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

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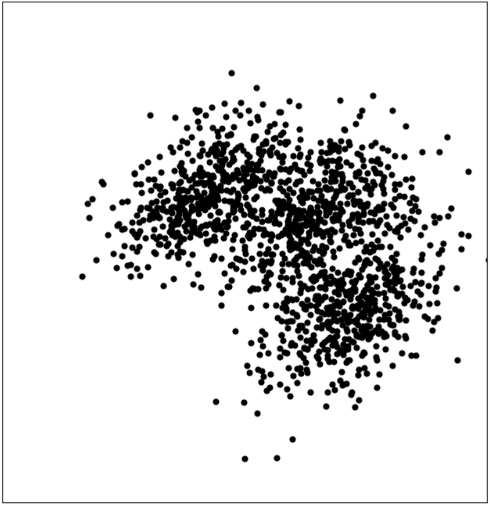
(Flat) Clustering



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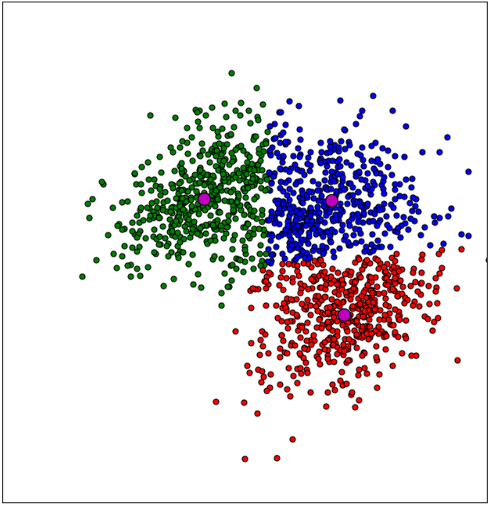
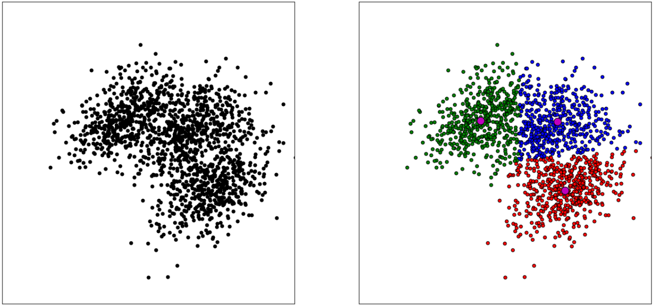


(Flat) Clustering: Objectives and Algorithms

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



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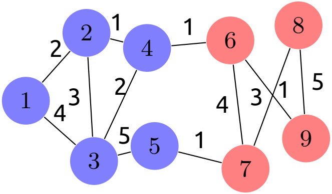
- Minimizing these objective functions is NP-hard
- Approximation algorithms are known

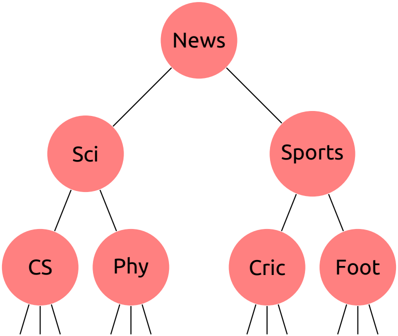
Clustering: Input as (Dis)-Similarity Graph



- 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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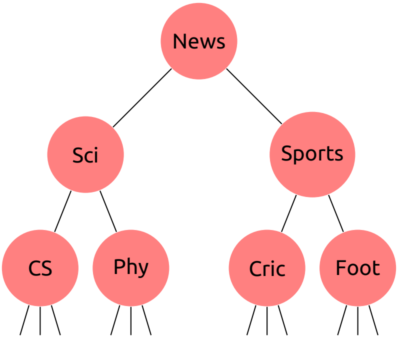

Will AI take over?

Someone finally figured out why neural nets work

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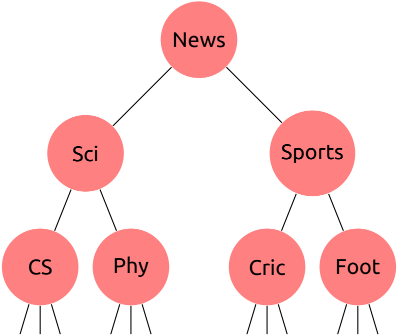

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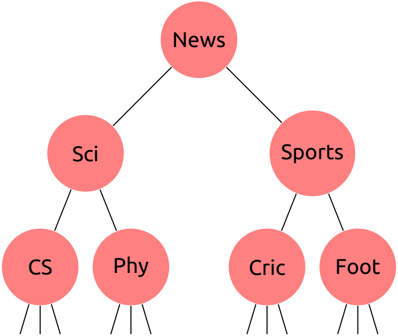

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Hierarchical Clustering in Practice: Linkage Algorithms

