# Machine Learning for Data Science (CS4786)
# Lecture 2

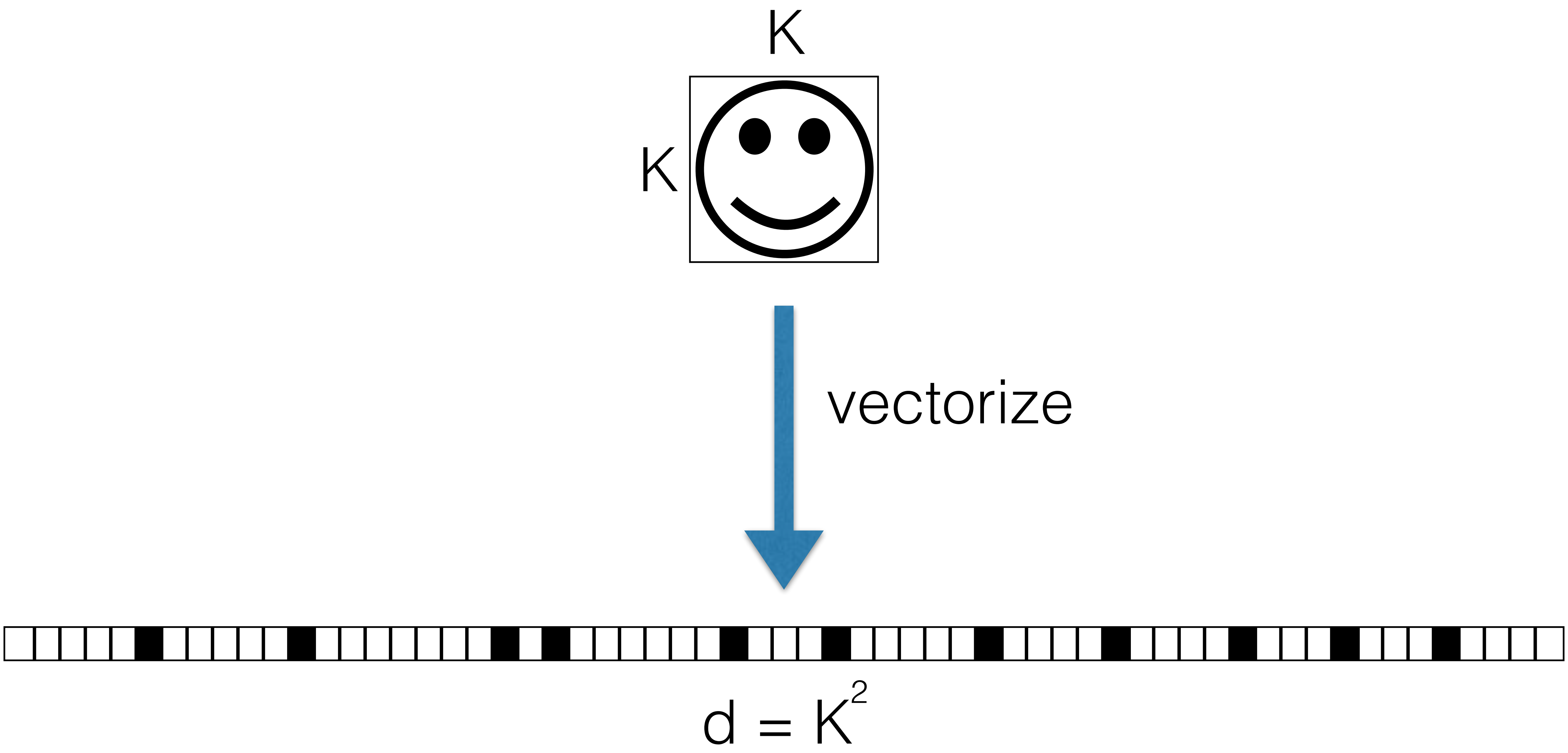
Clustering

Course Webpage :
http://www.cs.cornell.edu/Courses/cs4786/2017fa/

# Representing Data as Feature Vectors

- How do we represent data?
- Each data-point often represented as vector referred to as feature vector

# EXAMPLE: IMAGES



# Example: Text (Bag of Words)

***Documents:***

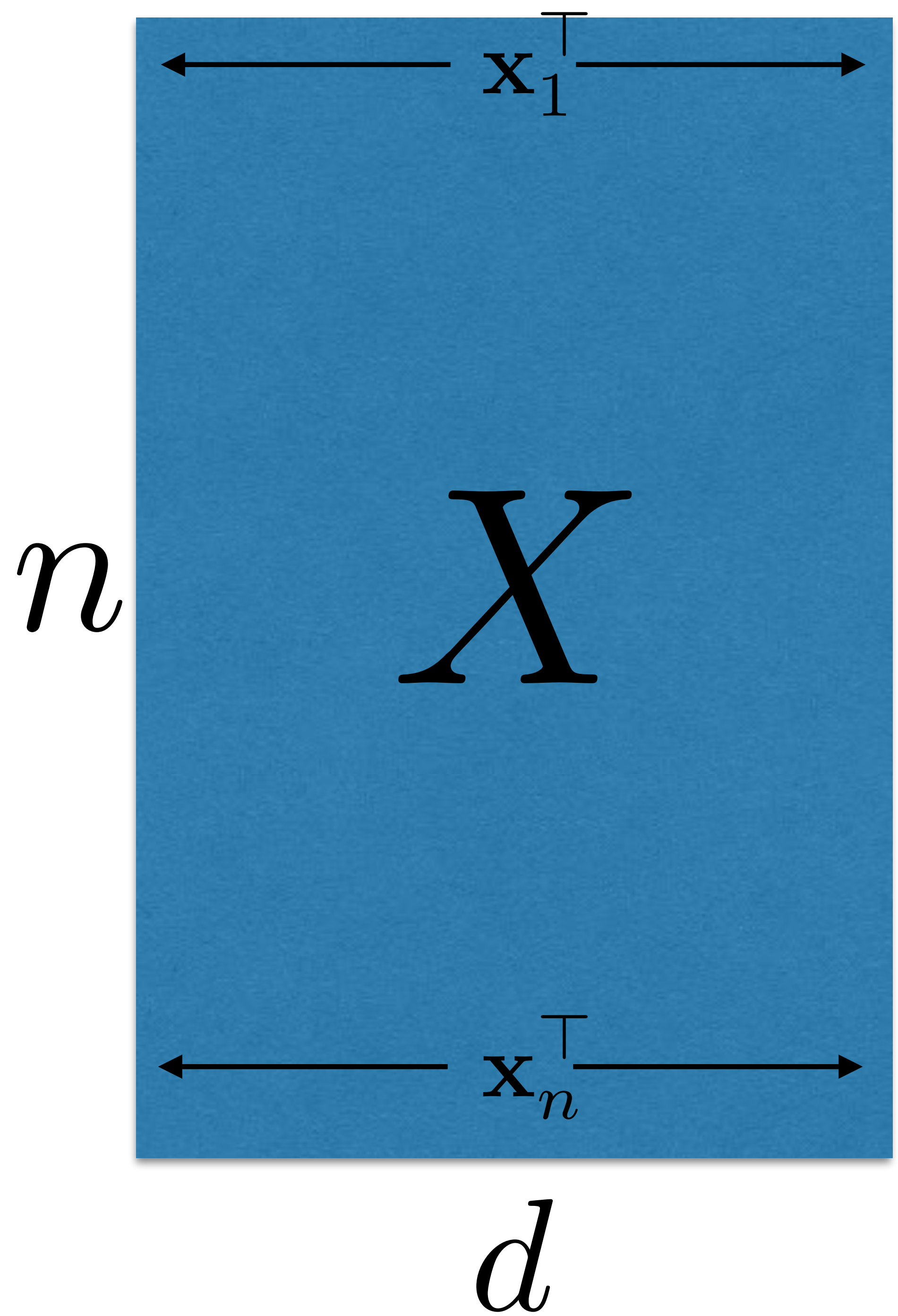
car
engine
hood
tires
truck
trunk

car
emissions
hood
make
model
trunk

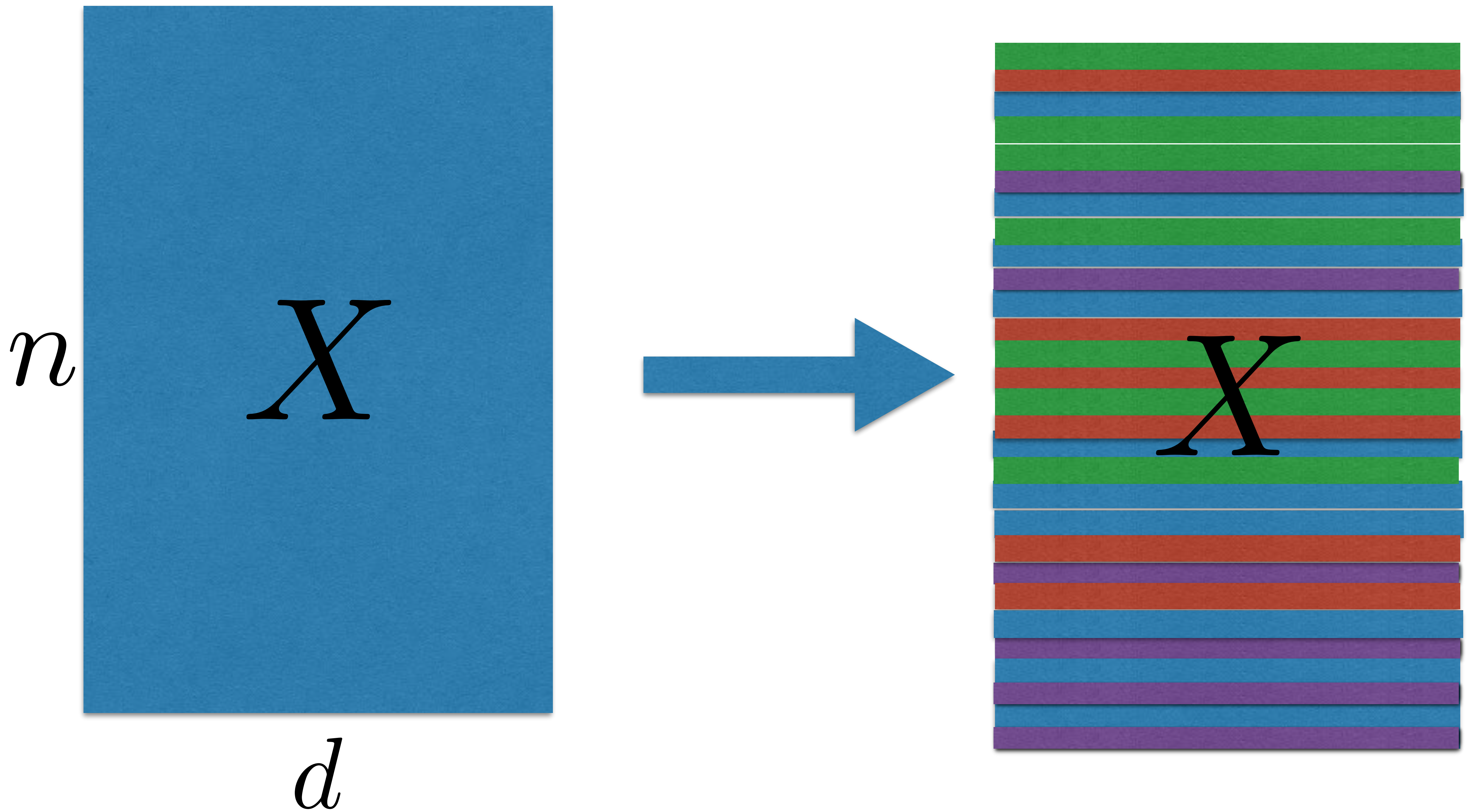
Chomsky
corpus
noun
parsing
tagging
wonderful

| car | Chomsky | corpus | emissions | engine | hood | make | model | noun | parsing | tagging | tires | truck | trunk | wonderful |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 0 |
| 1 | 0 | 0 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 1 |

