CPSC 340:
Machine Learning and Data Mining

Hierarchical Clustering

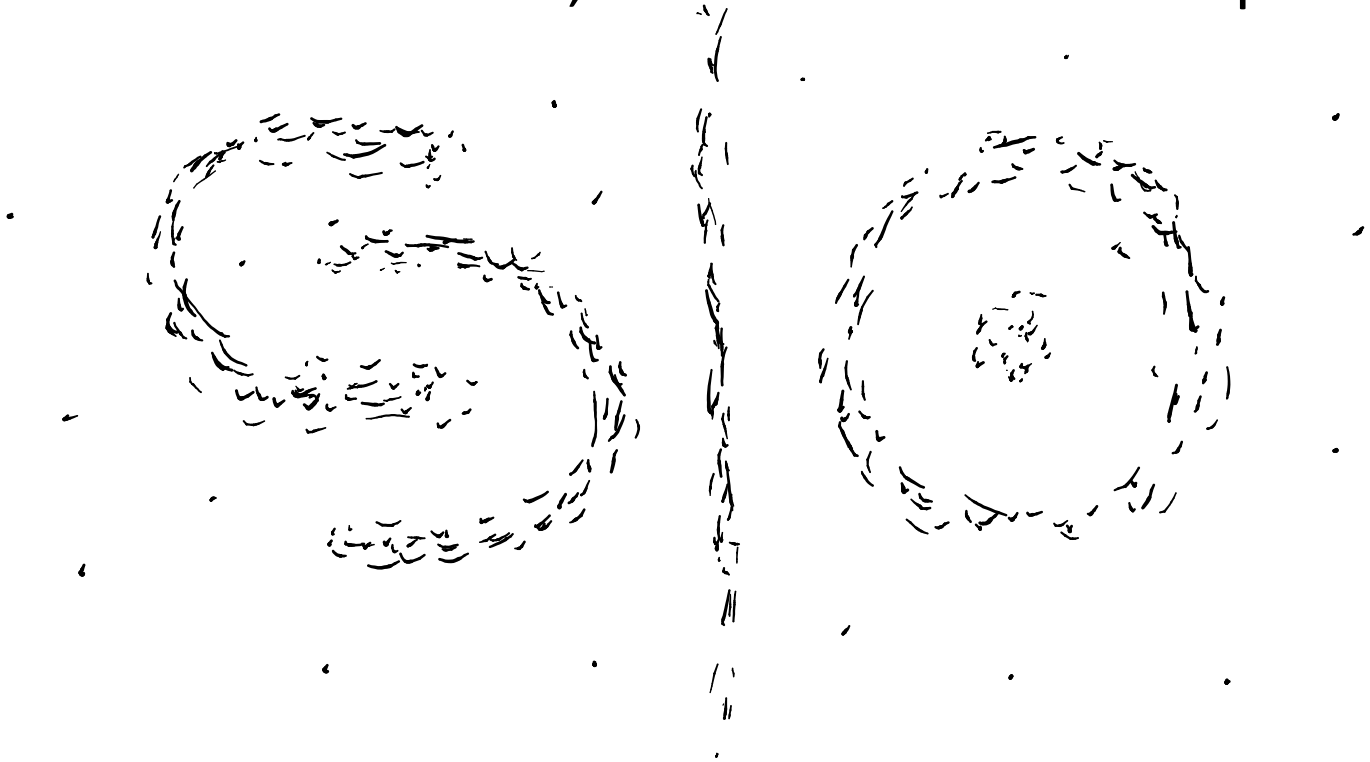
Fall 2016

Admin

- Assignment 1 :
  - 3 late days to hand it in before Friday.
  - 0 after that.
- Assignment 2 is out:
  - Due Friday of next week, but start early!
- Calculus and linear algebra terms to review for next week:
  - Vector addition and multiplication: $\alpha x + \beta y$.
  - Inner-product: $x^T y$.
  - Matrix multiplication: Xw.
  - Solving linear systems: $Ax = b$.
  - Matrix inverse: X^{-1}.
  - Norms: $||x||$.
  - Gradient: $\nabla f(x)$.
  - Stationary points: $\nabla f(x) = 0$.
  - Convex functions: $f''(x) \geq 0$.

Last Time: Density-Based Clustering

- We discussed density-based clustering:
  - Non-parametric clustering method.
  - Based on finding connected regions of dense points.
  - Can find non-convex clusters, and doesn't cluster all points.



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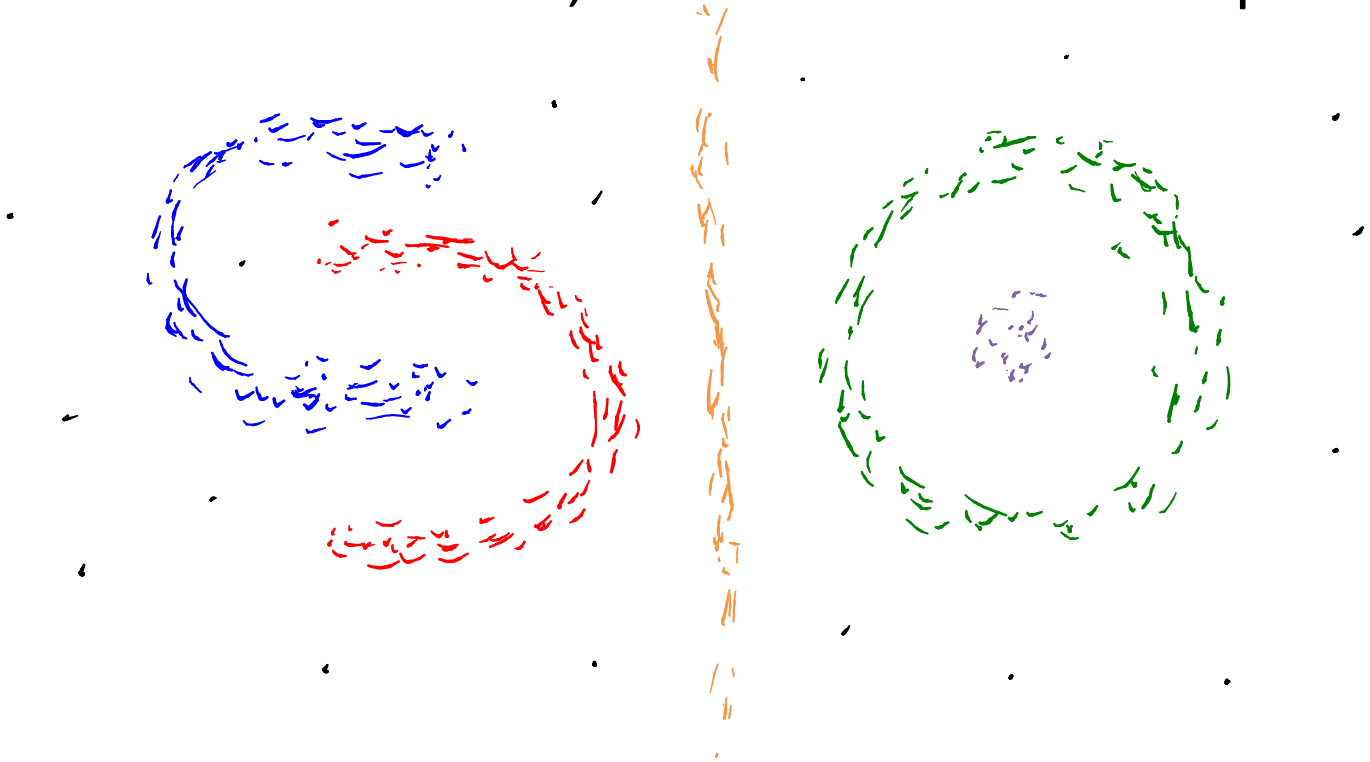


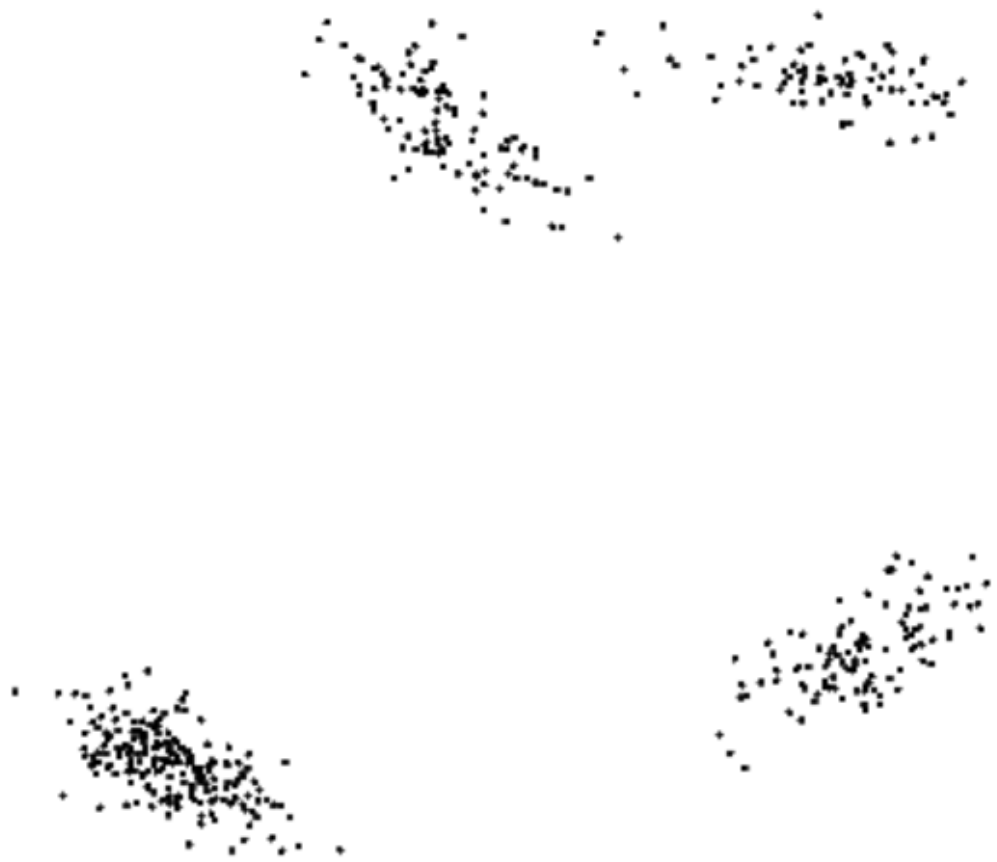
Cost of Density-Based Clustering

- Density-based clustering needs all points within "radius" distance.
  - What is the cost of this?

- Naïve approach to do this for all points:
  - Computing distance between 2 examples is O(d).
  - We have 'n' training examples, so there are $O(n^2)$ combinations.
  - Computing distance between all examples is $O(n^2d)$.
- Not feasible if 'n' is large.

