HIERARCHICAL CLUSTERING

An iterative improvement procedure for hierarchical clustering

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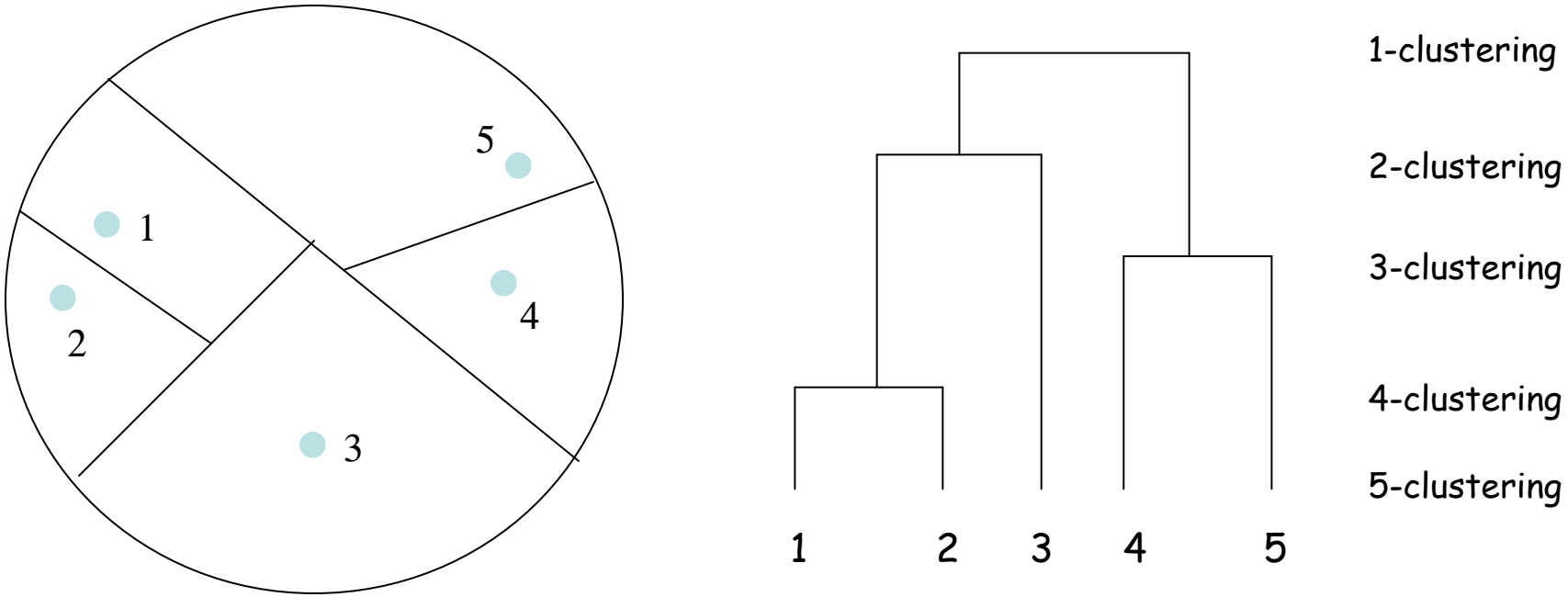
Why Hierarchical Clustering and Not Usual Clustering(K-means)?

- Obtain a hierarchy instead of an amorphous collection of groups
- No need to specify number of clusters
- Can view data at many levels of granularity, all at the same time
- Simple heuristics for constructing hierarchical clusterings

Hierarchical clustering

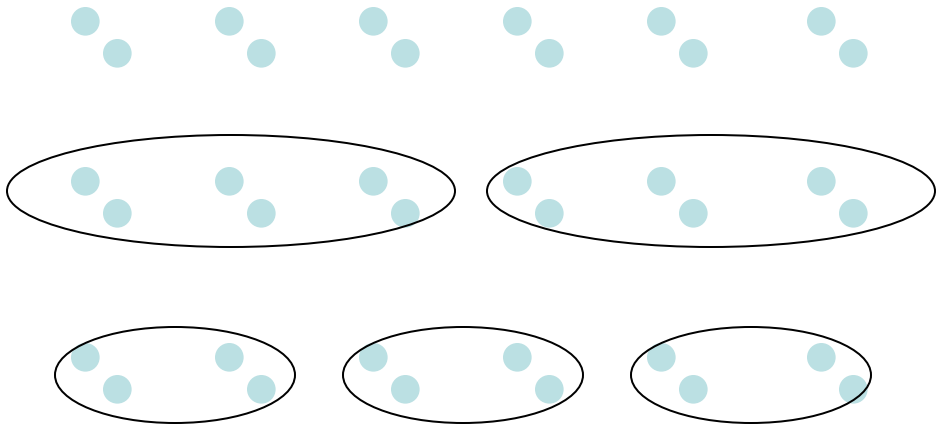
Recursive partitioning of a data set



Problem

The whole enterprise of hierarchical clustering could use some more justification.

e.g.



Conventional Hierarchical Techniques

- Agglomerative
- Divisive

Standard agglomerative heuristics

1. Initially each point is its own cluster.
2. Repeatedly merge the two "closest" clusters.

Need to define distance between clusters…

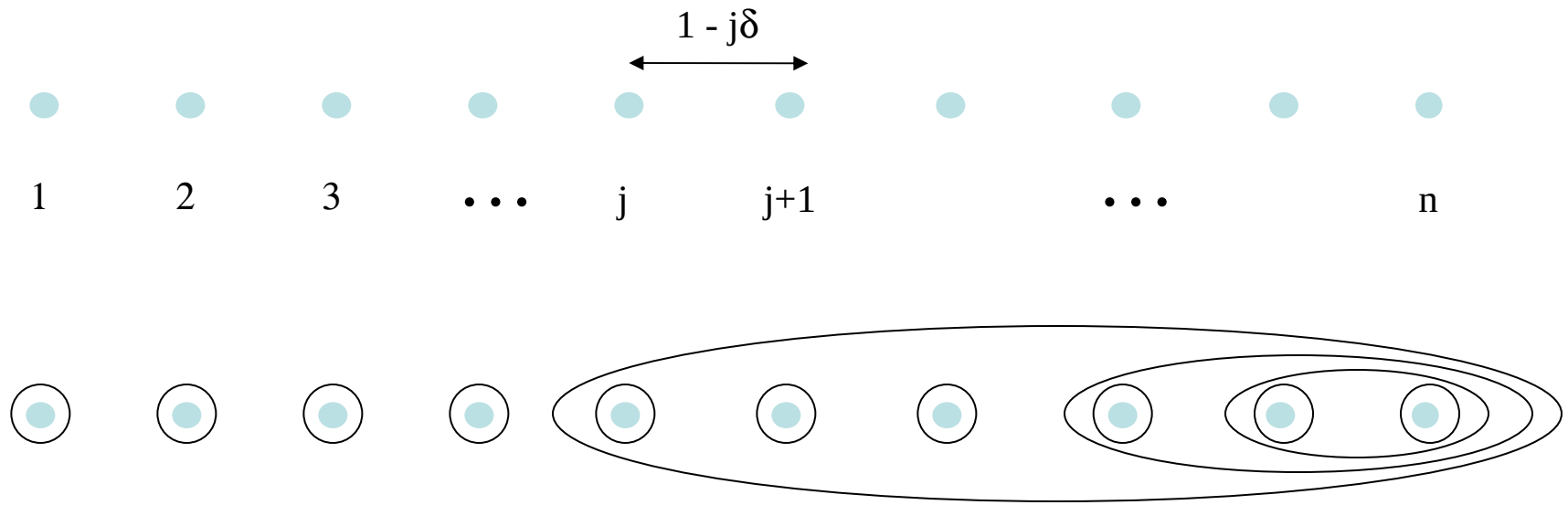
Single-linkage: distance between closest pair of points

Average-linkage: distance between centroids

Complete-linkage: distance between farthest pair

Single-linkage clustering

Chaining effect.



