Sublinear Algorithms for Hierarchical Clustering

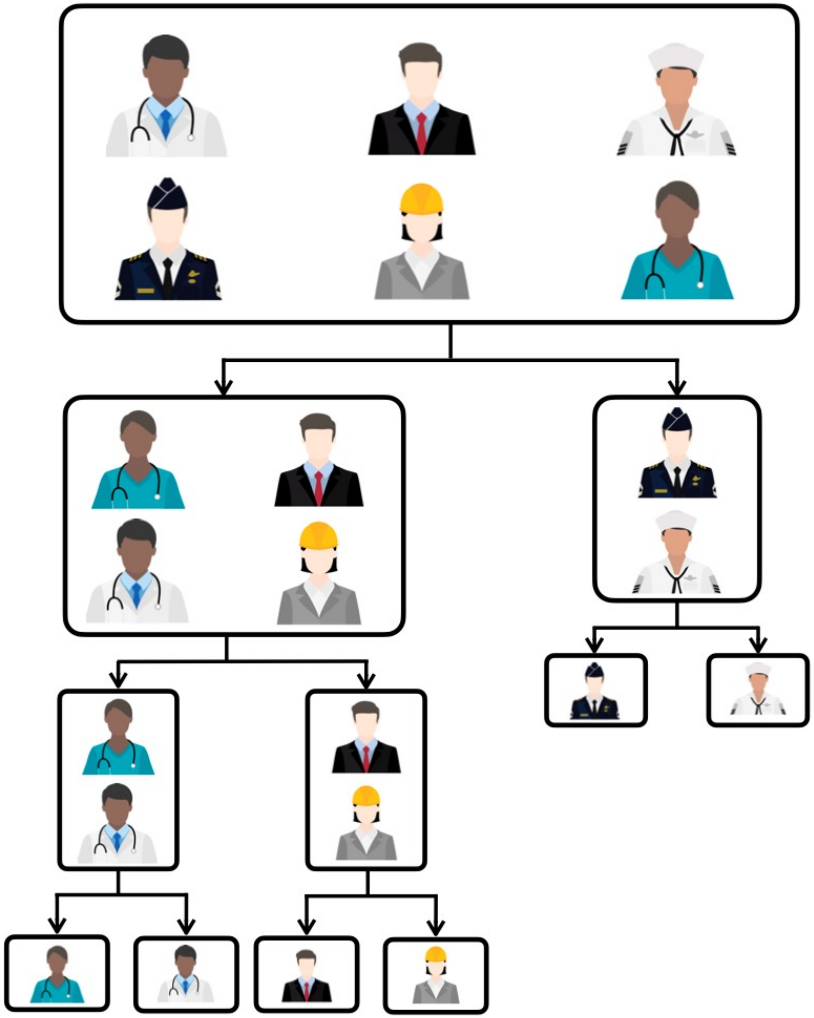
Sanjeev Khanna

University of Pennsylvania

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

Hierarchical Clustering

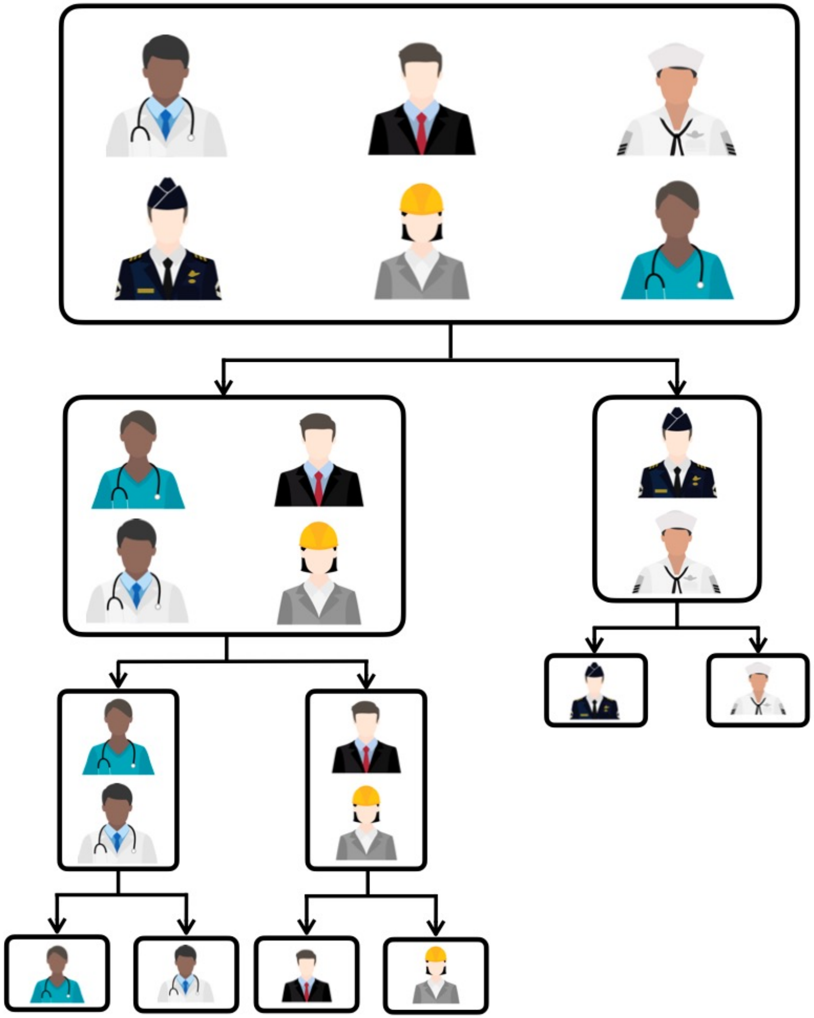
