HIERARCHICAL CLUSTERING

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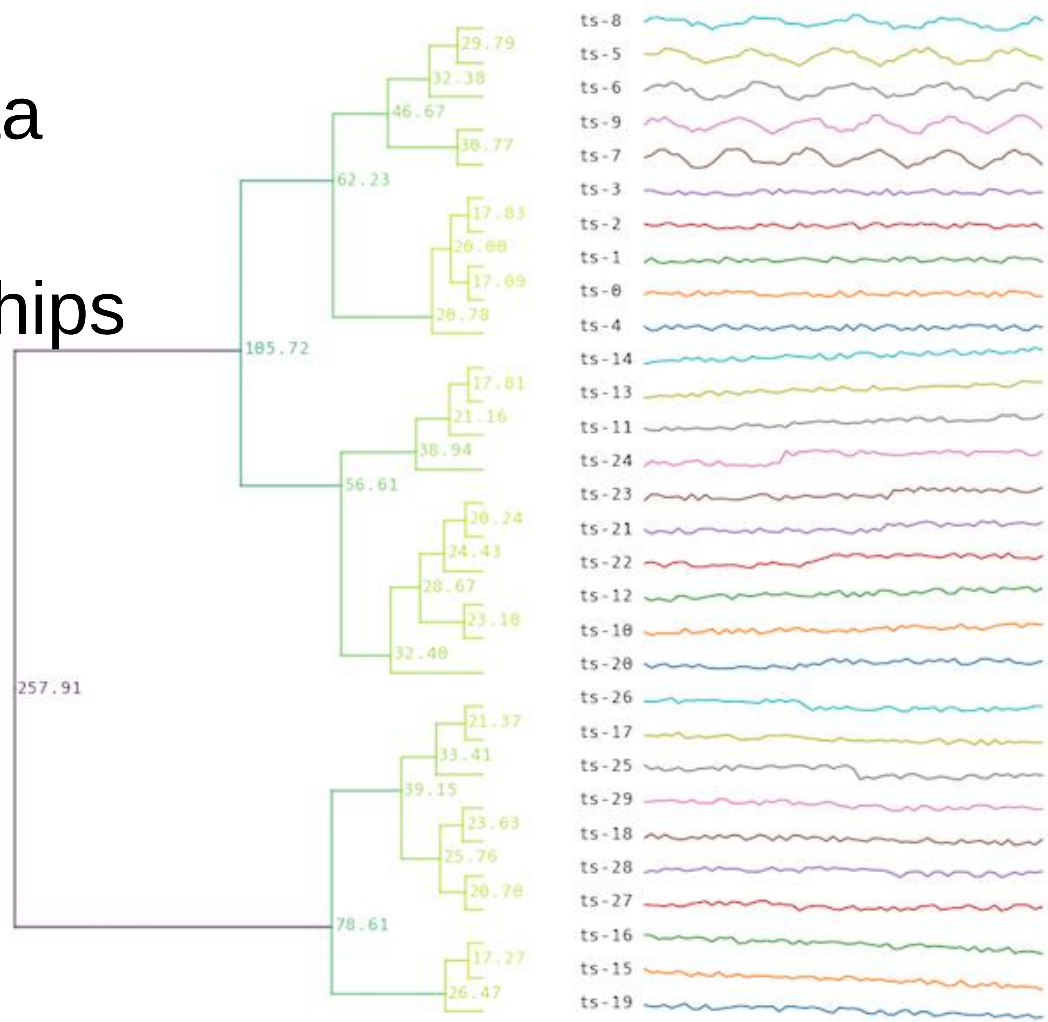
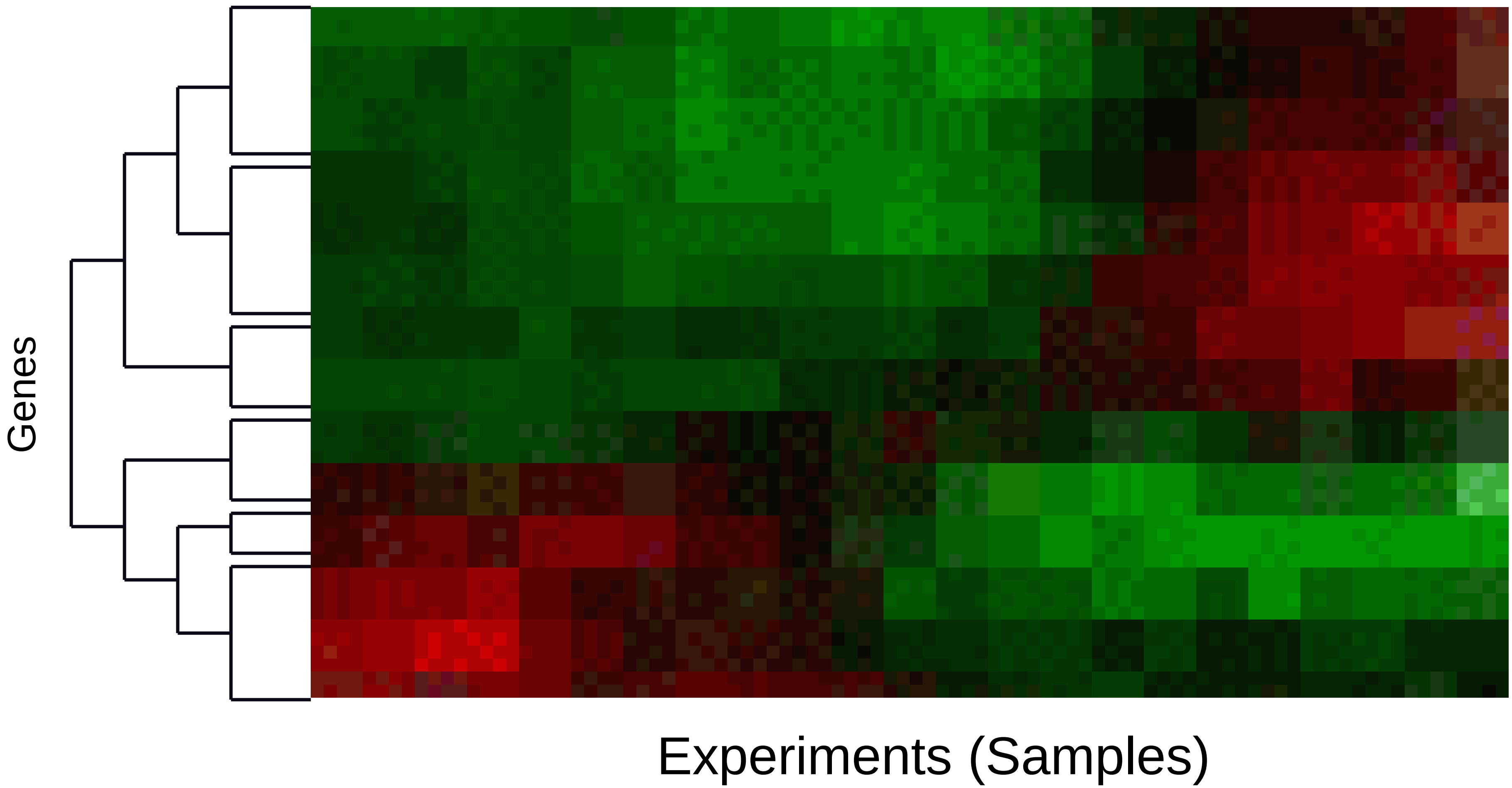
Hierarchical Clustering

- Model hierarchical structure in the data
- Captures relationships among clusters



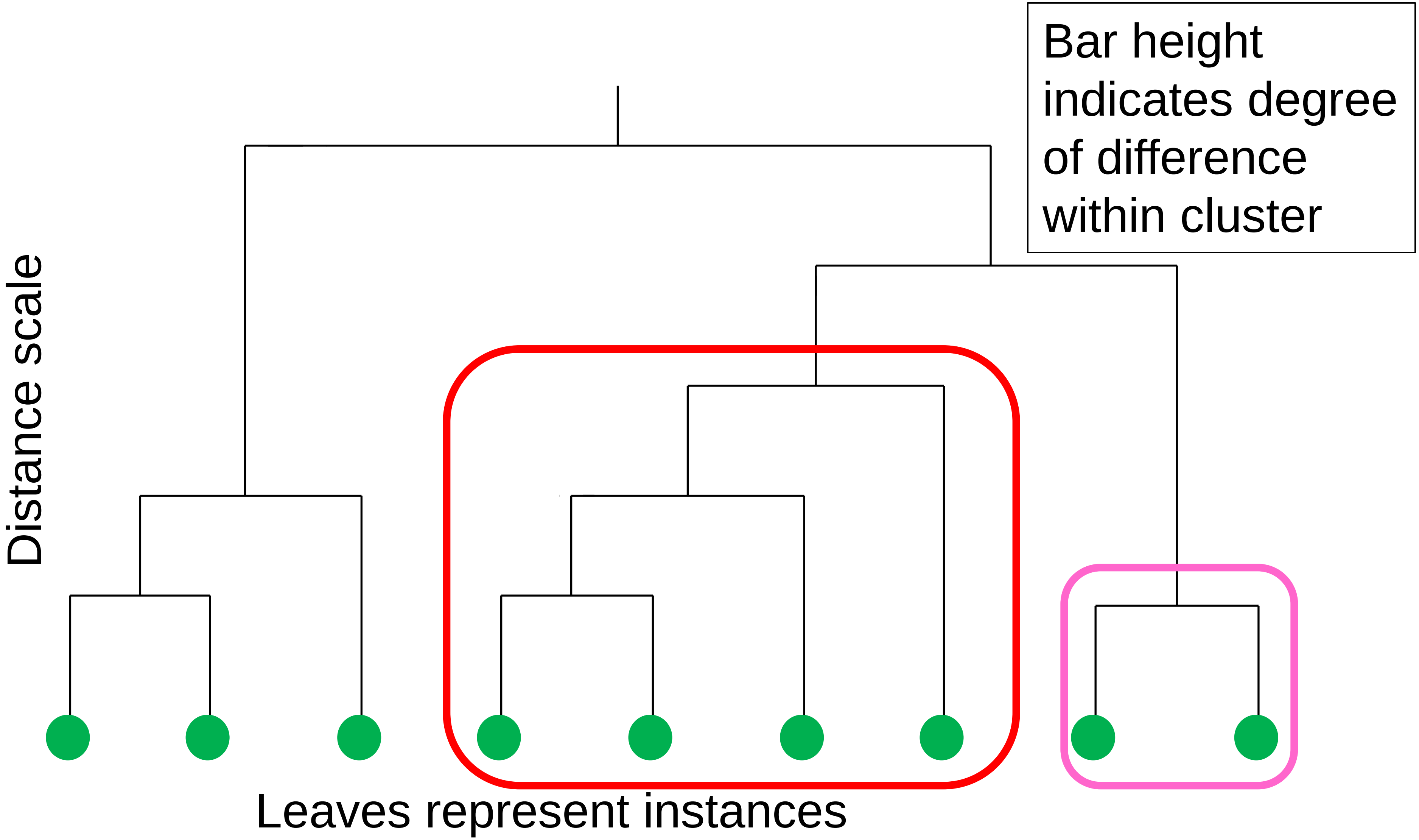
Example: Gene Expression

(Green = up-regulated, Red = down-regulated)



