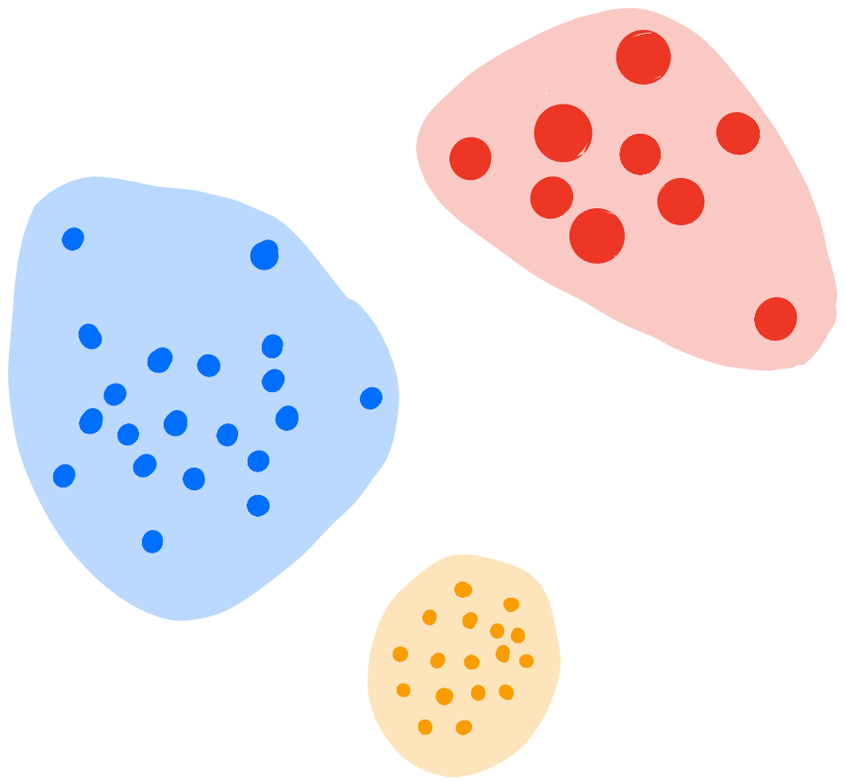
Introduction to clustering methods

Epid 814 - Marisa Eisenberg

Cluster Analysis

- What is a cluster?
    - A set of objects/data points, such that the objects in the set are more similar to one another than they are to the objects outside the set/other clusters.



Cluster Analysis

- Broadly used in data analysis, including machine learning
- **Clustering** (unsupervised) vs. **classification** (supervised)
- **Hard clustering** (every element belongs to only one cluster) vs. **fuzzy clustering** (every element has various probabilities of belonging to a given cluster)
- Some methods find the number of clusters, others use a predefined number of clusters

Cluster Analysis

- Wide range of methods—which is best depends on the data to be clustered. Not really one ‘best’ method across all settings.

- In general, we want:
  - High intra-cluster similarity, low inter-cluster similarity (how to determine similarity?)
  - Potential to discover hidden features (especially in high dimensional data)

Some general classes (or clusters haha) of clustering methods:

- **Partitioning** methods (e.g. k-means clustering & other centroid methods)
- **Hierarchical** clustering methods
- **Density-based** methods
- **Model or distribution-based** methods (e.g. Gaussian mixture models, latent class analysis)
- Network clustering methods (**community detection** methods)
- & many others!

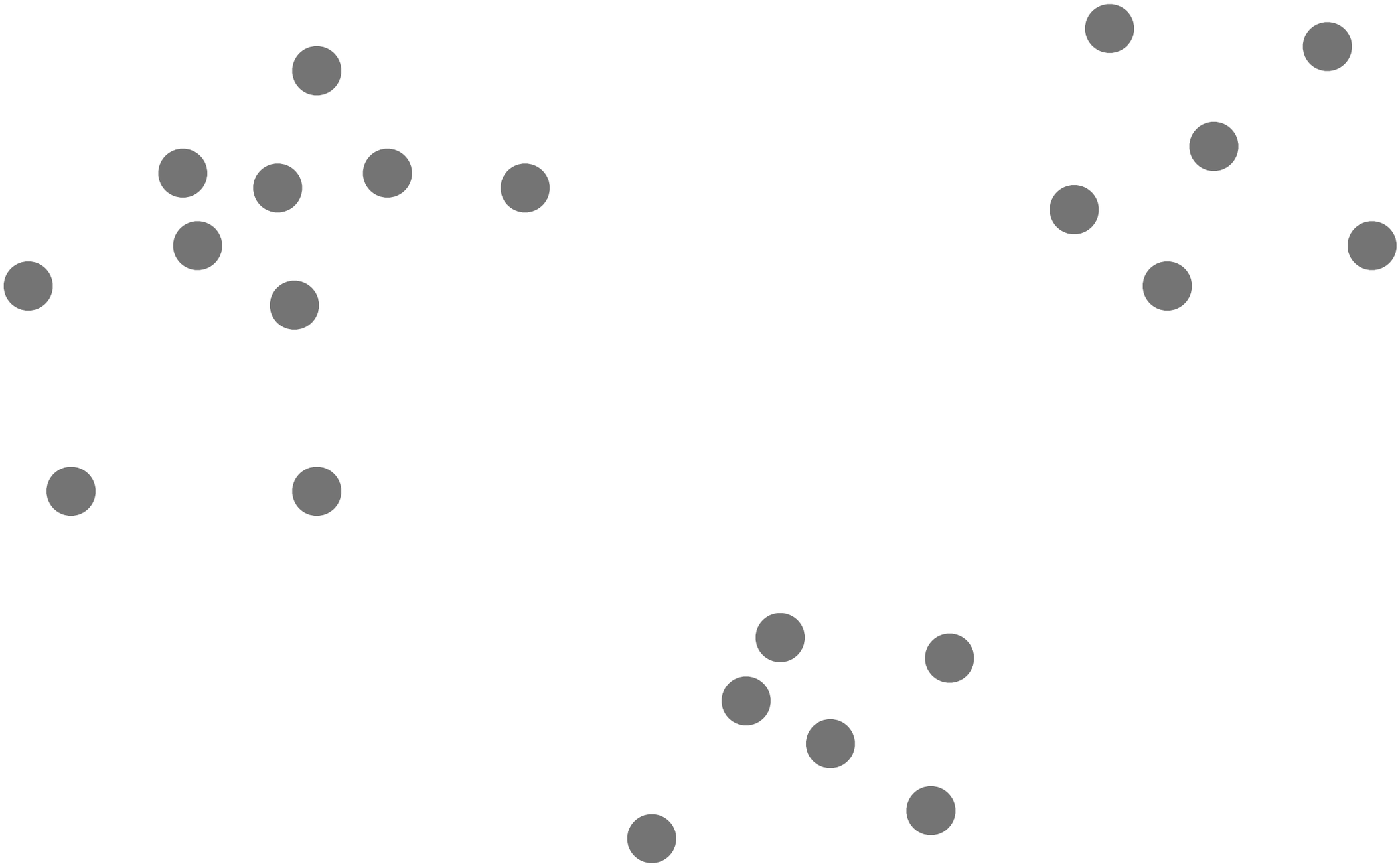
Partitioning methods

- General idea is often:
  - Construct a partition of the data into *k* clusters
  - Evaluate the resulting clusters and improve the partition
  - Repeat until optimal partition/clusters found
- Examples: k-means, k-medioids, k-modes (among many others)

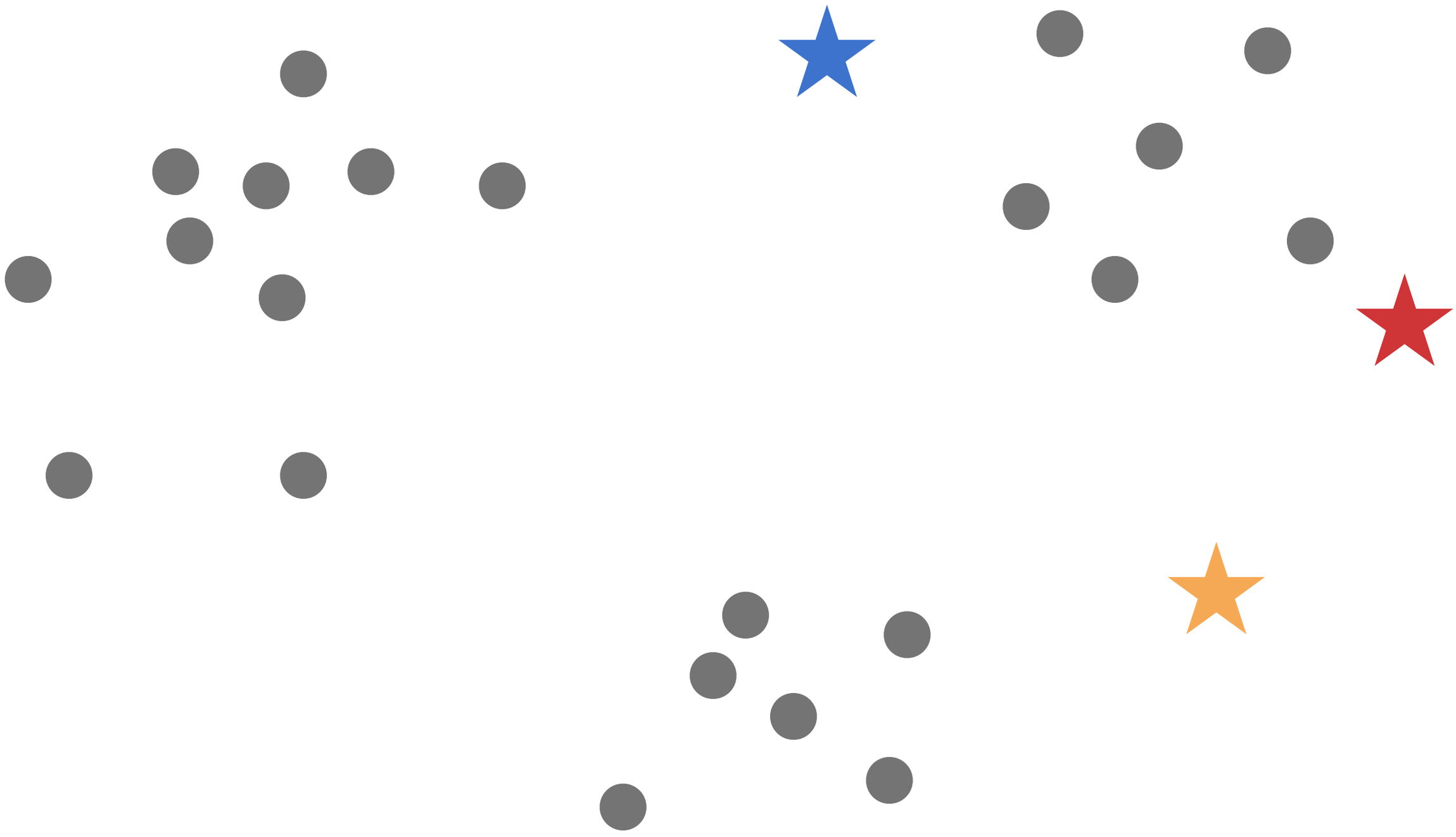
K-means clustering

- Select k centroids (means), and each data point is assigned to the nearest centroid
- This partitions the space into Voronoi cells, which are our clusters
- For each cluster, calculate the centroid of all points
- These become the new cluster centroids
- Reassign points to nearest centroid and repeat

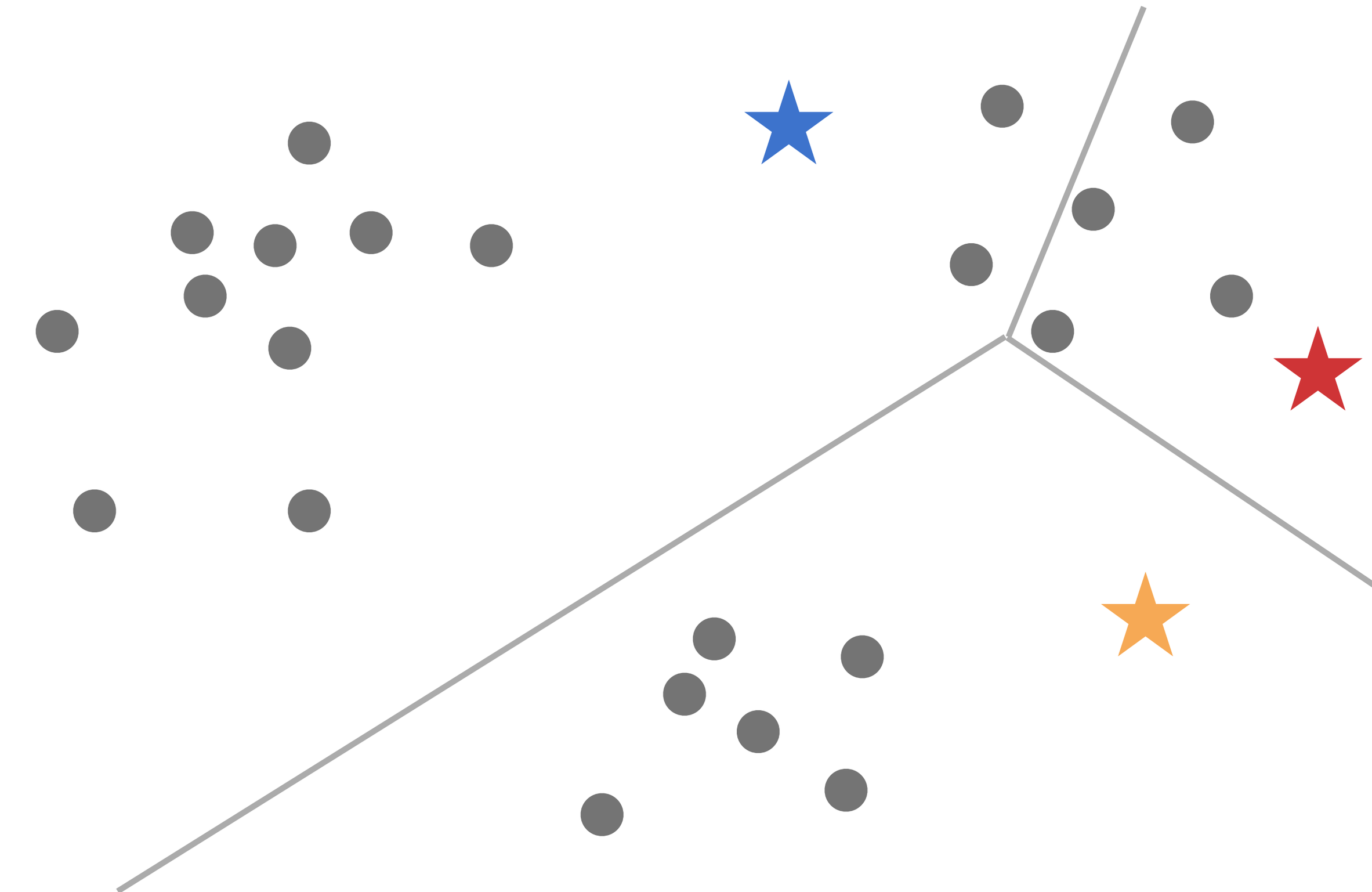
K-means clustering example



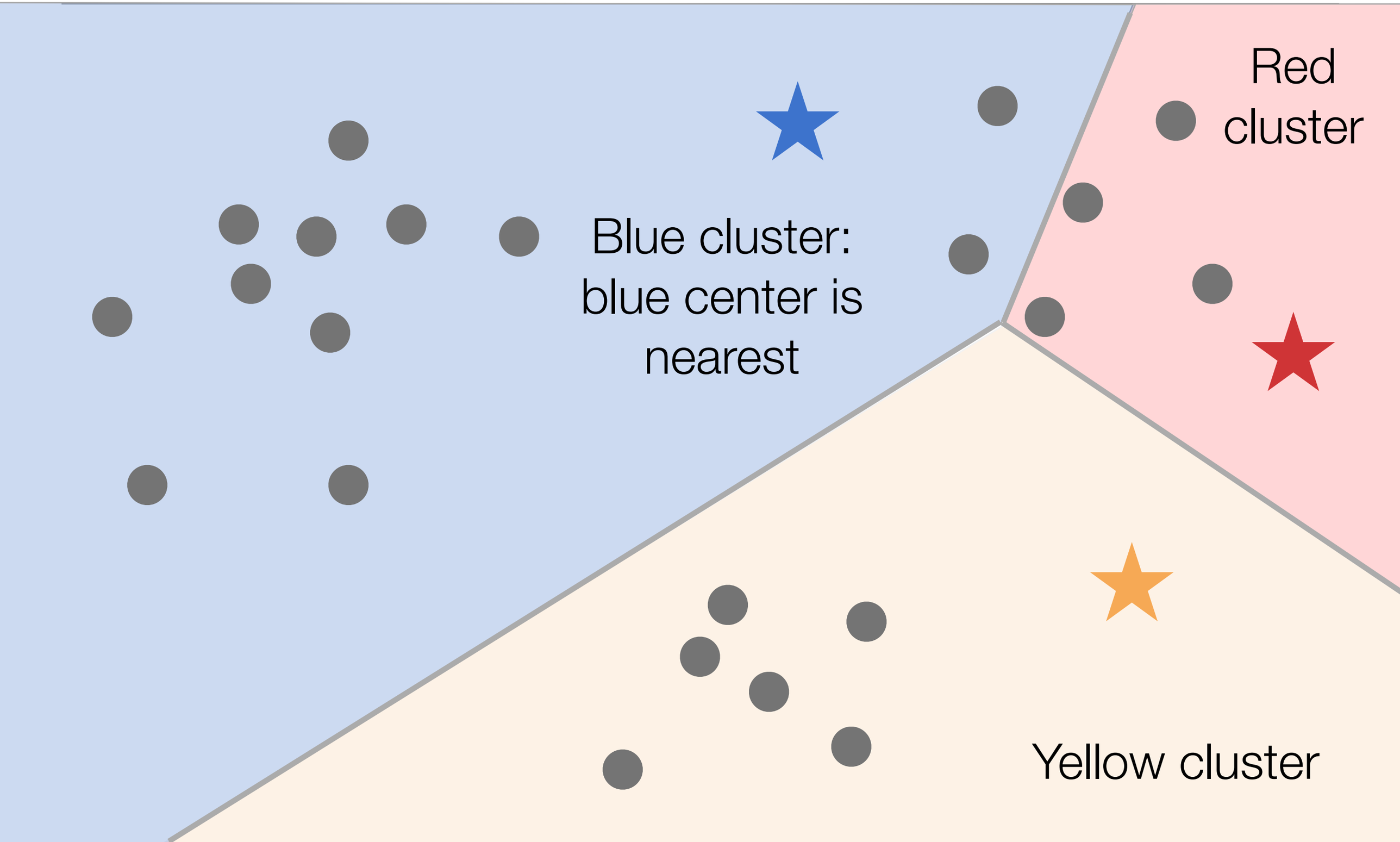
Randomly choose 3 cluster centers to start