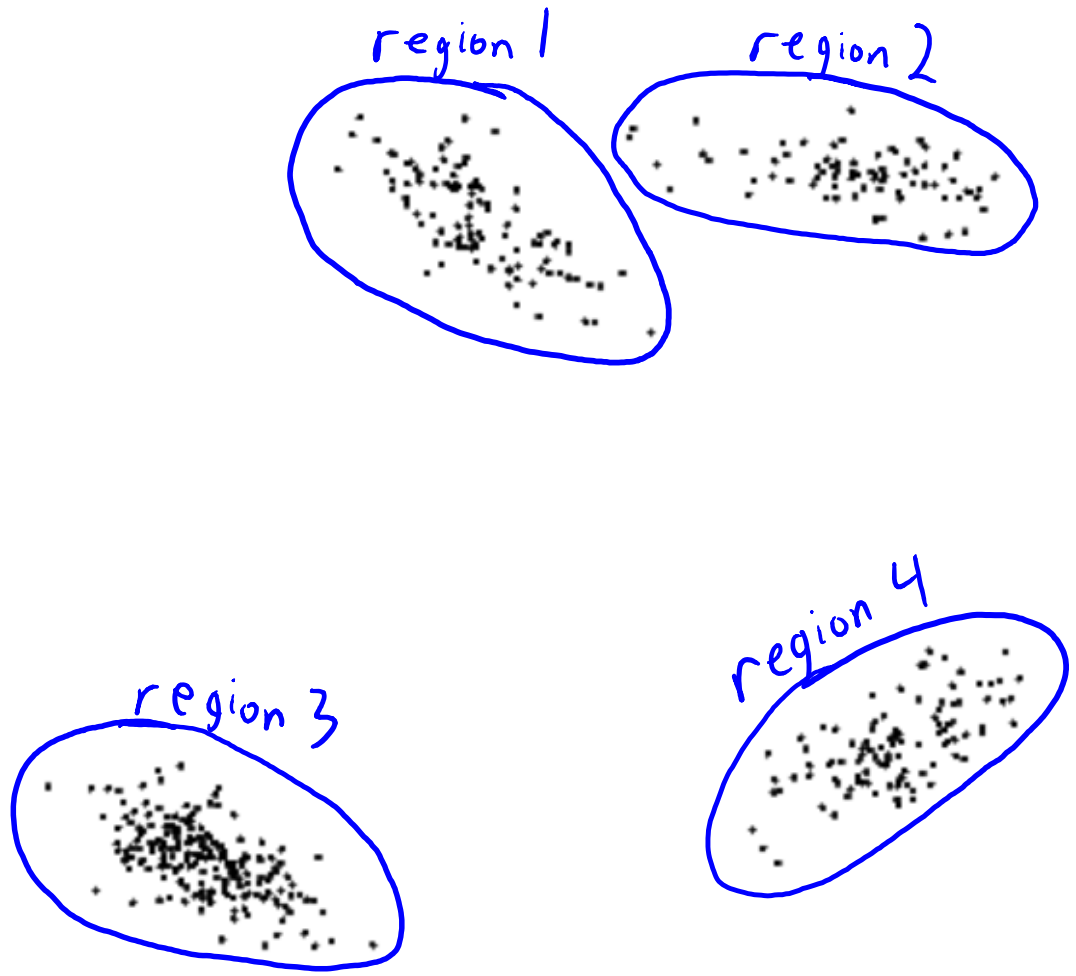
- How can we answer "closest points" queries when 'n' is large?

Distance-Based Pruning



Distance-Based Pruning

Divide objects into regions r_c.



Distance-Based Pruning

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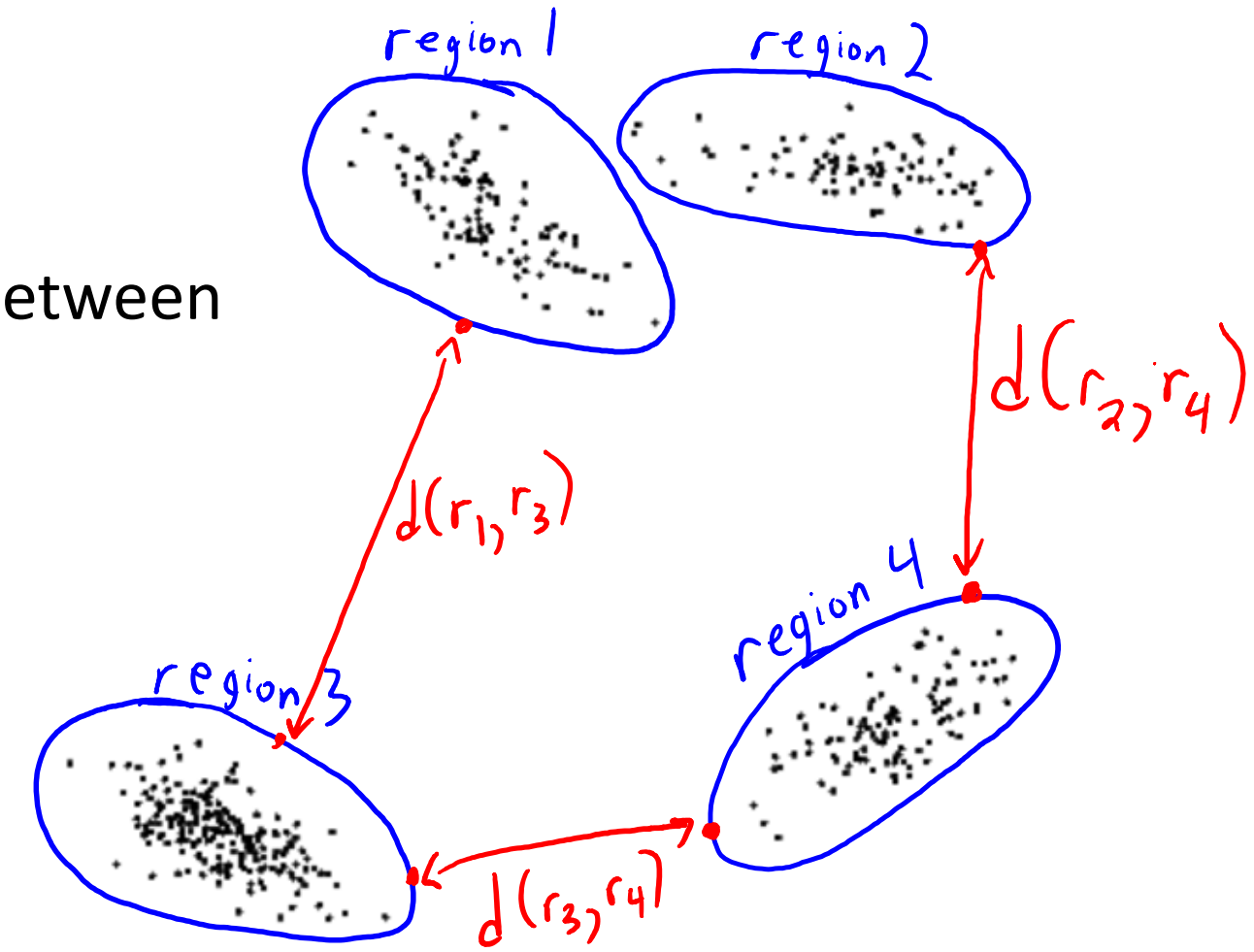
Let $d(r_i,r_j)$ be minimum distance between regions r_i and r_j.



Distance-Based Pruning

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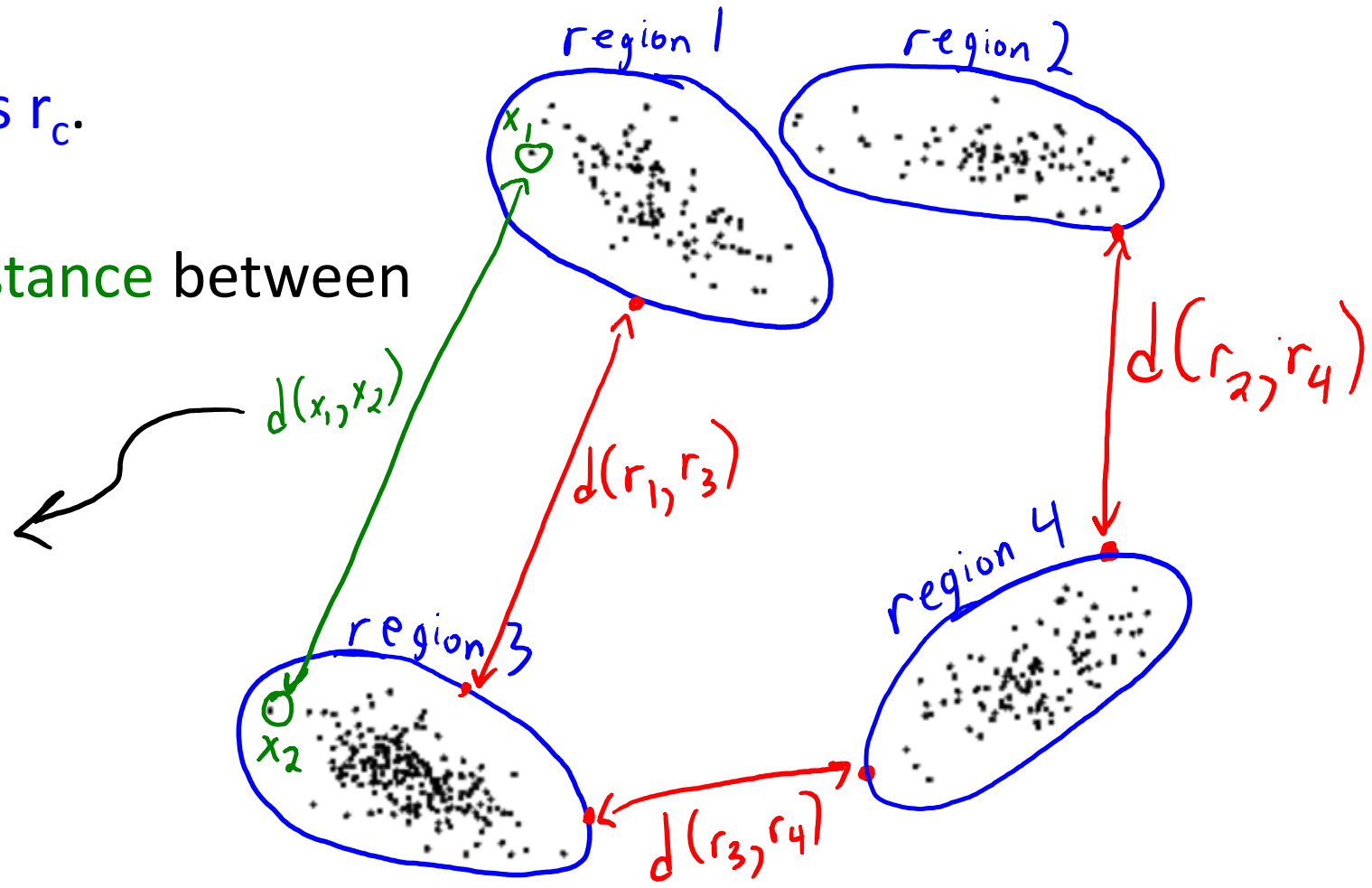
Notice that
$d(x_1,x_2) \geq d(r_1,r_3)$



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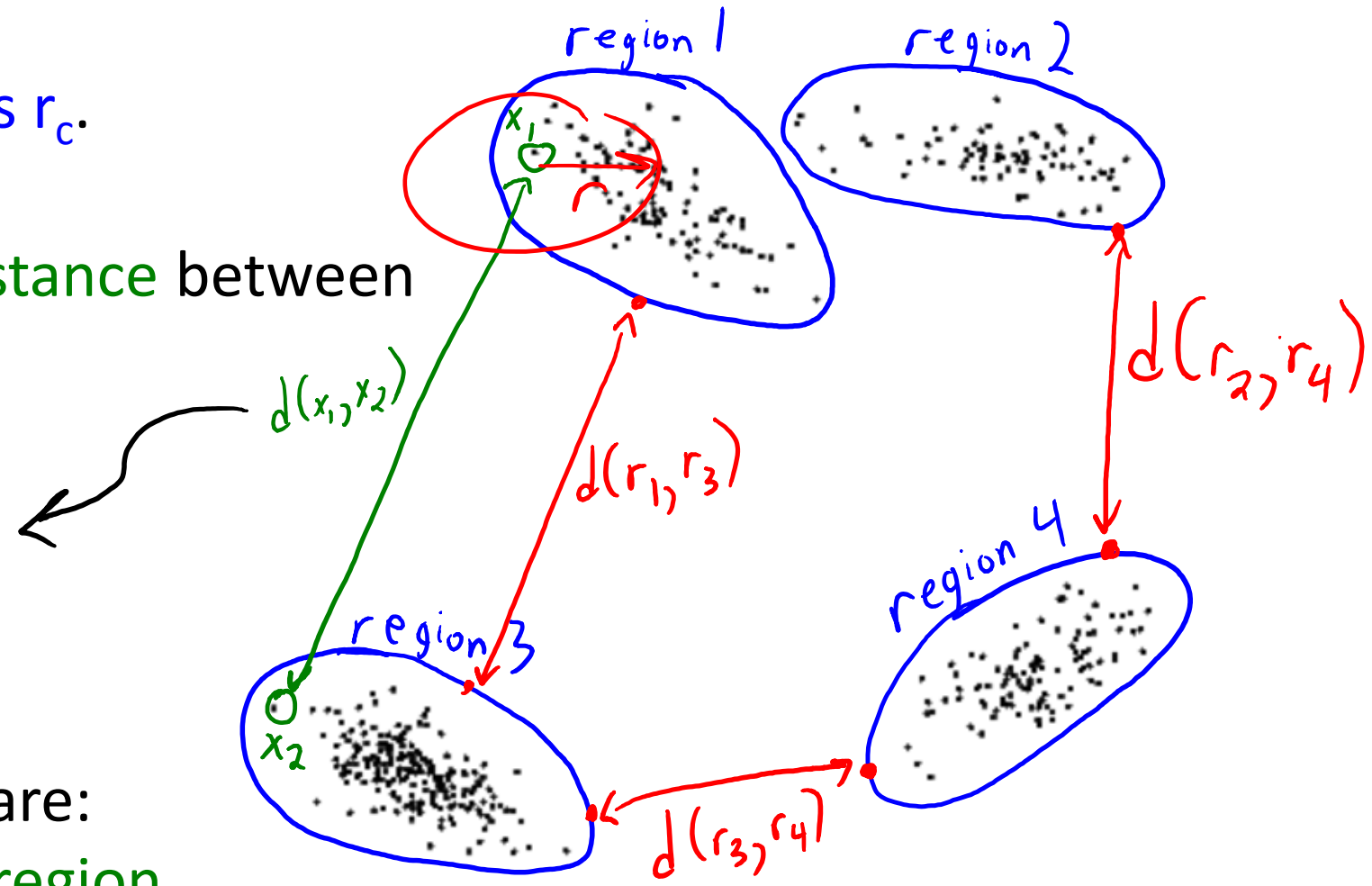

All points within radius "r" are:

- Points within same region.
- Points in "close" regions where $d(r_i,r_j) \leq r$.