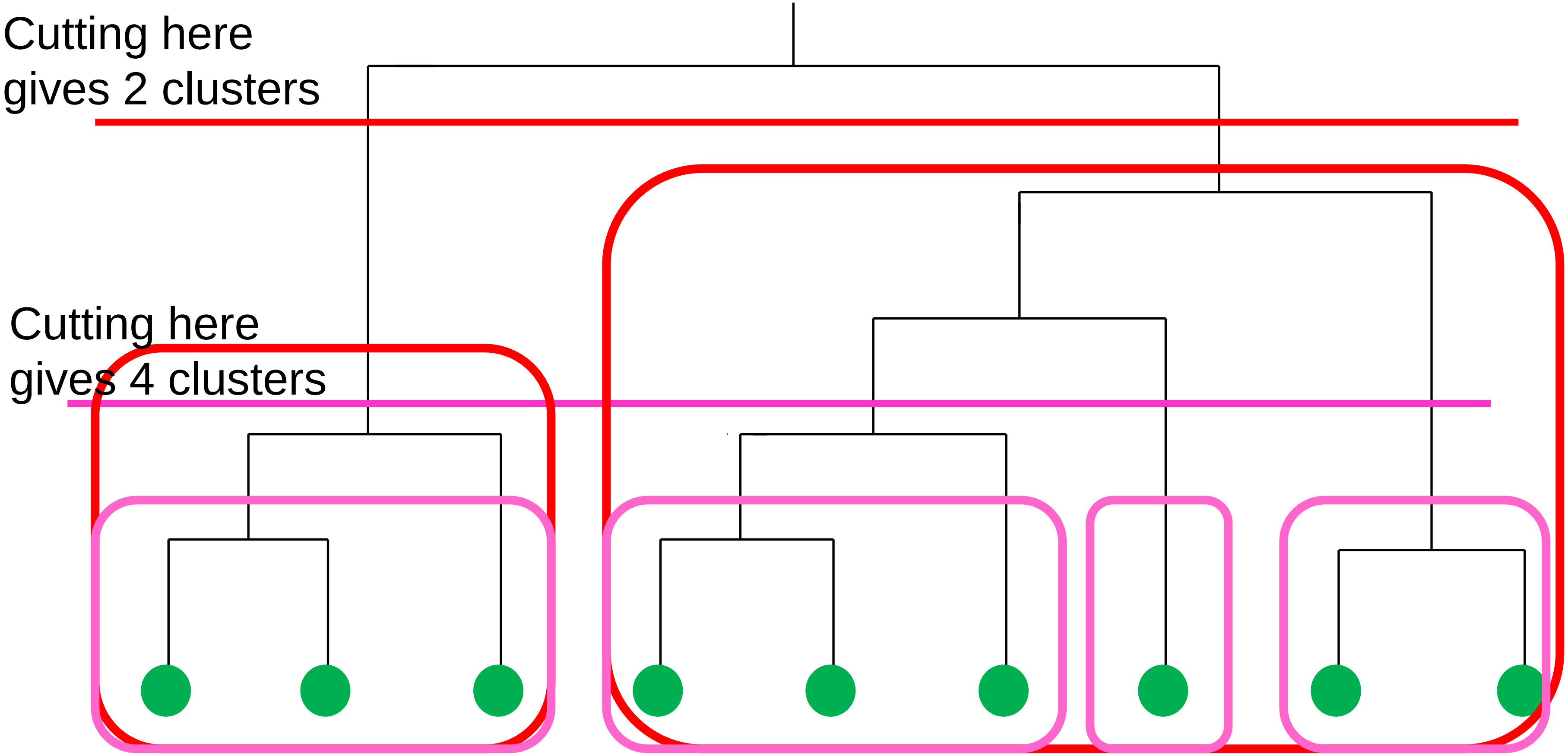
Basics

Hierarchical Clustering: Dendogram



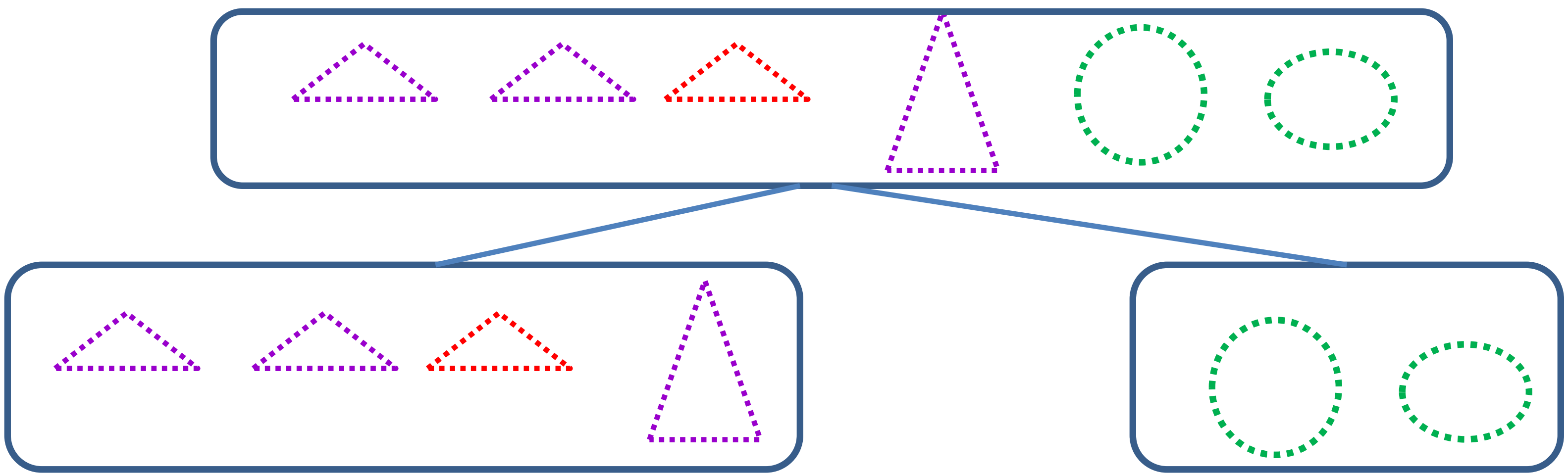
Note: Partitional Clustering from a Hierarchical Clustering

Can generate a partitional clustering from a hierarchical clustering by “cutting” the tree at some level

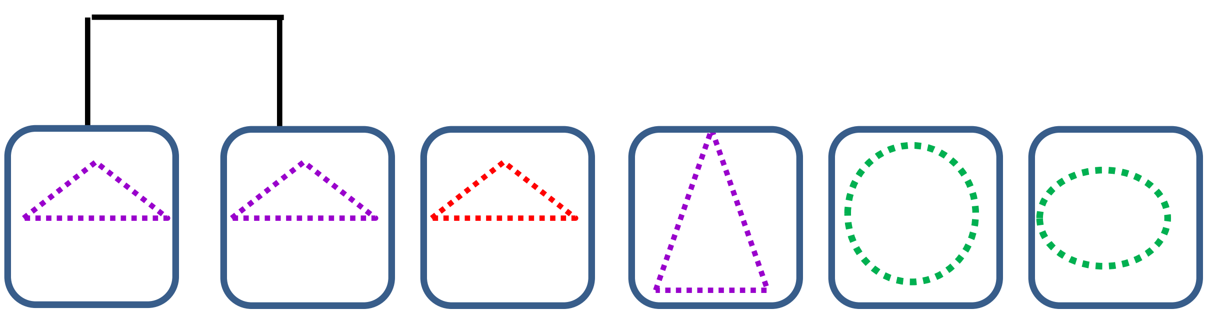


Hierarchical Clustering Approaches

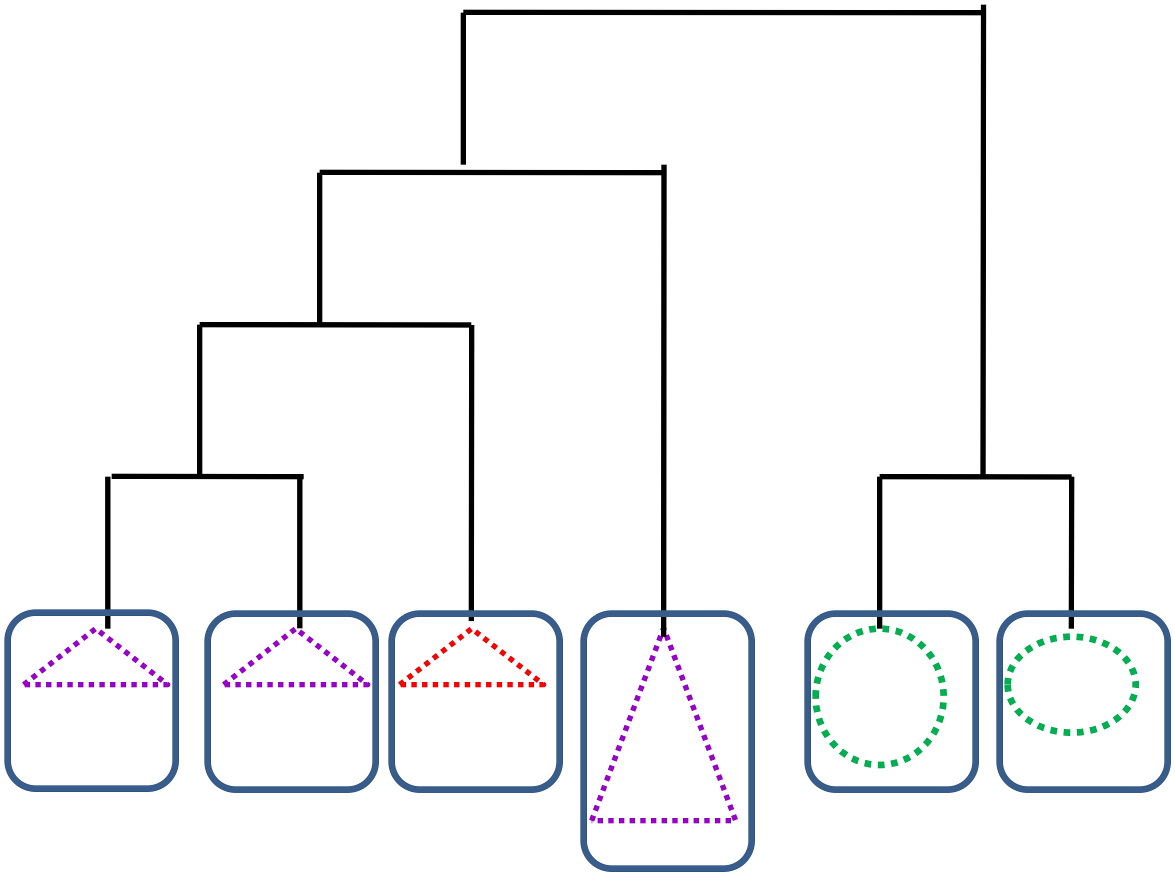
- Top-down or divisive



- Bottom-up or agglomerative



Bottom-Up Example



Bottom-Up Hierarchical Clustering

Given: instances $x_1,\ldots,x_n$

For i = 1 to n, $c_i = \{x_i\}$

$C = \{c_1,\ldots,c_n\}$

j = n

While |C| > 1

  j = j+1

  $(c_a,c_b) = \text{argmin dist}(c_a,c_b)$

  $c_j = c_a \cup c_b$

  add node to tree joining a and b

  $C = (C - \{c_a,c_b\}) \cup c_j$

Return tree with root node j

Key question: Measuring distance

Distance Matrix

$$D = \begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & \ddots & \\ d(n,1) & d(n,2) & d(n,3) & \cdots & 0 \end{bmatrix}$$

Initial Distance Matrix for a Data Set with 5 Examples

1) Form five clusters, one for each example
2) Compute pairwise distance between initial clusters (=pairwise distance between examples)

	1	2	3	4	5
1	**0**				
2	**7.4**	**0**			
3	**0.7**	**7.1**	**0**		
4	**7.3**	**0.3**	**7.0**	**0**	
5	**0.5**	**6.9**	**0.6**	**6.8**	**0**

Find Two Closest Clusters

	1	2	3	4	5
1	**0**				
2	**7.4**	**0**			
3	**0.7**	**7.1**	**0**		
4	**7.3**	**0.3**	**7.0**	**0**	
5	**0.5**	**6.9**	**0.6**	**6.8**	**0**

Smallest value in matrix

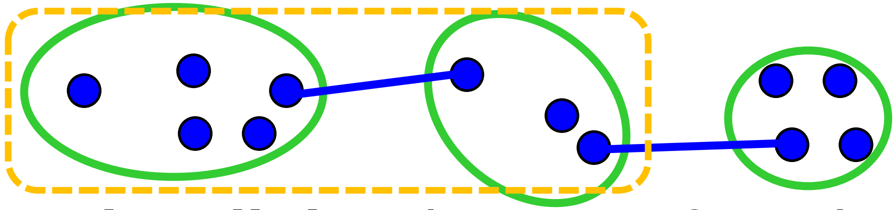
Update Distance Matrix

	1	(2,4)	3	5
1	**0**			
(2,4)	**?**	**0**		
3	**0.7**	**?**	**0**	
5	**0.5**	**?**	**0.6**	**0**

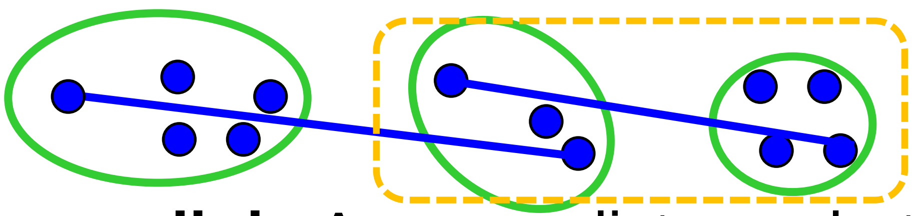
Question: What is the distance between the new cluster (2,4) and the other three clusters?