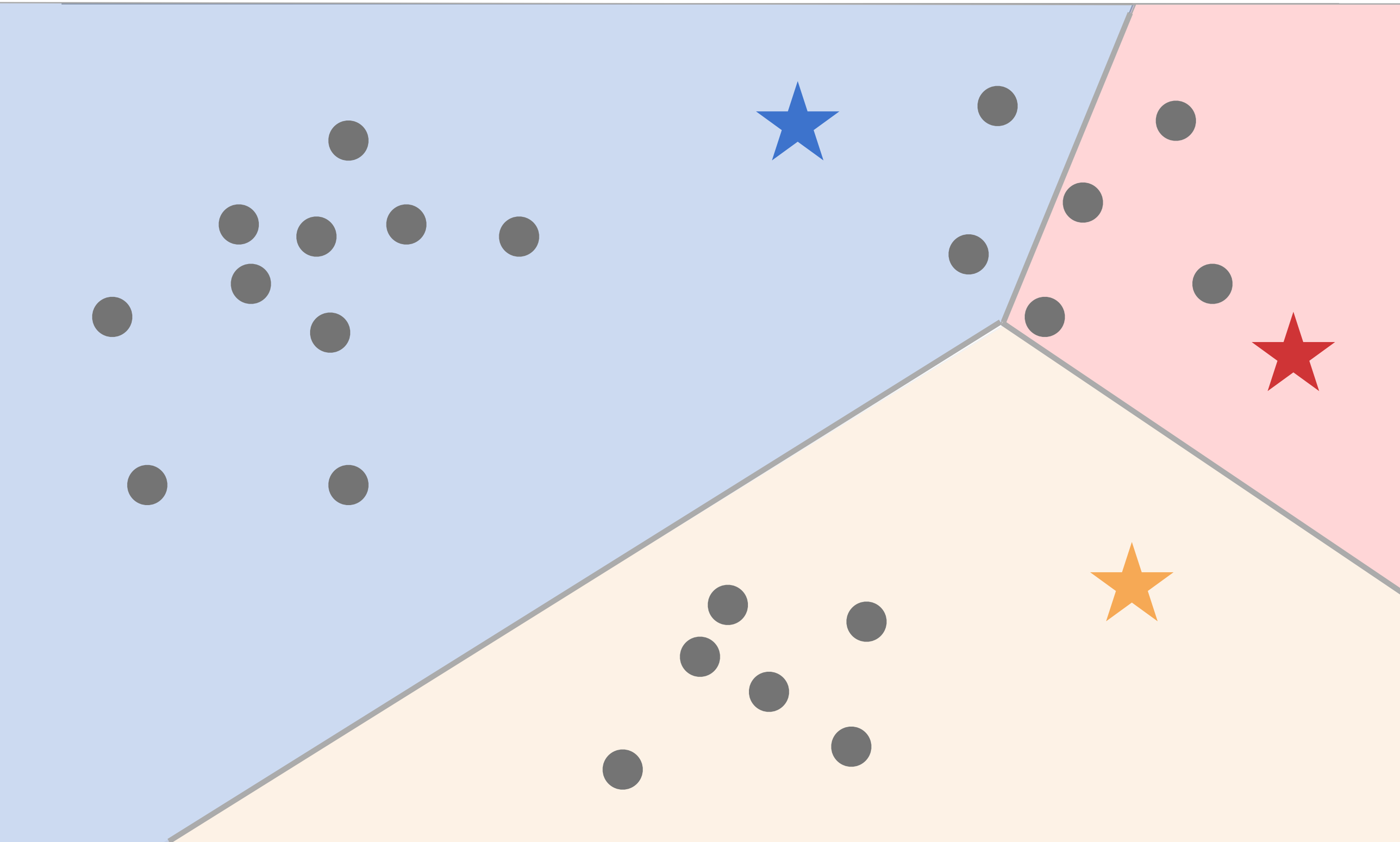
The cluster centers partition the space based on which center is nearest



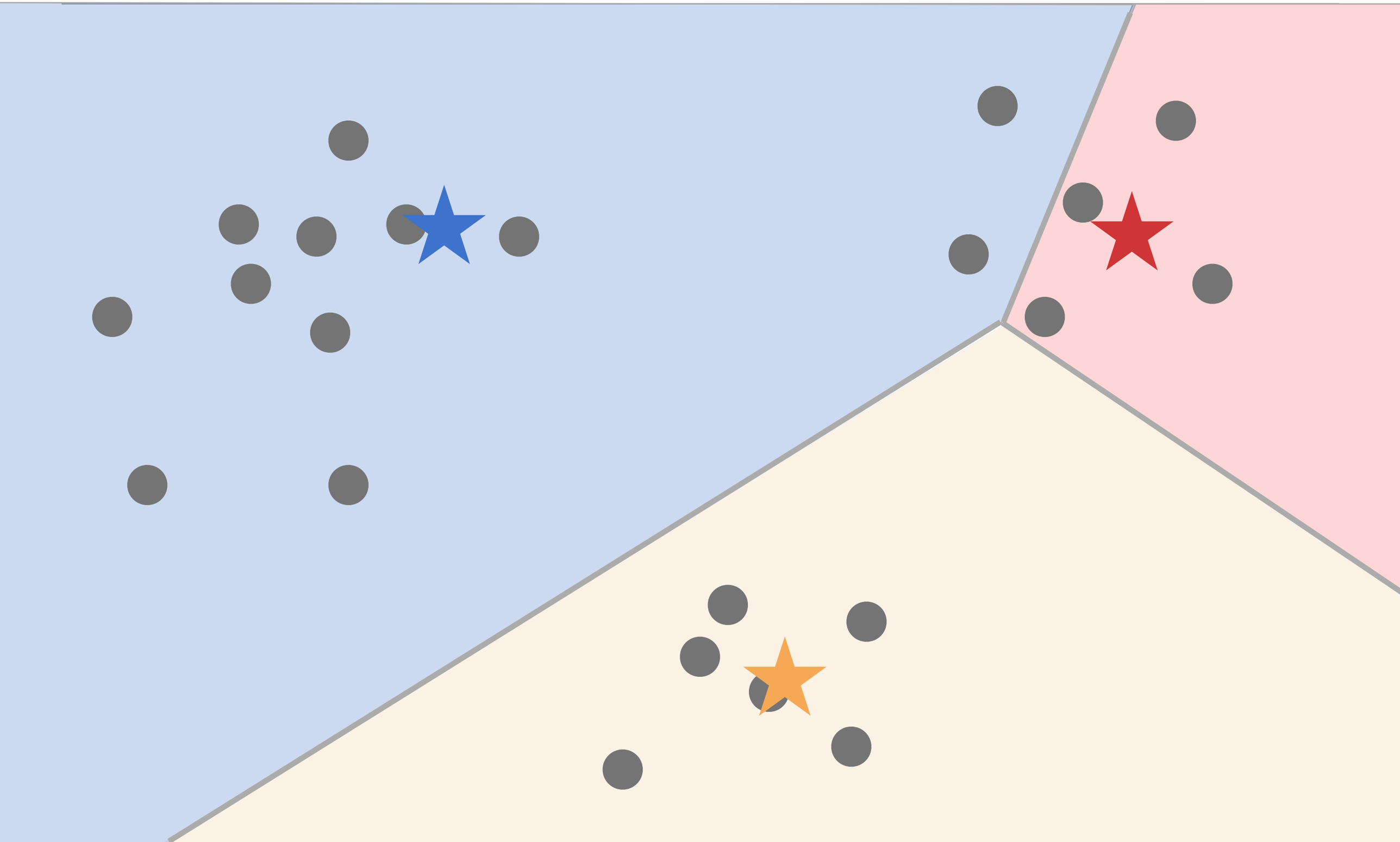
These are our starting **clusters**



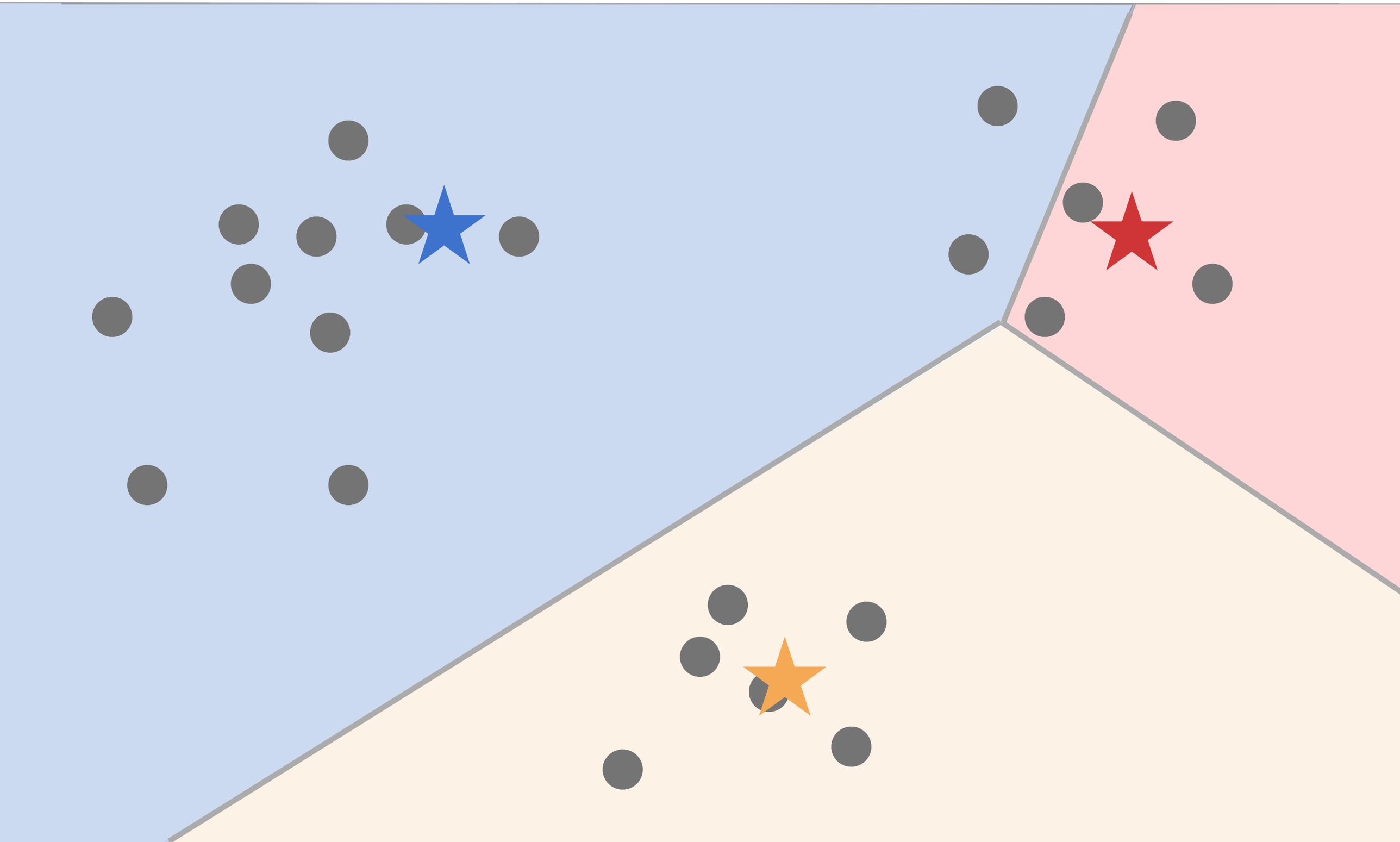
What are the means of the data points in each cluster?



These are the new centers.



Now which data points are closest to each center?



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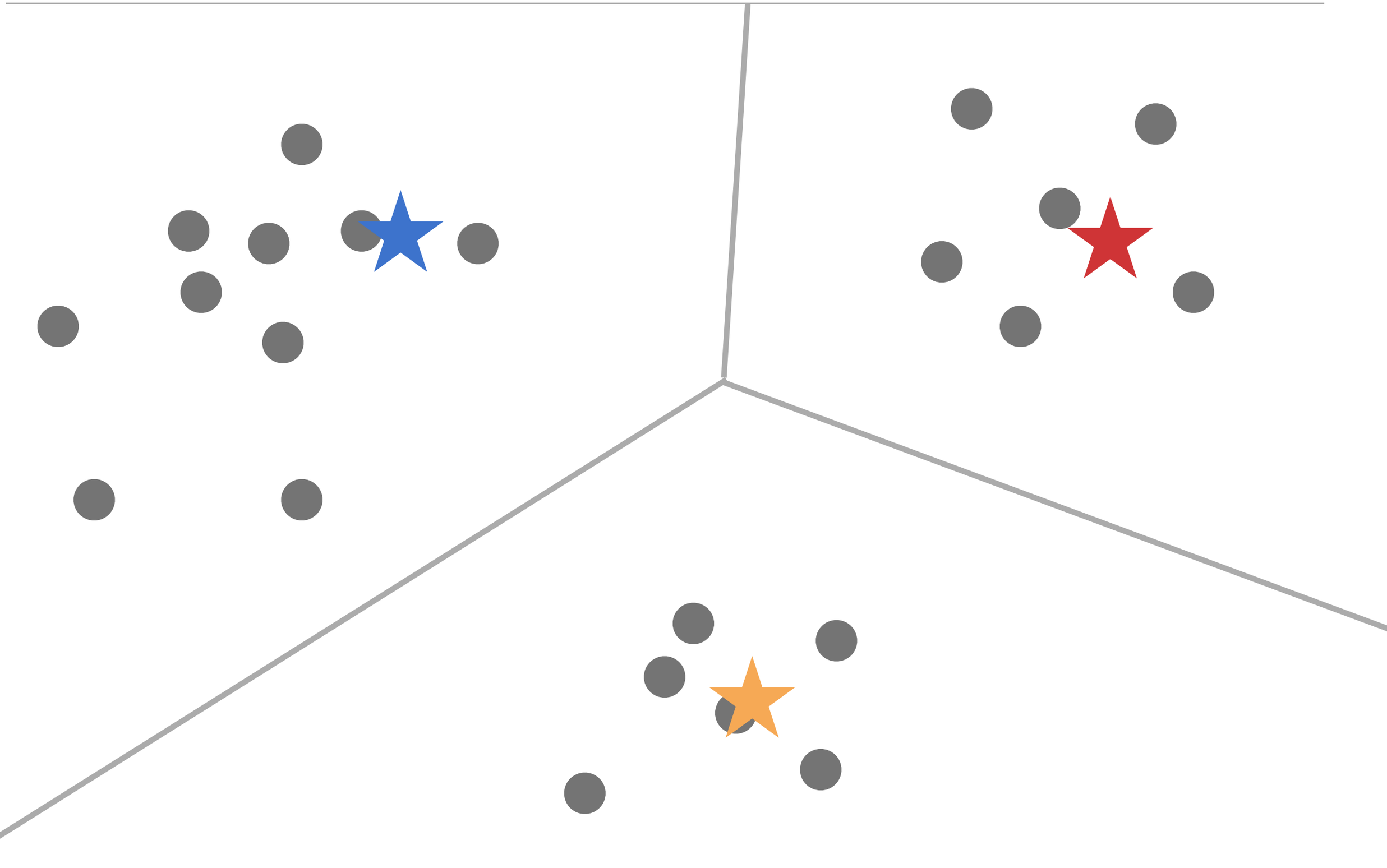
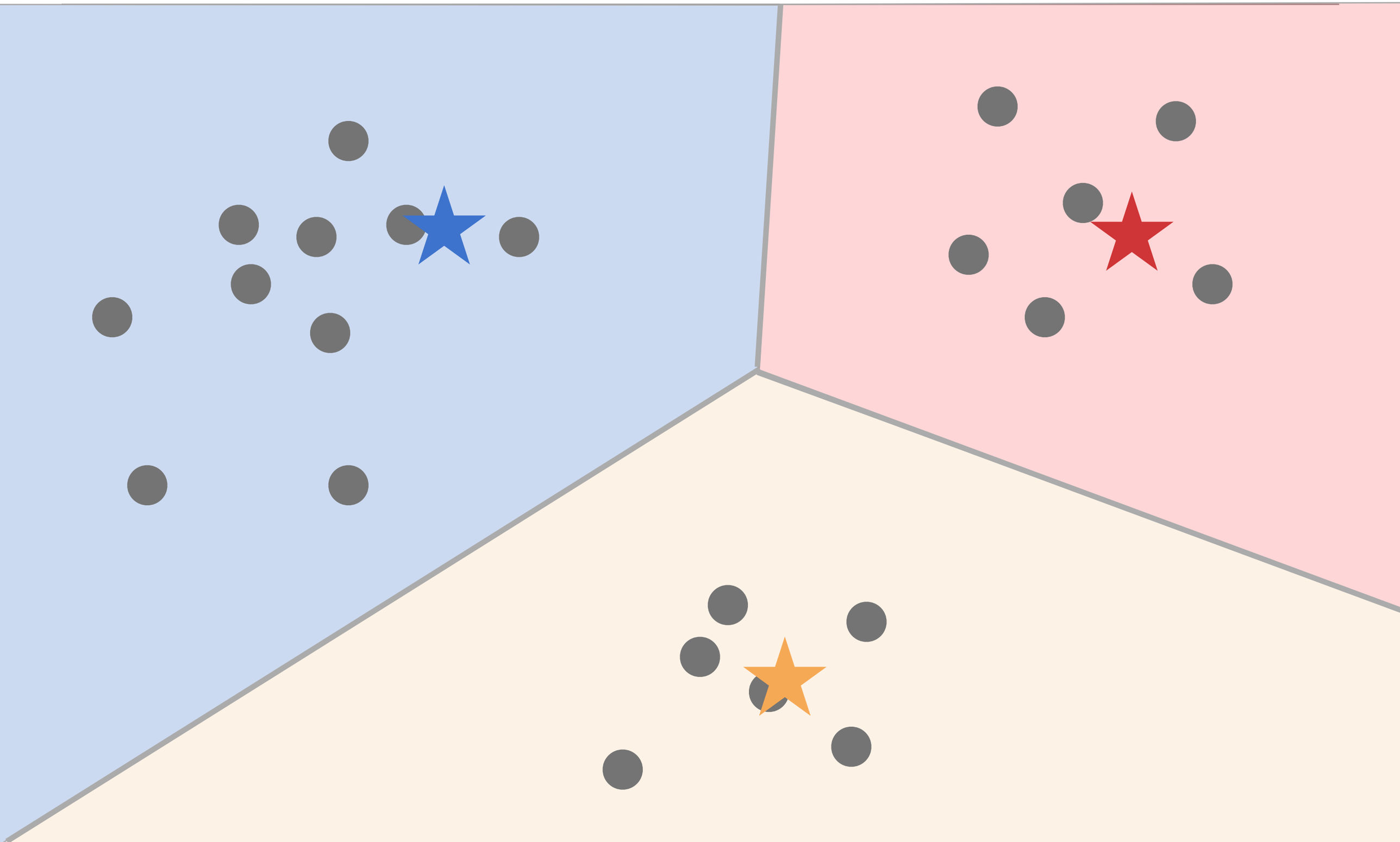
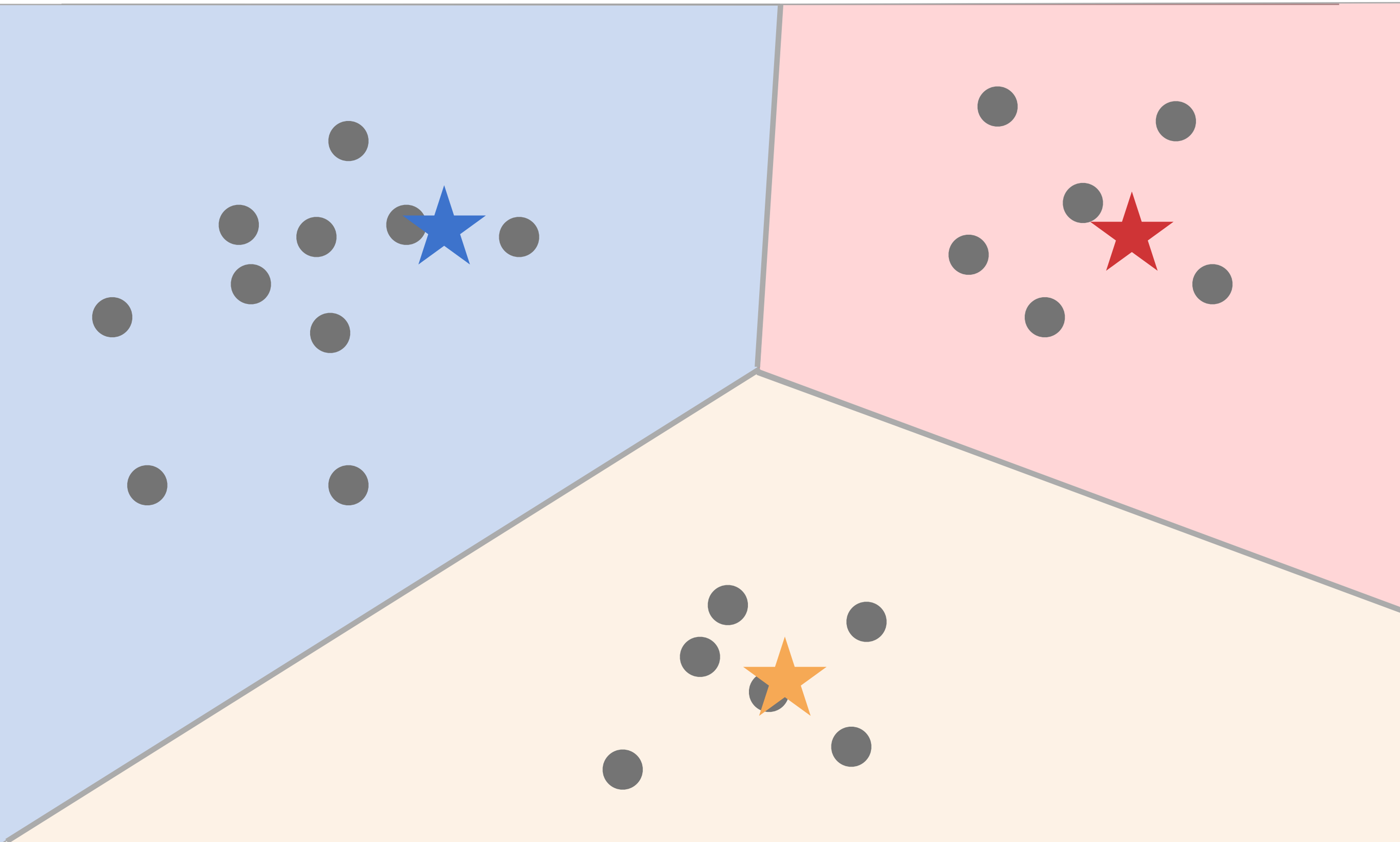


Redefine the clusters based on which center they're nearest



And repeat! Keep calculating the centers and redefining the clusters until they stop changing.



