# "algorithms for Big Data" 

## Lecture 4: Massively Parallel Computation

Slides at http://grigory.us/big-data-csclub.html

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## 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: Overview

## Graphs

## Vectors

## Basic

Connectivity
K-means

Correlation
Clustering

Single-Linkage
Clustering

## Cluster Computation (a la BSP)

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

Input: size $n \Rightarrow$

## $\Rightarrow$ Output



M machines

S space

## Cluster Computation (a la BSP)

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

Goal: Minimize $\boldsymbol{R}$. Ideally: $R=$ constant.
$\mathbf{S}$ space
$O\left(S^{1+o(1)}\right)$ time

## MapReduce-style computations

## YАНоО! 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 $O\left(\log _{s} n\right)$ 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 [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/
- $\sim$ 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/machinelearning/pricing/

73,000 total hours per month
VM class: regular
Instance type: f1-micro
Region: United States
Sustained Use Discount: 30\%
Effective Hourly Rate: \$0.0056
Estimated Component Cos \$4,905.60 per 1 year

730,000 total hours per month
VM class: regular
Instance type: f1-micro
Region: United States
Sustained Use Discount: 30\% ?
Effective Hourly Rate: $\$ 0.0056$
Estimated Component Co $\$ \$ 49,056.00$ per 1 year


7,300,000 total hours per month
VM class: regular
Instance type: f1-micro
Region: United States
Sustained Use Discount: 30\%

## Sorting: Terasort

- Sort Benchmark: http://sortbenchmark.org/
- Sorting $\boldsymbol{n}$ keys on $\boldsymbol{M}=\boldsymbol{O}\left(\boldsymbol{n}^{1-\boldsymbol{\epsilon}}\right)$ machines
- Would like to partition keys uniformly into blocks: first $\boldsymbol{n} / \boldsymbol{M}$, second $\boldsymbol{n} / \boldsymbol{M}$, etc.
- Sort the keys locally on each machine
- Build an approximate histogram:
- Each machine takes a sample of size $\boldsymbol{s}$
- All $\boldsymbol{M} * \boldsymbol{s} \leq \boldsymbol{S}=\boldsymbol{n}^{\boldsymbol{\epsilon}}$ samples are sorted locally
- Blocks are computed based on the samples
- By Chernoff: $\mathbf{M} * \boldsymbol{s}=O\left(\frac{\log \boldsymbol{n}}{\alpha^{2}}\right)$ samples suffice to compute all block sizes up to $\pm \boldsymbol{\alpha} \boldsymbol{n}$ error with high probability
- Take $\alpha=\frac{\boldsymbol{n}^{\epsilon-1}}{2}$ : $\operatorname{error} \mathrm{O}(\boldsymbol{S})$
- $\mathbf{M} * \boldsymbol{s}=\widetilde{O}\left(\boldsymbol{n}^{2-2 \epsilon}\right)=\boldsymbol{O}\left(\boldsymbol{M}^{2}\right) \leq \boldsymbol{O}\left(\boldsymbol{n}^{\epsilon}\right)$ for $\epsilon \geq 2 / 3$


## Algorithms for Graphs

- Dense graphs vs. sparse graphs
- Dense: $S \gg|V|$
- Linear sketching: one round
- "Filtering" (Output fits on a single machine) [Karloff, Suri Vassilvitskii, SODÁ10; Ene, Im, Moseley, KDD'11; Lattanzi, Moseley, Suri, Vassilvitskii, SPAA'11; Suri, Vassilvitskii, WWW'11]
- Sparse: $\boldsymbol{S} \ll|V|$ (or $\boldsymbol{S} \ll$ solution size)

Sparse graph problems appear hard (Big open question: connectivity in o $(\log n)$ rounds?)

vs.


## 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. $O\left(\log ^{\alpha} \mathrm{n}\right)$
3. $O\left(\mathrm{n}^{\alpha}\right)$
4. $O\left(2^{\alpha n}\right)$
5. Impossible

## Algorithm for Connectivity

- Version of Boruvka's algorithm:
- All vertices assigned to different components
- Repeat $O(\log \mathrm{n})$ 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


## 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 $i=1,2, \ldots, O(\log \mathrm{n})$ 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 $\pi$ ) vertex $\mathrm{w}^{\star}$ in $\Gamma\left(L_{w}\right)$.
- Mark w passive, relabel each vertex with label w by $\mathrm{w}^{\star}$.
- Output: set of connected components based on $\ell$.


## 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 $v$.
- If at least two different labels in the CC of $v$ then there is an edge $\left(v^{\prime}, \boldsymbol{u}\right)$ such that $\ell(v)=\ell\left(v^{\prime}\right)$ and $\ell\left(v^{\prime}\right) \neq \ell(\boldsymbol{u})$.
$-u$ marked as a leader with probability $1 / 2 \Rightarrow$ 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 $\pi$ ) vertex $\mathrm{w}^{\star} \in \Gamma\left(L_{w}\right)$
- 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]


## Algorithms for Graphs

- Dense graphs vs. sparse graphs
- Dense: $S \gg|V|$
- Linear sketching: one round, see [McGregor'14]
- "Filtering" (Output fits on a single machine) [Karloff, Suri Vassilvitskii, SODÁ10; Ene, Im, Moseley, KDD'11; Lattanzi, Moseley, Suri, Vassilvitskii, SPAA'11; Suri, Vassilvitskii, WWW'11]...
- Sparse: $\boldsymbol{S} \ll|V|$ (or $\boldsymbol{S} \ll$ solution size)

Sparse graph problems appear hard (Big open question: connectivity in o( $\log n$ ) rounds?)

vs.


