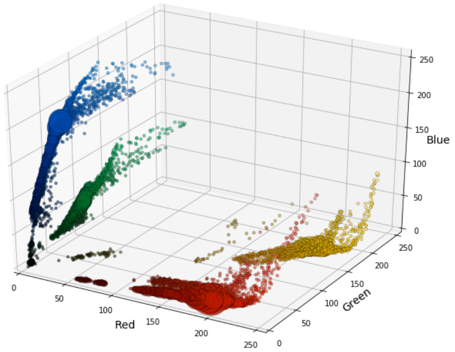
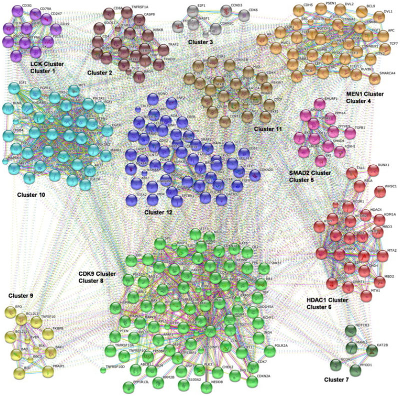
Clustering - Intro

Frederik Mallmann-Trenn
6CCS3AIN



- Goal: Points in the same cluster are ‘close’ and points of different clusters are ’far’

Application: Biological Networks



- Protein-Protein Interaction Networks (PPINs). See e.g., Rual et al Nature ’05 (+2500 citations)

Application: Recommendation Systems

- Similar users will buy similar items
- High dimensional data, how to find similar users? Clustering!

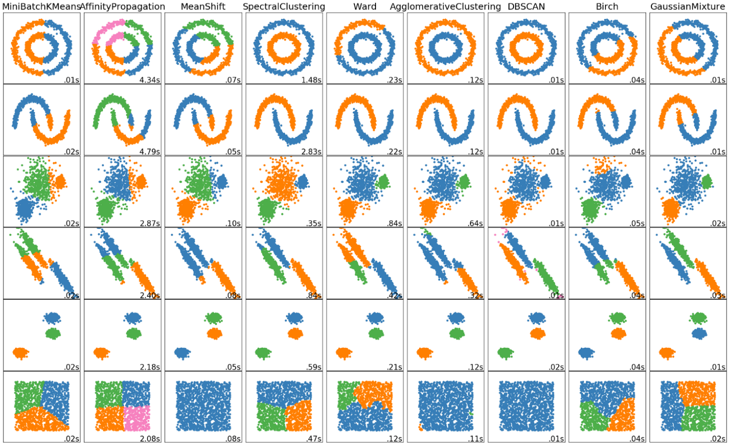
Other Applications

- Unsupervised learning (e.g., PCA)
- encoder-decoder neural network
- outlier detection applications such as detection of credit card fraud
- ....

Clustering Algorithm (incomplete)

- k-Means
- k-Median
- Agglomerative Clustering
  - Single-Linkage
  - Average-Linkage
  - Complete-Linkage
- Divisive Clustering
  - Sparsest-Cut

Clustering Algorithm Comparison



Source: https://towardsdatascience.com/

k-Means and k-Median

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k-Means

- Say we have n points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$.
- We want to partition them into k sets $S_1, S_2, \ldots, S_k$ such that the cost of the partition, $c(S_1, S_2, \ldots, S_k)$, is minimised:

$$c(S_1, S_2, \ldots, S_k) = \sum_{i=1}^{n} \left(\min_{j \in [k]} d(\mathbf{x}_i, \boldsymbol{\mu}_j) \right)^2,$$

where $\boldsymbol{\mu}_i$ is the mid-point of each cluster, i.e.,

$$\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{j \in S_i} \mathbf{x}_j$$

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- Note that $\mathbf{x}_i$ and $\boldsymbol{\mu}_i$ are vectors for $i \in [n]$.