Measuring the Distance Between Two Clusters

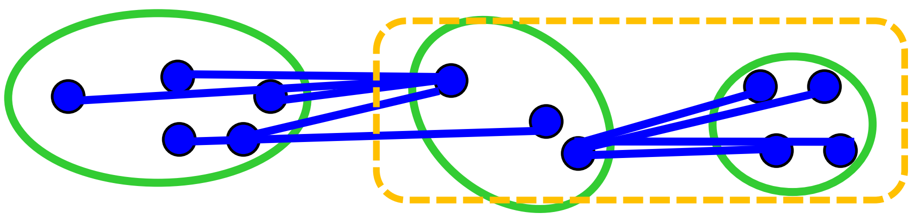
- **Single link:** Distance of two most similar instances: dist(c_u, c_v) = min{dist(a, b) | a∈c_u, b∈c_v}



- **Complete link:** Distance of two least similar instances: dist(c_u, c_v) = max{dist(a, b) | a∈c_u, b∈c_v}



- **Average link:** Average distance between instances: dist(c_u, c_v) = avg{dist(a, b) | a∈c_u, b∈c_v}



Efficient Distance Updates

- If we merged and c_u and c_v into c_j, we can determine distance to every other cluster:
  - Single link:

$$dist(c_j, c_k) = \min(dist(c_u, c_k), dist(c_v, c_k))$$

  - Complete link:

$$dist(c_j, c_k) = \max(dist(c_u, c_k), dist(c_v, c_k))$$

  - Average link:

$$dist(c_j, c_k) = \frac{|c_u| * dist(c_u, c_k) + |c_v| * dist(c_v, c_k)}{|c_u| + |c_v|}$$

Note: The linkage choice is a hyper parameter for the bottom-up clustering algorithm

Illustrative Example Updates for Each Linkage Criteria

Single

	2	4	(2,4)
1	7.4	7.3	**7.3**
3	7.1	7.0	**7.0**
5	6.9	6.8	**6.8**

min

Complete

	2	4	(2,4)
1	7.4	7.3	**7.4**
3	7.1	7.0	**7.1**
5	6.9	6.8	**6.9**

max

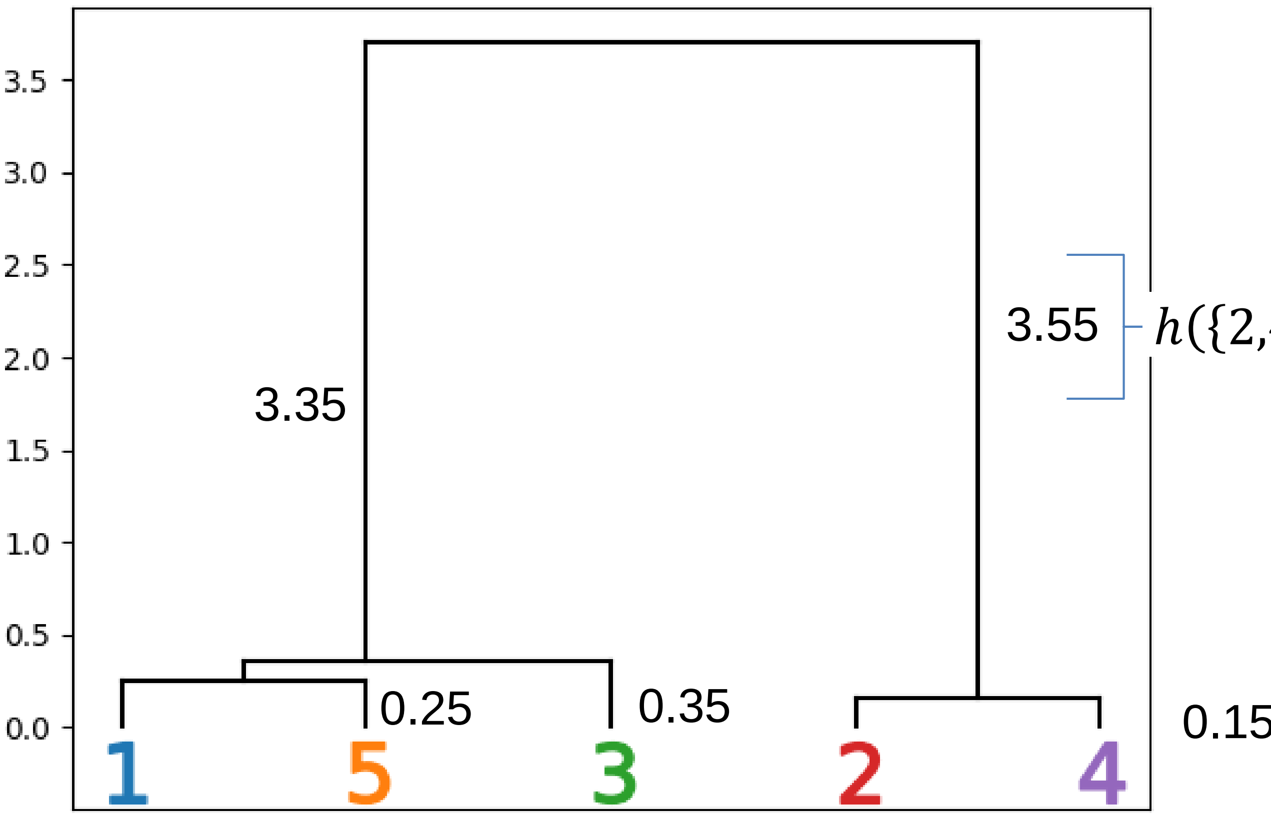
Average

	2	4	(2,4)
1	7.4	7.3	**7.35**
3	7.1	7.0	**7.05**
5	6.9	6.8	**6.85**

(Weighted) mean

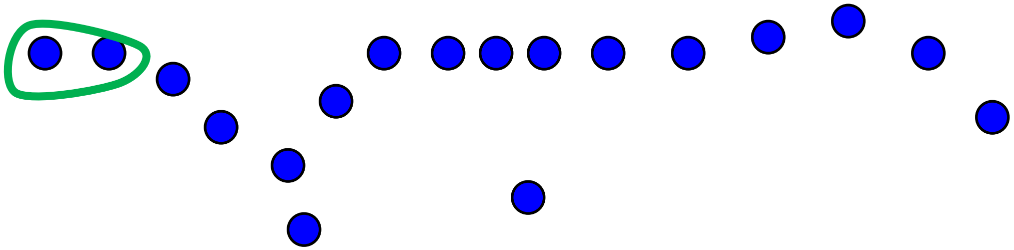
Complete Link Dendogram for Sample Dataset

$$\text{height} = \mathrm{h}(c_j, c_k) = \frac{dist(c_j, c_k)}{2}$$

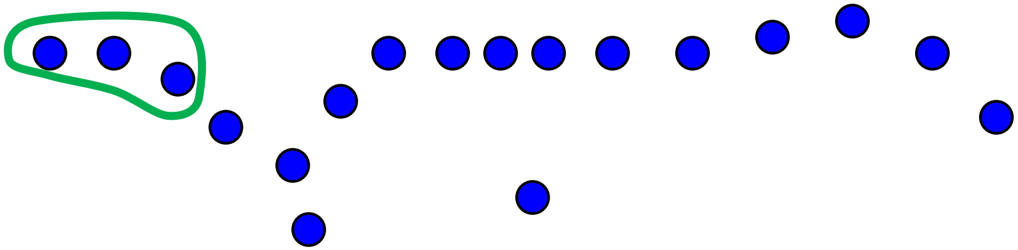


$$h(\{2,4\},\{1,5,3\}) - h\ (\{2\},\{4\})$$

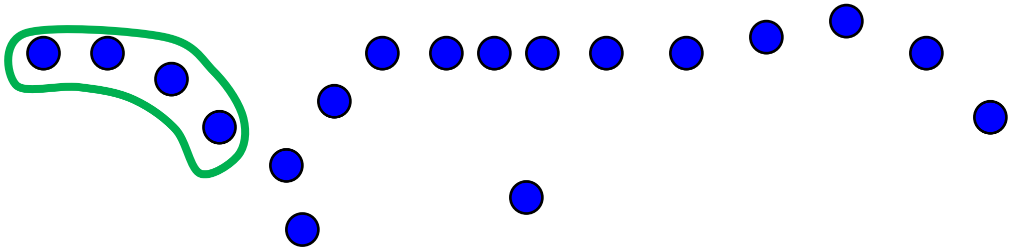
Single Link: Chaining



Single Link: Chaining

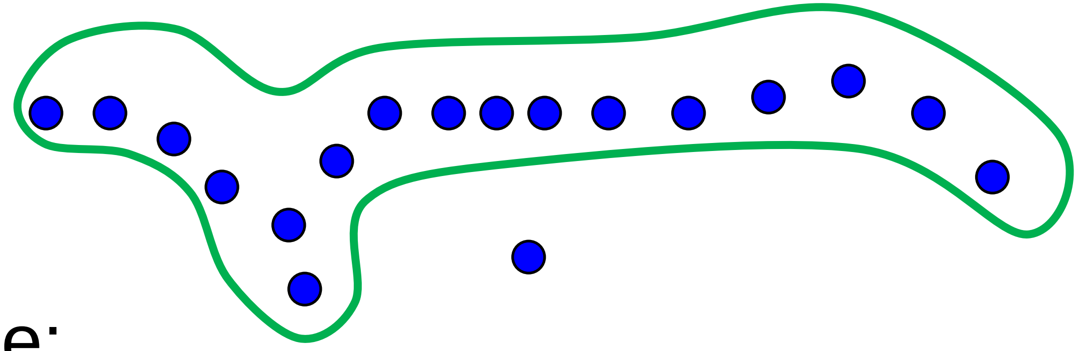


Single Link: Chaining



Single Link

- Chaining:



- Bottom line:
  - Simple, fast
  - Often low quality

Complete Link Hierarchical Summary

- Complexity: $O(n^3)$
  - $O(n^2)$ to build initial similarity matrix
  - $O(n)$ for the merges
- Fast algorithm: Requires $O(n^2)$ space
- Bottom line
  - Typically much faster than $O(n^3)$
  - Often good quality
  - No Chaining

Advanced Hierarchical Clustering

Other Hierarchical Clustering Methods

- Weaknesses of agglomerative clustering methods
  - **Do not scale well:** time complexity of at least $O(n^2)$, where n is the number of total objects
  - Can never undo what was done previously

- Integration of hierarchical with distance-based clustering
  - BIRCH: uses CF-tree and incrementally adjusts the quality of sub-clusters
  - CURE: selects well-scattered points from the cluster and then shrinks them towards the center of the cluster by a specified fraction

BIRCH: Balanced Iterative Reducing and Clustering using Hierarchies

- Incrementally construct a Clustering Feature (CF) tree
  - **Phase 1:** Scan DB to build an initial in-memory CF tree (each node: #points, sum, sum of squares)
  - **Phase 2:** use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree

- ***Scales linearly*****:** Finds a good clustering with a single scan

- ***Weaknesses:*** handles only numeric data, sensitive to order of data records

Definitions

- **Centroid:** $\mu = \frac{1}{N}\sum_{i=1}^{N} x_i$

Average along each dimension

- **Radius:** Average distance from member points to cluster centroid

$$R = \sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{d} (x_{ij} - \mu_j)^2}{N}}$$

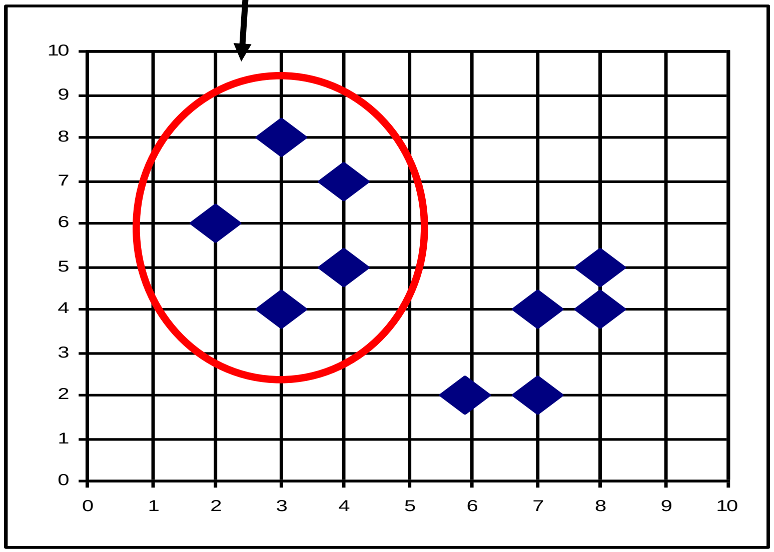
  - Captures tightness of cluster around centroid
  - Note: Math and verbal definition not 100% aligned, but these come directly from the paper

Cluster Feature Vector

- Given: $X_1, \ldots, X_n$, data points in a cluster where each with d-dimensions
- We define $\mathrm{CF} = (\mathrm{N}, \mathrm{LS}, \mathrm{SS})$, where
  - N: Number of data points
  - LS_j: $\sum_{i=1}^{n} x_{ij}$
  - SS_j: $\sum_{i=1}^{n} x_{ij}^2$
- Note: CFs are additive!
  - E.g., $\mathrm{CF}_1 + \mathrm{CF}_2 = (\mathrm{N}_1{+}\mathrm{N}_2, \mathrm{LS}_1{+}\mathrm{LS}_2, \mathrm{SS}_1{+}\mathrm{SS}_2)$

Cluster Feature Example

CF = (5, (16,30), (54,190))



(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

$LS_x = 3 + 2 + 4 + 4 + 3 = 16$

$LS_y = 4 + 6 + 5 + 7 + 8 = 30$

$SS_x = 3^2 + 2^2 + 4^2 + 4^2 + 3^2 = 54$

$SS_y = 4^2 + 6^2 + 5^2 + 7^2 + 8^2 = 190$

Comments

- $2d + 1$ values represent any number of points
  - d = number of dimensions
- **Average in each dimension j:** LS_j / N
- **Variance in each dimension *j*:** $(SS_j / N) - (LS_j / N)^2$
  - To get standard deviation take square root
- Can also compute the radius (next slide)

Radius Derivation

$$R = \sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{d}\,(x_{ij}-\mu_j)^2}{N}} = \sqrt{\frac{\sum_{j=1}^{d}\sum_{i=1}^{N}(x_{ij}^2\; - 2x_{ij}\mu_j + \mu_j^2)}{N}}$$

Definition of SS

Definition of LS

$$= \sqrt{\frac{\sum_{j=1}^{d}(\sum_{i=1}^{N} x_{ij}^2) - 2\mu_j\,(\sum_{i=1}^{N} x_{ij}) + (N\mu_j^2))}{N}}$$

