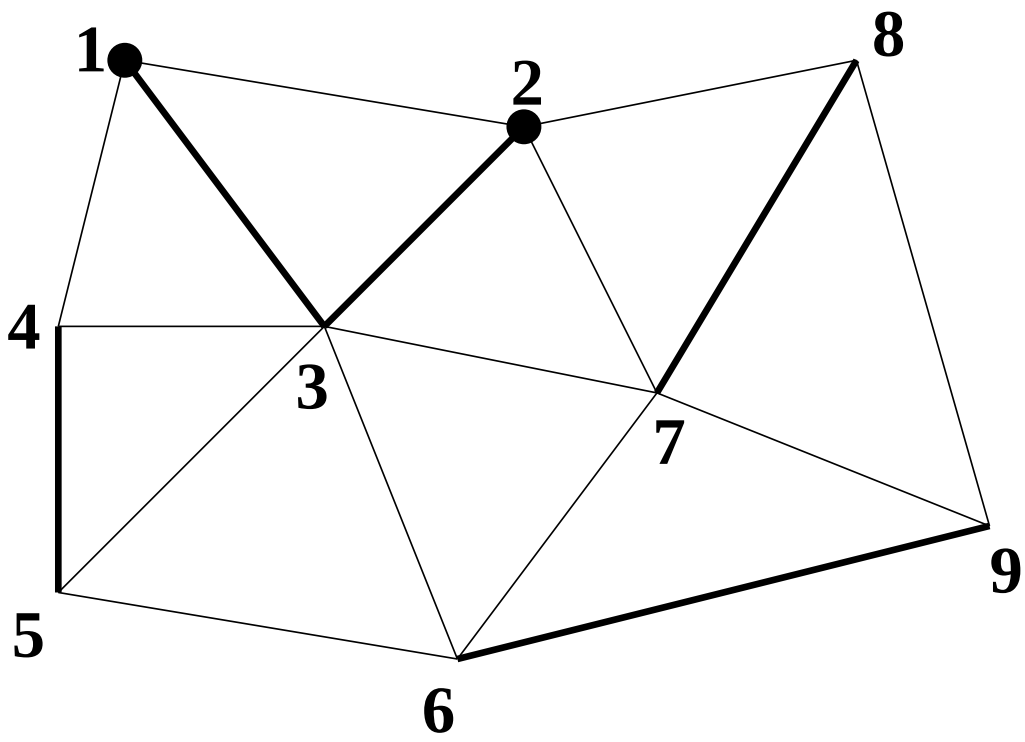
Suppose we match vertices simultaneously.

GPU matching problems



Vertices find an unmatched neighbour. . .

GPU matching problems



. . . but generate an invalid matching.

GPU matching

- To solve this we create two groups of vertices: **blue** and **red**.

GPU matching

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- **Blue** vertices propose.

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- Proposals that were responded to are matched.

GPU matching

- To solve this we create two groups of vertices: **blue** and **red**.
- **Blue** vertices propose.
- **Red** vertices respond.
- Proposals that were responded to are matched.
- Store matching in a map $\pi : V \rightarrow \mathbb{N}$:

$$\{u, v\} \in M \qquad \Longleftrightarrow \qquad \pi(u) = \pi(v).$$

GPU matching (implementation)

- The graph (neighbour ranges, indices, and weights) is stored as a triplet of 1D textures on the GPU.

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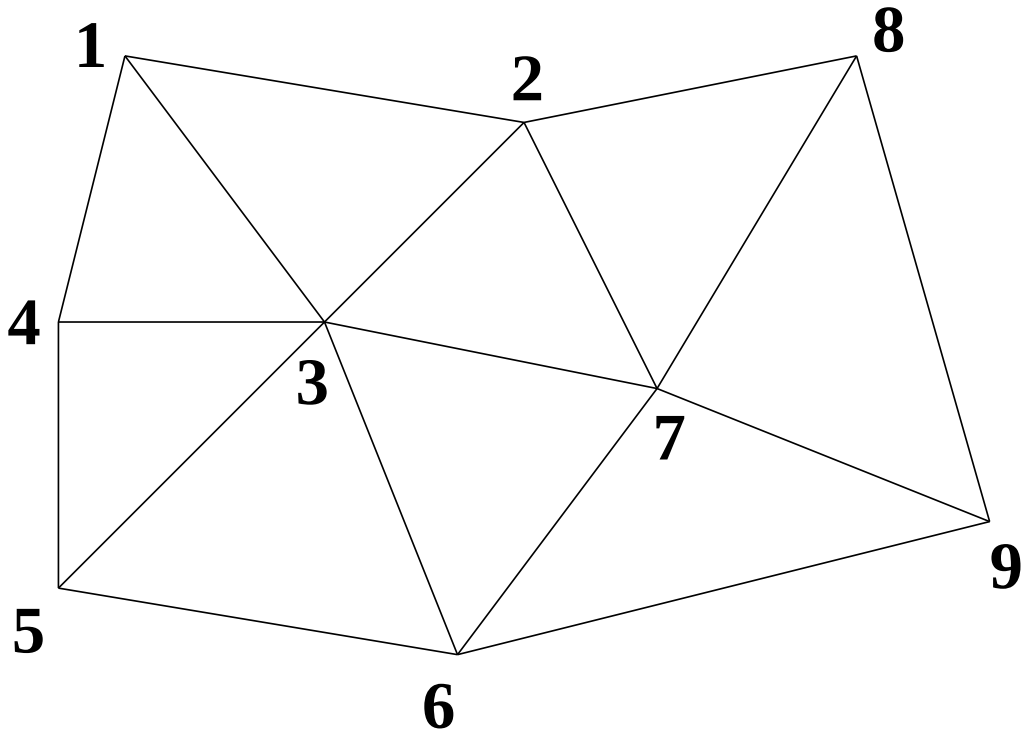
- We create one thread for each vertex in V.
- Each vertex $v \in V$ only updates
  - its colour/matching value $\pi(v)$;
  - and its proposal/response value $\sigma(v)$.
- Both π and σ are stored in 1D arrays in global memory.

GPU matching (algorithm)

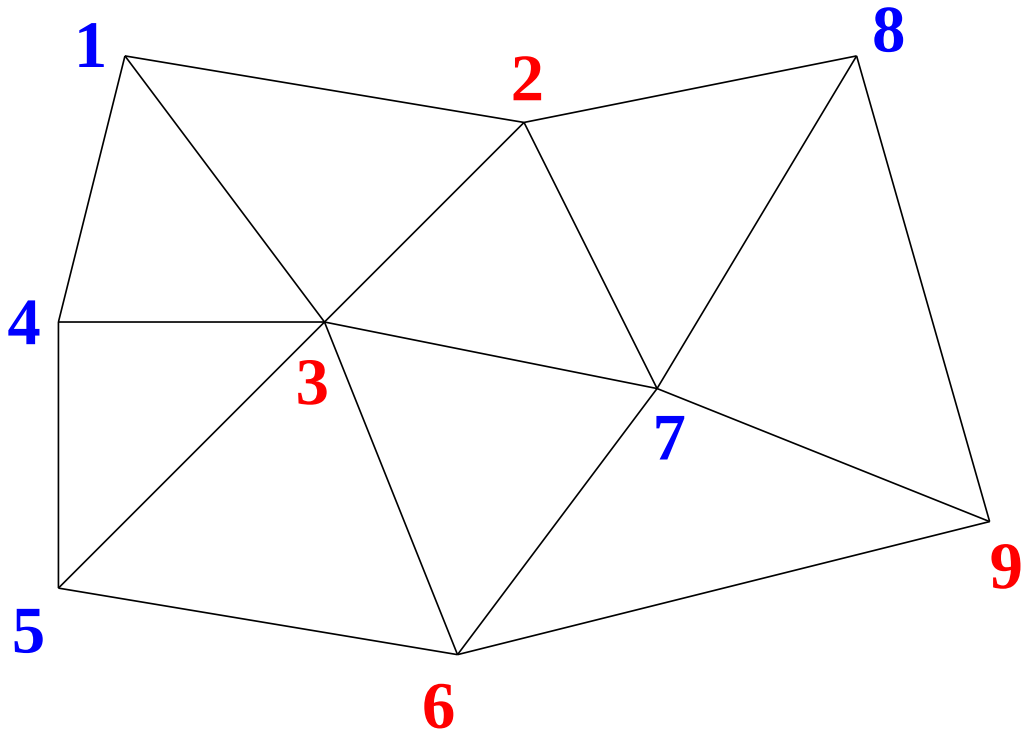
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	-	-	-	-	-	-	-	-	-
σ	-	-	-	-	-	-	-	-	-

