More Clustering

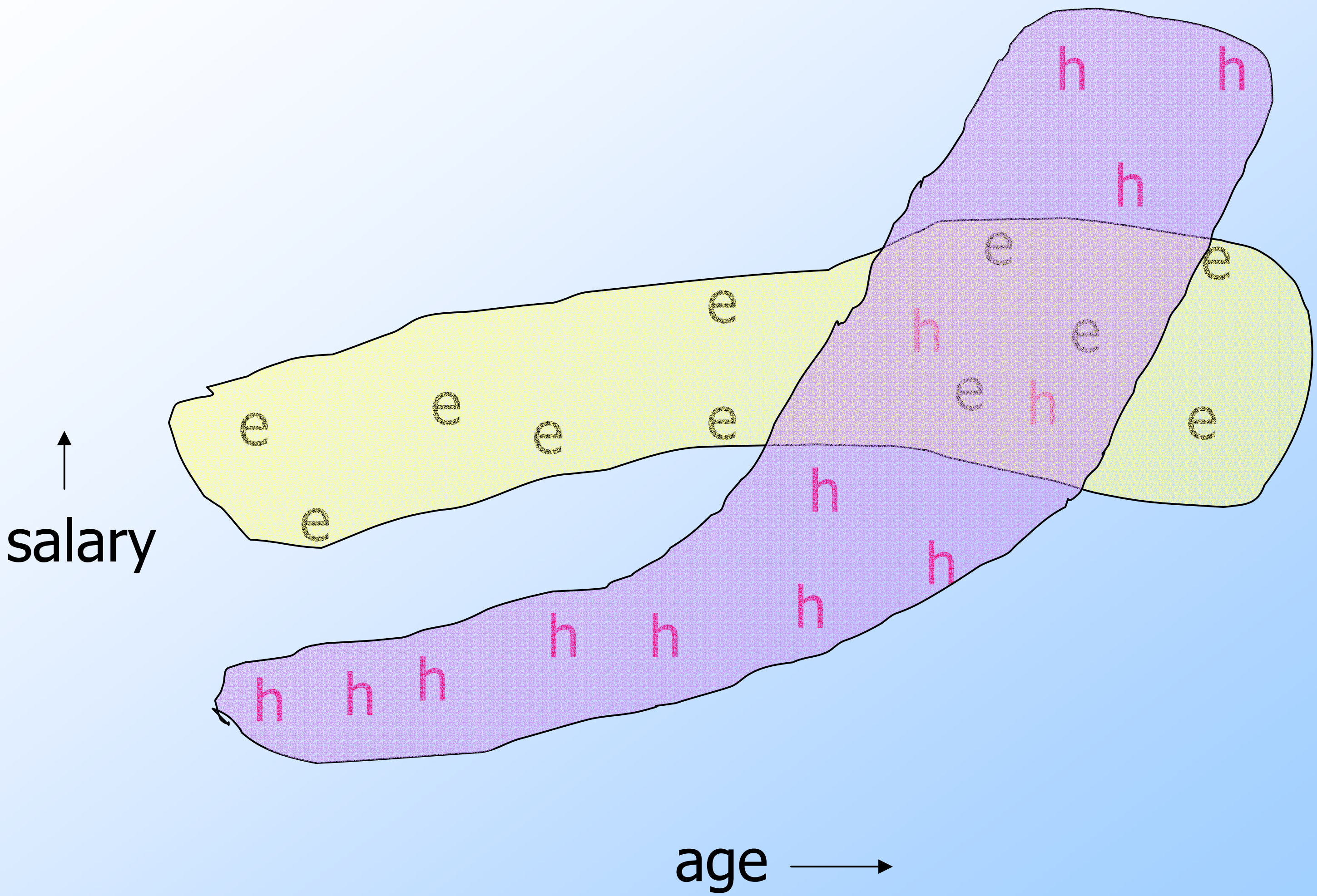
CURE Algorithm

Non-Euclidean Approaches

The CURE Algorithm

- Problem with BFR/*k* -means:
  - Assumes clusters are normally distributed in each dimension.
  - And axes are fixed --- ellipses at an angle are not OK.
- CURE:
  - Assumes a Euclidean distance.
  - Allows clusters to assume any shape.