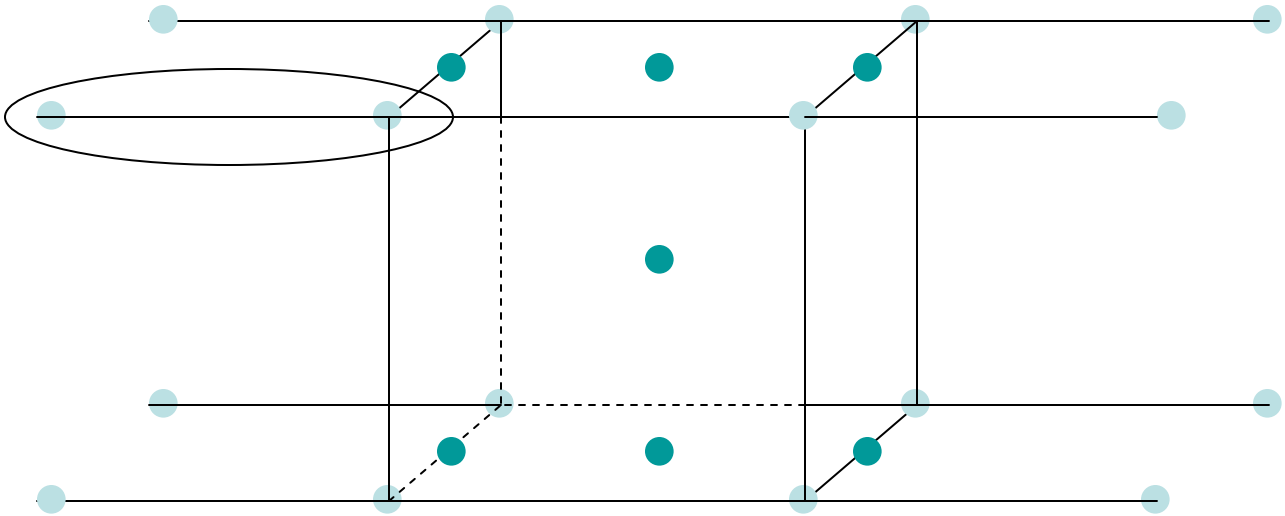
The *k*-clustering will have diameter about *n-k*, instead of *n/k*.

Complete-linkage clustering

Can similarly construct a bad case…

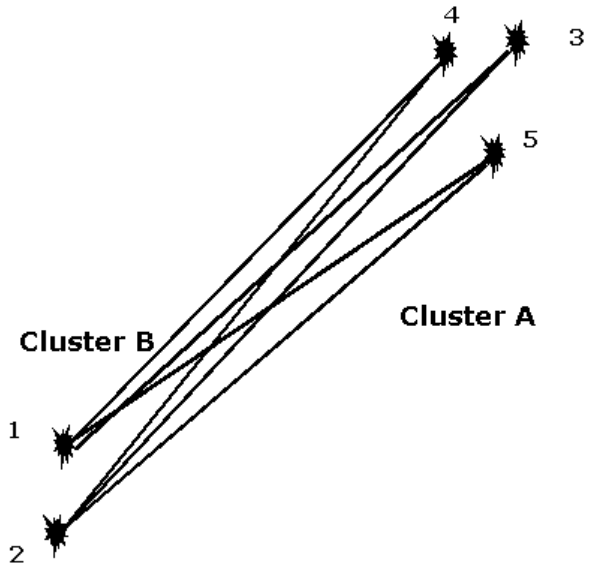
Average-linkage clustering

Points in d-dimensional space, $d = \log_2 k$, under an l_1 metric.



Final radius should be 1, instead is d.
Therefore: off by a factor of $\log_2 k$.

Average Linkage



The average linkage method avoids the extremes of either large clusters or tight compact clusters.

Average Linkage Cost Functions

- Sokal-Michener $\| \mu(S) - \mu(T) \|^2$
- $\frac{1}{|S| \cdot |T|} \sum_{x \in S, y \in T} \| x - y \|^2$
- Ward's Method: $\frac{|S| \cdot |T|}{|S| + |T|} \| \mu(S) - \mu(T) \|^2$

Divisive Methods

- Normalized Cut

  A binary partition is performed recursively increasing the similarity within cluster and dissimilarity between clusters

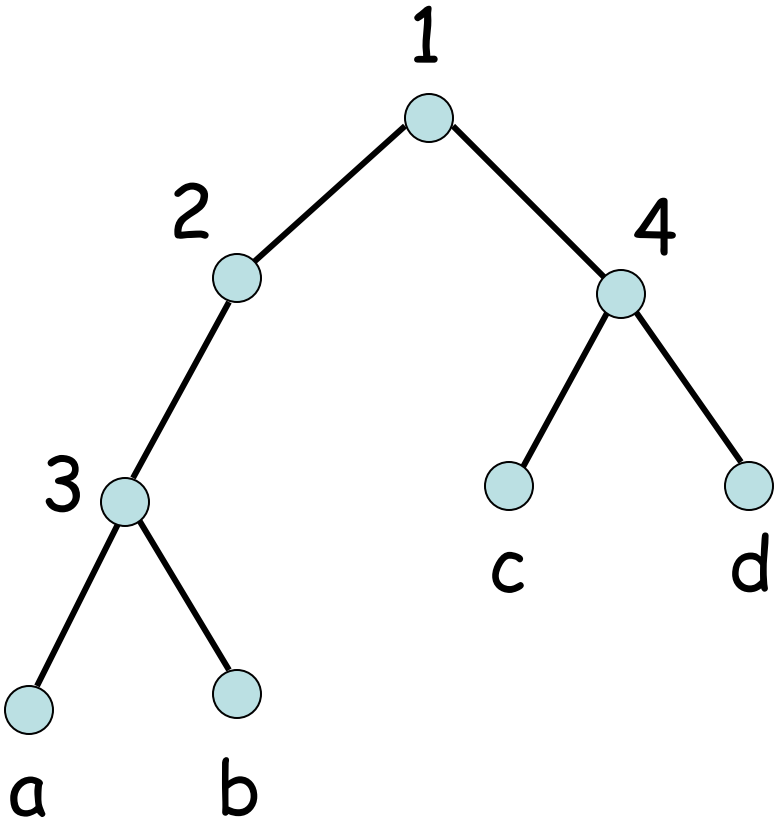
Evaluation of all agglomerative methods

- Can’t trace back
- Complexity at least $O(n^2)$

Goal:

- Local improvement algorithm for hierarchical clustering
- Hierarchical analog of k-means
- Key challenge: efficiency

Representation



Ordered binary tree

Large search space: given *n* data points,

$$\frac{n((n-1)!)^2}{2^{n-1}}$$

hierarchical clusterings

Cost of hierarchical clustering

- Let C_k be the set of k clusters $\{S_1, S_2, \ldots, S_k\}$ defined by a flat clustering. The k-means cost is:

$$\text{cost}(C_k) = \sum_{j=1}^{k} \sum_{x \in S_j} \left\| x - \mu(S_j) \right\|^2$$

