Hierarchical Clustering: Objectives & Algorithms

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Clustering

Flat Clustering

- Often data can be grouped together into subsets that are coherent, called clusters
- Data in the same cluster is typically more similar that data across different clusters

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Cluster the following news headlines in 3 categories

Will AI take over?
Google’s new AI wins against Bingo world champion
Black holes swallow stars whole according to new study
Neymar breaks his leg and stops playing football
France learns that cricket is not only an insect

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Football	Neymar breaks his leg and stops playing football
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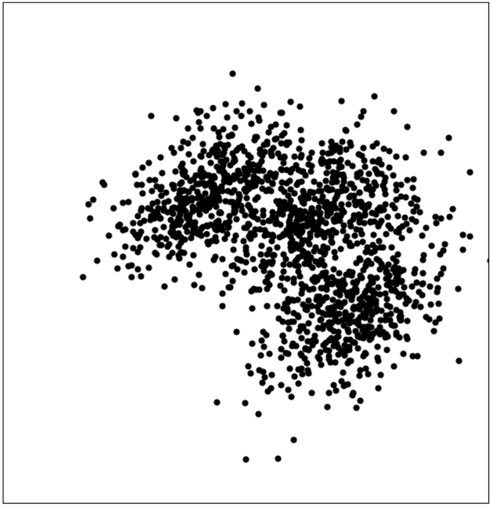
(Flat) Clustering



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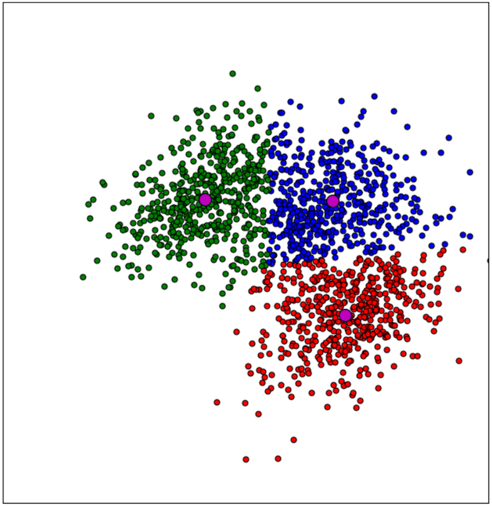
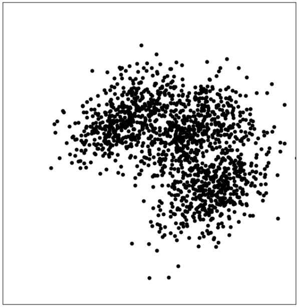


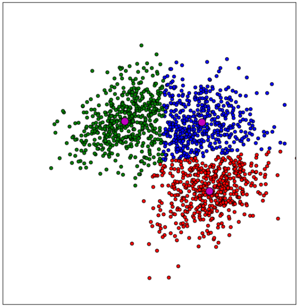
(Flat) Clustering: Objectives and Algorithms

Data lies in some metric space $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^D$

Find k points $\mu_1, \ldots, \mu_k$ that minimize, e.g.

1. k-median objective $\sum_{i=1}^{N} \left(\min_{j \in [k]} d(\mathbf{x}_i, \mu_j) \right)$
2. k-means objective $\sum_{i=1}^{N} \left(\min_{j \in [k]} d(\mathbf{x}_i, \mu_j) \right)^2$





(Flat) Clustering: Objectives and Algorithms

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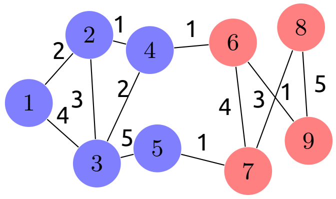
- Minimizing these objective functions is NP-hard
- Approximation algorithms are known

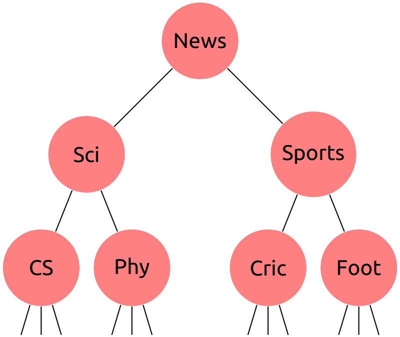
Clustering: Input as (Dis)-Similarity Graph



- Edge weights represent similarities
- Graph partitioning algorithms, e.g., mincut, sparsest cut, multi-way cut
- Many of these problems are NP-complete
- Approximation algorithms are widely studied
- Spectral partitioning algorithms can be highly efficient

Hierarchical Clustering

- Recursive partitioning of data at an increasingly finer granularity represented as a tree
- The leaves of the hierarchical cluster tree represent data.