k-Means

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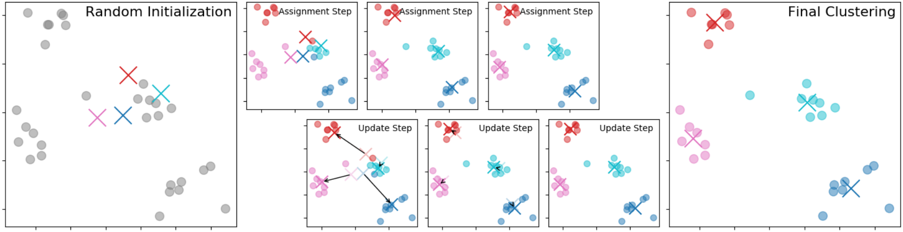
$$\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{j \in S_i} \mathbf{x}_j$$

- Note that $\mathbf{x}_i$ and $\boldsymbol{\mu}_i$ are vectors for $i \in [n]$.
- E.g., if $S_1 = \{\mathbf{x}_1, \mathbf{x}_2\}$ with $\mathbf{x}_1 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ and $\mathbf{x}_2 = \begin{pmatrix} 3 \\ 4 \end{pmatrix}$, then $\boldsymbol{\mu}_1 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$

k-Means

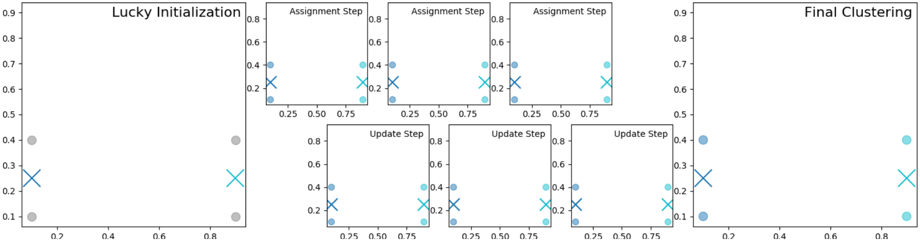
1. Select k cluster centres arbitrarily.
2. Repeat until convergence:
   2.1 Assignment Step:
      2.1.1 Assign each point to the cluster with the nearest mean
      2.1.2 $S_i = \{\mathbf{x}_j \mid d(\mathbf{x}_j, \boldsymbol{\mu}_i) \leqslant d(\mathbf{x}_i, \boldsymbol{\mu}_\ell)$ for all $\ell \in [k]\}$, where each point is assigned to exactly one cluster S_i.
   2.2 Update Step:
      2.2.1 Recalculate the mean point of the cluster
      2.2.2 $\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{j \in S_i} \mathbf{x}_j$

k-Means



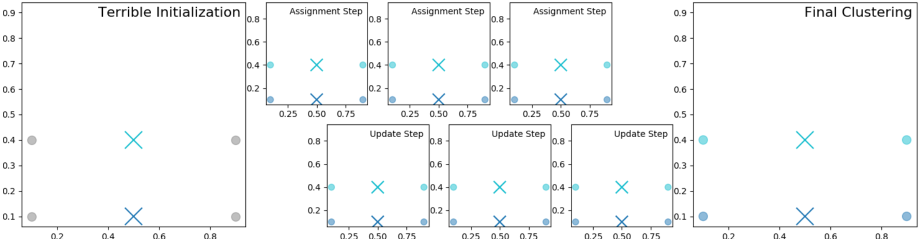
Random Initialization
Assignment Step
Assignment Step
Assignment Step
Update Step
Update Step
Update Step
Final Clustering

k-Means: Example with Optimal Instance



- Consider this example with four points.
- The optimal cluster is shown.

k-Means



- We can see that if we start with sub-optimal clusters, and we never change them!
- This can be made arbitrarily bad (by increasing the width of the rectangle).

k-Means++

- The way this can be solved is by using k-Means++
- It can be shown that the approximation factor is at most $O(\log k)$.

k-Means++

1. Set the first centre to be one of the input points chosen uniformly at random, i.e., $\boldsymbol{\mu}_1 = uniform(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$
2. For cluster $i = 2$ to k:
   2.1 For each point $\mathbf{x}_j$ compute the distance to the nearest centre, i.e., calculate $d_j = \min_\ell d(\mathbf{x}_j, \boldsymbol{\mu}_\ell)$
   2.2 Open a new centre at a point using the weighted probability distribution that is proportional to d_j^2. That is,

$$\Pr(\text{new centre in } \mathbf{x}_j) = \frac{d_j^2}{\sum_\ell d_\ell^2}$$

3. Continue with k-Means

k-Median

- Say we have n points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$.
- We want to partition them into k sets $S_1, S_2, \ldots, S_k$ such that the cost of the partition, $c(S_1, S_2, \ldots, S_k)$, is minimised:

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where $\boldsymbol{\mu}_i$ is the mid-point of each cluster, i.e.,

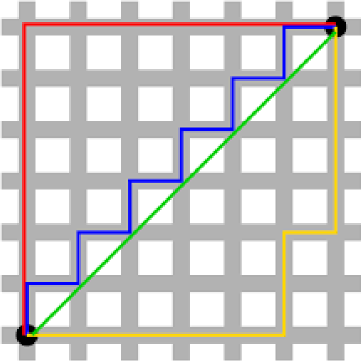
$$\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{j \in S_i} \mathbf{x}_j$$

- Recall that k-Means uses

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

-

k-Median

- K-Means minimises the Euclidean/geometric distance
- K-Medians minimises the Manhattan distance
- 
- Source: Wikipedia

Hierarchical Clustering

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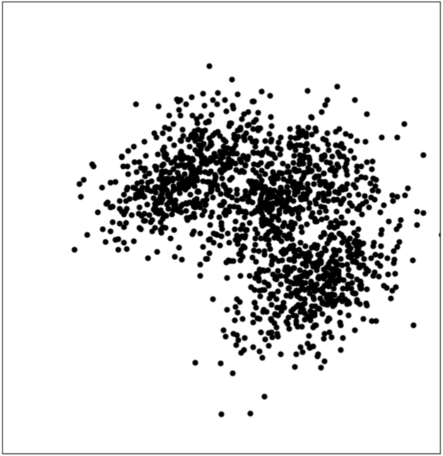
How should we choose k?



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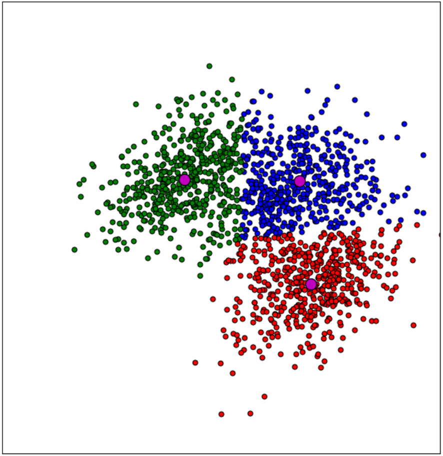
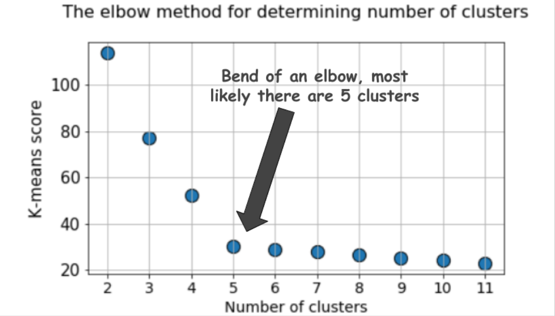


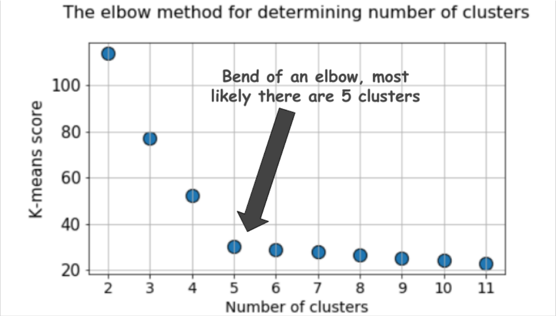
Elbow method



Source: https://towardsdatascience.com/

- The more clusters the better the lower the cost/score
- Of course we could have one cluster per datapoint, but that does not really help
- One way of strike a good tradeoff is to use the elbow method

Elbow method



Source: https://towardsdatascience.com/

- The more clusters the better the lower the cost/score
- Of course we could have one cluster per datapoint, but that does not really help
- One way of strike a good tradeoff is to use the elbow method
- A natural definition: Pick the $k \in \{2, 3, \ldots, n-1\}$ that maximises $cost_{k-1}/cost_k$, where $cost_j$ is the cost of the clustering with j clusters
- $k = 1$ and $k = n$ are ruled out as they result in trivial clusters