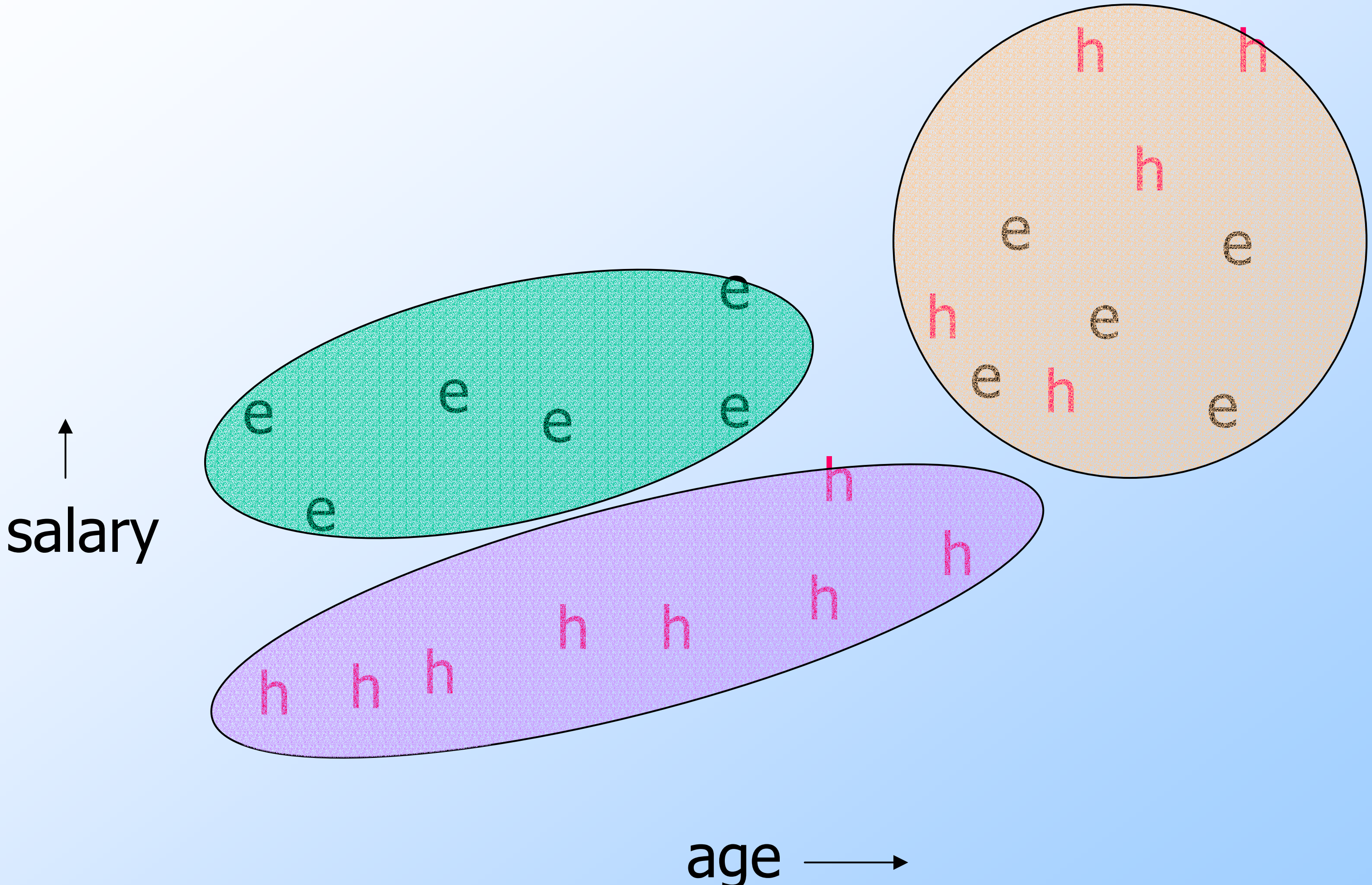
Example: Stanford Faculty Salaries



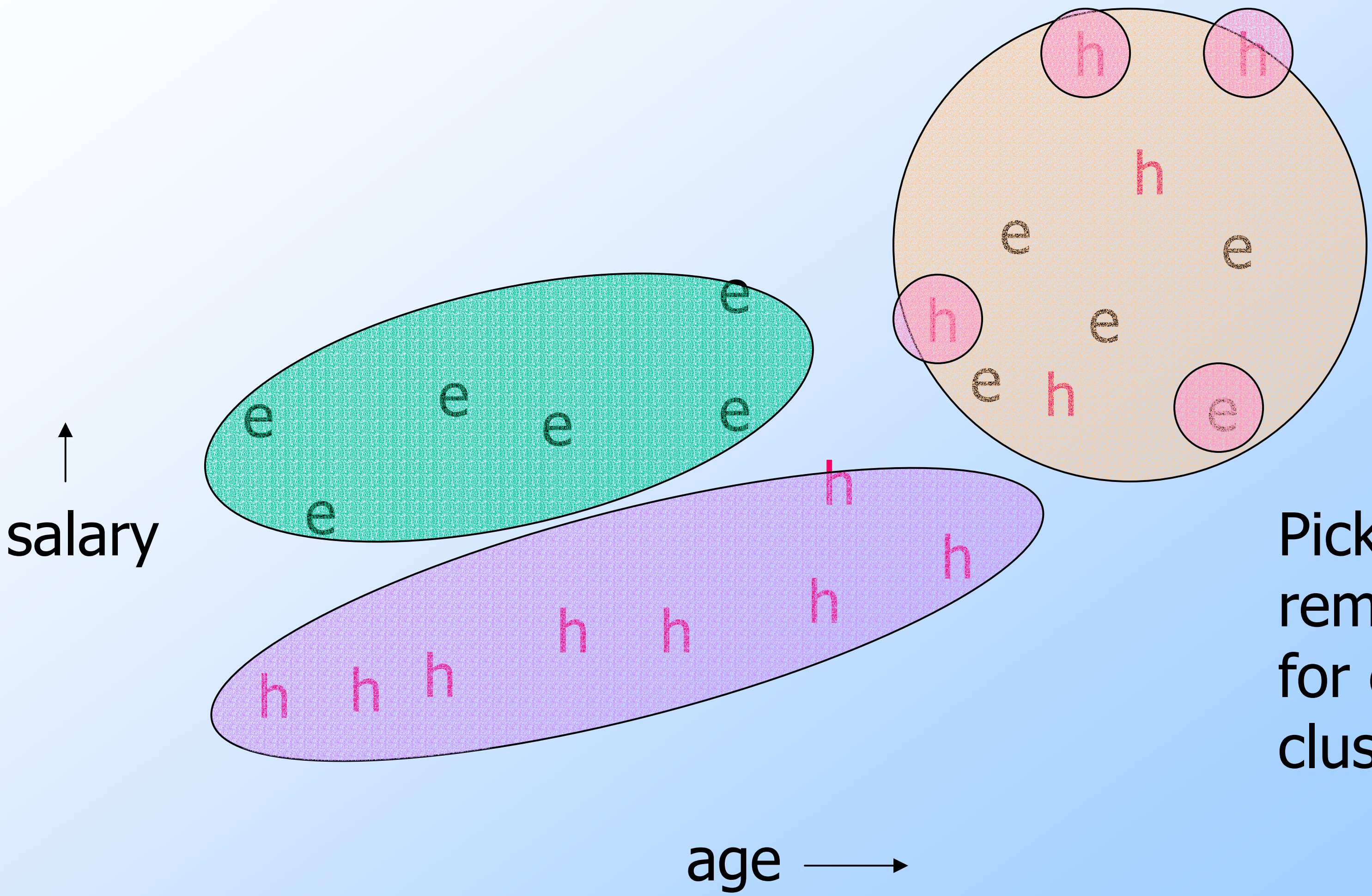
Starting CURE

1. Pick a random sample of points that fit in main memory.
2. Cluster these points hierarchically --- group nearest points/clusters.
3. For each cluster, pick a sample of points, as dispersed as possible.
4. From the sample, pick representatives by moving them (say) 20% toward the centroid of the cluster.

