Sublinear Algorithms for Hierarchical Clustering

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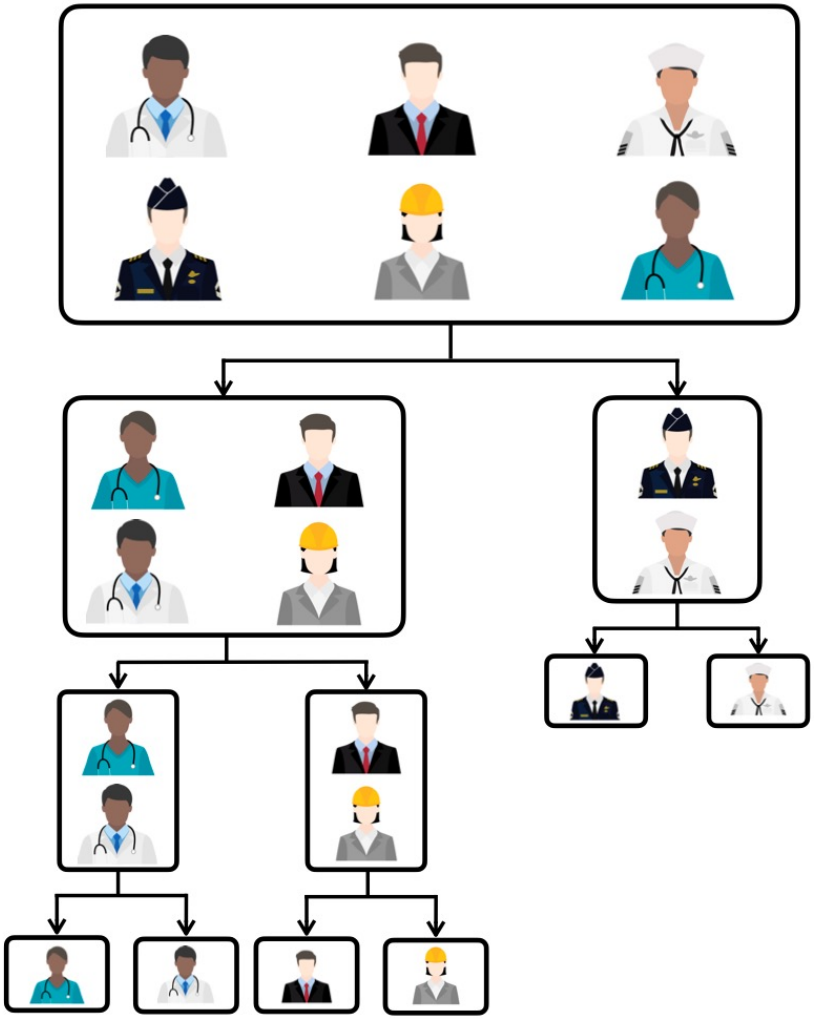
Joint work with Arpit Agarwal (Columbia), Huan Li (Penn), and Prathamesh Patil (Penn).

Hierarchical Clustering

A technique to cluster data into a multilevel hierarchy based on similarity.

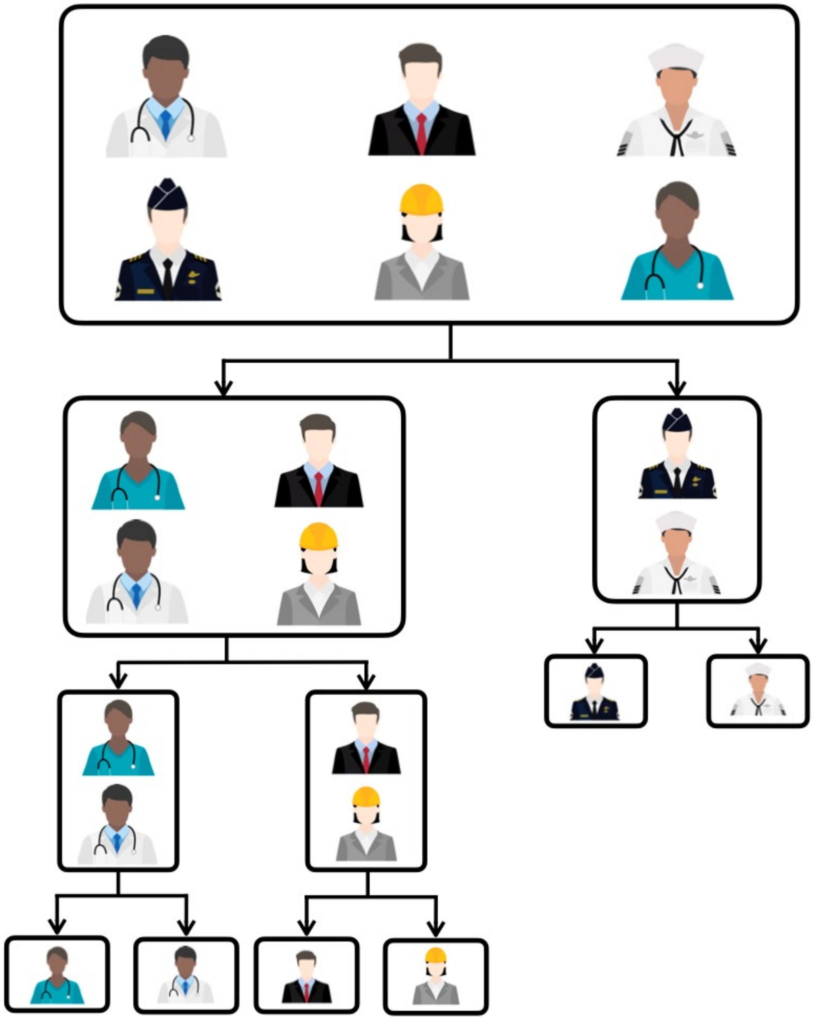


Hierarchical Clustering

A technique to cluster data into a multilevel hierarchy based on similarity. It arranges data as a rooted tree such that

-- the root represents the entire data set, and each leaf corresponds to a unique data point.