A technique to cluster data into a multilevel hierarchy based on similarity.



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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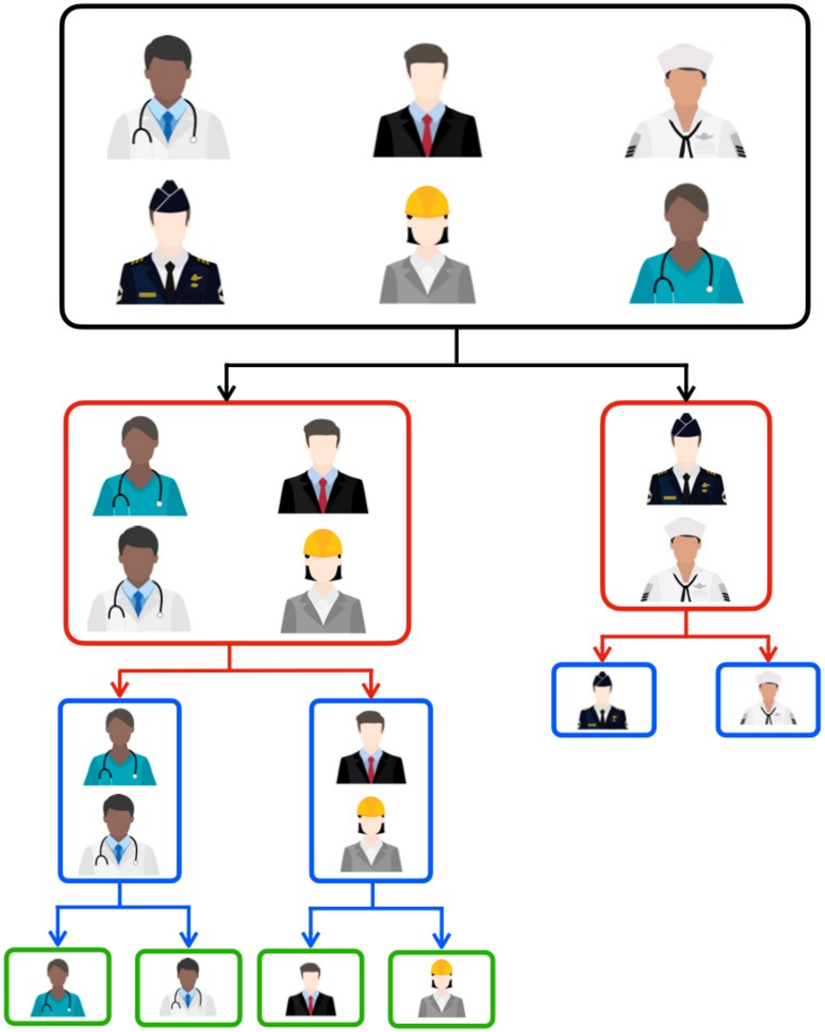
Clusters data at multiple levels of granularity simultaneously.



