Clustering on Clusters 2049: Massively Parallel Algorithms for Clustering Graphs and Vectors

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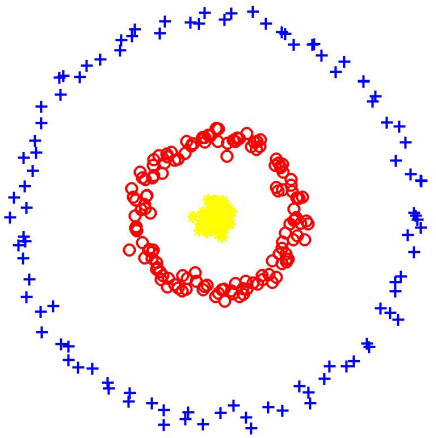
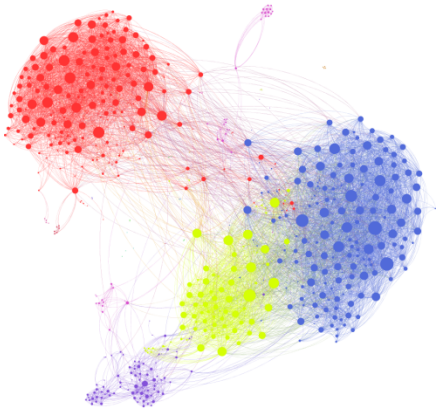


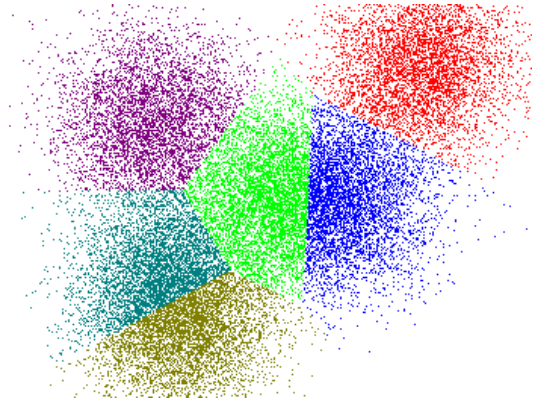
Grigory Yaroslavtsev

http://grigory.us

Clustering on Clusters: Overview

- Algorithm design for massively parallel computing
  - Blog: http://grigory.us/blog/mapreduce-model/
- MPC algorithms for graphs
  - Connectivity
  - Correlation clustering
- MPC algorithms for vectors
  - K-means
  - Single-linkage clustering
- Open problems and directions



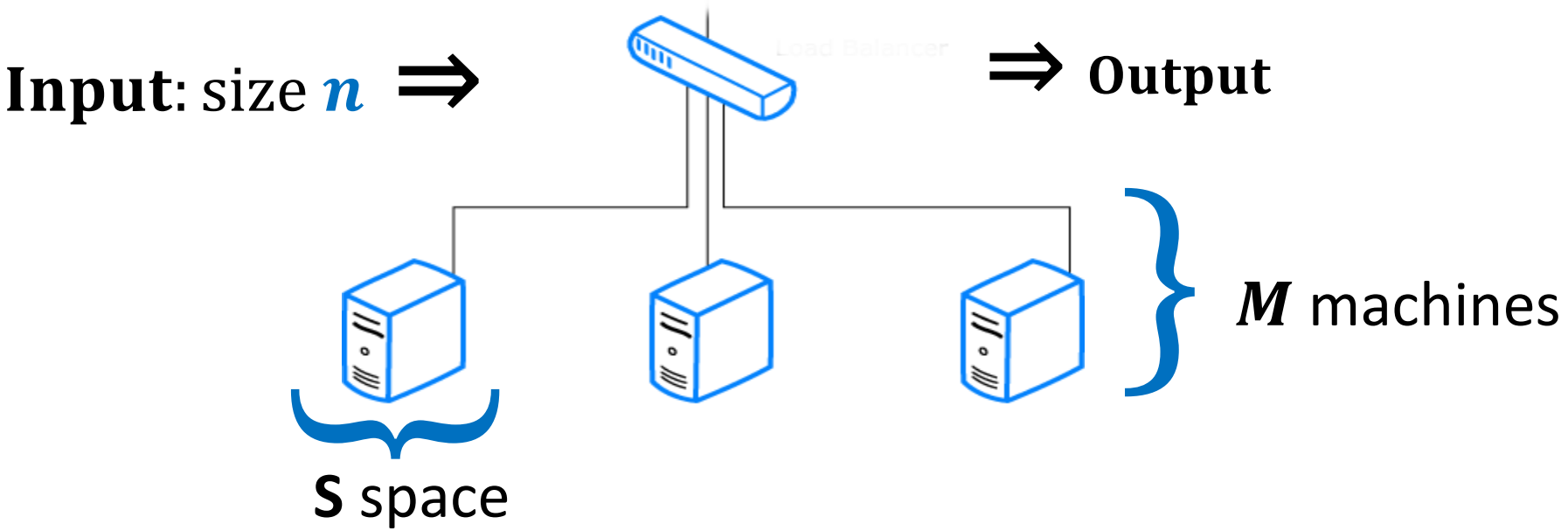


Clustering on Clusters 2049: Overview

	Graphs	Vectors
Basic	Connectivity **Connectivity++**	K-means **--**
Advanced	Correlation Clustering **Single-Linkage Clustering**	MST **Single-Linkage Clustering**

Cluster Computation (a la BSP)

- **Input**: size **n** (e.g. **n** = billions of edges in a graph)
- $\boldsymbol{M}$ **M**achines, $\boldsymbol{S}$ **S**pace (RAM) each
  - Constant overhead in RAM: $\boldsymbol{M} \cdot \boldsymbol{S} = O(\boldsymbol{n})$
  - $\boldsymbol{S} = \boldsymbol{n}^{1-\epsilon}$, e.g. ϵ = 0.1 or ϵ = 0.5 ($\boldsymbol{M} = \boldsymbol{S} = O(\sqrt{\boldsymbol{n}})$)
- **Output**: solution to a problem (often size O($\boldsymbol{n}$))
  - Doesn't fit in local RAM ($\boldsymbol{S} \ll \boldsymbol{n}$)