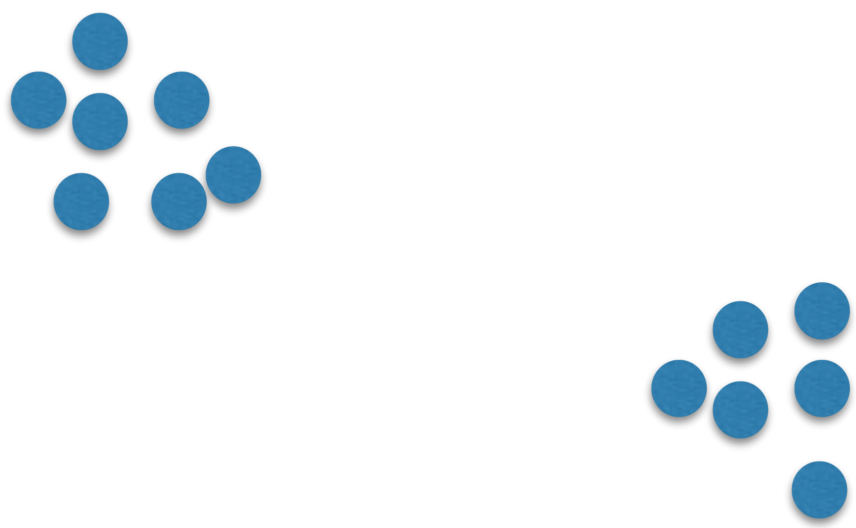
# Representing Data as Feature Vectors



# CLUSTERING

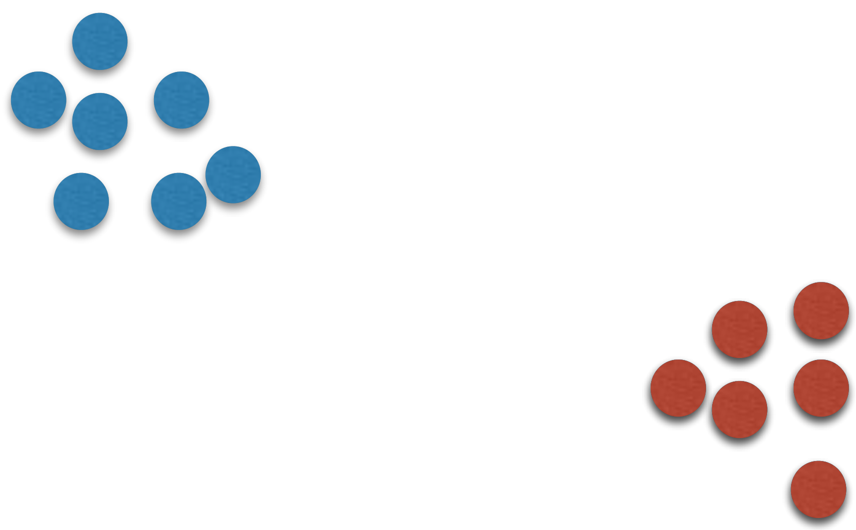


# Examples



What are the clusters?

# Examples



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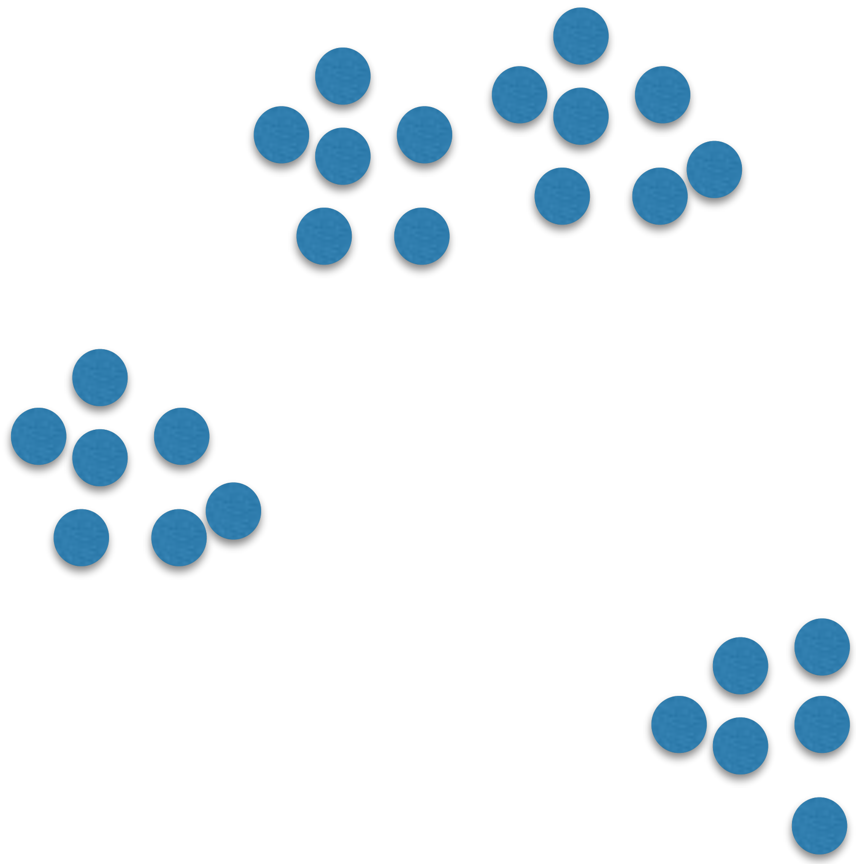
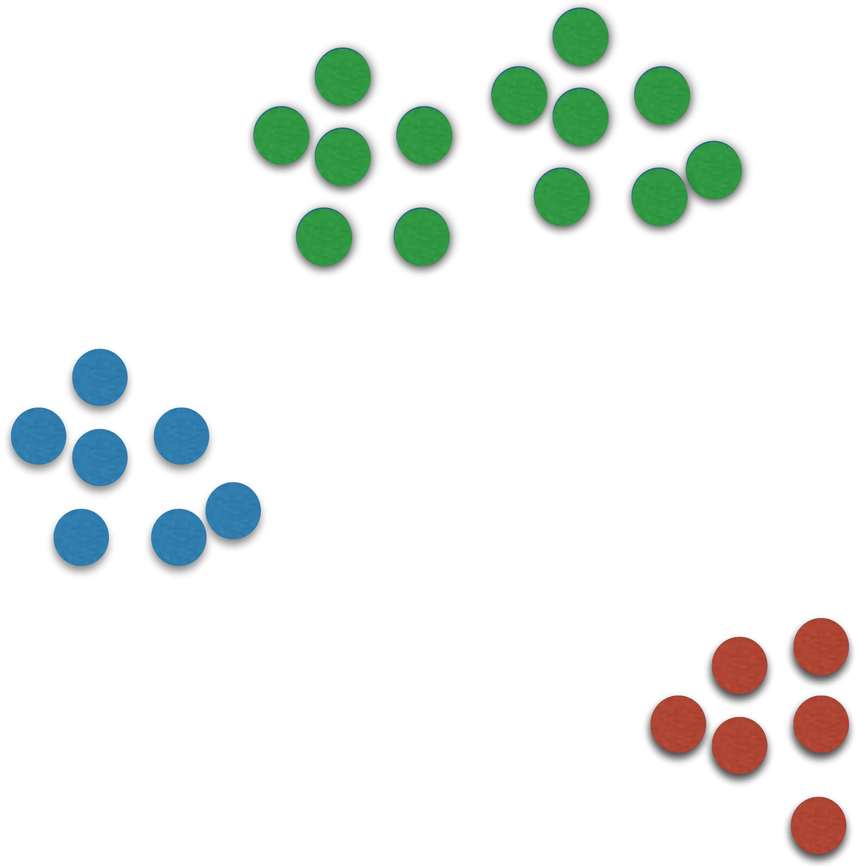
# Examples



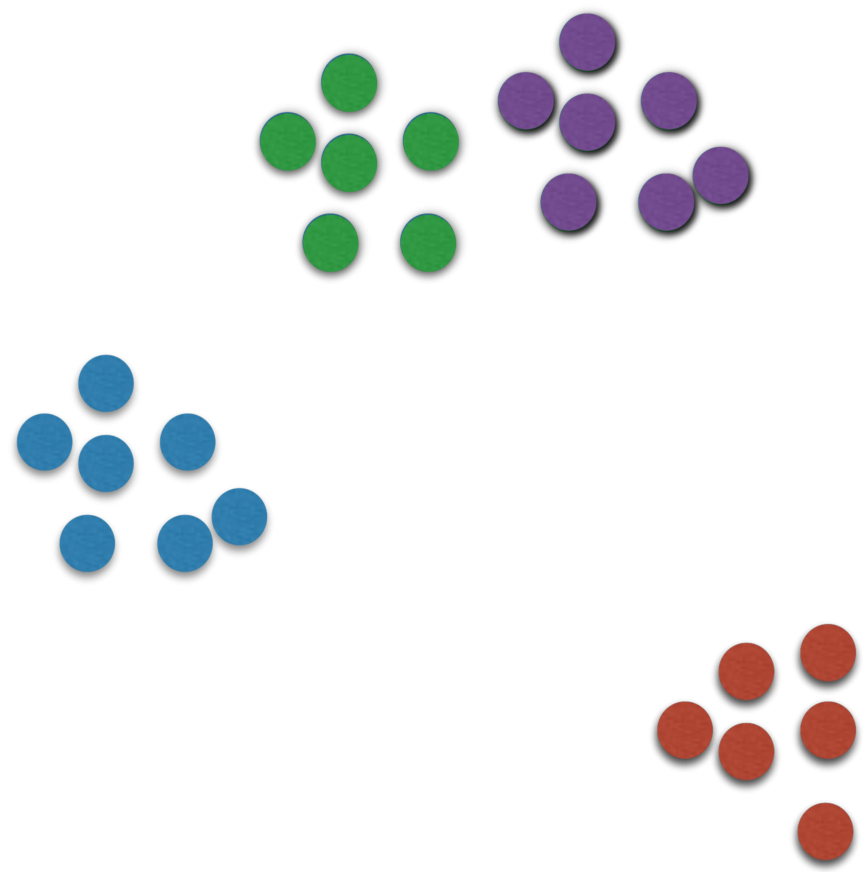
What are the clusters?