(skip comparing points in far-apart regions)

Square-Shaped Regions

- A computationally-nice way to define “regions” for 2D data:
  - Squares with side length of ‘r’.

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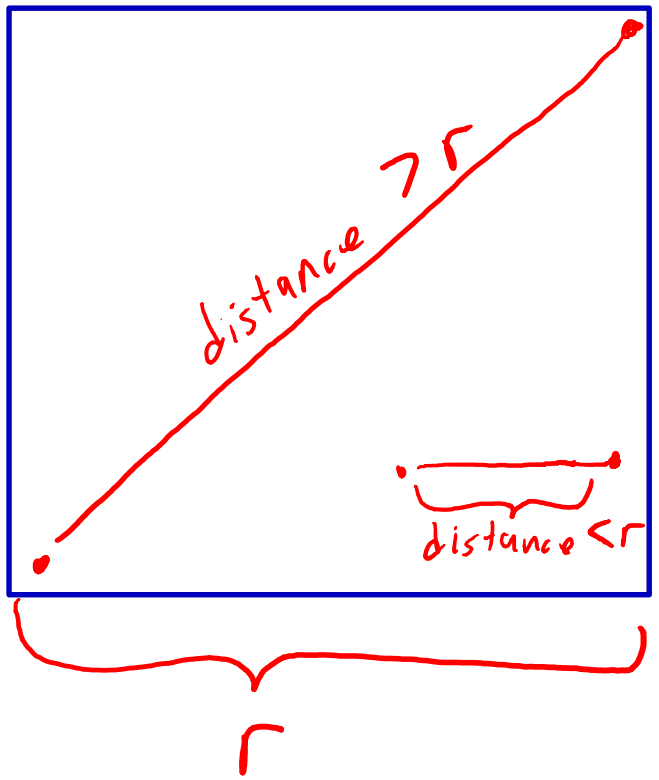
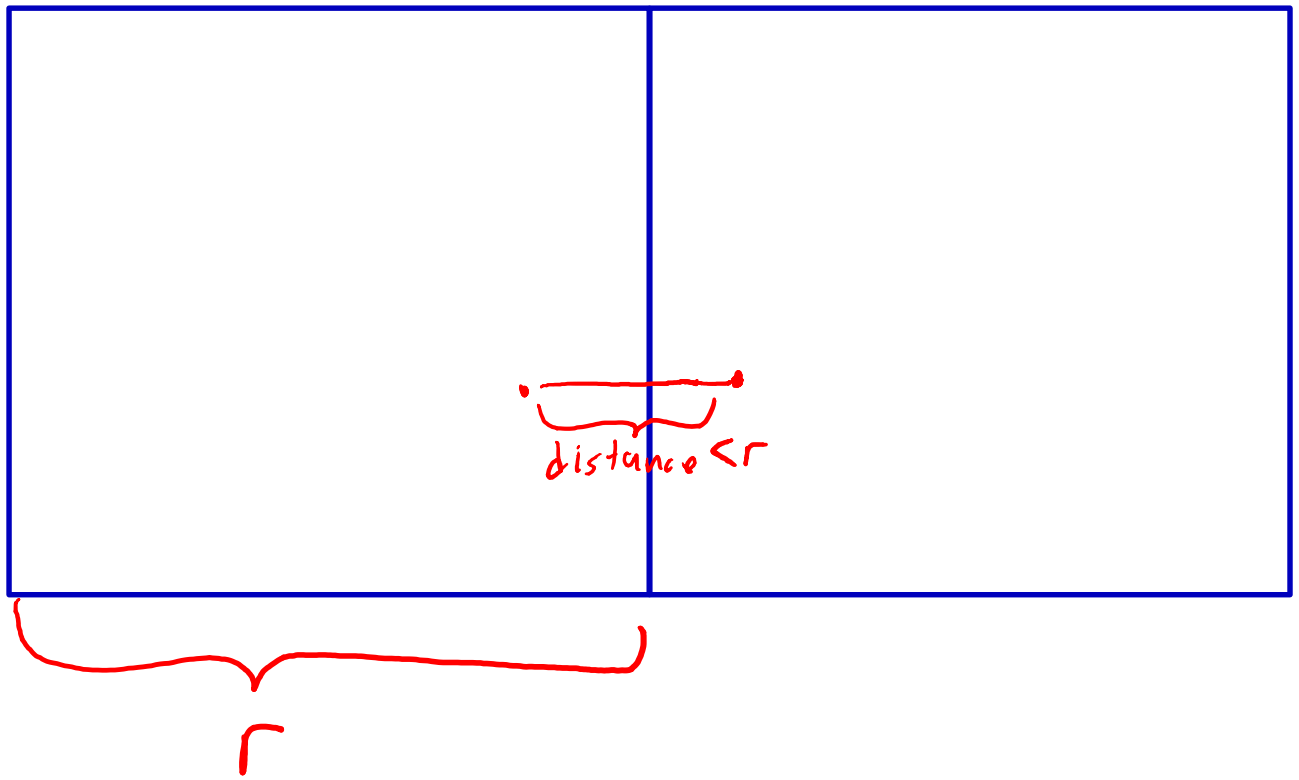


Points in same square can have distance less than ‘r’.

Square-Shaped Regions

- A computationally-nice way to define “regions” for 2D data:
  - Squares with side length of ‘r’.

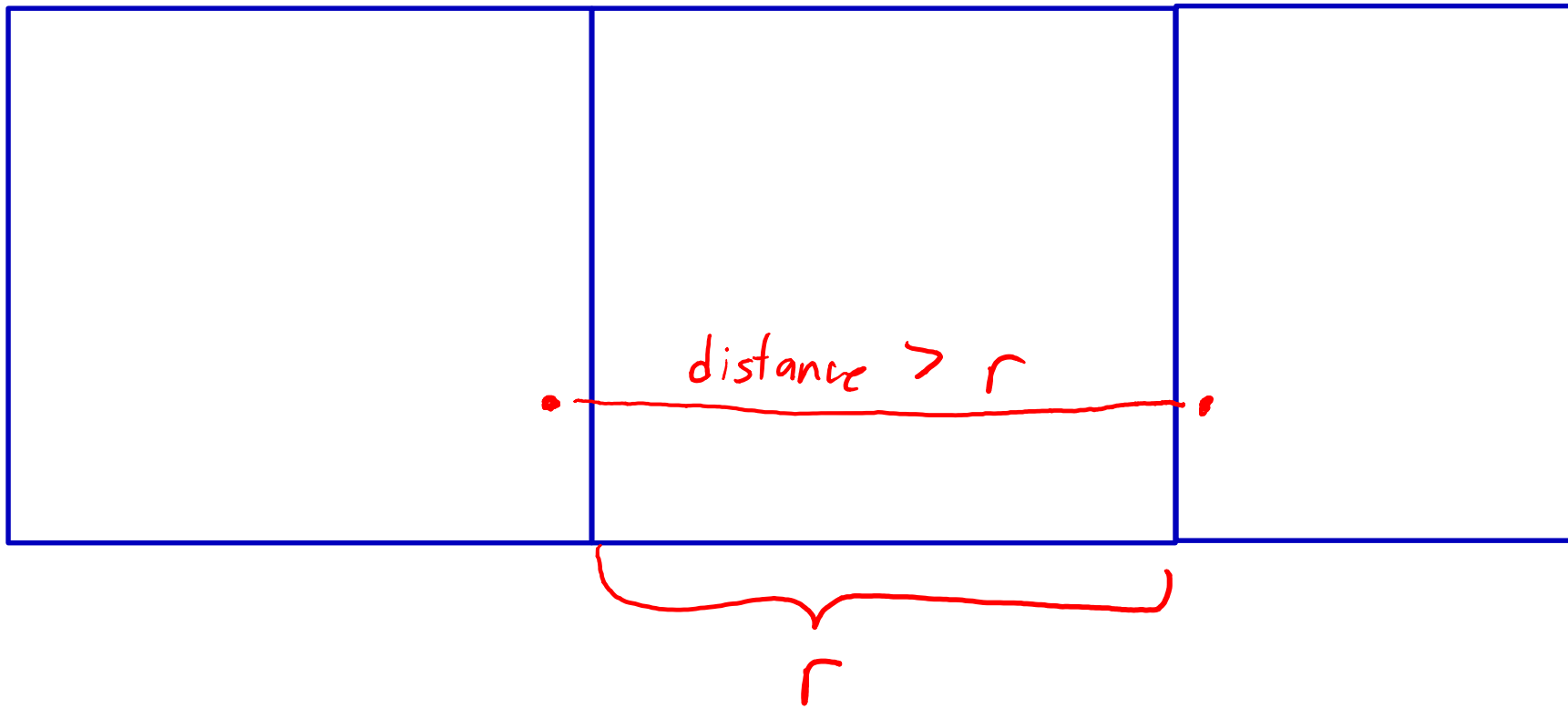
Points in adjacent squares can distance less than distance ‘r’.



Square-Shaped Regions

- A computationally-nice way to define “regions” for 2D data:
  - Squares with side length of ‘r’.

Points in non-adjacent squares must have distance more than ‘r’.

