Photo by Unsplash user @foodiesfeed

BBM406

Fundamentals of Machine Learning

Lecture 21:

Clustering
K-Means

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Erkut Erdem // Hacettepe University // Spring 2021

Last time… **Boosting**

- **Idea:** given a weak learner, run it multiple times on (reweighted) training data, then let the learned classifiers vote
- On each iteration t:
  - weight each training example by how incorrectly it was classified
  - Learn a hypothesis – h_t
  - A strength for this hypothesis – a_t
- Final classifier:
  - A linear combination of the votes of the different classifiers weighted by their strength $H(X) = \text{sign}\left(\sum \alpha_t h_t(X)\right)$
- **Practically useful**
- **Theoretically interesting**

slide by Aarti Singh & Barnabas Poczos

Last time.. **The AdaBoost Algorithm**

0) Set $\tilde{W}_i^{(0)} = 1/n$ for $i = 1, \ldots, n$

1) At the m^{th} iteration we find (any) classifier $h(\mathbf{x}; \hat{\theta}_m)$ for which the *weighted classification error* ϵ_m

$$\epsilon_m = 0.5 - \frac{1}{2}\left(\sum_{i=1}^{n} \tilde{W}_i^{(m-1)} y_i h(\mathbf{x}_i; \hat{\theta}_m)\right)$$

is better than chance.

2) The new component is assigned votes based on its error:

$$\hat{\alpha}_m = 0.5 \log(\,(1 - \epsilon_m)/\epsilon_m\,)$$

3) The weights are updated according to (Z_m is chosen so that the new weights $\tilde{W}_i^{(m)}$ sum to one):

$$\tilde{W}_i^{(m)} = \frac{1}{Z_m} \cdot \tilde{W}_i^{(m-1)} \cdot \exp\{\, -y_i \hat{\alpha}_m h(\mathbf{x}_i; \hat{\theta}_m)\,\}$$