# Examples



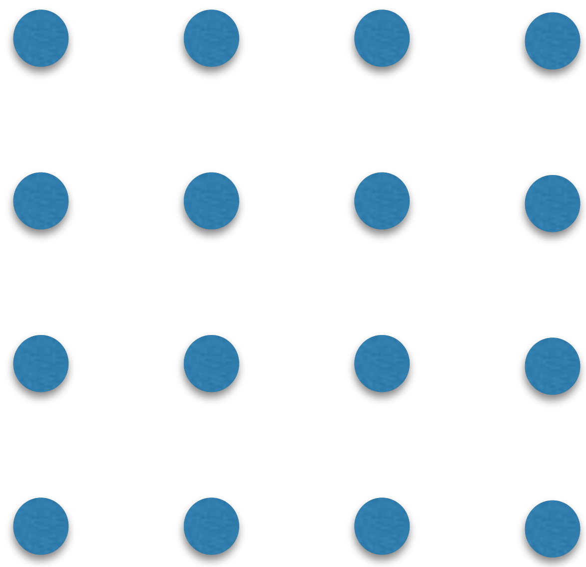
What are the clusters?

# Examples



What are the clusters?

# Examples



What are the clusters?

# Clustering

- Grouping sets of data points s.t.
  - points in same group are similar
  - points in different groups are dissimilar
- A form of unsupervised classification where there are no predefined labels

# Some Notations

- $K$ary clustering is a partition of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ into $K$ groups
- For now assume the magical $K$ is given to use
- Clustering given by $C_1, \ldots, C_K$, the partition of data points.
- Given a clustering, we shall use $c(\mathbf{x}_t)$ to denote the cluster identity of point $\mathbf{x}_t$ according to the clustering.
- Let $n_j$ denote $|C_j|$, clearly $\sum_{j=1}^{K} n_j = n$.

How do we formalize a good clustering objective?

# How do we formalize?

Say dissimilarity$(\mathbf{x}_t, \mathbf{x}_s)$ measures dissimilarity between $\mathbf{x}_t$ & $\mathbf{x}_s$

Given two clustering $\{C_1, \ldots, C_K\}$ (or $c$) and $\{C'_1, \ldots, C'_K\}$ (or $c'$)

How do we decide which is better?

- points in same cluster are not dissimilar
- points in different clusters are dissimilar

# Clustering Criterion

- Minimize total within-cluster dissimilarity

$$M_1 = \sum_{j=1}^{K} \sum_{s,t \in C_j} \text{dissimilarity}(x_t, x_s)$$

- Maximize between-cluster dissimilarity

$$M_2 = \sum_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$

- Maximize smallest between-cluster dissimilarity

$$M_3 = \min_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$

- Minimize largest within-cluster dissimilarity

$$M_4 = \max_{j \in [K]} \max_{s,t \in C_j} \text{dissimilarity}(x_t, x_s)$$

# Clustering Criterion

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$$M_4 = \max_{j \in [K]} \max_{s,t \in C_j} \text{dissimilarity}(x_t, x_s)$$

How different are these criteria?

# Clustering Criterion

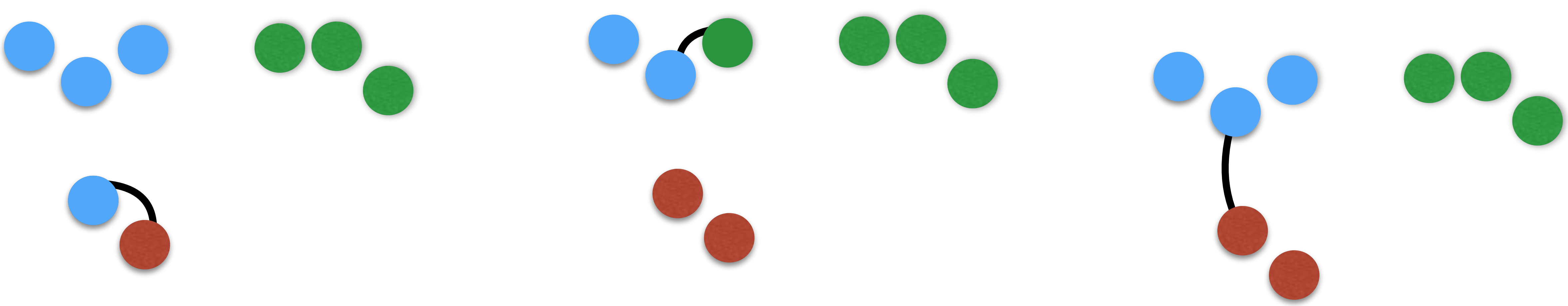
- minimizing $M_1 \equiv$ maximizing $M_2$

# Clustering

- Multiple clustering criteria all equally valid
- Different criteria lead to different algorithms/solutions
- Which notion of distances or costs we use matter

# Lets Build an Algorithm

$$M_3 = \min_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$



# Single Link Clustering

- Initialize $n$ clusters with each point $\mathbf{x}_t$ to its own cluster
- Until there are only $K$ clusters, do
  1. Find closest two clusters and merge them into one cluster

$$\text{dissimilarity}(C_i, C_j) = \min_{t \in C_i, s \in C_j} \text{dissimilarity}(\mathrm{x}_t, \mathrm{x}_s)$$

# Demo

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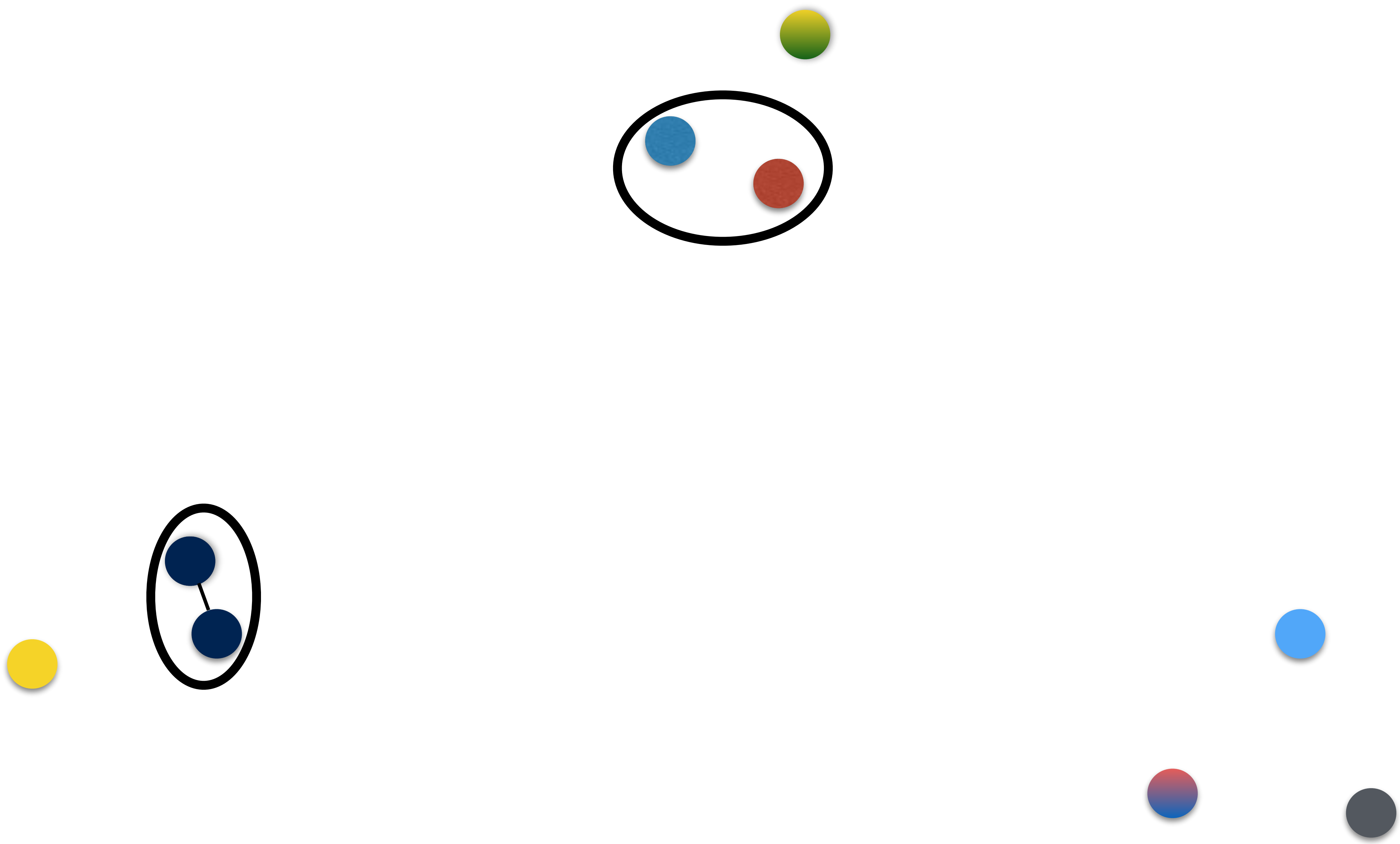