Example: Initial Clusters

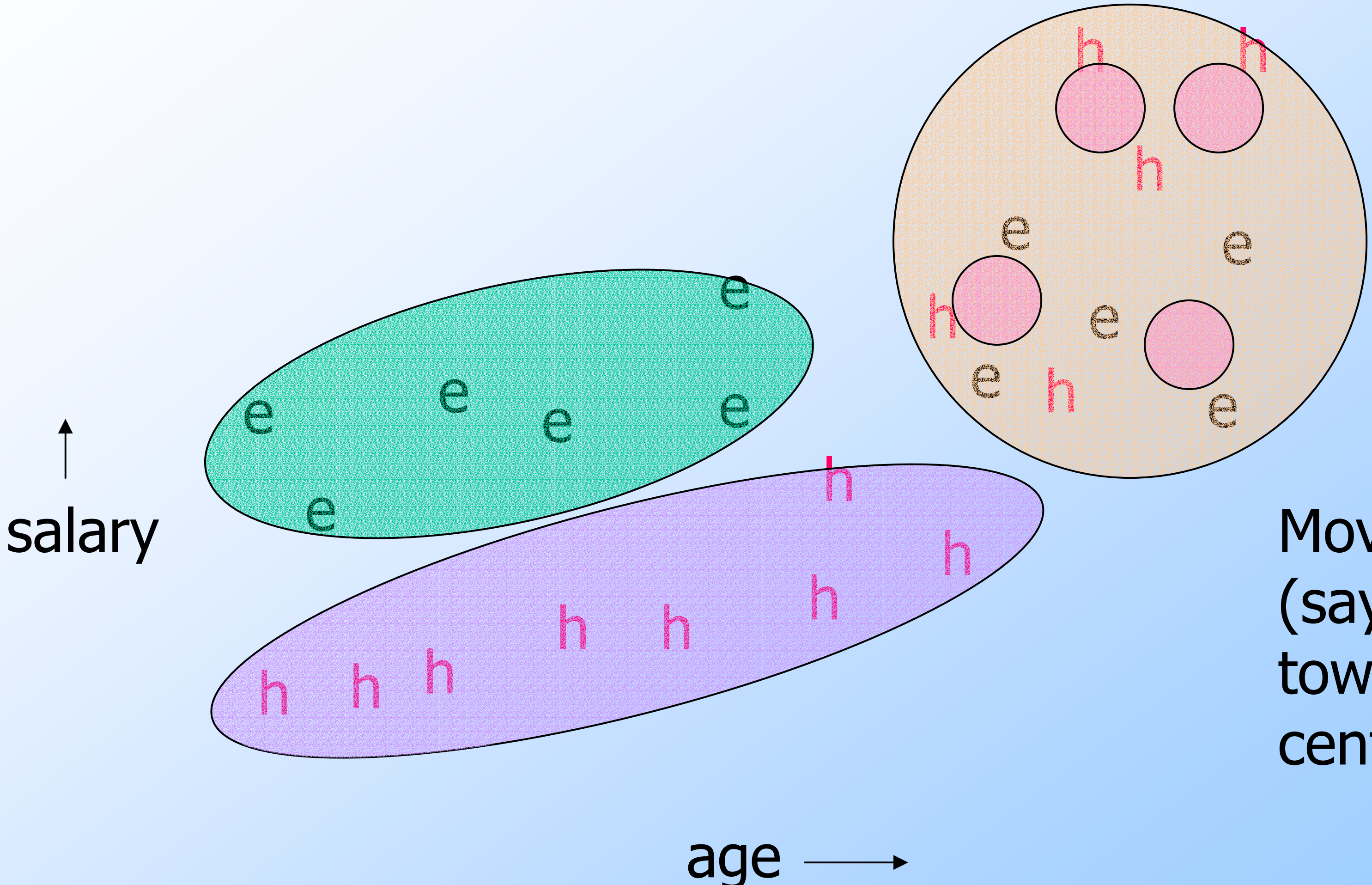


Example: Pick Dispersed Points



Pick (say) 4 remote points for each cluster.

Example: Pick Dispersed Points



Move points (say) 20% toward the centroid.

Finishing CURE

- Now, visit each point *p* in the data set.
- Place it in the "closest cluster."
  - Normal definition of "closest": that cluster with the closest (to *p*) among all the sample points of all the clusters.

Curse of Dimensionality

- One way to look at it: in large-dimension spaces, random vectors are perpendicular. Why?
  - Argument #1: Lots of 2-dim subspaces. There must be one where the vectors' projections are almost perpendicular.
  - Argument #2: Expected value of cosine of angle is 0.

Cosine of Angle Between Random Vectors

- Assume vectors emanate from the origin (0,0,…,0).
- Components are random in range [-1,1].
- $(a_1,a_2,\ldots,a_n).(b_1,b_2,\ldots,b_n)$ has expected value 0 and a standard deviation that grows as $\sqrt{n}$.
- But lengths of both vectors grow as $\sqrt{n}$.
- So dot product around $\sqrt{n}/ (\sqrt{n} * \sqrt{n}) = 1/\sqrt{n}$.

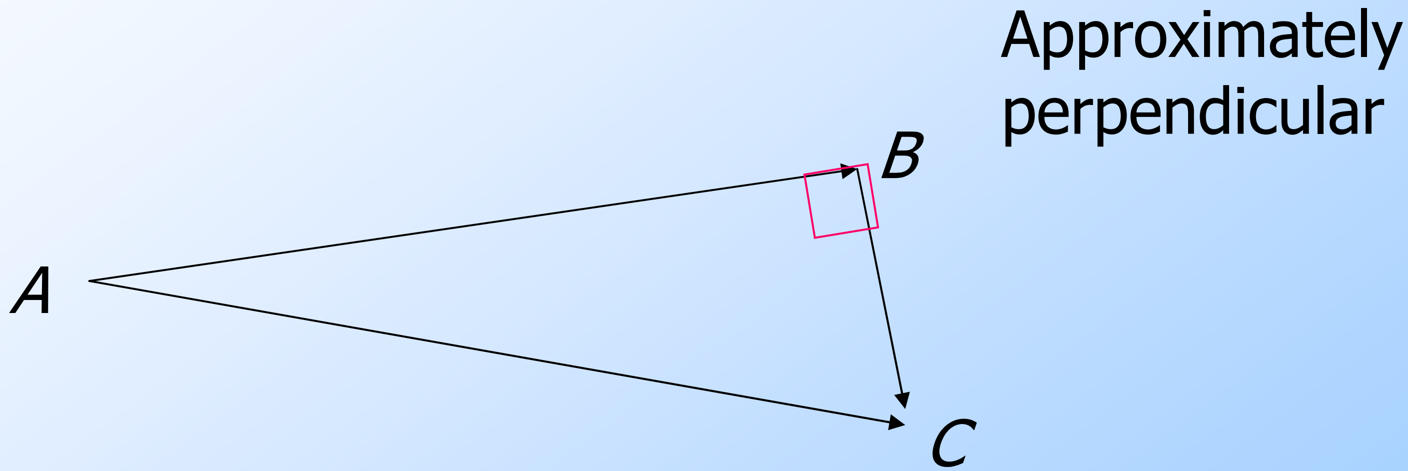
Random Vectors --- Continued

- Thus, a typical pair of vectors has an angle whose cosine is on the order of $1/\sqrt{n}$.
- As $n \to \infty$, that's 0; i.e., the angle is about 90°.

Interesting Consequence

- Suppose "random vectors are perpendicular," even in non-Euclidean spaces.
- Suppose we know the distance from A to B, say $d(A,B)$, and we also know $d(B,C)$, but we don't know $d(A,C)$.
- Suppose B and C are fairly close, say in the same cluster.
- What is $d(A,C)$?