-- each internal node corresponds to a cluster containing its descendant leaves



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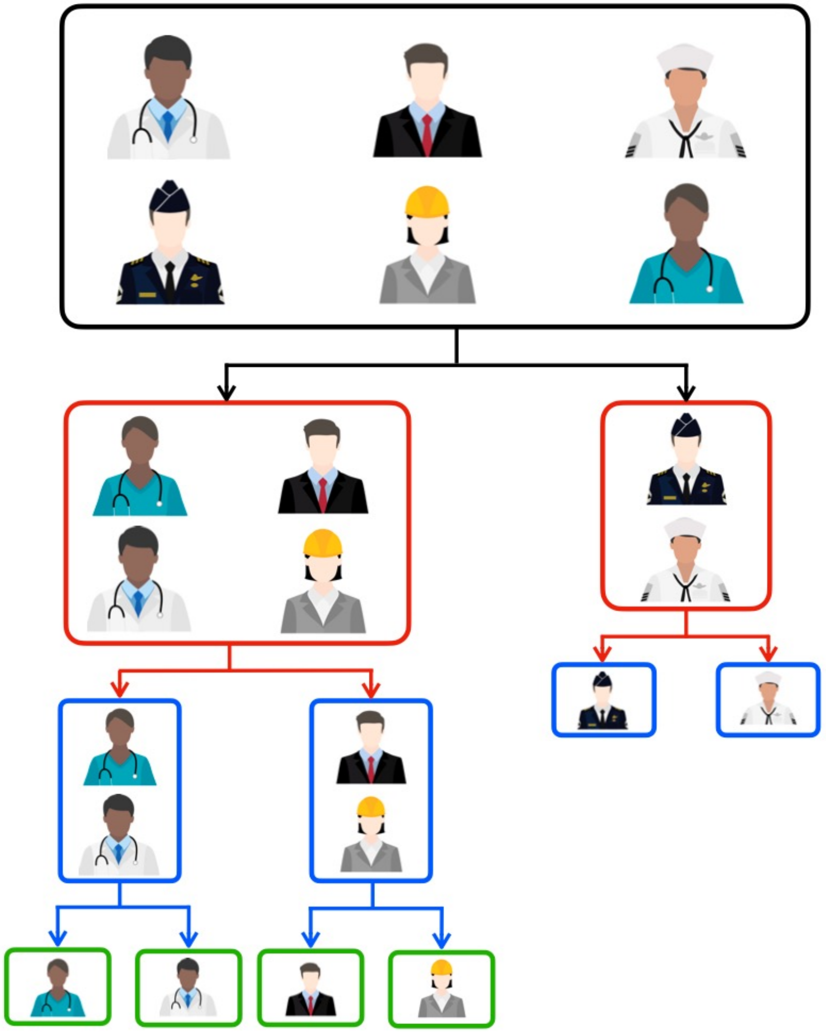
Clusters data at multiple levels of granularity simultaneously.



The Hierarchical Clustering Problem

Dasgupta (2016) introduced the following formalization:

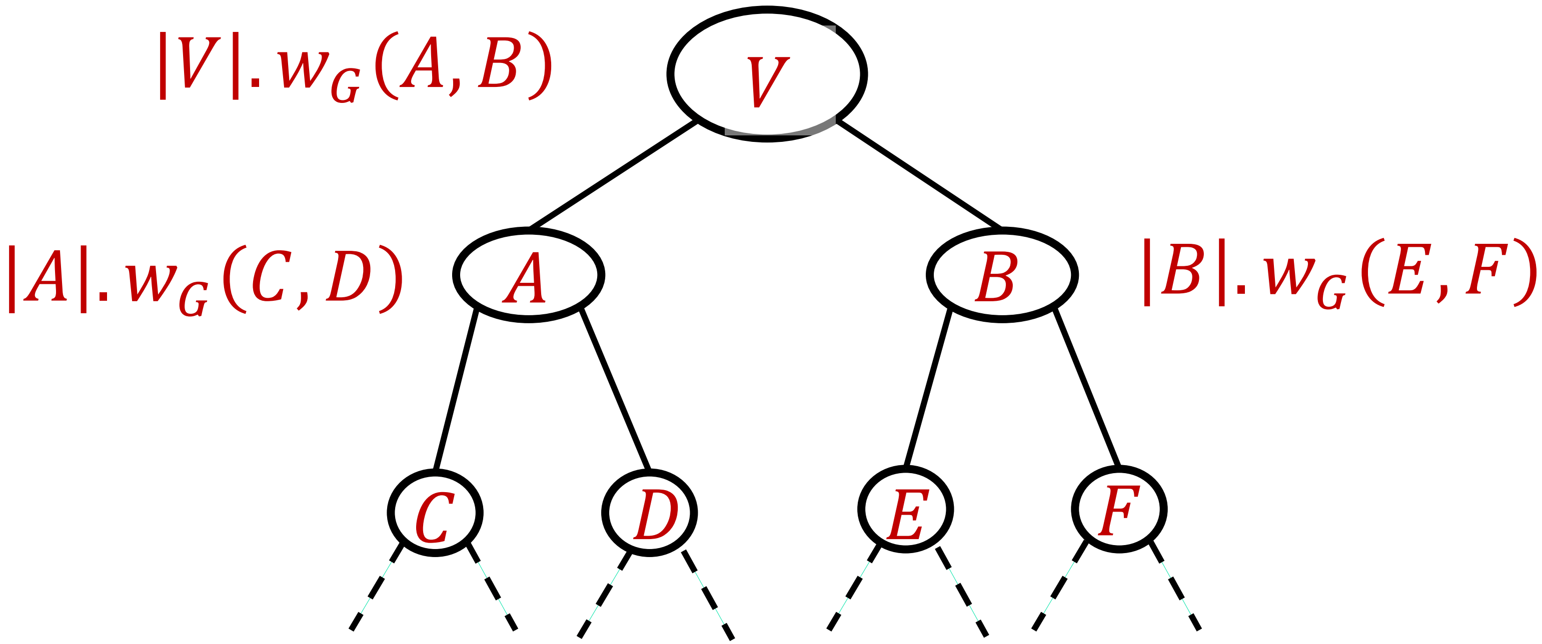
- Input: A weighted graph whose vertices correspond to data points and whose edges capture similarity between the data points.
- The cost of any HC tree T is given by

$$\text{Cost}(T) = \sum_{\text{splits } S \to (S_l, S_r) \text{ in } T} \left(|S| \cdot w_G(S_l, S_r) \right)$$

where $w_G(S_l, S_r)$ = total weight of edges going from S_l to S_r.

Goal: Find a tree that minimizes this cost.