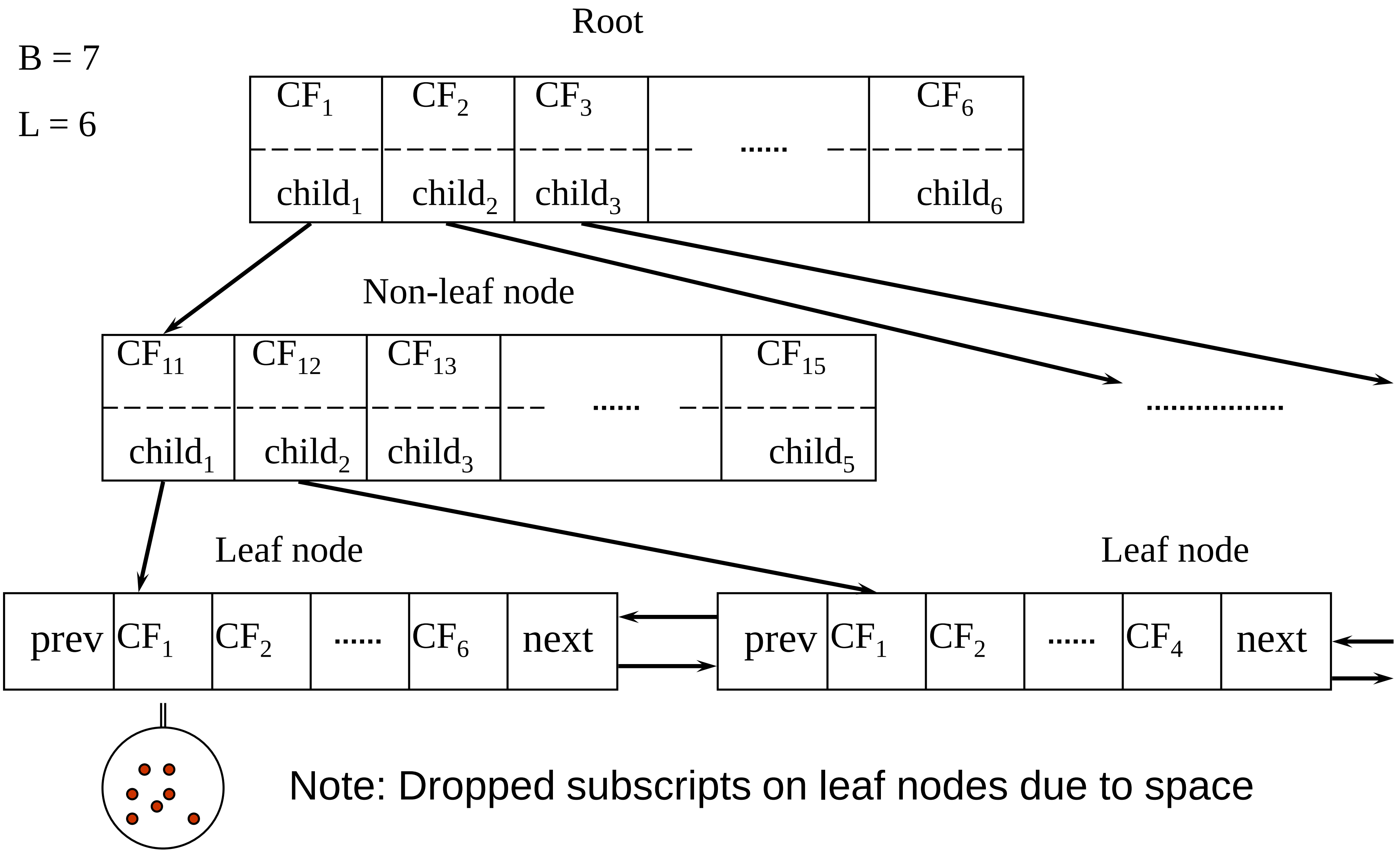
Definition of centroid

$$= \sqrt{\frac{\sum_{j=1}^{d} SS_j - 2\,\frac{LS_j}{N}\,LS_j + N\left(\frac{LS_j}{N}\right)^2}{N}}$$

Cluster Feature Tree

- A CF-tree is a height-balanced tree with two parameters:
  - Branching factor (non leaf nodes B, leaf nodes, L)
  - Threshold T
- Each non leaf node has the form [CF_i, $child_i$]
- Each leaf node has CF
  - Set of CFs
  - Two pointers: prev and next
- Radius of a subcluster under a leaf node can not exceed the threshold T

CF Tree



Note: Dropped subscripts on leaf nodes due to space

CF-Tree Construction

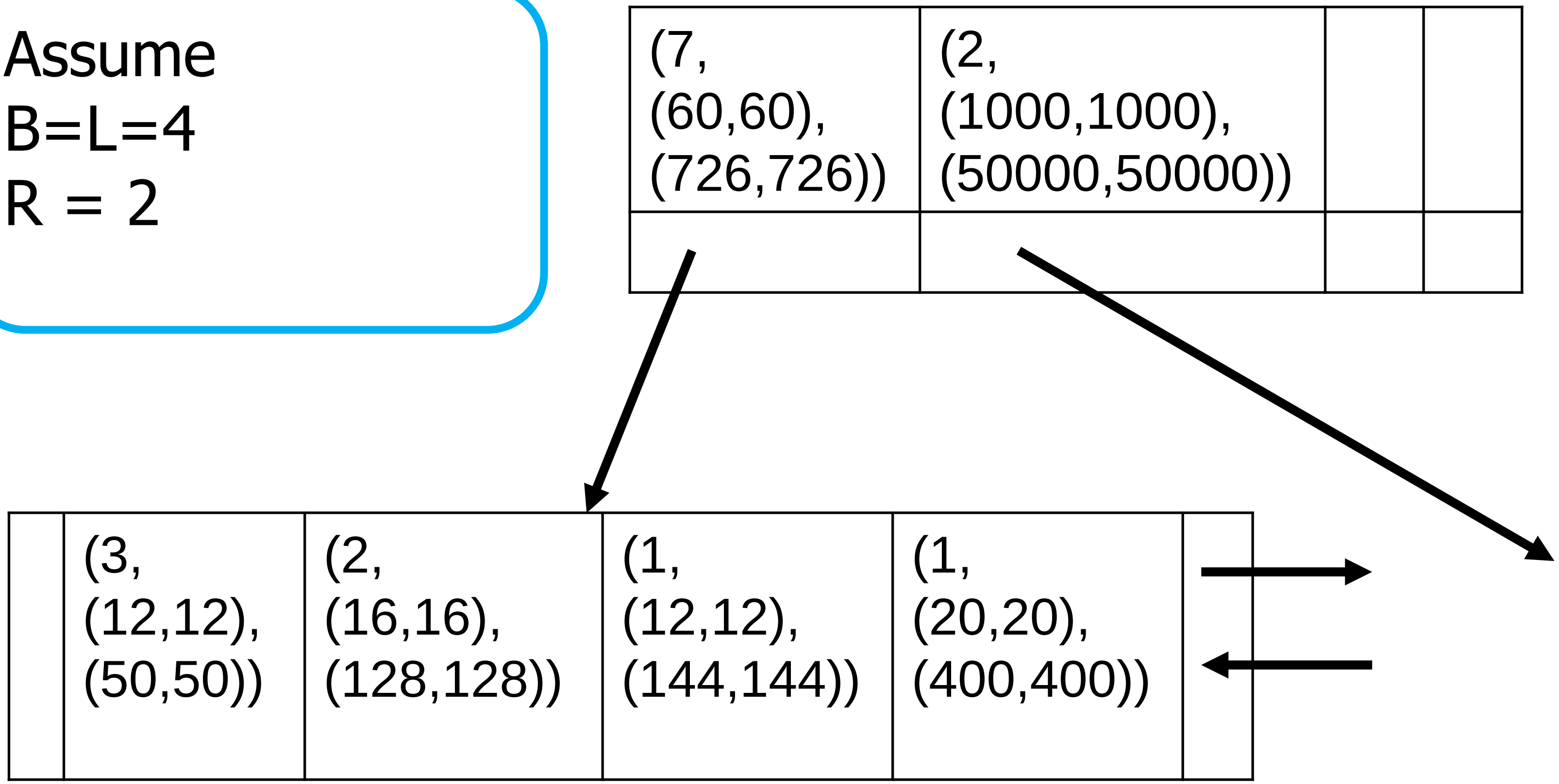
- Scan data set and insert the incoming data instances into the CF tree one by one
- Each instance is inserted into the closest subcluster under a leaf node
- If insertion causes subcluster radius to exceed threshold, then create new subcluster

CF-Tree Construction

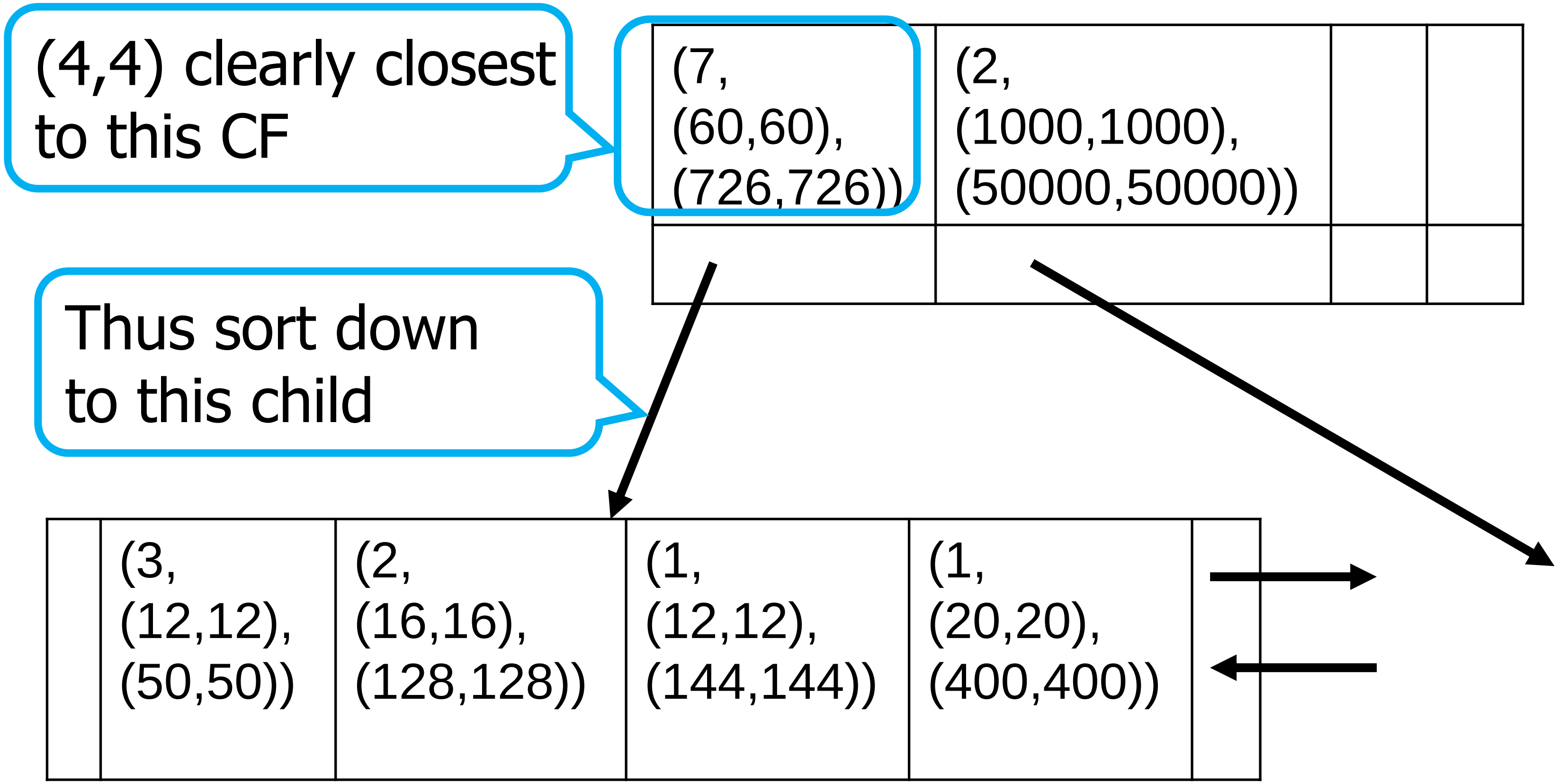
- The new subcluster may cause its parent to exceed branching factor
- If so, split leaf node
  - Identifying the pair of subclusters with largest inter-cluster distance
  - Divide by proximity to these two subclusters
- If this split clause non-leaf node to exceed branching factor, then recursively split
- If the root node is split, then the height of the CF tree is increased by one