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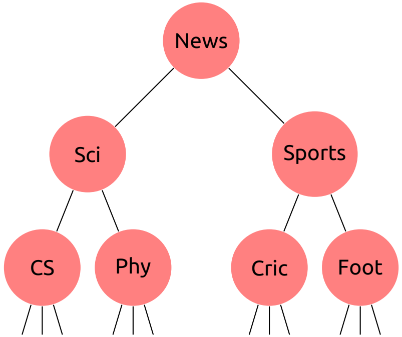

Will AI take over?

Someone finally figured out why neural nets work

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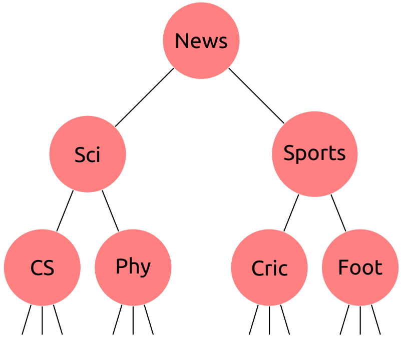

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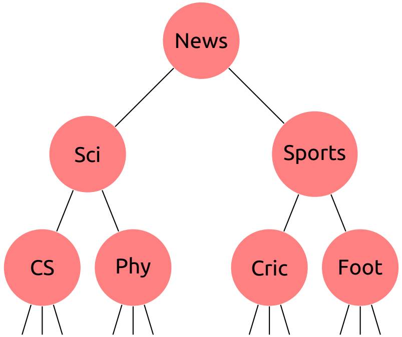

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Hierarchical Clustering in Practice: Linkage Algorithms

- We are given pairwise similarities between (some) pairs of datapoints

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- Repeatedly merge most similar clusters
- Builds up cluster tree bottom-up

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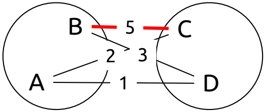
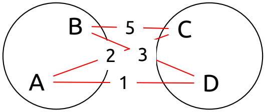
Single Linkage



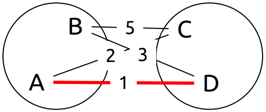
Similarity: 5

Average Linkage



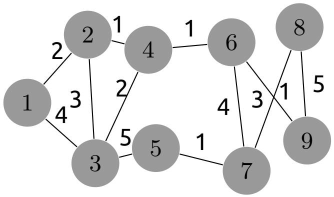
Similiarity: 2.75

Complete Linkage

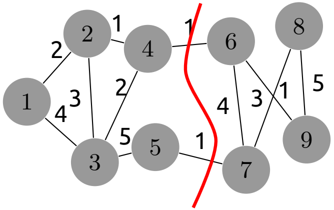


Similiarity: 1

Hierarchical Clustering: Divisive Heuristics



Hierarchical Clustering: Divisive Heuristics



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  - Split using bisection k-means
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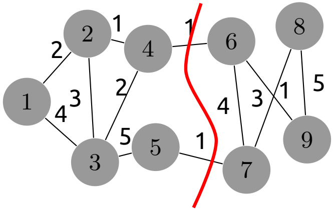
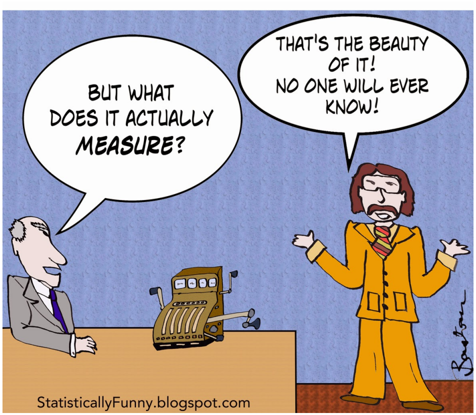


- Find a partition of the input similarity graph (or set of points)
  - Split using bisection k-means
  - Split using sparsest cut
- Recurse on each part
- Builds cluster-tree top-down

What are these algorithms actually doing?