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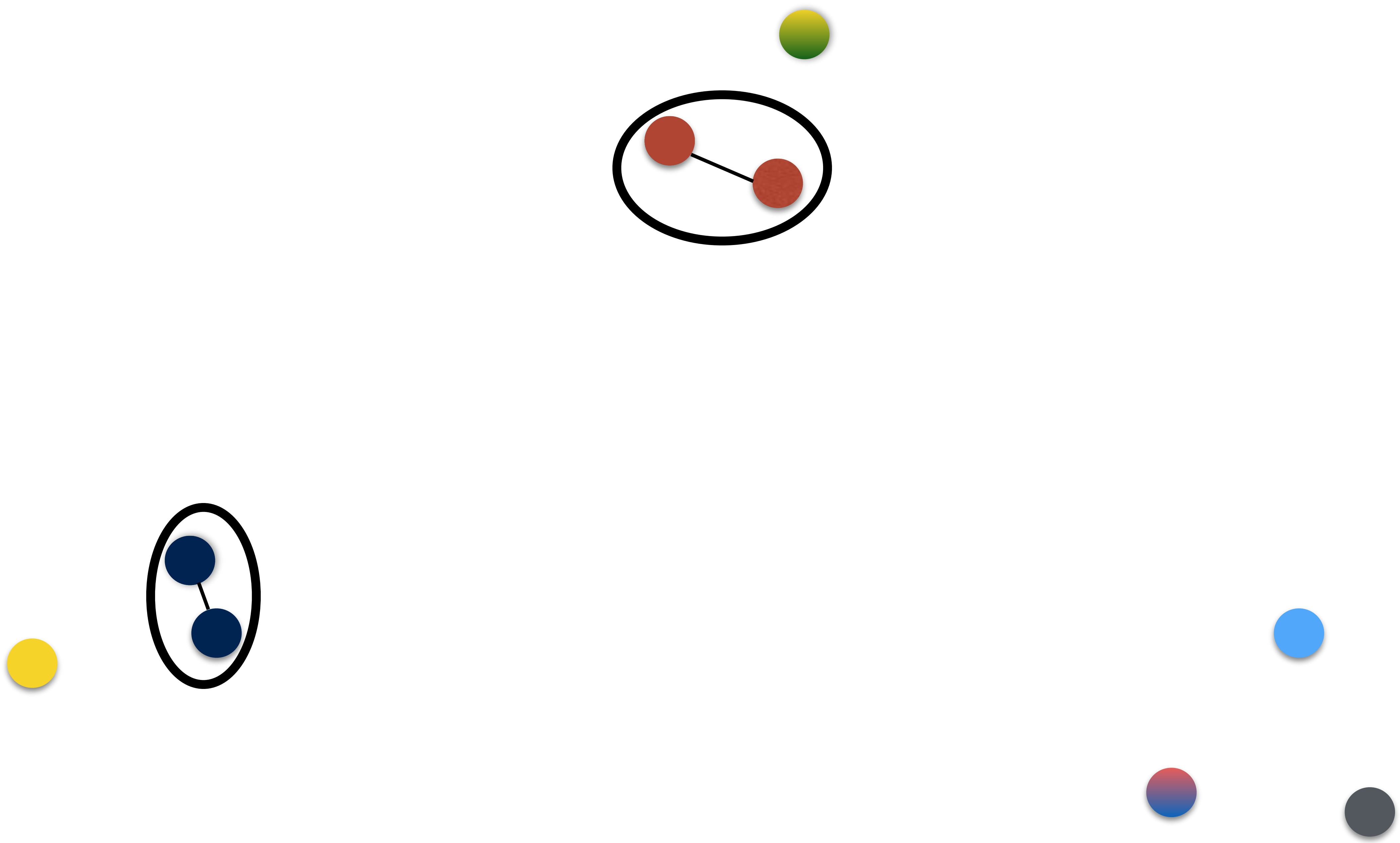

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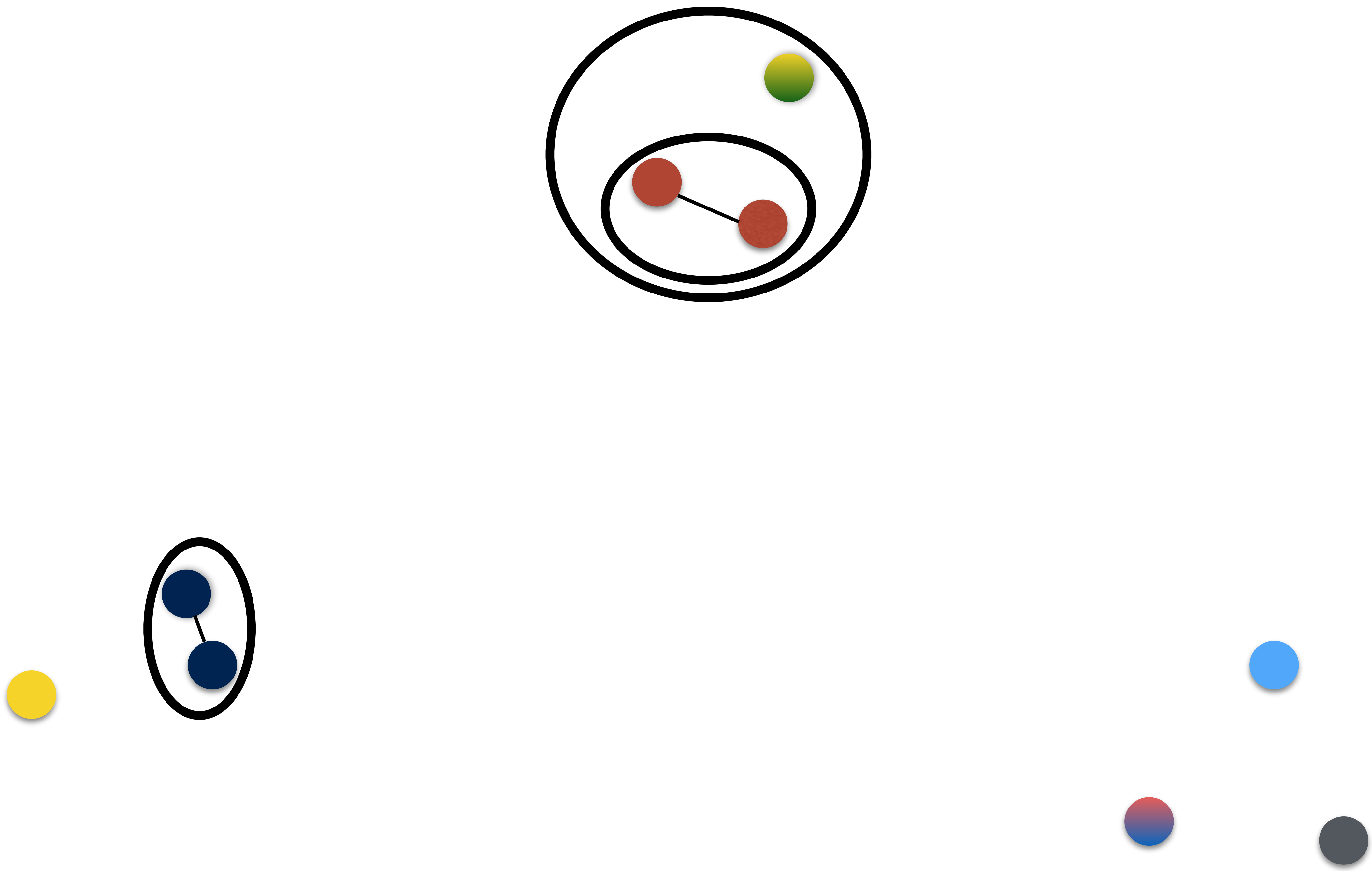

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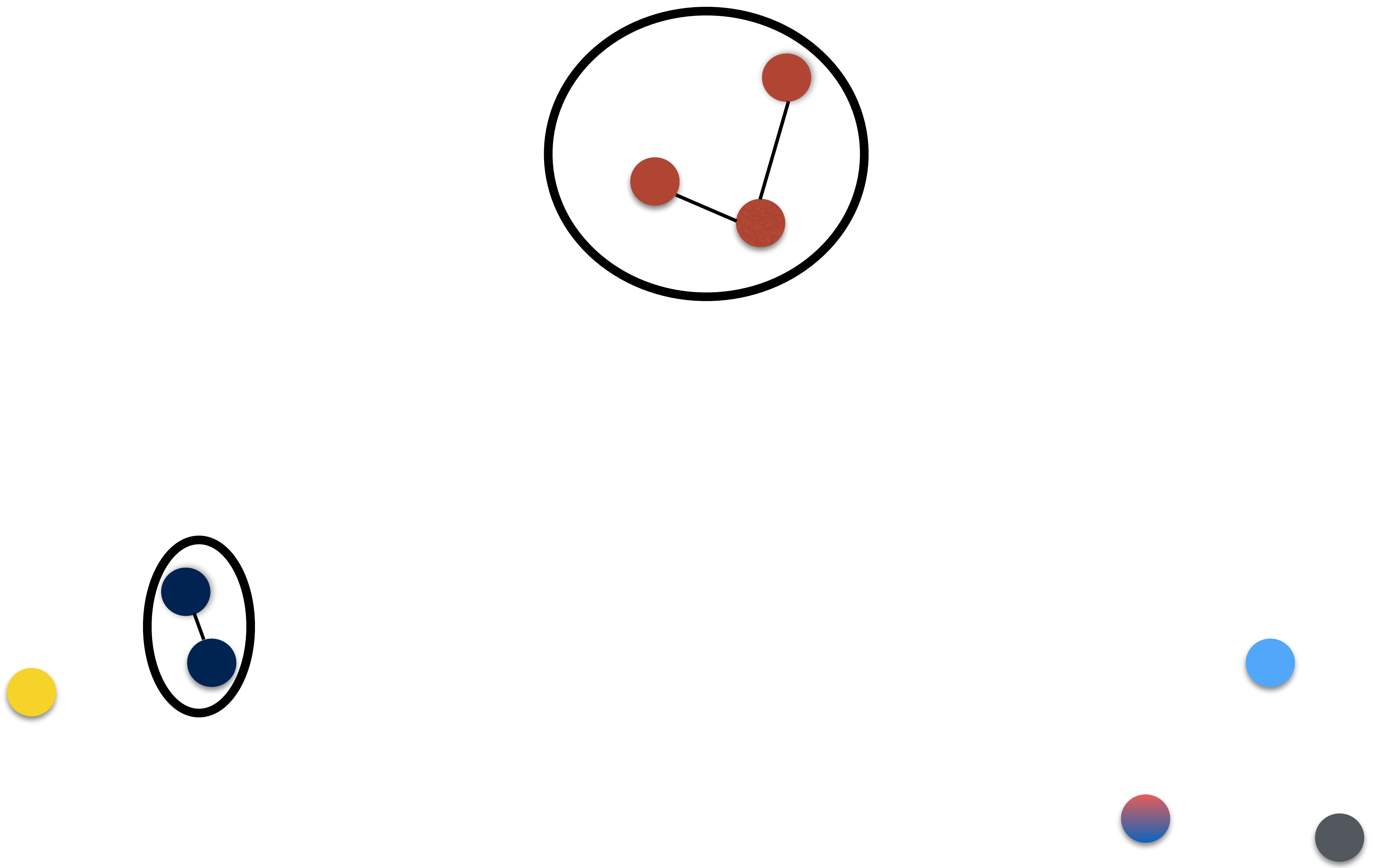