Diagram of Situation



Assuming points lie in a plane:

$d(A,B)^2 + d(B,C)^2 = d(A,C)^2$

Important Point

- Why do we assume AB is perpendicular to AC, and not that either of the other two angles are right-angles?
  1. AB and AC are not "random vectors"; they each go to points that are far away from A and close to each other.
  2. If AB is longer than AC, then it is angle ACB that is right, but both ACB and ABC are approximately right-angles.

Dealing With a Non-Euclidean Space

- Problem: clusters cannot be represented by centroids.
- Why? Because the "average" of "points" might not be a point in the space.
- Best substitute: the *clustroid* = point in the cluster that minimizes the sum of the squares of distances to the points in the cluster.

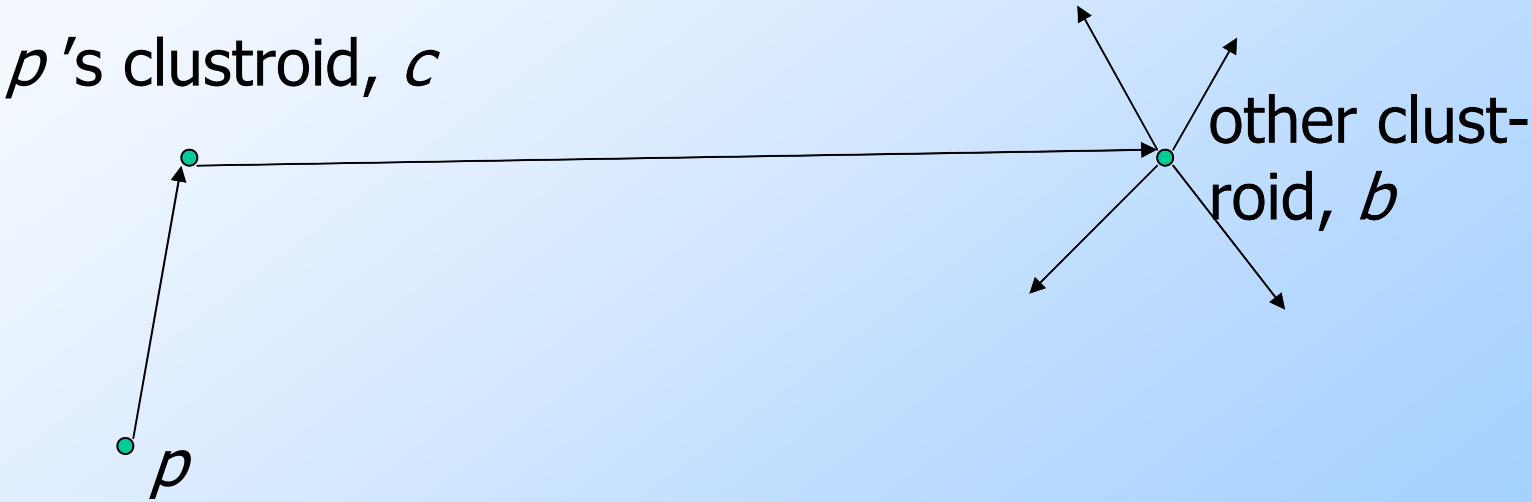
Representing Clusters in Non-Euclidean Spaces

- Recall BFR represents a Euclidean cluster by N, SUM, and SUMSQ.
- A non-Euclidean cluster is represented by:
  - N.
  - The clustroid.
  - Sum of the squares of the distances from clustroid to all points in the cluster.

Example of CoD Use

- Problem: in non-Euclidean space, we want to decide whether to merge two clusters.
  - Each cluster represented by *N*, clustroid, and "SUMSQ."
  - Also, SUMSQ for each point in the cluster, even if it is not the clustroid.
- Merge if SUMSQ for new cluster is "low."

Estimating SUMSQ



Suppose *p* Were the Clustroid of Combined Cluster

- It's SUMSQ would be the sum of:
  1. Old SUMSQ(p) [for old cluster containing p].
  2. SUMSQ(b) plus $d(p,b)^2$ times number of points in b's cluster.
- Critical point: vector p -> b assumed perpendicular to vectors from b to all other points in its cluster --- justifies (2).

Combining Clusters --- Continued

- We can thus estimate SUMSQ for each point in the combined cluster. Take the point with the least SUMSQ as the clustroid of the new cluster --- provided that SUMSQ is small enough.

The GRGPF Algorithm

- From Ganti et al. --- see reading list.
- Works for non-Euclidean distances.
- Works for massive (disk-resident) data.
- Hierarchical clustering.
- Clusters are grouped into a tree of disk blocks (like a B-tree or R-tree).