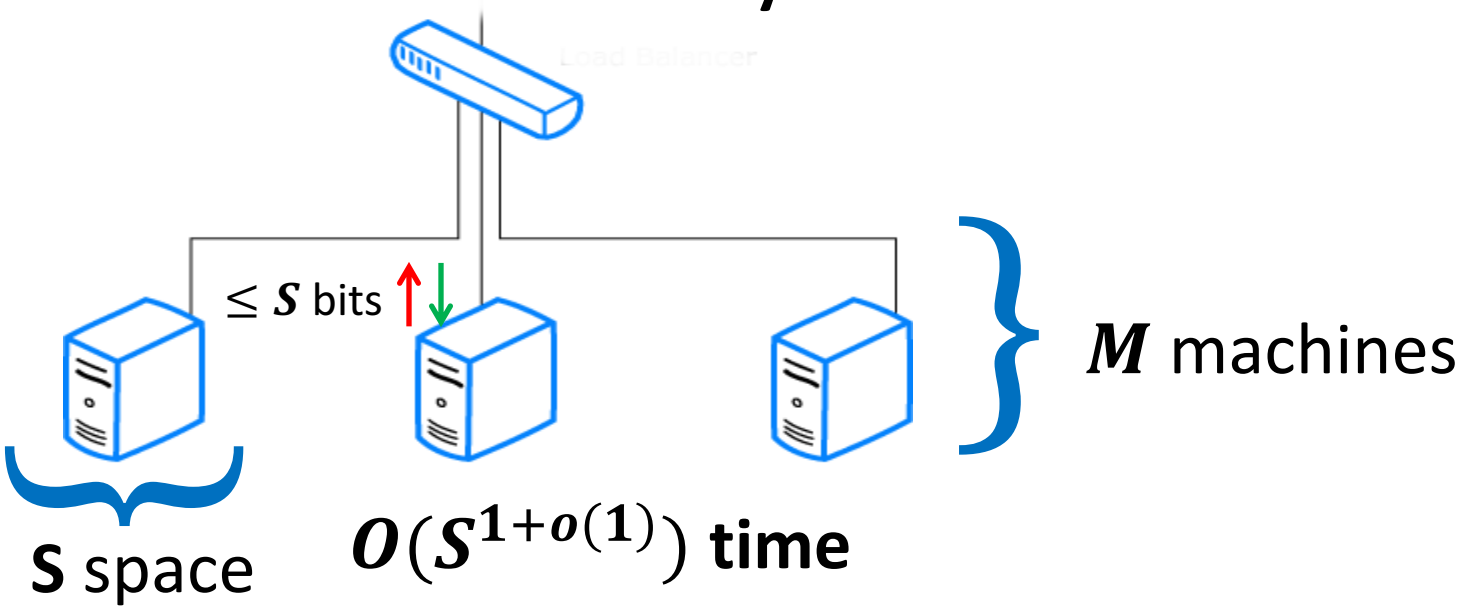


Cluster Computation (a la BSP)

- Computation/Communication in $\boldsymbol{R}$ rounds:
  - Every machine performs a **near-linear time** computation => Total user time $O(\boldsymbol{S^{1+o(1)}R})$
  - Every machine **sends/receives at most $\boldsymbol{S}$ bits** of information => Total communication $O(\boldsymbol{nR})$.

Goal: Minimize $\boldsymbol{R}$.

Ideally: $\boldsymbol{R}$ = constant.

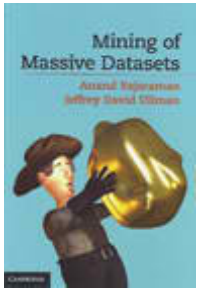


MapReduce-style computations

YAHOO! Google

What I won't discuss today

- PRAMs (**shared memory**, multiple processors) (see e.g. [Karloff, Suri, Vassilvitskii'10])
  - Computing XOR requires $\widetilde{\Omega}(\log n)$ rounds in CRCW PRAM
  - Can be done in $O(\log_s n)$ rounds of MapReduce
- Pregel-style systems, Distributed Hash Tables (see e.g. Ashish Goel's class notes and papers)
- Lower-level implementation details (see e.g. Rajaraman-Leskovec-Ullman book)



Models of parallel computation

- **Bulk-Synchronous Parallel Model** (BSP) **[Valiant,90]**

  Pro: Most general, generalizes all other models

  Con: Many parameters, hard to design algorithms

- **Massive Parallel Computation** [Andoni, Onak, Nikolov, **Y.** '14] [Feldman-Muthukrishnan-Sidiropoulos-Stein-Svitkina'07, Karloff-Suri-Vassilvitskii'10, Goodrich-Sitchinava-Zhang'11, ..., Beame, Koutris, Suciu'13]

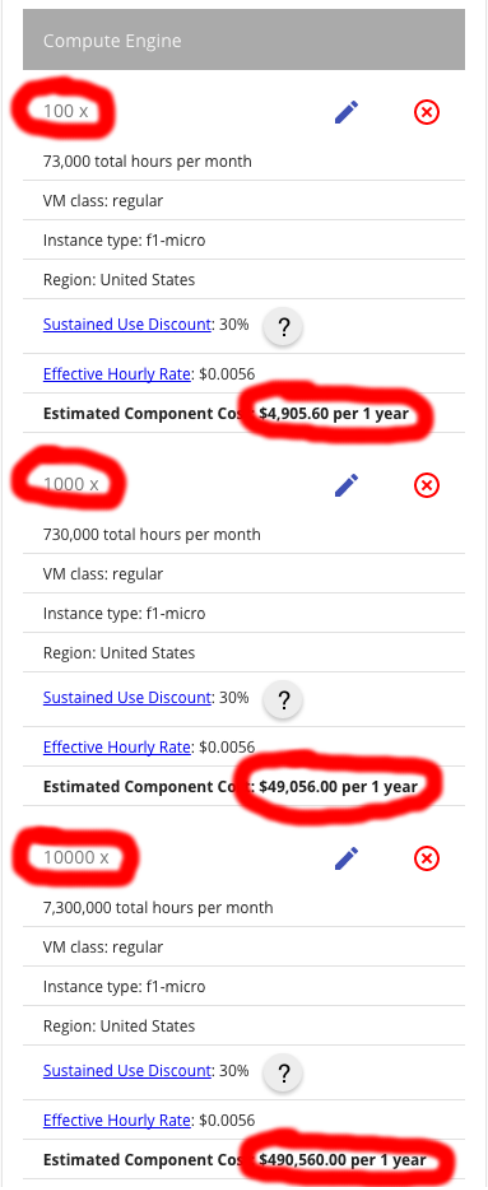
  Pros:

  - Inspired by **modern** systems (Hadoop, MapReduce, Dryad, Spark, Giraph, …)
  - Few parameters, **simple** to design algorithms
  - **New algorithmic ideas**, robust to the exact model specification
  - **# Rounds** is an information-theoretic measure => can prove unconditional results