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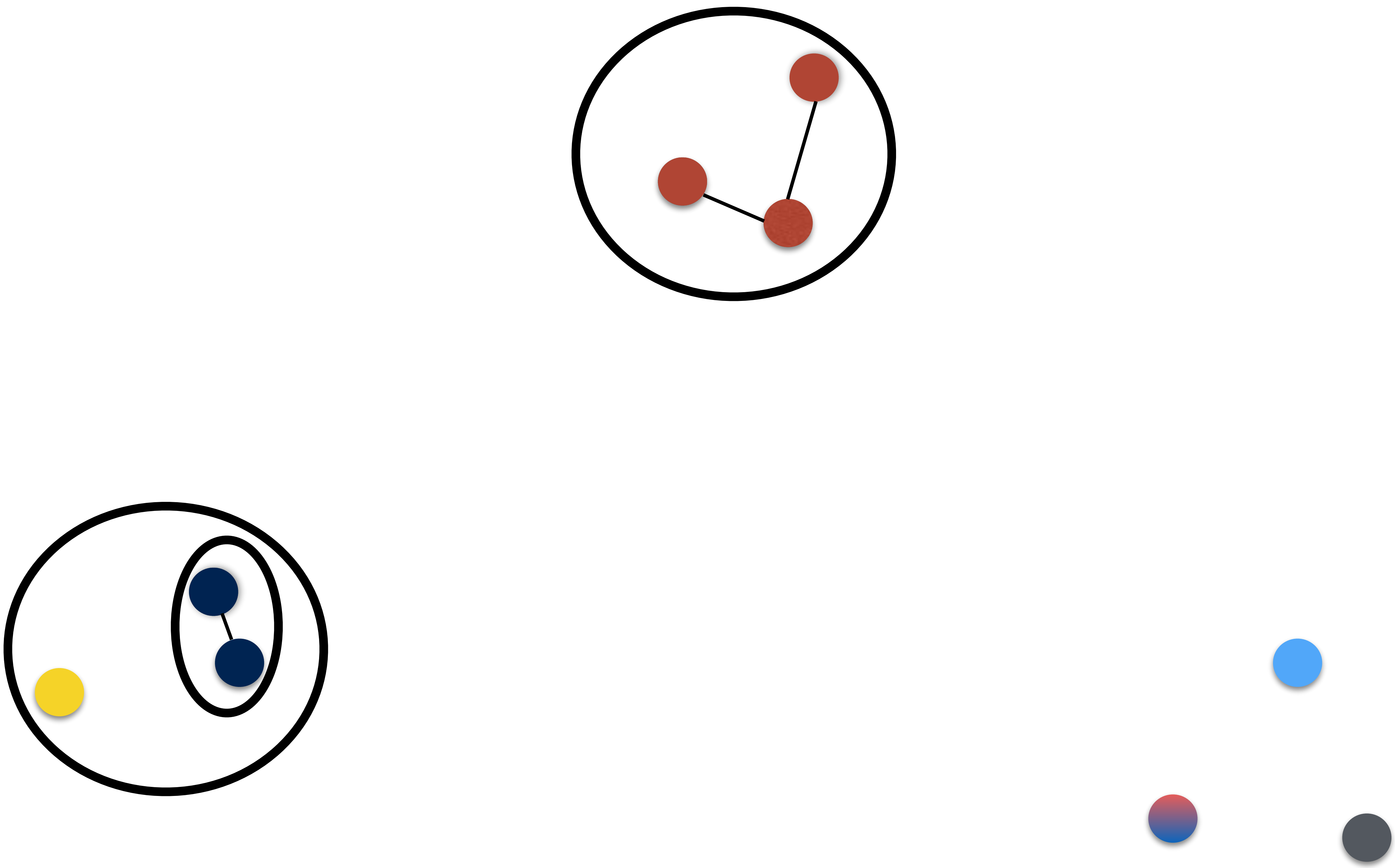

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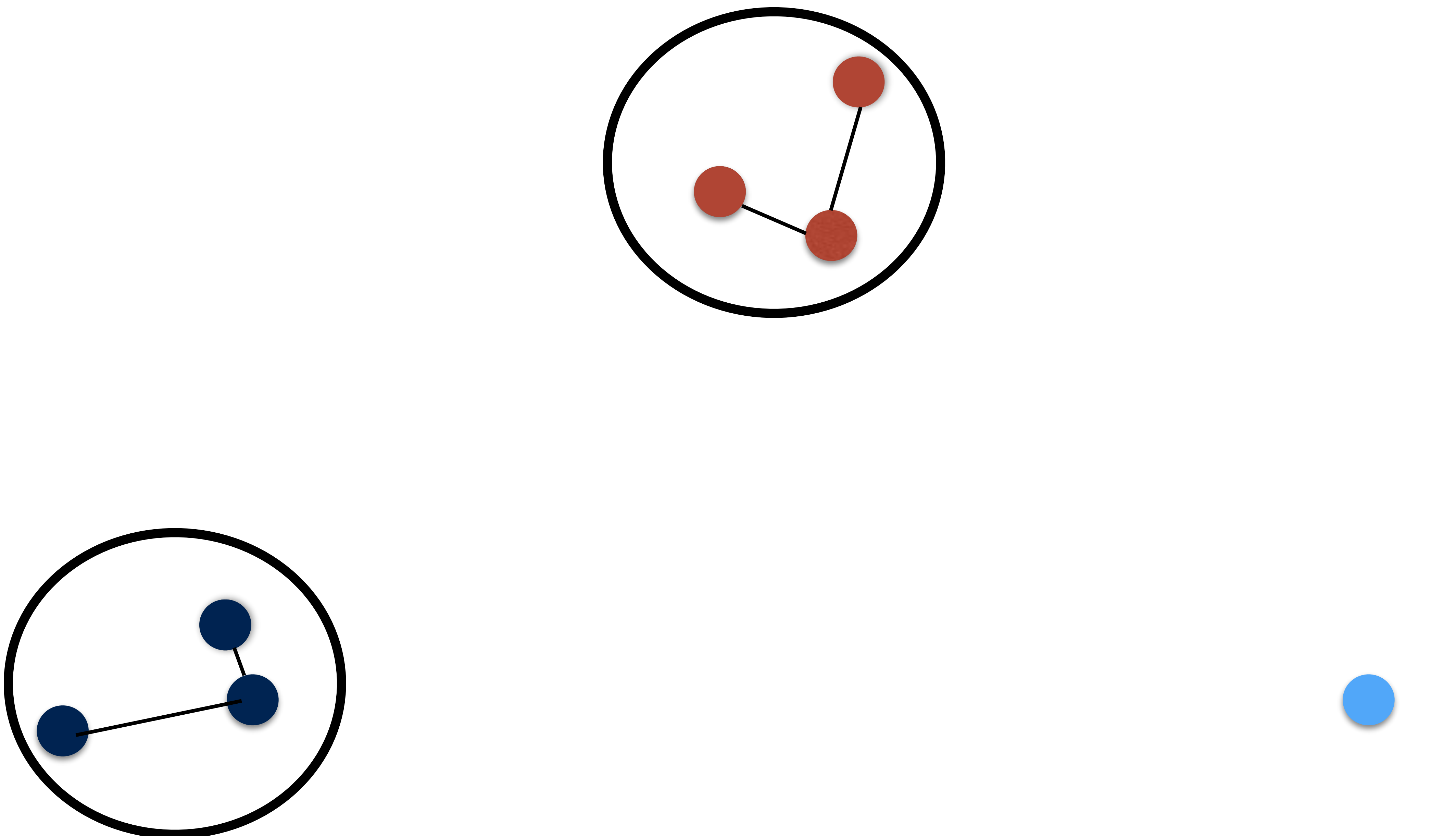

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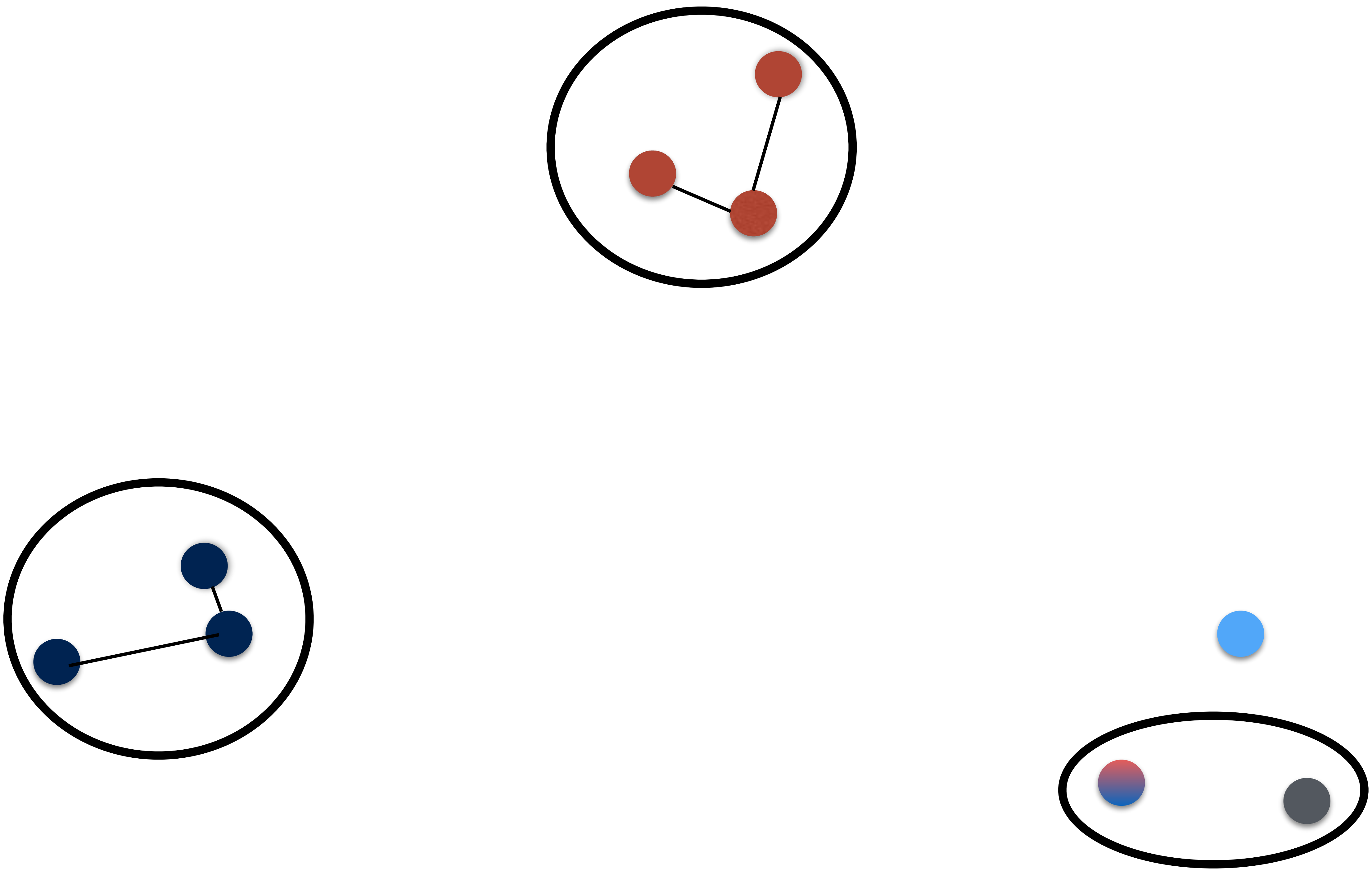