The Hierarchical Clustering Problem

Dasgupta (2016) introduced the following formalization:

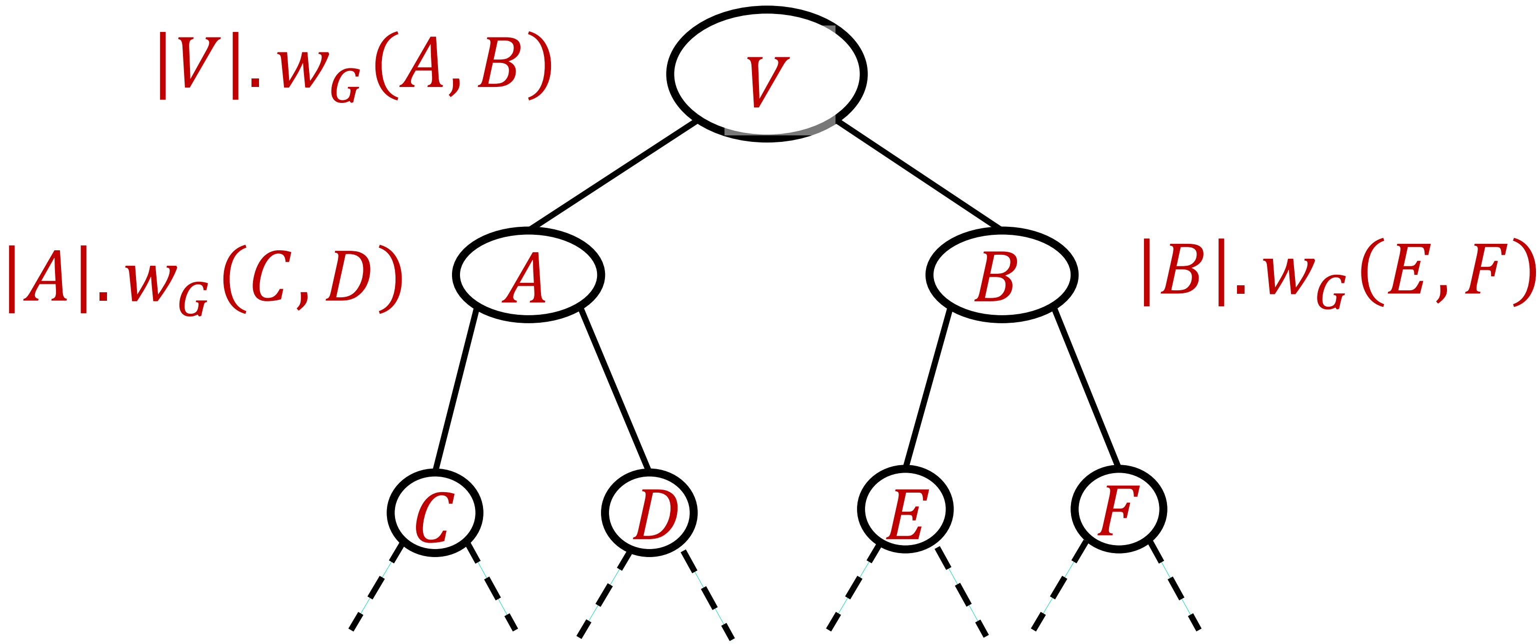
- Input: A weighted graph whose vertices correspond to data points and whose edges capture similarity between the data points.
- The cost of any HC tree T is given by

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

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

Goal: Find a HC tree T that minimizes this cost.

The Hierarchical Clustering Problem



The cost function incentivizes cutting high weight similarity edges only 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 hierarchical tree first separates out these components.
  - When the input graph is a clique, all trees should have the same cost – no particular cluster hierarchy should 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

(n = # of vertices; m = # of edges)

- The problem of finding an optimal 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].