GPU matching (algorithm)

Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	-	-	-	-	-	-	-	-	-

GPU matching (algorithm)

Colour
Propose
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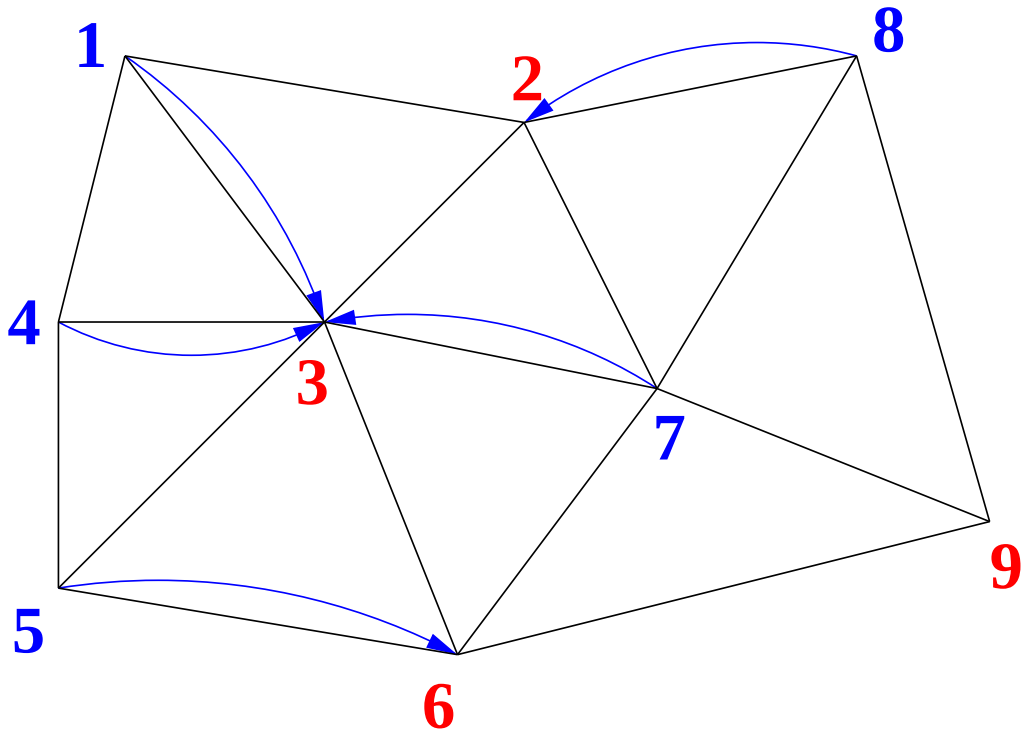
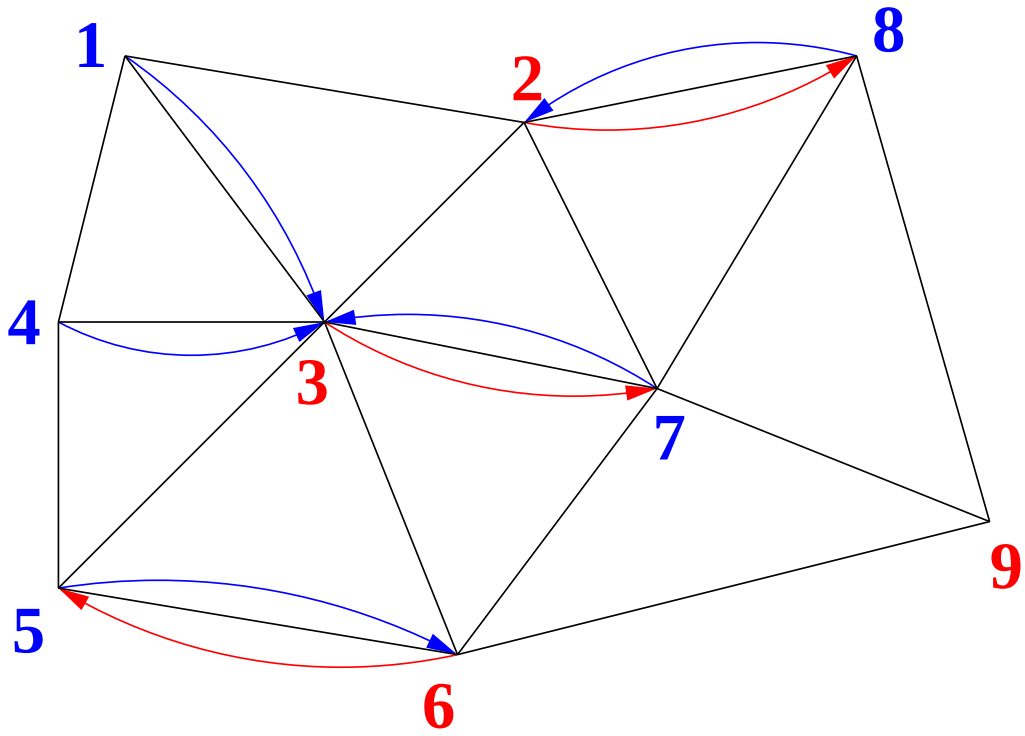


	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	3	-	-	3	6	-	3	2	-

GPU matching (algorithm)

Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	3	8	7	3	6	5	3	2	-

GPU matching (algorithm)

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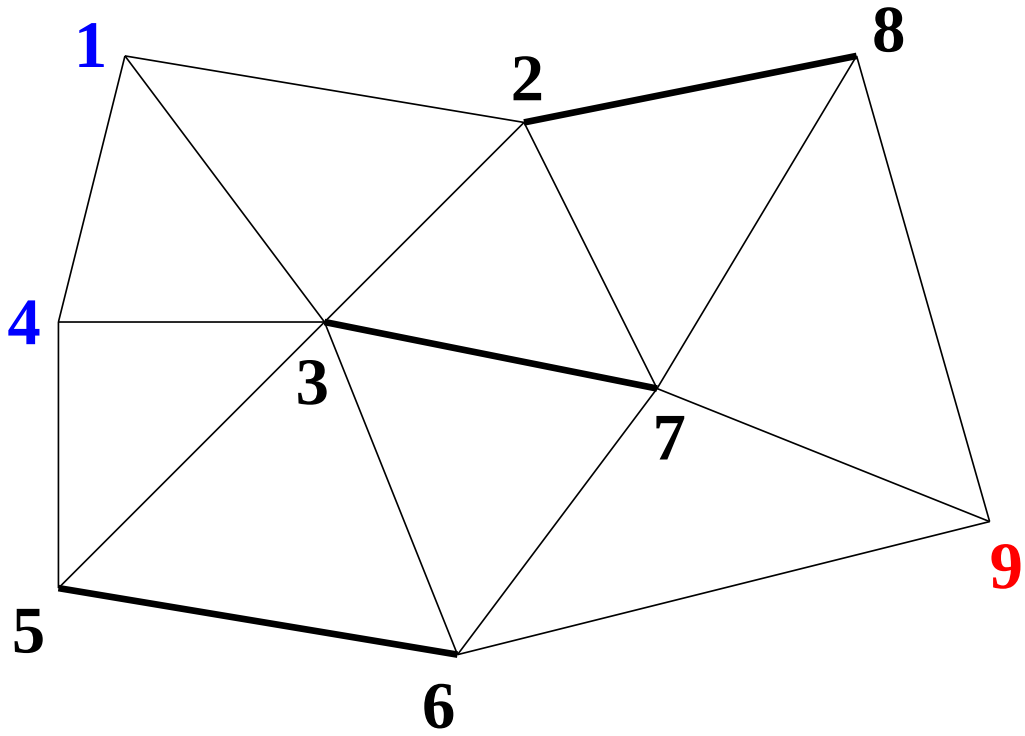