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

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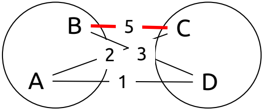
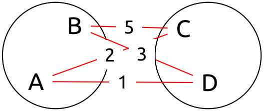
Single Linkage



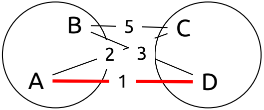
Similarity: 5

Average Linkage



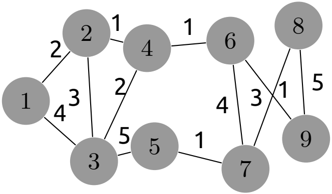
Similiarity: 2.75

Complete Linkage



Similiarity: 1

Hierarchical Clustering: Divisive Heuristics



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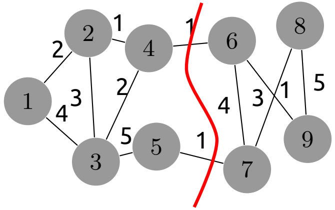

- Find a partition of the input similarity graph (or set of points)
  - Split using bisection k-means
  - Split using sparsest cut

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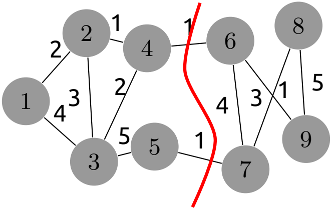
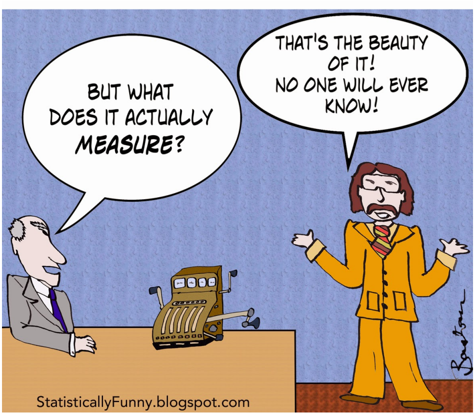


- Find a partition of the input similarity graph (or set of points)
  - Split using bisection k-means
  - Split using sparsest cut
- Recurse on each part
- Builds cluster-tree top-down

What are these algorithms actually doing?



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
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  "The lack of an objective function has prevented a theoretical understanding"

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  - Thus, comparisons between hierarchical clustering algorithms are only qualitative
- [Dasgupta '16]

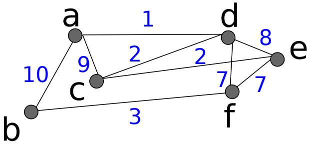
  "The lack of an objective function has prevented a theoretical understanding"

- 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

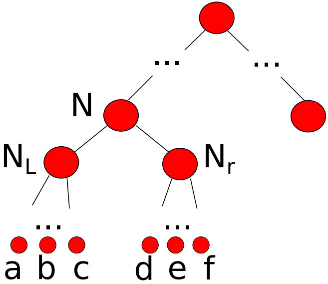
Cost of the output: Sum of the costs of the nodes of T

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 $N_R\}$

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



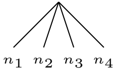
Cost of N = $(3 + 3) \cdot (1 + 2 + 2 + 3)$

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

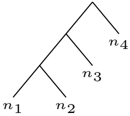
Dasgupta’s Cost Function

Some Desirable Properties

- Using binary trees can always reduce cost



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



cost = $(n_1 + n_2) w(A_1, A_2) + \cdots + + (n_1 + n_2 + n_3 + n_4) w(A_1 \cup A_2 \cup A_3, A4)$

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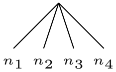

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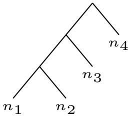

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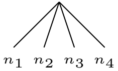

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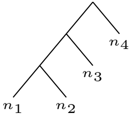

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- For unit-weight cliques, all binary trees have the same cost

- 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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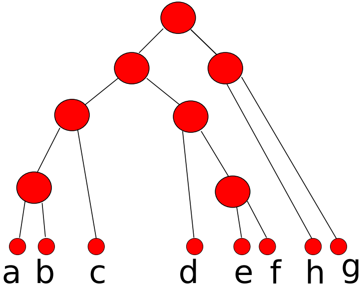
Admissible Cost Function

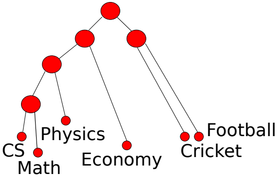
If the input has an underlying "ground-truth" hierarchical clustering tree,

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.

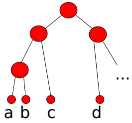
Inputs with an Underlying "Ground-Truth" Hierarchical Clustering

Ultrametrics to generate ground-truth inputs:

Assume that the data elements $x_1, \ldots, x_n$ 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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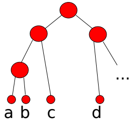

> A weighted graph G is a ground-truth input if there exists an ultrametric and a non-increasing function f such that similarity $(u, v) = f(d(x_u, x_v)), \forall u, v$.

The tree represents the ground-truth hierarchical clustering.