Sublinear Algorithms

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

Based on the computing platform, we may want algorithms that are sublinear in time, space, or communication.

We will consider optimization of 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 input graph.

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

- The graph can be accessed via following queries:
  - Degree queries: What is the degree of a vertex v?
  - Pair queries: Is (u, v) an edge?
  - Neighbor queries: Output 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: minimize the time needed to process the queries to output 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 size of the graph.
- Computation proceeds in rounds where in each round, a machine can send and receive limited information from other machines (not exceeding its memory). At the end, a designated machine (coordinator) outputs the answer.

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.

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

- $O(n+m)$ 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

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

- For any fixed $\epsilon > 0$, we can get an $O(\sqrt{\log n})$-approximate solution in $n^{1+\epsilon}$ time [Sherman 09] and [Chen, Kyng, Liu, Peng, Probst Gutenberg, Sachdeva 22].
- We can get similar guarantees for the weighted case, if we assume a suitable graph representation.

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 for a graph G, the cost of T is given by

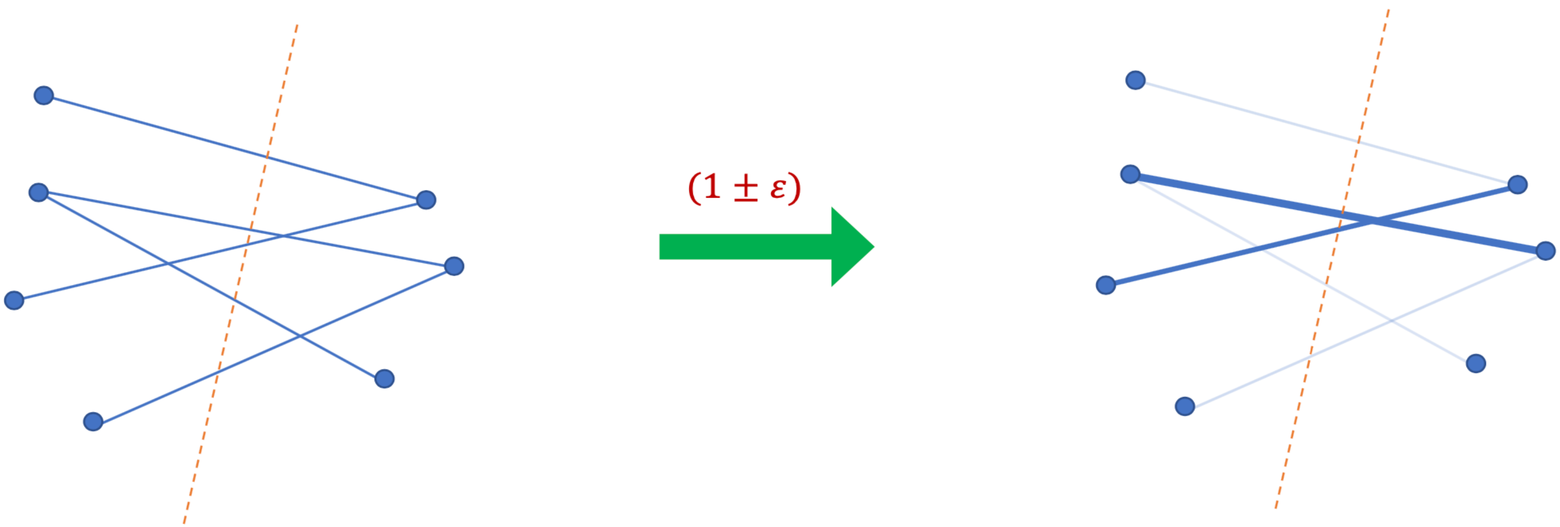
Cost(T) = $\sum_{\text{splits } S \to (S_l, S_r) \text{ in } T} \left(|S| \cdot w_G(S_l, S_r) \right)$

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

Natural idea: Work with an approximate cut sparsifier of G.

Cut Sparsifiers

Given a graph G, a $(1 \pm \varepsilon)$ -cut sparsifer is a sparse subgraph G' of G that preserves every cut in G to within a $(1 \pm \varepsilon)$ factor.