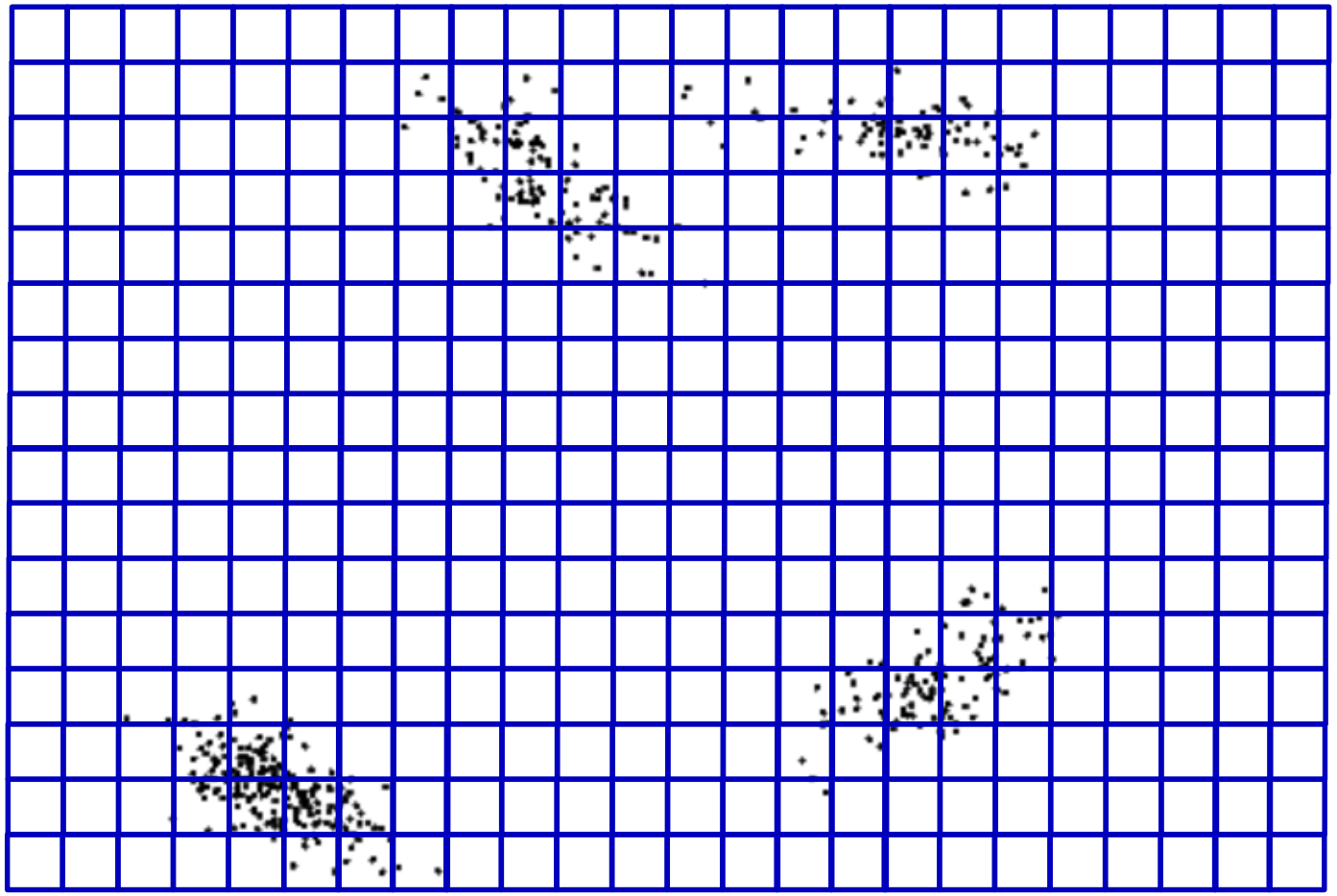


Grid-Based Pruning

- Assume we want to find objects within a distance of ‘r’.

Divide space into squares of length r.

Assign (“hash”) each object to its square region.



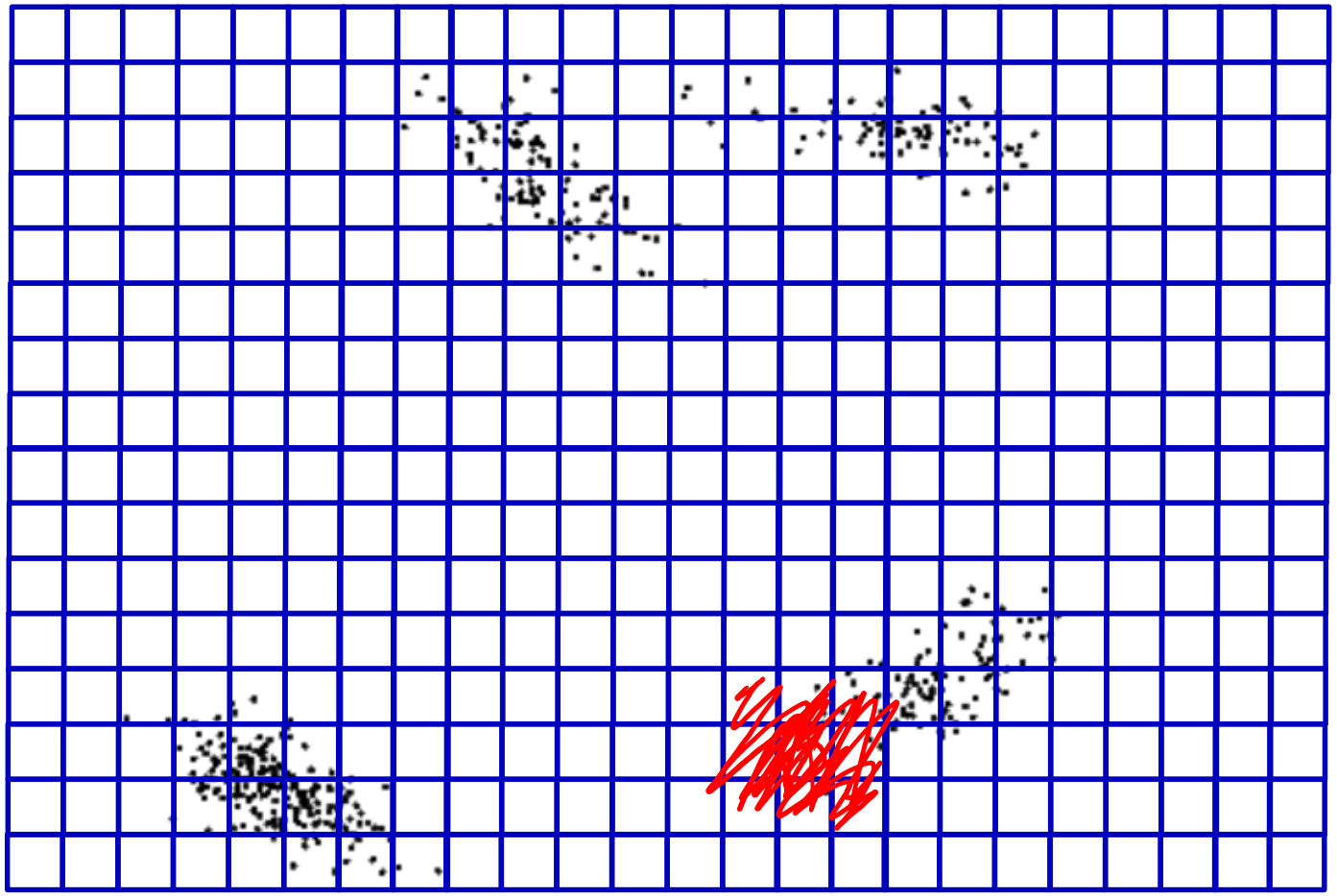
Grid-Based Pruning

- Assume we want to find objects within a distance of ‘r’.

Divide space into squares of length r.

Assign (“hash”) each object to its square region.

- Only check objects in same and adjacent regions.

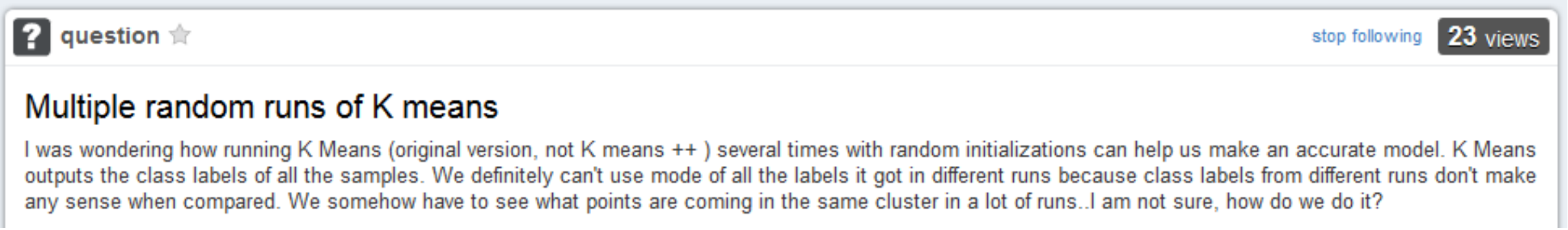


Grid-Based Pruning Discussion

- Grid-based pruning also works for L_1-norm and L_∞-norm.
- Similar ideas can be used for other "closest point" calculations:
  - K-nearest neighbours (finding closest training examples).

- But we again have the "curse of dimensionality":
  - Hyper-cubes of length 'r' are tiny: few points will fall into each cube.
  - Number of adjacent cubes increases exponentially:
    - 8 in 2D, 26 in 3D, 80 in 4D, 252 in 5D, 3^d-1 in n-D.
- Better "regions" in high-dimensions (but still bad in worst case):
  - Quad-trees, R-trees, ball-trees.
- Approximate methods:
  - Locality sensitive hashing (random transformation to low-dimensional problem).

Ensemble Clustering


question

stop following 23 views

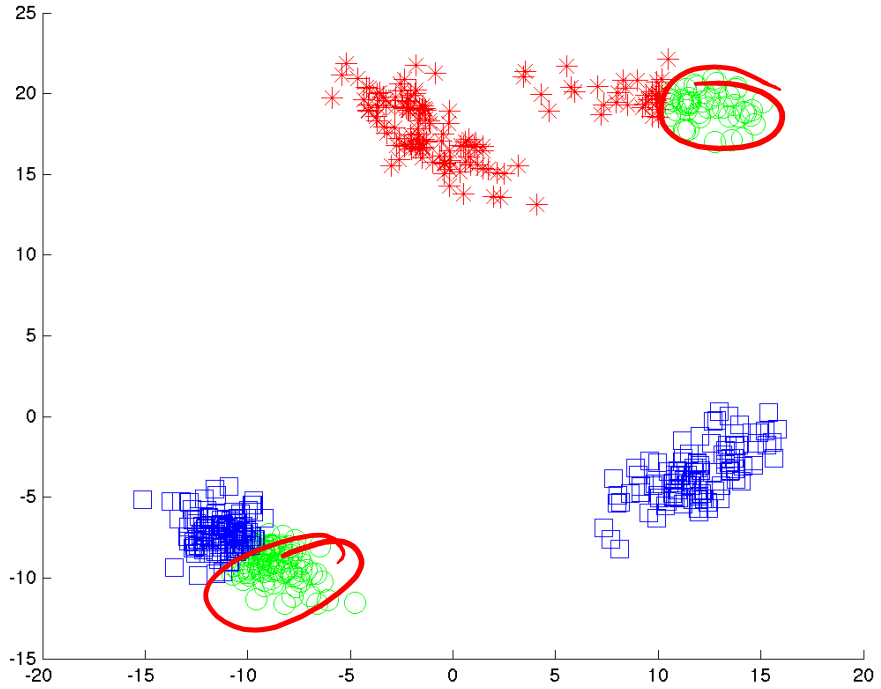
Multiple random runs of K means

I was wondering how running K Means (original version, not K means ++) several times with random initializations can help us make an accurate model. K Means outputs the class labels of all the samples. We definitely can't use mode of all the labels it got in different runs because class labels from different runs don't make any sense when compared. We somehow have to see what points are coming in the same cluster in a lot of runs..I am not sure, how do we do it?

- We can consider ensemble methods for clustering.
  - "Consensus clustering"
- It's a good/important idea:
  - Bootstrapping is widely-used.
  - "Do clusters change if the data was slightly different?"
- But we need to be careful about how we combine models.

Ensemble Clustering

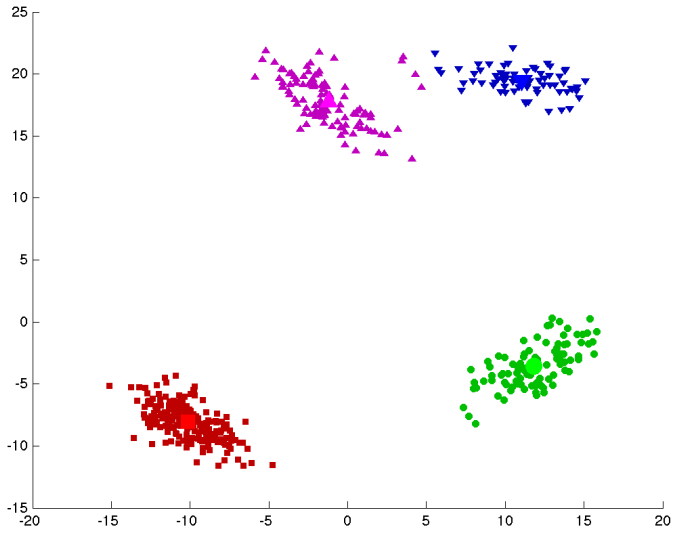
- E.g., run k-means 20 times and then cluster using the mode.
- Normally, averaging across models doing different things is good.