  Con: sometimes not enough to model more complex behavior

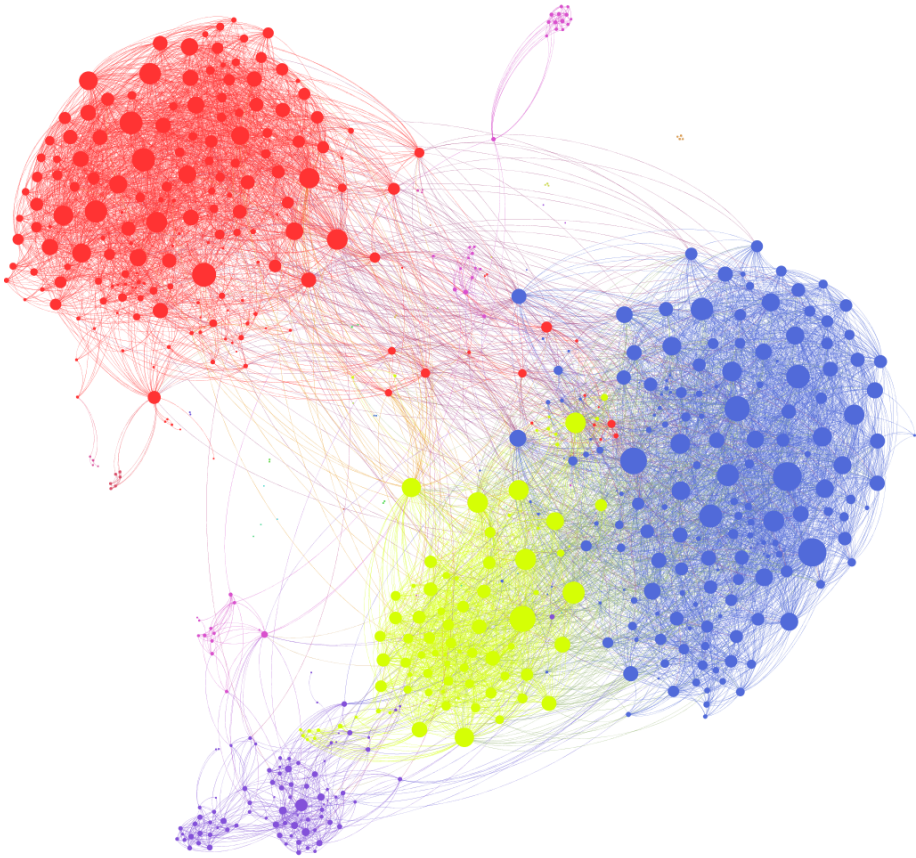
Business perspective

- Pricings:
  - https://cloud.google.com/pricing/
  - https://aws.amazon.com/pricing/
- ~Linear with **space** and **time** usage
  - 100 machines: 5K $/year
  - 10000 machines: 0.5M $/year
- You pay **a lot more** for using provided algorithms
  - https://aws.amazon.com/machine-learning/pricing/



Part 1: Clustering Graphs

- Applications:
  - Community detection
  - Fake account detection
  - Deduplication
  - Storage localization
  - …

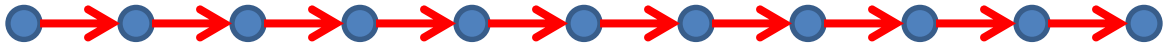


Problem 1: Connectivity

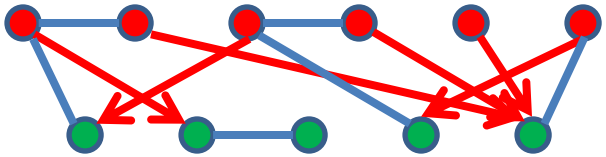
- **Input**: **n** edges of a graph (arbitrarily partitioned between machines)
- **Output**: is the graph connected? (or # of connected components)
- **Question:** how many rounds does it take?
  1. $O(1)$
  2. $O(\log^{\alpha} \mathbf{n})$
  3. $O(\mathbf{n}^{\alpha})$
  4. $O(2^{\alpha \mathbf{n}})$
  5. Impossible

Algorithm for Connectivity

- Version of **Boruvka's algorithm**:
  - All vertices assigned to different components
  - Repeat $O(\log |V|)$ times:
    - Each component chooses a neighboring component
    - All pairs of chosen components get merged
- How to avoid **chaining**?



- If the graph of components is bipartite and only one side gets to choose then no chaining



- **Randomly** assign components to the sides

Algorithms for Graphs: Graph Density

- **Dense**: $\boldsymbol{S} \gg |V|$, e.g. $\boldsymbol{S} \geq |V|^{3/2}$
- Semi-**dense**: $\boldsymbol{S} = \Theta(|V|)$
- Sparse: $\boldsymbol{S} \ll |V|$, e.g. $\boldsymbol{S} \leq |V|^{1/2}$

Algorithms for Graphs: Graph Density

- **Dense**: $\boldsymbol{S} \gg |V|$, e.g. $\boldsymbol{S} \geq |V|^{3/2}$
  - Linear sketching: one round, see [McGregor'14]
    - Workshop at Berkeley tomorrow: http://caml.indiana.edu/linear-sketching-focs.html

- "Filtering" [Karloff, Suri Vassilvitskii, SODA'10; Ene, Im, Moseley, KDD'11; Lattanzi, Moseley, Suri, Vassilvitskii, SPAA'11; Suri, Vassilvitskii, WWW'11]…

Algorithms for Graphs: Graph Density

- Semi-**dense** Graphs: $\boldsymbol{S} = \Theta(|V|)$ [Avdyukhin, **Y.**]
  - Run Boruvka's algorithm for $O(\sqrt{\log |V|})$ rounds
  - # Vertices reduces down to $\frac{|V|}{2^{\sqrt{\log |V|}}}$
  - Repeat $O(\sqrt{\log |V|})$ times:
    - Compute a spanning tree of locally stored edges
    - Put $2^{\sqrt{\log |V|}}$ such trees per machine

Algorithms for Graphs: Graph Density

- Sparse: $\boldsymbol{S} \ll |V|, \boldsymbol{S} \leq |V|^{1/2}$
- Sparse graph problems appear hard
  - **Big open question**: connectivity in $o(\log |V|)$ rounds?
  - Probably no: [Roughgarden, Vassilvitskii, Wang'16]
- "One Cycle vs. Two Cycle" Problem
  - Distinguish one cycle from two in $o(\log |V|)$ rounds?

Other Connectivity Algorithms

- [Rastogi,Machanavajjhala,Chitnis, Das Sarma'13]
  - D = graph diameter

Algorithm	MR Rounds	Communication per round
Hash-Min	D	$O(\|V\| + \|E\|)$
Hash-to-all	Log D	$O(\|V\|^2 + \|E\|)$
Hash-to-Min	$O(\log \|V\|)$ for paths	$\tilde{O}((\|V\| + \|E\|))$ for paths
Hash-Greater-to-Min	O(log n)	O(|V| + |E|)

Graph-Dependent Connectivity Algs?

- **Big question:** connectivity in $O(\log\ D)$ rounds with $\tilde{O}(|V| + |E|)$ communication per round?
- [Rastogi et al'13] conjectured that Hash-to-Min can achieve this
- [Avdyukhin, **Y.'17**]:
  - Hash-to-Min takes $\Omega(D)$ rounds
- **Open problem:** better connectivity algorithms if we parametrize by graph expansion?
- Other work: [Kiveris et al. '14]

What about clustering?

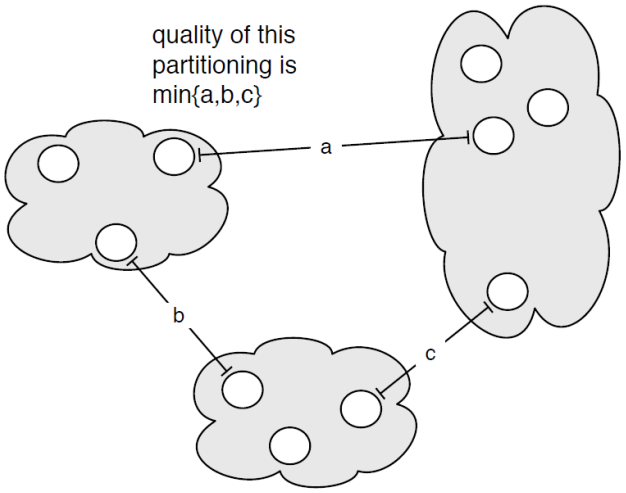
- ≈same ideas work for Single-Linkage Clustering
- Using connectivity as a primitive can preserve cuts in graphs [Benczur, Karger'98]
  - Construct a graph with O(n log n) edges
  - All cut sizes are preserved with a factor of 2
- Allows to run clustering algorithms that use cuts in the objective using this sparse graph