[Benczúr-Karger '96] Any graph has a $(1 \pm \varepsilon)$-cut sparsifier that contains $O(\frac{n \log n}{\varepsilon^2})$ edges, and is computable in $\tilde{O}(n+m)$ time.

Cut Sparsifiers

- A cut sparsifier for G clearly suffices to find a good top-level partition of the vertex set.

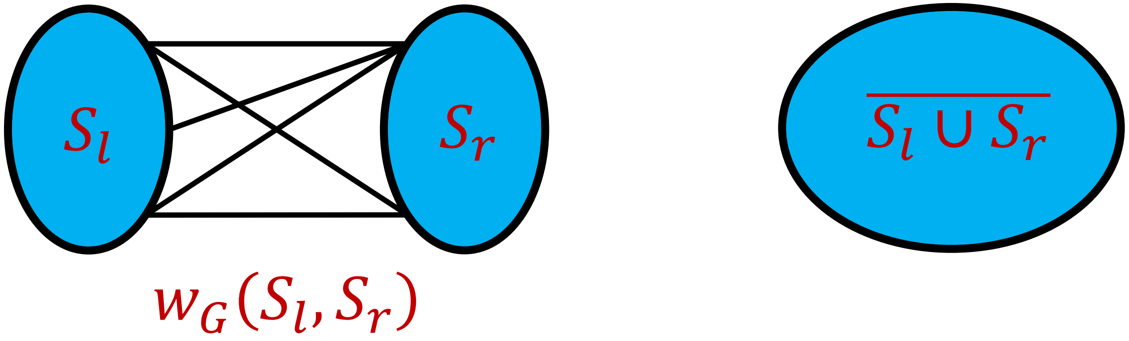
- But what we really need is something more general: cut sparsifiers for vertex-induced subgraphs of G that arise as problem instances at intermediate nodes!

- Concretely, suppose we have a set S of vertices at some intermediate node and we wish to know the cost of partitioning S into two sets S_l, S_r : this depends only on edges between S_l and S_r.

Graph Sparsification for HC

For any pair of disjoint sets S_l, S_r, we can express $w_G(S_l, S_r)$ in terms of cuts in G:

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

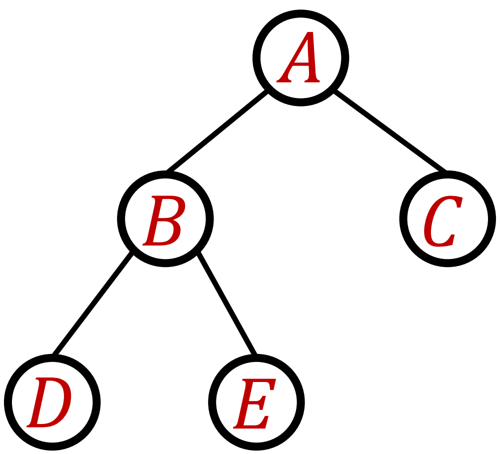


Problem: Expressing $w_G(S_l, S_r)$ as difference of approximately preserved values, can result in unbounded error.

Graph Sparsification for HC

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

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 expressed as a non-negative weighted combination of cuts in the original graph.

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

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

Follows from [Ahn, Guha, McGregor 12].

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.

The linear sketching scheme used in [Ahn, Guha, McGregor 12] can be adapted to show the following as well.

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.

Application to Sublinear Time?

Unfortunately, constructing a cut sparsifier necessarily requires $\Omega(n + m)$ queries (even for testing connectivity).

To get around this, we will work with a relaxed notion of cut sparsifiers that will prove much easier to construct, and will turn out to be sufficient for our purpose.

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

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

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

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

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

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 to hierarchical clustering?
- 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 HC 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's focus on this density regime, (i.e. $m \gg n^{3/2}$) and we will design a $\tilde{O}(n/\varepsilon^2)$ query algorithm to get a $(\epsilon, O(1))$-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 an 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 (choose G' to be a random graph of constant degree).

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 $(1+\epsilon)w_G(S) + (1+\epsilon).O(min\{|S|, |\bar{S}|\})$.