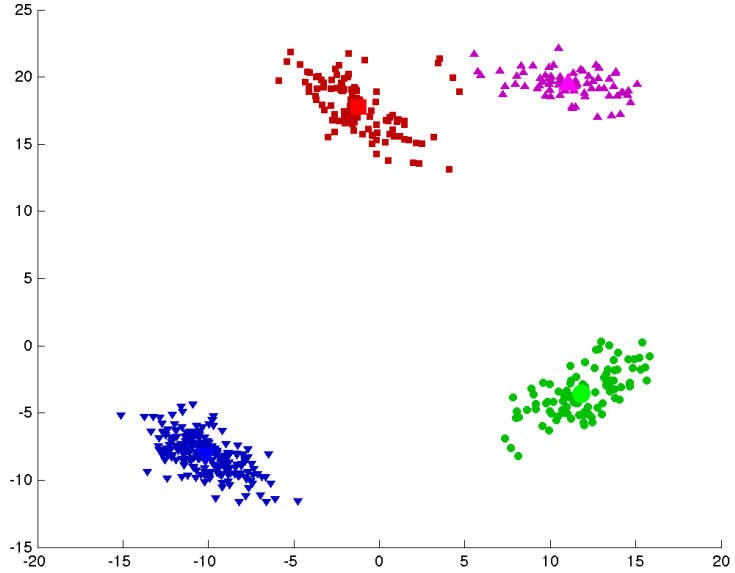


- But this is a bad ensemble method: worse than k-means on its own.

Label Switching Problem

- This doesn't work because of label switching:
  - The cluster labels are meaningless.
  - We could get same clustering with permuted labels:

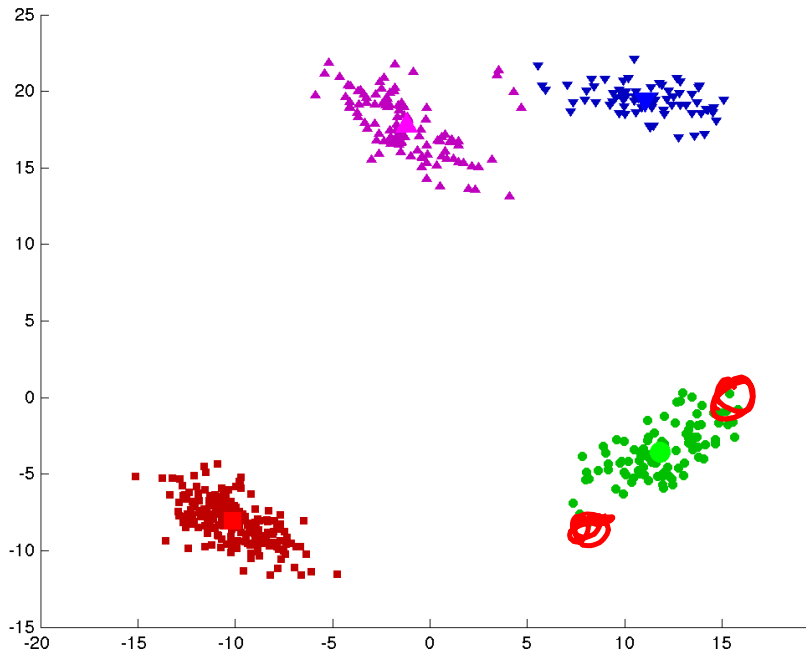


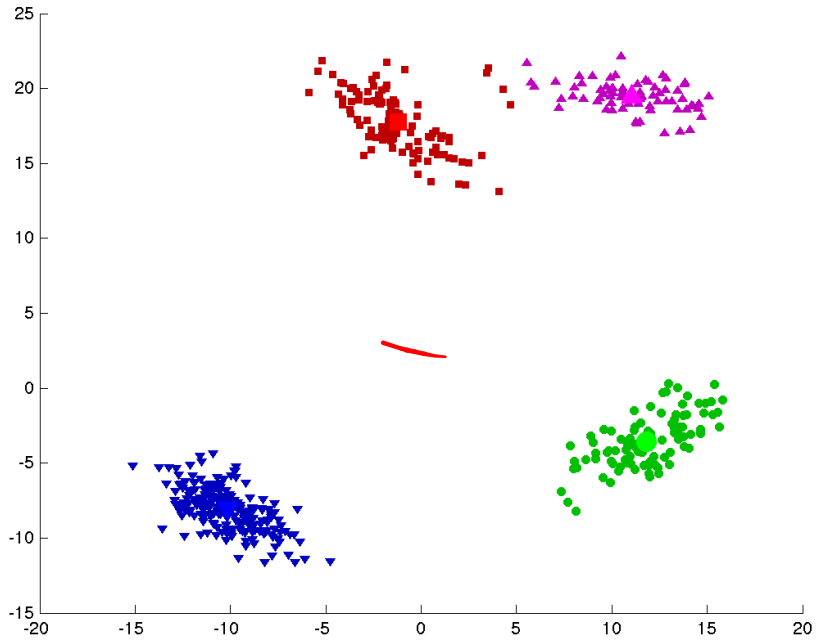


  - All clusters become equally likely as number of initializations increases.

Addressing Label Switching Problem

- Ensembles can't depend on label "meaning":
  - Don't ask "is point x_i in red square cluster?", which is meaningless.
  - Ask "is point x_i in the same cluster as x_j?", which is meaningful.





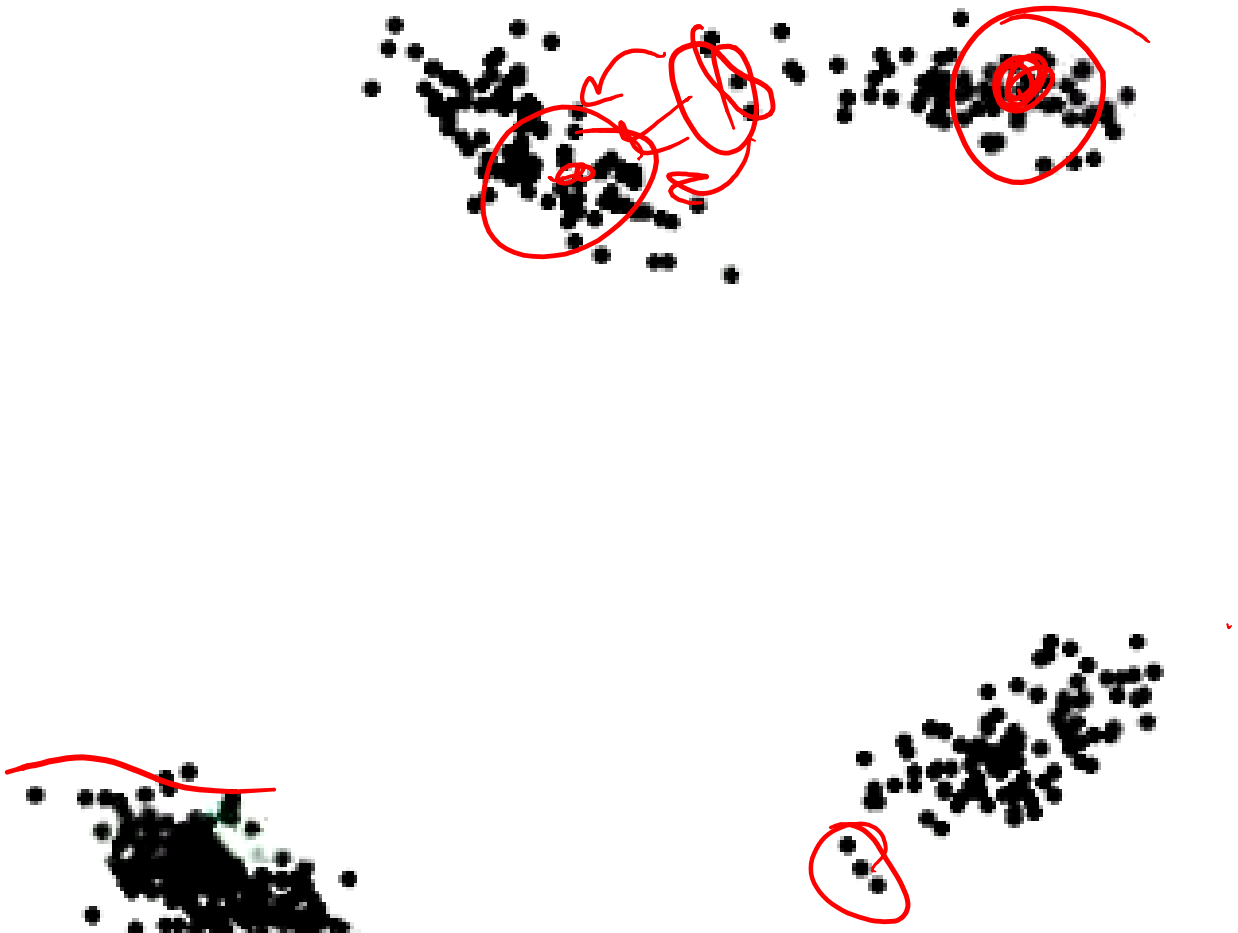
UBClustering Algorithm

- Let's define a new ensemble clustering method: UBClustering.

1. Run k-means with 't' different random initializations.
2. For each object i and j:
   - Count the number of times x_i and x_j are in the same cluster.
   - Define p(i,j) = count(x_i in same cluster as x_j)/t.
3. Put x_i and x_j in the same cluster if p(i,j) > 0.5.

- Like DBSCAN merge clusters in step 3 if i or j are already assigned.
  - You can implement this with a DBSCAN code (just changes "distance").
  - Each x_i has an x_j in its cluster with p(i,j) > 0.5.
  - Some points are not assigned to any cluster.

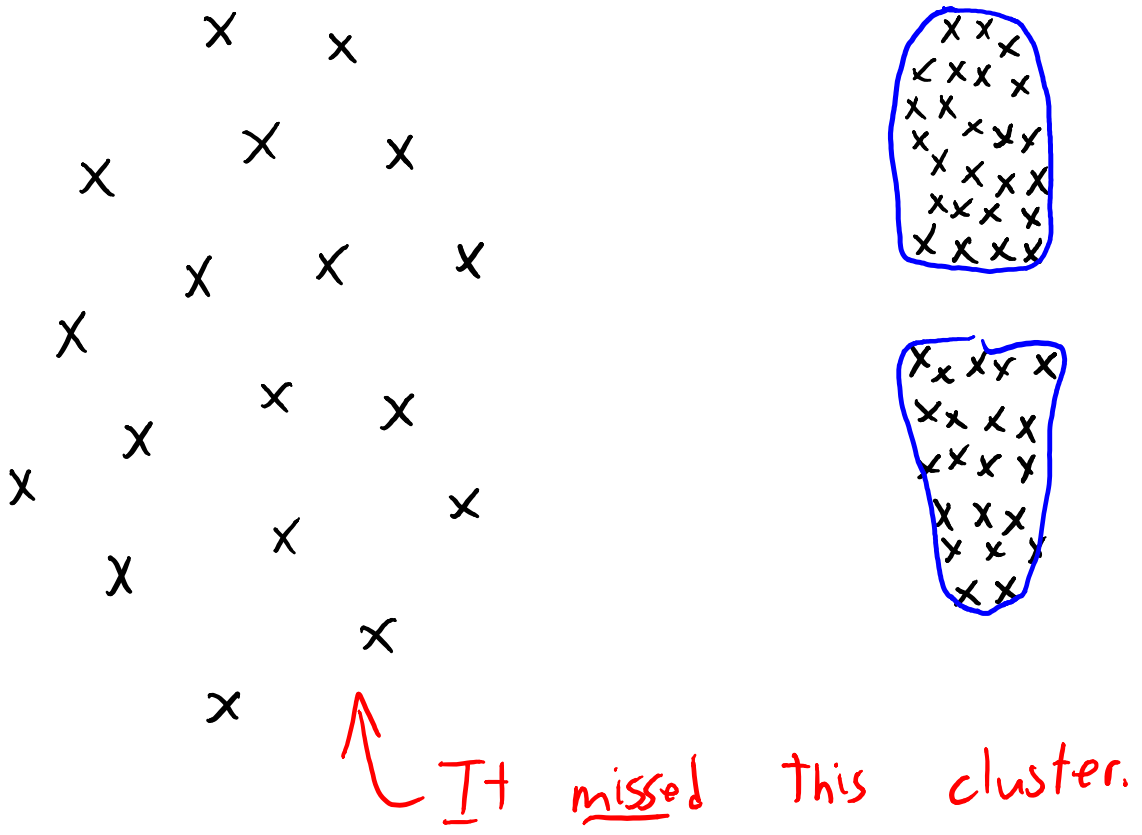
UBClustering Algorithm



It looks like DBSCAN, but far-away points will be assigned to a cluster if they always appear in same cluster as other points.