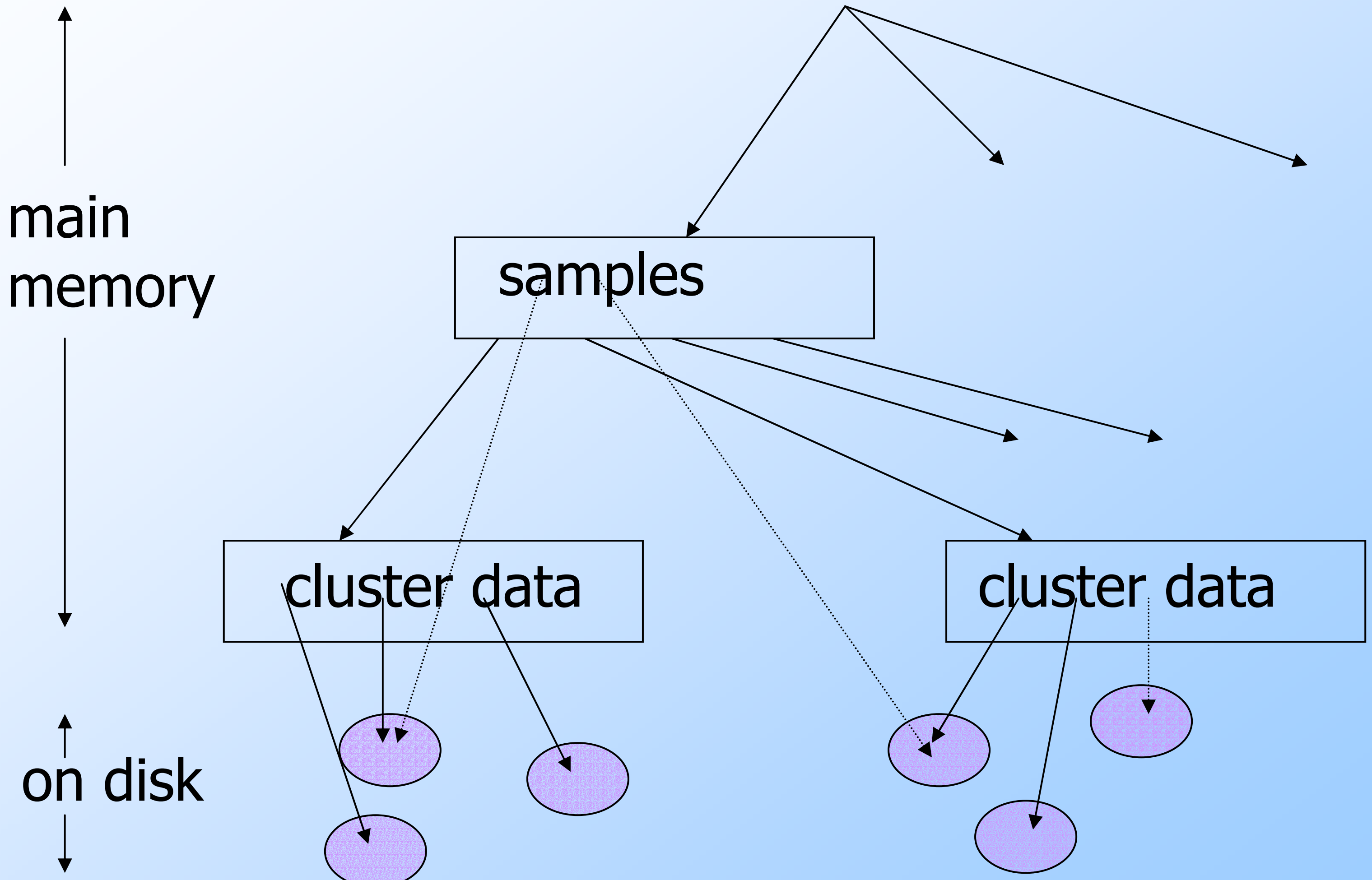
Information Retained About a Cluster

1. *N*, clustroid, SUMSQ.
2. The *p* points closest to the clustroid, and their values of SUMSQ.
3. The *p* points of the cluster that are furthest away from the clustroid, and their SUMSQ's.

At Interior Nodes of the Tree

- Interior nodes have samples of the clustroids of the clusters found at descendant leaves of this node.
- Try to keep clusters on one leaf block close, descendants of a level-1 node close, etc.
- Interior part of tree kept in main memory.

Picture of the Tree



Initialization

- Take a main-memory sample of points.
- Organize them into clusters hierarchically.
- Build the initial tree, with level-1 interior nodes representing clusters of clusters, and so on.
- All other points are inserted into this tree.

Inserting Points

- Start at the root.
- At each interior node, visit one or more children that have sample clustroids near the inserted point.
- At the leaves, insert the point into the cluster with the nearest clustroid.

Updating Cluster Data

- Suppose we add point X to a cluster.
- Increase count N by 1.
- For each of the $2p + 1$ points Y whose SUMSQ is stored, add $d(X,Y)^2$.
- Estimate SUMSQ for X.

Estimating SUMSQ(X)

- If C is the clustroid, SUMSQ(X) is, by the CoD assumption:
  $Nd(X,C)^2$ + SUMSQ(C)
  - Based on assumption that vector from X to C is perpendicular to vectors from C to all the other nodes of the cluster.
- This value may allow X to replace one of the closest or furthest nodes.

Possible Modification to Cluster Data

- There may be a new clustroid --- one of the *p* closest points --- because of the addition of *X*.
- Eventually, the clustroid may migrate out of the *p* closest points, and the entire representation of the cluster needs to be recomputed.