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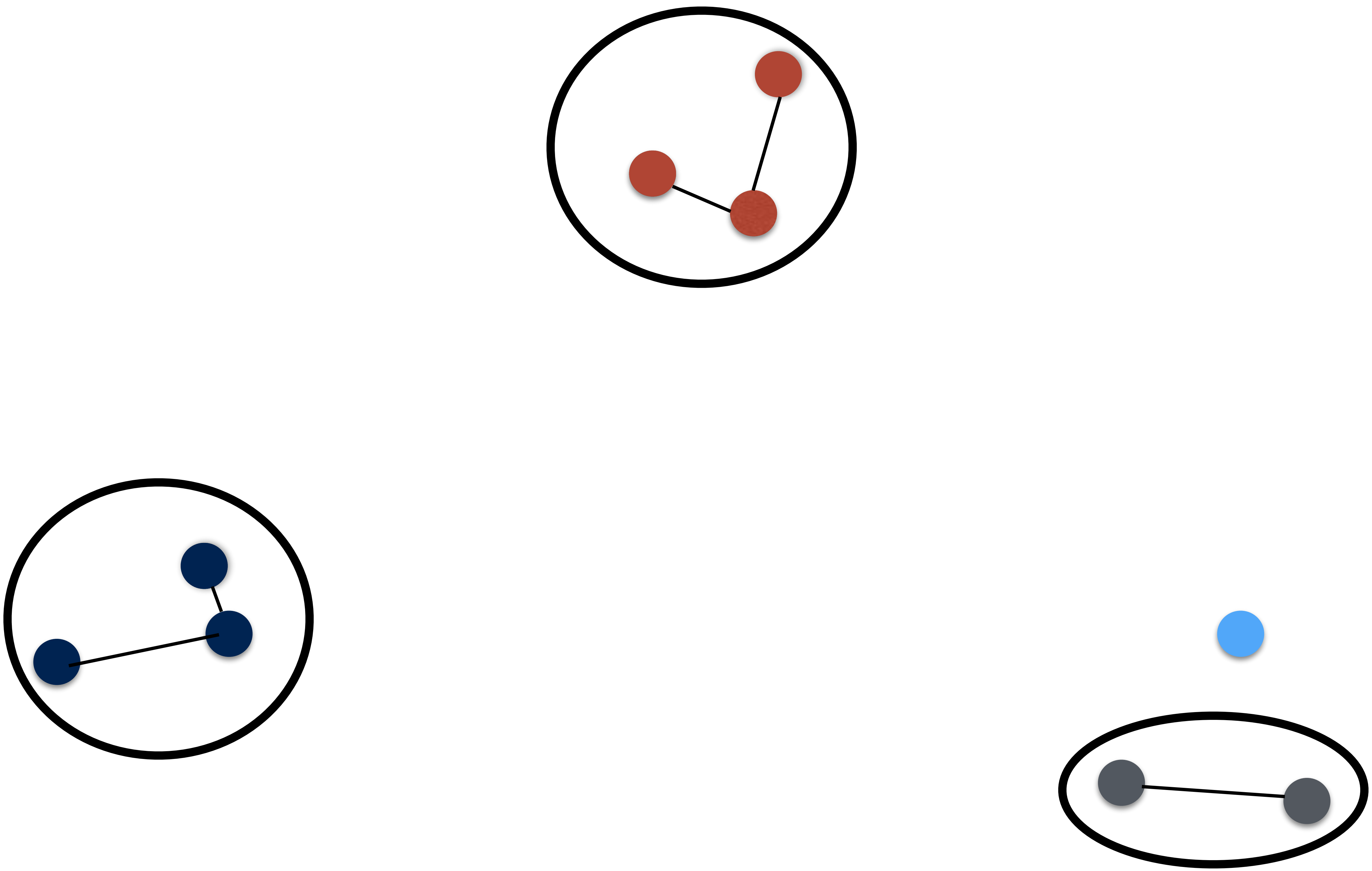

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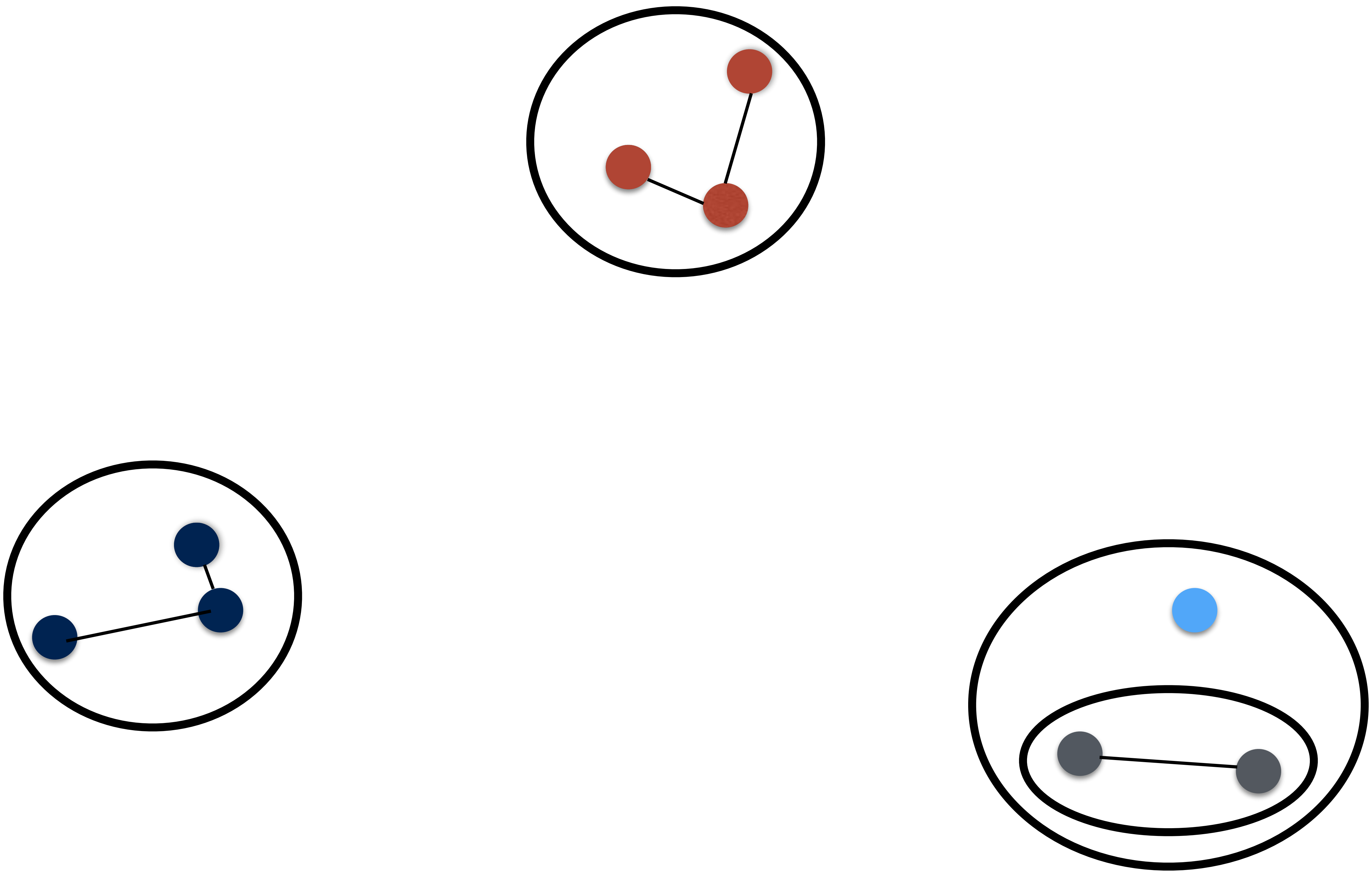

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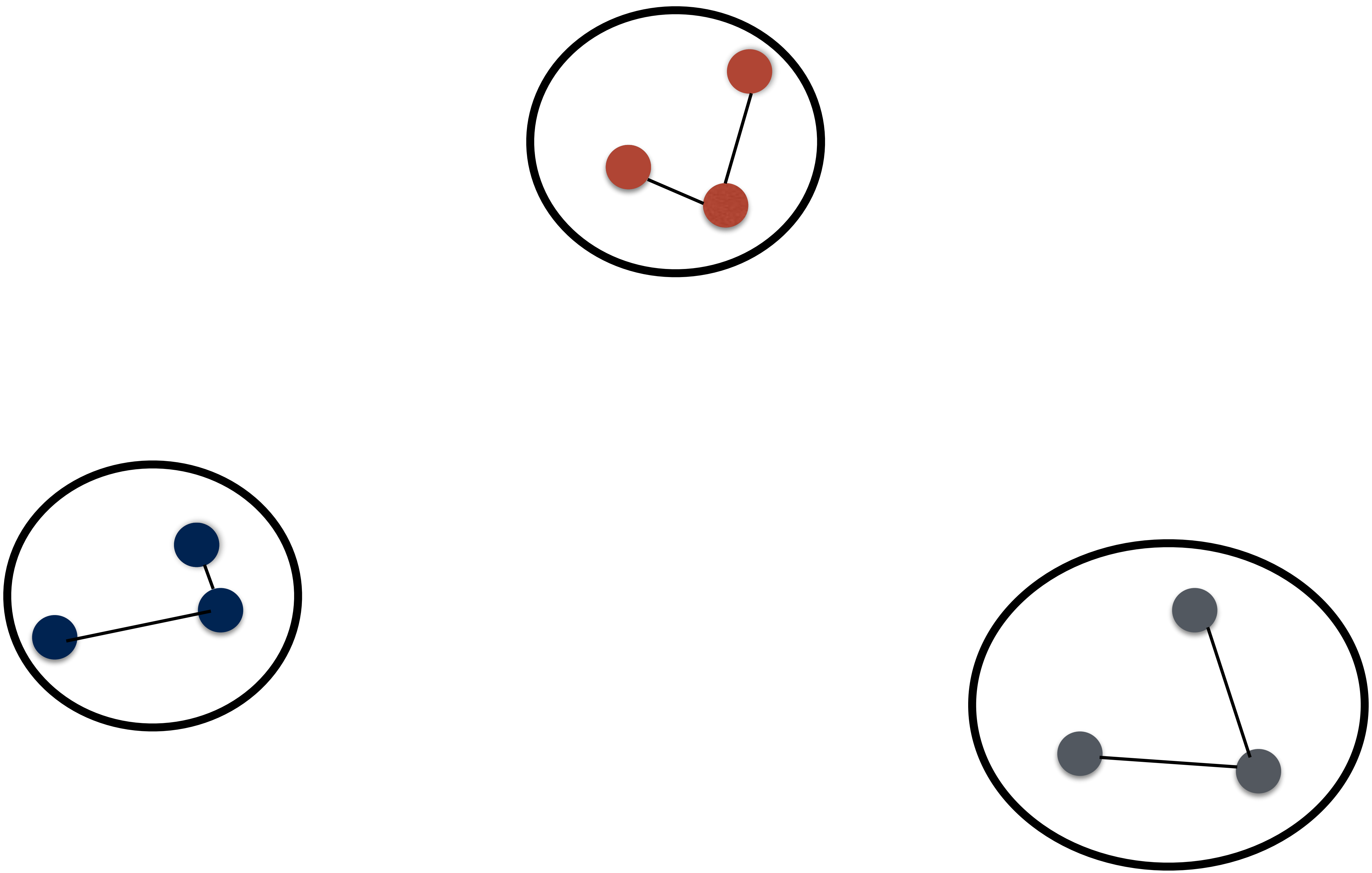