Example: Insert (4,4) into CF Tree

Assume
B=L=4
R = 2



Example: Insert (4,4) into CF Tree



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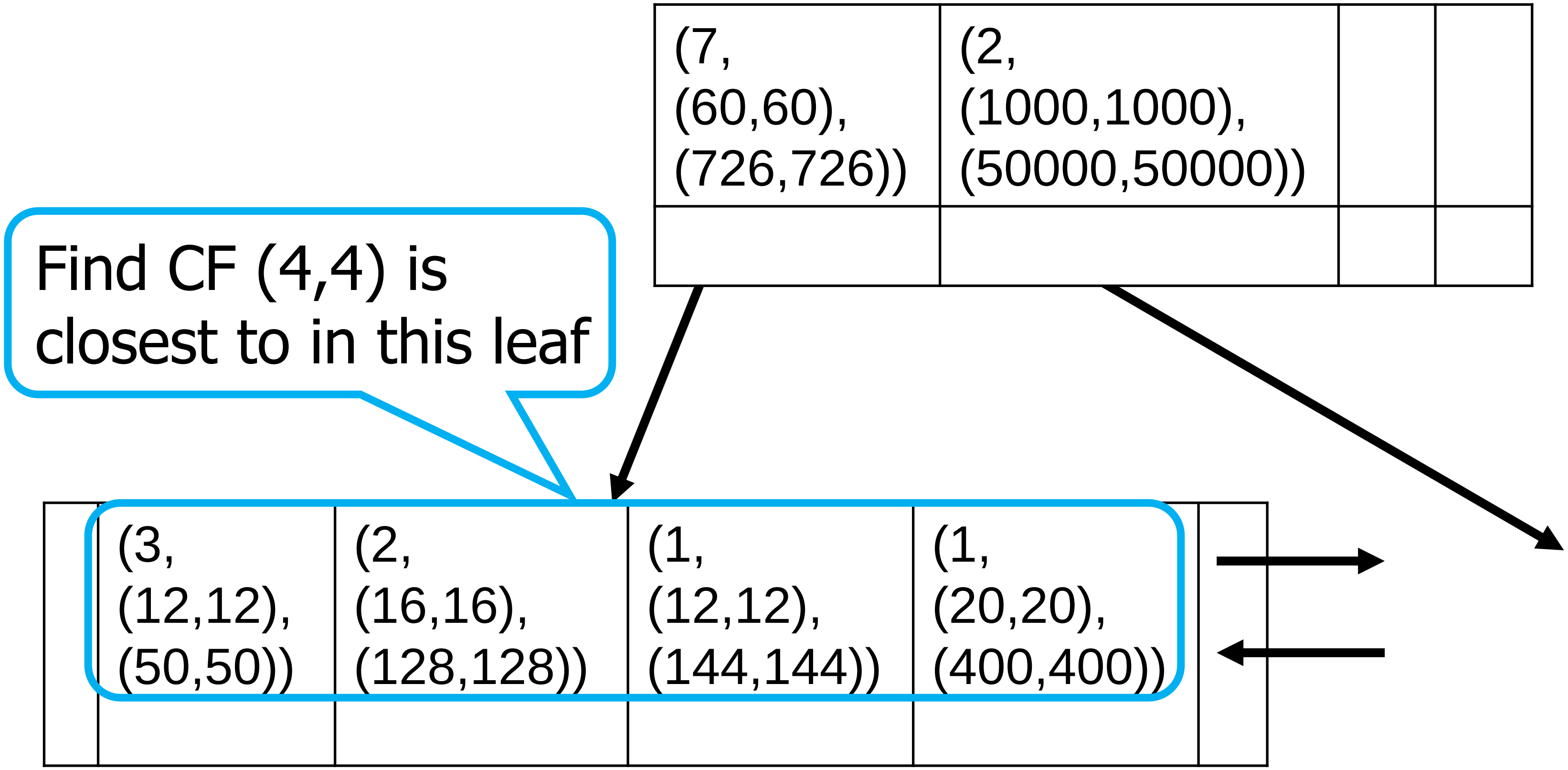
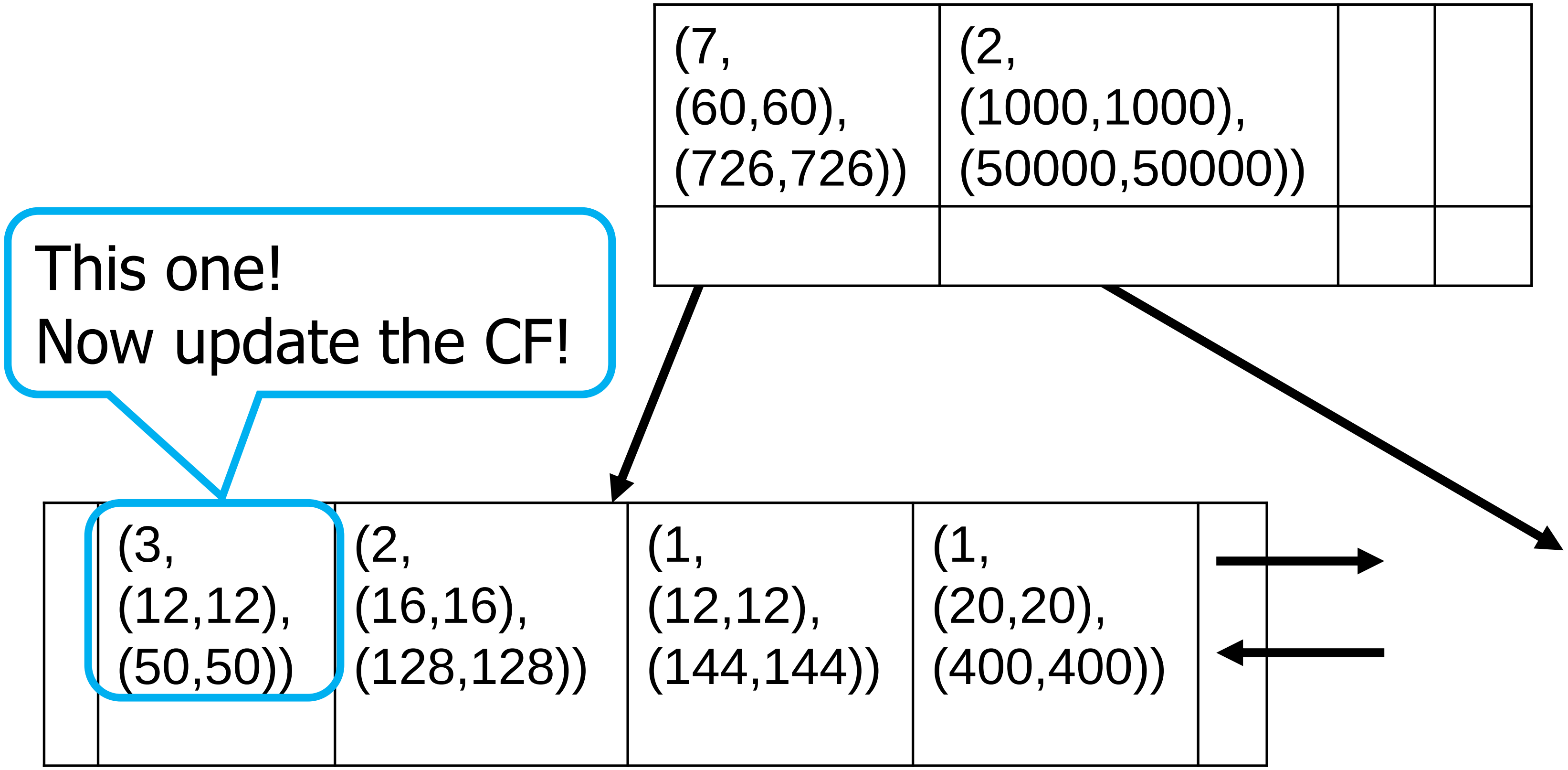
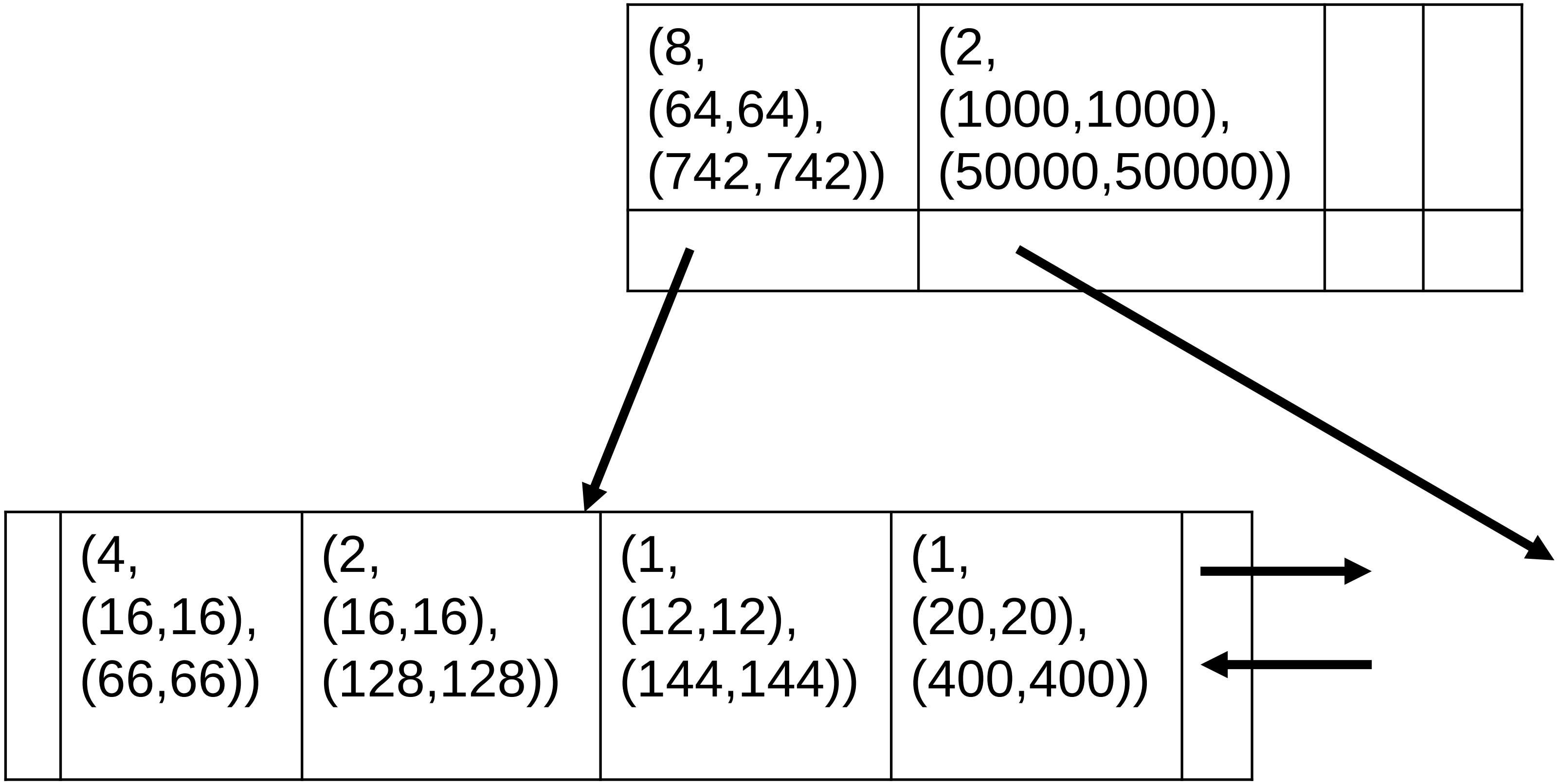