The Hierarchical Clustering Problem



The cost function incentivizes cutting high weight similarity edges deeper down the tree.

Why this Cost Function?

- Dasgupta (2016) motivates this cost function as having several desirable properties :
  - When the data consists of a collection of connected components, an optimal tree starts by building a hierarchy that separates the components.
  - When the input graph is a clique, all trees should have the same cost – no particular cluster hierarchy is to be favored.
  - It recovers the desirable solution for some models of planted cluster partitions.
- Cohen-Addad et al. (2019) take an axiomatic approach to characterize good cost functions in general.
- We will focus on the Dasgupta objective in this talk.

The Hierarchical Clustering Problem

- The problem of finding the best HC tree is NP-hard.
- Assuming Small Set Expansion (SSE) conjecture, no $O(1)$–approximation possible [Charikar-Chatziafratis 17].
- A natural algorithm called recursive sparsest cut gives $O(\alpha)$–approximation where $\alpha = O(\sqrt{\log n})$ is the sparsest cut approximation guarantee [Charikar-Chatziafratis 17], [Cohen-Addad et al. 19].

Useful fact: At expense of an $O(1)$–loss in approximation ratio, we can assume that each binary partition is roughly balanced.

Sublinear Algorithms

Can we match the best-known approximation guarantees for hierarchical clustering via sublinear algorithms?

Based on the computational platform, we may want sublinear query/time, space, or communication algorithms.

We will consider all three resources.

Sublinear Space Algorithms

Streaming Model of Computation

- The graph is presented as a stream of edges.
- The algorithm has limited memory to store information about the edges seen in the stream.
- A natural model when the input is either generated ``on the fly'' or is stored on a sequential access device, like a disk.
- The algorithm no longer has random access to the input.

Goal is to design algorithms that use space that is much smaller than the size of the graph.

Sublinear Query/Time Algorithms

Query Model of Computation

- Degree queries: What is the degree of a vertex v?
- Pair queries: Is (u, v) an edge?
- Neighbor queries: Who is the k_{th} neighbor of a vertex v?

Goal is to design algorithms that compute by performing only a few queries – much smaller than the size of the graph.

Additional goal: efficiently process the queries to recover a good HC tree.

Sublinear Communication Algorithms

MPC Model of Computation (Massively Parallel Computation)

- The edges of the graph are partitioned across multiple machines in an arbitrary manner.
- Each machine has small memory – much smaller than the input.
- Computation proceeds in rounds where in each round, a machine can send and receive limited information to other machines (not exceeding its memory).

Goal is to compute in a small number of rounds using only machines with small memory.

Our Results

- There are efficient sublinear algorithms for hierarchical clustering in all three models of computation.
- There are also nearly matching lower bounds that show these algorithms are essentially best possible.

Notation: We will use n to denote the number of vertices and m to denote the number of edges.

Results 0: Sublinear Space Algorithms

Theorem 0: Given a weighted graph G as a stream of edges, there is an $\tilde{O}(n)$ space algorithm to find a $(1+o(1))$–approximate hierarchical clustering of G.

- The approximation guarantee above is better than $O(\sqrt{\log n})$ because the model allows unbounded computation time. It is $O(\sqrt{\log n})$ in poly-time.
- It is also easy to show that $\Omega(n)$ space is necessary to obtain any $\tilde{O}(1)$-approximation.
- The algorithm also works for dynamic streams.

Results 1: Sublinear Communication Algorithms (MPC Model)

Theorem 1: Given a weighted graph G with edges partitioned across machines with $\tilde{O}(n)$ memory, can find a $(1 + o(1))$–approximate hierarchical clustering of G in 2 rounds.

Theorem 2: No randomized 1-round protocol using machines with $n^{4/3-\epsilon}$ memory for any $\epsilon > 0$, can output an $\tilde{O}(1)$ –approximate hierarchical clustering even on unweighted graphs.

Results 2: Sublinear Query/Time Algorithms

Theorem 3: Given an unweighted graph G with m edges, there is an algorithm that outputs a $(1+o(1))$–approximate hierarchical clustering of G using

- $\tilde{O}(n+m)$ queries if $m \leq n^{4/3}$.
- $\tilde{O}(n+m/\alpha^3)$ queries if $m = \alpha . n^{4/3}$ for some $\alpha \geq 1$.

The query bound starts becoming sublinear once m exceeds $n^{4/3}$, and then drops to $\tilde{O}(n)$ queries once $m \geq n^{3/2}$.

Results 2: Sublinear Query/Time Algorithms

- By investing an additional $n^{1+\tau+o(1)}$ time over the query complexity, we can get an $O(\sqrt{\log n/\tau})$-approximate solution [Sherman 09] and [Chen, Kyng, Liu, Peng, Probst Gutenberg, Sachdeva 22].
- We can get similar guarantees for the weighted case, assuming a suitable graph representation.

Theorem 4: The query complexity achieved by the algorithm in Theorem 3 is essentially optimal for every edge density.

Related Recent Work

Assadi, Chatziafratis, Lacki, Mirrokkni, and Wang (2022)

- Focuses on estimating the HC value in sublinear in n space, and shows several negative results.
- Also gives algorithms for finding a $\Theta(1)$–approximate HC tree in the streaming and the MPC model – this is slightly weaker than $(1 + o(1))$–approximation that we get.

Kapralov, Kumar, Lattanzi, Mousavifar (2022)

- Focuses on estimating the HC value in sublinear queries in (k, ϵ)-clusterable graphs: input is k expanders with outer conductance bounded by ϵ.
- $O(\sqrt{\log k})$–approximation in $poly(k).\, n^{\frac{1}{2}+O(\epsilon)}$ queries.

Sublinear Algorithms

Graph Sparsification for HC

Given any HC tree T, the cost of T is given by

Cost$(G,T) = \sum_{\text{splits } S \to (S_l, S_r) \text{ in } T} \left(|S| \cdot w_G(S_l, S_r) \right)$

where $w_G(S_l, S_r)$ = total weight of edges going from S_l to S_r.