- We define the cost of a hierarchical clustering as the weighted sum of the n clusterings defined by the hierarchy

$$\text{hcost} = \sum_{i=1}^{n} w_k \, \text{cost}(C_k)$$

Features of the cost function

- Based on *k*-means cost function
- Inherently emphasizes smaller *k*
- Weights can be set to emphasize particular *k*
- Using properties of Euclidean distance: $O(n)$ time to calculate

General Algorithm Idea

Use state space search methods to optimize criterion function

Two local moves:

- Keep the ordering fixed and restructure tree optimally

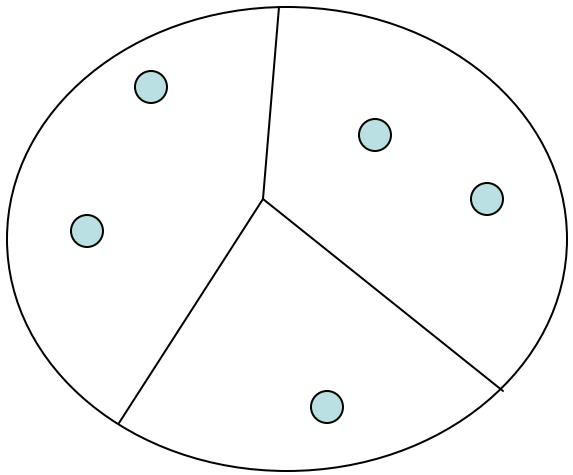
NP-Hard?

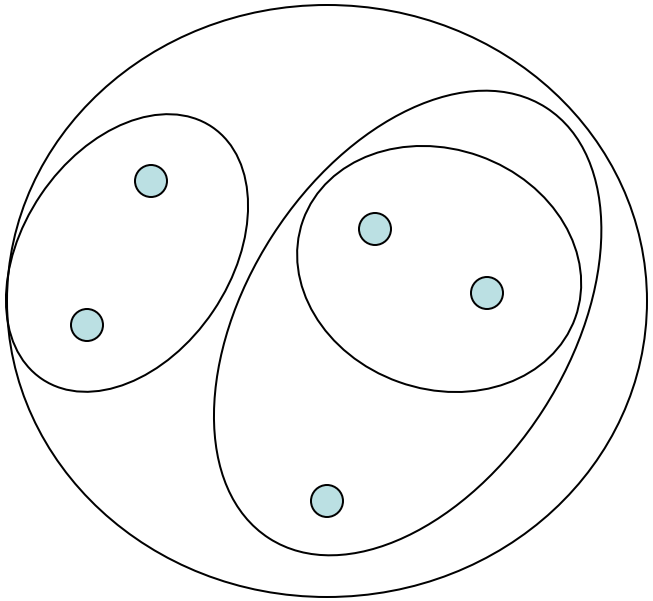
- Keep structure fixed and reorder split order of internal nodes optimally

scheduling algorithm

Analogy with *k*-means

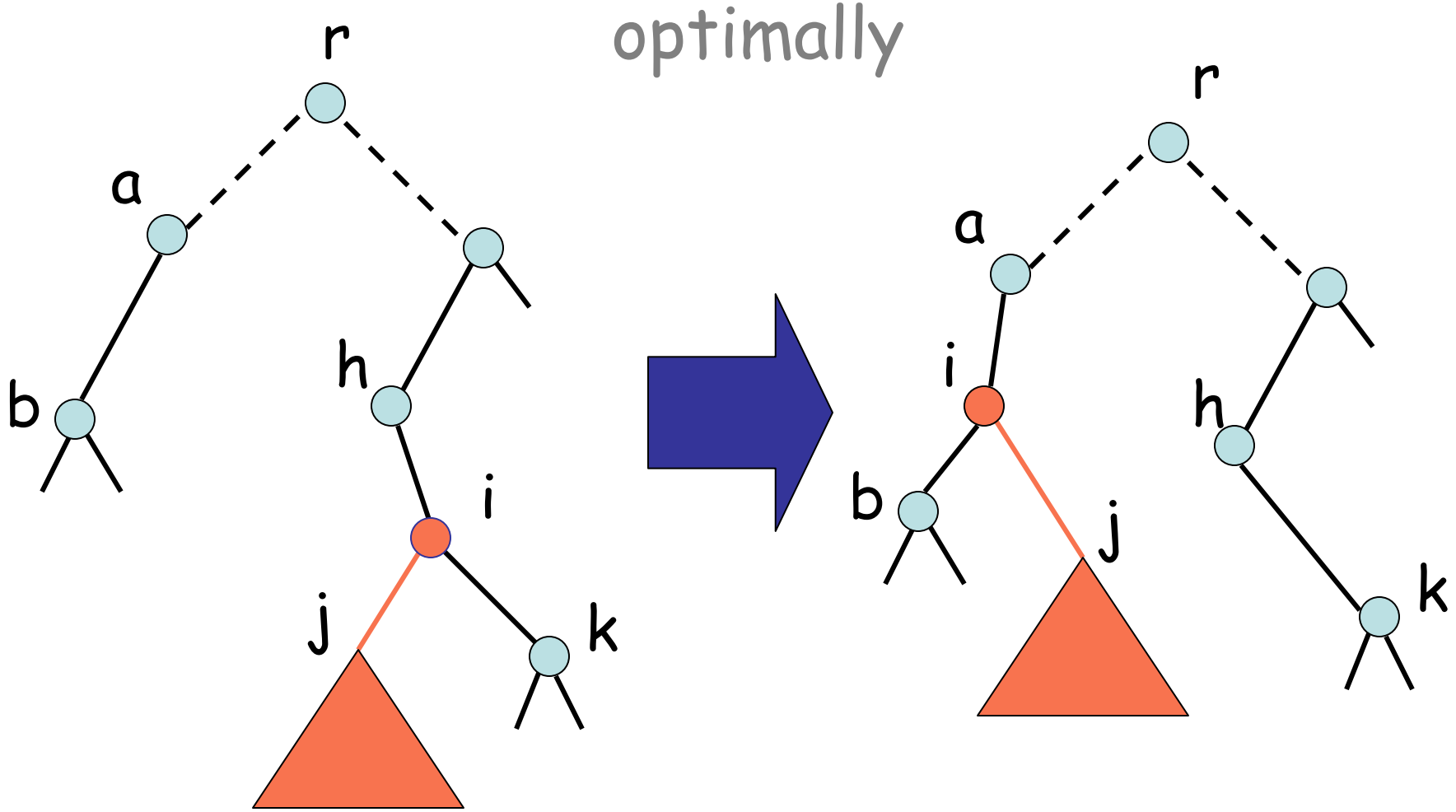
- Keep the means fixed and optimize the partitioning
- Keep the partition fixed and recompute means





The Graft:

Keep the ordering fixed and restructure tree optimally



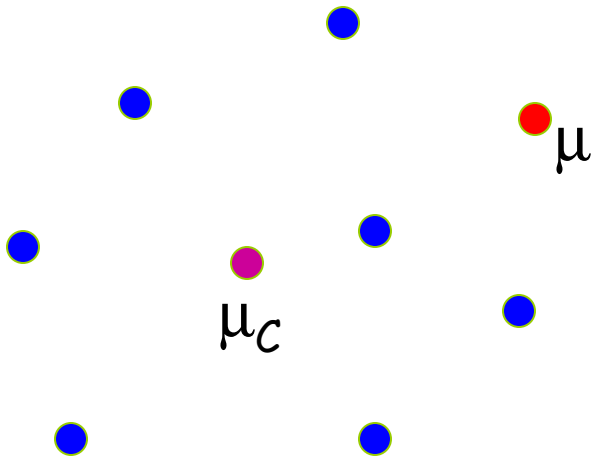
Making the graft efficient

Key idea: Rewrite the hierarchical clustering cost *locally*, as a sum of contributions from individual tree edges.