## Problem 2: Correlation Clustering

- Inspired by machine learning at WhizBang ${ }_{\text {LABS }}$
- 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
- $\approx$ 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],...
- $\approx$ 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 cluster ing


## 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 $p \cup N(p)$, where $N(p)$ is the set of neighbors of $p$
- 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 $O\left(\log ^{2} n / \epsilon\right)$ rounds [Chierichetti, Dalvi, Kumar, KDD'14]
- Algorithm: while the graph is not empty
- $\boldsymbol{D}=$ current maximum degree
- Activate each node independently with prob. $\epsilon / D$
- 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 $\mathrm{O}\left(\frac{\log ^{2} n}{\epsilon}\right)$ rounds
- Fact: Activation process induces close to uniform marginal distribution of the pivots
$\Rightarrow$ analysis similar to regular pivot gives $(3+\epsilon)$ approximation


## Part 2: Clustering Vectors

- Input: $v_{1}, \ldots, v_{n} \in \mathbb{R}^{d}$
- Feature vectors in ML, word embedings in NLP, etc.
- (Implicit) weighted graph of pairwise distances
- Applications:
- Same as before + Data visualization



## Problem 3: K-means

- Input: $v_{1}, \ldots, v_{n} \in \mathbb{R}^{d}$
- Find $\boldsymbol{k}$ centers $c_{1}, \ldots, c_{k}$
- Minimize sum of squared distance to the closest center:

$$
\sum_{i=1}^{n} \min _{j=1}^{k}\left\|v_{i}-c_{j}\right\|_{2}^{2}
$$

- $\left\|v_{i}-c_{j}\right\|_{2}^{2}=\sum_{t=1}^{d}\left(v_{i t}-c_{j t}\right)^{2}$
- NP-hard


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

- $C=\left\{c_{1}, \ldots, c_{t}\right\}$ (collection of centers)
- $d^{2}(v, C)=\min _{j=1}^{k}\left\|v-c_{j}\right\|_{2}^{2}$

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

- Pick $c_{1}$ uniformly at random from the data
- Pick centers $c_{2} \ldots, c_{k}$ sequentially from the distribution where point $v$ has probability

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

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

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

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

- Solve $k$-means for these $\mathrm{O}(k \log \psi)$ points locally
- Thm. If final step gives $\alpha$-approximation $\Rightarrow O(\alpha)$-approximation overall


## Problem 4: Single Linkage Clustering

- [Zahn'71] Clustering via Minimum Spanning Tree: k clusters: remove $k-1$ longest edges from MST
- Maximizes minimum intercluster distance

[Kleinberg, Tardos]



## Large geometric graphs

- Graph algorithms: Dense graphs vs. sparse graphs
- Dense: $S \gg|V|$.
- Sparse: $S \ll|V|$.
- Our setting:
- Dense graphs, sparsely represented: $0(n)$ 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)
- $R=\log _{s} n=\mathrm{O}(1)$ rounds $\left(S=n^{\boldsymbol{\Omega}(\mathbf{1})}\right)$


## $O(\log n)-\mathrm{MST}$ in $R=O(\log n)$ rounds

- Assume points have integer coordinates $[0, \ldots, \Delta]$, where $\Delta=O\left(n^{2}\right)$.

Impose an $O(\log n)$-depth quadtree Bottom-up: Foreach cellin thequadtreem

- compute optimum MSTs in subeclls
- Use only one feresintative frompeach cell on the next level



## $\epsilon L$-nets

- $\epsilon L$-net for a cell C with side length $L$ :

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

Bottom-up: For each cell in the quadtree

- Compute optimum MSTs in subcells
- Use $\epsilon L$-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:
 O(1)-apprqximation per level



## Randomly shifted quadtree

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

Impose a randomly shifted quadtree (top cell length $\mathbf{2 \Delta}$ )
Bottom-up: For each cell in the quadtree

- Compute optimum MSTs in subcells
- Use $\epsilon L$-net from each cell on the next level



## Pay 5 instead of 4 <br> $\operatorname{Pr}[$ Baadeut $]=\Omega(1)$

## $(1+\boldsymbol{\epsilon})-\mathrm{MST}$ 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


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

$$
\operatorname{Pr}[\text { Bad Cut }]=\boldsymbol{O}(\epsilon)
$$

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

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


$$
\sqrt{M}=n^{\Omega(1)}
$$

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


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

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

$$
\mathbb{E}_{P}[\mathbf{A L G}] \leq(1+O(\epsilon \operatorname{ld})) \mathbf{O P T}
$$

## Proof (sketch):

- $\Delta_{P}(u, v)=$ cell length, which first partitions $(u, v)$
- New weights: $w_{P}(u, v)=\|u-v\|_{2} \dagger \epsilon \Delta_{P}(u, v)$
$\|u-v\|_{2} \leq E_{P}\left[w_{P}(u, v)\right] \leq(1+O(\epsilon\| \| v)) p((u, v)\rangle \|_{2}$
- Our algorithmimpiements Kiruskal for weights $\boldsymbol{w}_{\boldsymbol{P}}$


## Technical Details

$(1+\epsilon)-\mathrm{MST}$ :

- "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 $\epsilon$-net is $O\left(\frac{d}{\epsilon}\right)^{d}$ )
- Generalizes to bounded doubling dimension


## 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:

| CIS |
| :---: |
| CIS 700: |
| KEEP CALM |
| CRUN |
| DATA IN O(N) |

$\Psi$
CSCI B609:
KEEP CALM
AND
DIG
FOUNDATIONS of
DATA SCIENCE