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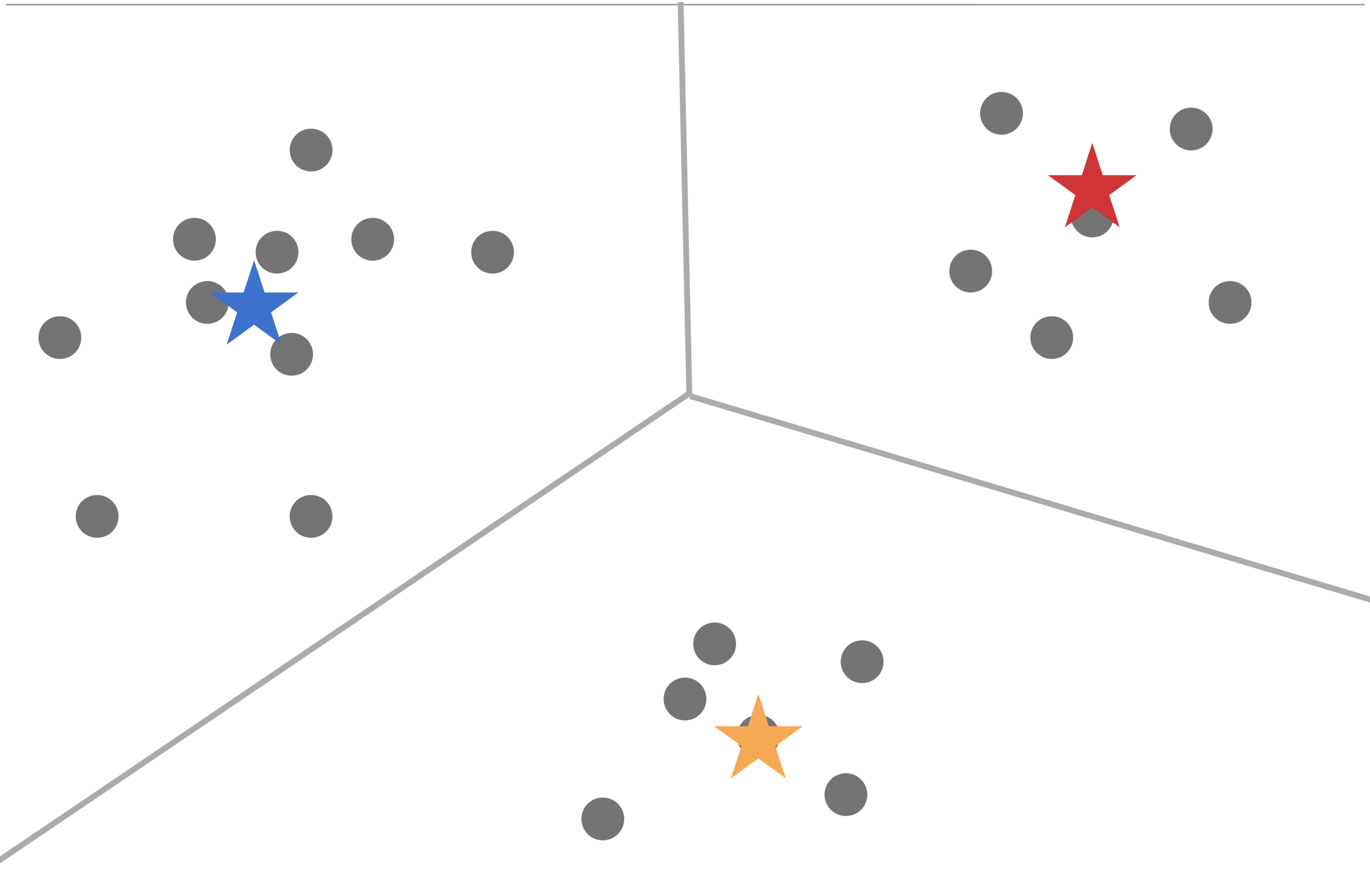
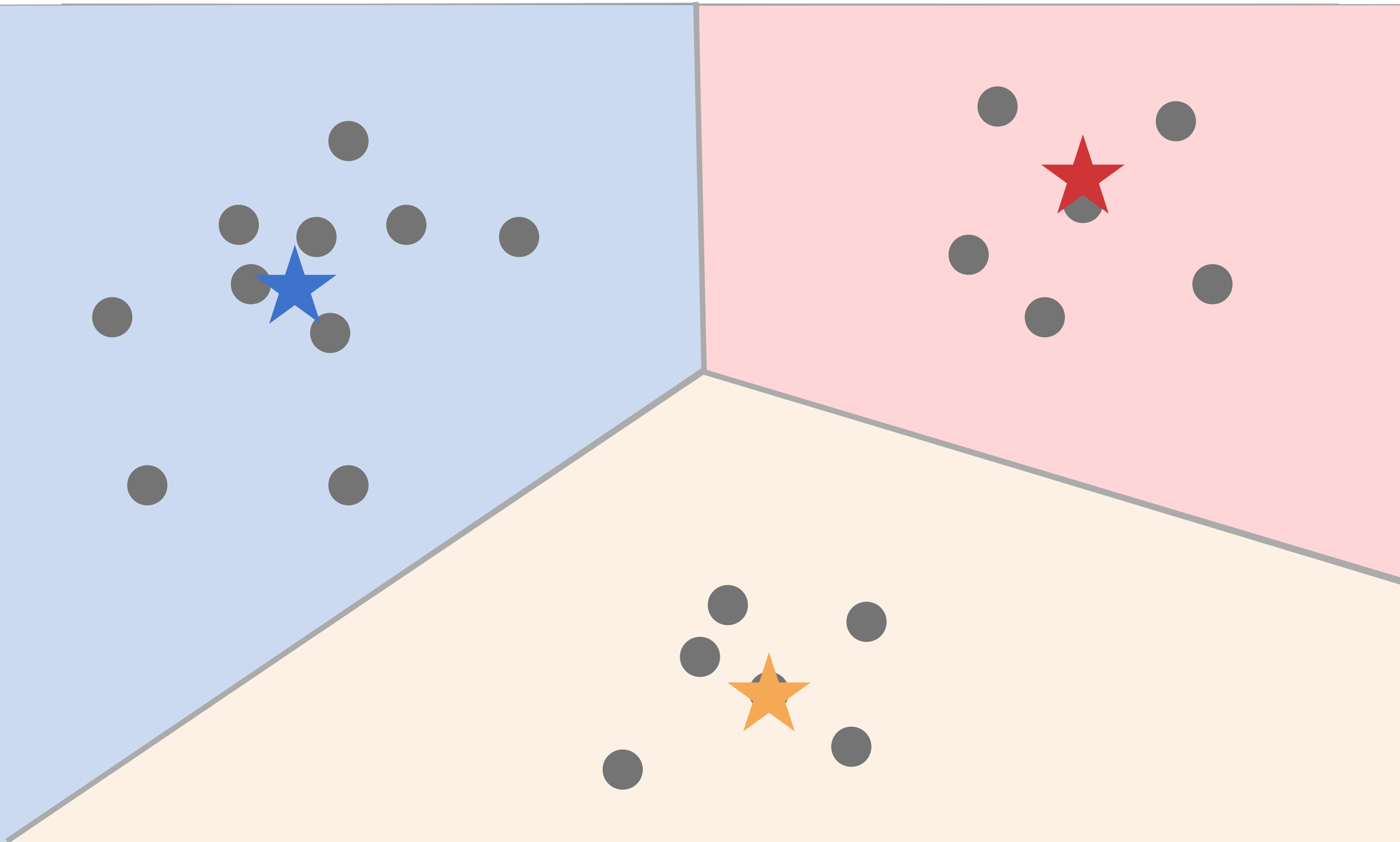
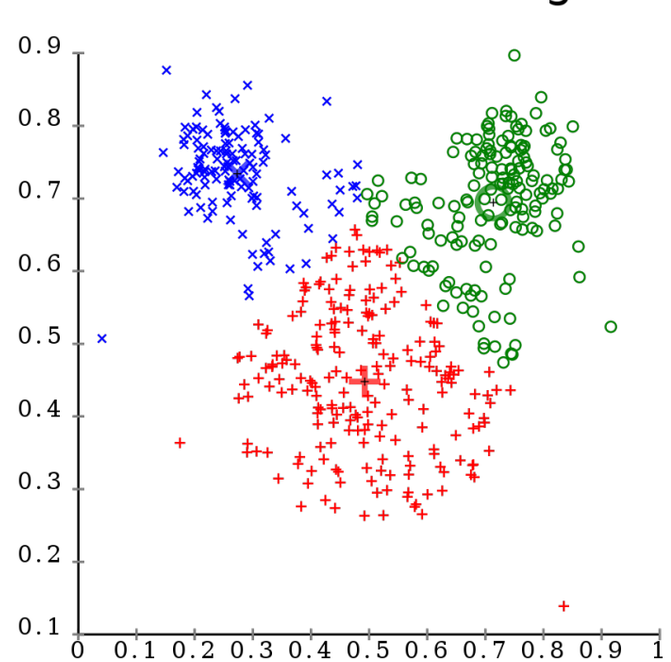


The results once the clusters and centers are fixed are your final k-means clusters.



K-means clustering

- Relatively efficient
- Can converge to local optima (e.g. depending on starting points)
- Have to specify k (number of clusters)
- Cannot make clusters with non-convex shapes
- Tends toward equal sized clusters
- How to handle categorical data? (e.g. can use k-modes)



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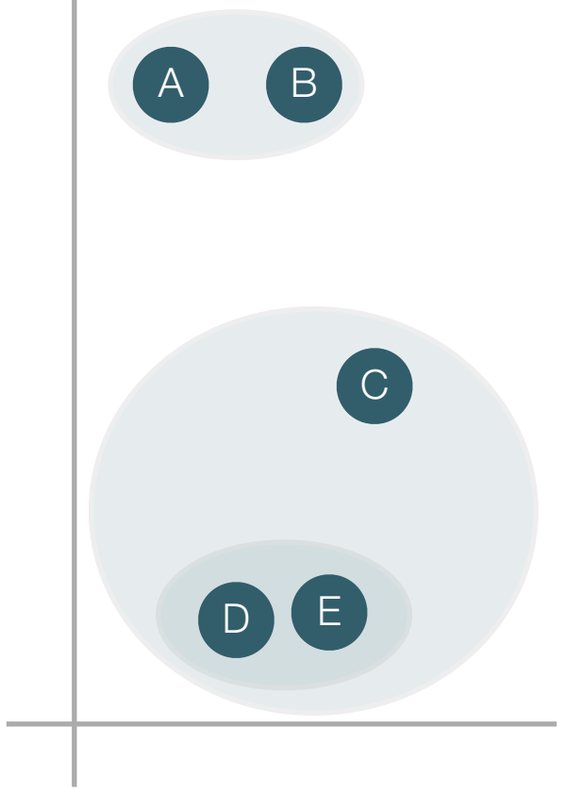
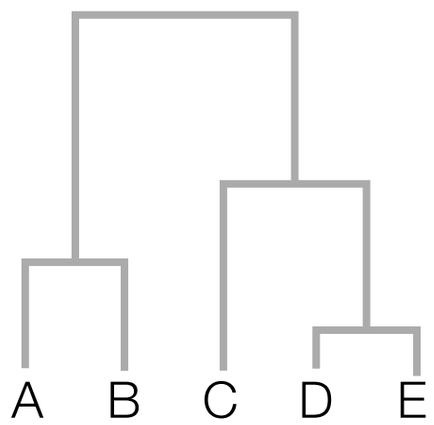
Hierarchical clustering methods

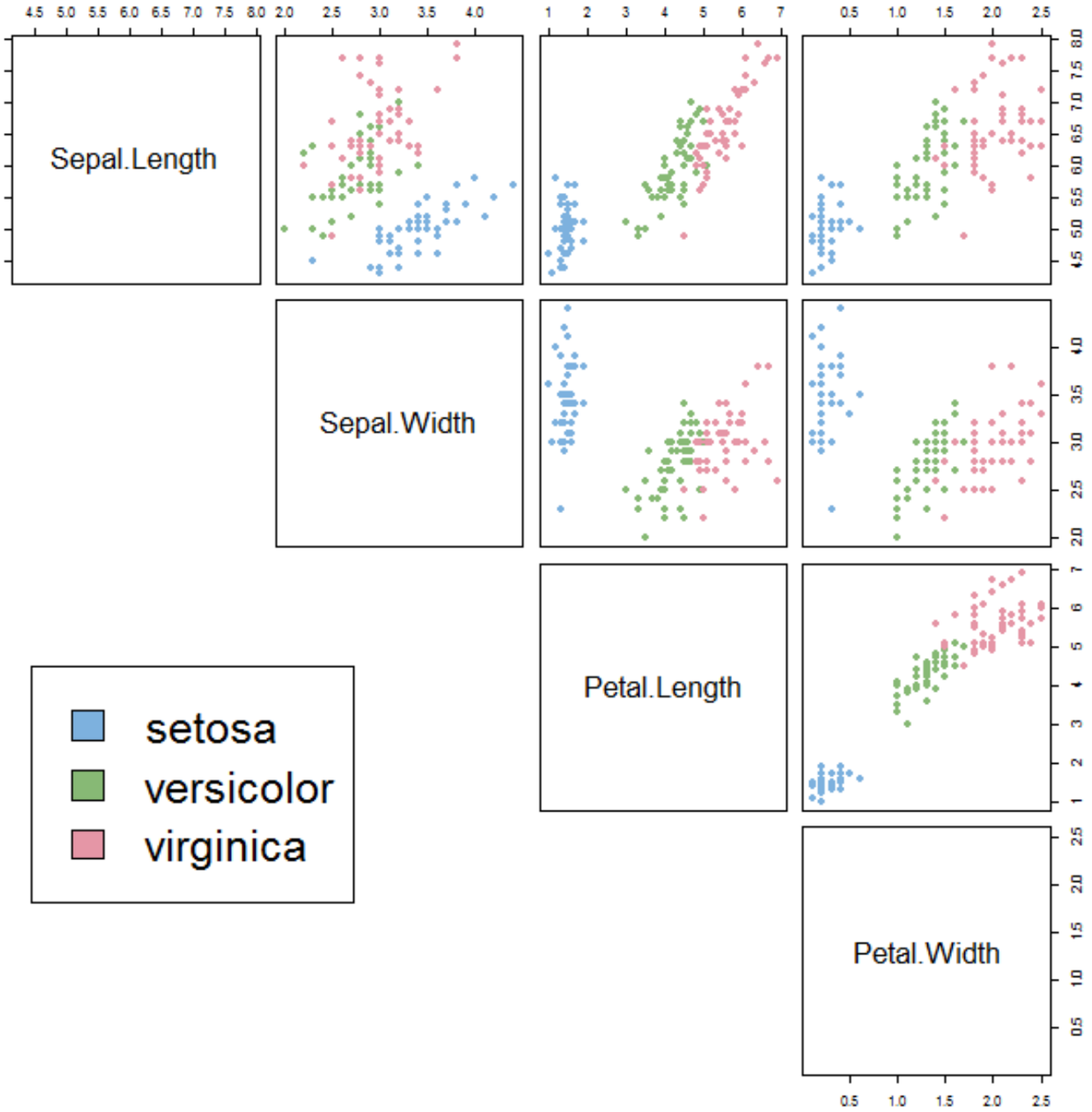
- Agglomerative approach to clustering
    - Starts with small clusters (e.g. individual points) and then merges based on distance
- Divisive approach does the reverse (all one cluster then split into smaller ones)
- Many different approaches with different distance measurements, etc.

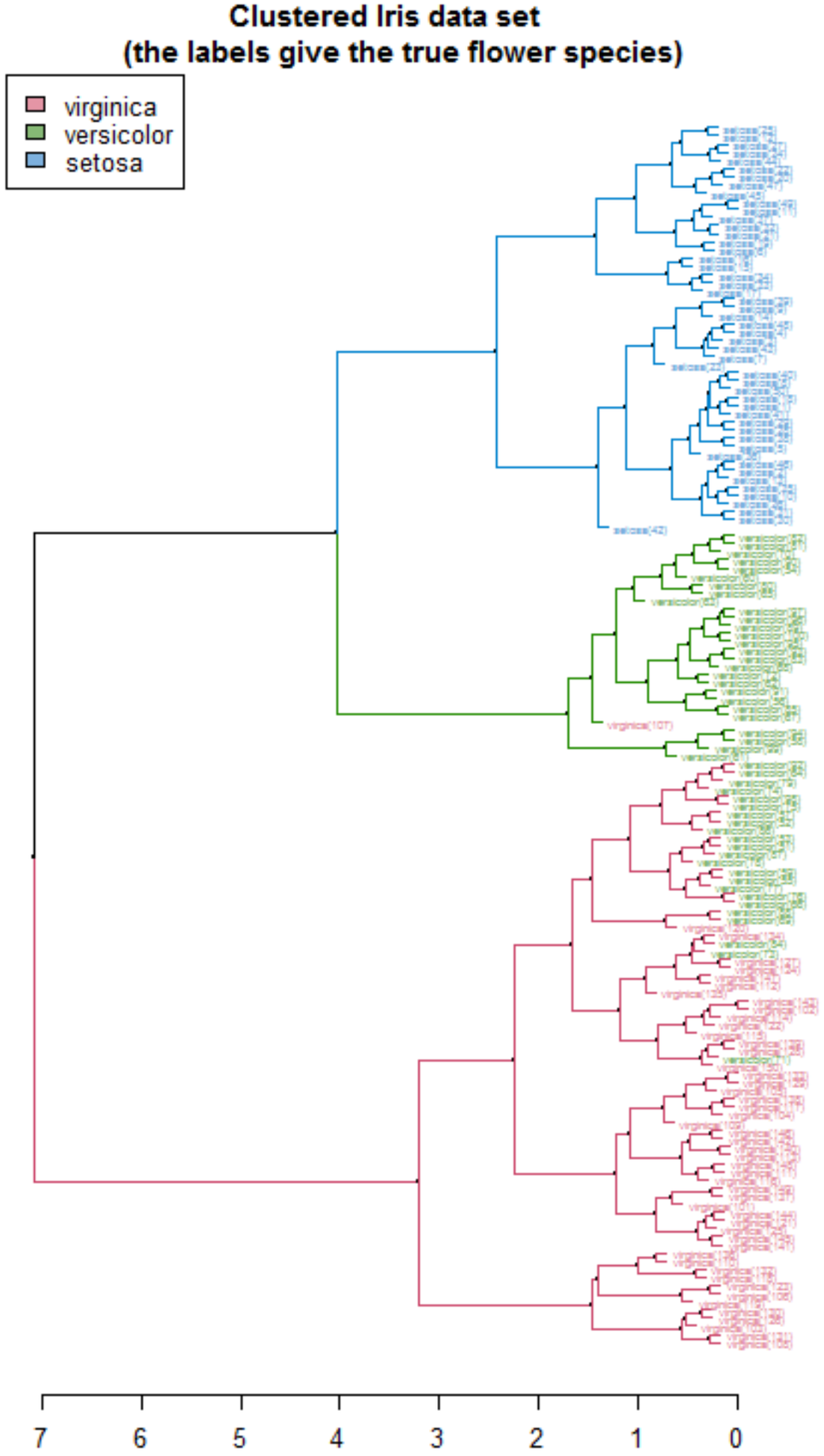
Hierarchical clustering example





- Start with all single point clusters
- Merge the two nearest clusters—forms a new cluster
- Merge the next two nearest clusters, etc.
- How to decide cluster distances? (What metric, do we use nearest point distance, furthest, centroid?)
- Capture clusters as a dendrogram—can choose resolution of clusters as desired





https://cran.r-project.org/web/packages/dendextend/vignettes/Cluster_Analysis.html

Hierarchical clustering

- Slow for larger data sets
- Useful for finding substructures/subclusters in data
- Assumes every data point is relevant/part of the clusters
- How to choose level of granularity?