Single Linkage Clustering

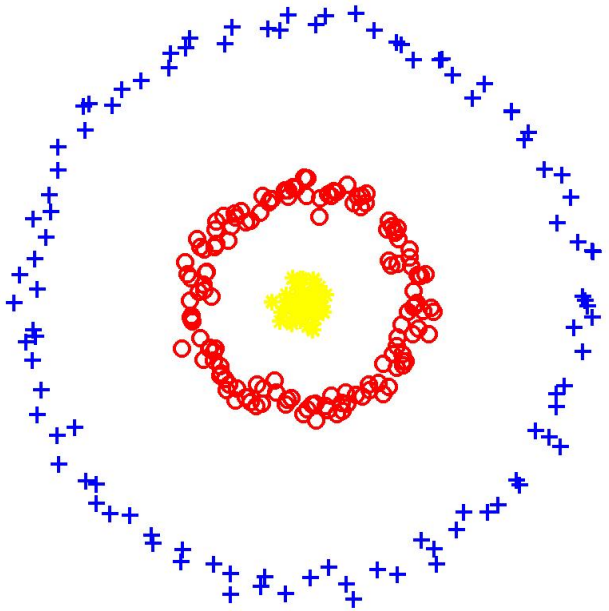
- [Zahn'71] **Clustering** via Minimum Spanning Tree:

k clusters: remove $\boldsymbol{k-1}$ longest edges from MST

- Maximizes **minimum** intercluster distance

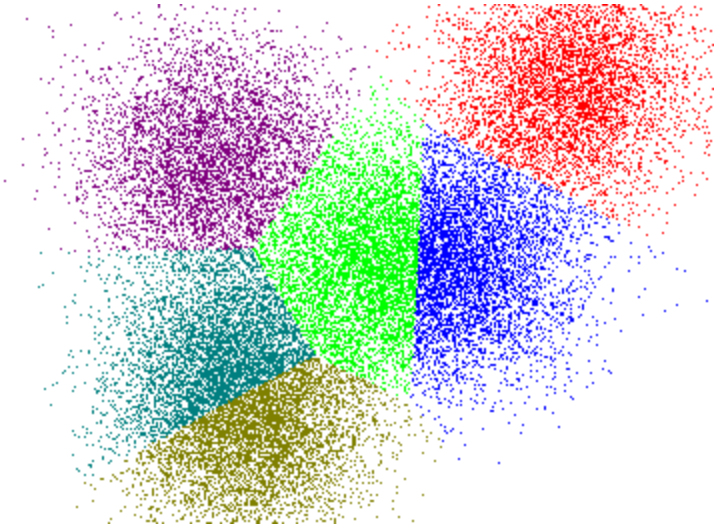


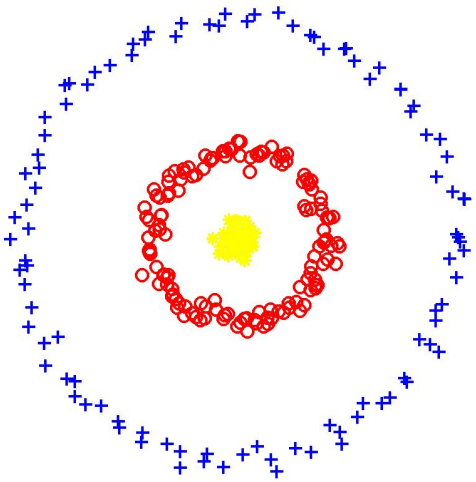
[Kleinberg, Tardos]



Part 2: Clustering Vectors

- Input: $v_1, \ldots, v_n \in \mathbb{R}^d$
  - Feature vectors in ML, word embeddings in NLP, etc.
  - (Implicit) weighted graph of pairwise distances
- Applications:
  - Same as before + Data visualization





Large geometric graphs

- Graph algorithms: **Dense graphs** vs. sparse graphs
  - **Dense**: $S \gg |V|$.
  - Sparse: $S \ll |V|$.

- **Our setting:**
  - Dense graphs, sparsely represented: $O(n)$ space
  - Output doesn't fit on one machine ($S \ll n$)
- **Today:** $(1+\epsilon)$-approximate MST [Andoni, Onak, Nikolov, **Y.**]
  - $d = 2$ (easy to generalize)
  - $R = \log_S n = O(1)$ rounds ($S = n^{\Omega(1)}$)

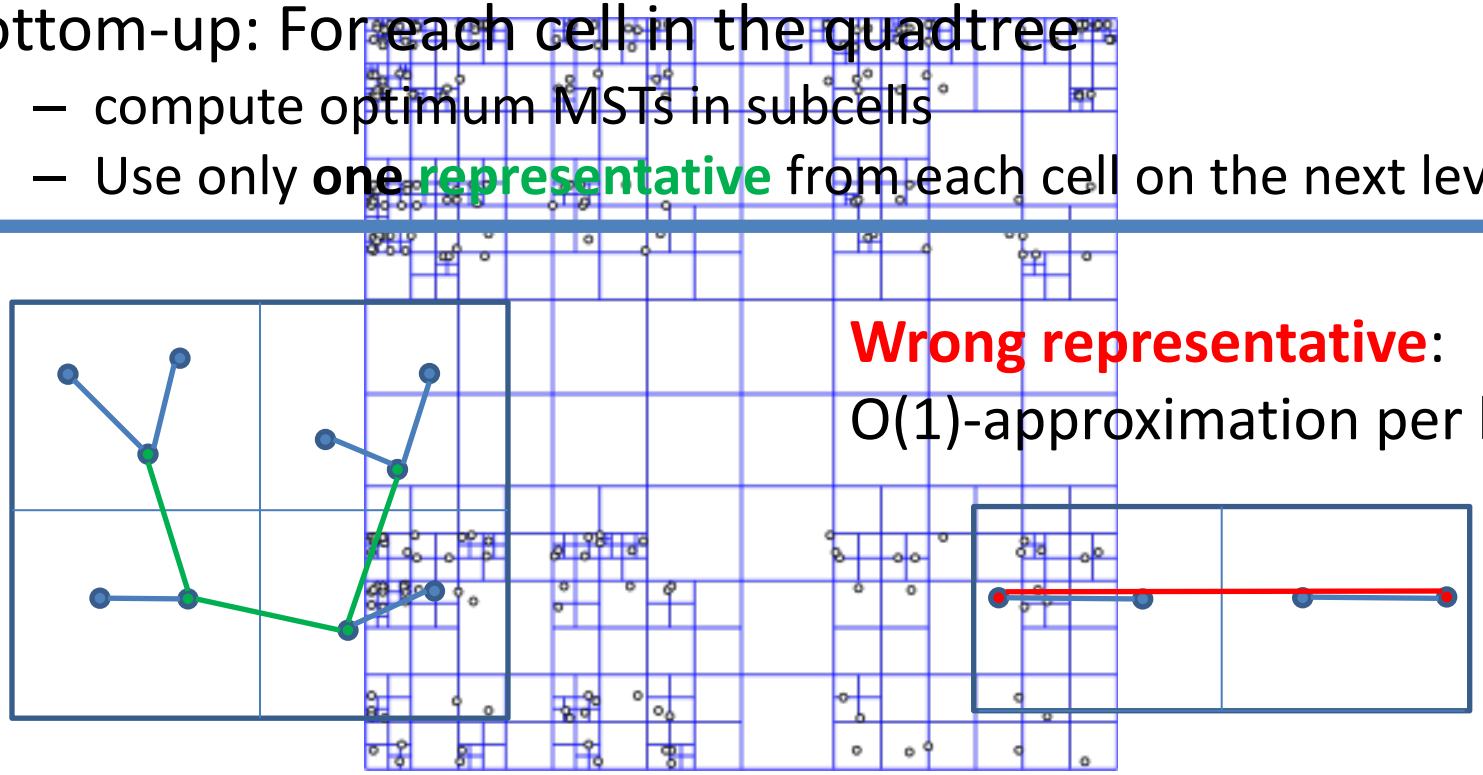
$O(\log n)$-MST in $R = O(\log n)$ rounds

- Assume points have integer coordinates $[0, \dots, \Delta]$, where $\Delta = O(n^2)$.