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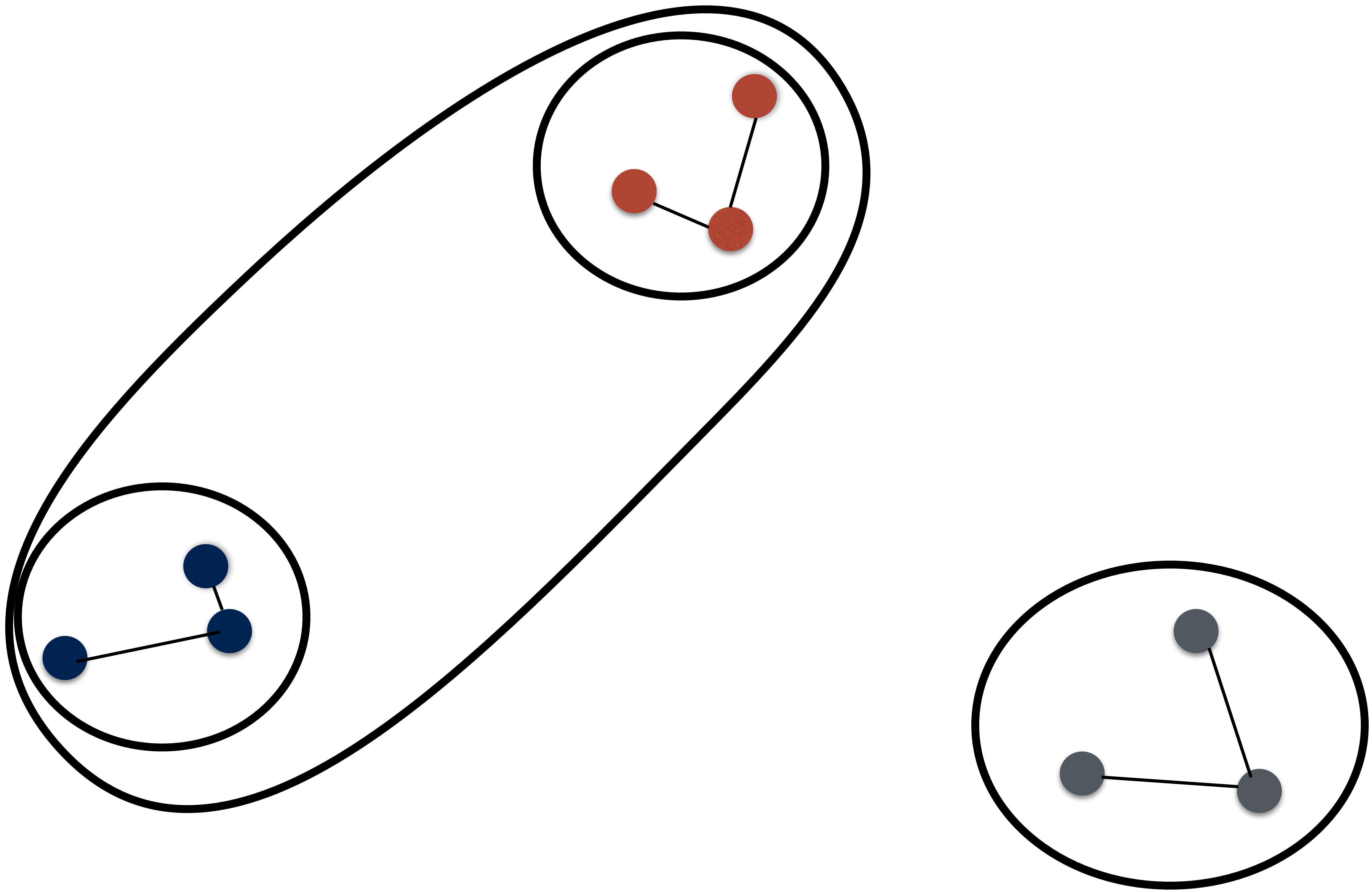

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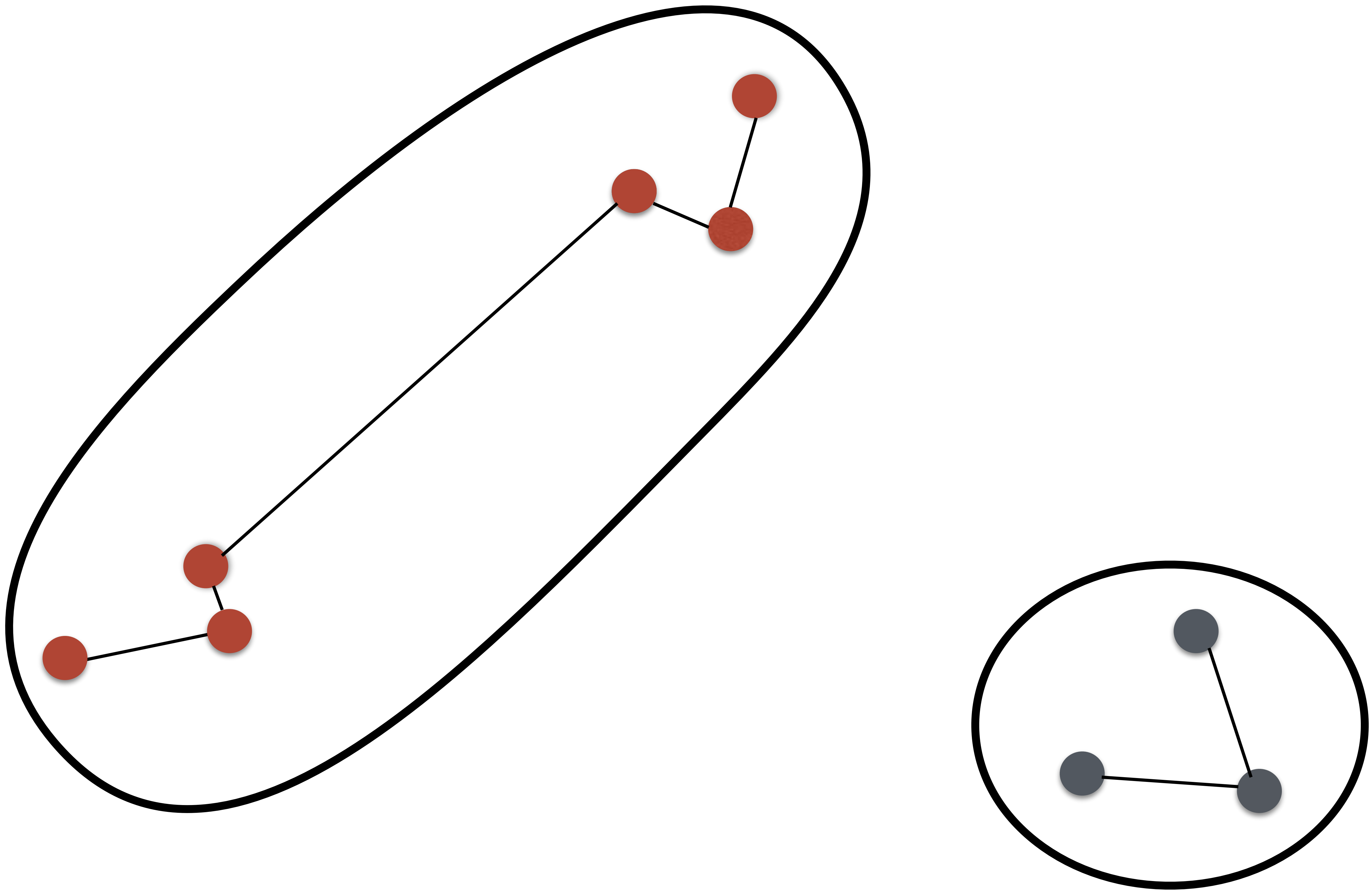