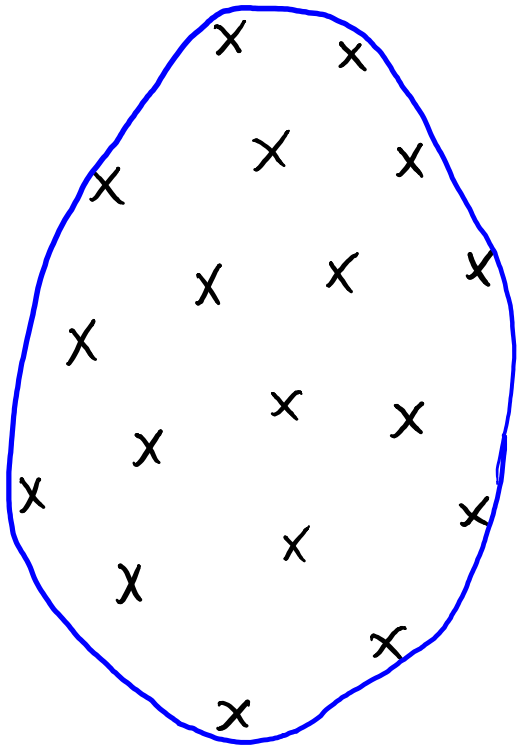
Differing Densities

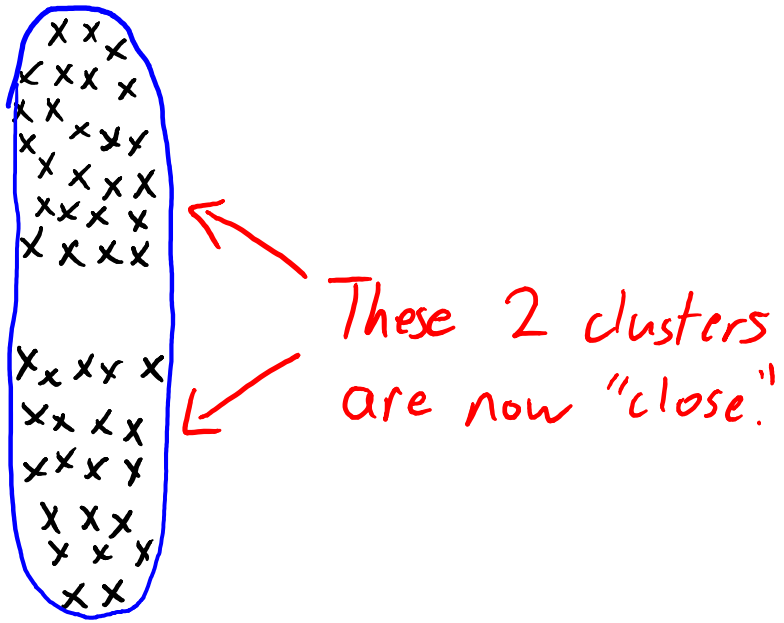
- Consider density-based clustering on this data:



Differing Densities

- Increase the radius and run it again:

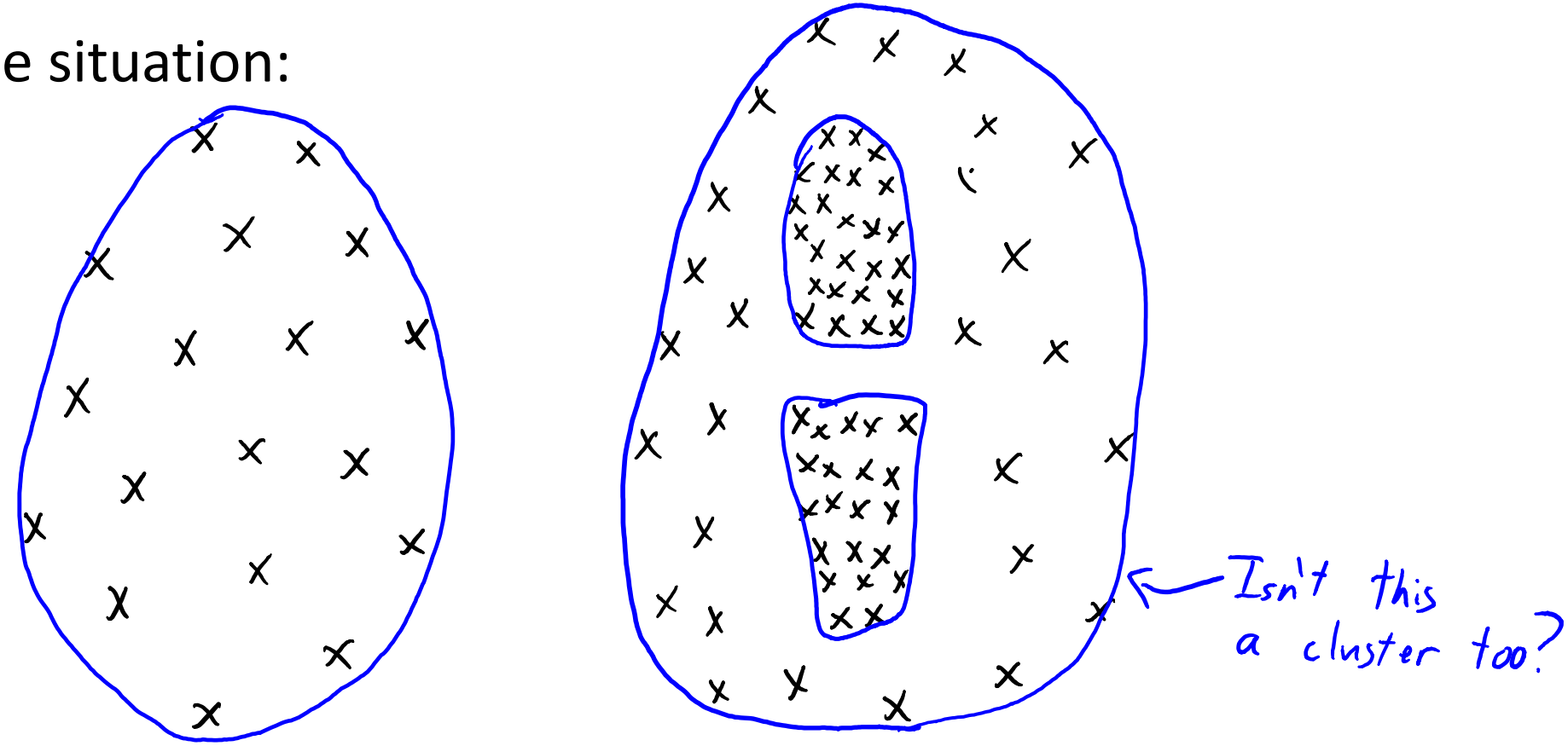




- There may no density-level that gives you 3 clusters.

Differing Densities

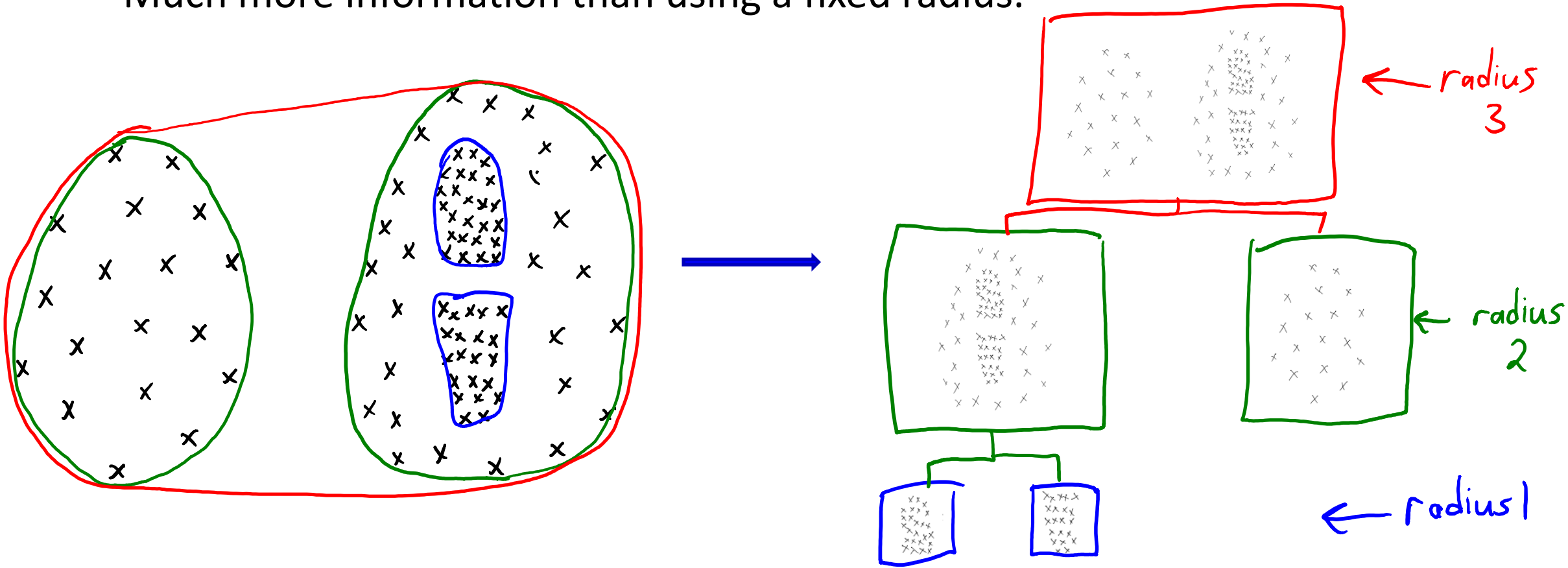
- Here is a worse situation:



- Now you need to choose between coarse/fine clusters.
- Instead of fixed clustering, we often want hierarchical clustering.

Density-Based Hierarchical Clustering

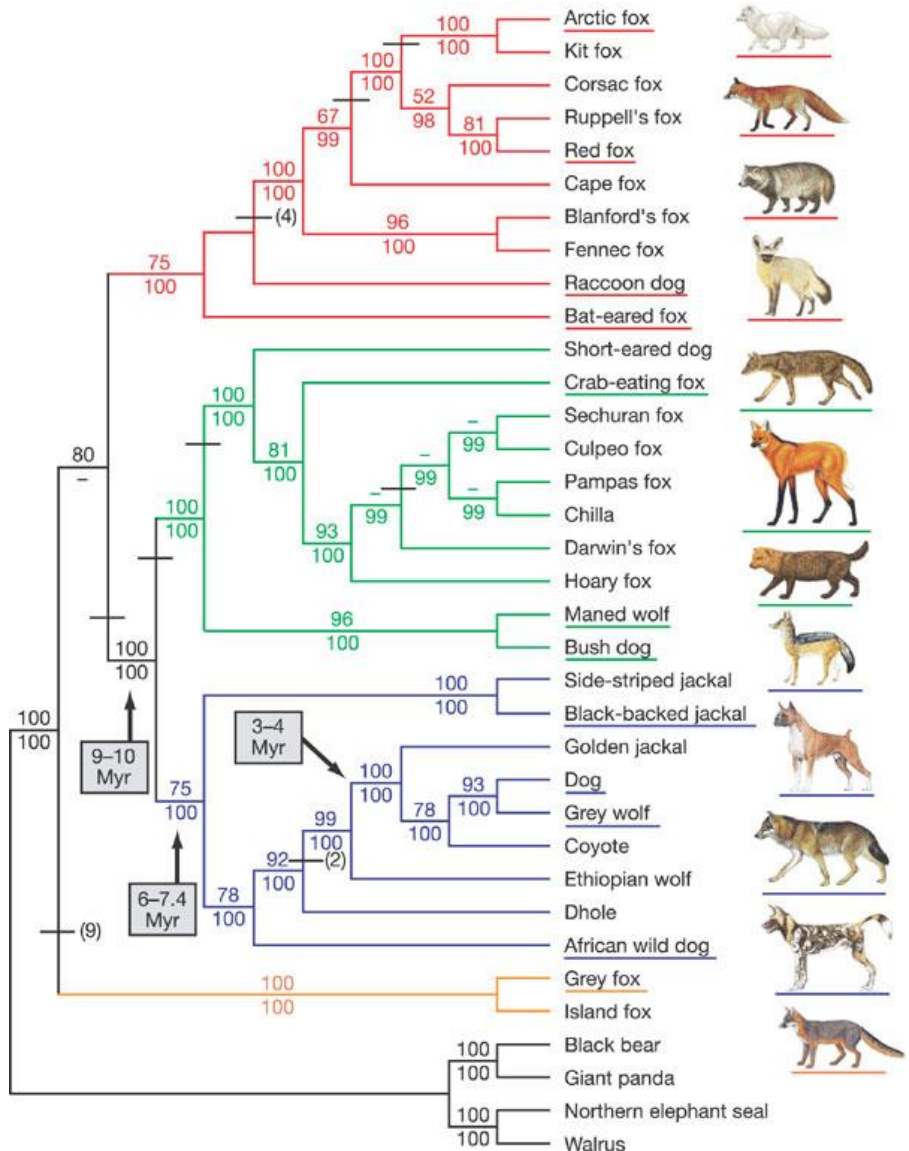
- A simple way to make a hierarchical DBSCAN:
  - Fix minPoints, record clusters as you vary the radius.
  - Much more information than using a fixed radius.