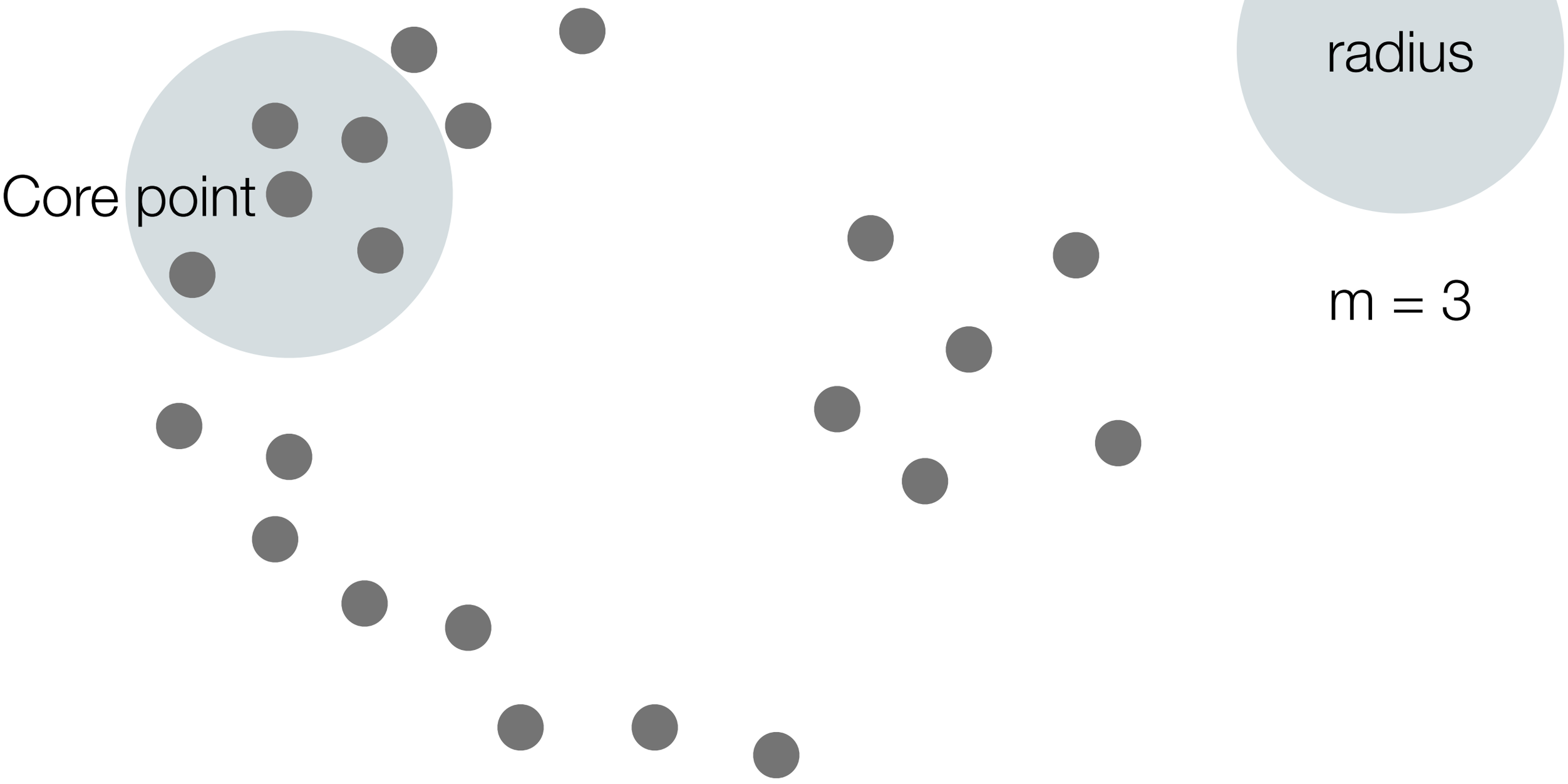
Density-based clustering

- Decides clusters based on density of points
- Not every point need be assigned a cluster—some can be considered noise or outliers
- One of the most commonly used algorithms is DBSCAN (Density-Based Spatial Clustering of Applications with Noise)

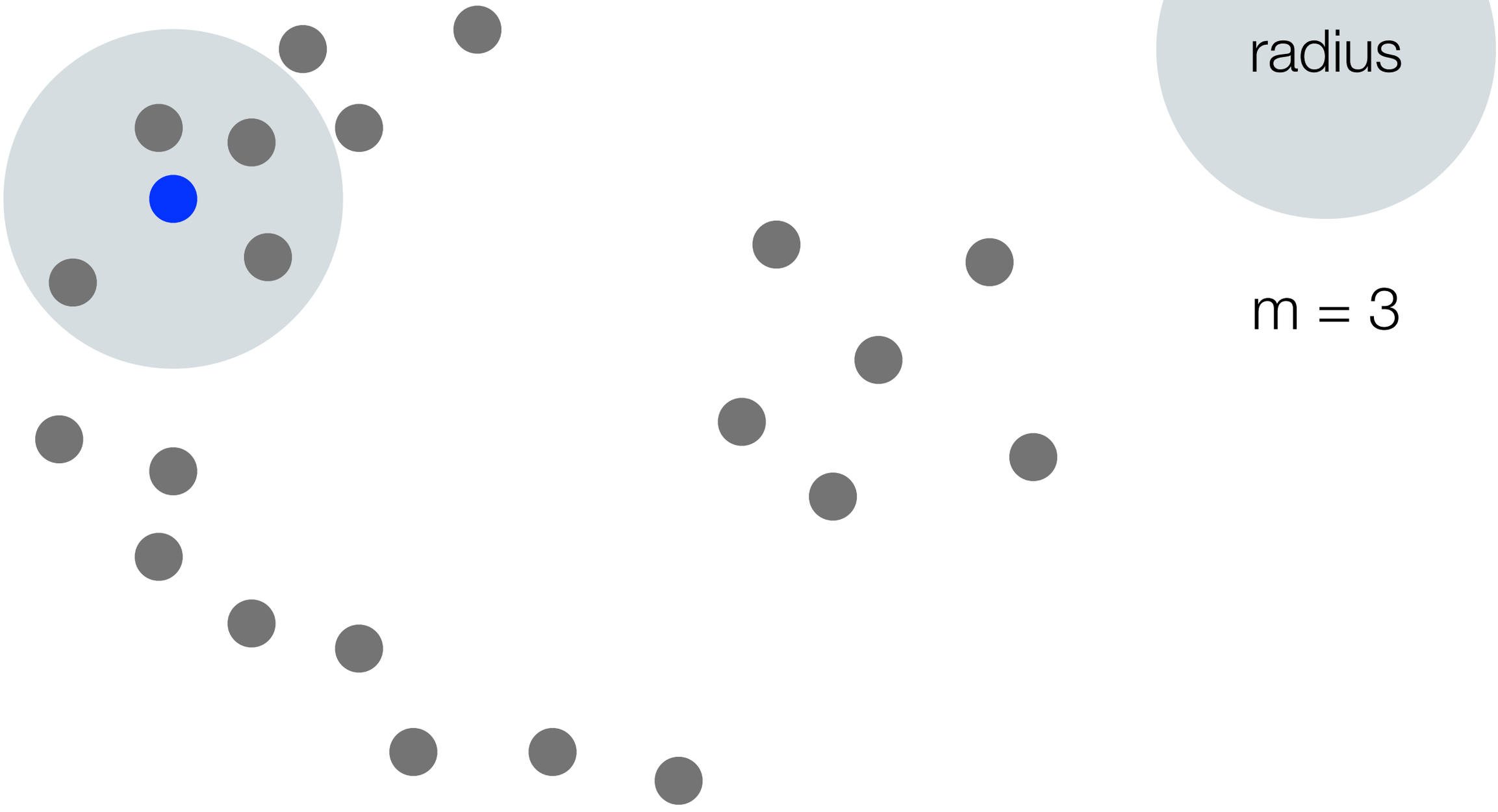
DBSCAN

- Choose a radius *r* and a minimum number of points *m*
- Classify each point as a:
  - **Core point** - has at least *m* other points within radius *r*
  - **Border point** - does not have *m* points within radius *r*, but is **reachable** a core point *p* - i.e. can be connected to data point *p* by a chain of core points each within radius *r* of the next point
  - **Outlier** - neither core nor border

DBSCAN example



DBSCAN example

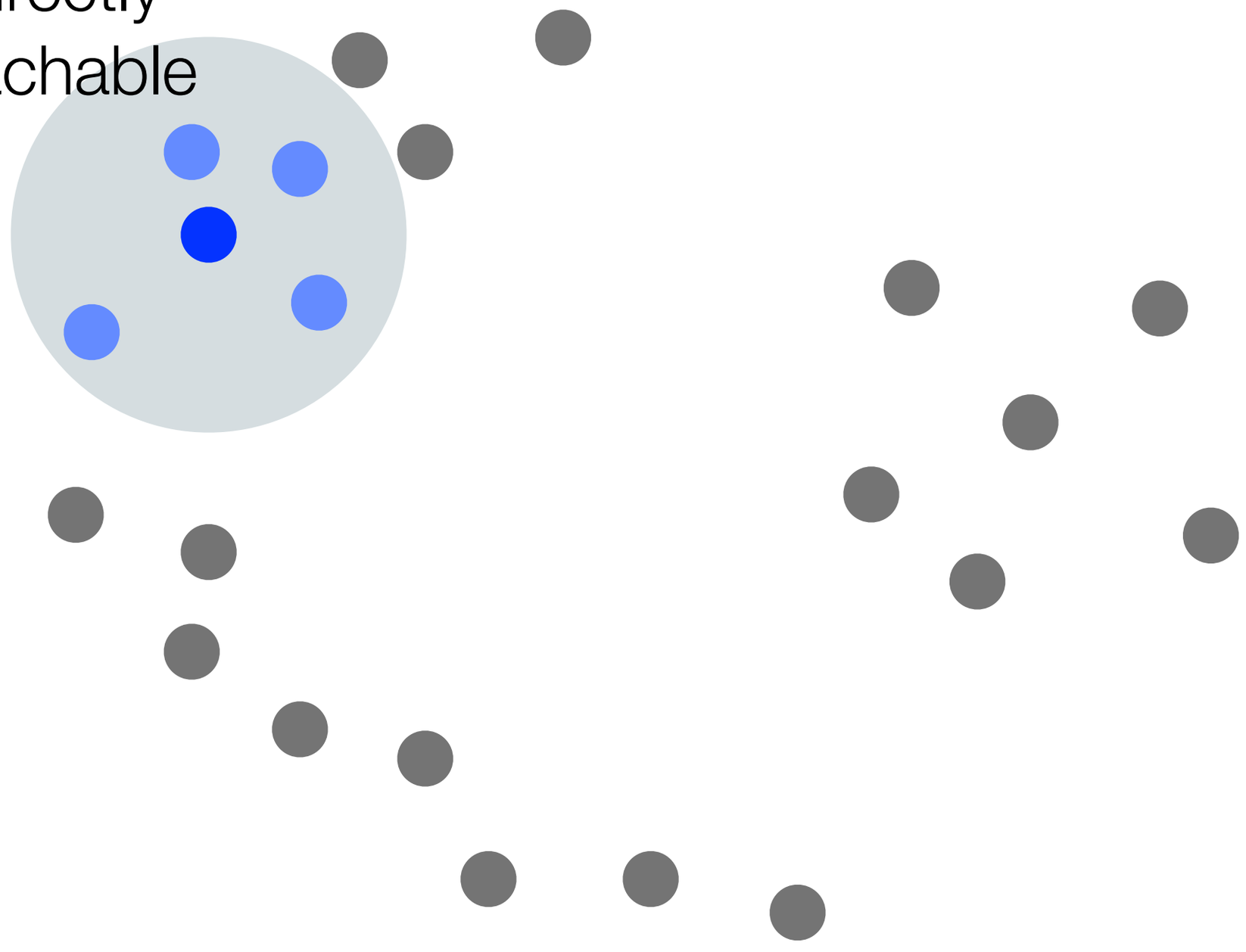


DBSCAN example

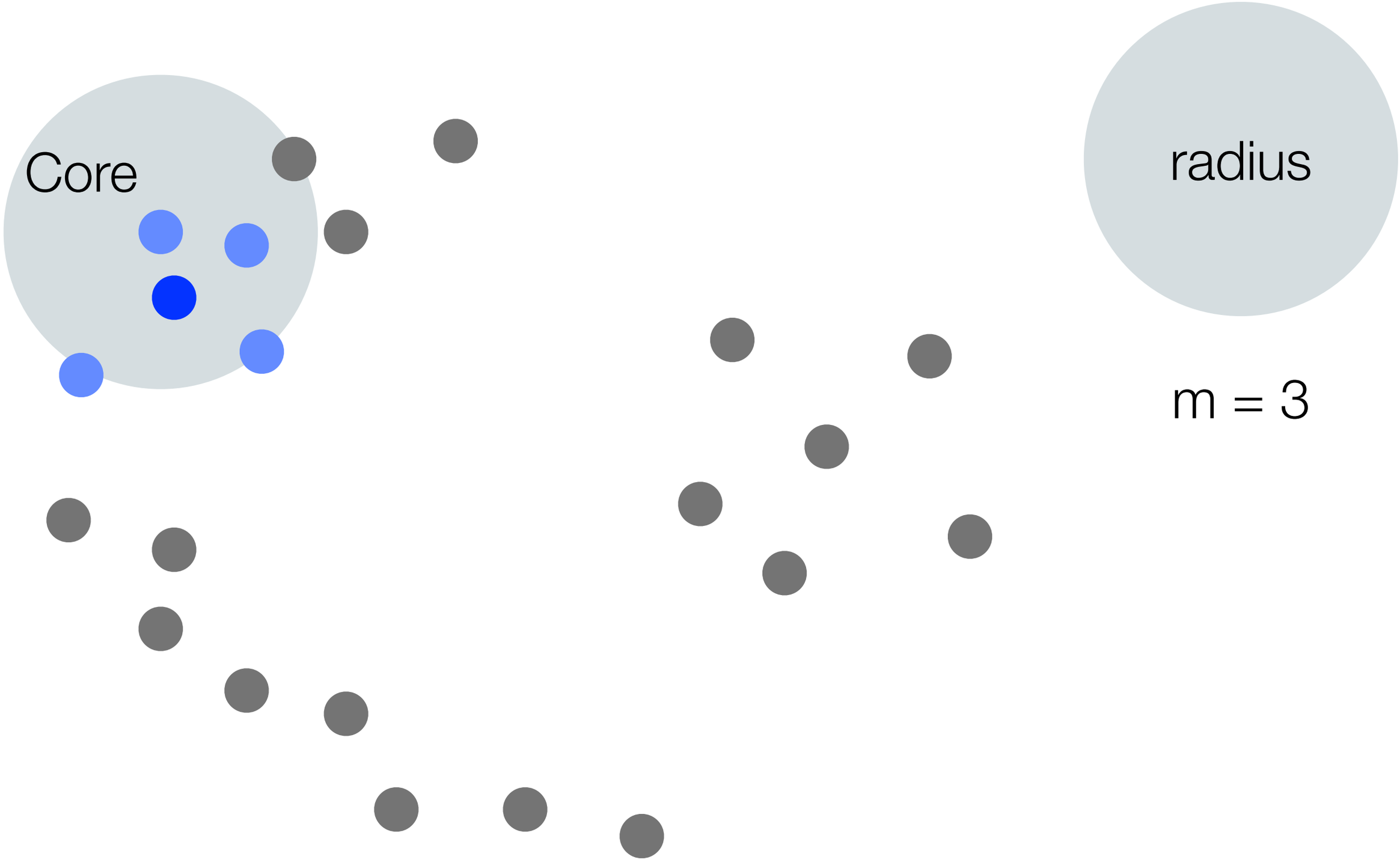
Directly reachable

radius

m = 3



DBSCAN example



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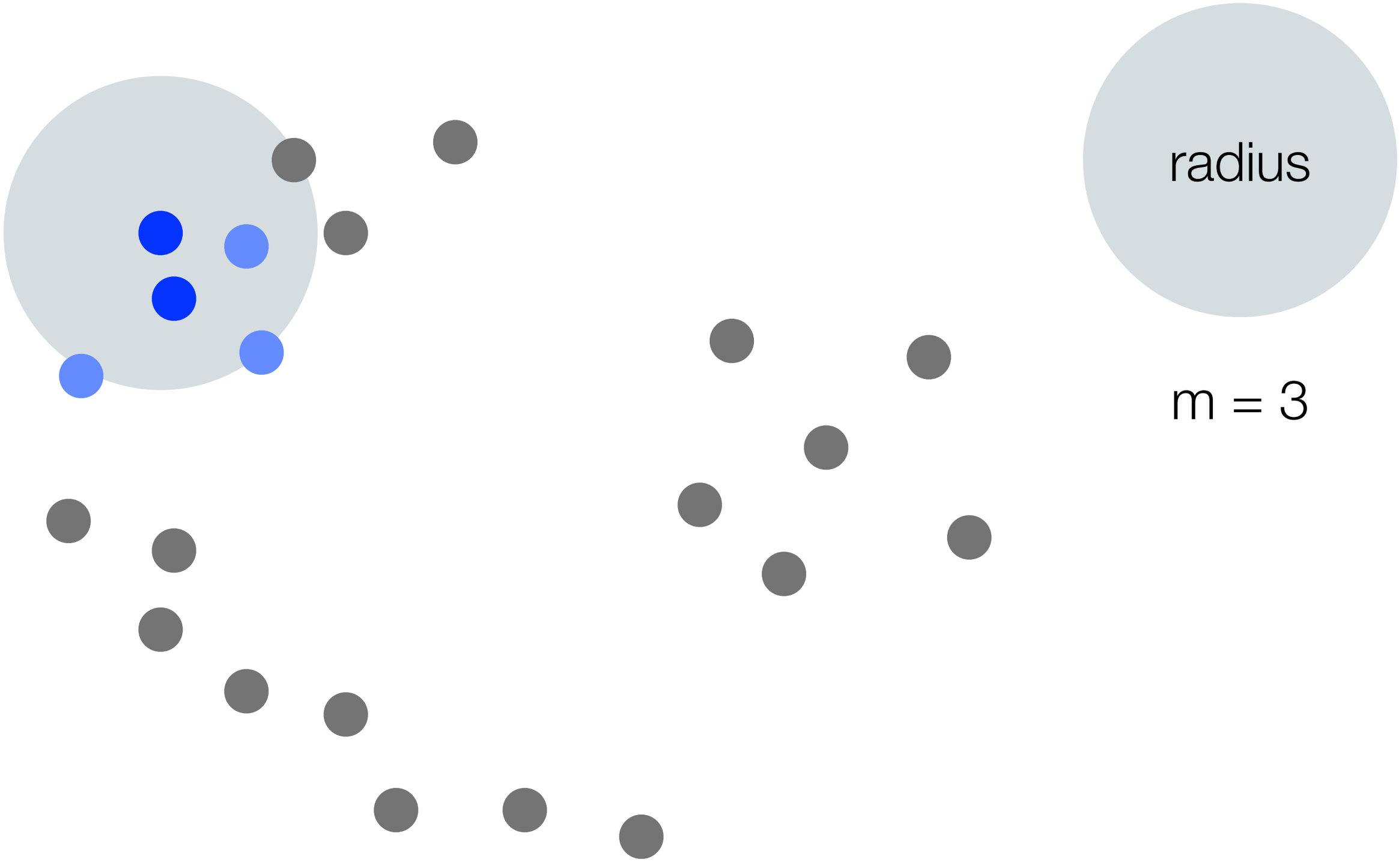