	1	2	3	4	5	6	7	8	9
π	**b**	2	3	**b**	5	5	3	2	**r**
σ	3	8	7	3	6	5	3	2	-

GPU matching (algorithm)

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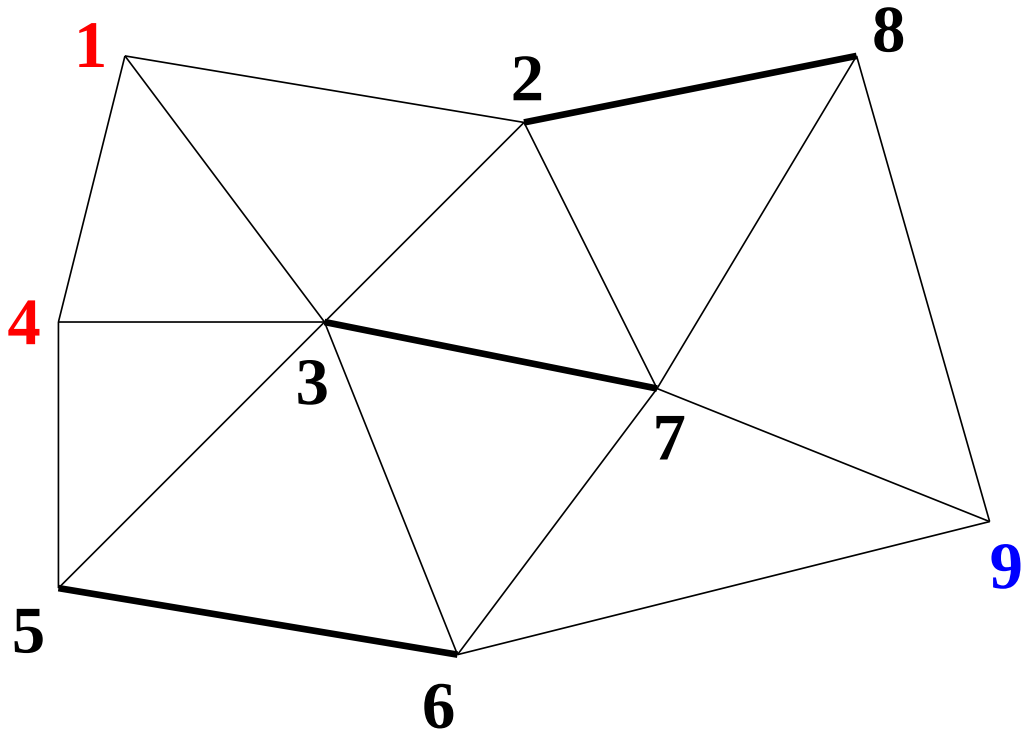
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**b**
σ	3	8	7	3	6	5	3	2	-

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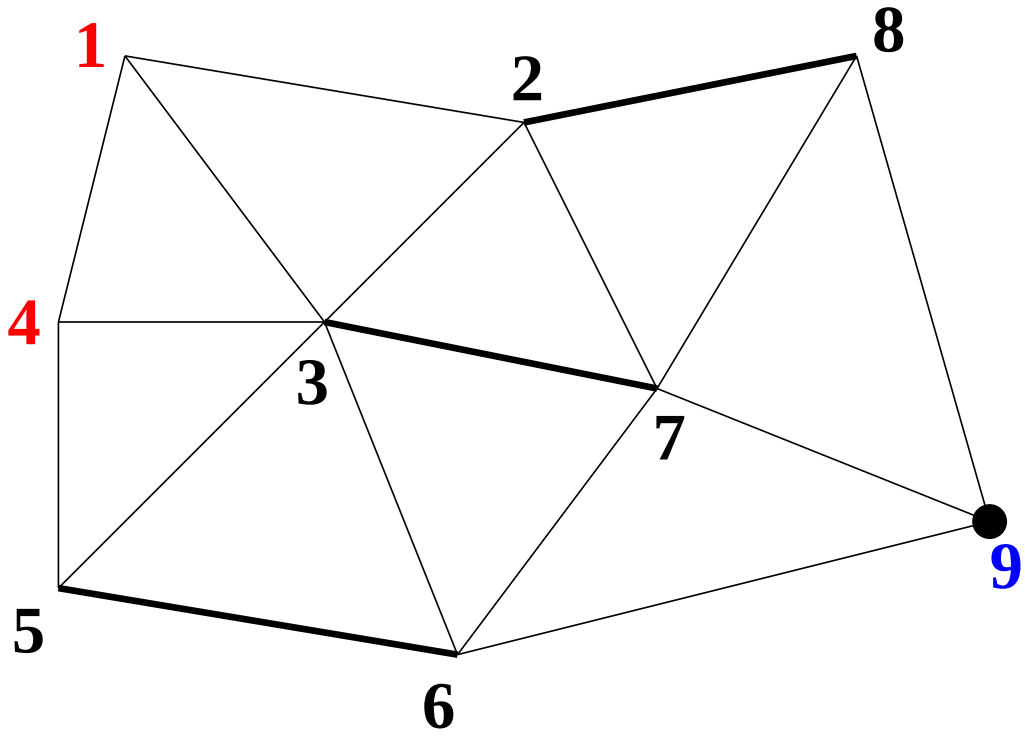

	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**b**
σ	-	-	-	-	-	-	-	-	**d**

GPU matching (algorithm)