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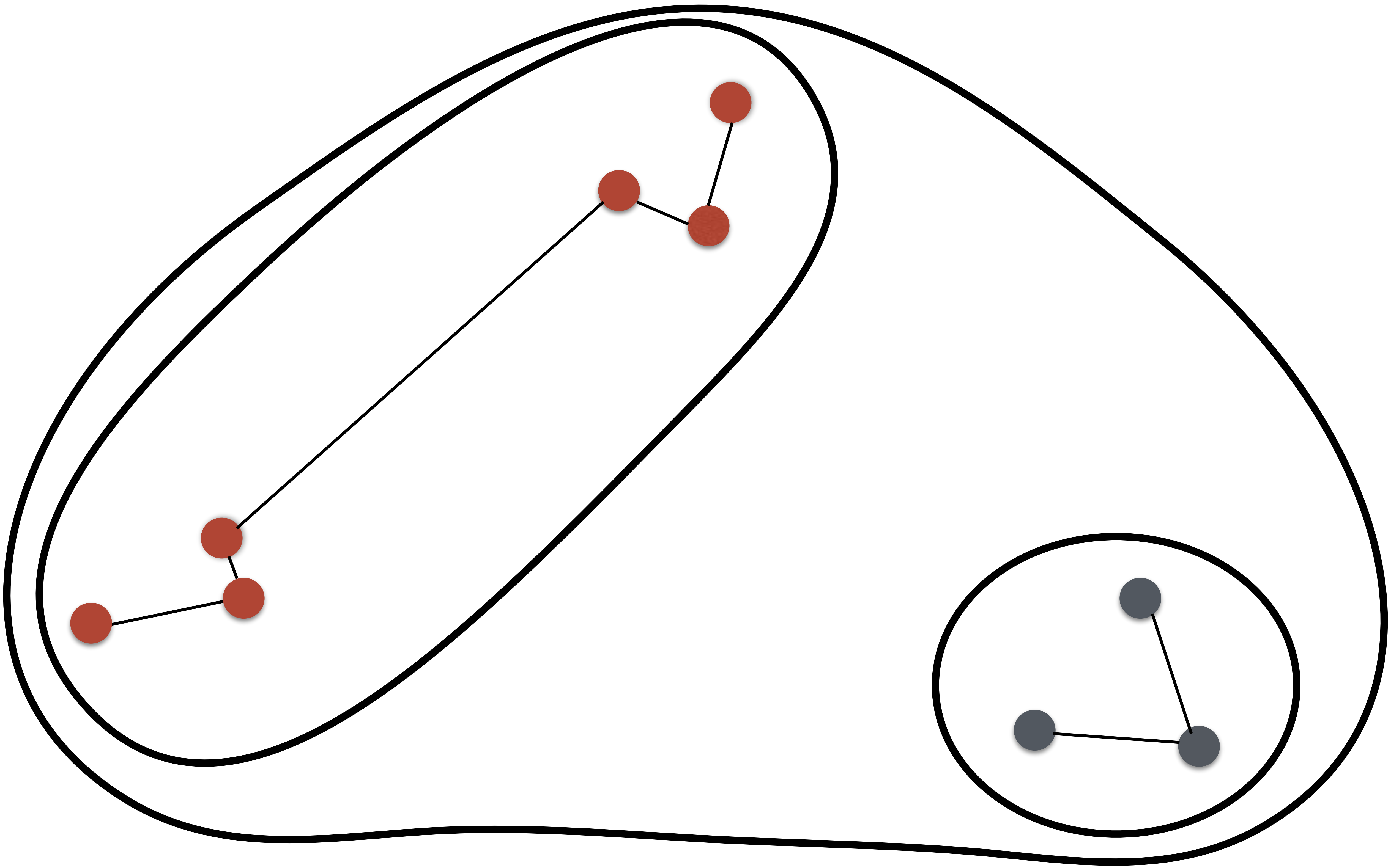

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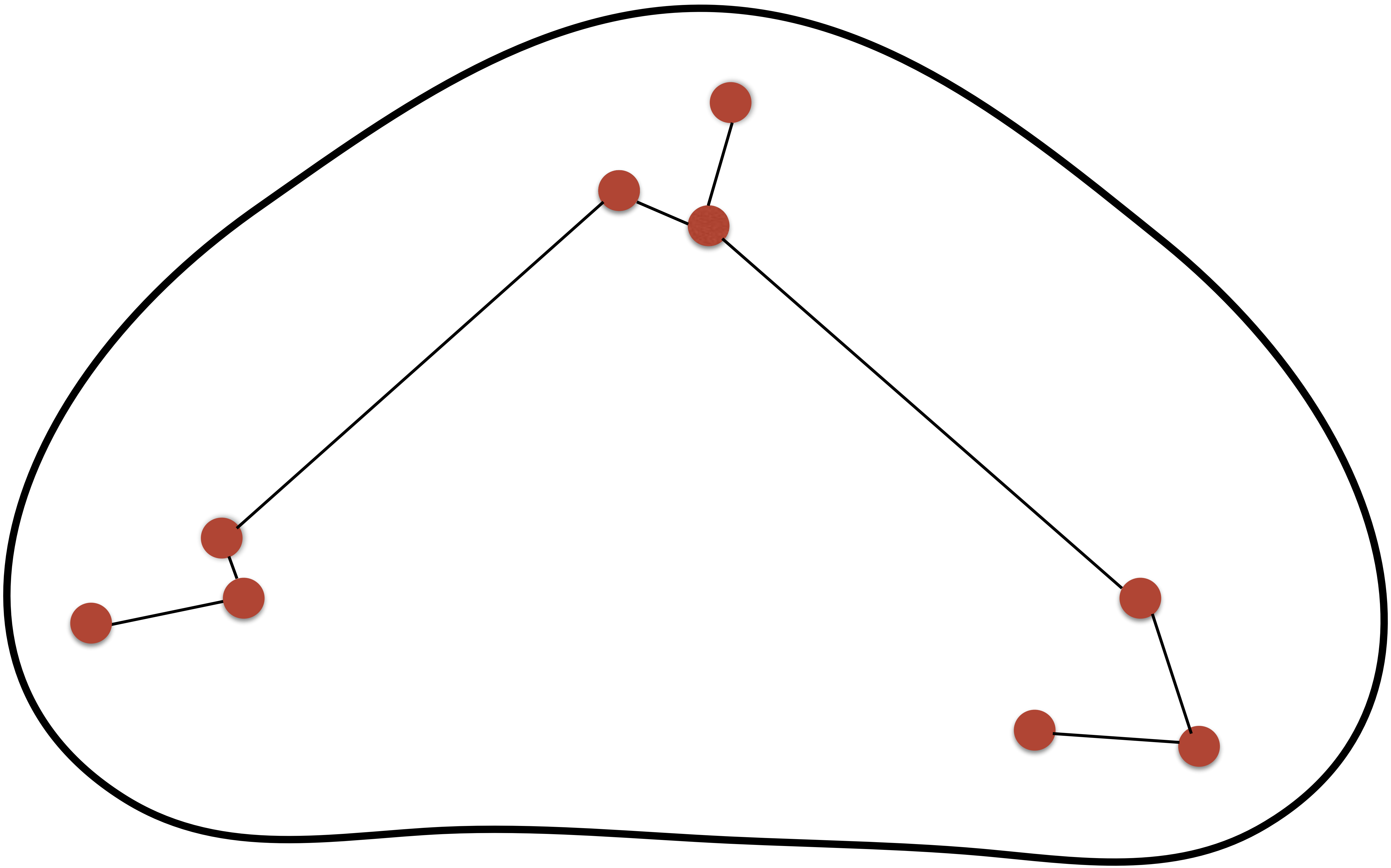


# Single Link Objective

Objective for single-link:

$$M_3 = \min_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$

Single link clustering is optimal for above objective!

# Single Link Objective

Proof:

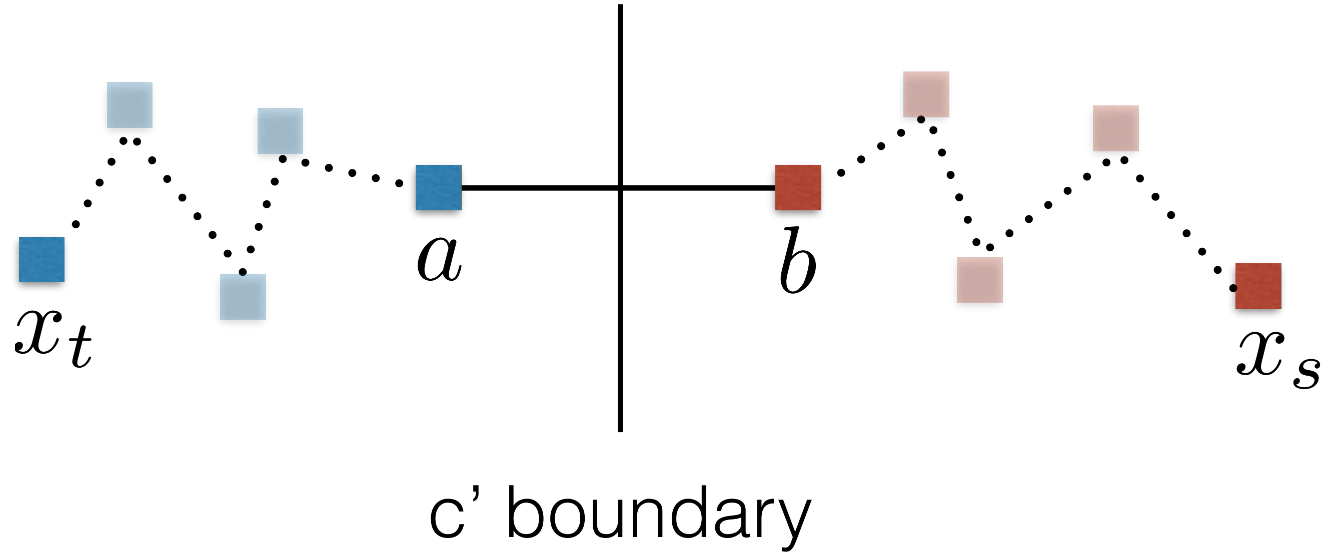
Say $c$ is solution produced by single-link clustering

Key observation:

$$\min_{t,s:c(x_i)\neq c(x_j)} \text{dissimilarity}(x_i, x_j) >$$ Distance of points merged (on the tree)

Say $c' \neq c$ then,

$$\exists\ t, s \text{ s.t. } c'(x_t) \neq c'(x_s) \text{ but } c(x_t) = c(x_s)$$



# Clustering Criterion

- Minimize average dissimilarity within cluster

$$M_6 = \sum_{j=1}^{K} \frac{1}{|C_j|} \sum_{s \in C_j} \text{dissimilarity}\left(\mathbf{x}_s, C_j\right)$$

$$= \sum_{j=1}^{K} \frac{1}{|C_j|} \sum_{s \in C_j} \left( \sum_{t \in C_j, t \neq s} \text{dissimilarity}\left(\mathbf{x}_s, \mathbf{x}_t\right) \right)$$

$$= \sum_{j=1}^{K} \frac{1}{|C_j|} \sum_{s \in C_j} \left( \sum_{t \in C_j, t \neq s} \|\mathbf{x}_s - \mathbf{x}_t\|_2^2 \right)$$

- Minimize within-cluster variance: $\mathbf{r}_j = \frac{1}{n_j} \sum_{\mathbf{x} \in C_j} \mathbf{x}$

$$M_5 = \sum_{j=1}^{K} \sum_{t \in C_j} \|\mathbf{x}_t - \mathbf{r}_j\|_2^2$$

# Clustering Criterion

- minimizing $M_5 \equiv$ minimizing $M_6$

# Lets build an Algorithm

$$M_5 = \sum_{j=1}^{K} \sum_{t \in C_j} \left\| \mathbf{x}_t - \mathbf{r}_j \right\|_2^2$$

$$\text{where } \mathbf{r}_j = \frac{1}{|C_j|} \sum_{t \in C_j} \mathbf{x}_t$$

# K-means Clustering

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^1$ randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \ldots, n\}$, set cluster identity of the point

$$\hat{c}^m(\mathbf{x}_t) = \underset{j \in [K]}{\text{argmin}} \|\mathbf{x}_t - \hat{\mathbf{r}}_j^m\|$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^{m+1} = \frac{1}{|\hat{C}_j^m|} \sum_{t \in \hat{C}_j^m} \mathbf{x}_t$$

  3. $m \leftarrow m + 1$