Splitting and Merging Clusters

- Maintain a threshold for the *radius* of a cluster = $\sqrt{(\text{SUMSQ}/N)}$.
- Split a cluster whose radius is too large.
- Adding clusters may overflow leaf blocks, and require splits of blocks up the tree.
  - Splitting is similar to a B-tree.
  - But try to keep locality of clusters.

Splitting and Merging --- (2)

- The problem case is when we have split so much that the tree no longer fits in main memory.
- Raise the threshold on radius and merge clusters that are sufficiently close.

Merging Clusters

- Suppose there are nearby clusters with clustroids *C* and *D*, and we want to consider merging them.
- Assume that the clustroid of the combined cluster will be one of the *p* furthest points from the clustroid of one of those clusters.

Merging --- (2)

- Compute SUMSQ(X) [from the cluster of C] for the combined cluster by summing:
  1. SUMSQ(X) from its own cluster.
  2. SUMSQ(D) + $N[d(X,C)^2 + d(C,D)^2]$.
     - Uses the CoD to reason that the distance from X to each point in the other cluster goes to C, makes a right angle to D, and another right angle to the point.

Merging --- Concluded

- Pick as the clustroid for the combined cluster that point with the least SUMSQ.
- But if this SUMSQ is too large, do not merge clusters.
- Hope you get enough mergers to fit the tree in main memory.

Fastmap

- Not a clustering algorithm --- rather, a method for applying *multidimensional scaling*.
  - That is, mapping the points onto a small-dimension space, so the CoD does not apply.

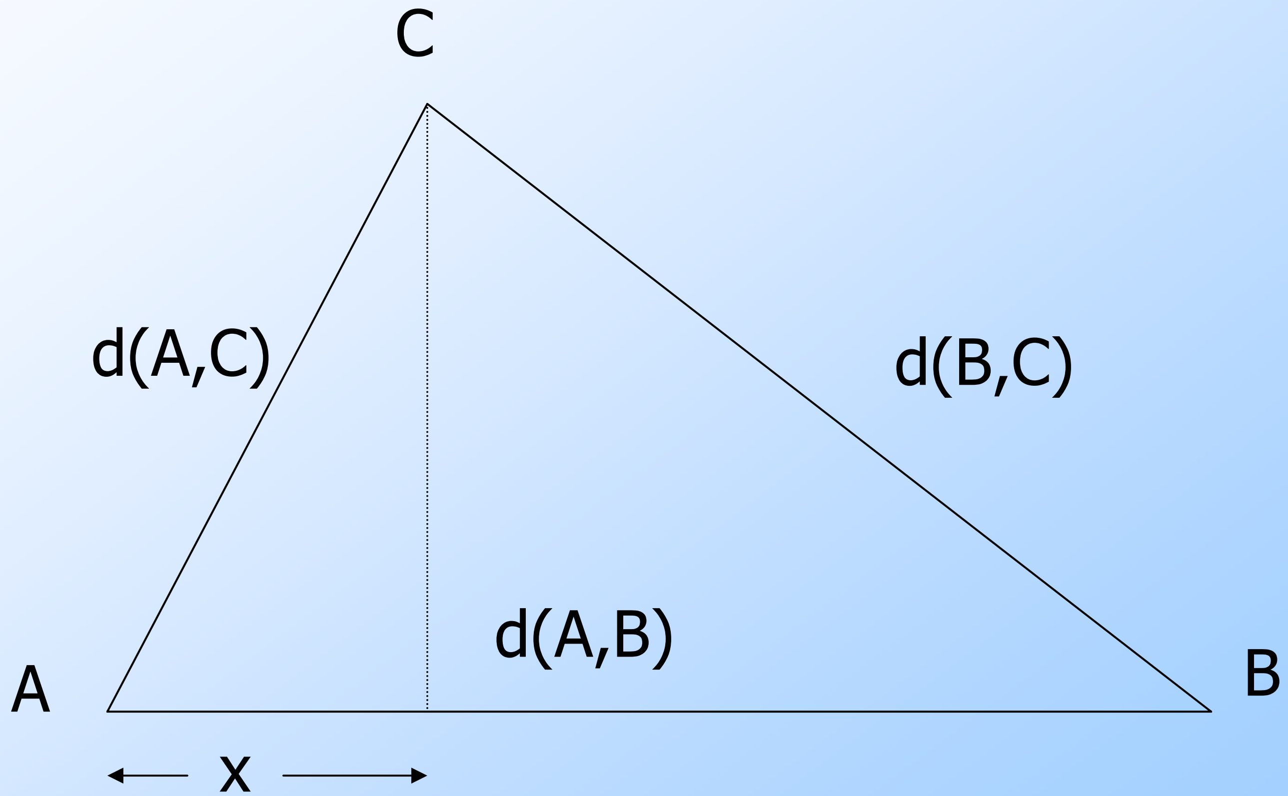
Fastmap --- (2)

- Assumes non-Euclidean space.
  - But like GRGFP pretends it is working in 2-dimensional Euclidean space when it is convenient to do so.
- Goal: map *n* points in much less than $O(n^2)$ time.
  - I.e., you cannot compute distances between each pair of points and place points in k-dim. space to minimize error.