Application: Phylogenetics

- We sequence genomes of a set of organisms.
- Can we construct the “tree of life”?

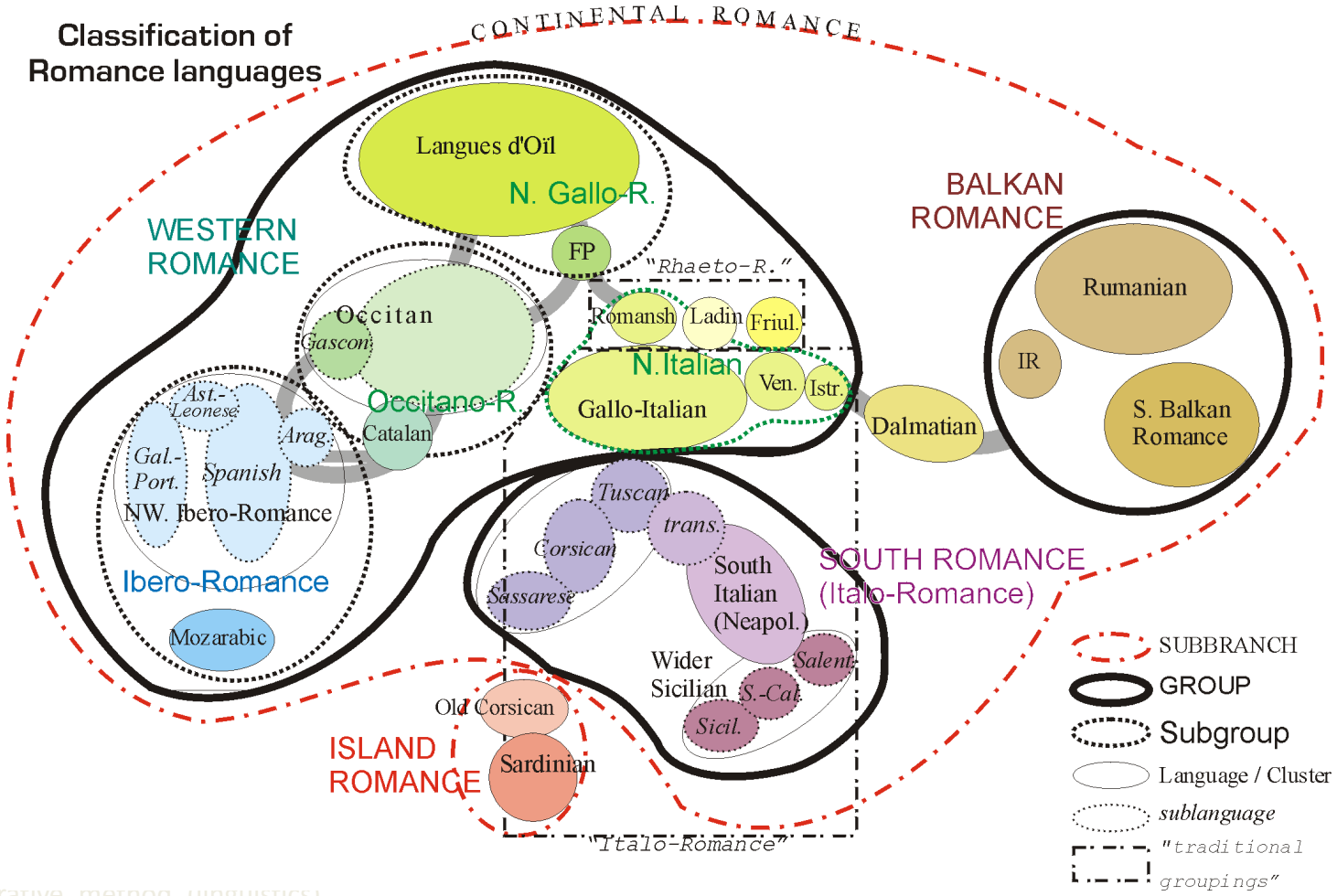
- Comments on this application:
  - On the right are individuals.
  - As you go left, clusters merge.
  - Merges are ‘common ancestors’.
  - “Distance”: approximation of change needed.
  - Line lengths: approximate amount of change.
  - Numbers: #clusterings across bootstrap samples.
  - ‘Outgroups’ (walrus, panda) are a sanity check.



http://www.nature.com/nature/journal/v438/n7069/fig_tab/nature04338_F10.html

Application: Phylogenetics

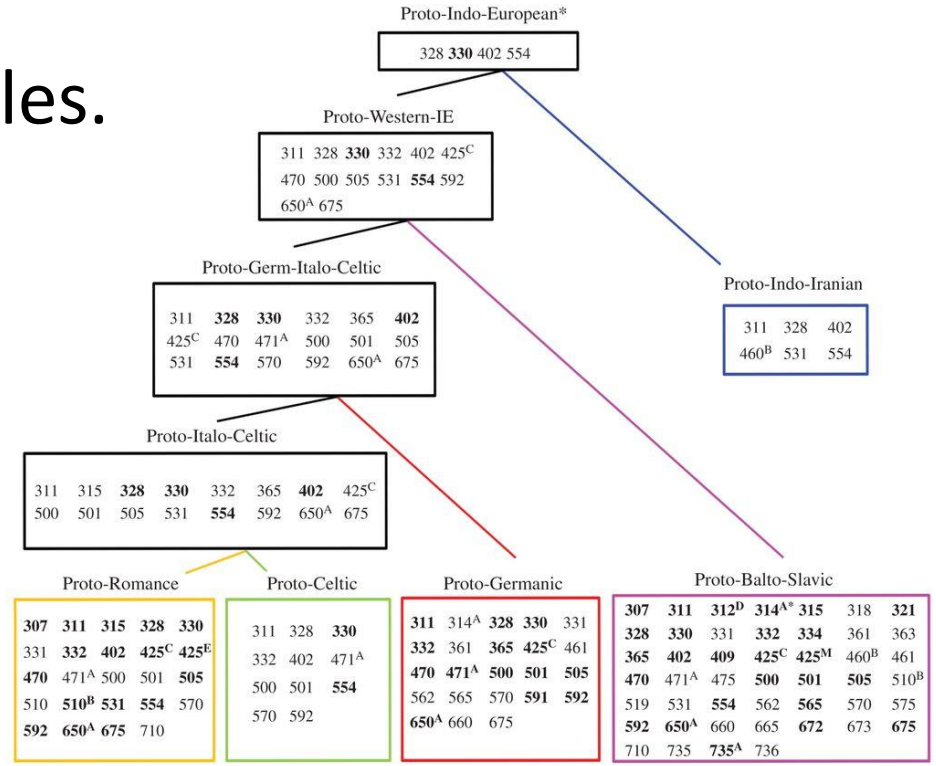
- Comparative method in linguistics studies evolution of languages:



https://en.wikipedia.org/wiki/Comparative_method_(linguistics)

Application: Phylogenetics

- Paper from January on evolution of fairy tales.
  - Evidence that “Devil and the Smith” goes back to bronze age.
  - “Beauty and the Beast” published in 1740, but might be 2500-6000 years old.

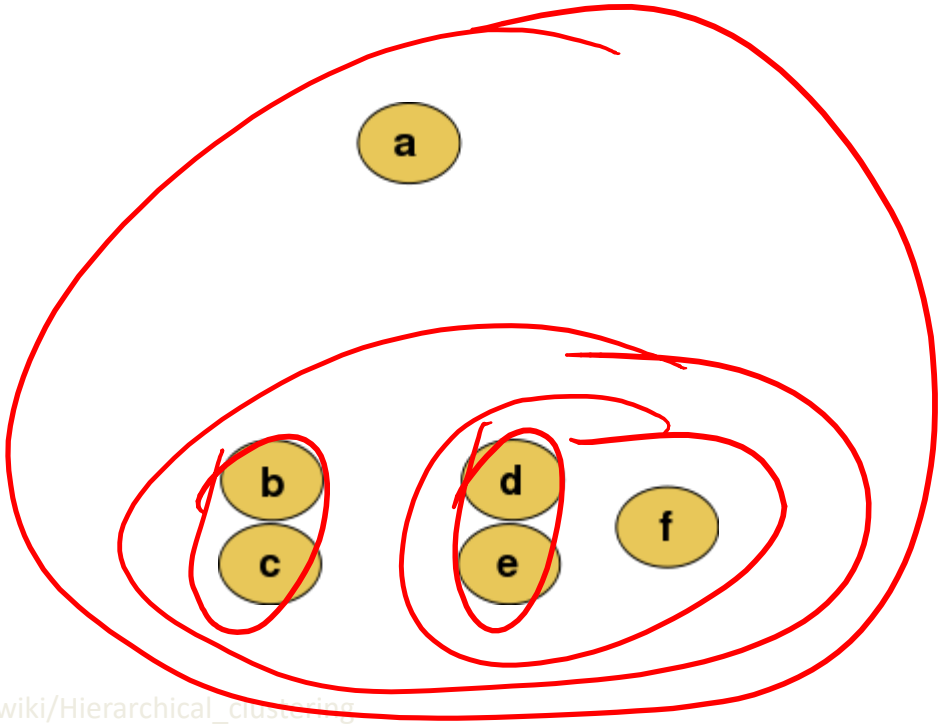


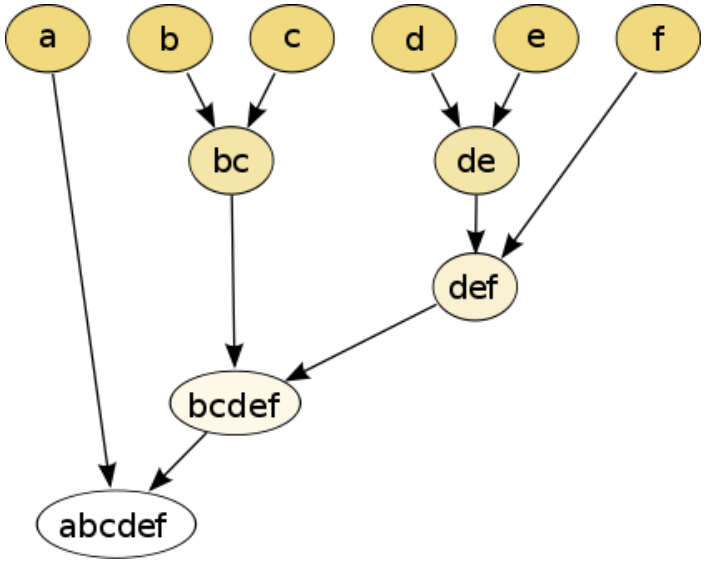
International tale types

307	The Princess in the Coffin	**409**	The Girl as Wolf	**562**	The Spirit in the Blue Light
311	Rescue by Sister	**425C**	Beauty and the Beast	**565**	The Magic Mill
312D	Rescue by the Brother	**425E**	The Enchanted Husband	**570**	The Rabbit-Herd
314A	The Shepherd and the Giants	**425M**	The Snake Bridegroom	**575**	The Prince's Wings
314A*	Animal Helper in the Flight	**460B**	The Journey	**591**	The Thieving Pot
315	The Faithless Sister	**461**	Three Hairs	**592**	The Dance Among Thorns
318	The Faithless Wife	**470**	Friends in Life and Death	**650A**	Strong John
321	Eyes Recovered from Witch	**471A**	The Monk and the Bird	**660**	The Three Doctors
328	The Boy Steals Ogre's Treasure	**475**	The Man as the Heater	**665**	The Man who Flew and Swam
330	The Smith and the Devil	**500**	Supernatural Helper	**672**	The Serpent's Crown
331	The Spirit in the Bottle	**501**	The Three Old Spinning Women	**673**	The White Serpent's Flesh
332	Godfather Death	**505**	The Grateful Dead	**675**	The Lazy Boy
334	Household of the Witch	**510**	Cinderella and Peau d'Âne	**710**	Our Lady's Child
361	Bear Skin	**510B**	Peau d'Asne	**735**	The Rich and the Poor Man
363	The Corpse-Eater	**519**	The Strong Woman as Bride	**735A**	Bad Luck Imprisoned
365	The Dead Bridegroom	**531**	The Clever Horse	**736**	Luck and Wealth
402	The Animal Bride	**554**	The Grateful Animals		

Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: agglomerative clustering.
  1. Starts with each point in its own cluster.
  2. Each step merges the two “closest” clusters.
  3. Stop when everything is in one big cluster.





https://en.wikipedia.org/wiki/Hierarchical_clustering

Agglomerative (Bottom-Up) Clustering

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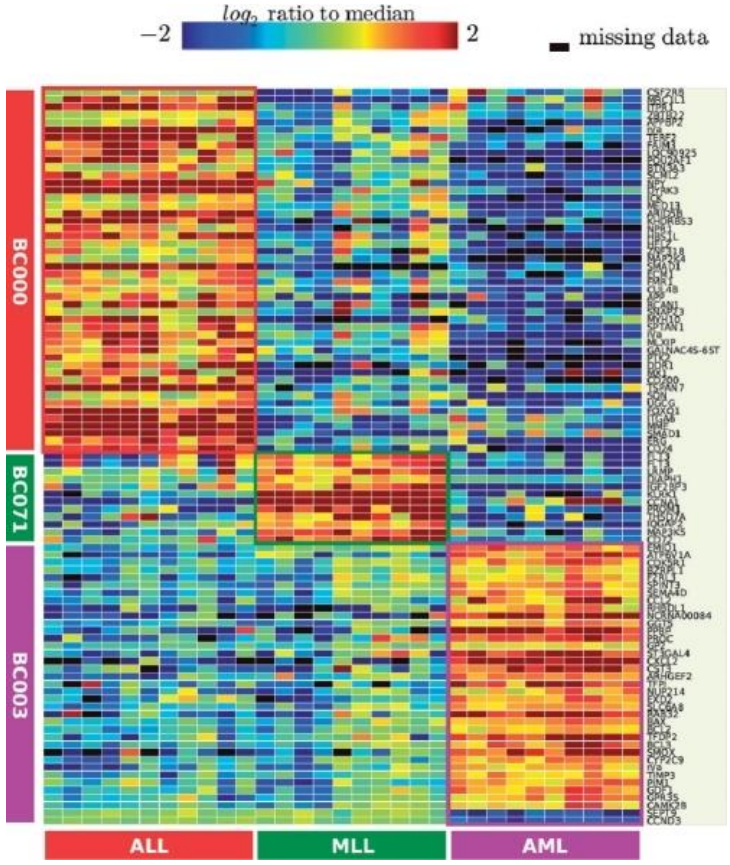
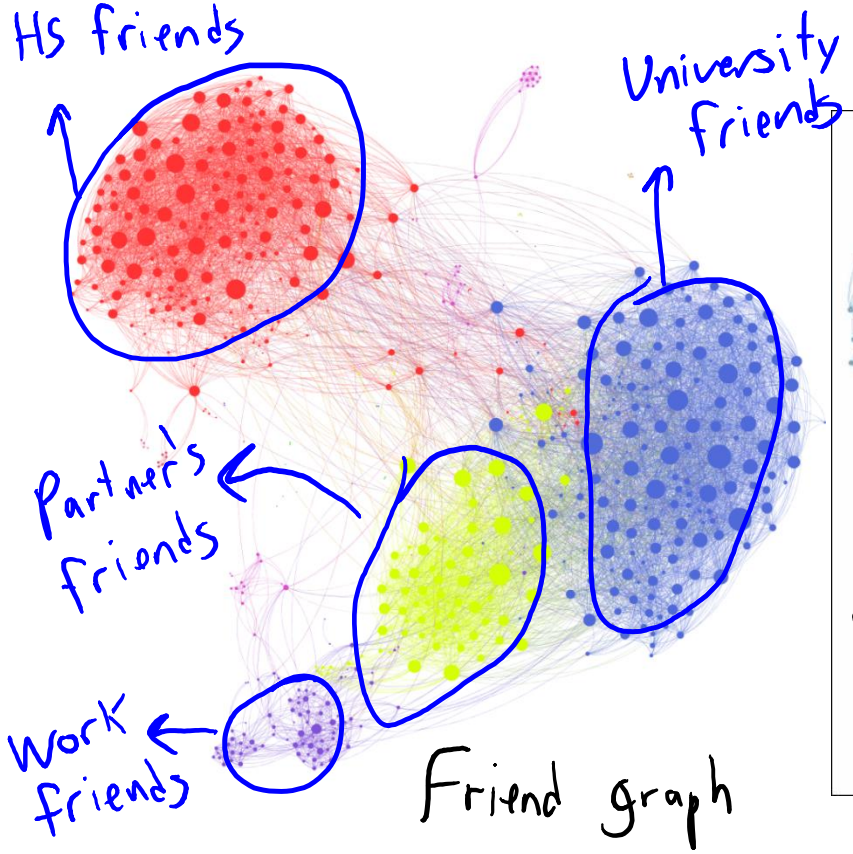
  1. Starts with each point in its own cluster.
  2. Each step merges the two “closest” clusters.
  3. Stop when everything is in one big cluster.
- How do you define “closest” clusters?
  - Average-link: average distance between points in clusters.
  - Single-link: minimum distance between points in clusters.
  - Complete-link: maximum distance between points in clusters.
  - Ward’s method: minimize within-cluster variance.
- Reinvented by different fields under different names (UPGMA).
  - Popular implementation: BIRCH.

Other Clustering Methods

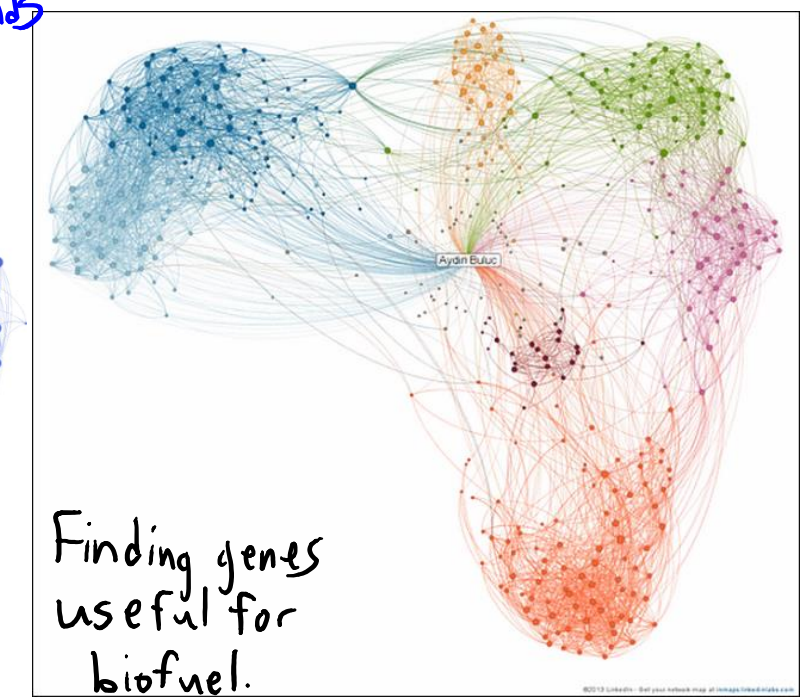
- Mixture models:
  - Probabilistic clustering.
- Mean-shift clustering:
  - Finds local “modes” in density of points.
- Bayesian clustering:
  - A variant on ensemble methods.
  - Averages over models/clustering, weighted by “prior” belief in the model/clustering.
- Biclustering:
  - Simultaneously cluster objects and features.
- Spectral clustering and graph-based clustering:
  - Clustering of data described by graphs.



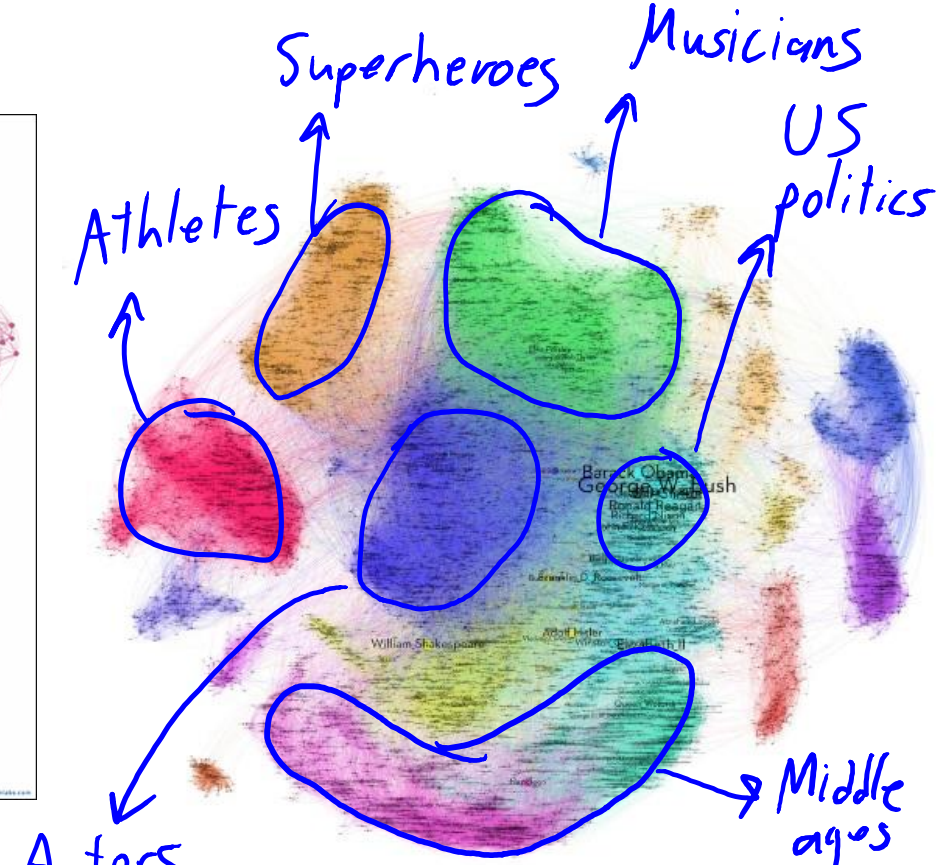
Graph-Based Clustering Methods



Friend graph



Finding genes useful for biofuel.



Wikipedia links

https://griffsgraphs.wordpress.com/tag/clustering/
http://ascr-discovery.science.doe.gov/2013/09/sifting-genomes/
https://www.hackdiary.com/2012/04/05/extracting-a-social-graph-from-wikipedia-people-pages/

Summary

- Region-based pruning: speeds up “closest point” calculations.
- Ensemble clustering: combines multiple clusterings.
  - Can work well but need to account for label switching.
- Hierarchical clustering: more informative than fixed clustering.
- Agglomerative clustering: sequentially merges clusters.

- Next time: discovering a hole in the ozone layer.

Bonus Slide: Divisive (Top-Down) Clustering

- Start with all objects in one cluster, then start dividing.
- E.g., run k-means on a cluster, then run again on resulting clusters.
  - A clustering analogue of decision tree learning.