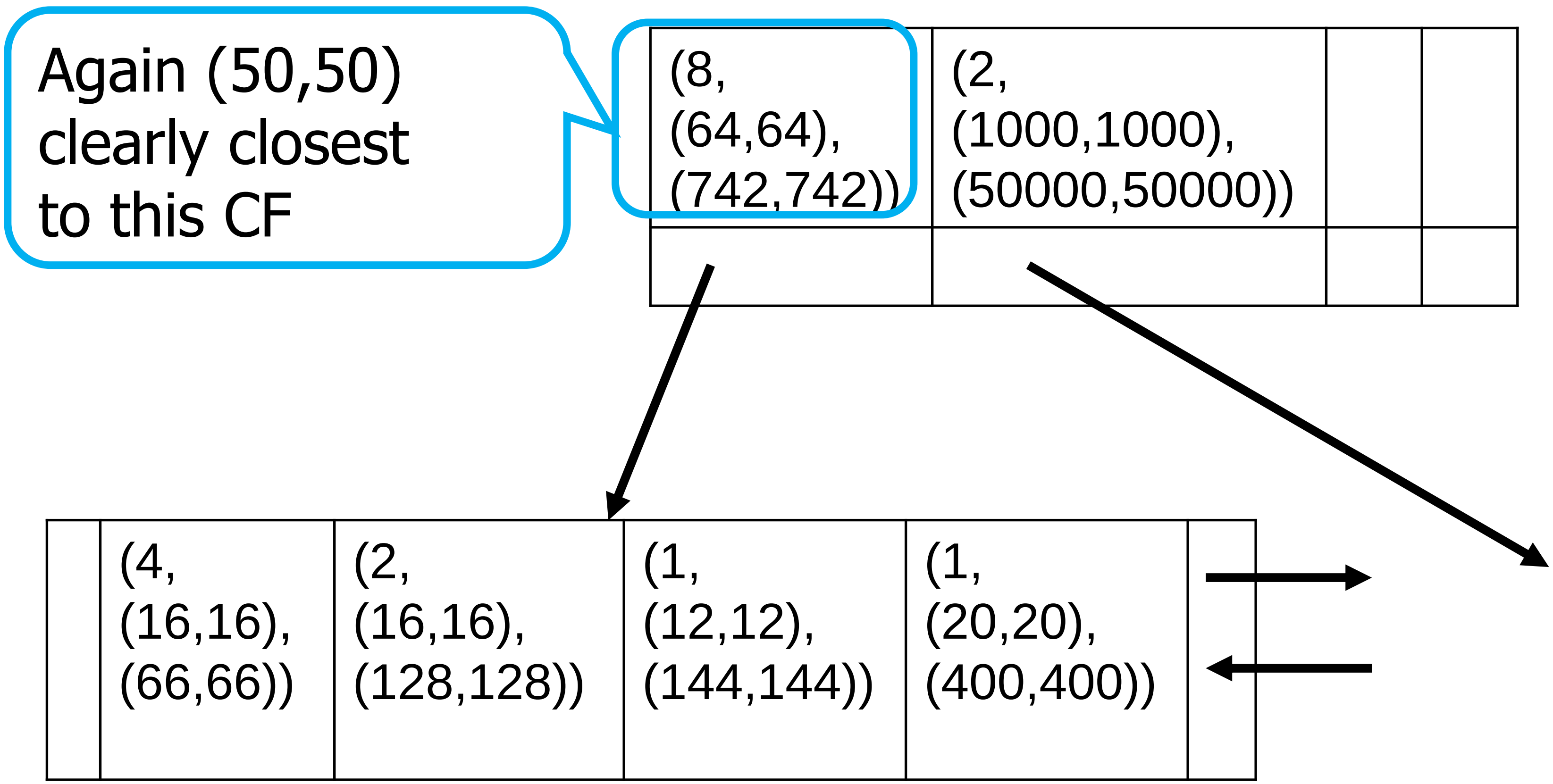
Example: Insert (4,4) into CF Tree



Example: Result After Inserting (4,4) into CF Tree



Now Insert (50,50) into CF Tree



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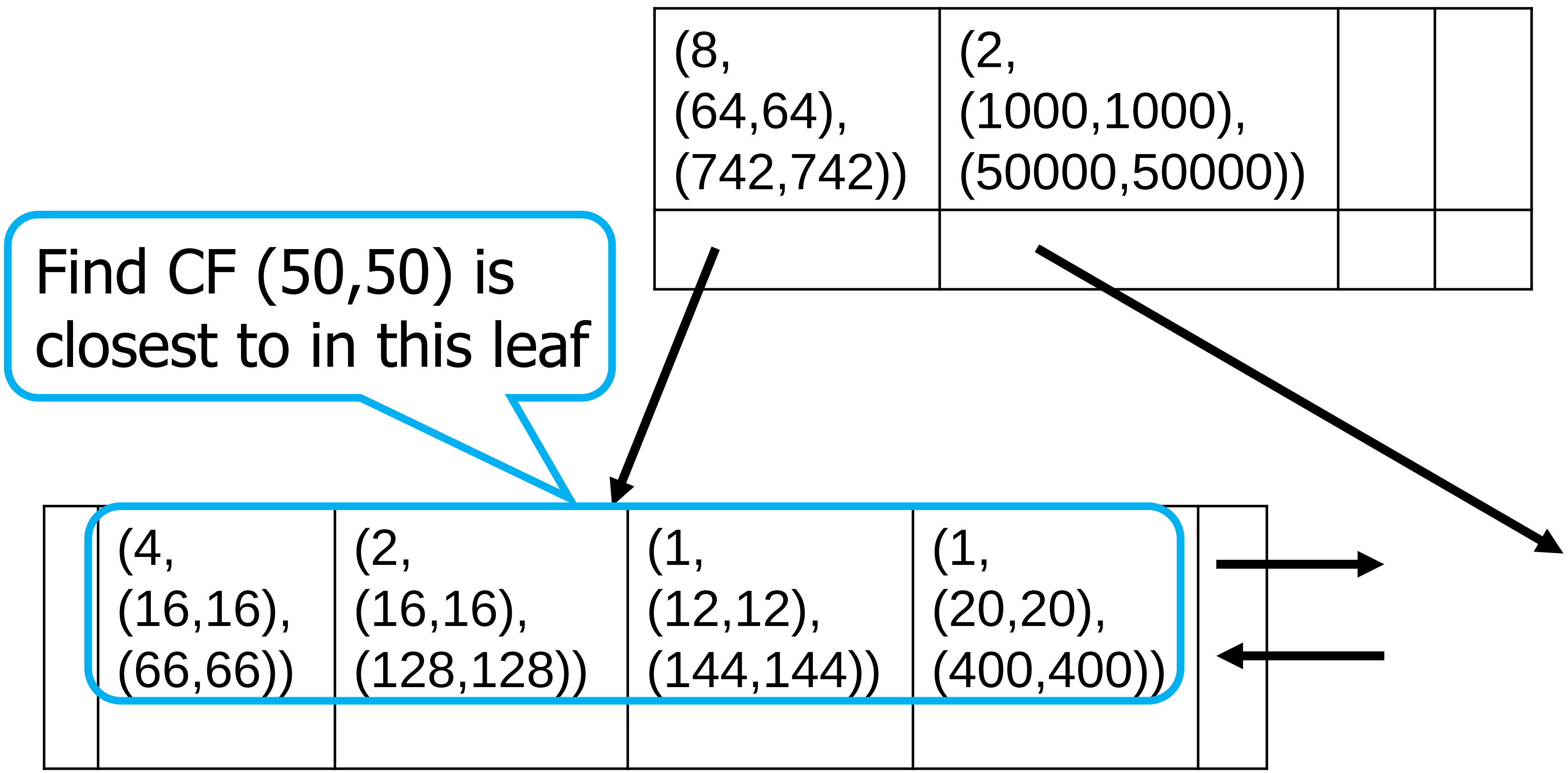

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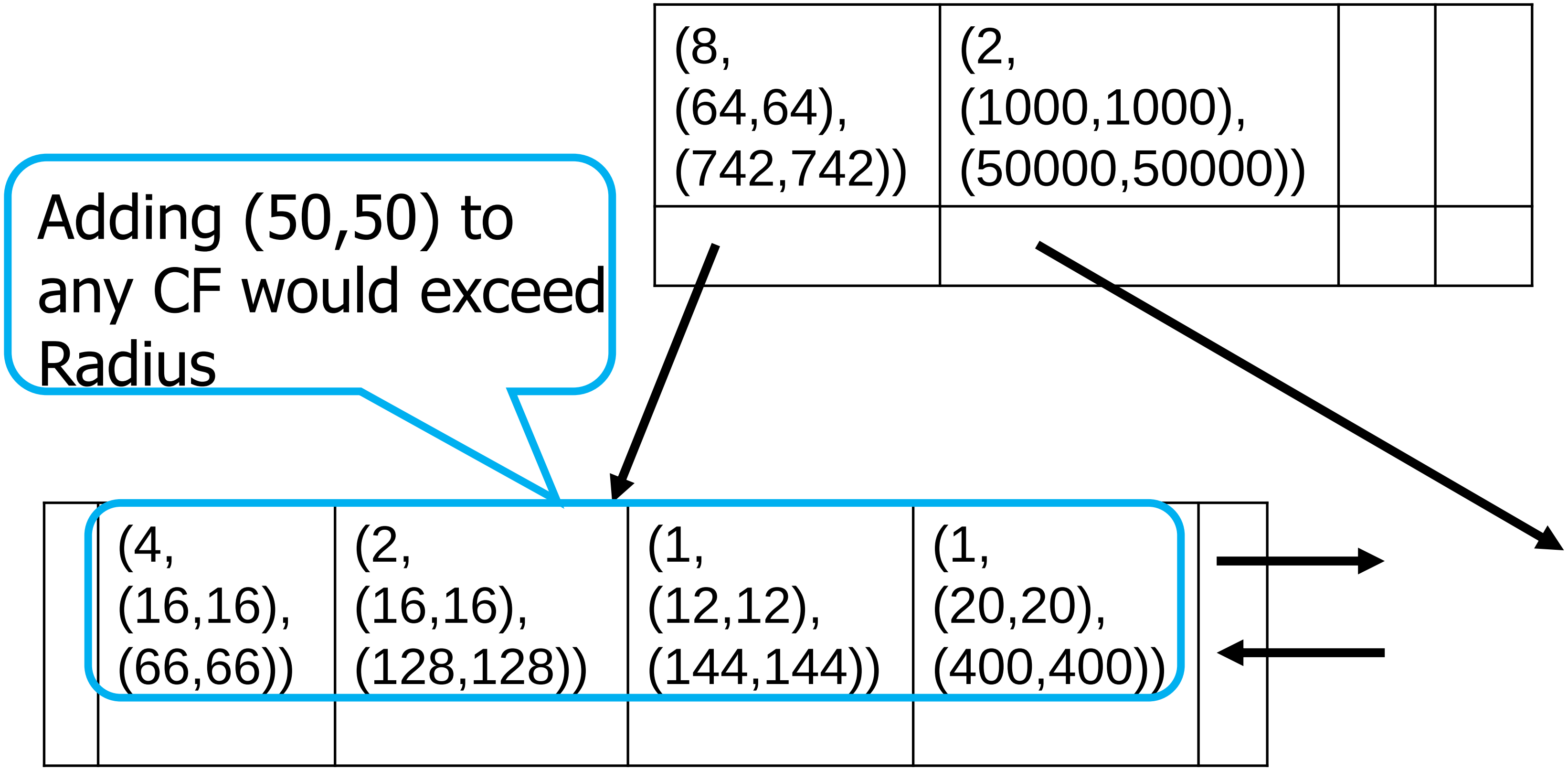

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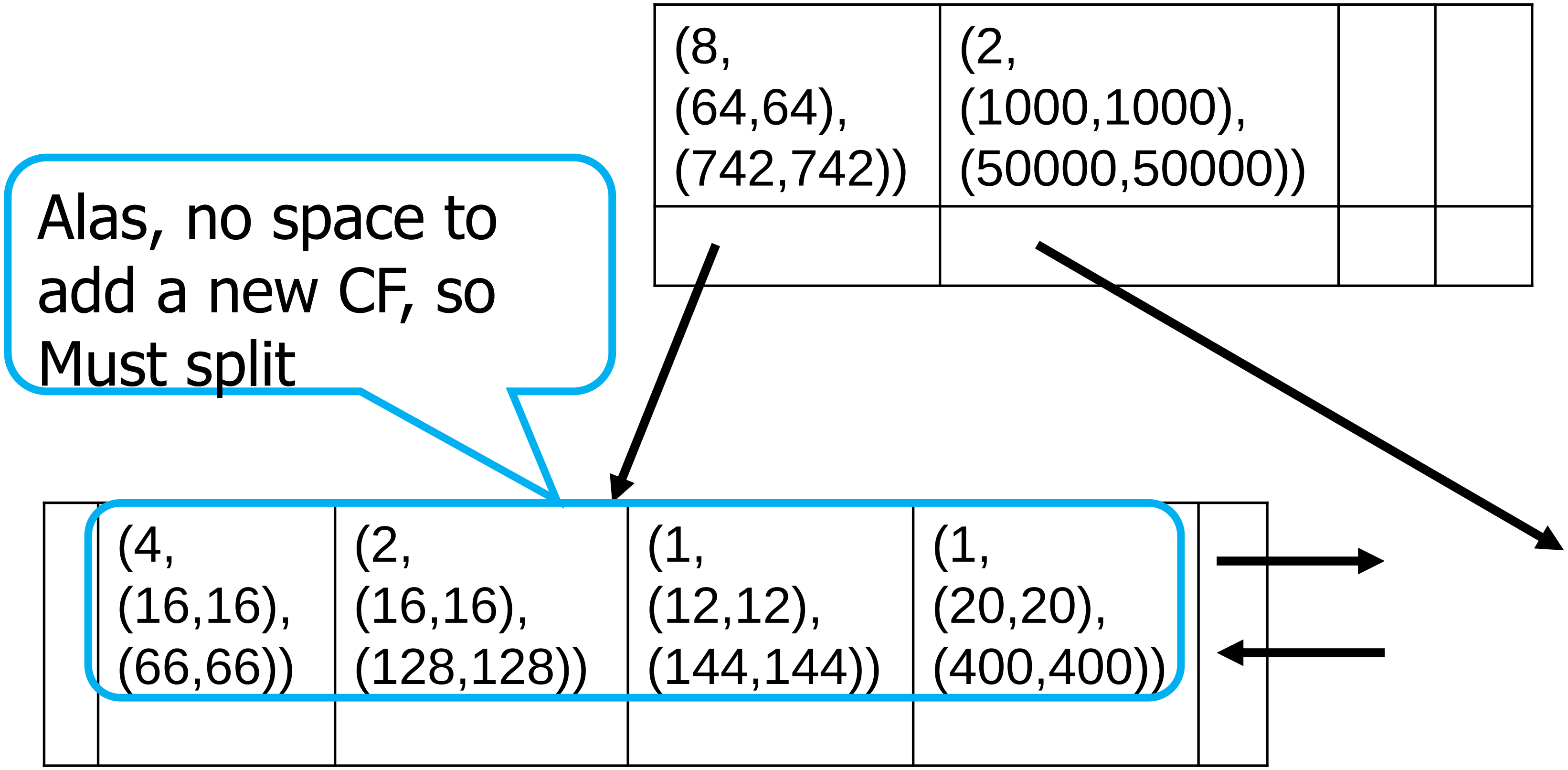
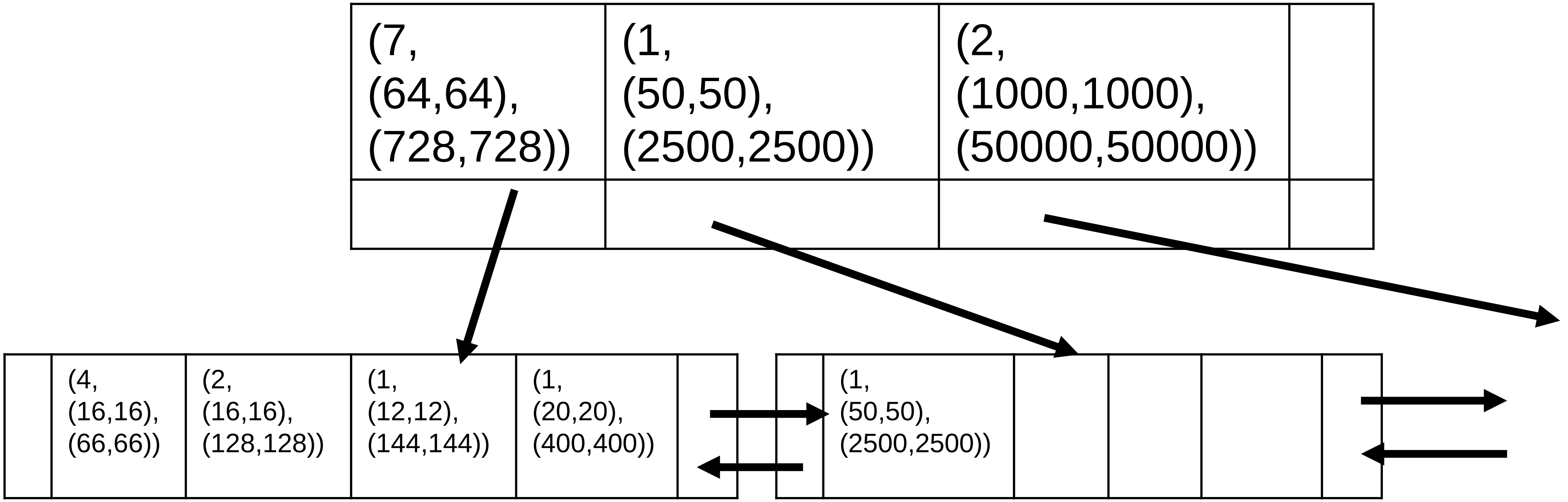
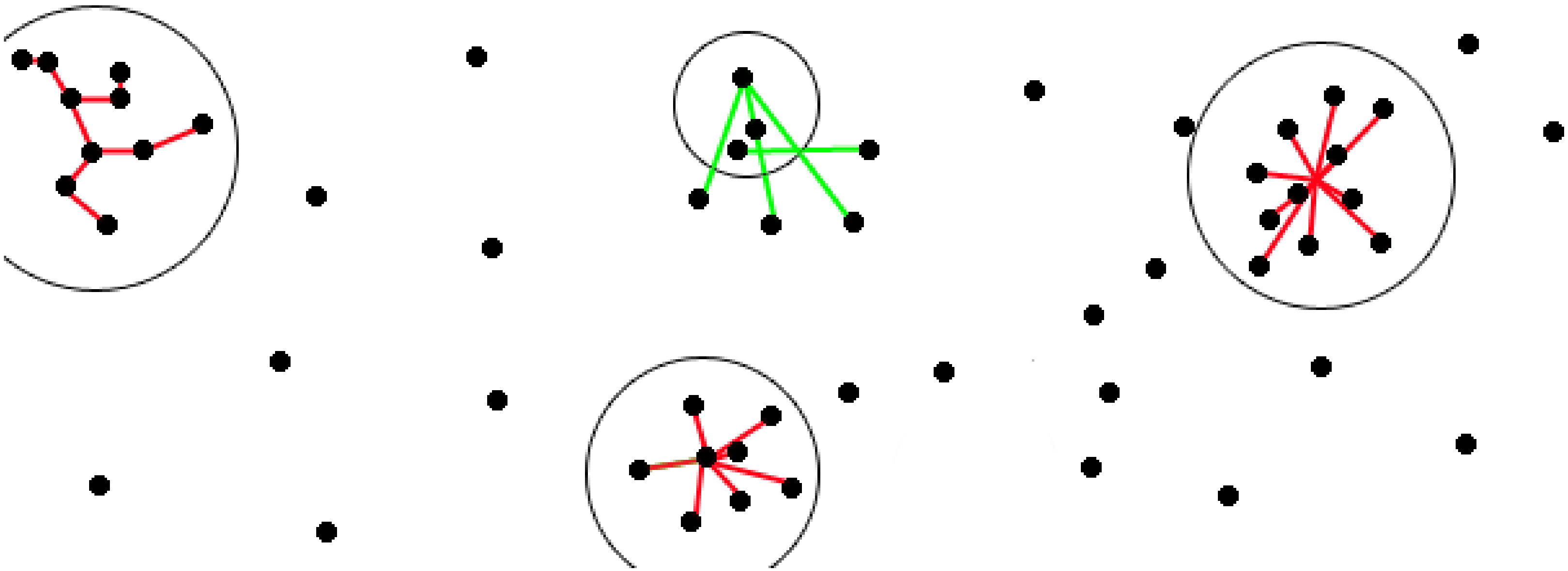