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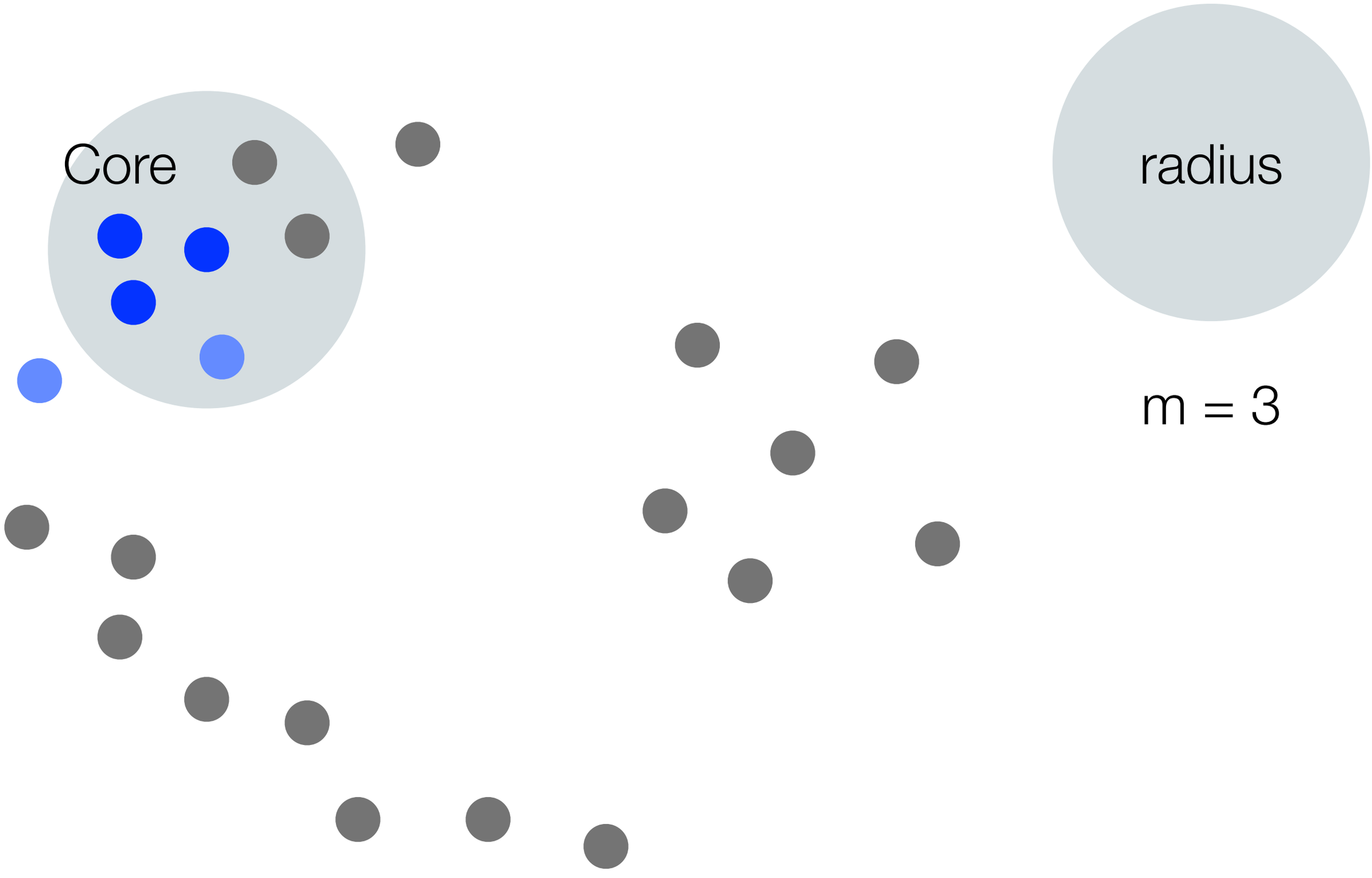

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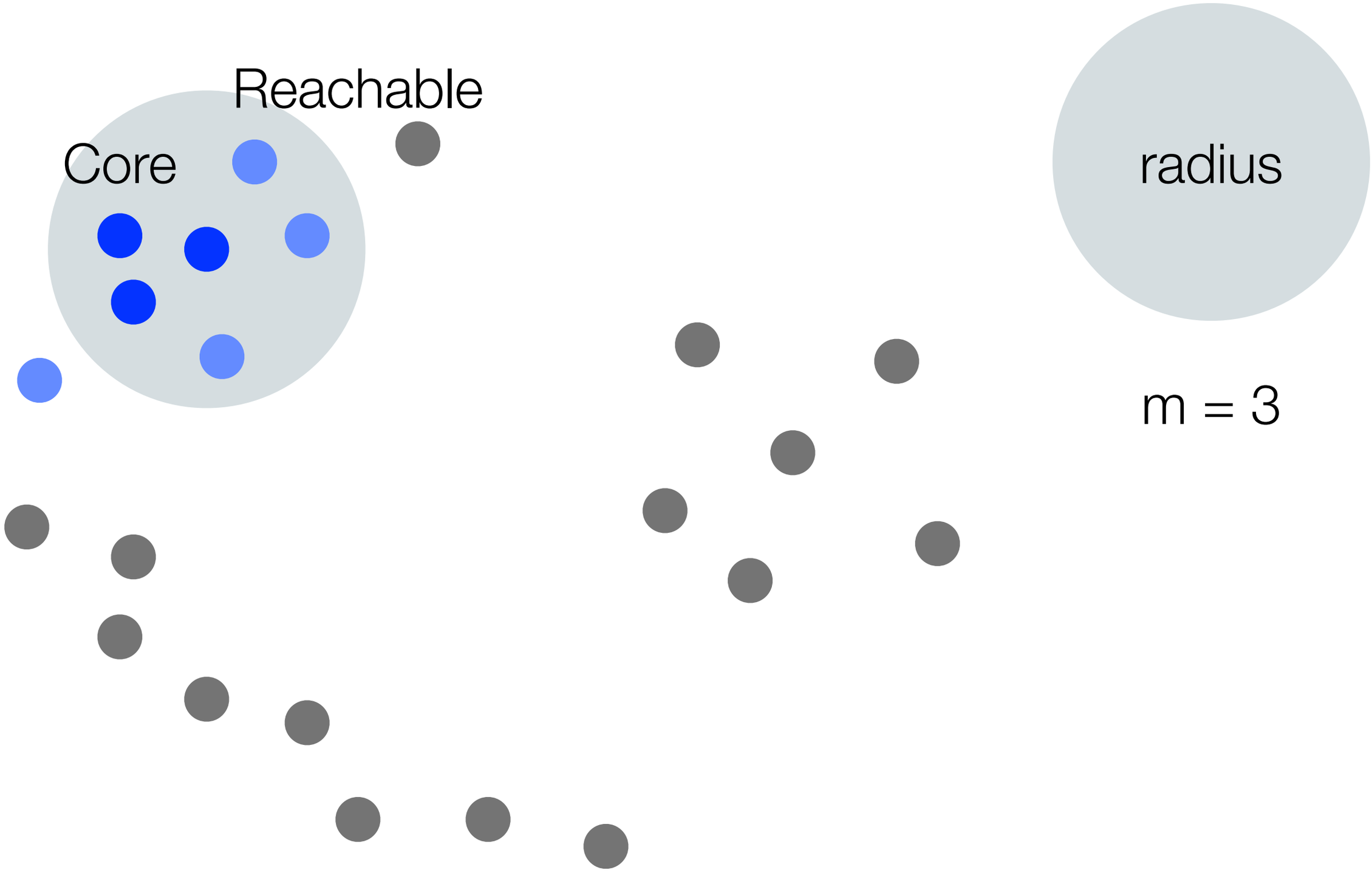

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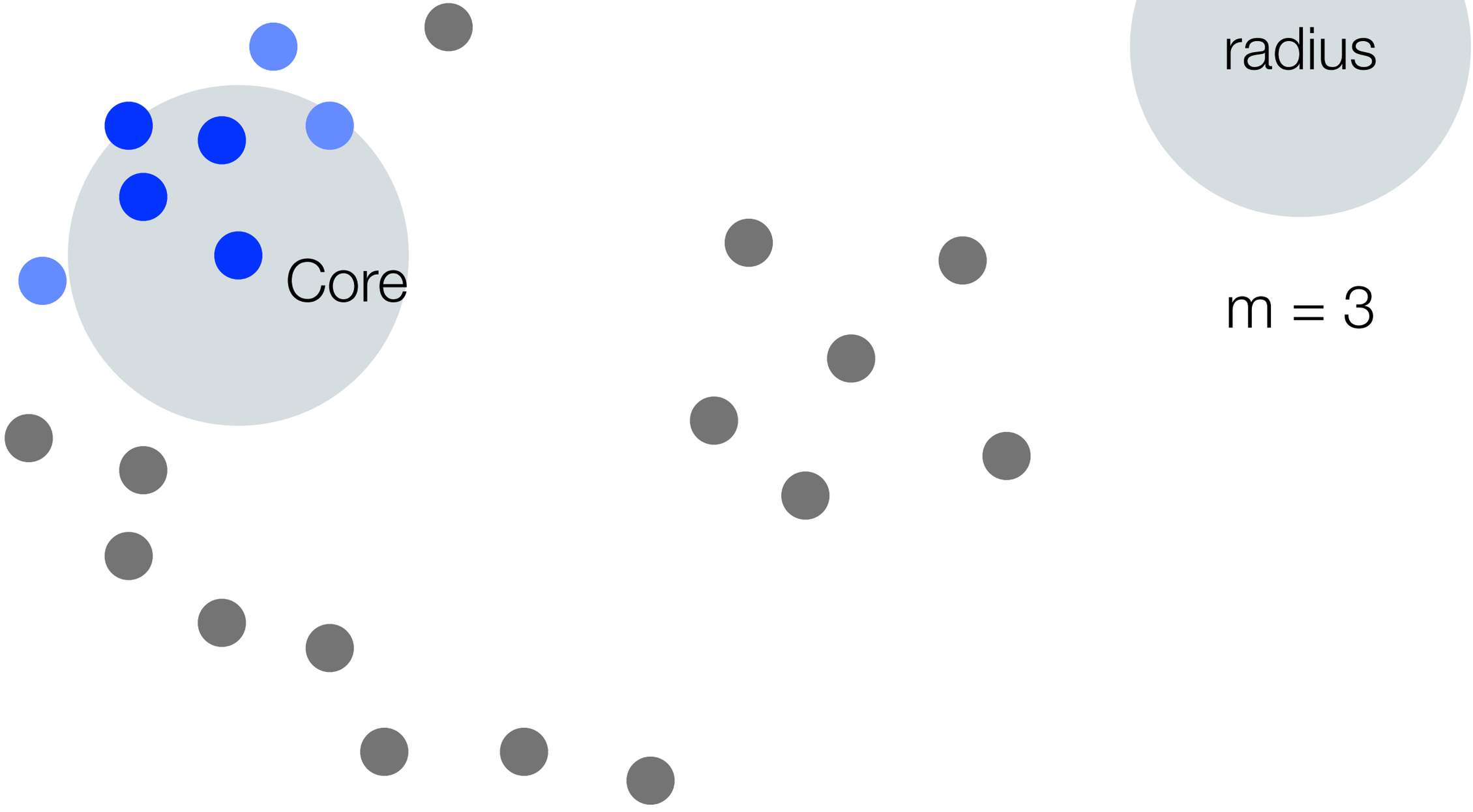

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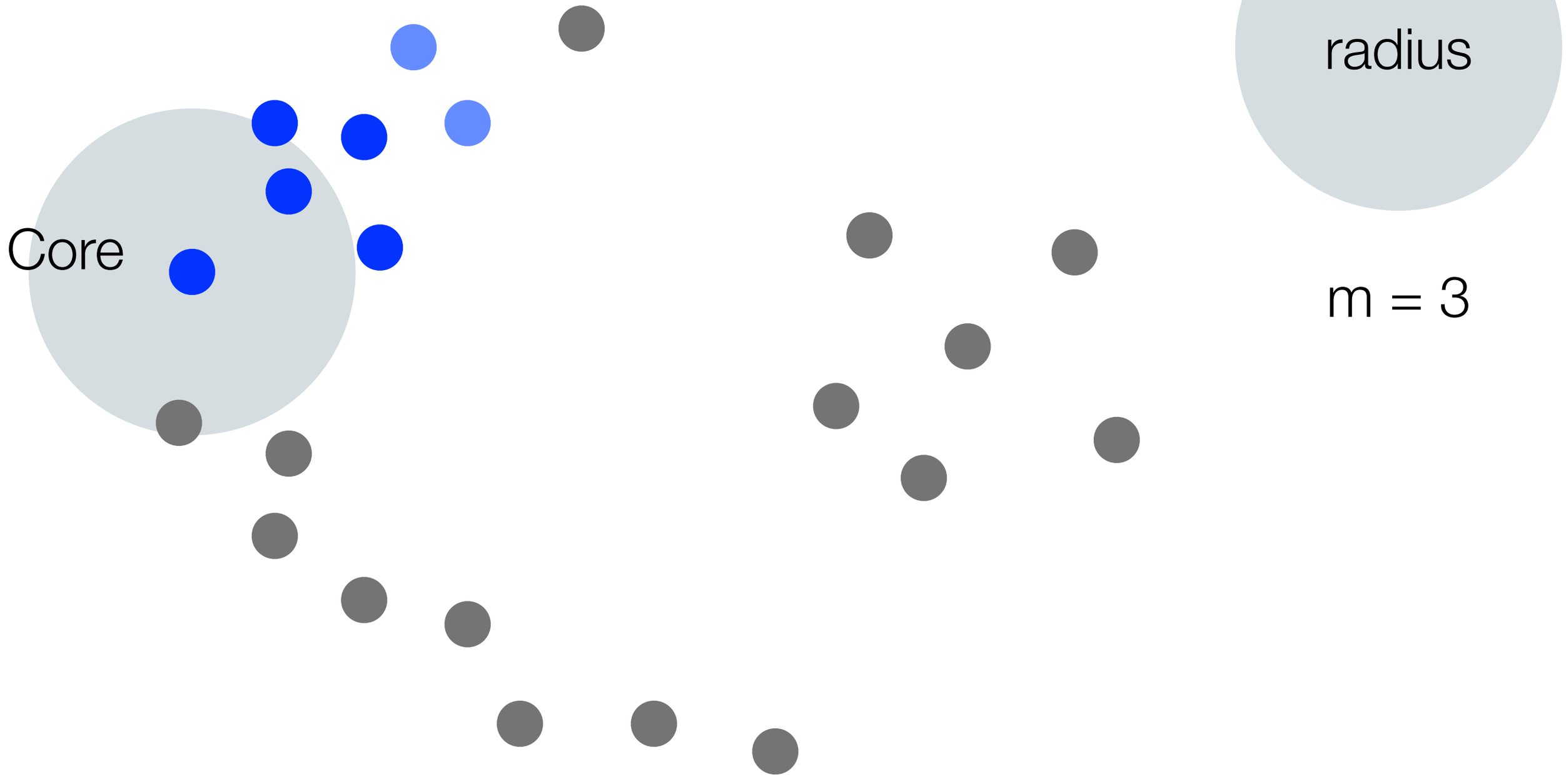

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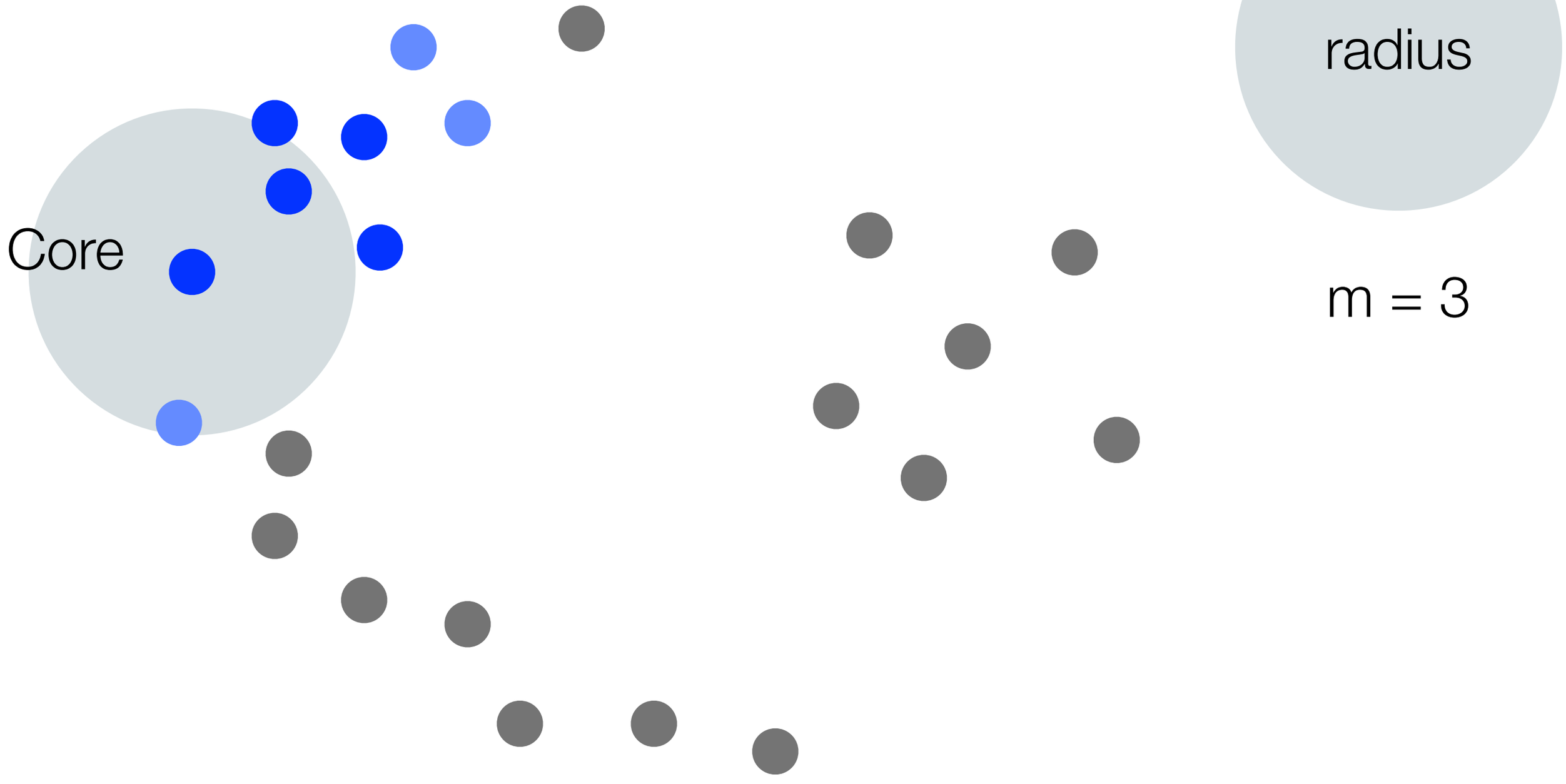