Natural idea: Work with an approximate cut sparsifier of G.
For any pair of disjoint sets X, Y, we can express $w_G(X, Y)$ in terms of cuts in G:

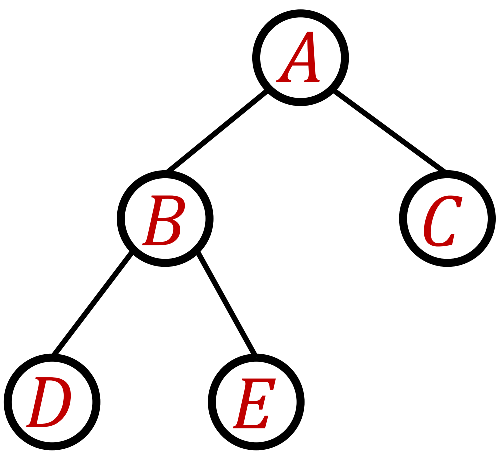
$w_G(S_l, S_r) = \frac{1}{2} . (w_G(S_l, \overline{S_l}) + w_G(S_r, \overline{S_r}) - w_G(S_l \cup S_r, \overline{S_l \cup S_r}))$.

Problem: Expressing $w_G(S_l, S_r)$ as difference of approximately preserved values, can result in unbounded error.

Graph Sparsification for HC

$w_G(S_l, S_r) = \frac{1}{2}.\left(w_G(S_l, \overline{S_l}) + w_G(S_r, \overline{S_r}) - w_G(S_l \cup S_r, \overline{S_l \cup S_r})\right).$

Observation: If we fix any HC tree, the negative term at any node appears with a strictly larger positive coefficient at the parent of the node.



$|A|.\frac{1}{2}.(\, w_G(B, \bar{B}) + w_G(C, \bar{C}) - w_G(A, \bar{A})\,)$

$|B|.\frac{1}{2}.(\, w_G(D, \bar{D}) + w_G(E, \bar{E}) - w_G(B, \bar{B})\,)$

Note that $|A| > |B|$.

Graph Sparsification for HC

Upshot: The cost of any tree T can be written as

$$\sum_{\text{splits } S\to(S_l,S_r) \text{ in } T} \frac{1}{2}.\left(|S_r|.\, w_G\,(S_l,\overline{S_l}) + |S_l|.\, w_G(S_r,\overline{S_r})\right) + \sum_v w_G(\, v, \bar{v})\,)$$

We get a blackbox reduction to cut sparsifiers.

To get a $(1 + o(1))$-approximate hierarchical clustering, it suffices to construct a $(1 + o(1))$–approximate cut sparsifier.

Now we can just focus on accomplishing this task in various models of computation.

Immediate Applications

Corollary (Thm 0): There is an $\tilde{O}(n)$ space dynamic streaming algorithm that outputs a $(1 + o(1))$ –approximate hierarchical clustering of a weighted graph.

Corollary (Thm 1): There is a 2-round MPC algorithm with $\tilde{O}(n)$ space per machine that outputs a $(1 + o(1))$–approximate hierarchical clustering of a weighted graph.

Both results basically follow from [Ahn, Guha, McGregor 12].

Application to Sublinear Time?

Constructing a cut sparsifier necessarily requires $\Omega(m)$ queries (even for connectivity).

We will work with a relaxed notion of cut sparsifiers that will prove much easier to construct.

A Relaxed Notion of Cut Sparsifiers

A graph $H(V, E')$ is an (ϵ, δ)-sparsifier of a graph $G(V, E)$ if for any cut $(S, \bar{S})$, we have

$$(1-\epsilon)w_G(S) \leq w_H(S) \leq (1+\epsilon)w_G(S) + \delta.\min\{|S|, |\bar{S}|\}$$

The usual notion of cut sparsifiers gives an $(\epsilon, 0)$-sparsifier.

Lemma: If H is an (ϵ, δ)-sparsifier of a graph G then for any HC tree T, we have

$$(1-\epsilon)cost_G(T) \leq cost_H(T) \leq (1+\epsilon)cost_G(T) + O(\delta.n^2)$$

High-level Plan for Sublinear Time

We will focus on unweighted graphs.

- Show that larger the δ, the easier it is to compute an (ϵ, δ)-sparsifier.
- But how large can we make δ to still get a $(1 + o(1))$ – approximation?
- Identify an easy to compute lower bound C for optimal HC cost, and set $\delta = o\left(\frac{C}{n^2}\right)$ to get $(1 + o(1))$–approximation.

High-level Plan for Sublinear Time

Lemma: The cost of hierarchical clustering on any unweighted graph G with n vertices and m edges is $\Omega(\frac{m^2}{n})$.

Example: Suppose G is any graph with $m \gg n^{3/2}$ edges, then optimal tree cost is $\gg n^2$.

So if we set $\delta = O(1)$, then the $O(\delta. n^2)$ additive error term is negligible because optimal tree cost is $\gg n^2$.

Let us focus on this density regime, and we will design a $\tilde{O}(n/\varepsilon^2)$ query algorithm to construct an $(\epsilon, O(1))$-sparsifier.

Constructing an $(\epsilon, O(1))$-sparsifier

[Spielman-Srivastava 11]

One way to construct an $(\epsilon, 0)$-sparsifier of G:

sample $O(n \log n/\epsilon^2)$ times each edge $e = (u, v)$ with probability p_e proportional to $R(u, v)$ = effective resistance between u and v.

Difficulty: How to estimate effective resistances in sublinear time?

Fix: Add a constant degree expander G' to G.

Constructing an $(\epsilon, O(1))$-sparsifier

Observation: Any $(\epsilon, 0)$-sparsifier for the graph $H = G \cup G'$ is an $(\epsilon, O(1))$-sparsifier for the graph G.

For any cut $(S, \bar{S})$, its size in any $(\epsilon, 0)$-sparsifier of H

- is at least $(1 - \epsilon)w_G(S)$, and
- at most $(1 + \epsilon)w_G(S) + O(1 + \epsilon).min\{|S|, |\bar{S}|\}$

New Goal: Construct an $(\epsilon, 0)$-sparsifier of the graph H.

An $(\epsilon, 0)$-sparsifier of the Graph H

What have we gained by shifting the focus to H instead of G?