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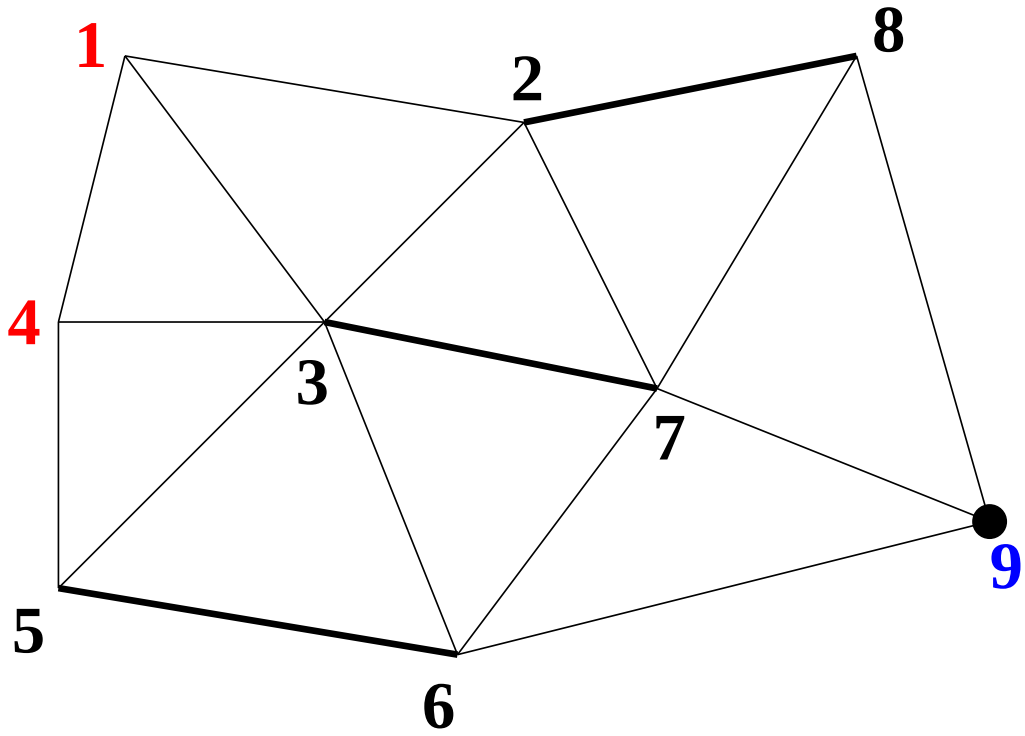
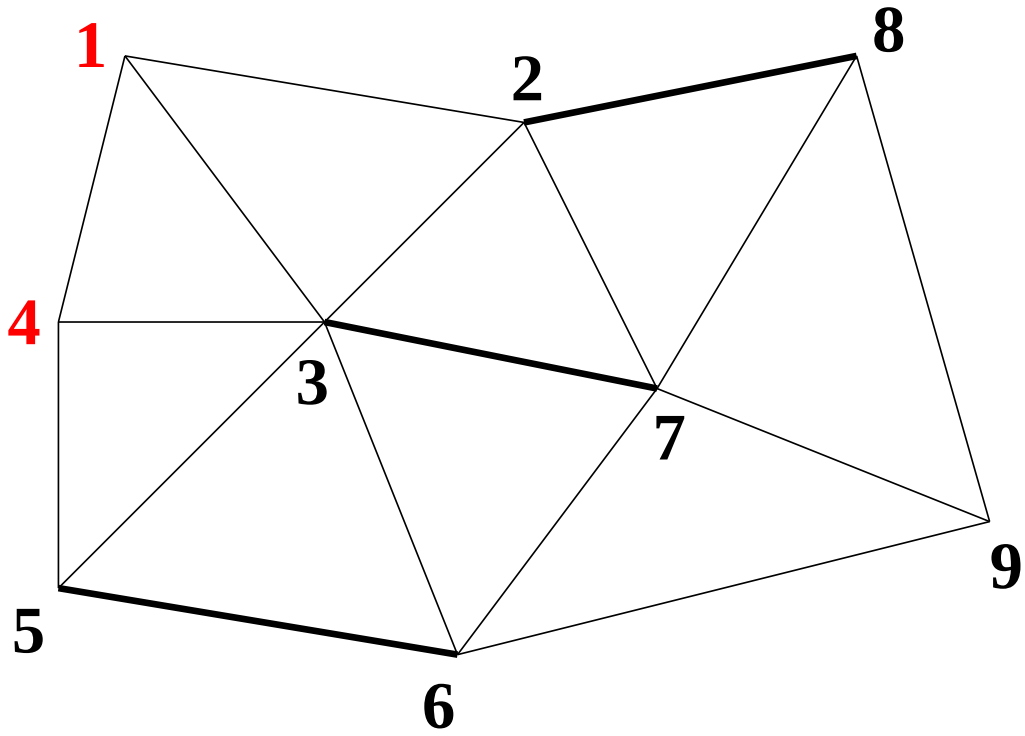
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**b**
σ	-	-	-	-	-	-	-	-	**d**

GPU matching (algorithm)

Colour
Propose
Respond
Match



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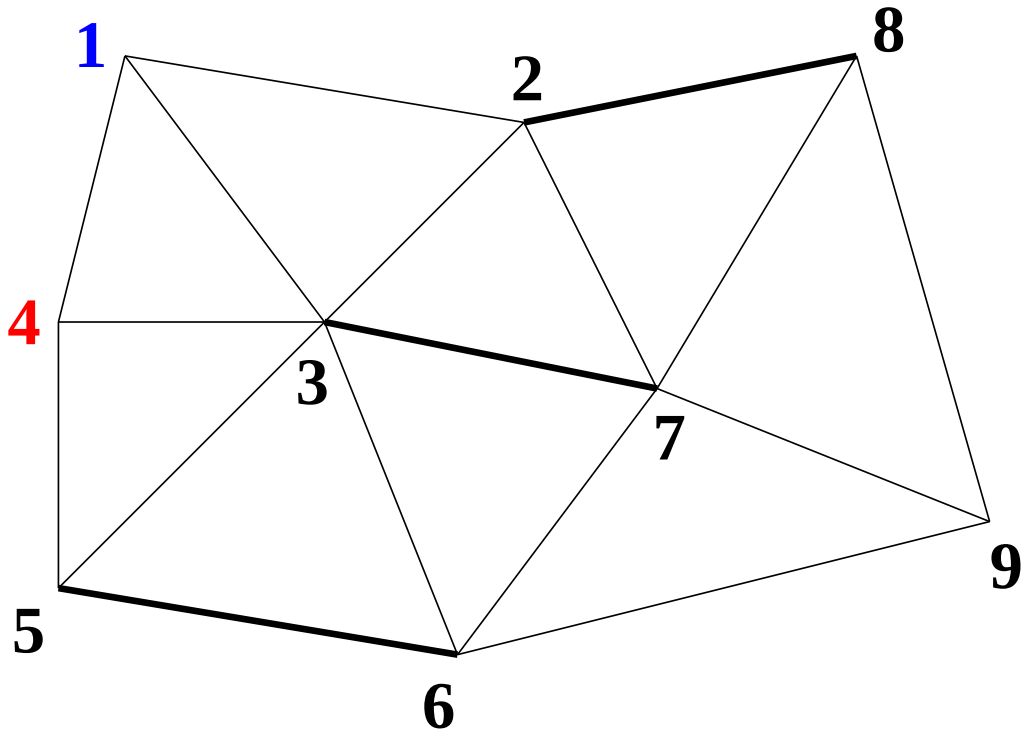

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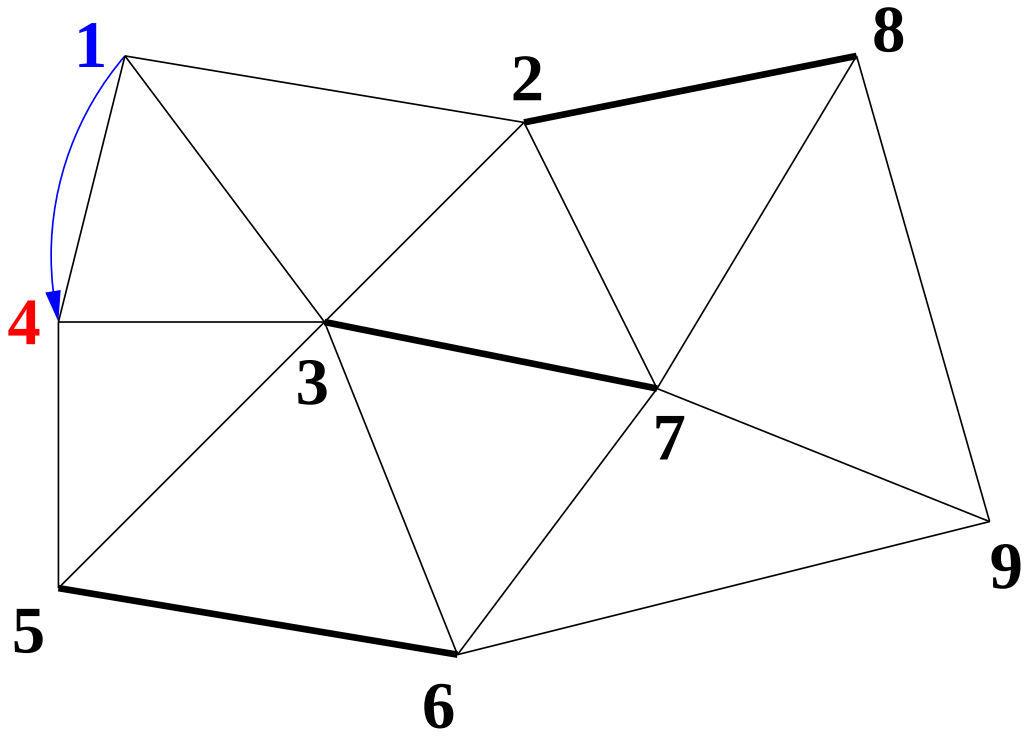