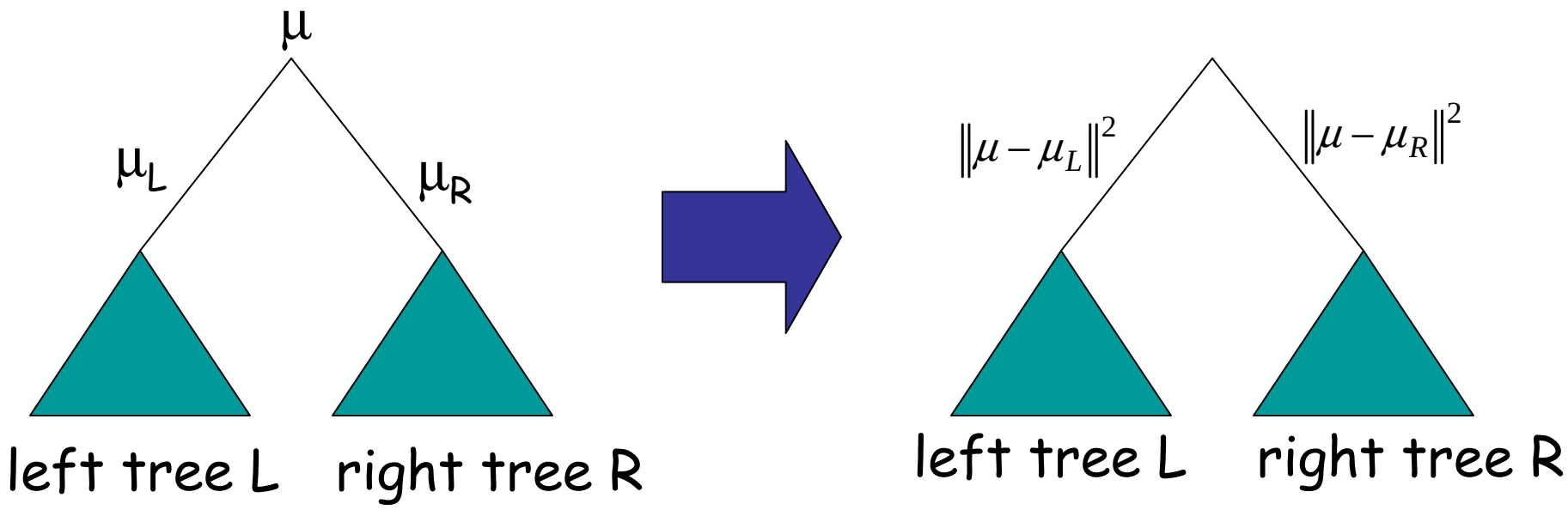
This can be done by exploiting special properties of squared Euclidean distance.

Lemma: Suppose cluster C has mean μ_C; then for any other point μ,

$$\sum_{x \in C} \|x - \mu\|^2 = \sum_{x \in C} \|x - \mu_C\|^2 + |C| \cdot \|\mu - \mu_C\|^2$$



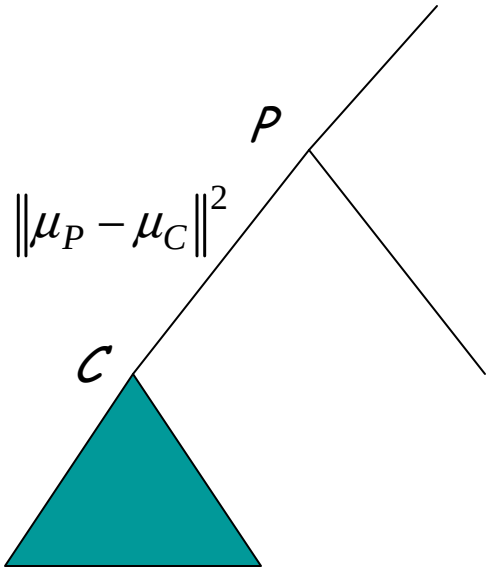
Calculating *k*-means cost by counting tree edges



$$\text{cost}(L \cup R) = |L| * \|\mu - \mu_L\|^2 + \sum_{x \in L} \|x - \mu_L\|^2 + |R| * \|\mu - \mu_R\|^2 + \sum_{x \in R} \|x - \mu_R\|^2$$

$$= |L| * \|\mu - \mu_L\|^2 + \text{cost}(L) + |R| * \|\mu - \mu_R\|^2 + \text{cost}(R)$$

Counting edges for criterion function:



Recall: $\text{hcost} = \sum_{i=1}^{n} w_k \, \text{cost}(C_k)$

This is in fact just a linear combination of lengths of tree edges. The coefficient for the edge between *P* and *C* is:

$$\left|T_C\right| * \sum_{i=1}^{\sigma(p)-1} w_i$$

O(n) computation time

Optimal location for a sub-tree

Pick any subtree. What's the best place to move it (using a "graft"), while respecting split numbers?

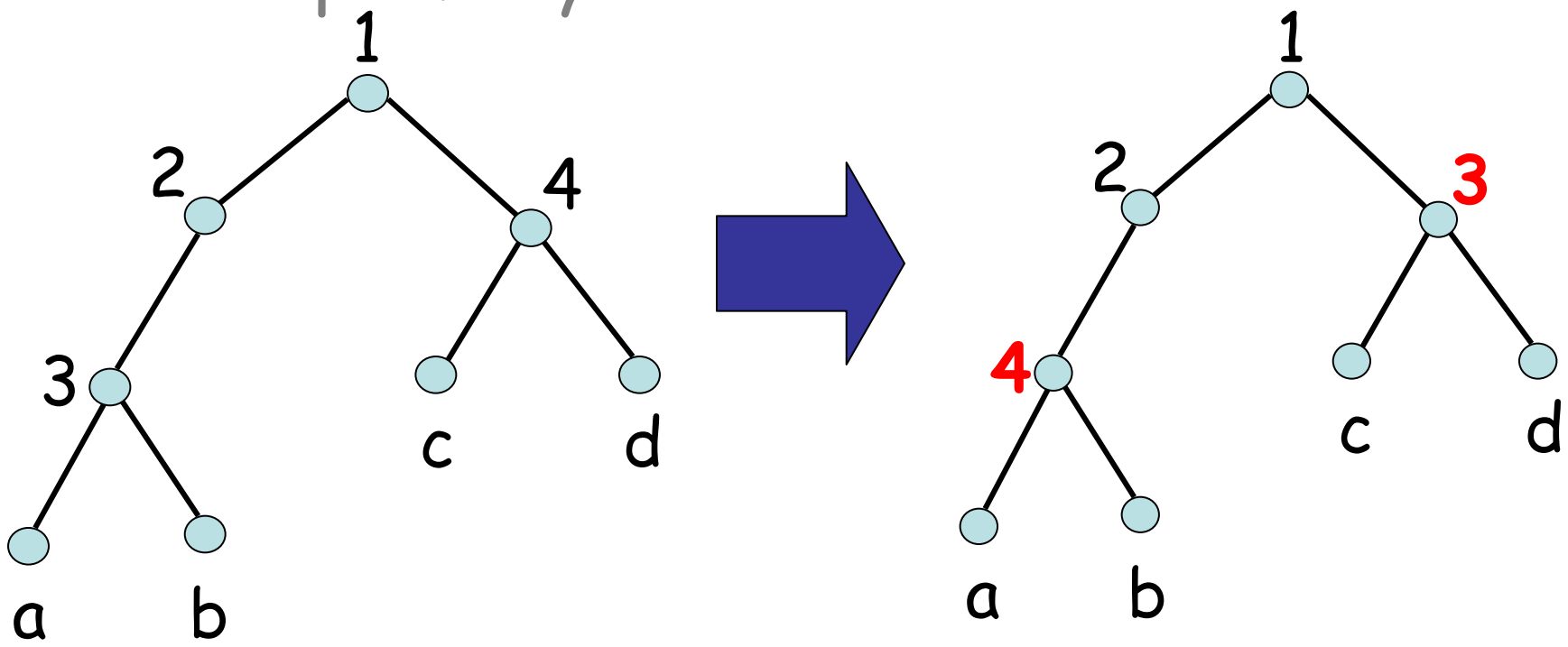
Can be determined in just *O(n)* time:

Upward pass: compute change in cost due to removing subtree

Downward pass: calculate change in cost for each potential location

Reordering internal nodes

Keep structure fixed and reorder split order of internal nodes optimally



Optimal internal node ordering

Key idea: Each split in the tree reduces the clustering cost (i.e.. finer approximation to the data). We want to place the best splits early on… this is a *scheduling* problem! (board example)

Optimal split ordering

- Let $g(\cdot)$ be the reduction in cost of splitting cluster rooted at x, T_x: $g(T_x) = \text{cost}(T_x) - (\text{cost}(T_L) + \text{cost}(T_R))$
- Overall hierarchical clustering cost is a time-weighted sum of these:

$$\text{hcost} = \frac{1}{n} \sum_{x \in V} \sigma(x) g(x)$$

where $\sigma(x)$ is the time (1 to n) at which T_x is split.

A scheduling algorithm

Choose order $\sigma(\cdot)$ of splits.

Greedy choice based on $g(\cdot)$ doesn't work – a split whose immediate benefit is small might nevertheless enable future good splits.

Horn [1972]: next subtree T to split is the one which maximizes $\frac{1}{|T|}\sum_{z \in T} g(z)$

Can be implemented in $O(n \log n)$ time.

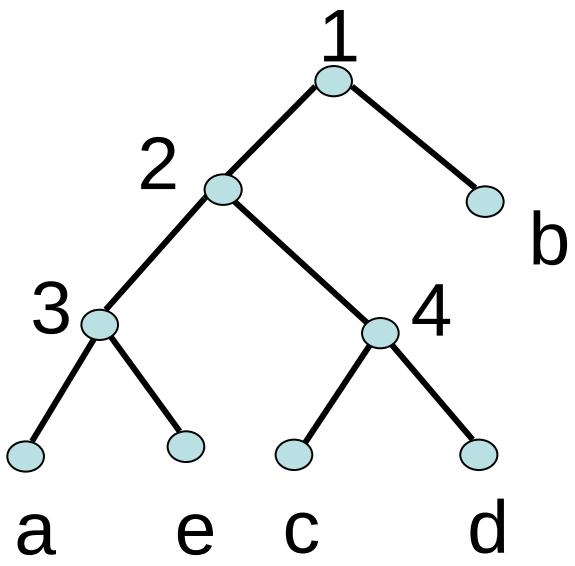
Final Algorithm

Iterate between two local moves

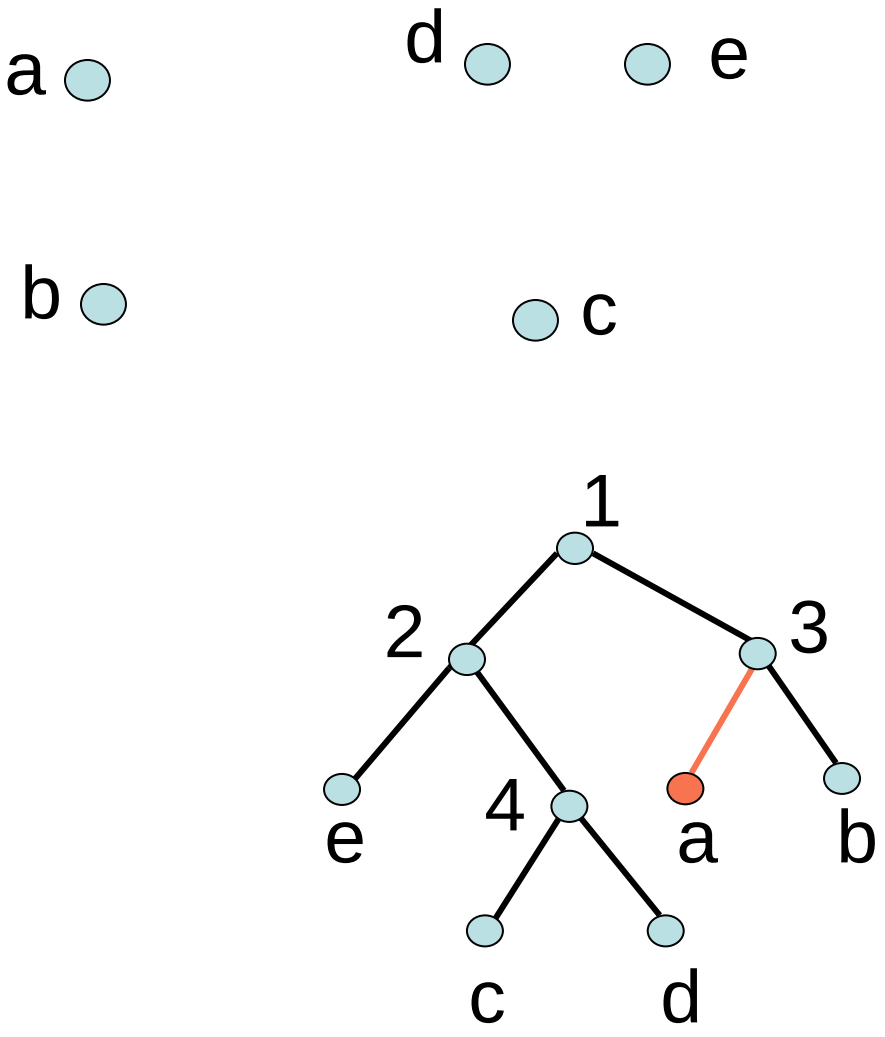
- Keep structure fixed and reorder split order of internal nodes optimally $O(n \log n)$
- Optimally relocate r sub-trees:

$O(r\ n) \rightarrow O(n)$, since $r<n$

Example

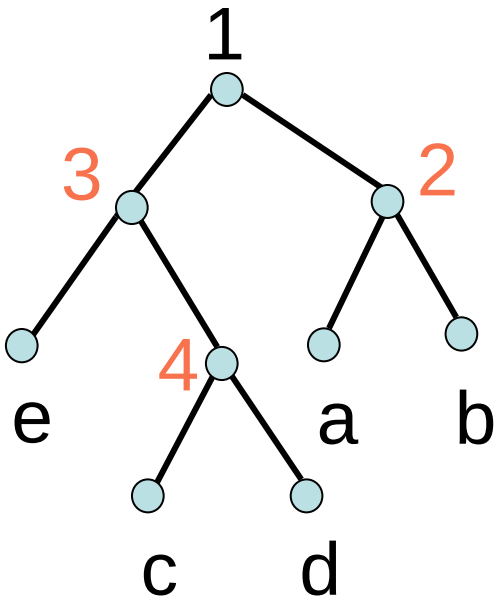


Initial tree: cost 62.25

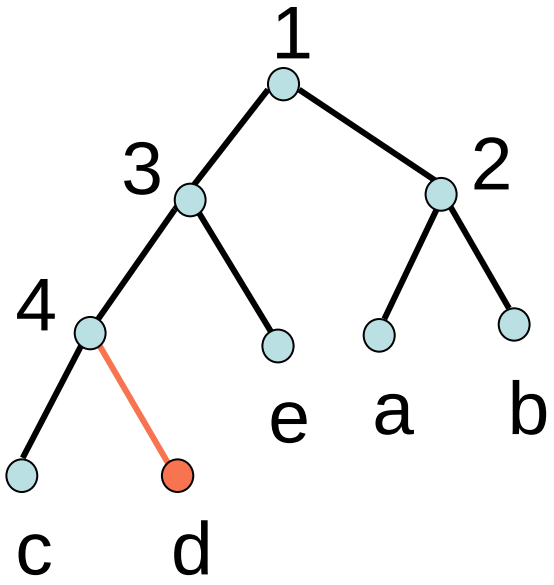


After graft: 27.0

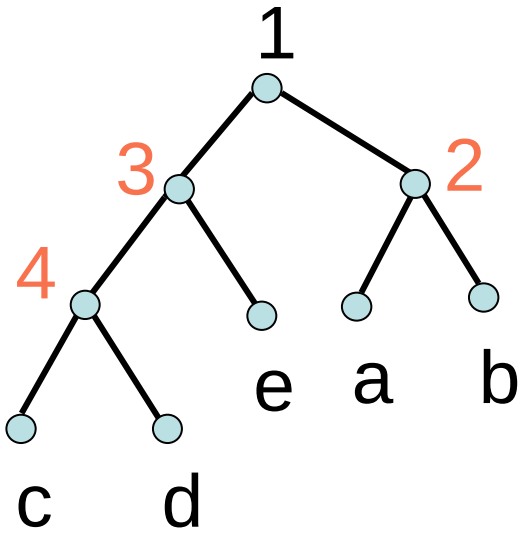
Example, continued



After reordering:
cost 25.5



Graft



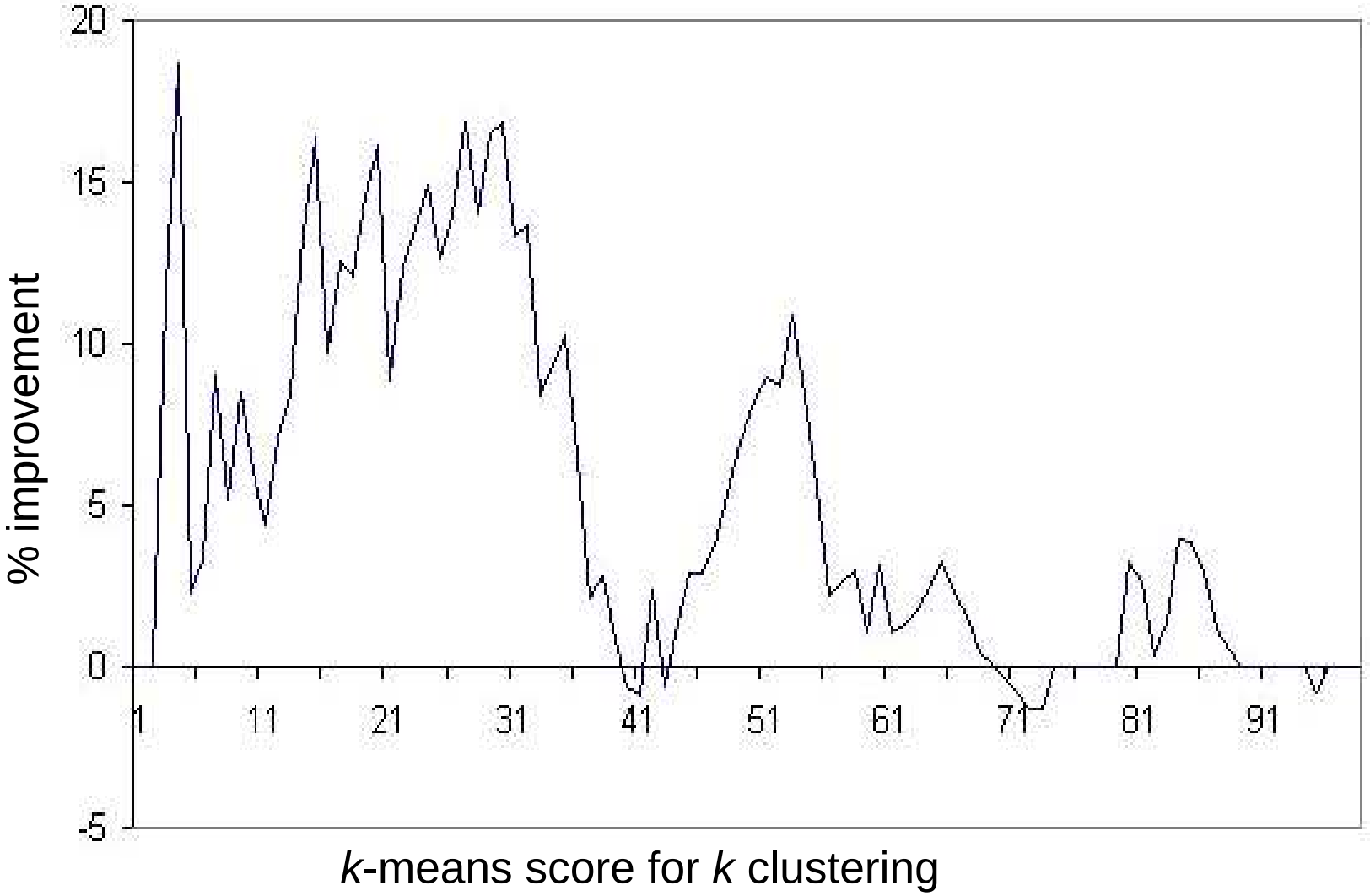
Final tree:
cost 21.0

Improvement over average linkage

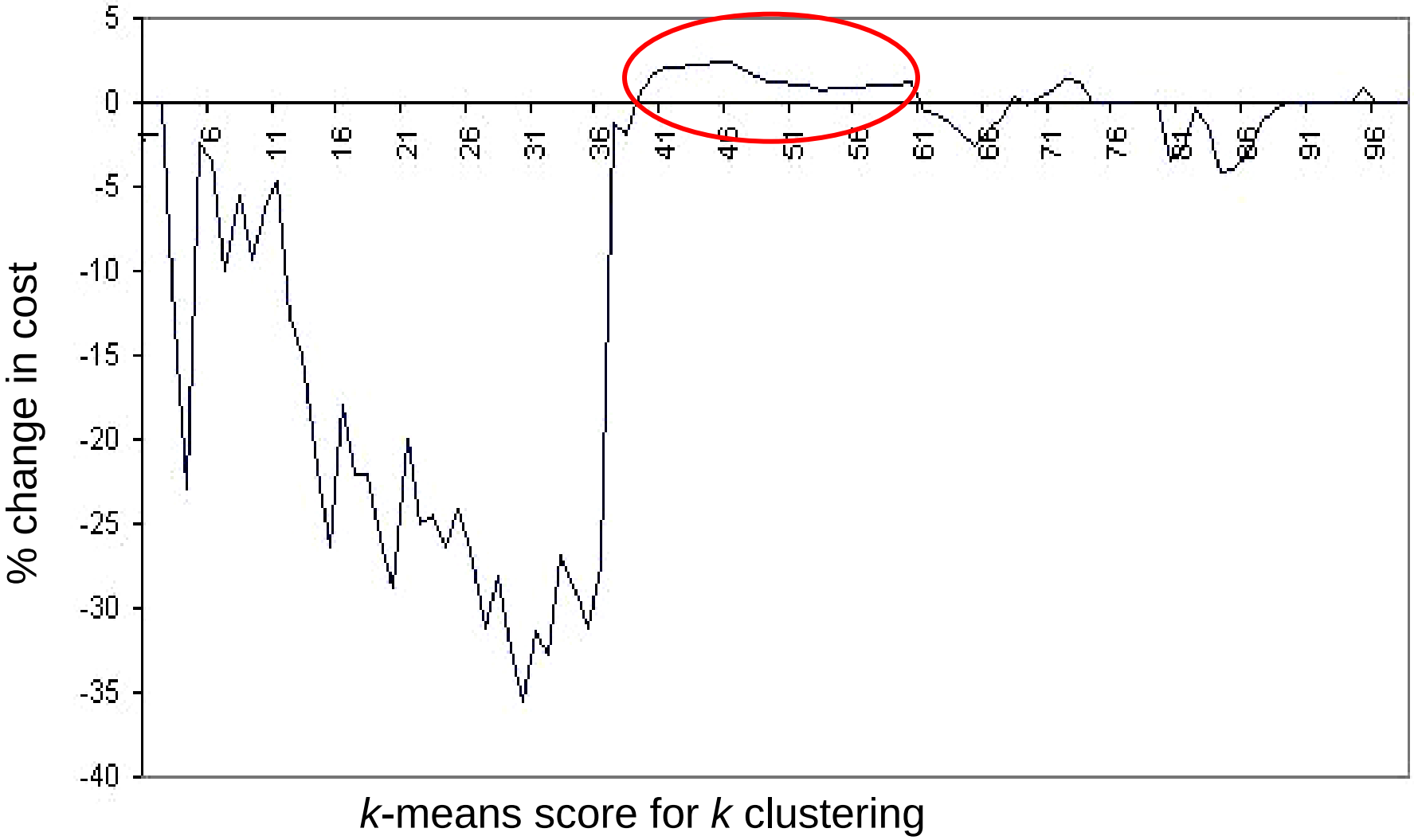
	Iterative algorithm, initialized with average linkage	Iterative algorithm, initialized randomly	Annealed algorithm, initialized with average linkage	Average linkage
20 points	21.59 8 iterations	Best: 20.88 Worst: 24.56	Best: 20.88	21.99
100 points	411.83 233 iterations	Best: 430.35 Worst: 449.38	NA	444.15

- Random and annealed methods find better optima