After Inserting (50,50) into CF Tree



Traditional Algorithms

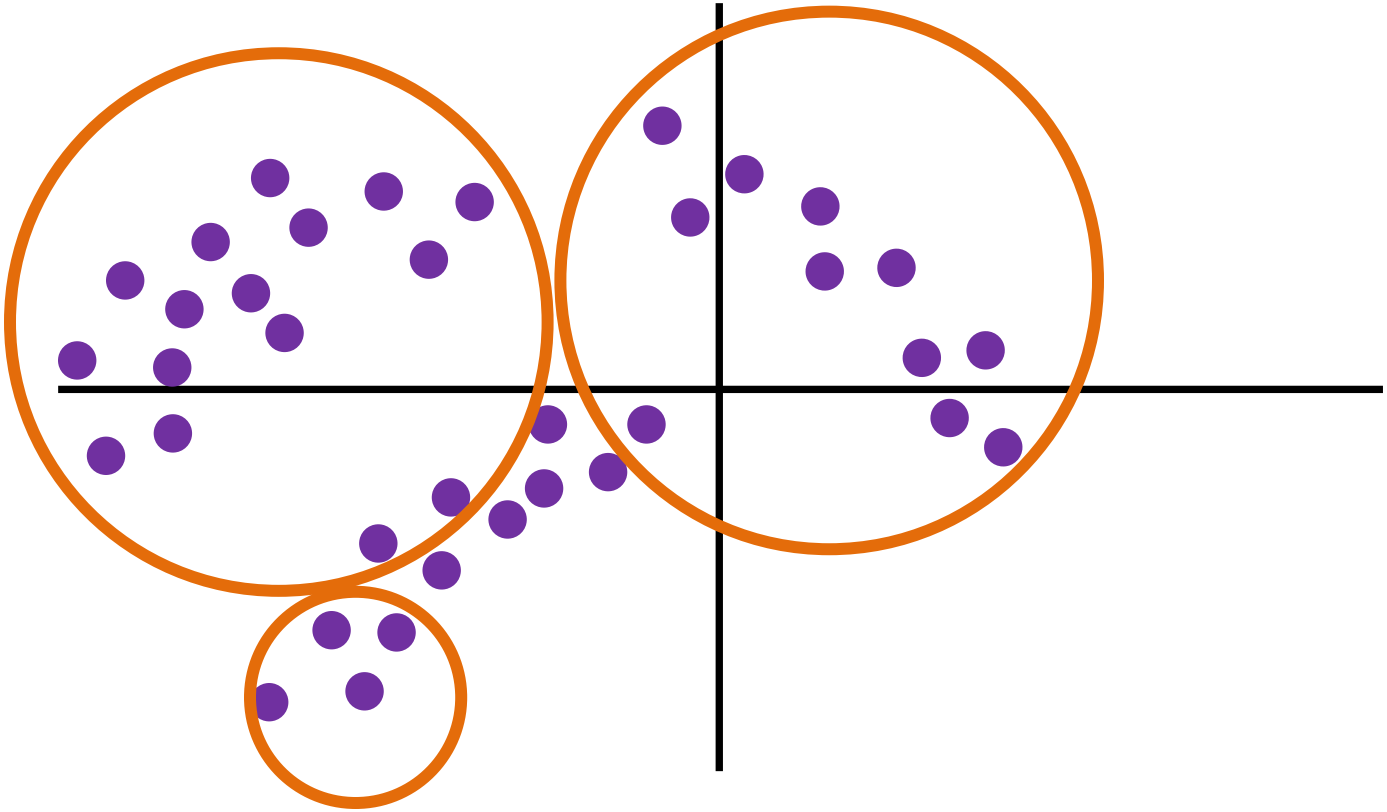


All-Points Based | Centroid Based

d_{min}, d_{max} | d_{avg}, d_{mean}

What Would BIRCH Do?

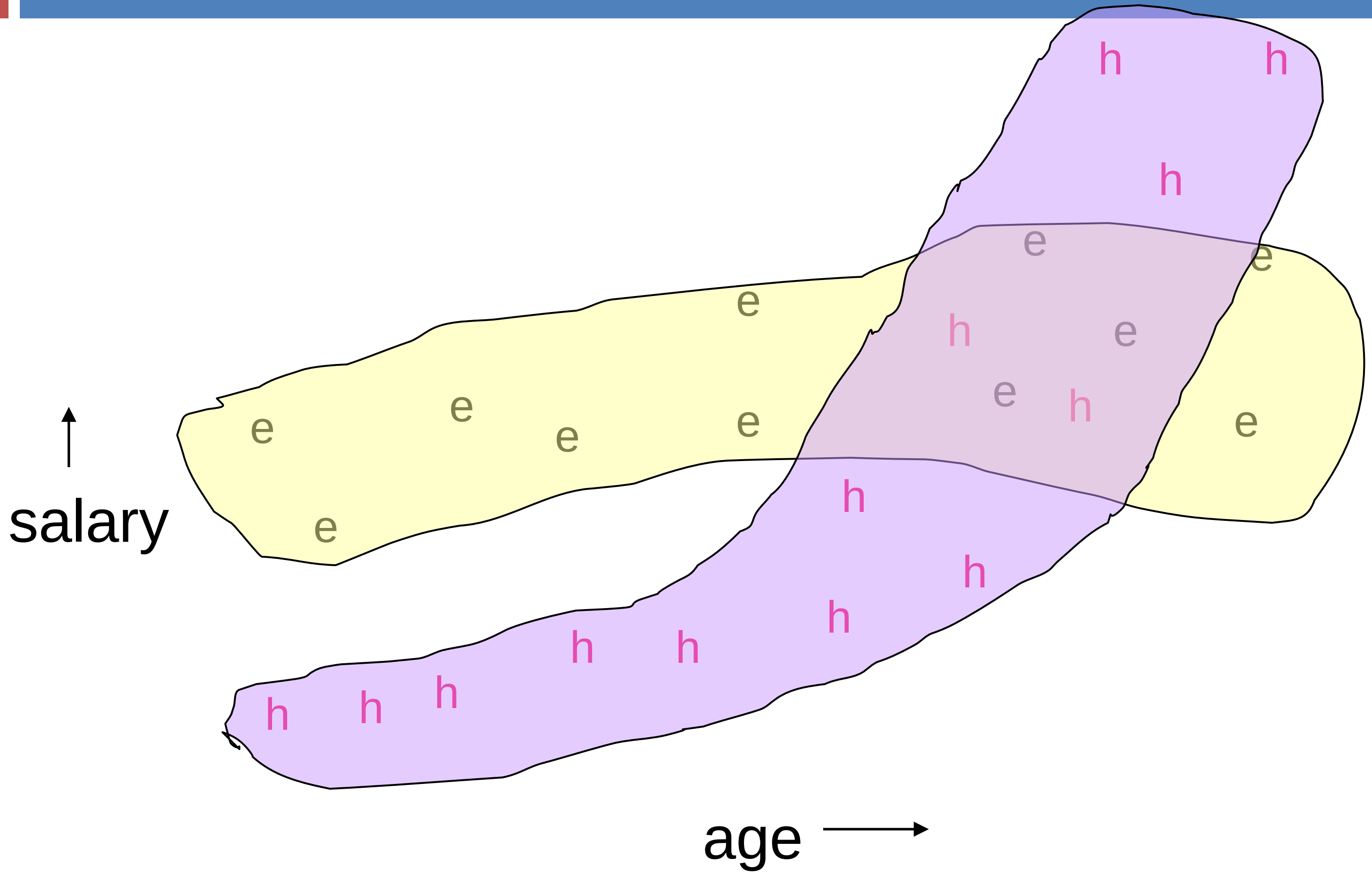
- **BIRCH assumes:**
  - Clusters are normally distributed in each dimension
  - Axes are fixed: Ellipses at an angle are ***not*** ***OK***



Clustering Using Representatives (CURE)

- Cluster definition: Set of representative points
  - Enables clusters of differing shapes
- Requires an Euclidean space
- Two-pass (hierarchical) clustering approach
  - Pass 1: Clustering of subset of data to pick “representative” points
  - Pass 2: Assign all points to clusters