Impose an $O(\log n)$-depth quadtree

Bottom-up: For each cell in the quadtree

- compute optimum MSTs in subcells
- Use only **one representative** from each cell on the next level



Wrong representative:
O(1)-approximation per level

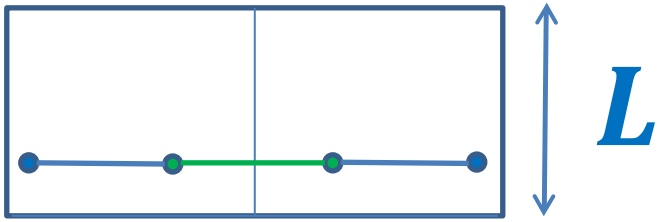
ϵL-nets

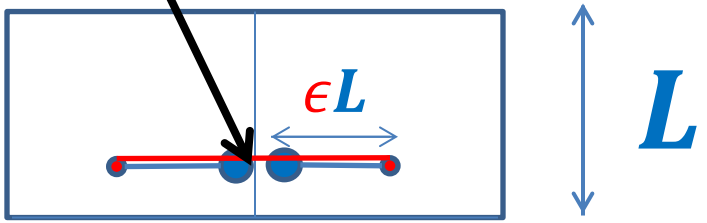
- ϵL-net for a cell C with side length L:
  Collection **S** of vertices in C, every vertex is at distance <= ϵL from some vertex in **S**. (Fact: Can efficiently compute ϵ-net of size $O\left(\frac{1}{\epsilon^2}\right)$)

Bottom-up: For each cell in the quadtree
- Compute optimum MSTs in subcells
- Use ϵL-net from each cell on the next level

- **Idea**: Pay only $O(\epsilon L)$ for an **edge** cut by cell with side L
- Randomly shift the quadtree:
  $\Pr[cut\ edge\ of\ length\ \ell\ by\ L] \leq \ell / L$ — charge errors
  O(1)-approximation per level

Wrong representative





Randomly shifted quadtree

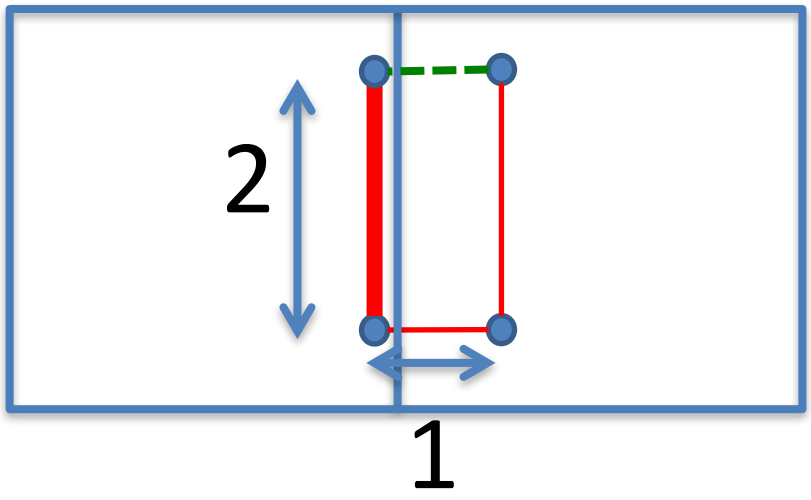
- Top cell shifted by a random vector in $[0, \boldsymbol{L}]^2$

Impose a **randomly shifted** quadtree (top cell length $\boldsymbol{2\Delta}$)

Bottom-up: For each cell in the quadtree

– Compute optimum MSTs in subcells

– Use $\boldsymbol{\epsilon L}$-net from each cell on the next level



Pay **5** instead of **4**

Bad Cut

Pr[Bad Cut] = Ω(1)

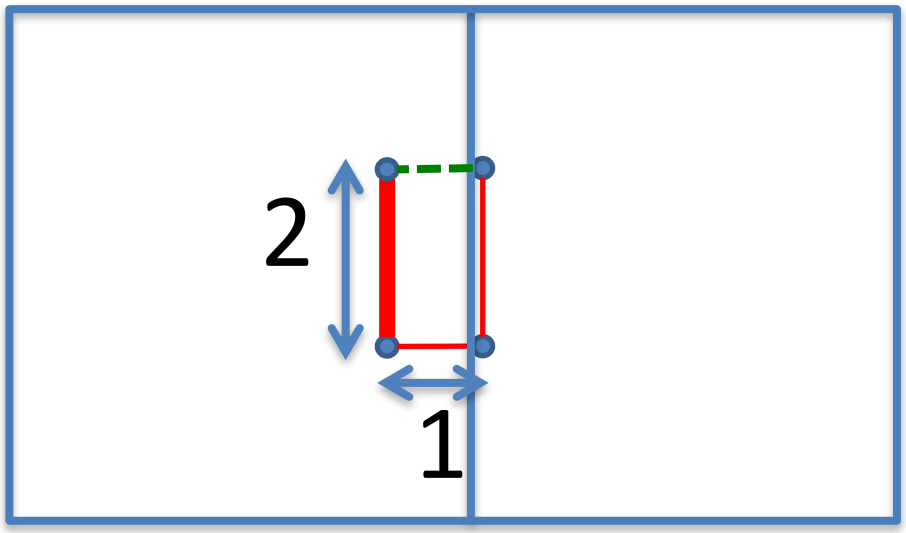
$(1+\epsilon)$-MST in $\mathbf{R} = O(\log\ n)$ rounds

- **Idea:** Only use short edges inside the cells

Impose a **randomly shifted** quadtree (top cell length $\frac{2\Delta}{\epsilon}$)

Bottom-up: For each node (cell) in the quadtree

- compute optimum Minimum Spanning **Forests** in subcells, **using edges of length $\leq \epsilon L$**
- Use only $\epsilon^2 L$-net from each cell on the next level

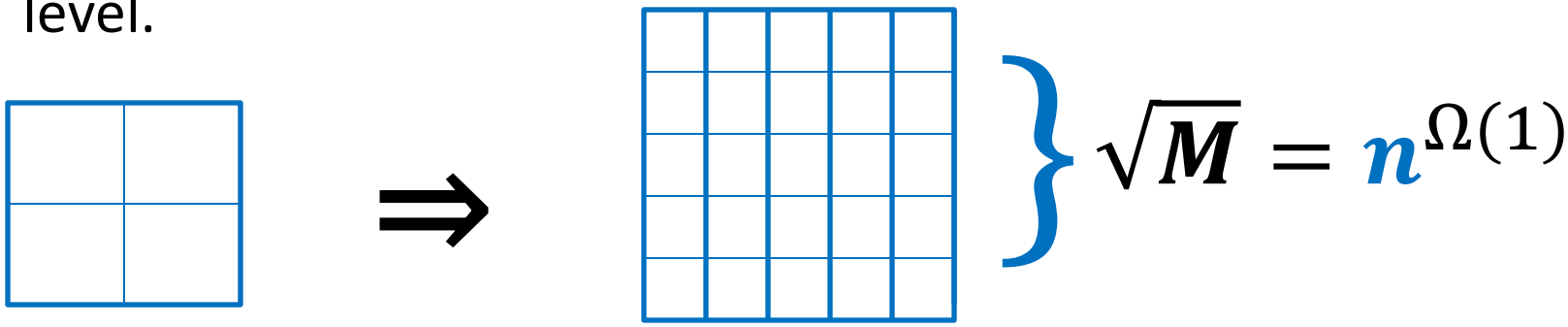


$$L = \Omega\left(\frac{1}{\epsilon}\right)$$

Pr[Bad Cut] = $O(\epsilon)$

$(1+\epsilon)$-MST in $\mathbf{R} = O(1)$ rounds

- $O(\log n)$ rounds => O($\log_S n$) = O(1) rounds
  - Flatten the tree: ($\sqrt{M}\times\sqrt{M}$)-grids instead of (2x2) grids at each level.