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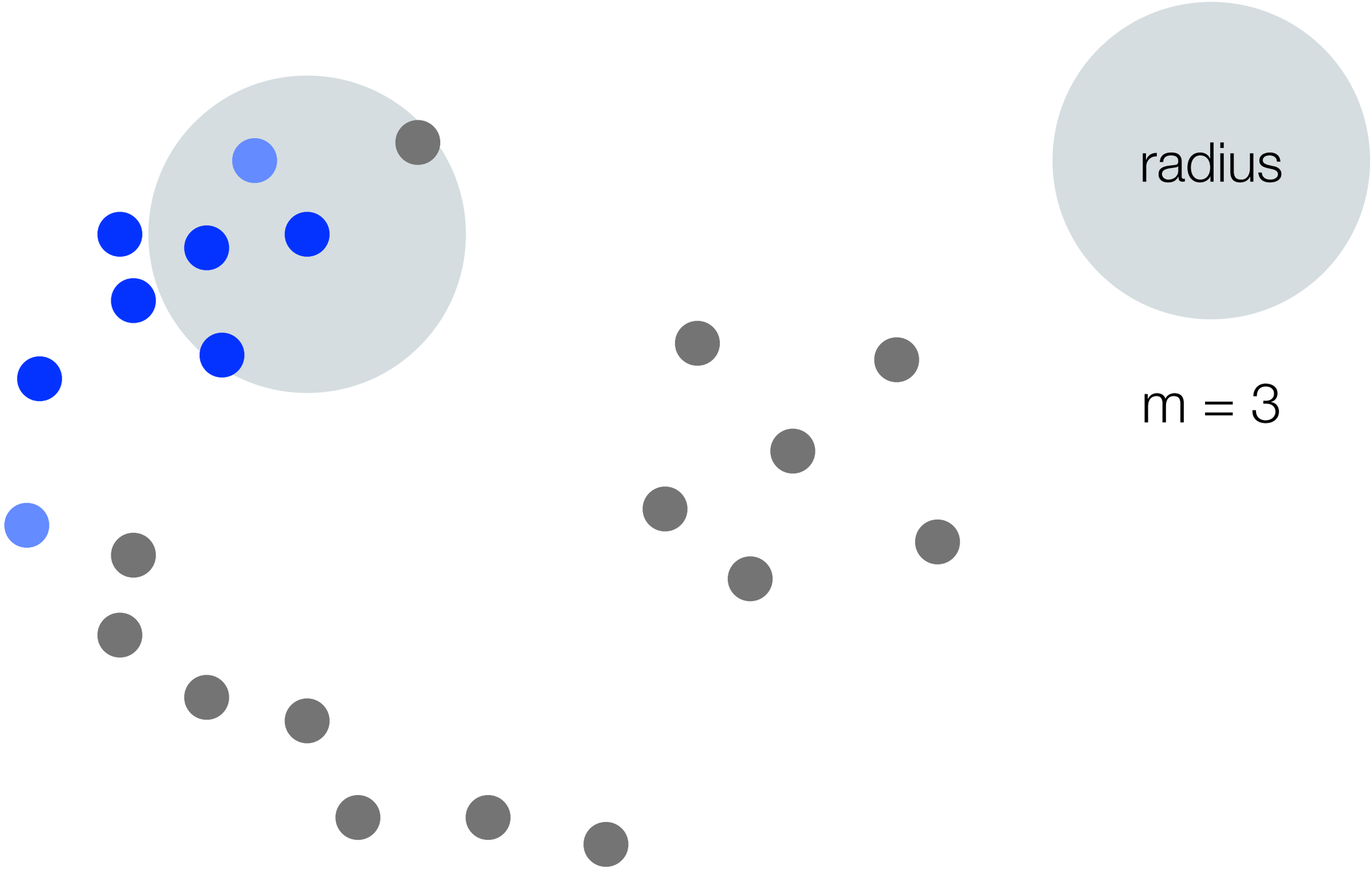

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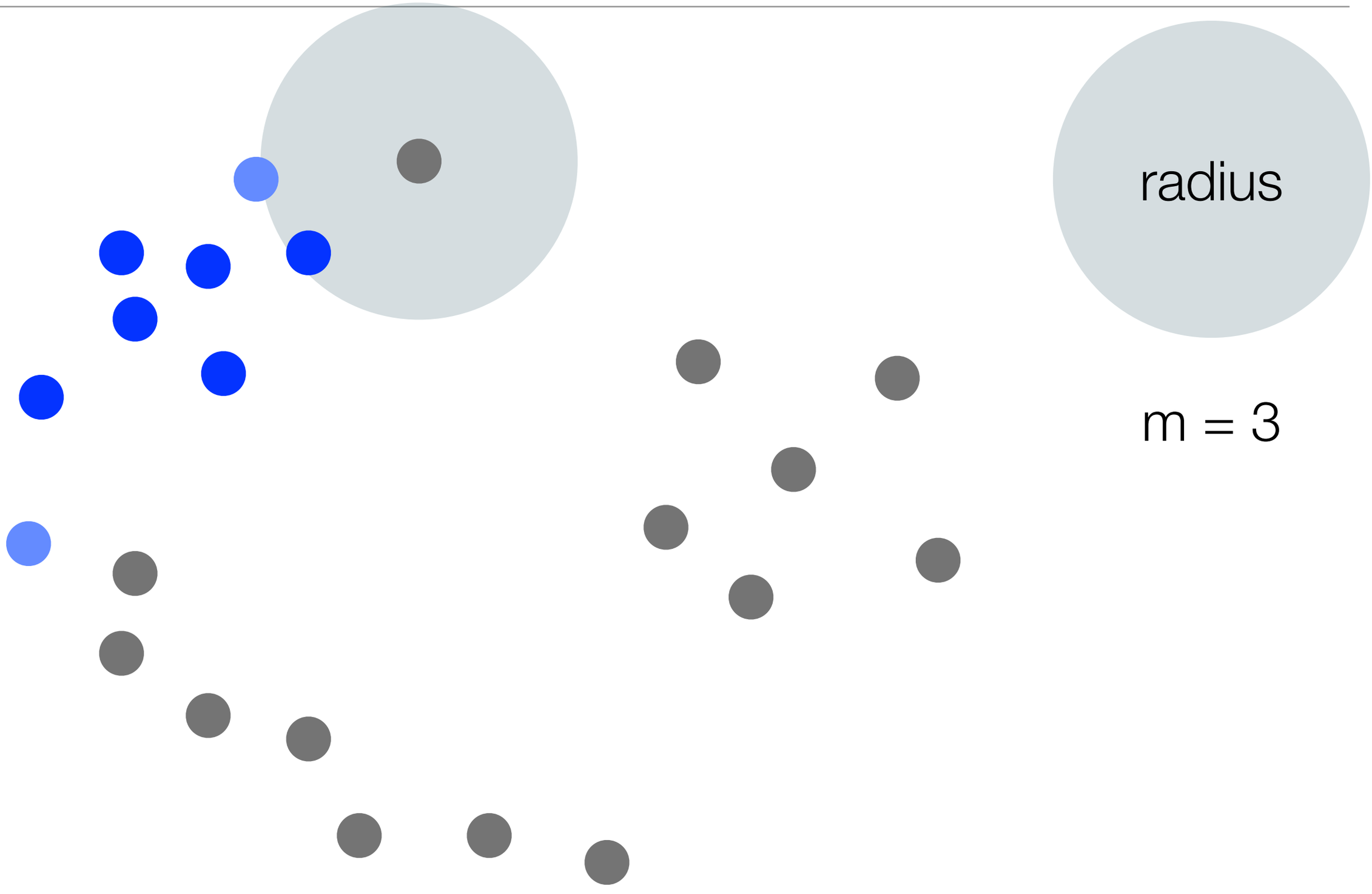

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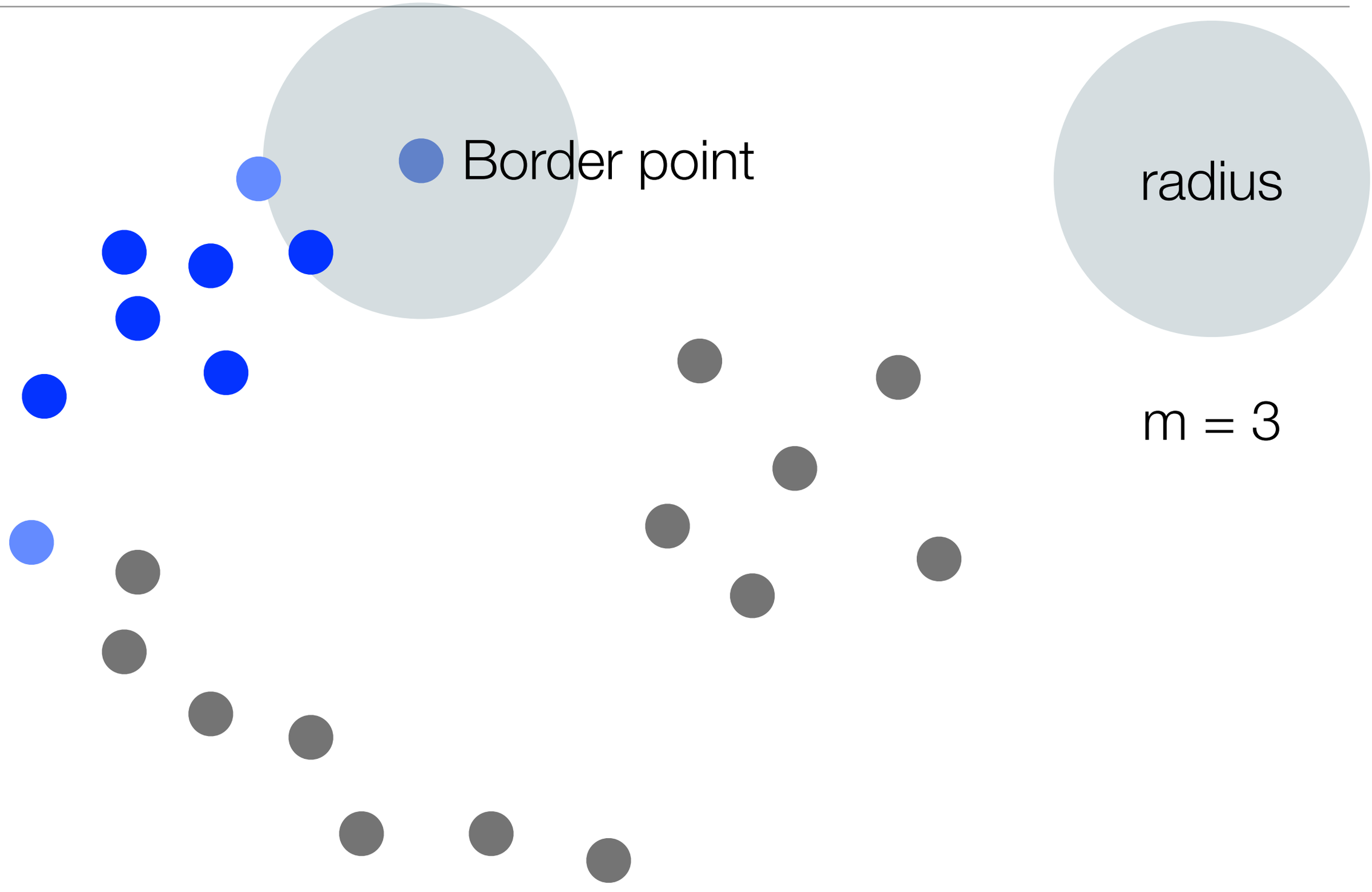

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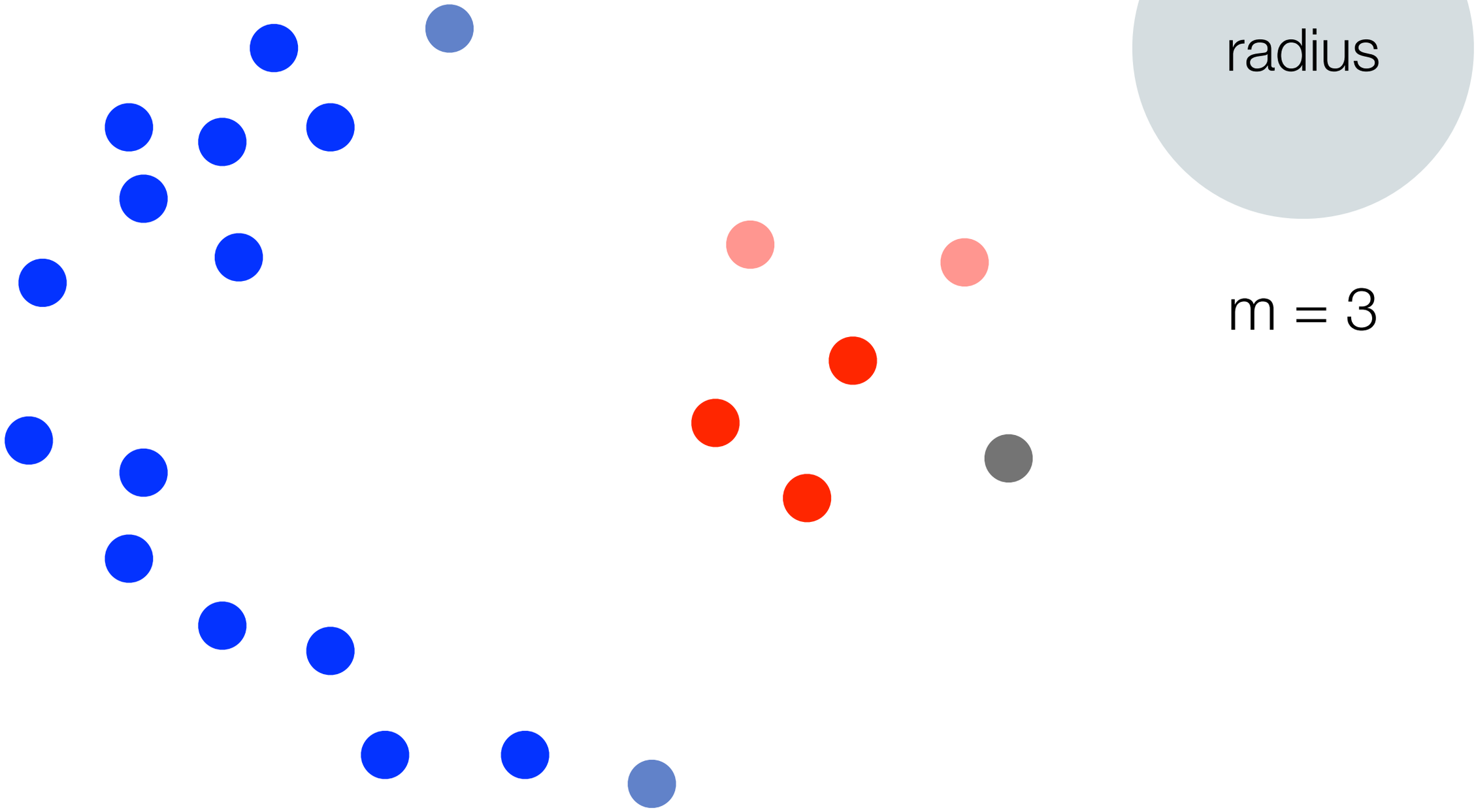

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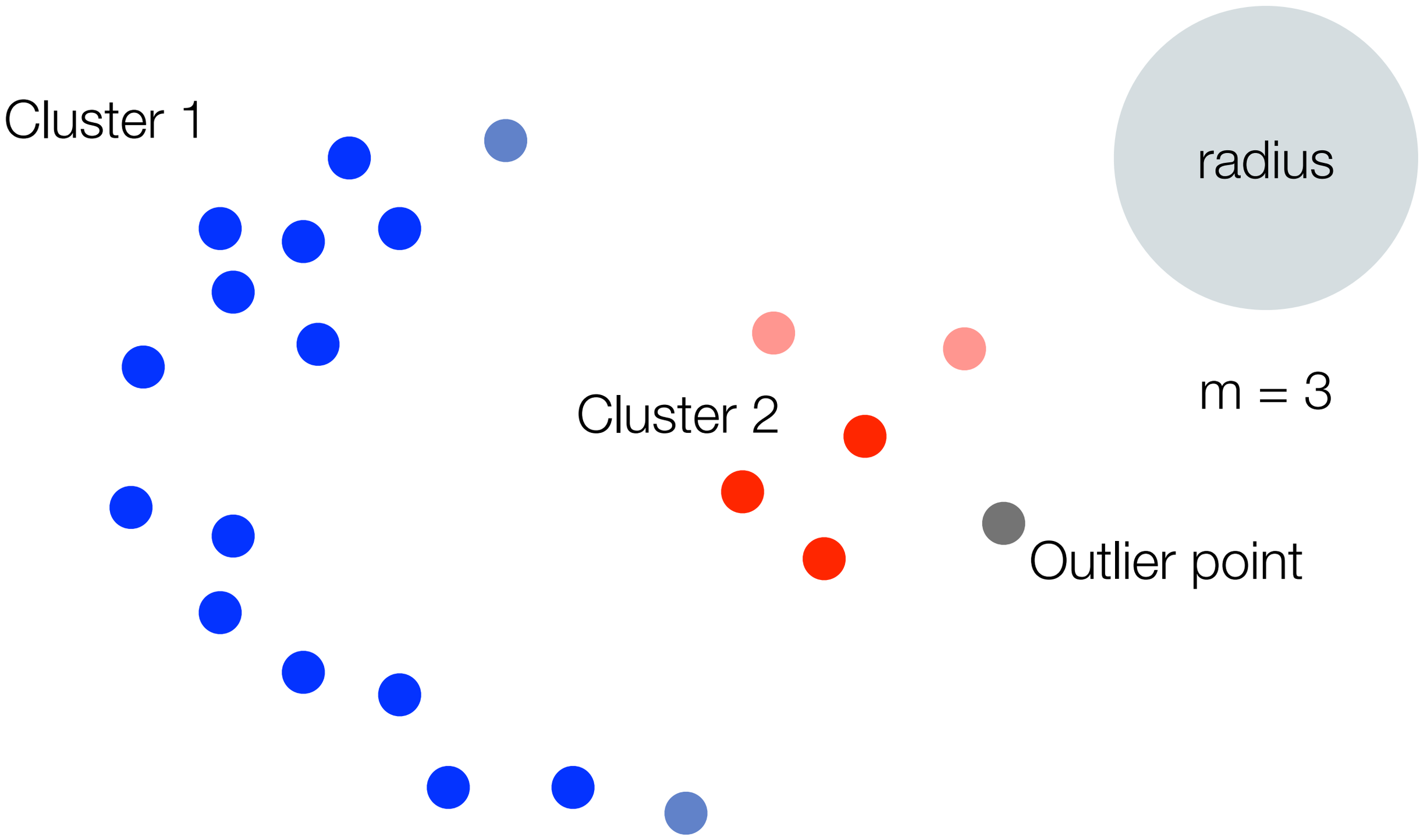