Fastmap --- Key Idea

- Create a "dimension" in non-Euclidean space by:
  1. Pick a pair of points A and B that are far apart.
     - Start with random A; pick most distant B.
  2. Treat AB as an "axis" and project all points onto AB, using the law of cosines.

Projecting Point C Onto AB

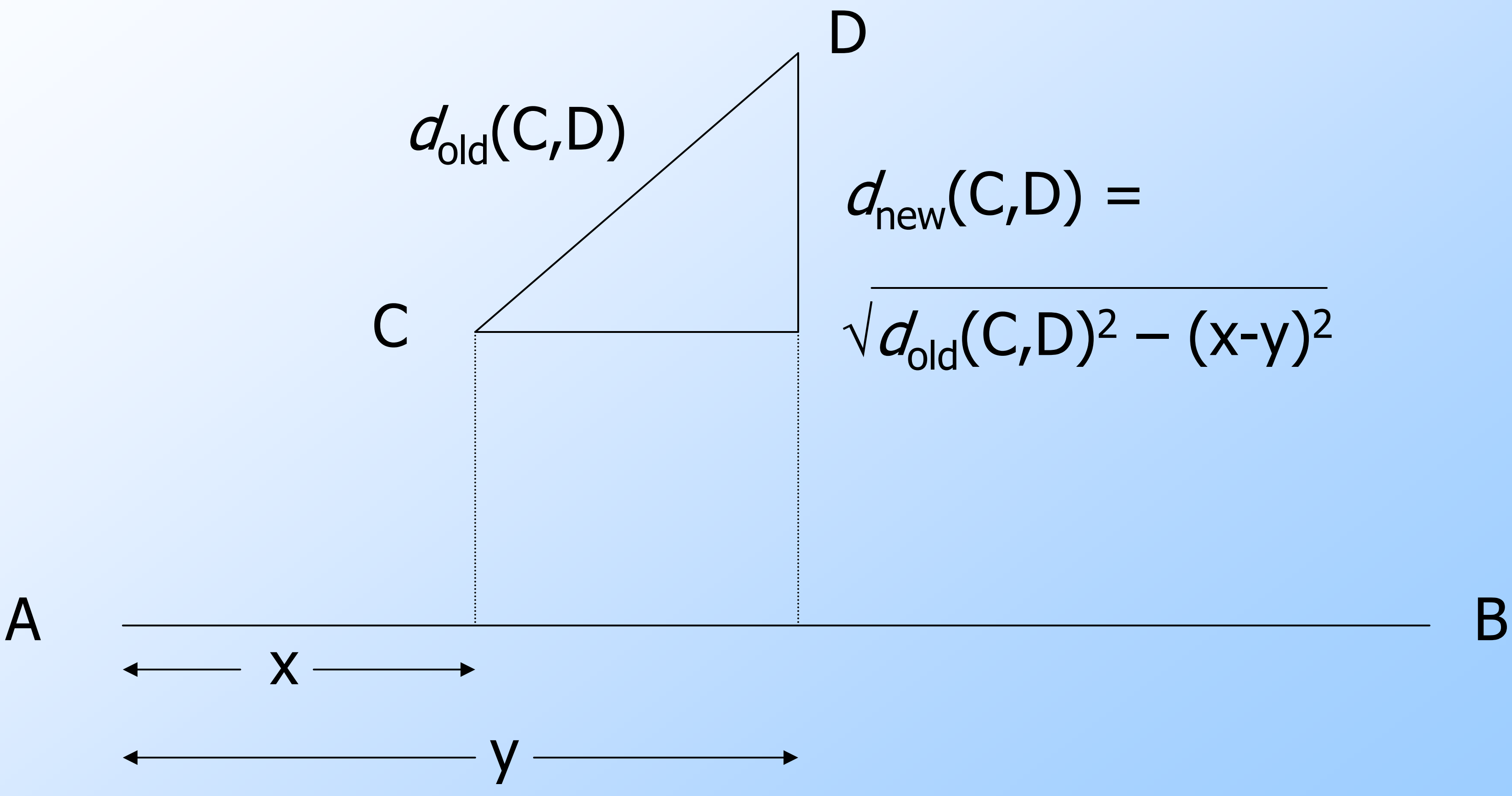


$$x = [d^2(A,C) + d^2(A,B) - d^2(B,C)]/2d(A,B)$$

Revising Distances

- Having computed the position of every point along the *pseudo-axis* AB, we need to lower the distances between points in the "other dimensions."

Picture



But …

- We can’t afford to compute new distances for each pseudo-dimension.
  - It would take O(n^2) time.
- Rather, for each pseudo-dimension, store the position along the pseudo-axis for each point, and adjust the distance between points by square-subtract-sqrt only when needed.
  - I.e., one of the points is an axis-end.

Fastmap --- Summary

- Pick a number of dimensions *k*.

```
FOR i = 1 TO k DO BEGIN
  Pick a pseudo-axis AiBi;
  Compute projection of each
    point onto this pseudo-axis;
END;
```

- Each step is O(ni); total O(nk^2).