- Simulated annealing is much more consistent than local search with random initialization
- Number of iterations to converge grows with data size

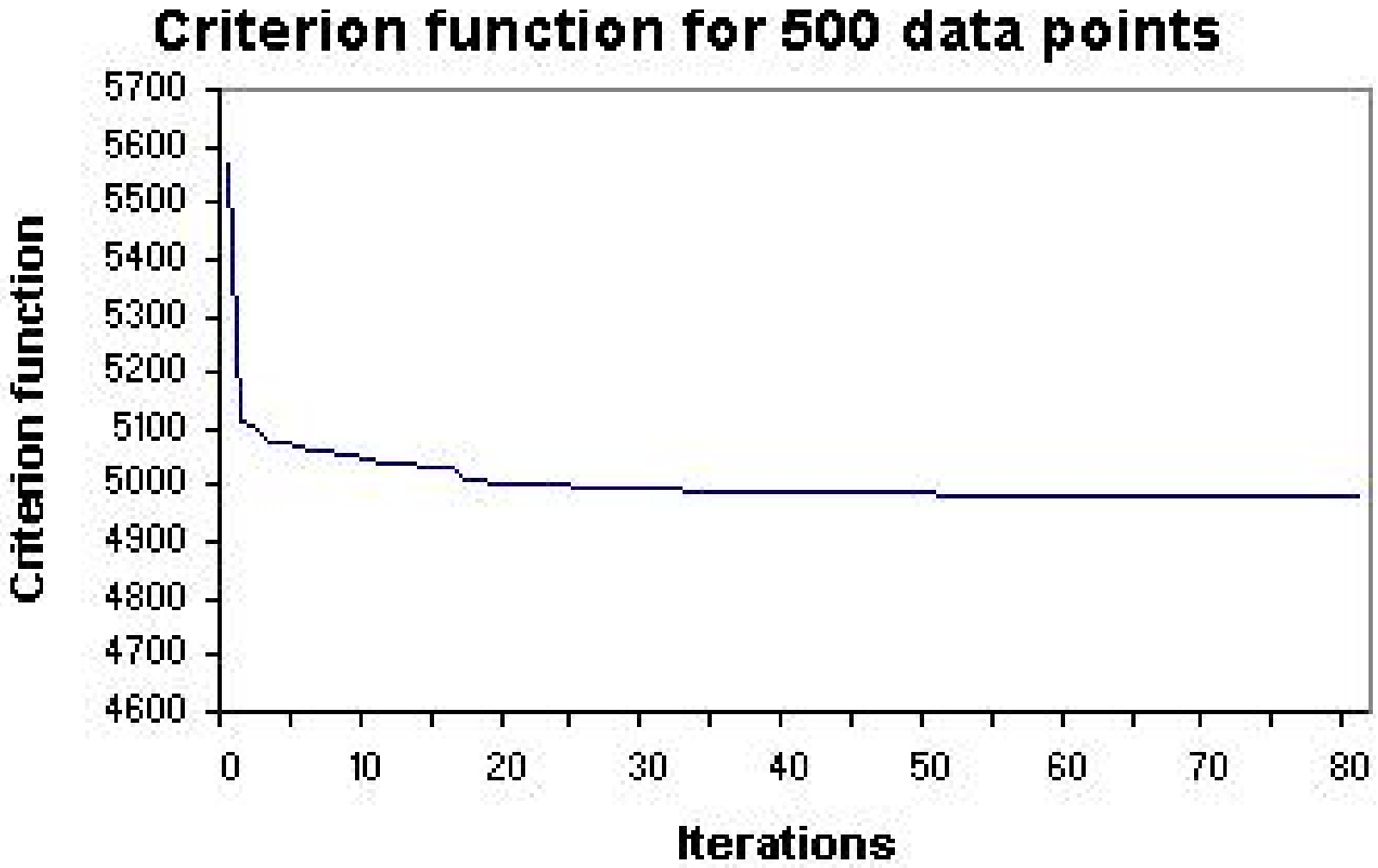
Improvement over average linkage



Weighted (40 – 60) vs. uniform



Convergence



Applications

- Gene Expression Analysis
- Microarray Data
- Image Segmantation
- Desease Classification

Summary

There is a basic existence question about hierarchical clustering which needs to be addressed:

must there always exist a hierarchical clustering in which, for each k, the induced k-clustering is close to optimal?

It turns out the answer is yes.

(see S. Dasgupta and P.M. Long)

Summary

In fact, there is a simple, fast algorithm to construct such hierarchical clusterings.