Flat Clustering

- So far we tried to assign the points to k clusters.
- We haven't assumed any structure among the clusters

Clustering

The problem with flat clustering is that it's flat

Example: Cluster the following news headlines in 3 categories

Clustering

The problem with flat clustering is that it's flat

Example: Cluster the following news headlines in 3 categories

- Deepmind's AlphaBingo wins world championship
- Black holes swallow stars whole according to new study
- Someone didn't dope
- Researcher finally figured out the rules of cricket

Clustering

The problem with flat clustering is that it's flat

Example: Cluster the following news headlines in 3 categories

CS	• Deepmind's AlphaBingo wins world championship
Physics	• Black holes swallow stars whole according to new study
Sports	• Someone didn't dope
Sports	• Researcher finally figured out the rules of cricket

Clustering

The problem with flat clustering is that it's flat

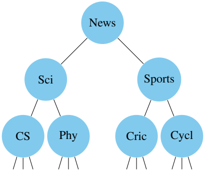
Example: Cluster the following news headlines in 3 categories

Science	• Deepmind's AlphaBingo wins world championship
Science	• Black holes swallow stars whole according to new study
Cycling	• Someone didn't dope
Cricket	• Researcher finally figured out the rules of cricket

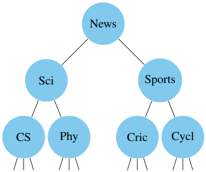
Structure is lost ...

Hierarchical Clustering

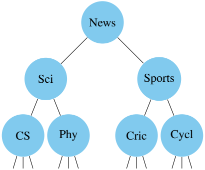
- Recursive partitioning of data at increasingly finer granularity represented as a tree
- The leaves of the hierarchical cluster tree represent data.



Hierarchical Clustering



Hierarchical Clustering



- Google's AlphaBingo wins world champinship
- Someone finally figured out why neural nets work
- Black holes swallow stars whole according to new study
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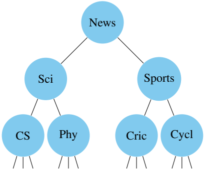
Hierarchical Clustering



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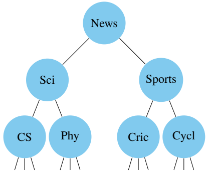

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Physics	•Black holes swallow stars whole according to new study
Cycling	•Someone didn't dope
Cricket	•Researcher finally figured out the rules of cricket

Hierarchical Clustering Algorithms

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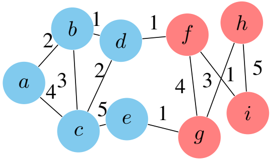
How are hierarchical clusters obtained in practice?

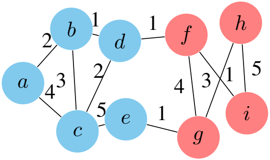
- Agglomerative clustering (bottom up)
  - Initially place each data point in its own clusters
  - Repeatedly merge most similar clusters
- Divisive clustering (top down)
  - Split using bisection k-means (or sparsest cut)
  - Recurse on each part

Agglomerative Clustering



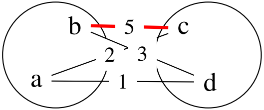
- An edge can mean similarity or dissimilarity
- In this lecture we'll only consider similarities.
- A high similarity value means that the corresponding two nodes are very similar and should be in the same cluster

Agglomerative Clustering



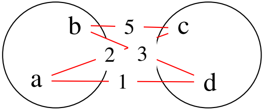
- Each node starts in a separate cluster
- The similarity between two clusters $C_1 = \{a, b\}$, $C_2 = \{c, d\}$ is

Single Linkage



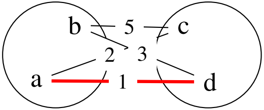
Similarity: 5

Average Linkage



Similiarity: 2.75

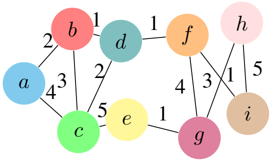
Complete Linkage



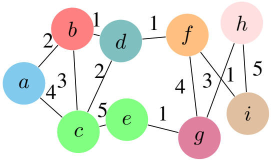
Similiarity: 1

Single-Linkage

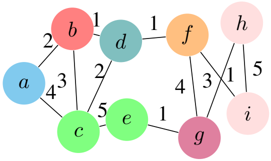
Round 0:



Round 1:

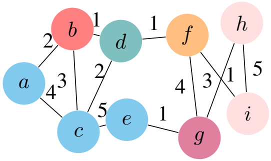


Round 2:

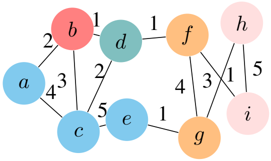


Single-Linkage

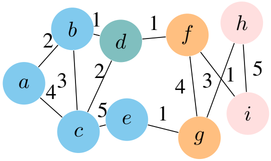
Round 3:



Round 4:

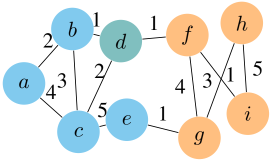


Round 5:

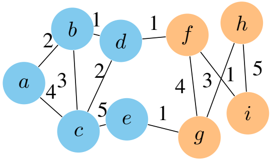


Single-Linkage

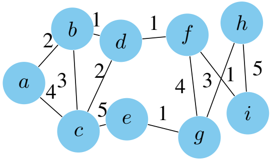
Round 6:



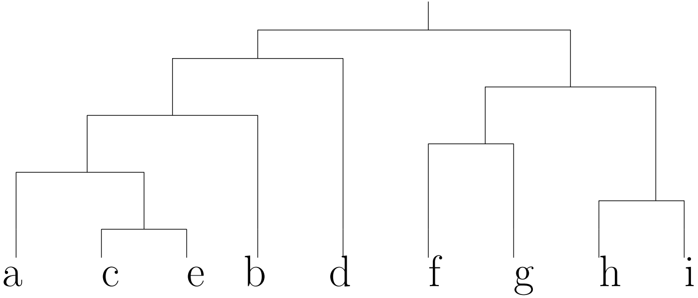
Round 7:



Round 8:

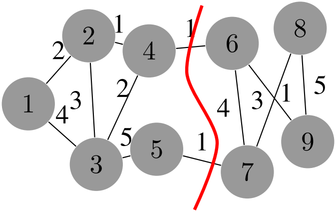


Hierarchical Clustering: Dendogram



- The obtained merges can be represented in a dendogram

Hierarchical Clustering: Divisive Heuristics



- 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

Sparsest cut

- Given a graph with nodes V and edges in $E \subset V \times V$
- The sparsity of a cut $\phi(S)$, is given by

$$\phi(S) = \frac{E(S, \bar{S})}{\min(|S|, |\bar{S}|)},$$

  where $E(S, \bar{S})$ is the sum of weights of edges crossing the cut. Here $\bar{S} = V \backslash S$.
- The sparsest cut of a graph is given by the S^* that minimises $\phi(S^*)$, i.e.,

$$\phi(S^*) = \min_S \phi(S)$$

Hierarchical Clustering Objective

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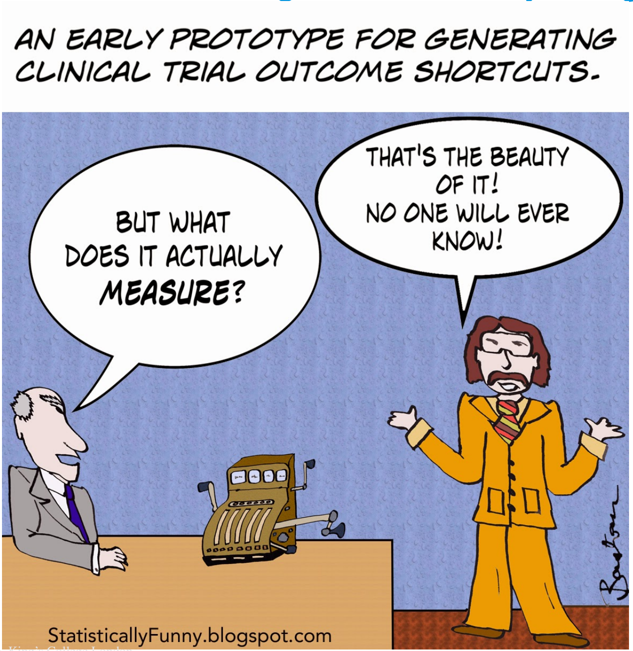
What are the hierarchical algorithms actually doing?