BUT WHAT DOES IT ACTUALLY *MEASURE?*
THAT'S THE BEAUTY OF IT! NO ONE WILL EVER KNOW!
StatisticallyFunny.blogspot.com

What quantity are these algorithms optimizing?

- For flat clustering, algorithms designed to optimize some objective function
    - We can decide quantitatively which one is the best
- For hierarchical clustering, algorithms have been studied procedurally
    - Thus, comparisons between hierarchical clustering algorithms are only qualitative

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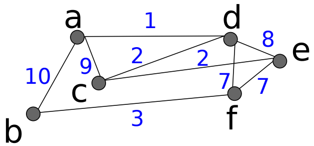
  "The lack of an objective function has prevented a theoretical understanding"
- Dasgupta introduced an objective function to model the hierarchical clustering problem

Dasgupta's Cost Function

Input: a weighted similarity graph G

- Edge weights represent similarities



Output: T a tree with leaves labelled by nodes of G

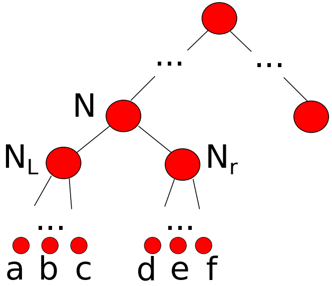
Cost of the output: Sum of the costs of the nodes of T

Cost of a node N of the tree:

$A = \{u \mid u$ is leaf of subtree rooted at $N_L\}$

$B = \{v \mid v$ is leaf of subtree rooted at $N_R\}$

$$\mathrm{cost}(N) = (|A| + |B|) \cdot \sum_{\substack{u \in A \\ v \in B}} \text{similarity}(u, v)$$



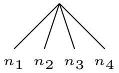
Cost of N = $(3+3) \cdot (1+2+2+3)$

Intuition: Better to cut a high similarity edge at a lower level

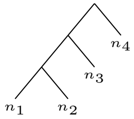
Dasgupta's Cost Function

Some Desirable Properties

- Using binary trees can always reduce cost



cost = $(n_1 + \cdots + n_4) \cdot$
$(w(A_1, A_2) + \cdots + w(A_3, A_4))$



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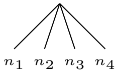

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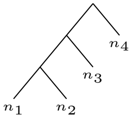

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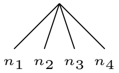

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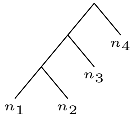

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- Disconnected components must be separated first
- For unit-weight cliques, all binary trees have the same cost
- For planted partition random graphs, the optimal tree first separates according to the partition

Cost Functions: An Axiomatic Approach

- Are there other suitable cost functions?
- What properties should cost functions satisfy?

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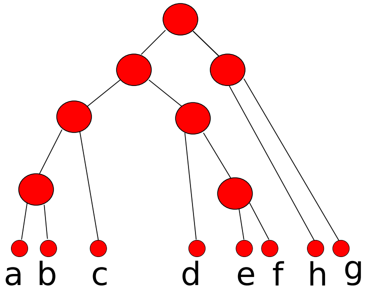
Admissible Cost Function

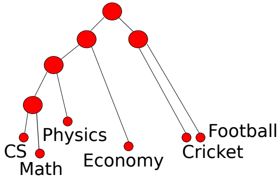
If the input has an underlying "ground-truth" hierarchical clustering tree,

then any tree should be optimal with respect to the cost function if and only if it is a "ground-truth" tree.

Inputs with an Underlying "Ground-Truth" Hierarchical Clustering

There exists a hierarchical clustering of the input,





such that:

- similarity(a, b) $>$ similarity(a, c) $>$ similarity(b, f),
- similarity(a, c) = similarity(b, c).

We want

> If the input graph has such an underlying structure then the above tree is the optimal one w.r.t. the cost function.