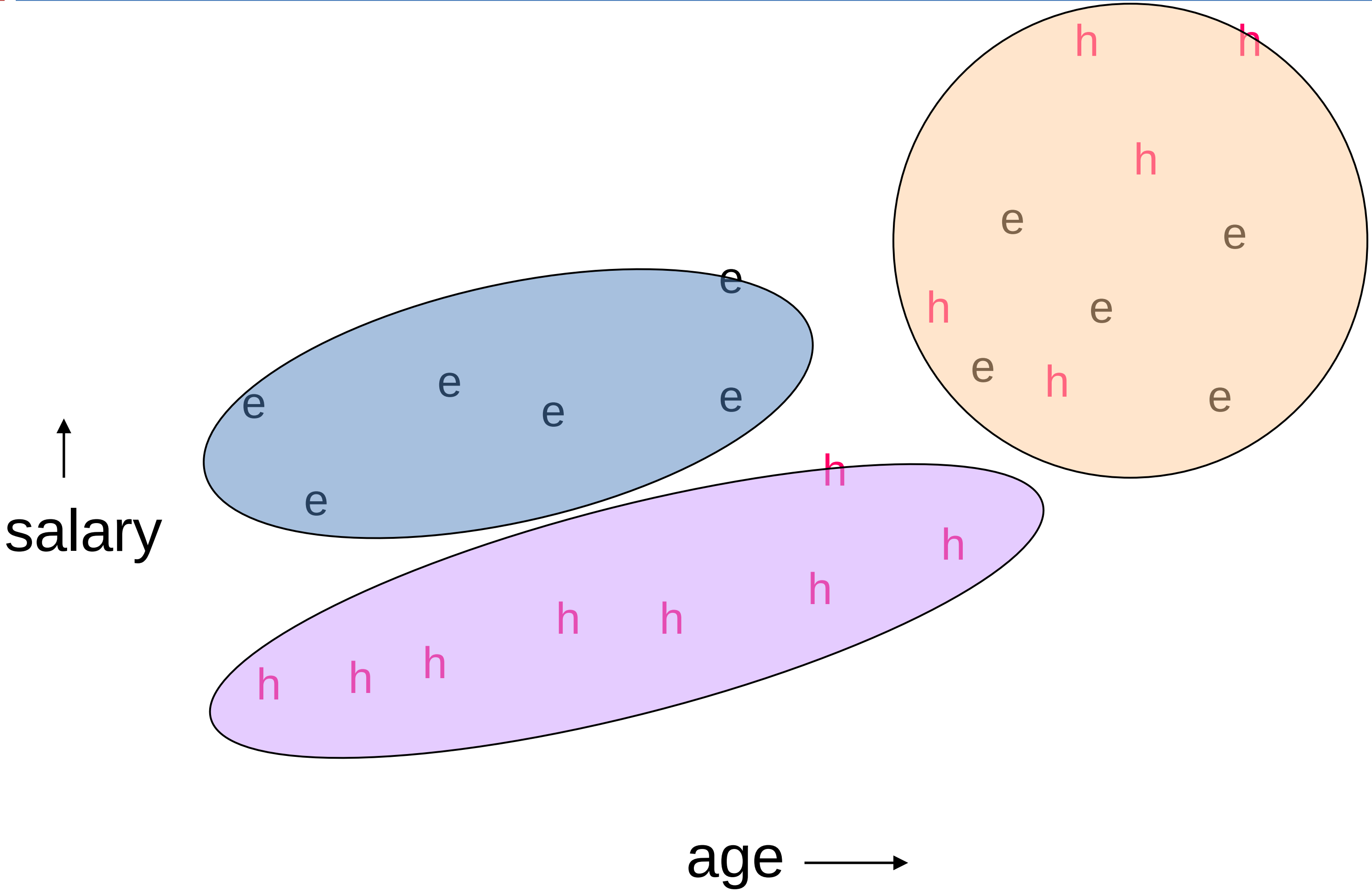
Example: Stanford Salaries



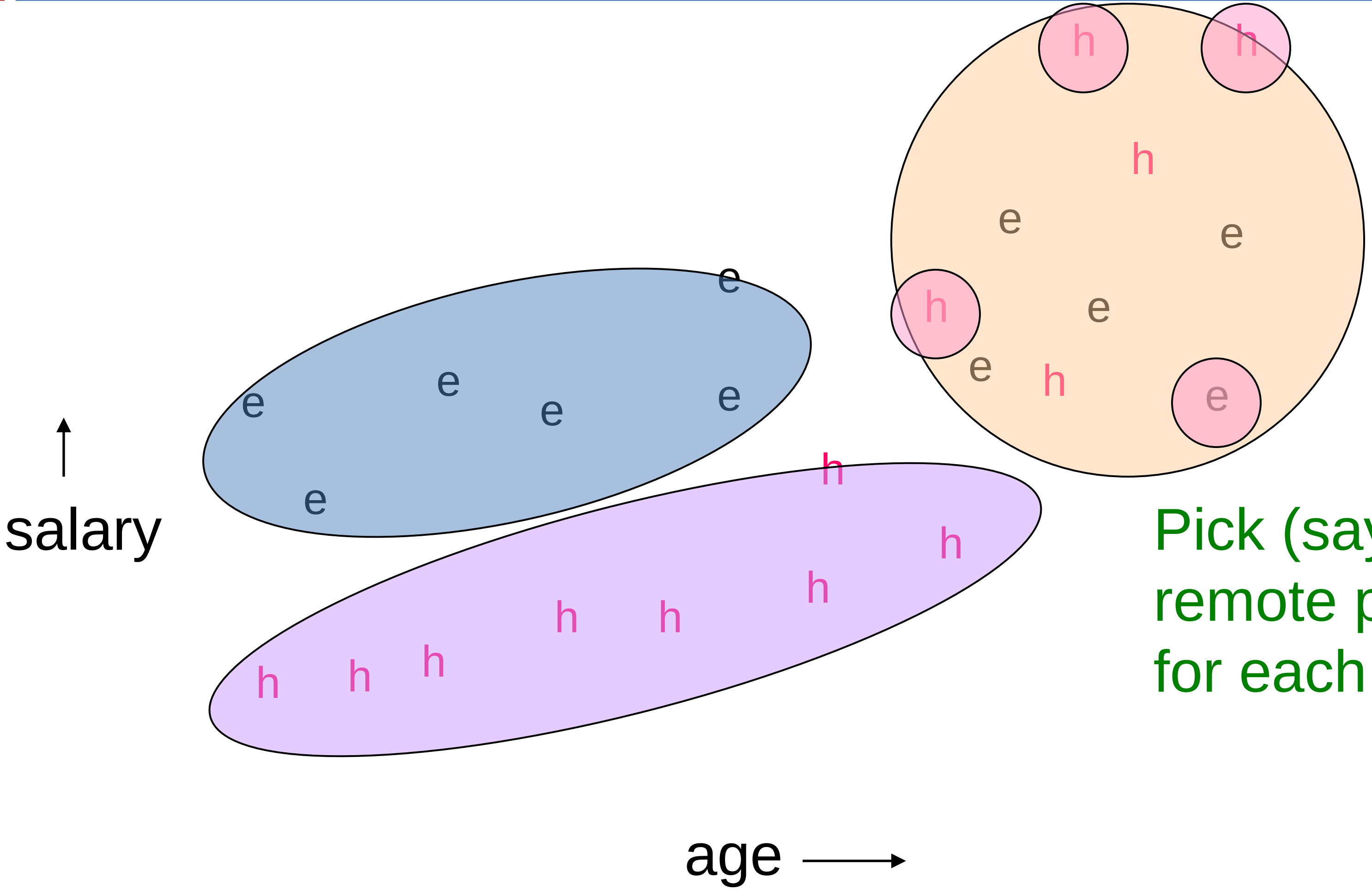
Pass 1

- Randomly sample of data that fits in memory
- Find initial clusters: Hierarchically cluster the data sample
- For each cluster, pick representative points
  - Select subset of points, as dispersed as possible to represent cluster
  - Move these points towards cluster center (e.g., shrink 20% towards mean)

Example: Initial Clusters

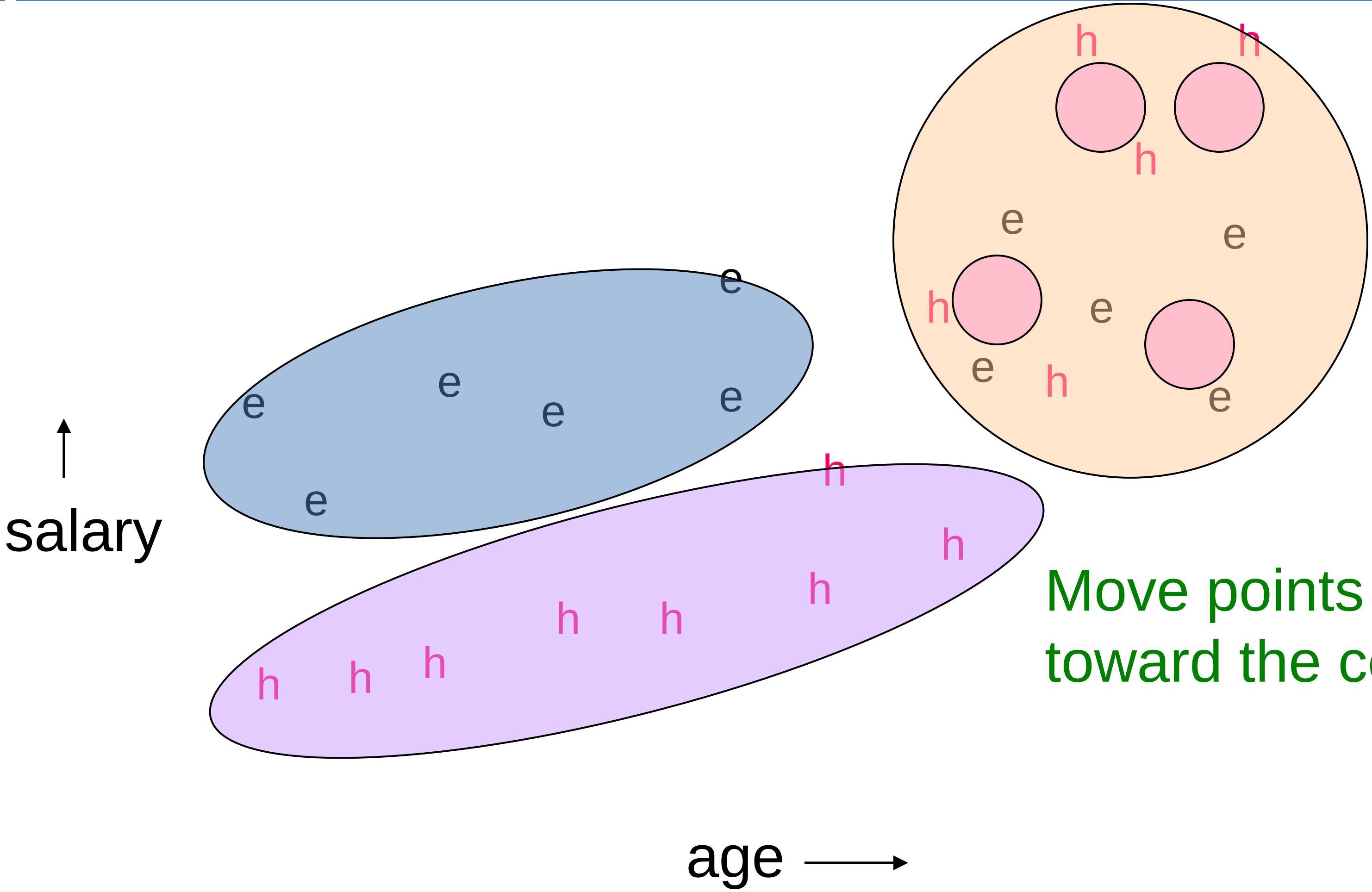


Example: Pick Dispersed Points



Pick (say) 4 remote points for each cluster.

Example: Pick Dispersed Points

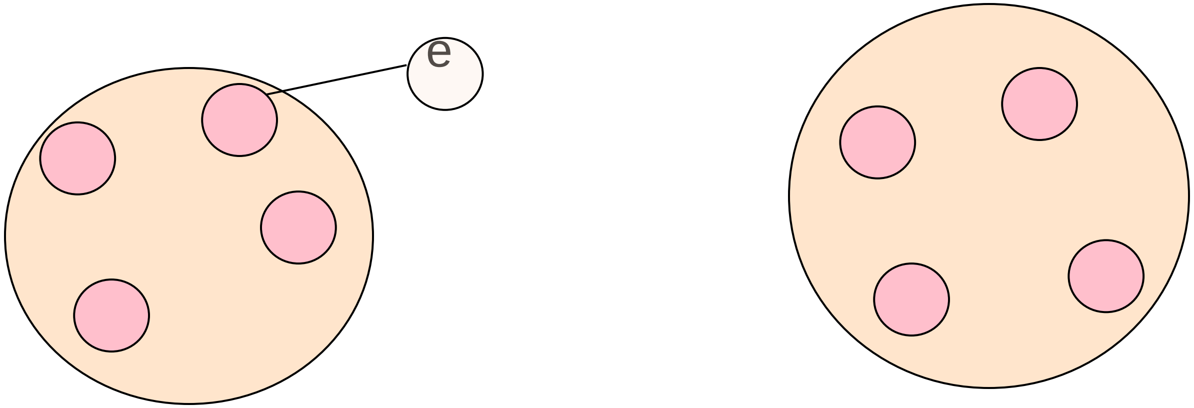


Move points (say) 20% toward the centroid.

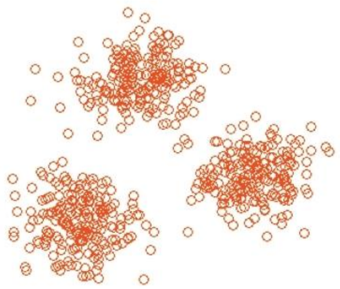
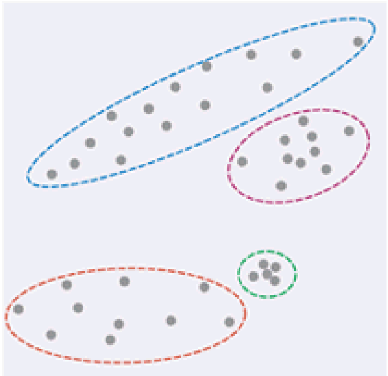
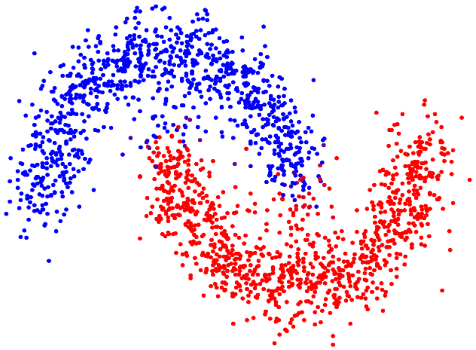
Pass 2

- Scan entire data set

- Assign each example e to "closest" cluster
  - Standard metric determines closest
  - Done by finding representative with smallest distance to e



BIRCH vs. CURE Summary

BIRCH		CURE
		
Fixed axes, normally distributed in each dimension	Rotated axes	Non-ellipsoid shape

Summary

- Hierarchical clustering models hierarchical structure among the examples
- Typically learned in a bottom-up manner
  - Linkage and distance are key parameters
  - Scalability is a key concern
- Advanced algorithms improve efficiency
- Shapes that can be represented are algorithm dependent

Questions?

- CURE slides from MMDS.org