Impose a **randomly shifted** ($\sqrt{M}\times\sqrt{M}$)-tree

Bottom-up: For each node (cell) in the tree

- compute optimum MSTs in subcells via edges of length $\leq \epsilon L$
- Use only $\epsilon^2 L$-net from each cell on the next level

Single-Linkage Clustering [Y., Vadapalli]

- **Q**: Single-linkage clustering from $(1+\epsilon)$-MST?
- **A: No**, a fixed edge can be arbitrarily distorted

- **Idea:**
  - Run $O(\log n)$ times & collect all $(1+\epsilon)$-MST edges
  - Compute MST of these edges using Boruvka
  - Use this MST for k-Single Linkage Clustering for all k

- Overall: O(log n) rounds of MPC instead of O(1)
- **Q**: Is this actually necessary?
- **A: Most likely yes**, i.e. yes, assuming sparse connectivity is hard

Single-Linkage Clustering [Y., Vadapalli]

- **Conj 1**: Sparse Connectivity requires $\Omega(\log |V|)$
- **Conj 2**: "1 cycle vs. 2 cycles" requires $\Omega(\log |V|)$
- Under ℓ_p-Distances:

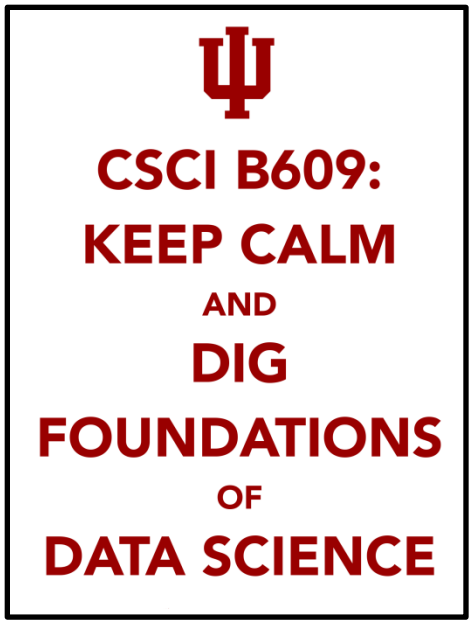
Distance	Approximation	Hardness under Conjecture 1*	Hardness under Conjecture 2*
Hamming	Exact	2	3
ℓ_1	$(1+\epsilon)$	2	3
ℓ_2	$(1+\epsilon)$	$1.41 - \epsilon$	$1.84 - \epsilon$
ℓ_∞	$(1+\epsilon)$	2	

Thanks! Questions?

- Slides will be available on **http://grigory.us**
- More about algorithms for massive data:

http://grigory.us/blog/

- More in the classes I teach:



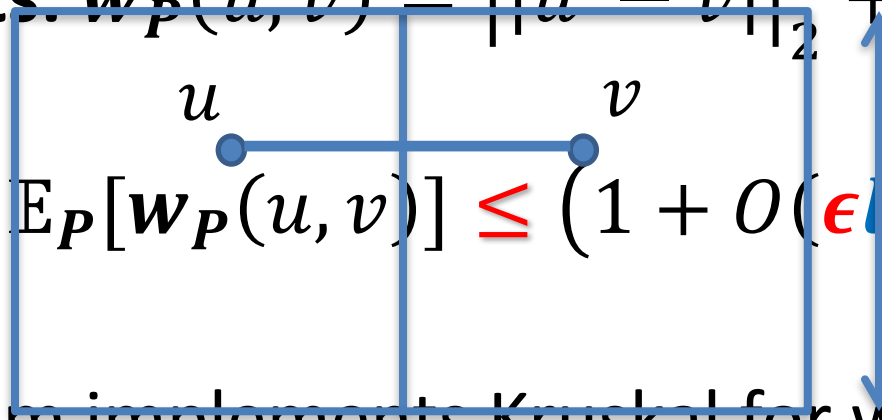
$(1+\epsilon)$-MST in $\mathbf{R} = O(1)$ rounds

Theorem: Let $l = \#$ levels in a random tree P

$$\mathbb{E}_P[\mathbf{ALG}] \leq \big(1 + O(\epsilon l d)\big)\mathbf{OPT}$$

Proof (sketch):

- $\Delta_P(u,v)$ = cell length, which first partitions (u,v)
- **New weights:** $w_P(u,v) = ||u-v||_2 + \epsilon\Delta_P(u,v)$



$$||u-v||_2 \leq \mathbb{E}_P[w_P(u,v)] \leq \big(1 + O(\epsilon l d)\big)\,||u-v||_2$$

- Our algorithm implements Kruskal for weights w_P

Technical Details

$(1+\epsilon)$-**MST**:

- "**Load balancing**": partition the tree into parts of the same size
- **Almost linear time locally**: Approximate Nearest Neighbor data structure [Indyk'99]
- Dependence on dimension **d** (size of ϵ-net is $O\left(\frac{d}{\epsilon}\right)^{d}$)
- Generalizes to bounded **doubling dimension**

Algorithm for Connectivity: Setup

Data: **n** edges of an undirected graph.

Notation:

- $\pi(v) \equiv$ unique id of v
- $\Gamma(S) \equiv$ set of neighbors of a subset of vertices S.

Labels:

- Algorithm assigns a label $\ell(v)$ to each v.
- $L_v \equiv$ the set of vertices with the label $\ell(v)$ (invariant: subset of the connected component containing v).

Active vertices:

- Some vertices will be called **active** (exactly one per L_v).

Algorithm for Connectivity

- Mark every vertex as **active** and let $\ell(v) = \pi(v)$.
- For phases $i = 1,2, \ldots, O(\log \mathbf{n})$ do:
  - Call each **active** vertex a **leader** with probability 1/2. If v is a **leader**, mark all vertices in L_v as **leaders**.
  - For every **active** **non-leader** vertex w, find the smallest **leader** (by π) vertex $\mathrm{w}^\star$ in $\Gamma(L_w)$.
  - Mark w **passive**, relabel each vertex with label w by $\mathrm{w}^\star$.
- **Output**: set of connected components based on ℓ.