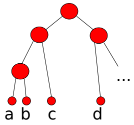
Inputs with an Underlying "Ground-Truth" Hierarchical Clustering

Ultrametrics to generate ground-truth inputs:

Assume that the data elements $x_1, \dots, x_n$ lie in some ultrametric:

$$d(x_i, x_j) \leq \max(d(x_i, x_\ell), d(x_j, x_\ell)) \quad \forall i, j, \ell$$

can be represented as a weighted tree:



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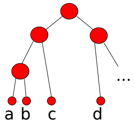

A weighted graph G is a ground-truth input if there exists an ultrametric and a non-increasing function f such that similarity $(u,v) = f(d(x_u, x_v)), \forall u, v$.

The tree represents the ground-truth hierarchical clustering.

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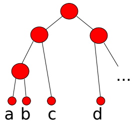

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Theorem: All the algorithms used in practice output the ground-truth hierarchical clustering on a ground-truth input.

Admissible Cost Functions

Ground-Truth Input

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Admissible Costs Functions

For any ground-truth input, a tree is optimal if and only if it is a ground-truth tree (i.e.: the ultrametric tree).

Theorem

A cost function of the form $\sum_{N \in T} \text{Cut}(N_L, N_R) \cdot g(N_L, N_R)$ is admissible if and only if

(i) g is symmetric, *i.e.*, $g(|A|, |B|) = g(|B|, |A|)$

(ii) g is increasing, *i.e.*, $g(|A| + 1, |B|) \geq g(|A|, |B|)$

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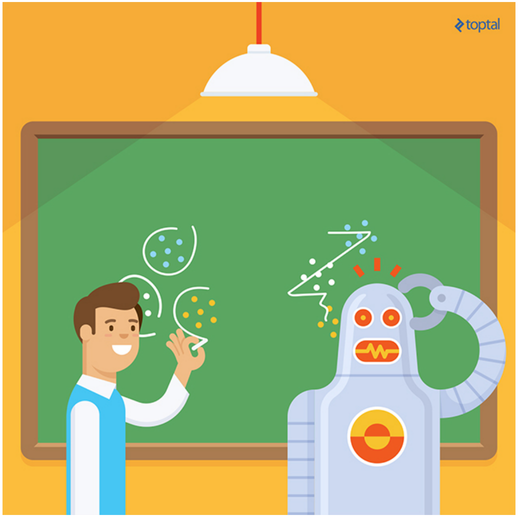
- Rest of Talk: Focus on Dasgupta's cost function

Algorithms



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Solution 1: Find approximation algorithms
Solution 2: Beyond worst-case analysis

Hope: Recursive Sparsest Cut

Algorithm: Recursive Sparsest Cut

Input: Weighted graph $G = (V, E, w)$

$\{A, V \setminus A\} \leftarrow$ cut with sparsity $\leq \phi \cdot \min_{S \subseteq V} \frac{w(S, V \setminus S)}{|S| \cdot |V \setminus S|}$

Recurse on subgraphs $G[A]$, $G[V \setminus A]$ to obtain trees T_A, $T_{V \setminus A}$

Output: Return tree whose root has subtrees T_A, $T_{V \setminus A}$

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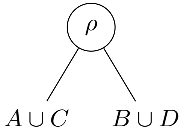
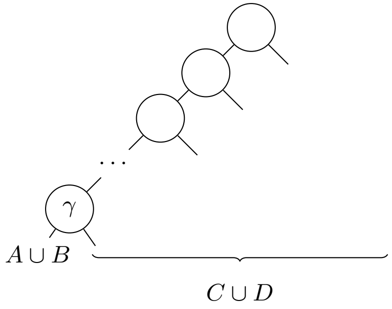
- For Dasgupta's cost function, $O(\log n \cdot \phi)$-approximation [Dasgupta '16]
- Current best known value for ϕ is $O(\sqrt{\log n})$ [ARV '09]
- We show $O(\phi)$-approximation (also independently [CC '17])