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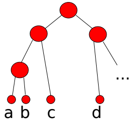

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Theorem: All the algorithms used in practice output the ground-truth hierarchical clustering on a ground-truth input.

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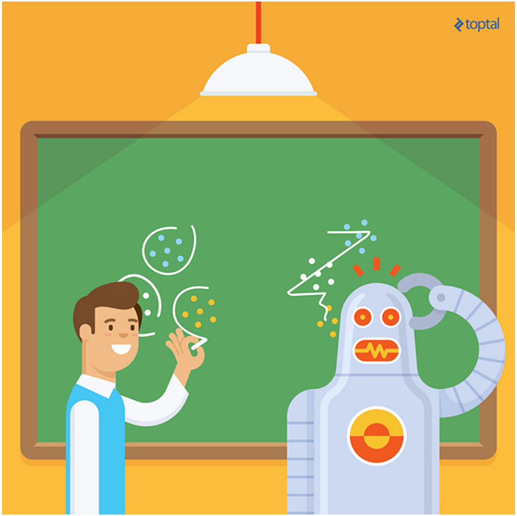
- Rest of Talk: Focus on Dasgupta's cost function

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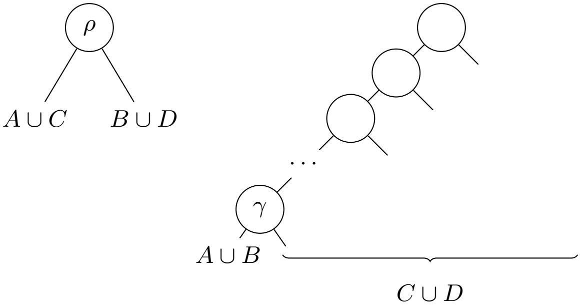
- For Dasgupta's cost function, $O(\log n \cdot \phi)$-approximation [Dasgupta '16]
- Current best known value for ϕ is $O(\sqrt{\log n})$ [ARV '09]
- We show $O(\phi)$-approximation (also independently [CC '17])

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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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?

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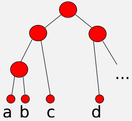
What is a reasonable model for real-world inputs?

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

Generate graphs using ultrametrics:
Take an ultrametric,

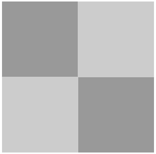


Generate an unweighted edge u, v with probability $f(\text{dist}(u, v))$ for some non-increasing function $f : \mathbb{R}_+ \mapsto [0, 1]$.

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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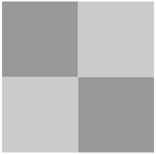
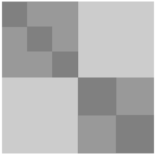


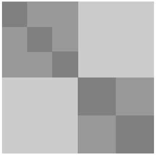
Hierarchical Clustering

- 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

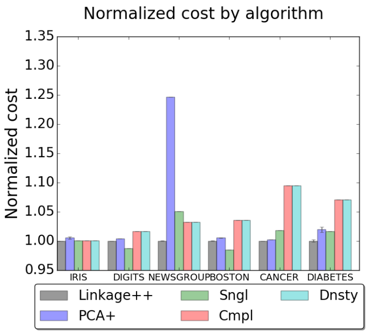
Back to practice

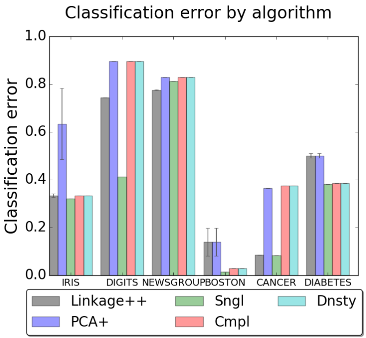
Evaluation of algorithms on synthetic (planted hierarchical random graphs) and a few UCI datasets

Report Dasgupta cost and classification error for various algorithms

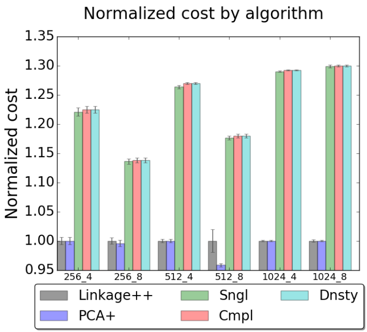
- Linkage++
- PCA+ (perform PCA and then average linkage)
- Sngl (Single linkage directly on graph)
- Cmpl (Complete linkage directly on graph)
- Dnsty (Average linkage directly on graph)

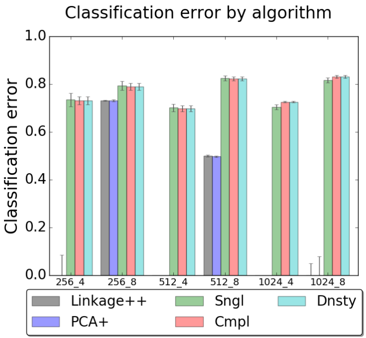
Experimental Results: UCI Datasets





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