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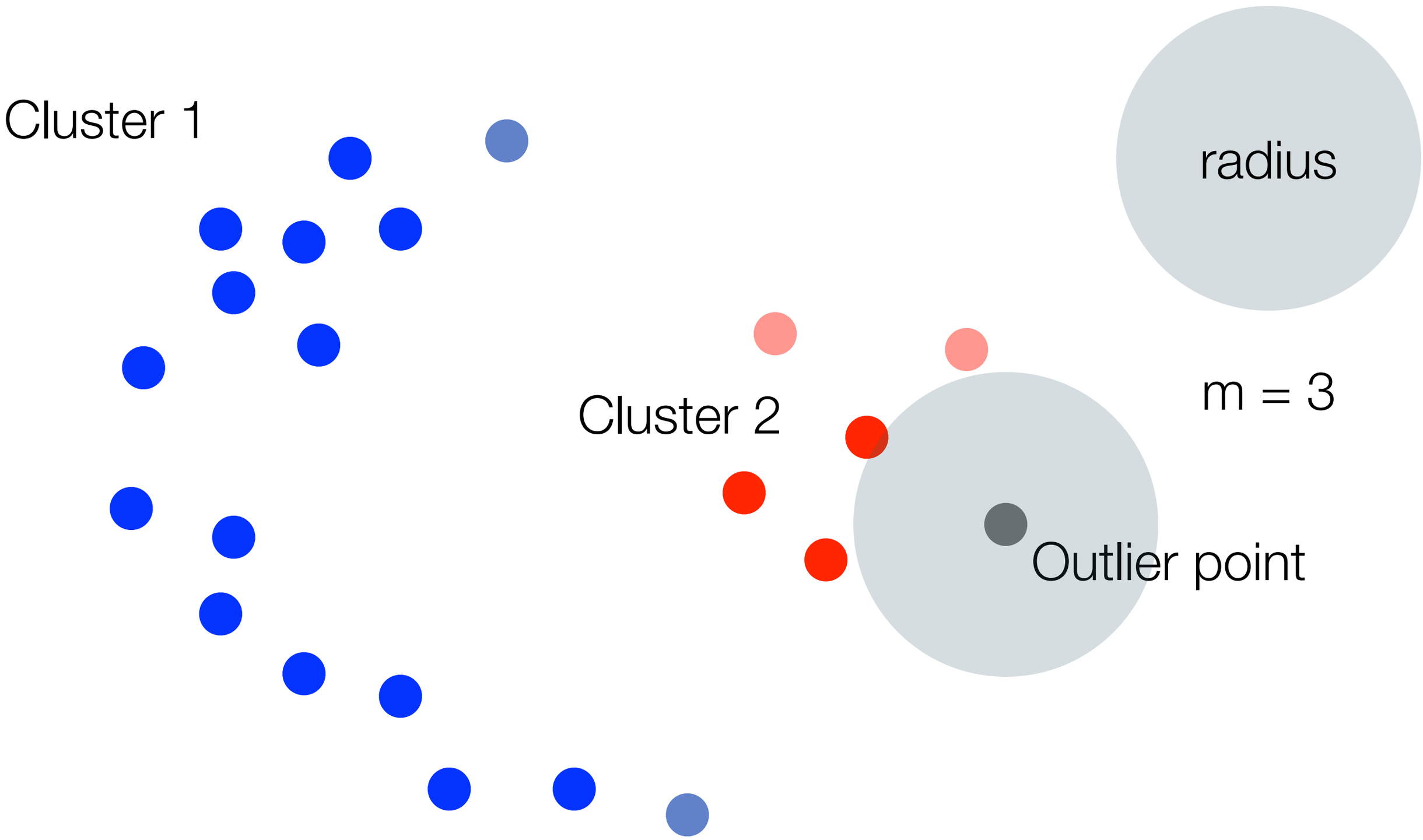
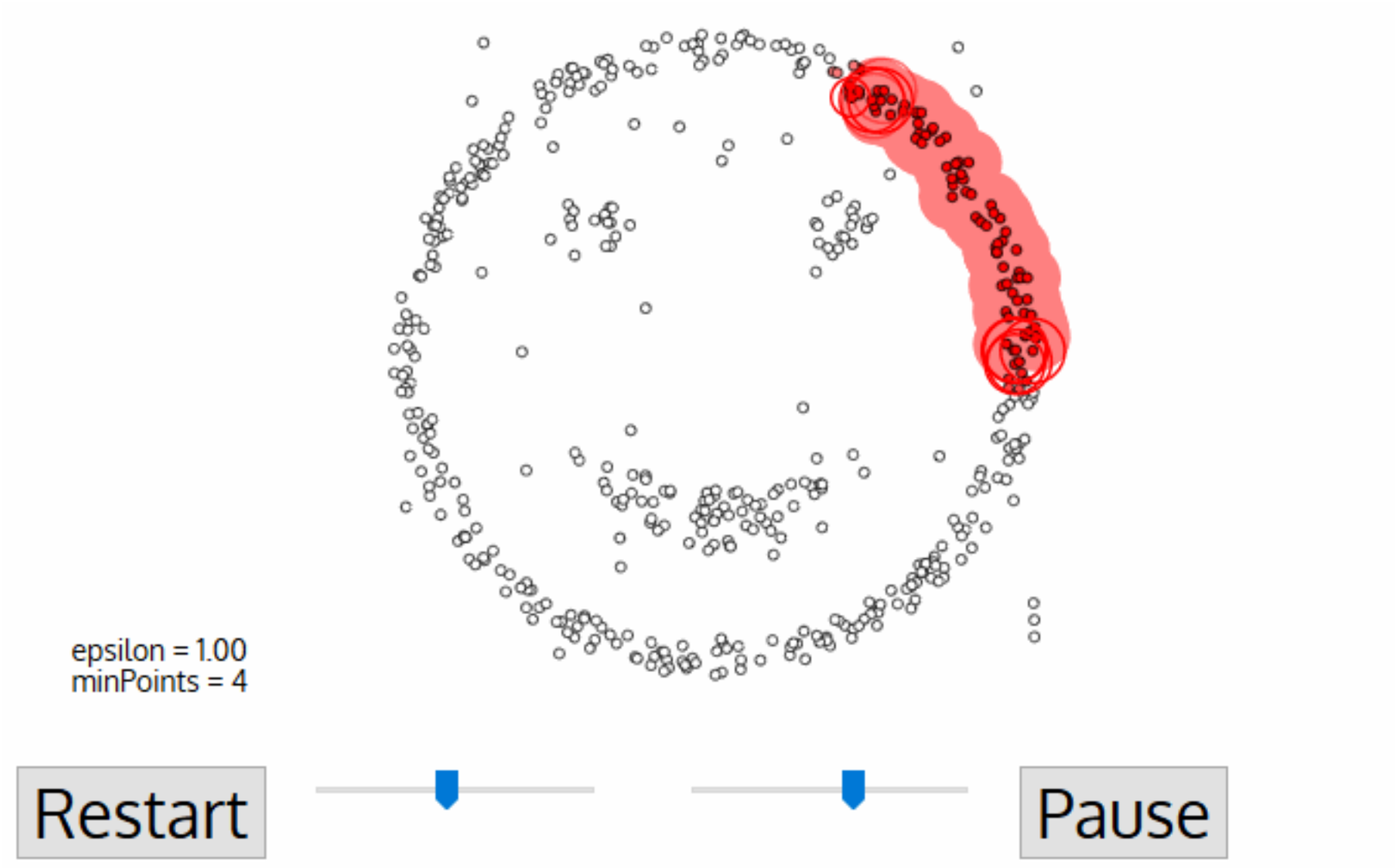


DBSCAN



https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68

DBSCAN

- Can find non-convex clusters
- Automatically determines number of clusters needed
- Not every point goes into a cluster (handles outliers/noise; however can be a drawback if you want to assign all points to a cluster)
- Tends to find/work best with clusters of similar density
- How to choose radius & min points? There are rules of thumb but can be tricky! Often use min points = 2 x dim, for radius, can us elbow plot of a k-distance graph, but harder to say)

Model based methods: Gaussian Mixture Models

- Assumes the data points come from a combination of multivariate gaussians

- This seems restrictive but is often no more so than other methods (e.g. k-means in some sense assumes a centroid and resulting Voronoi diagram govern the data)

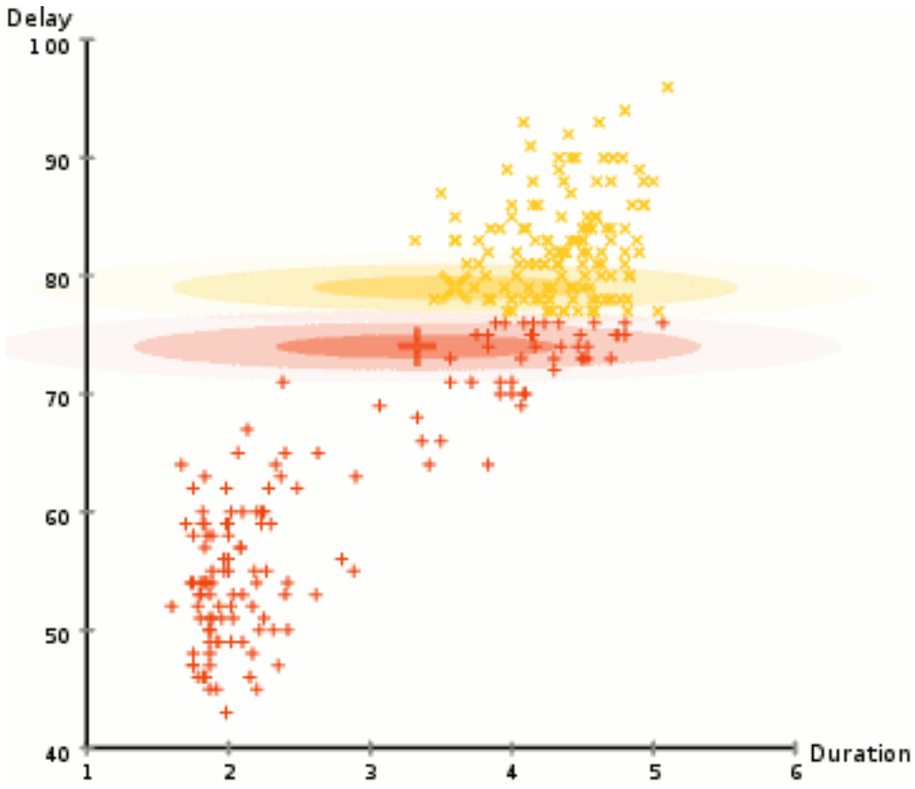
- Each data point has a probability of belonging to each cluster

- Often fit via expectation maximization (a type of maximum likelihood approach)

Model based methods: Gaussian Mixture Models

- Select number of clusters (number of gaussians to fit)
- Randomly initialize them (or better yet, use a method to pick a good starting guess)
- Compute the probability that each data point is in each cluster (based on the value of the gaussian at that point)
- Compute new parameters (μ,σ) for each gaussian that maximize this probability
- Repeat last two steps above until convergence

Model based methods: Gaussian Mixture Models



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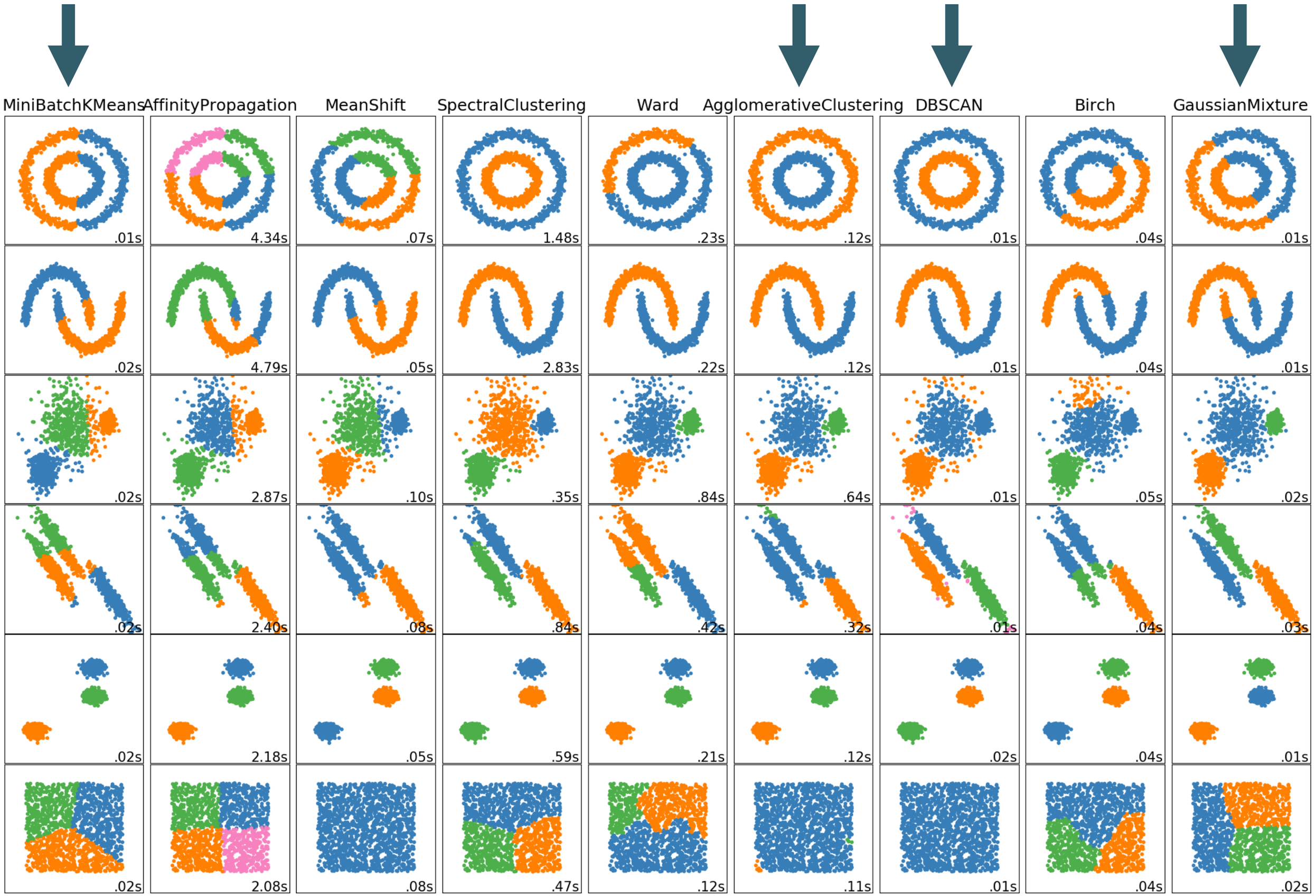
Clustering methods

- Many different approaches! These are just a few examples

- Different methods behave better/worse on different data sets

- Testing how well a clustering method behaves can be difficult, especially in high dimensions and/or without ground truth information



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Resources

- https://en.wikipedia.org/wiki/Cluster_analysis
- https://en.wikipedia.org/wiki/DBSCAN
- https://medium.com/predict/three-popular-clustering-methods-and-when-to-use-each-4227c80ba2b6
- https://blog.dominodatalab.com/topology-and-density-based-clustering/
- https://shapeofdata.wordpress.com/2014/03/04/k-modes/
- https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68

Clustering in networks

- Many different ways to look at clustering

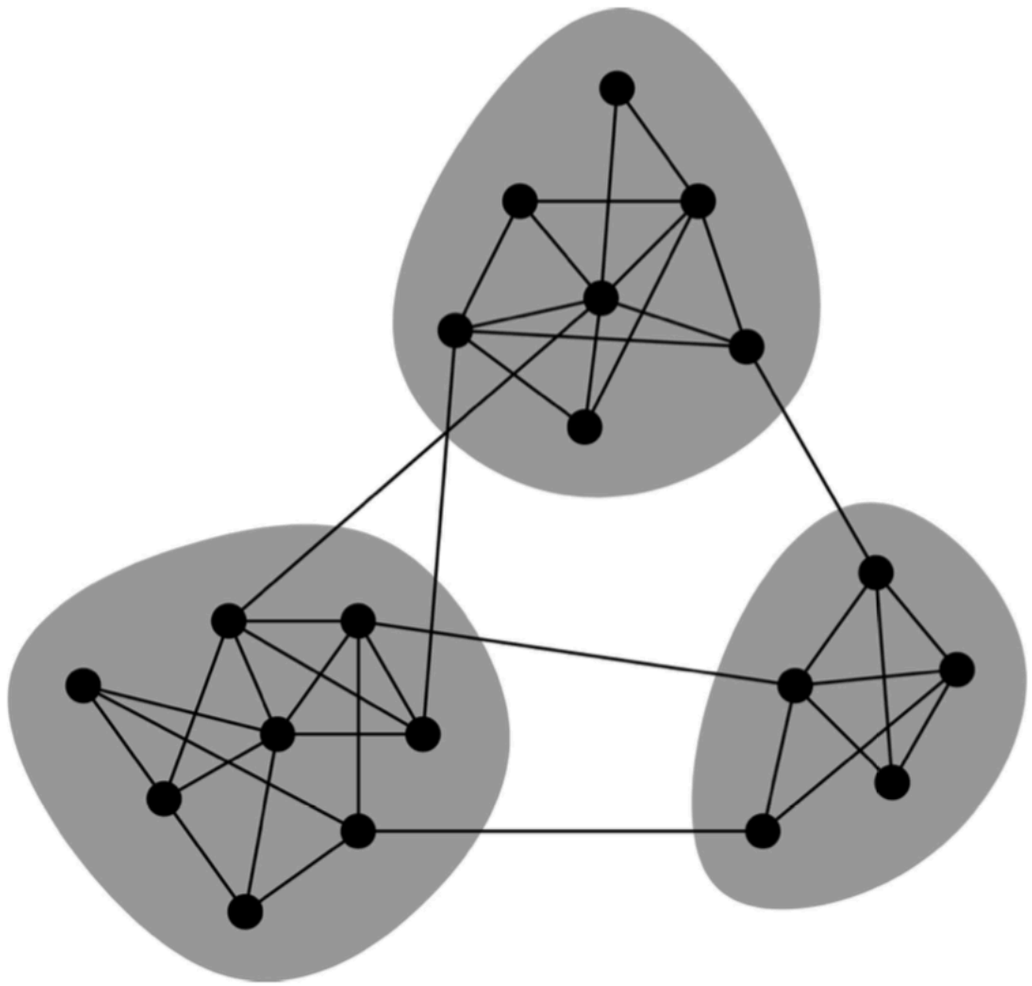
- Community detection - finding clusters (groups) of nodes that are highly connected within the group and less connected between groups (i.e. clustering, where similarity is based on connectivity)

- How do node traits (degree, covariates) cluster based on edges? E.g. do smokers tend to be friends with other smokers? Do individuals cluster by popularity

Network methods: **modularity** maximization

- Community (cluster) detection approach for networks

- Looks for groups of nodes that have more within-group edges than would be expected from a random graph with the same degree for each node