	1	2	3	4	5	6	7	8	9
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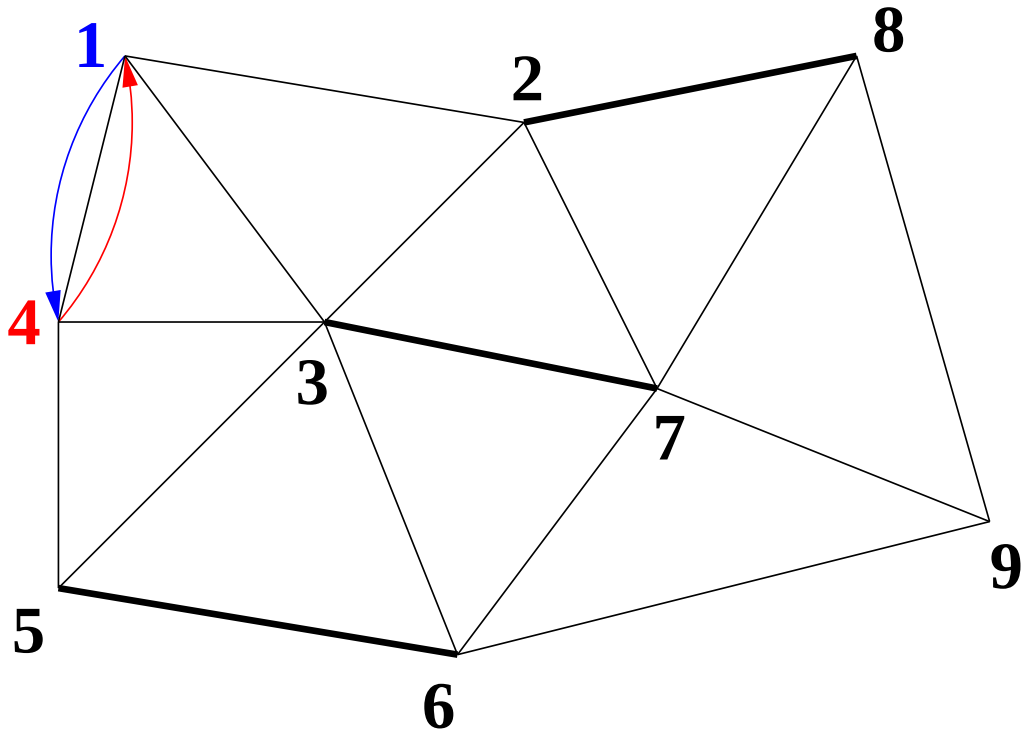

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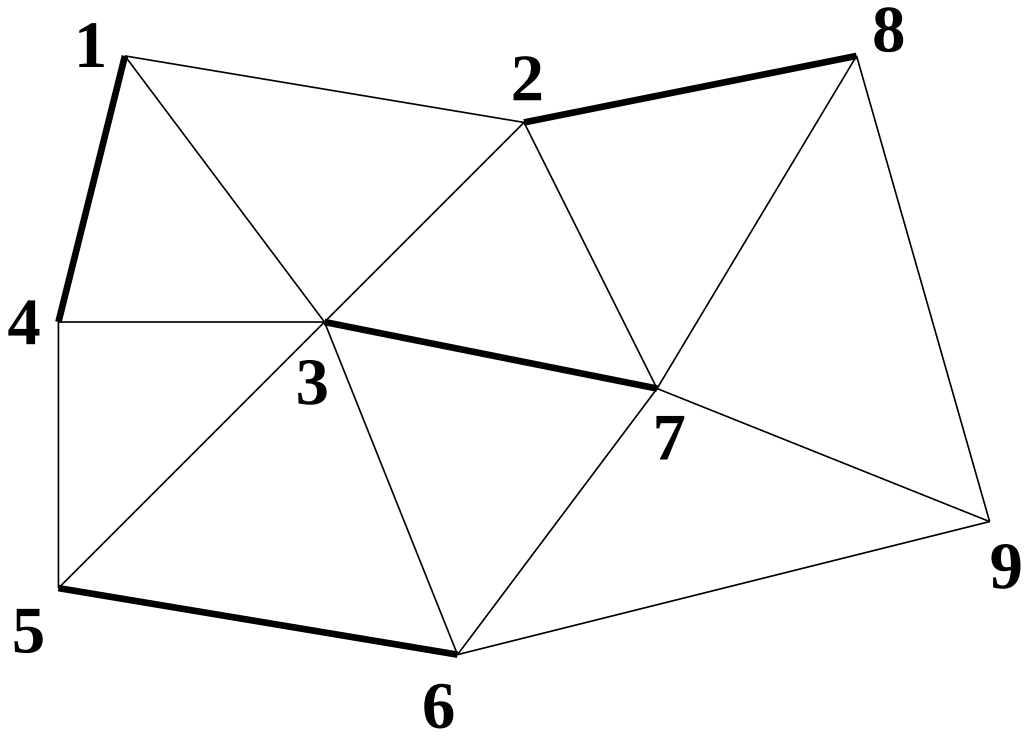