Proof Sketch

Tree T output by the algorithm



Optimal Tree T^*



$$\frac{w(A \cup C, B \cup D)}{|A \cup C| \cdot |B \cup D|} \leq \phi \frac{w(A \cup B, C \cup D)}{|A \cup B| \cdot |C \cup D|} = \Theta(\phi \cdot \frac{w(A \cup B, C \cup D)}{n^2})$$

$$\mathrm{cost}(\rho) = (|A| + |B| + |C| + |D|) \cdot w(A \cup C, B \cup D) = n \cdot w(A \cup C, B \cup D)$$

$\mathrm{cost}(\gamma$ and ancestors$) \geq (|A| + |B|) \cdot w(A \cup B, C \cup D) \geq n/3 \cdot w(A \cup B, C \cup D)$

Charge the cost of ρ to the edges of $(A \cup B, C \cup D)$

Proof Sketch

Lemma

The total charge (due to all nodes of T) for any edge (u, v) is at most $\frac{9}{2}\phi \min\{\frac{3}{2}|V(\mathsf{LCA}_{T^*}(u, v))|, n\}$

Proof by induction.

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The total charge (due to all nodes of T) for any edge (u, v) is at most $\frac{9}{2}\phi \min\{\frac{3}{2}|V(\mathsf{LCA}_{T^*}(u, v))|, n\}$

Proof by induction.

Lemma [Dasgupta '16]

For a tree T^*, $\text{cost}(T^*) = \sum_{(u,v)\in E} w((u, v)) \cdot |V(\mathsf{LCA}_{T^*}(u, v))|$

Combining the two lemmas shows that the recursive sparsest cut gives an $O(\phi)$-approximation

- For worst case inputs, Recursive Sparsest Cut gives $O(\phi)$-approximation
- Assuming the "Small Set Expansion Hypothesis", no polytime $O(1)$-approx.

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Real-world graphs are often not worst-case

Hierarchical Clustering: Random Graph Models

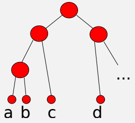
What is a reasonable model for real-world inputs?

Hierarchical Clustering: Random Graph Models

What is a reasonable model for real-world inputs?

In real world, inputs have some underlying, noisy ground-truth.

Generate graphs using ultrametrics:
Take an ultrametric,

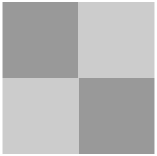


Generate an unweighted edge u, v with probability $f(\text{dist}(u, v))$ for some non-increasing function $f : \mathbb{R}_+ \mapsto [0, 1]$.

A generalization of the random graphs model for flat clustering

Flat Clustering

- Planted partition/block models
- Higher probability of edge between same part
- Lower probability of edge across different parts
- Adjacency matrix for graphs with 2 parts



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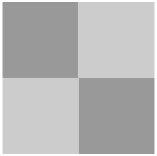
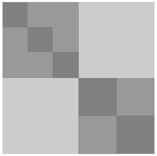


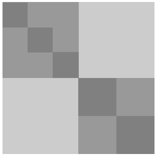
Hierarchical Clustering

- Planted hierarchy
- Higher probability of edge between nodes with deeper common ancestor
- Adjacency matrix for graphs with planted hierarchy



Hierarchical Clustering: Random Graph Models

- Random graphs with k-bottom level clusters (k can be function of n)
- Each bottom level cluster is sufficiently large
- Hidden (planted) hierarchical structure over the k bottom-level clusters



Can we identify a hierarchical cluster-tree that is an $O(1)$ or $(1+\epsilon)$-approximation w.r.t. Dasgupta's cost function for such randomly generated graphs?

Spectral Algorithm for Planted (Flat) Clusters

Probability Matrix

$$\begin{bmatrix} 0.6 & 0.6 & 0.6 & 0.3 & 0.3 & 0.3 \\ 0.6 & 0.6 & 0.6 & 0.3 & 0.3 & 0.3 \\ 0.6 & 0.6 & 0.6 & 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 & 0.6 & 0.6 & 0.6 \\ 0.3 & 0.3 & 0.3 & 0.6 & 0.6 & 0.6 \\ 0.3 & 0.3 & 0.3 & 0.6 & 0.6 & 0.6 \end{bmatrix}$$

Adjacency Matrix

$$\begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

- Probability matrix is low rank; adjacency matrix (realized graph) may be full rank
- Projecting adjacency matrix onto top k (e.g., 2) singular vectors reveals planted partition