Algorithm for Connectivity: Analysis

- If $\ell(u) = \ell(v)$ then u and v are in the same CC.
- **Claim:** Unique labels with high probability after $O(\log N)$ phases.
- For every CC # active vertices reduces by a constant factor in every phase.
  - Half of the active vertices declared as non-leaders.
  - Fix an active **non-leader** vertex $\boldsymbol{v}$.
  - If at least two different labels in the CC of v then there is an edge $(\boldsymbol{v'}, \boldsymbol{u})$ such that $\ell(\boldsymbol{v}) = \ell(\boldsymbol{v'})$ and $\ell(\boldsymbol{v'}) \neq \ell(\boldsymbol{u})$.
  - $\boldsymbol{u}$ marked as a **leader** with probability 1/2 ⇒ half of the active non-leader vertices will change their label.
  - Overall, expect 1/4 of labels to disappear.
  - After $O(\log N)$ phases # of active labels in every connected component will drop to one with high probability

Algorithm for Connectivity: Implementation Details

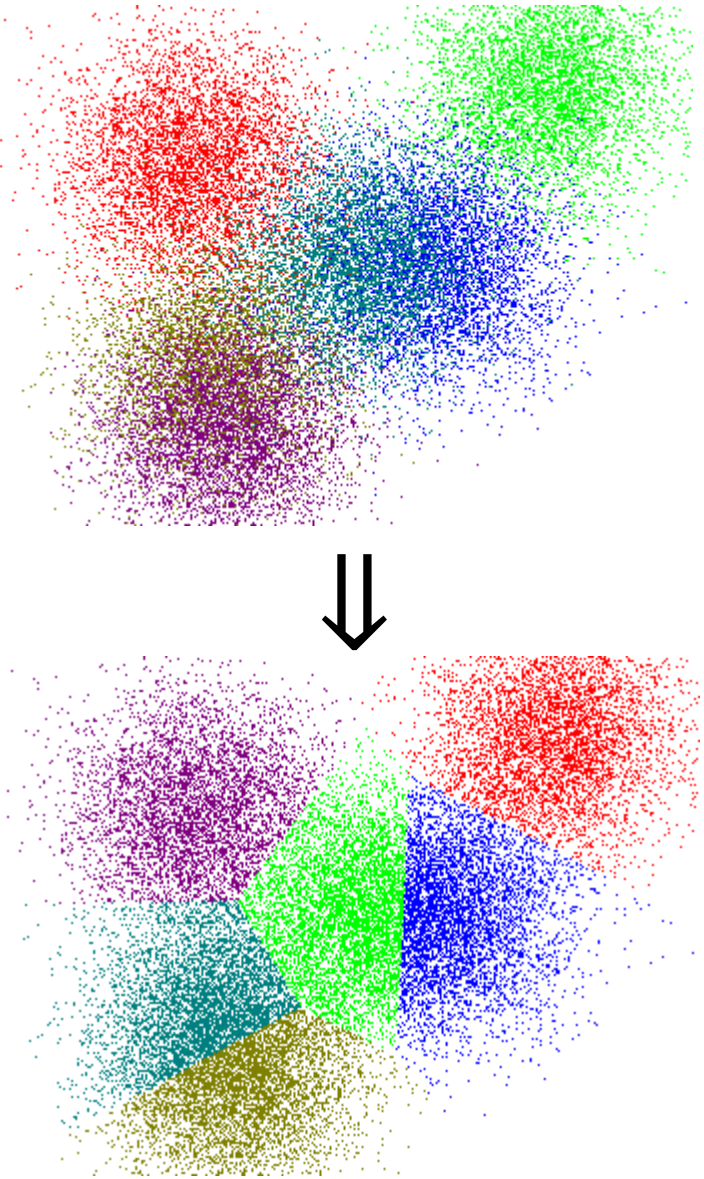
- Distributed data structure of size $O(|V|)$ to maintain labels, ids, leader/non-leader status, etc.
  - O(1) rounds per stage to update the data structure
- Edges stored locally with all auxiliary info
  - Between stages: use distributed data structure to update local info on edges
- For every **active non-leader** vertex w, find the smallest **leader** (w.r.t π) vertex $w^\star \in \Gamma(L_w)$
  - Each (**non-leader, leader**) edge sends an update to the distributed data structure
- Much faster with Distributed Hash Table Service (DHT) [Kiveris, Lattanzi, Mirrokni, Rastogi, Vassilvitskii'14]

Problem 3: K-means

- Input: $v_1, \ldots, v_n \in \mathbb{R}^d$
- Find k centers $c_1, \ldots, c_k$
- Minimize sum of squared distance to the closest center:

$$\sum_{i=1}^{n} \min_{j=1}^{k} ||v_i - c_j||_2^2$$

- $||v_i - c_j||_2^2 = \sum_{t=1}^{d} (v_{it} - c_{jt})^2$
- NP-hard



K-means++ [Arthur,Vassilvitskii'07]

- $C = \{c_1, \ldots, c_t\}$ (collection of centers)
- $d^2(v, C) = \min_{j=1}^{k} ||v - c_j||_2^2$

K-means++ algorithm (gives $O(\log \boldsymbol{k})$-approximation):

- Pick c_1 uniformly at random from the data
- Pick centers $c_2 \ldots, c_{\boldsymbol{k}}$ sequentially from the distribution where point v has probability

$$\frac{d^2(v, C)}{\sum_{i=1}^{n} d^2(v_i, C)}$$

K-means|| [Bahmani et al. '12]

- Pick $C = c_1$ uniformly at random from data
- Initial cost: $\psi = \sum_{i=1}^{n} d^2(v_i, c_1)$
- Do $O(\log \psi)$ times:
  - Add $O(\boldsymbol{k})$ centers from the distribution where point v has probability

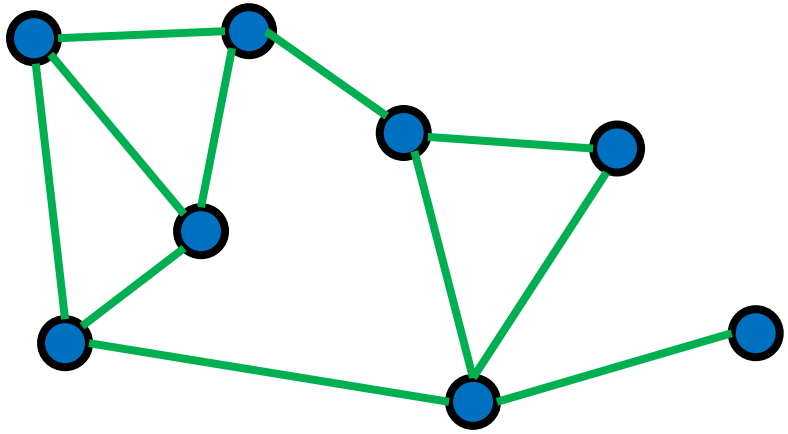
$$\frac{d^2(v, C)}{\sum_{i=1}^{n} d^2(v_i, C)}$$

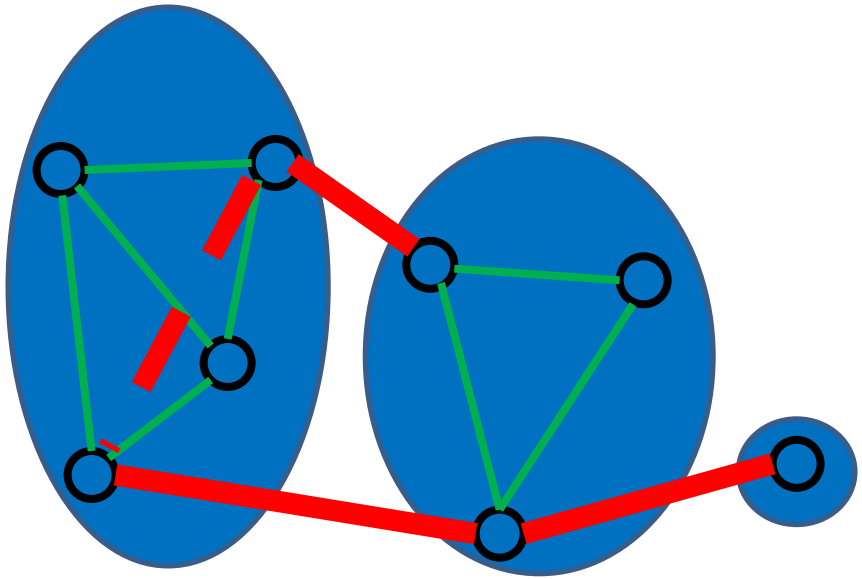
- Solve k-means for these O($\boldsymbol{k} \log \psi$) points locally