Observation: For any edge $e = (u, v)$, its effective resistance $R(u, v)$ in H satisfies

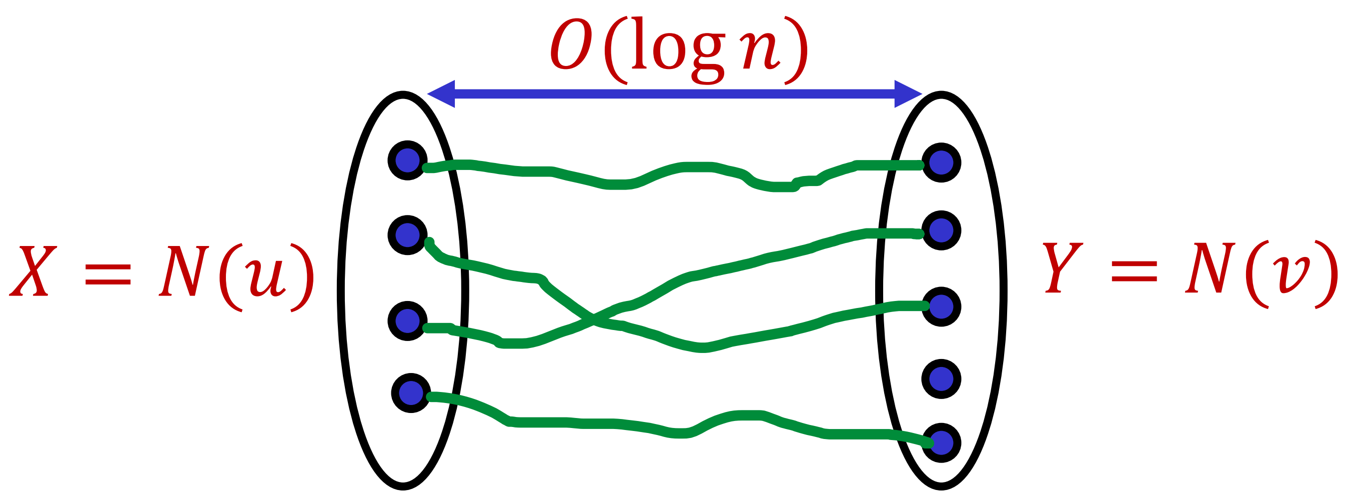
$$\frac{1}{\min\{\, d_H(u), d_H(v)\}} \le R(u, v) \le \frac{O(\log n)}{\min\{\, d_H(u), d_H(v)\}}$$

$R(u, v) \ge \frac{1}{\min\{\, d_H(u), d_H(v)\}}$ is easy.

An $(\epsilon, 0)$-sparsifier of the Graph H

More interesting direction: $R(u,v) \leq \frac{O(\log n)}{\min\{\, d_H(u), d_H(v)\}}$

In a constant degree expander, for any 2 sets X and Y, there are $\approx \min\{|X|, |Y|\}$ edge-disjoint paths of $O(\log n)$ length between X and Y [Frieze 01].



Constructing an $(\epsilon, O(1))$-sparsifier

We now have a very simple algorithm to construct an $(\epsilon, 0)$-sparsifier for the graph $H = G \cup G'$.

Repeat the following for $\tilde{O}(n/\epsilon^2)$ steps:

- sample a random vertex v.
- sample a random edge incident on v, and add it to the sparsifier.

Thus in $\tilde{O}(n/\epsilon^2)$ queries, we get a sparsified graph that gives a $(1+\epsilon)$–approximation to hierarchical clustering whenever the input graph contains $m \gg n^{3/2}$ edges.

General Case: An (ϵ, δ)-sparsifier

Add constant degree expander G' with edges of weight δ.

Observation: For any edge (u, v) in $H = G \cup G'$, we have

$$\frac{1}{\min\{ d_H(u), d_H(v)\}} \leq R(u, v) \leq \frac{O(\log n)}{\min\{ d_H(u), d_H(v)\}} \cdot \frac{1}{\delta}$$

Now construct an $(\epsilon, 0)$-sparsifier for the graph $H = G \cup G'$ by sampling as before for $\tilde{O}(n/\delta\epsilon^2)$ steps.

A variation of this expander idea was used by [Lee 14] for efficiently answering a single cut query with bounded additive error – we need this guarantee to hold for all cut queries.

Lower Bounds

Query Lower Bounds

Theorem: For any $\gamma \in (0, ½)$, there is a family of unweighted graphs with $m = \Theta(n^{1+\gamma})$ edges such that any randomized algorithm that outputs an $\tilde{O}(1)$–approximate hierarchical clustering for this family, requires $n^{\min\{1+\gamma, 2-2\gamma\}-o(1)}$ queries.

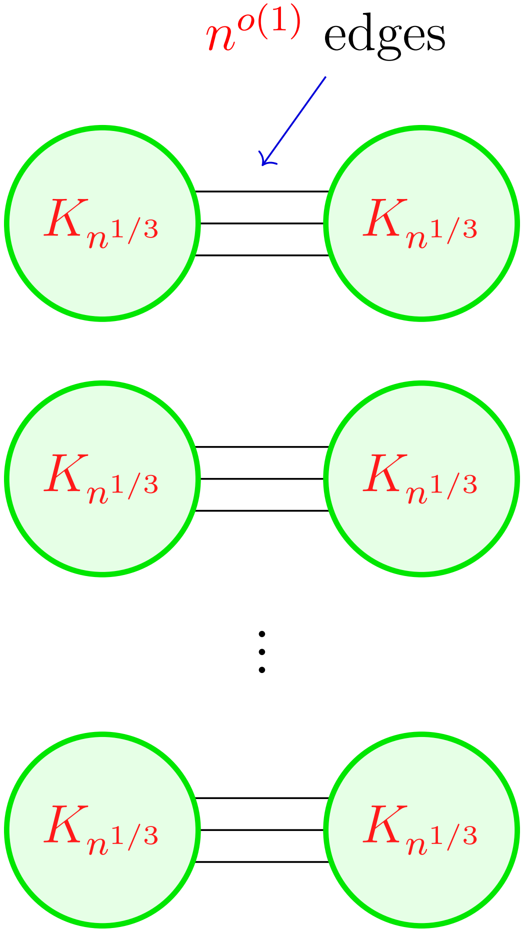
The lower bound

- remains $m^{1-o(1)}$ as m increases from n to $n^{4/3}$; and
- then gradually decreases from $n^{4/3-o(1)}$ to $n^{1-o(1)}$ as m increases from $n^{4/3}$ to $n^{3/2}$.