Spectral Algorithm: Random Hierarchical Graphs

Algorithm: Linkage++

Input: Graph $G = (V, E)$

- Project adjacency matrix A of G to top k- singular vectors to obtain $\mathbf{x}_i \in \mathbb{R}^k$ for every $i \in V$

- Perform single linkage on $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ using Euclidean distances in $\mathbb{R}^k$ until k clusters are obtained

- Perform single linkage on the k-clusters using edge density in G between these clusters

Output: Resulting hierarchical tree

Spectral Algorithm: Random Hierarchical Graphs

Theorem. Linkage++ Performance

Provided the following conditions hold:

- The smallest bottom-level cluster has $\tilde{\Omega}(\sqrt{n})$-nodes
- Each probability is $\omega(\sqrt{\log n/n})$

Then the Linkage++ outputs a tree with cost at most $(1+\epsilon)$opt with respect to the Dasgupta cost function with probability at least $1-o(1)$.

Spectral Algorithm: Random Hierarchical Graphs

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- Proof involves results from McSherry (2001) combined with analysis of linkage algorithms
- Different algorithm using semi-definite programming extends to wider ranges of semi-random graph models

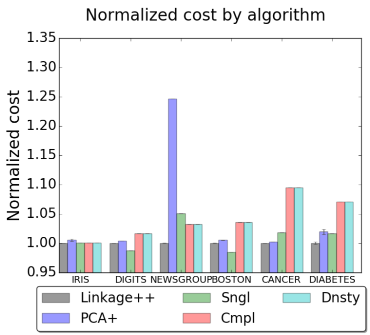
Back to practice

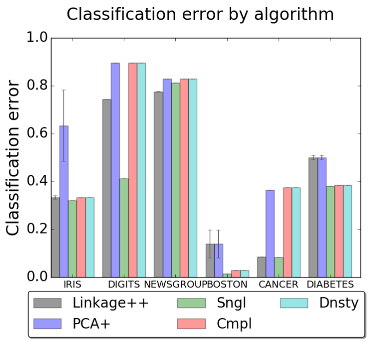
Evaluation of algorithms on synthetic (planted hierarchical random graphs) and a few UCI datasets

Report Dasgupta cost and classification error for various algorithms

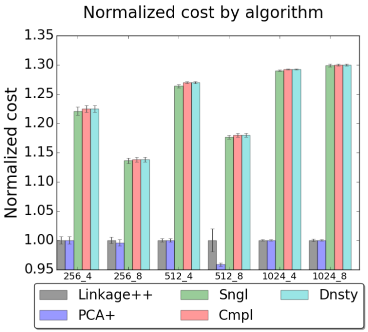
- Linkage++
- PCA+ (perform PCA and then average linkage)
- Sngl (Single linkage directly on graph)
- Cmpl (Complete linkage directly on graph)
- Dnsty (Average linkage directly on graph)

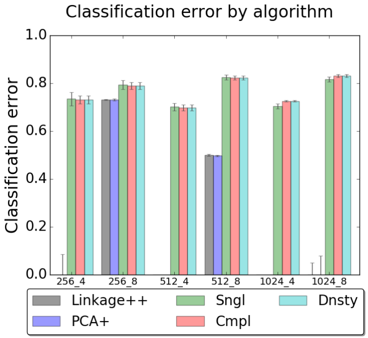
Experimental Results: UCI Datasets





Experimental Results: Synthetic Data





Conclusion

- Hierarchical clustering is a fundamental problem in data analysis that has mainly been studied through procedures rather than as an optimization problem
- Axiomatic study of admissible cost functions, provides a way to analyse quantitatively the performance of algorithms
- Efficient approximation algorithm for Dasgupta's cost function based on recursive sparsest-cut. Cannot get constant factor assuming SSEH.
- Beyond worst-case analyis:
  - Random graphs with planted hierarchies
  - Linkage++ (Spectral methods + linkage algorithms) gives $(1+\epsilon)$-approximation with high probability and efficient in practice

Open Questions

- Open Question: Improve the definition of real-world inputs for hierarchical clustering (maybe based on the stability conditions for flat clustering)
- Open Question: (semi-)streaming algorithms for real-world inputs