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?

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

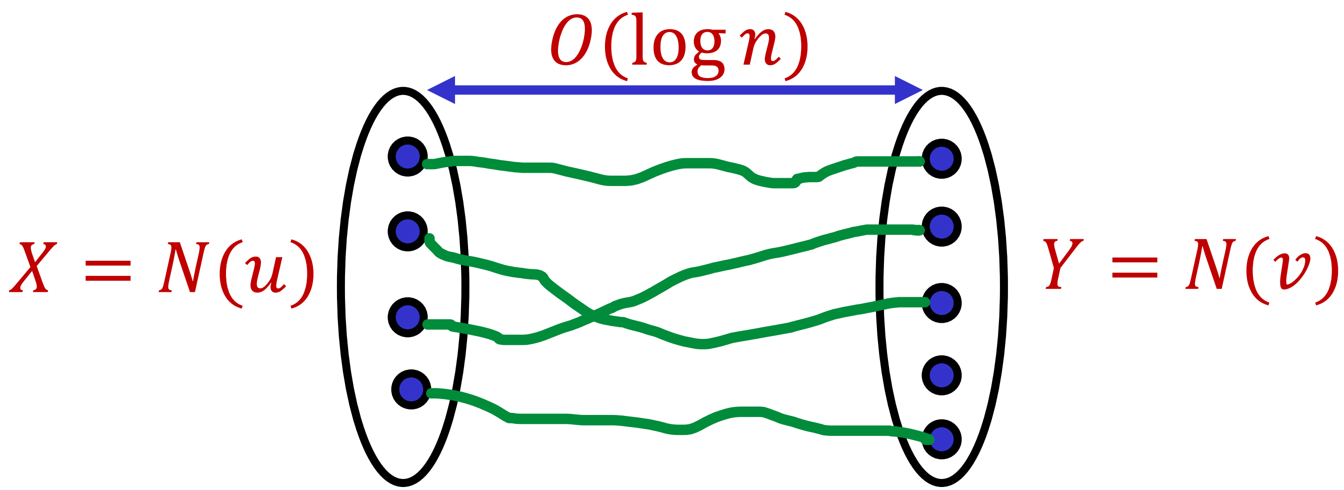
$$\frac{1}{\min\{ d_H(u), d_H(v)\}} \leq R(u, v) \leq \frac{O(\log n)}{\min\{ d_H(u), d_H(v)\}}$$

Addition of expander G' narrows down the resistance of each edge to within a narrow band that only depends on the degrees of its end-points!

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

In a constant degree expander, we can connect 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].

So u and v are connected by $\min\{d_H(u), d_H(v)\}$ paths of $O(\log n)$ length.



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: There is a family of unweighted graphs such that any randomized algorithm that outputs an $\tilde{O}(1)$–approximate hierarchical clustering for graphs in this family, needs at least:

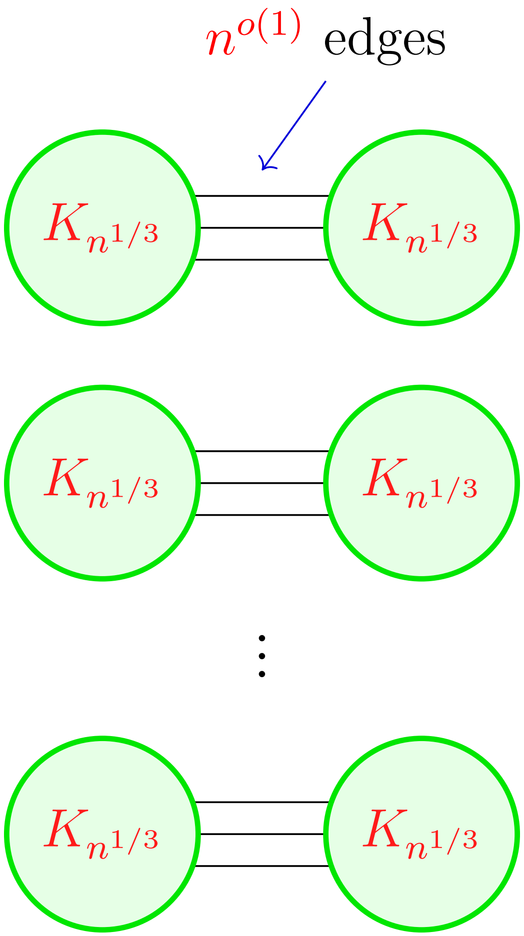
- $m^{1-o(1)}$ queries as m increases from n to $n^{4/3}$; and
- when $m = n^{\frac{4}{3}+\delta}$ for $\delta \in (0,1/6)$, it requires $\frac{m^{1-o(1)}}{\delta^3}$ queries.