slide by Jiri Matas and Jan Šochman

Today

- What is clustering?
- K-means algorithm

What is clustering

Clustering

- Grouping data according to similarity

slide by Tamara Broderick

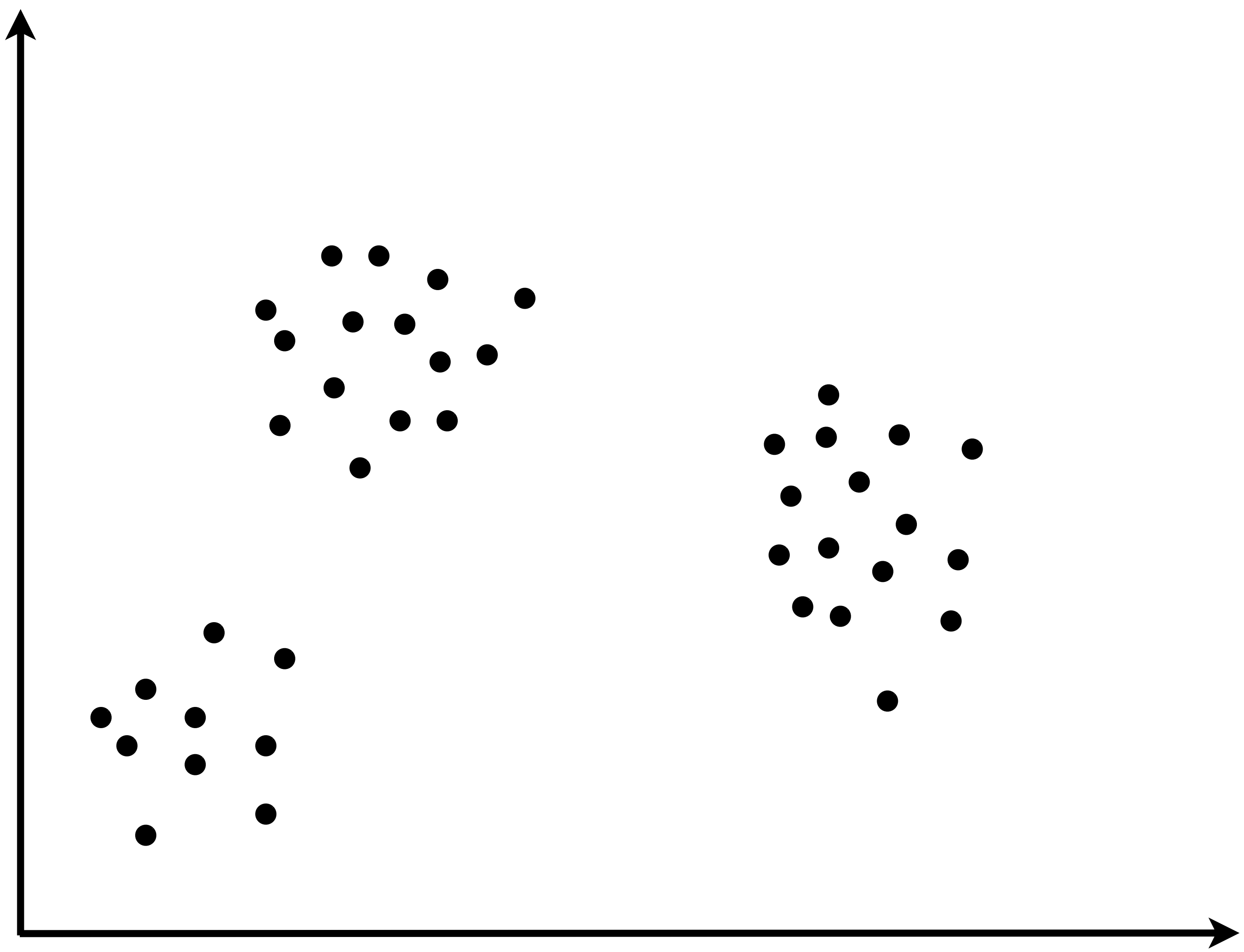
Clustering

- <u>Grouping</u> <u>data</u> according to <u>similarity</u>

slide by Tamara Broderick