- **Thm.** If final step gives $\boldsymbol{\alpha}$-approximation
  $\Rightarrow O(\boldsymbol{\alpha})$-approximation overall

Problem 2: Correlation Clustering

- Inspired by machine learning at WhizBang! LABS
- Practice: [Cohen, McCallum '01, Cohen, Richman '02]
- Theory: [**Blum, Bansal, Chawla '04**]

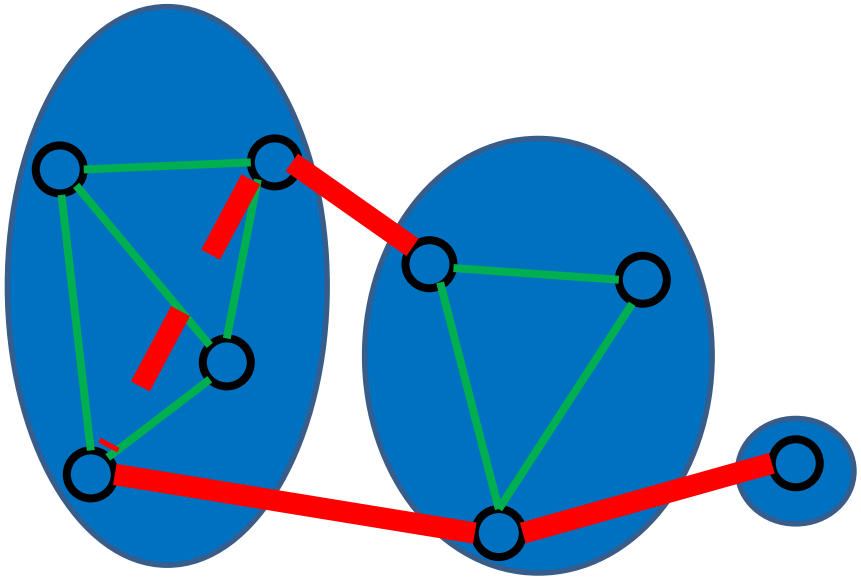




Correlation Clustering: Example

- **Minimize** # of **incorrectly** classified pairs:

  # Covered non-edges + # Non-covered edges



4 incorrectly classified =
1 covered non-edge +
3 non-covered edges

Approximating Correlation Clustering

- **Minimize** # of **incorrectly** classified pairs
  - ≈ 20000-approximation [Blum, Bansal, Chawla'04]
  - [Demaine, Emmanuel, Fiat, Immorlica'04],[Charikar, Guruswami, Wirth'05], [Ailon, Charikar, Newman'05] [Williamson, van Zuylen'07], [Ailon, Liberty'08],…
  - ≈ 2-approximation [Chawla, Makarychev, Schramm, **Y.** '15]
- **Maximize** # of **correctly** classified pairs
  - $(1-\epsilon)$-approximation [Blum, Bansal, Chawla'04]

Correlation Clustering

One of the most successful clustering methods:

- Only uses **qualitative information** about similarities
- **# of clusters unspecified** (selected to best fit data)
- Applications: document/image **deduplication** (data from crowds or black-box machine learning)
- **NP-hard** [Bansal, Blum, Chawla '04], admits **simple approximation algorithms** with good provable guarantees

Correlation Clustering

More:

- **Survey** [Wirth]
- **KDD'14** tutorial: "Correlation Clustering: From Theory to Practice" [Bonchi, Garcia-Soriano, Liberty] http://francescobonchi.com/CCtuto_kdd14.pdf
- **Wikipedia** article: http://en.wikipedia.org/wiki/Correlation_clustering

Data-Based Randomized Pivoting

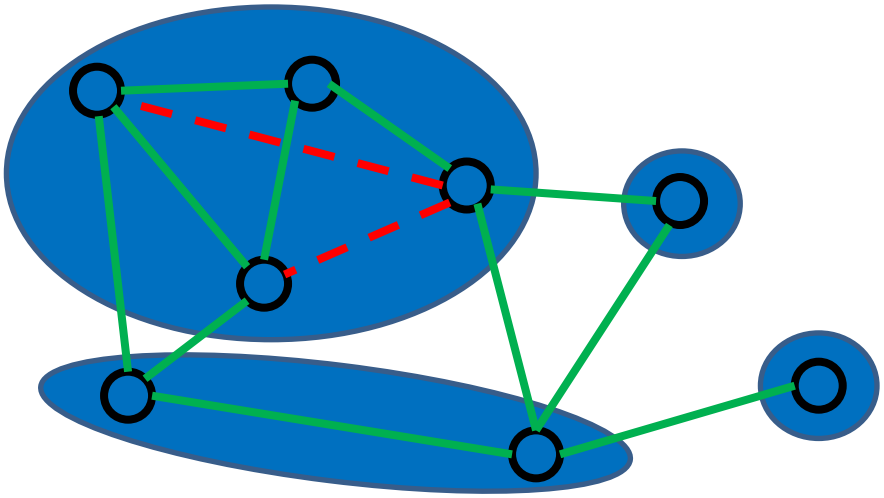
3-approximation (expected) [Ailon, Charikar, Newman]

Algorithm:

- Pick a random pivot vertex v
- Make a cluster $v \cup N(v)$, where $N(v)$ is the set of neighbors of v
- Remove the cluster from the graph and repeat

Data-Based Randomized Pivoting

- Pick a random pivot vertex $\boldsymbol{p}$
- Make a cluster $\boldsymbol{p} \cup N(\boldsymbol{p})$, where $N(\boldsymbol{p})$ is the set of neighbors of $\boldsymbol{p}$
- Remove the cluster from the graph and repeat



8 incorrectly classified =
2 covered non-edges +
6 non-covered edges

Parallel Pivot Algorithm

- $(3+\epsilon)$-approx. in $O(\log^2 n / \epsilon)$ rounds [Chierichetti, Dalvi, Kumar, KDD'14]
- Algorithm: while the graph is not empty
  - $\boldsymbol{D}$ = current maximum degree
  - Activate each node independently with prob. $\boldsymbol{\epsilon/D}$
  - Deactivate nodes connected to other active nodes
  - The remaining nodes are **pivots**
  - Create cluster around each pivot as before
  - Remove the clusters

Parallel Pivot Algorithm: Analysis

- **Fact:** Halves max degree after $\frac{1}{\epsilon}\log n$ rounds

  $\Rightarrow$ terminates in $O\left(\frac{\log^2 n}{\epsilon}\right)$ rounds

- **Fact:** Activation process induces **close to uniform** marginal distribution of the pivots

  $\Rightarrow$ analysis similar to regular pivot gives $(3+\epsilon)$-approximation