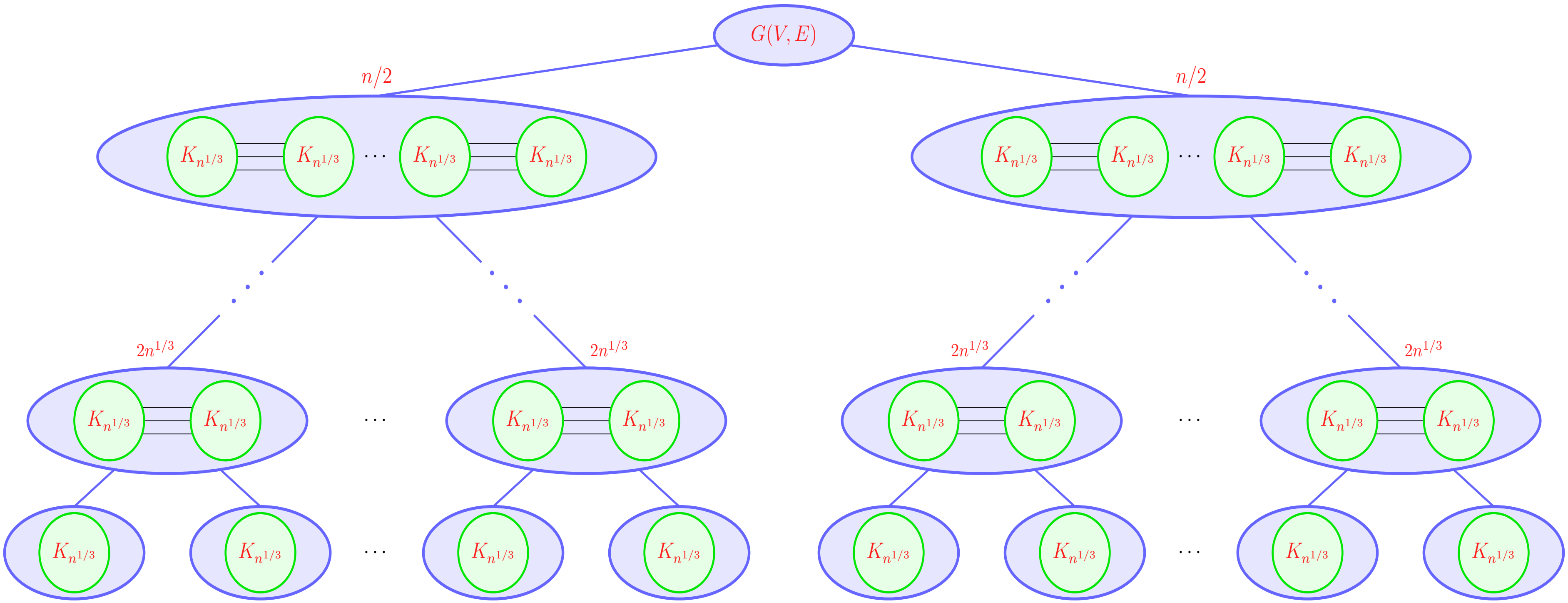
We will illustrate the lower bound idea for $\gamma = 1/3$, and show a lower bound of $n^{4/3-o(1)}$ queries.

$n^{4/3-o(1)}$ Query Lower Bound for $m = n^{4/3}$

$n^{2/3}$ randomly matched pairs of cliques



An Optimal Tree



Optimal clustering cost: $\Theta(n^{5/3})$

Lower Bound Idea

Consider any $\tilde{O}(1)$ –approximation algorithm A.

- Assume w.l.o.g. that the top-level partition is roughly balanced in the solution output by A.
- A must not cut too many clique matching edges at the top partition since penalty for each edge cut is n. So A must ``discover'' most of the meta-matching among the cliques.
- It takes about $n^{2/3-o(1)}$ queries to discover match of a given clique under M.
- We need to discover $\Omega(n^{2/3})$ matches in M, giving us an $n^{4/3-o(1)}$ query lower bound.

MPC Lower Bound

Theorem 2: No randomized 1-round protocol using machines with $n^{4/3-\epsilon}$ memory for any $\epsilon > 0$, can output an $\tilde{O}(1)$ – approximate hierarchical clustering even on unweighted graphs.

- The input graph is partitioned across $\approx n^{1/3}$ machines with $n^{4/3-\epsilon}$ memory for an arbitrarily small $\epsilon > 0$.
- We want to rule out recovery of an $\tilde{O}(1)$–approximate HC tree in one round of communication.