Clustering

- Grouping <u>data</u> according to similarity

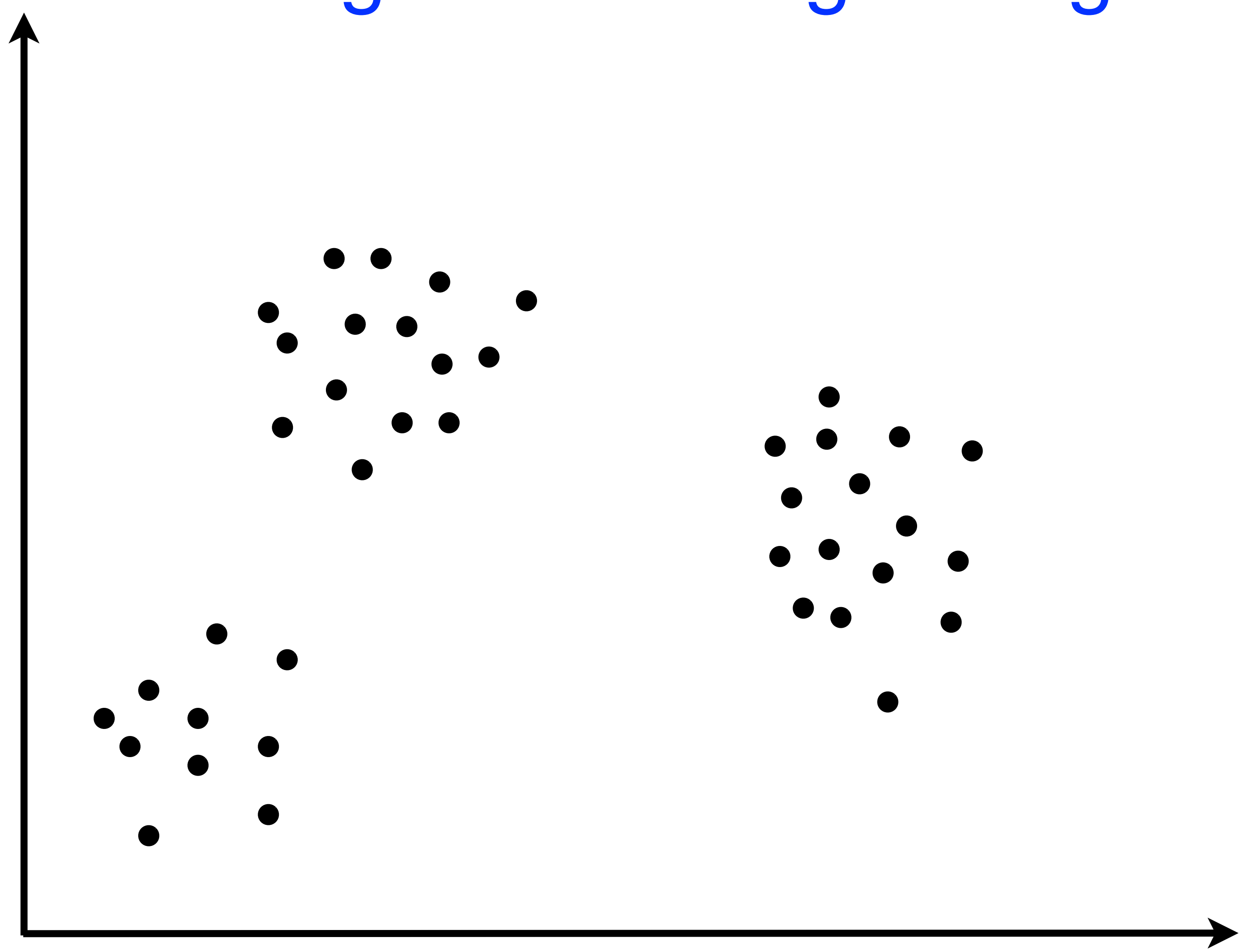


slide by Tamara Broderick

Clustering

- Grouping data according to similarity

e.g. archaeological dig



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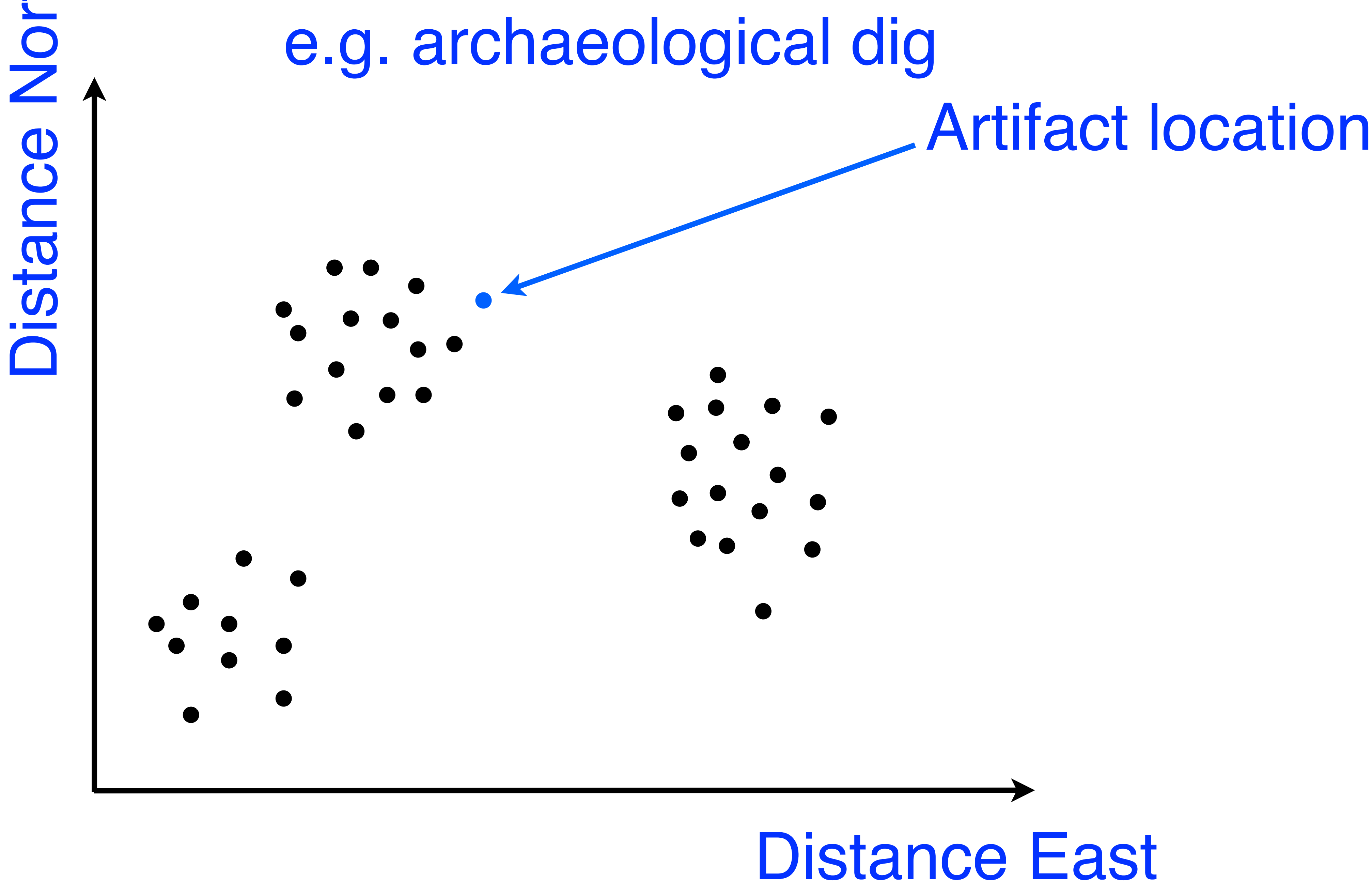