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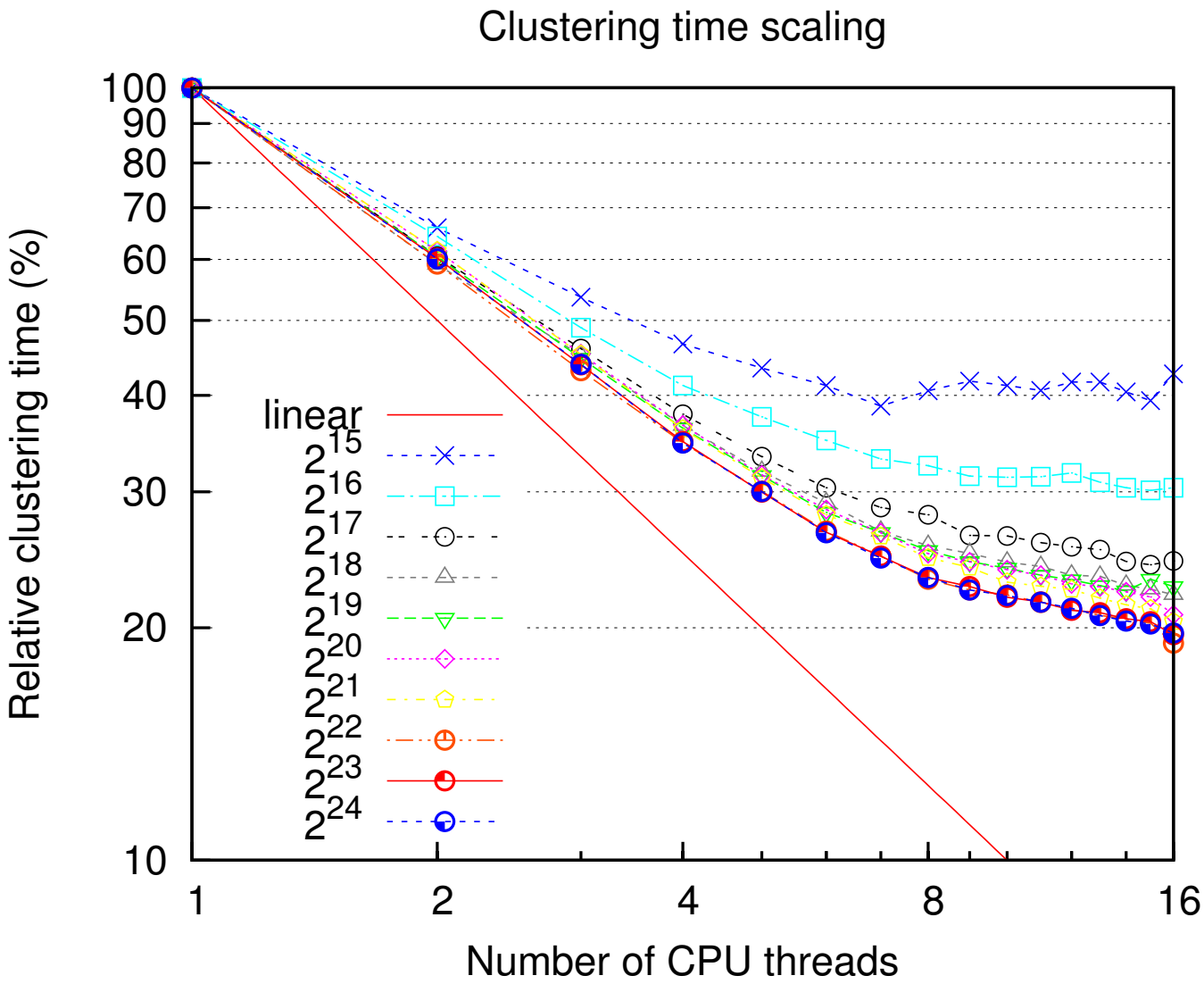
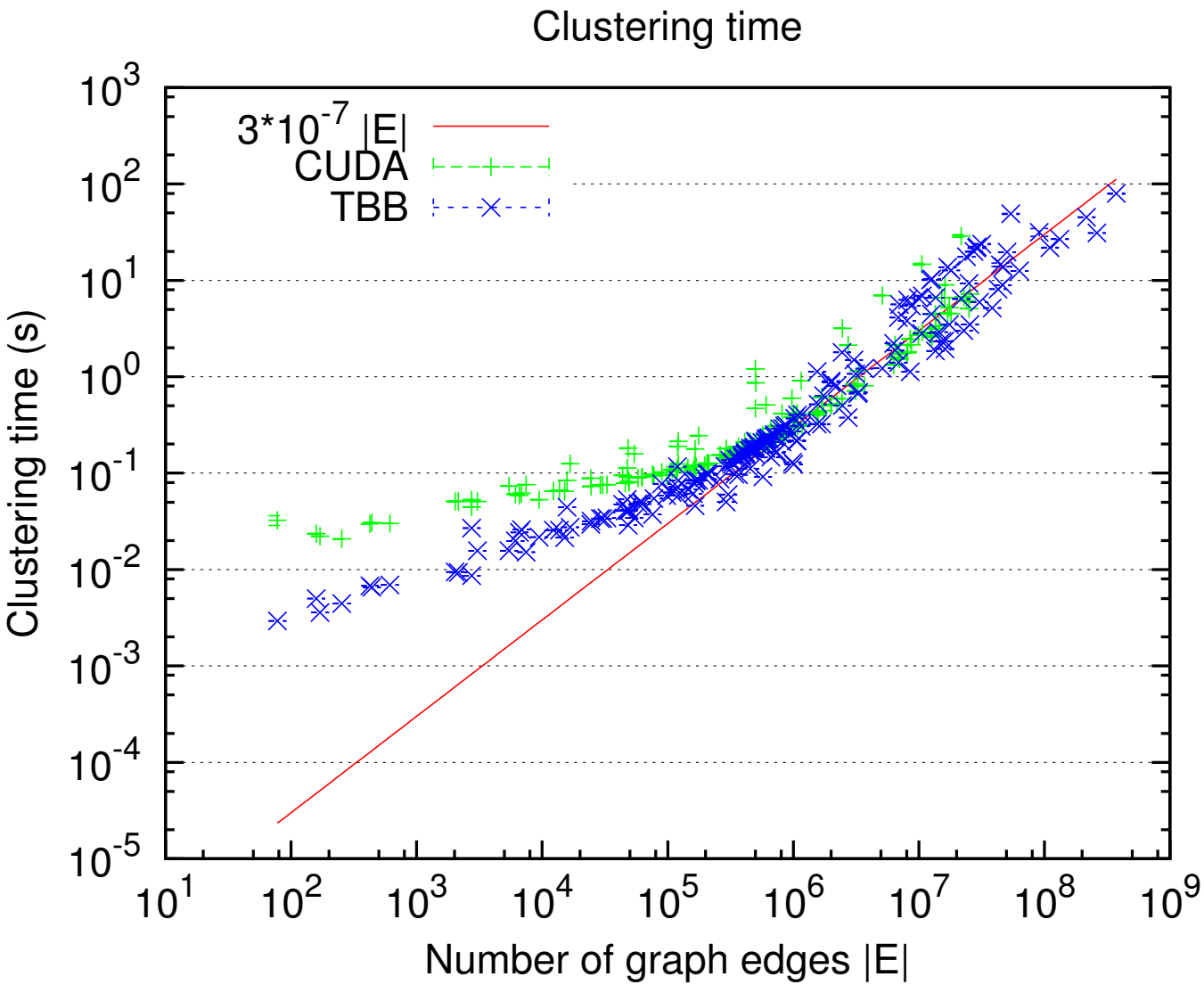
- Test set: 10th DIMACS challenge.
- Test hardware: dual quad-core Xeon E5620 and an NVIDIA Tesla C2050 (thanks: the Little Green Machine project).

Results (scaling)



Results (time)



Results (quality)

	$\|V\|$	$\|E\|$	CUDA	TBB	Ovelgönne et al. (2010)
karate	34	78	0.363	0.383	0.412
jazz	198	2,742	0.314	0.369	0.444
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- Lower quality, because we do not use local refinement.

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- TBB: `uk-2002`, $|V| = 18{,}520{,}486$, $|E| = 261{,}787{,}258$, modularity 0.974 clustering in 31 seconds.

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- The algorithm is very fast, but quality could be improved by parallel local refinement.

Questions

$\exists$ any questions?

Modularity

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- But this leads to $\mathcal{C} = \{V\}$ as optimal solution!

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- Cut all edges and reconnect vertices randomly, then

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- Modularity measures how much better we do than the random case:

$$\text{mod}(\mathcal{C}) := \sum_{i=1}^{k} \left(e_{i\,i} - a_i^2 \right).$$

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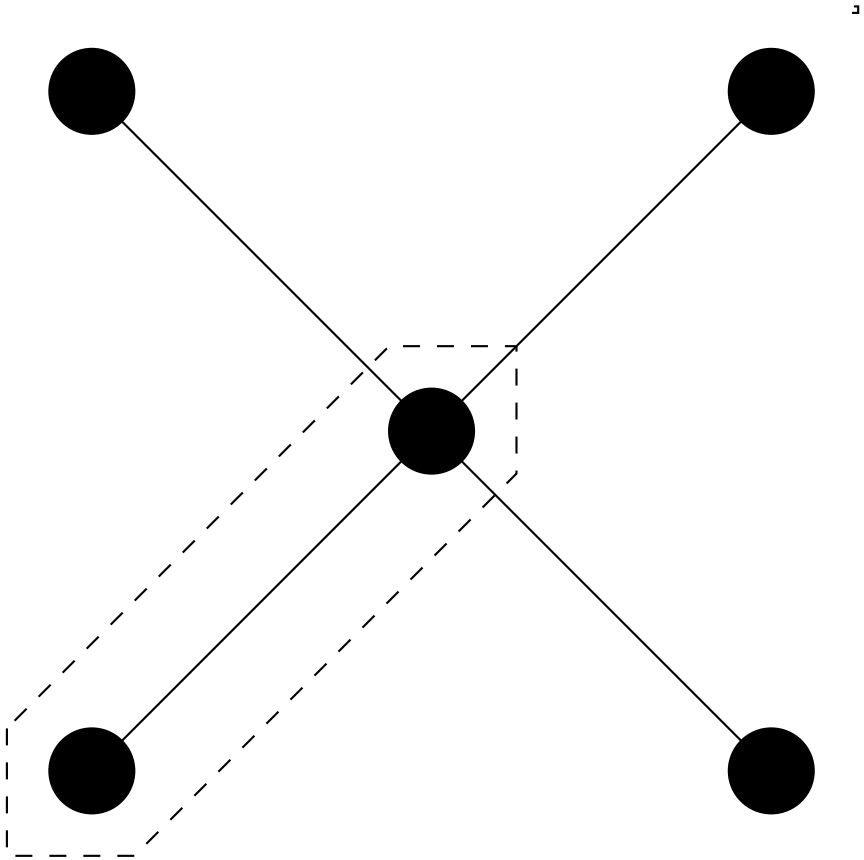
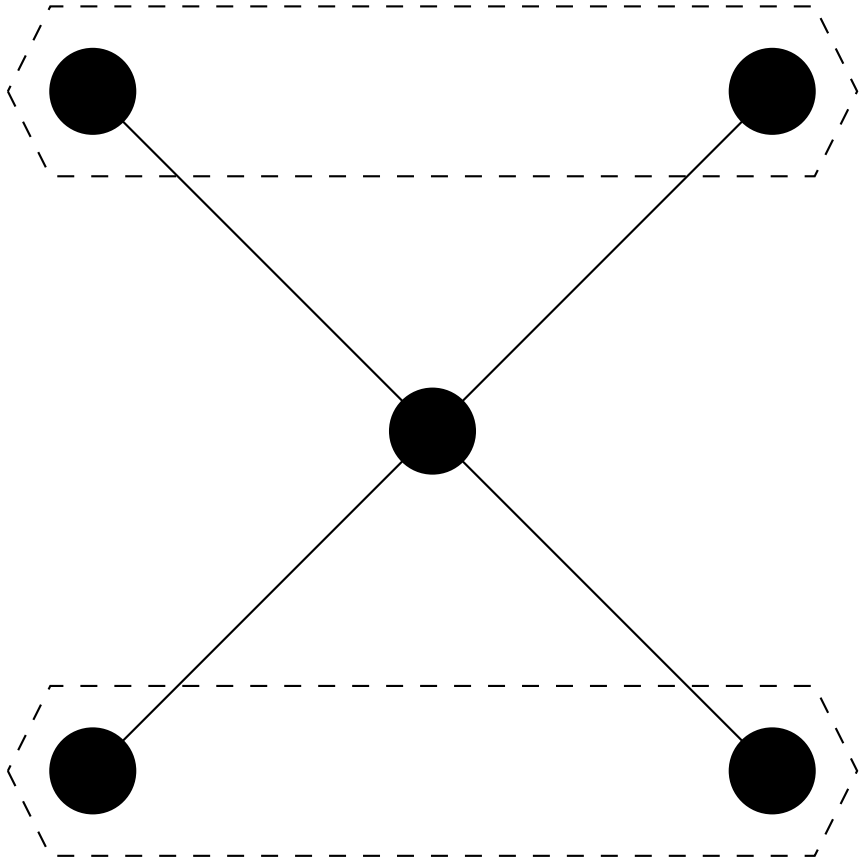
- Modularity maximisation fails to resolve small communities (Kumpula et al., 2007).

Star graphs



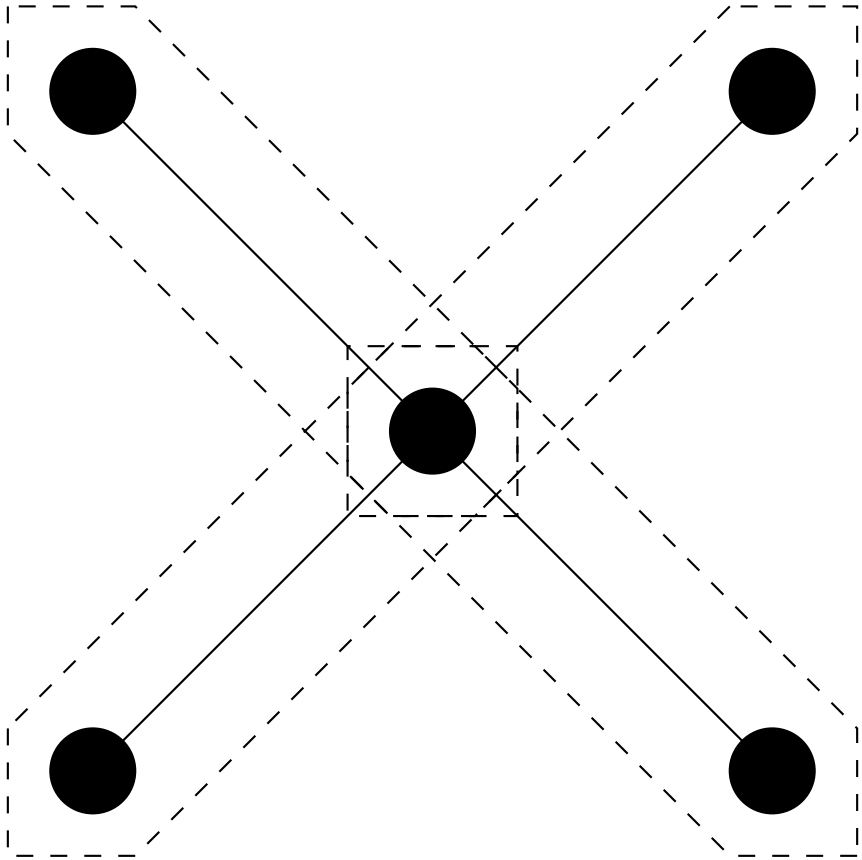
Agglomerative clustering slows down on star graphs.

Star graphs



Merging vertices with the same neighbours is bad for clustering.

Star graphs



So we merge multiple satellites to the same centre.

Centre potential

- To identify star centres and satellites, we propose a centre potential.

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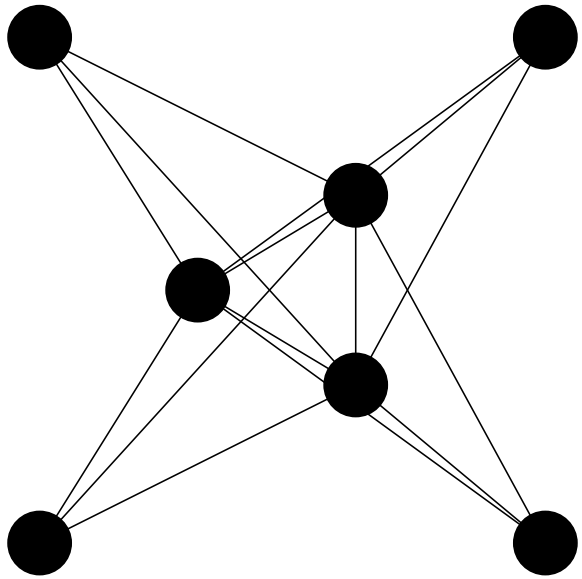
- We use $\mathrm{cp}(\cdot)$ to identify satellites and match these to centres.

Centre potential



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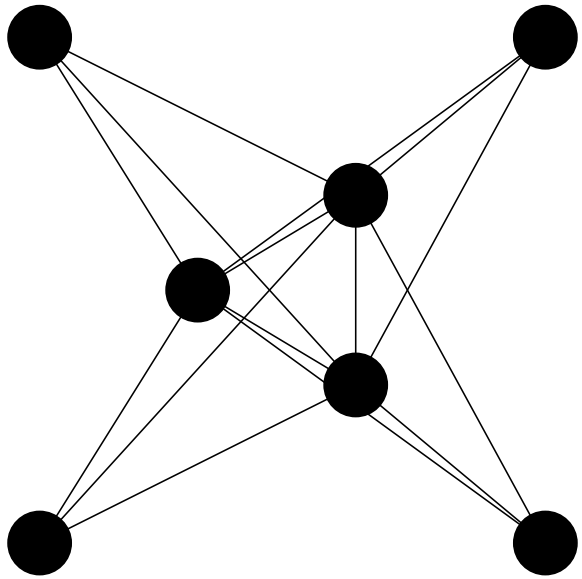