MPC Lower Bound

$|V_1| = |V_2| = n.$

Union of $\approx n^{1/3}$ bipartite cliques of size $\approx n^{2/3}$

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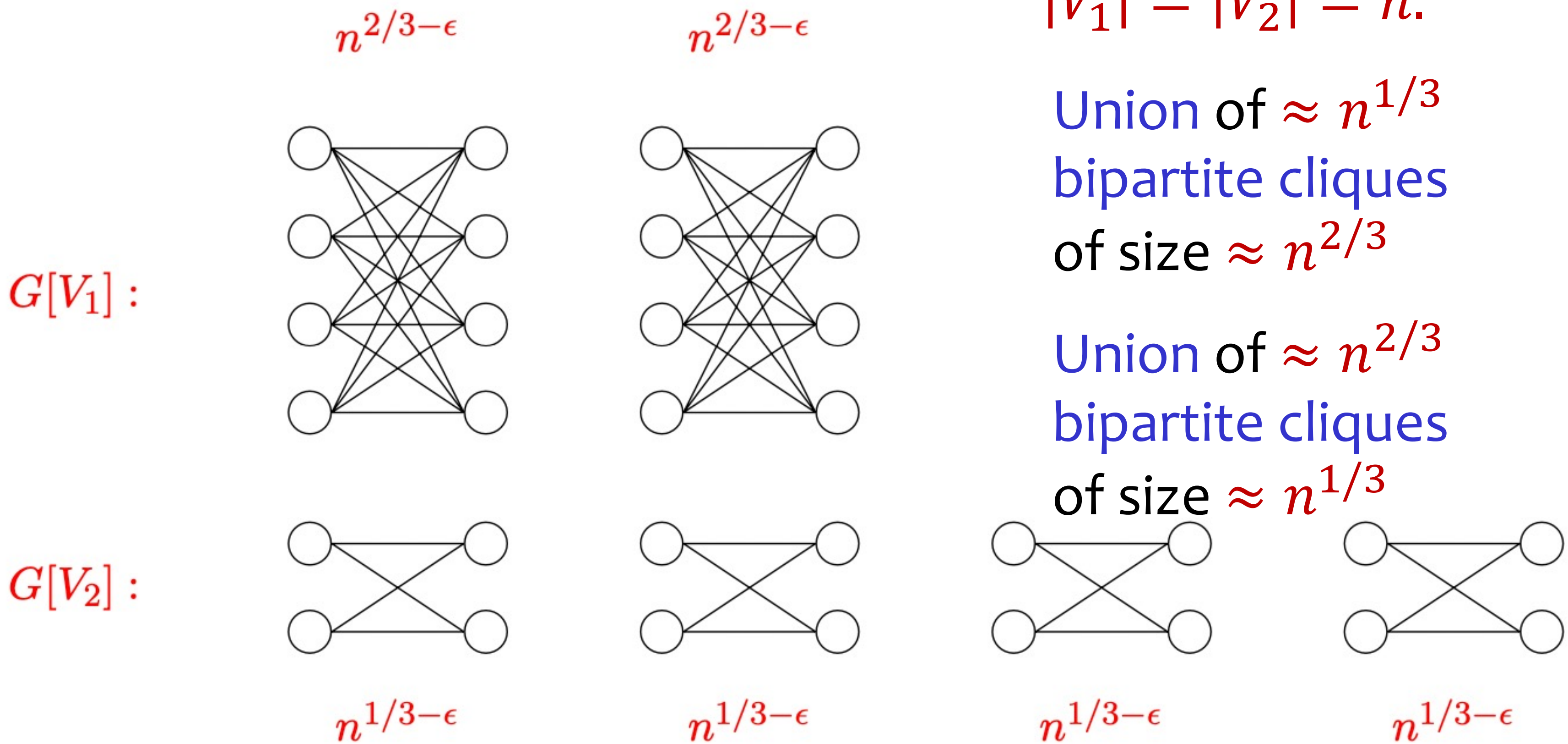
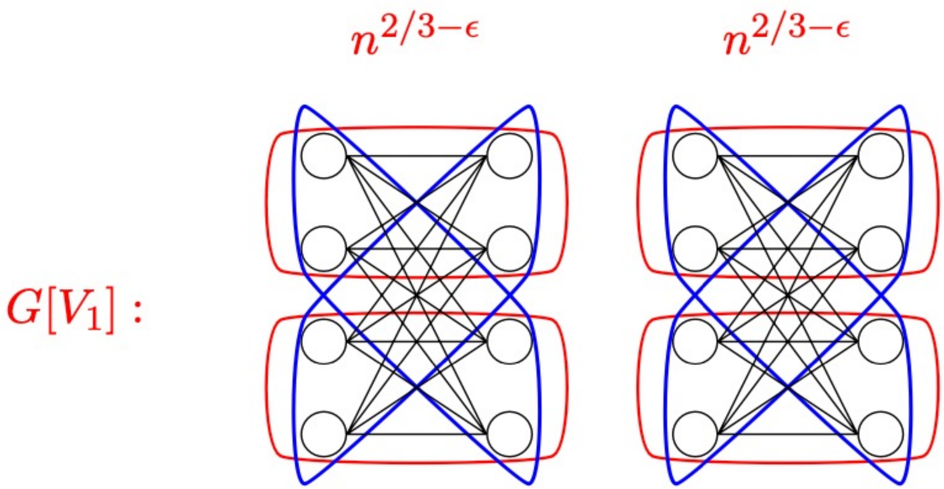
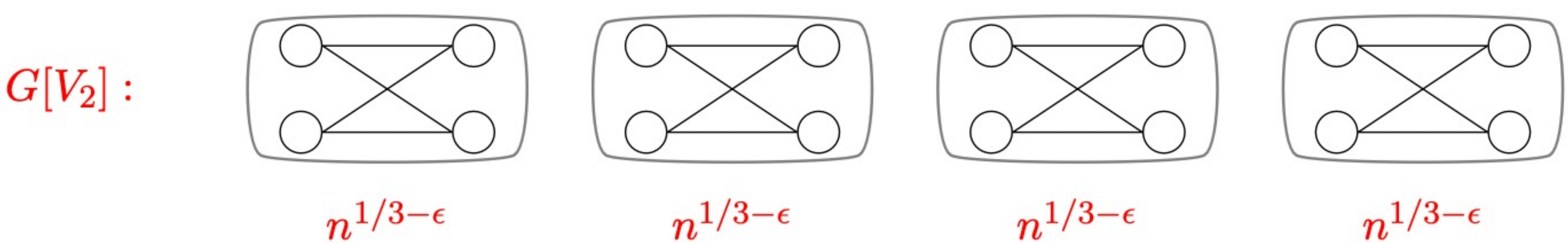


So $\Theta(n^{5/3})$ edges are partitioned across $\approx n^{1/3}$ machines.