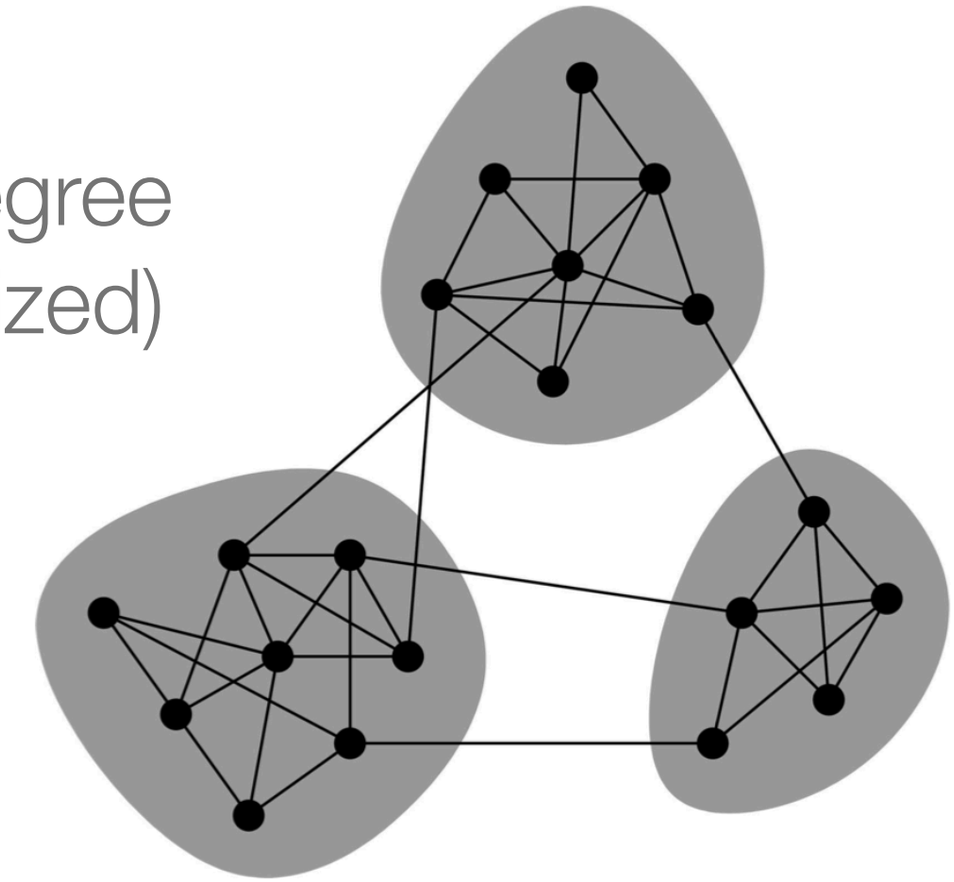
Modularity and community structure in networks. M. E. J. Newman. PNAS 2006, 103 (23) 8577-8582; DOI: 10.1073/pnas.0601602103

Modularity

- Modularity compares observed community edges to what would be expected at random

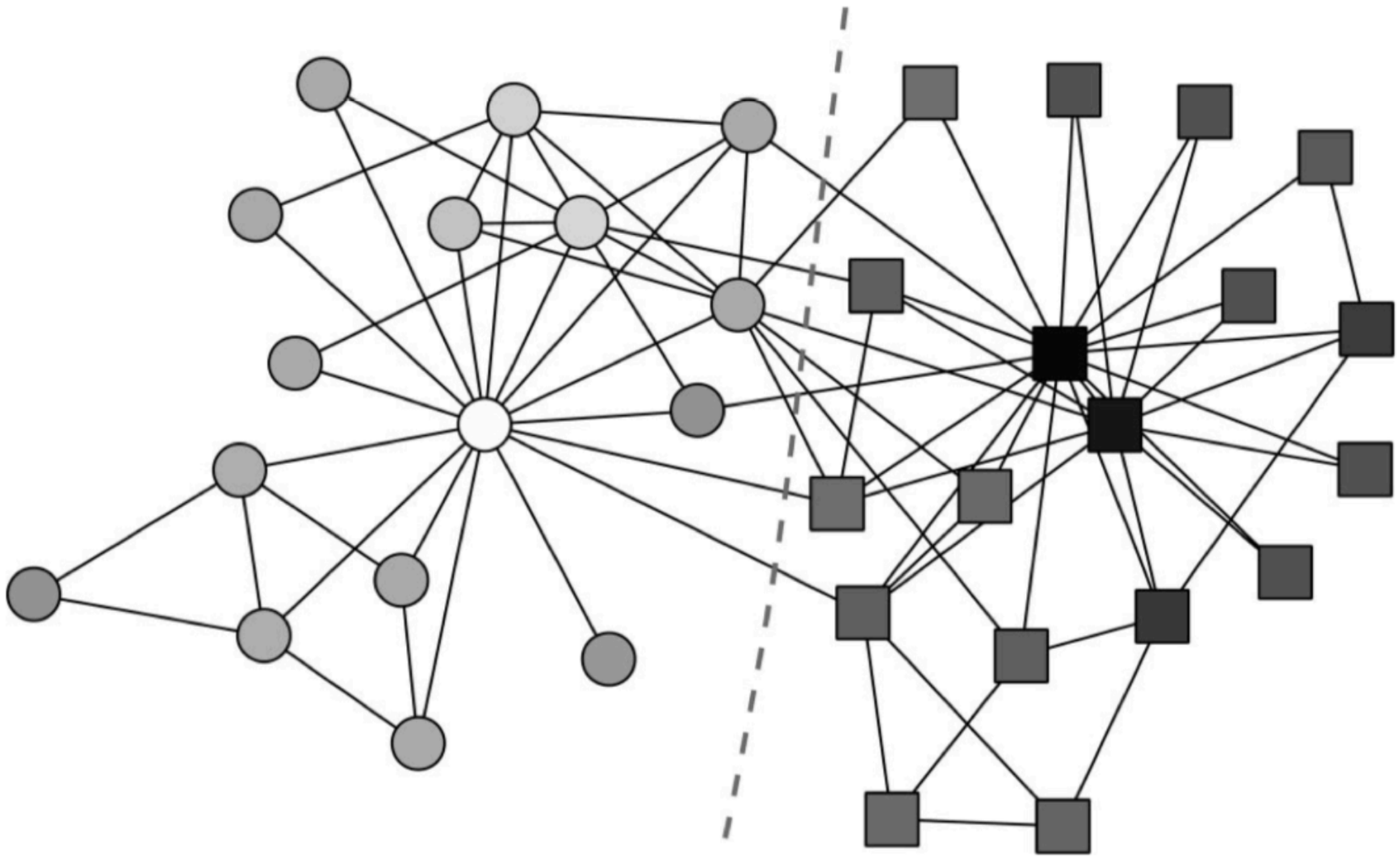
- Modularity is the fraction of within-group edges minus the fraction expected at random (if degree conserved but edges are randomized)

- Modularity-based community detection: find community groupings that maximize modularity



Newman, Mark EJ. "Modularity and community structure in networks." *PNAS* 103.23 (2006): 8577-8582.

Karate club example



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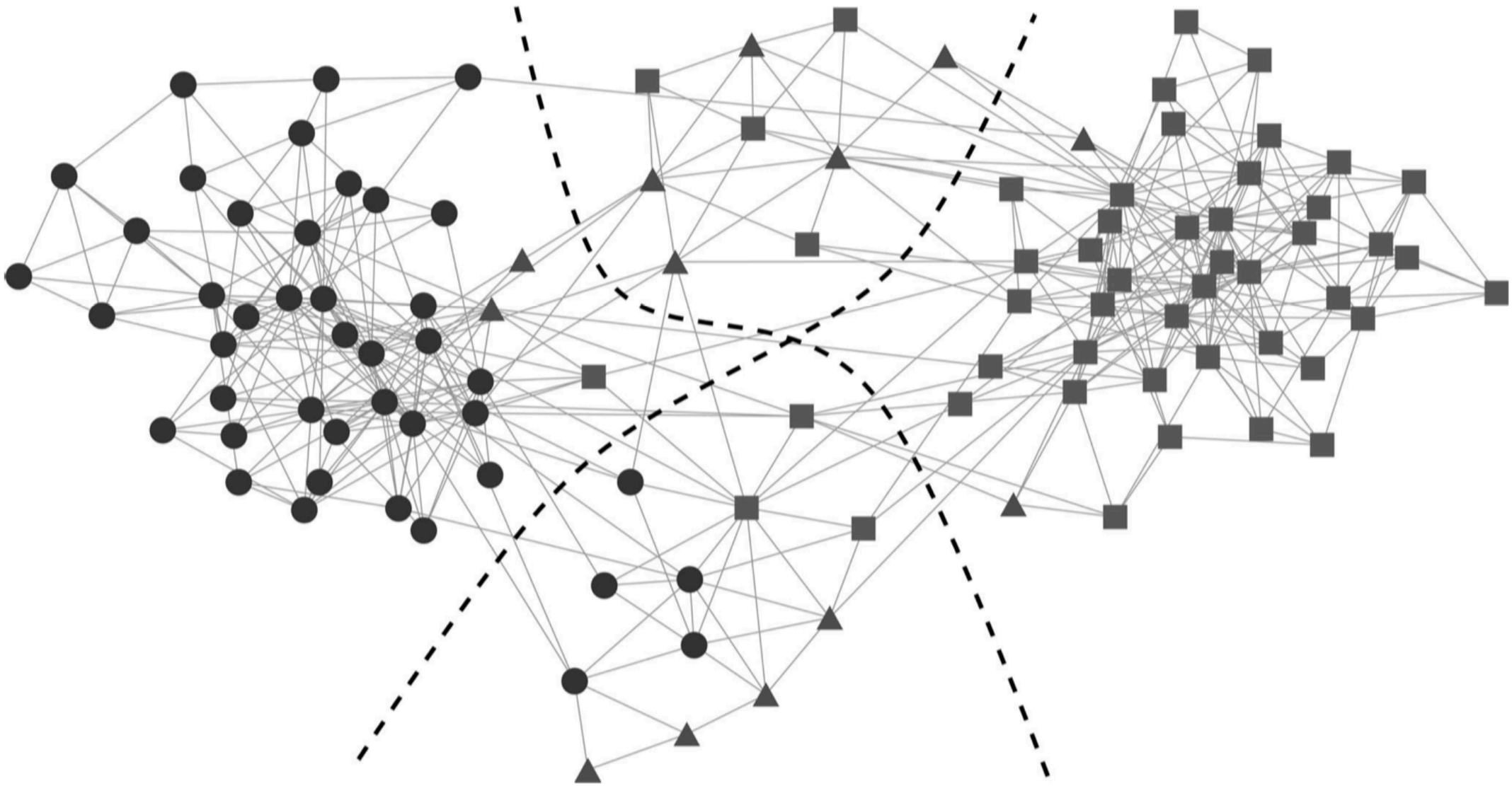
Political books



Newman, Mark EJ. "Modularity and community structure in networks." *PNAS* 103.23 (2006): 8577-8582.

Modularity

- Can be slow/difficult to maximize—spectral methods have made much faster

- Resolution limit - as the network grows larger, it is harder for modularity-based community detection methods to find small communities

Network methods: **assortativity**

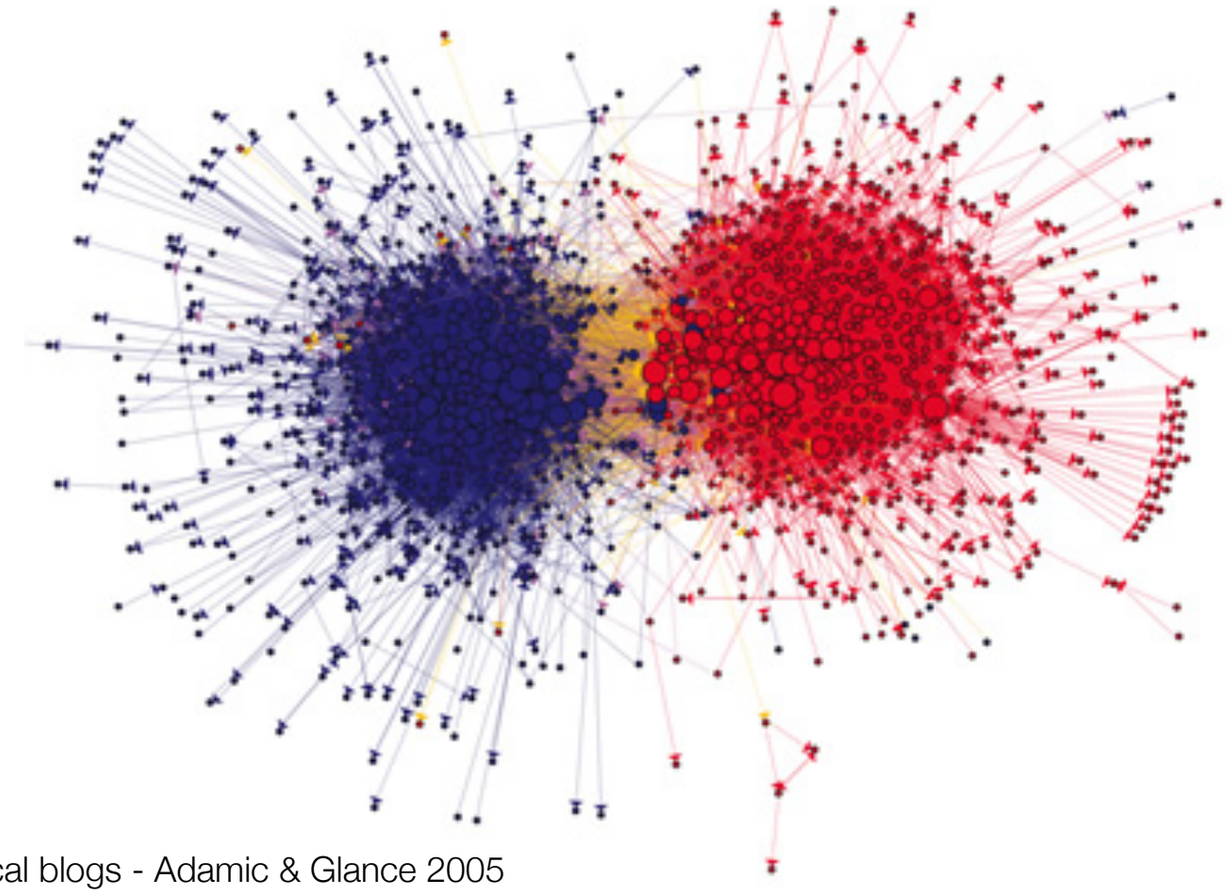
- **Assortativity** - measures network-level tendency for nodes to to attach to similar nodes

- Not really for cluster (community) detection, so much as to evaluate how clustered a given property is on the network

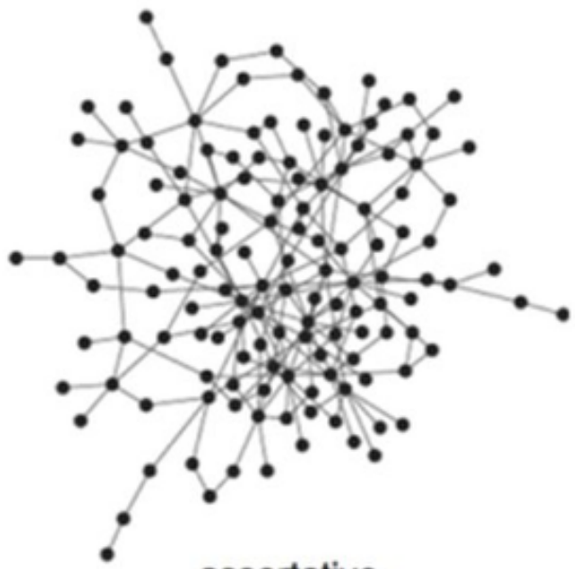
- Often look at clustering of degree, but can be other properties (e.g. how is the network clustered by gender, vaccination, smoking behaviors, etc.)

Assortativity

- Heterosexual networks - highly dissassortative by gender
- Social/sexual networks often assortative on a range of demographic, degree, behavioral traits - ‘birds of a feather flock together’



Political blogs - Adamic & Glance 2005



assortative

disassortative

Assortativity

- Calculate fraction of edges between nodes of the same type/value, compare to what would be expected from a random network

- Ranges from -1 (dissassortative) to 1 (assortative)

    - But min value (most dissassortative) is between -1 and 0 depending on the composition of the network

M. E. J. Newman, Mixing patterns in networks Physical Review E, 67 026126, 2003

Assortativity

- Consider a case where we have discrete characteristics on the nodes

- Define a mixing matrix with entries e_{ij} given by the fraction of the total edges linking type *i* to type *j*

- Let a_i and b_i be the total fractions of each end type that we have ($a_i = b_i$ for undirected graphs)

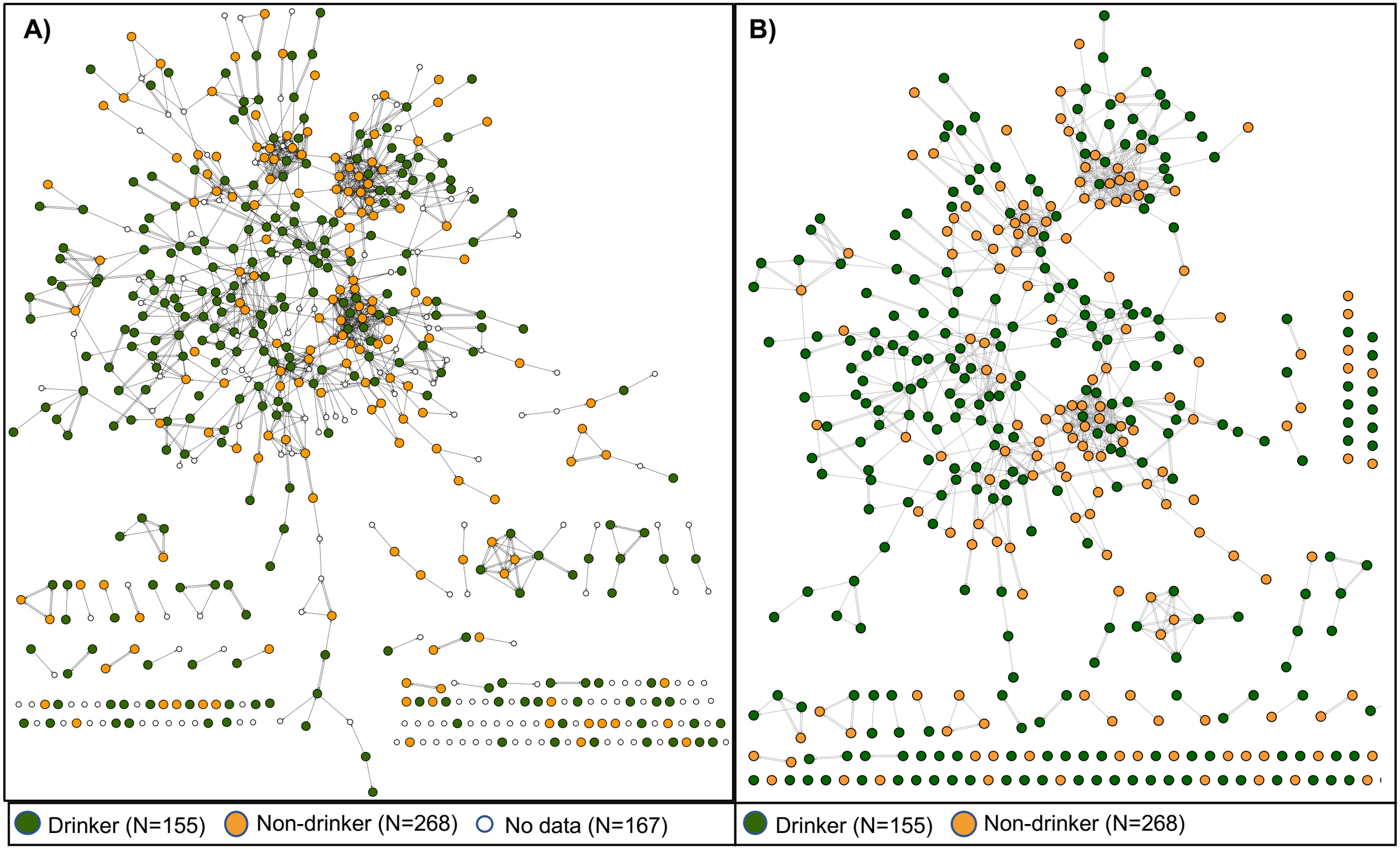
- Note that $\sum_{ij} e_{ij} = 1, \quad \sum_{j} e_{ij} = a_i, \quad \sum_{i} e_{ij} = b_j$

Assortativity

- Defined based on a mixing matrix - entries are the fraction of edges in a network linking type i to type j

$$r = \frac{\sum_i e_{ii} - \sum_i a_i b_i}{1 - \sum_i a_i b_i} = \frac{\mathbf{Tre} - ||\mathbf{e}^2||}{1 - ||\mathbf{e}^2||},$$

- For degree assortativity (and other scalar variables), assortativity is the Pearson correlation coefficient of degree between pairs of linked nodes



Ali Walsh Dissertation, 2019 (assortativity 0.2)