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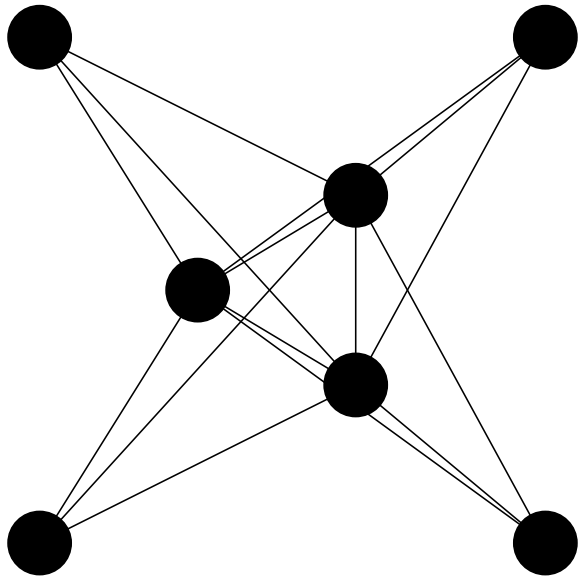

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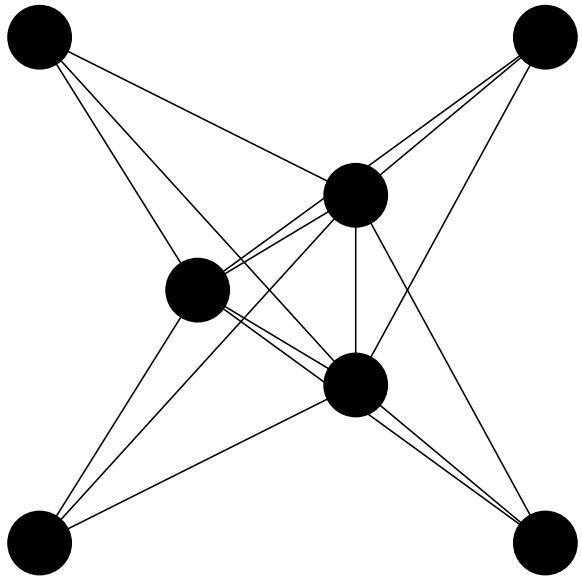

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$$\text{cp(centre)} \geq \frac{4}{3} \qquad \text{and cp(centre)} \to \infty \text{ as } k \to \infty.$$

Colouring vertices

- To colour vertices $v \in V$, we use for a fixed $p \in [0, 1]$

$$\pi(v) = \begin{cases} \textbf{blue} & \text{with probability } p, \\ \textbf{red} & \text{with probability } 1 - p. \end{cases}$$

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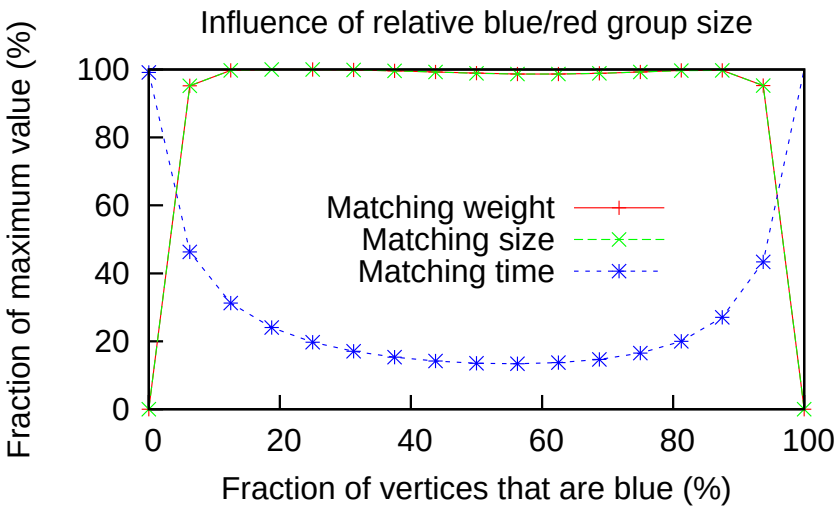
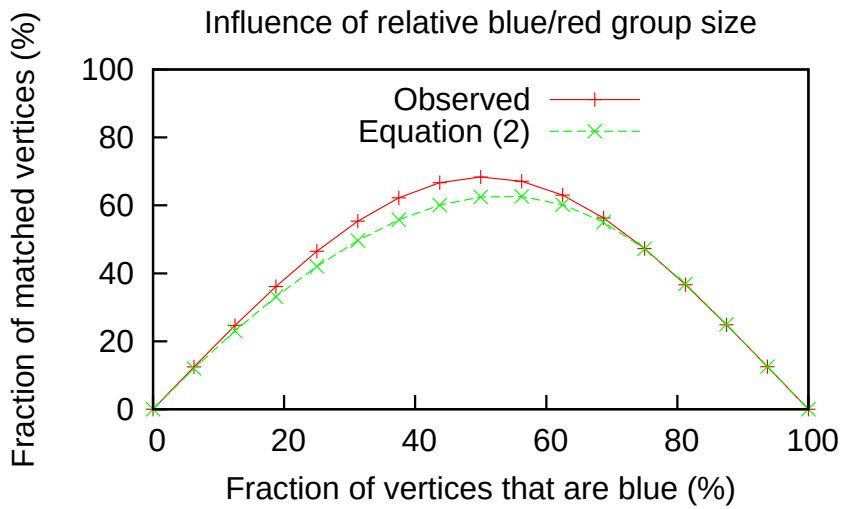
- How to choose p? Maximise the number of matched vertices.
- For a large random graphs, the expected fraction of matched vertices can be approximated by (independent of edge density)

$$2\,(1-p)\left(1 - e^{-\frac{p}{1-p}}\right).$$

Choosing p





We should choose $p \approx 0.53406$.

Choosing p

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- For a random graph with n vertices, we can approximate (independent of edge density)

$$\lim_{n\to\infty} \frac{2\,E(N(n))}{n} \approx 2\,(1-p)\left(1 - e^{-\frac{p}{1-p}}\right).$$

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$$\approx n(1-p) \left(1 - \left(1 - \frac{p\, d}{1 + (1-p)\,(d\,(n-1) - 1)}\right)^{n-1}\right).$$

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  - $$\zeta'(v') = \sum_{\pi(v)=v'} \zeta(v)$$ (sum vertex weights),
  - $\pi(u) = \pi(v)$ if and only if $\mu(u) = \mu(v)$ (compress μ to π).

GPU coarsening (implementation)

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- View G as a collection of adjacency lists for each vertex.
- First, we create π and π^{-1} from μ.
- Then, we create the new adjacency lists and weights for G'.
- Use μ, π, π^{-1}, and a bookkeeping array ρ in global GPU memory.

GPU coarsening (algorithm)

ρ	1	2	3	4	5	6	7	8	9	10	11	12
μ	9	2	3	22	9	9	22	2	3	3	2	4
π^{-1}												
π												

Initialise ρ sequentially and store μ.

GPU coarsening (algorithm)

ρ	1	2	3	4	5	6	7	8	9	10	11	12
μ	9	2	3	22	9	9	22	2	3	3	2	4
π^{-1}												
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Sort by increasing μ-value (`sort_by_key`).

GPU coarsening (algorithm)

ρ	2	8	11	3	9	10	12	1	5	6	4	7
μ	2	2	2	3	3	3	4	9	9	9	22	22
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ρ	2	8	11	3	9	10	12	1	5	6	4	7
μ	2	2	2	3	3	3	4	9	9	9	22	22
π^{-1}												
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Determine different matched groups (`adjacent_not_equal`).

GPU coarsening (algorithm)

ρ	2	8	11	3	9	10	12	1	5	6	4	7
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π^{-1}												
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Extract boundaries for π^{-1} (`copy_index_if_nonzero`).

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Perform scan to find π indices (`inclusive_scan`).

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ρ	2	8	11	3	9	10	12	1	5	6	4	7
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μ	1	1	1	2	2	2	3	4	4	4	5	5
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