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Clustering

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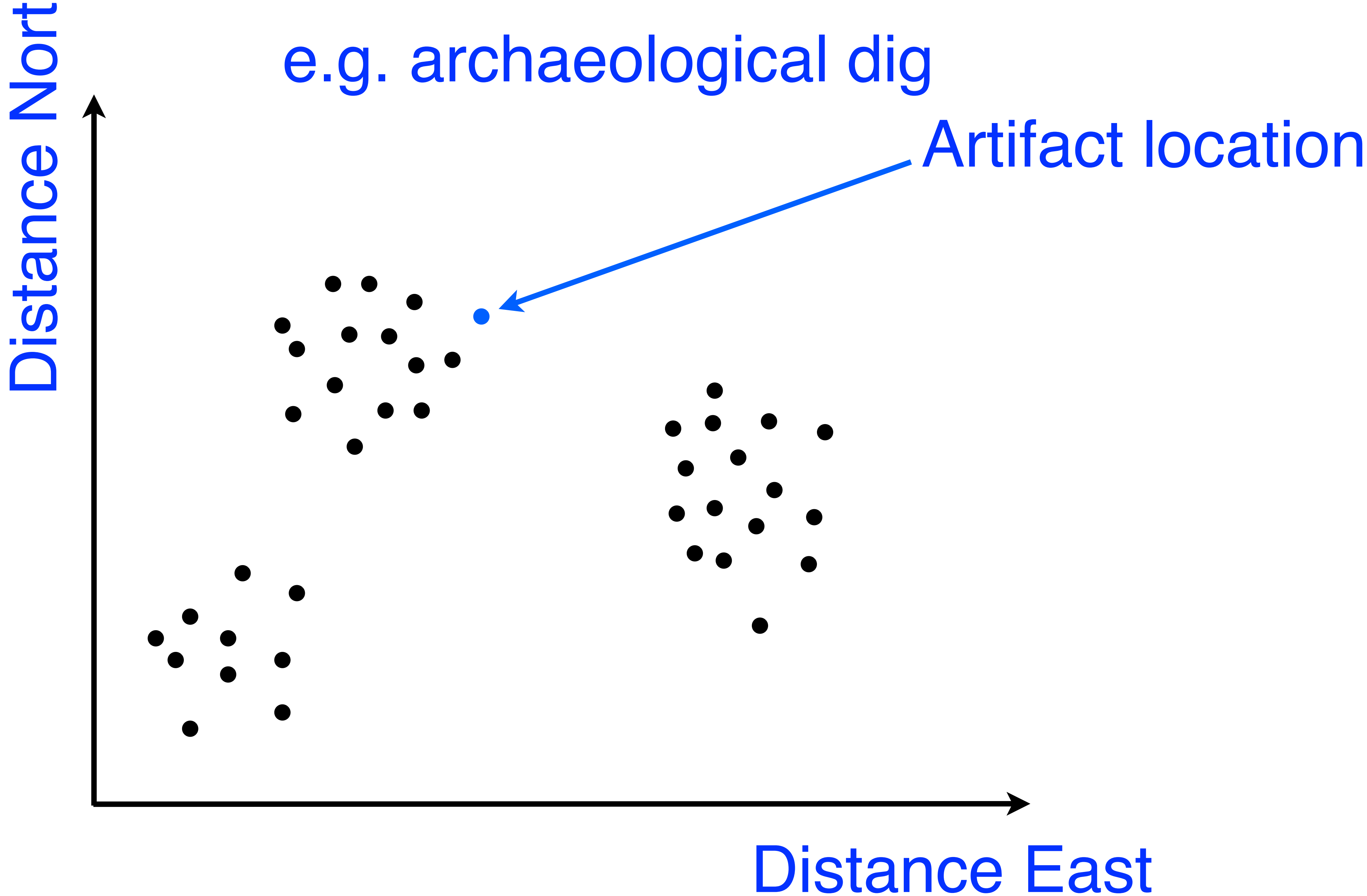