(Thus the lower bound gradually decreases from $n^{4/3-o(1)}$ to $n^{1-o(1)}$ as m increases from $n^{4/3}$ to $n^{3/2}$.)

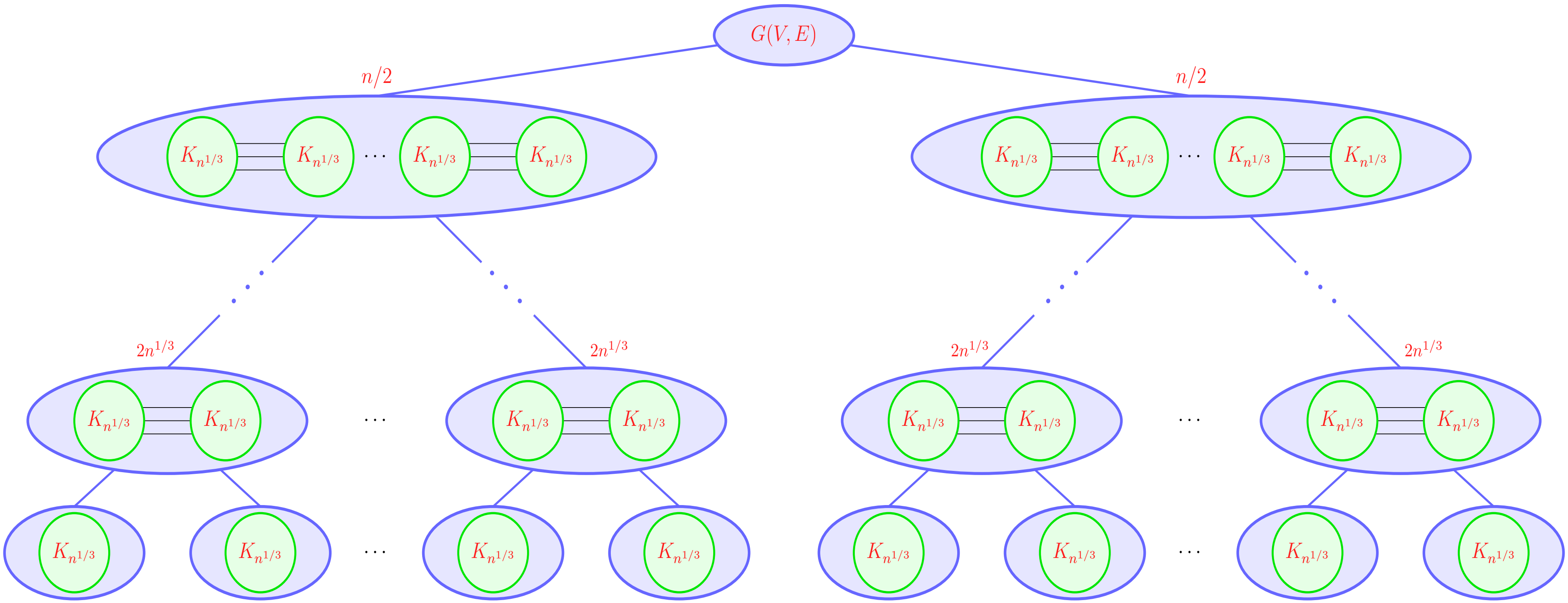
We will illustrate the lower bound idea for $m = n^{\frac{4}{3}}$, and show a lower bound of $n^{4/3-o(1)}$ queries.

$n^{4/3-o(1)}$ 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.

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 guarantees 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 !