What quantity are these algorithms optimizing?

- For flat clustering, algorithms designed to optimize some objective function
  - Remember:
    for **flat clustering** the goal was to 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 $\sum_{i=1}^{N} \left(\min_{j \in [k]} d(\mathbf{x}_i, \mu_j) \right)^2$
- For hierarchical clustering, algorithms have been studied procedurally
  - Thus, comparisons between hierarchical clustering algorithms are only qualitative!

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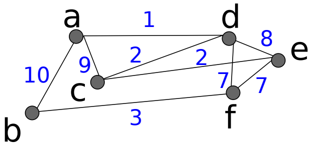
- For hierarchical clustering, algorithms have been studied procedurally
  - Thus, comparisons between hierarchical clustering algorithms are only qualitative!
- [Dasgupta '16]
  "The lack of an objective function has prevented a theoretical understanding"
- Dasgupta introduced an objective function to model the hierarchical clustering problem

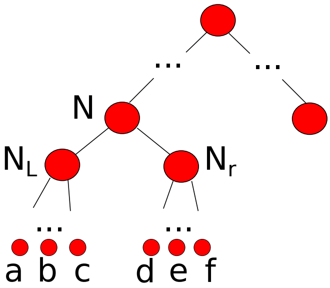
Dasgupta's Cost Function

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:

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

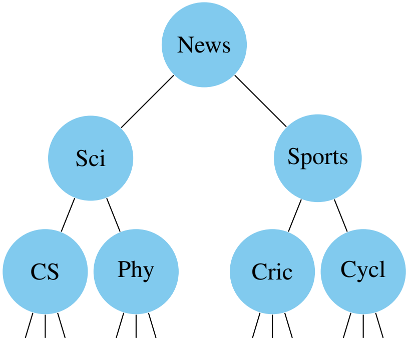
$R = \{v \mid v$ is leaf of subtree rooted at $N_R\}$

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

The total cost is the sum of costs of all subtrees.

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

Results

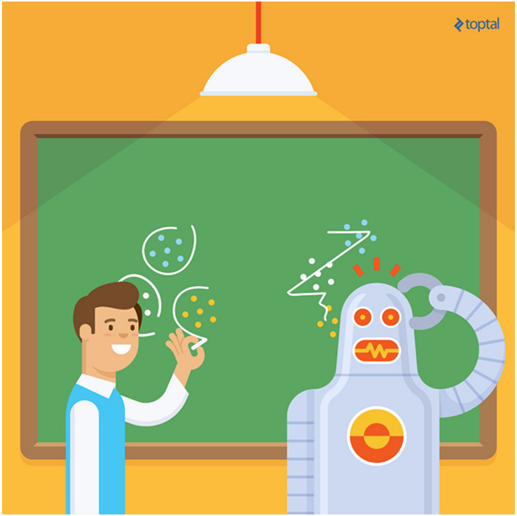


Hierarchical Clustering: Objective Functions and Algorithms
Vincent Cohen-Addad, Varun Kanade, Frederik Mallmann-Trenn, Claire Mathieu
JACM 2019

Result 1: Is Dasgupta the only reasonable function?

- We characterize the set of ‘good’ objective functions based on axioms.
  - Disconnected components must be separated first
  - Symmetry
  - Only the ‘true’ hierarchical clustering should minimize the cost function (if there is one).
- In some sense Dasgupta is the most natural

Result 2: Algorithms



Hope: Recursive Sparsest Cut

- Dissimilarity graph:
  - We show Avg. Linkage has a $3/2$-approximation factor
  - We also show that other practical algorithms have a $\Omega(n^{1/4})$-approximation factor

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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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  - We show $O(\phi)$-approximation
  - Improves the $O(\log n \cdot \phi)$-approximation [Dasgupta '16]
  - Current best known value for ϕ is $O(\sqrt{\log n})$ [ARV '09]

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

Real-world graphs are often not worst-case