MPC Lower Bound

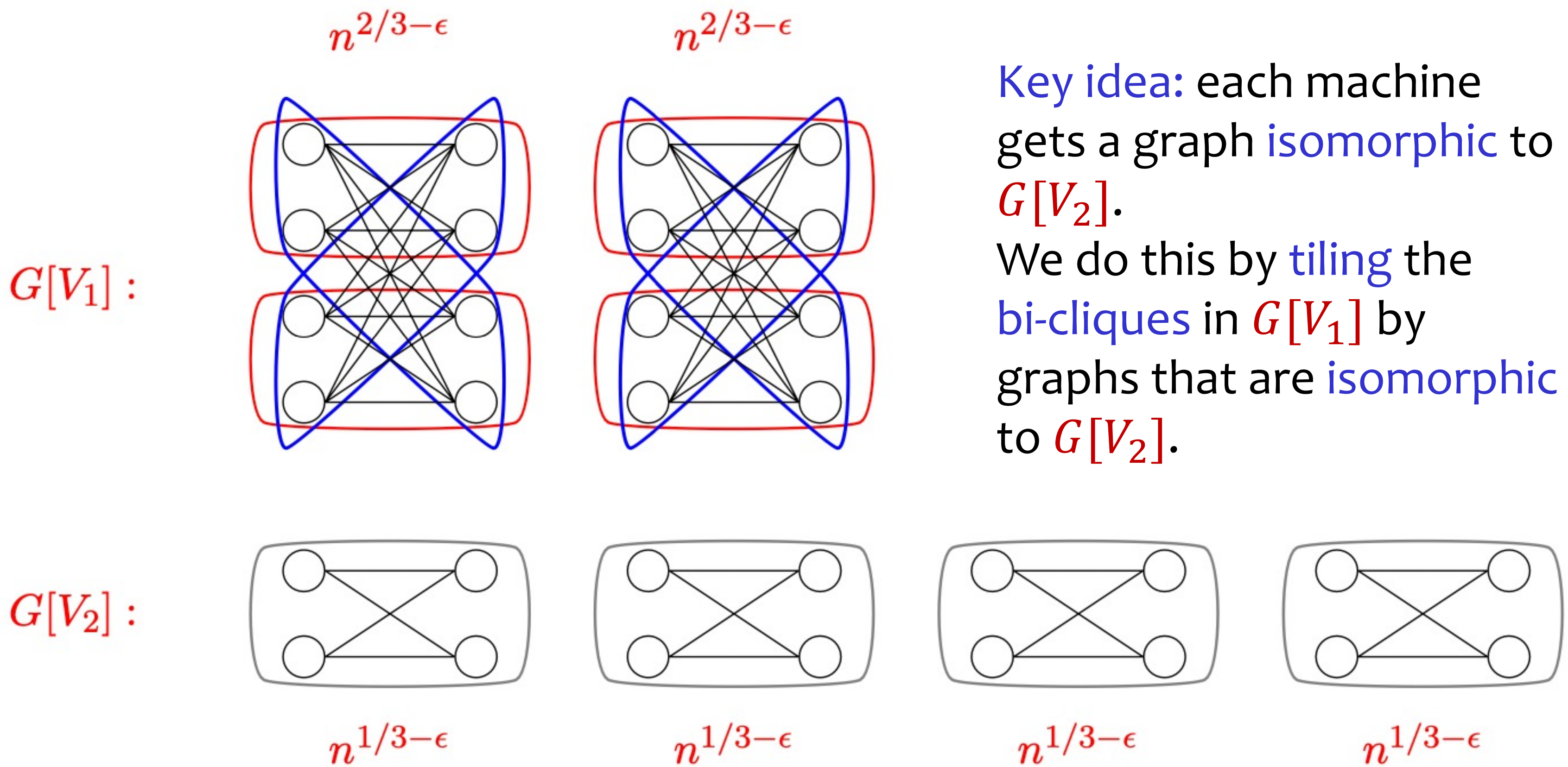


Key idea: each machine gets a graph isomorphic to $G[V_2]$.
We do this by tiling the bi-cliques in $G[V_1]$ by graphs that are isomorphic to $G[V_2]$.



A machine can not tell locally whether it received the blue cliques, the red cliques, or the graph $G[V_2]$ itself.

MPC Lower Bound



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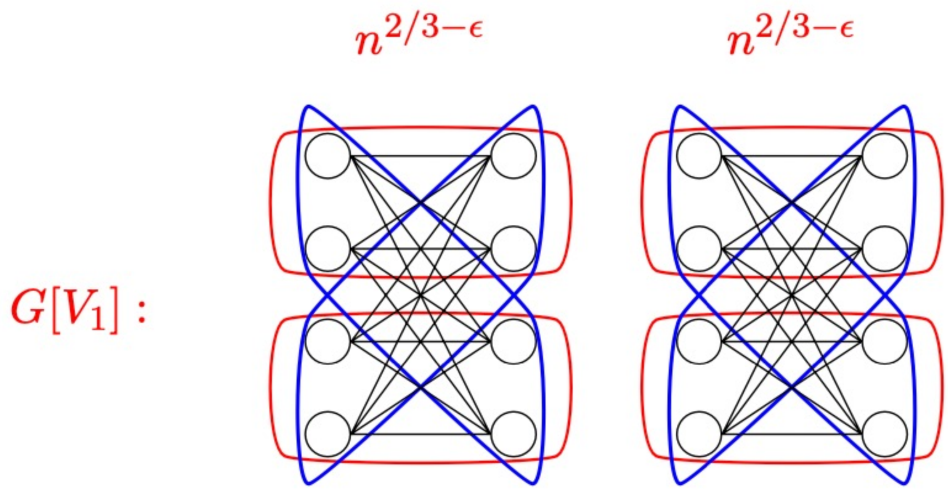
Any $\tilde{O}(1)$–approximate solution must discover how the vertices are partitioned across the cliques in $G[V_2]$.

MPC Lower Bound



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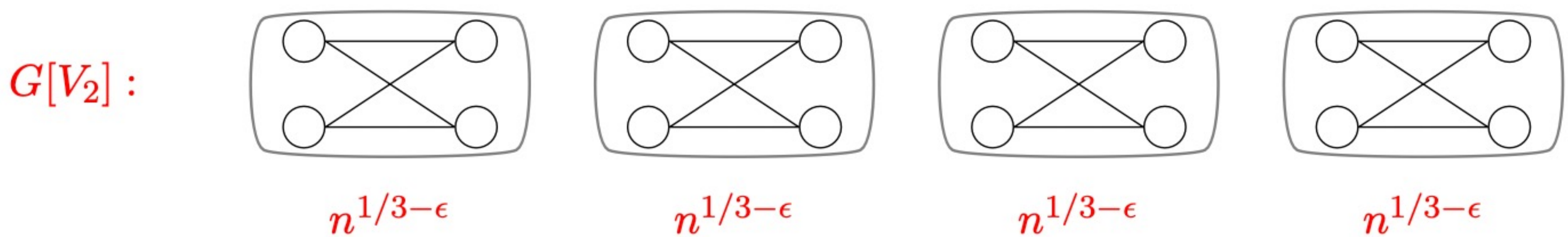

So each of the $n^{1/3}$ machines needs to send $\Omega(n)$ bits of information to the coordinator – this is much more than the coordinator's memory.

Concluding Remarks

- We designed near-optimal sublinear algorithms for hierarchical clustering in the query model, streaming, and MPC model.
- The main algorithmic ingredient:
  - a relaxed notion of cut sparsifiers that is easy to compute in various computational models.
- We also establish lower bounds that almost match the performance of our algorithms.
- An interesting direction is to understand if there is a separation between the queries needed to estimate the value and finding a clustering in general graphs.

Thank you !