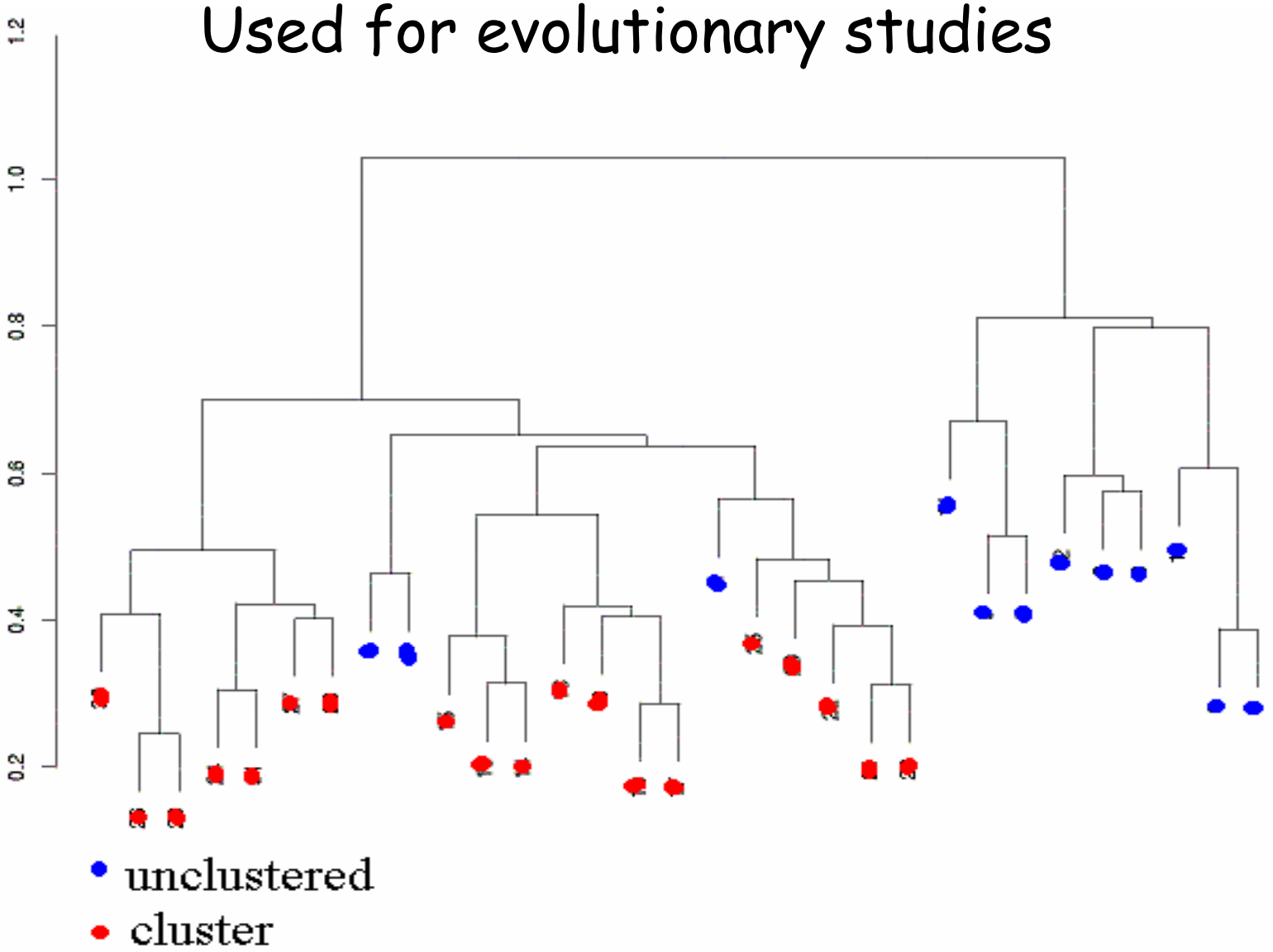
Meanwhile, the standard agglomerative heuristics do not always produce close-to-optimal clusterings.

Discussion

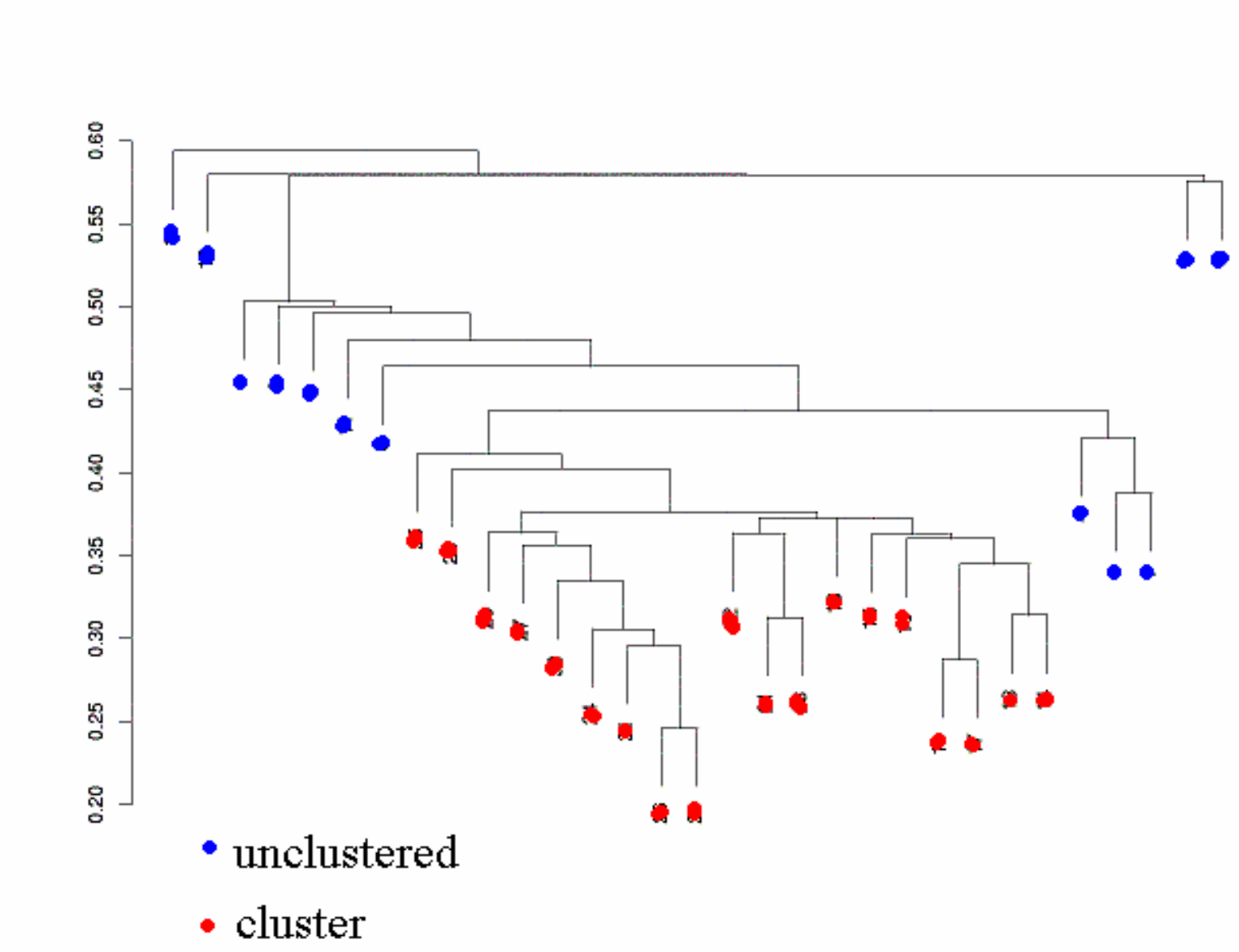
- Other cost functions for clustering.
- Local improvement procedures for hierarchical clustering?

Single linkage (Nearest Neighbor)

Used for evolutionary studies



Complete linkage (FN)



Ward's method (information loss)