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Clustering

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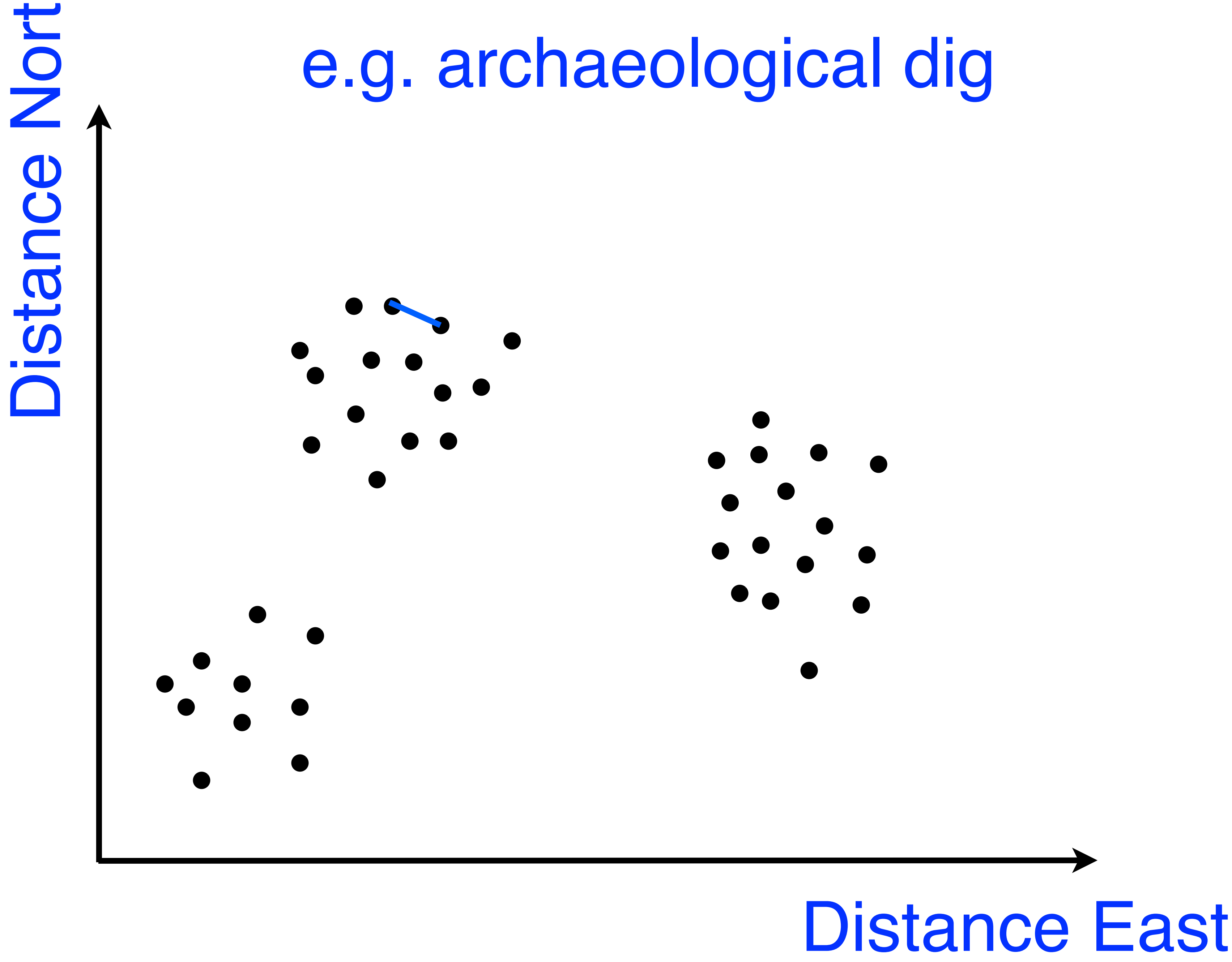

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Clustering

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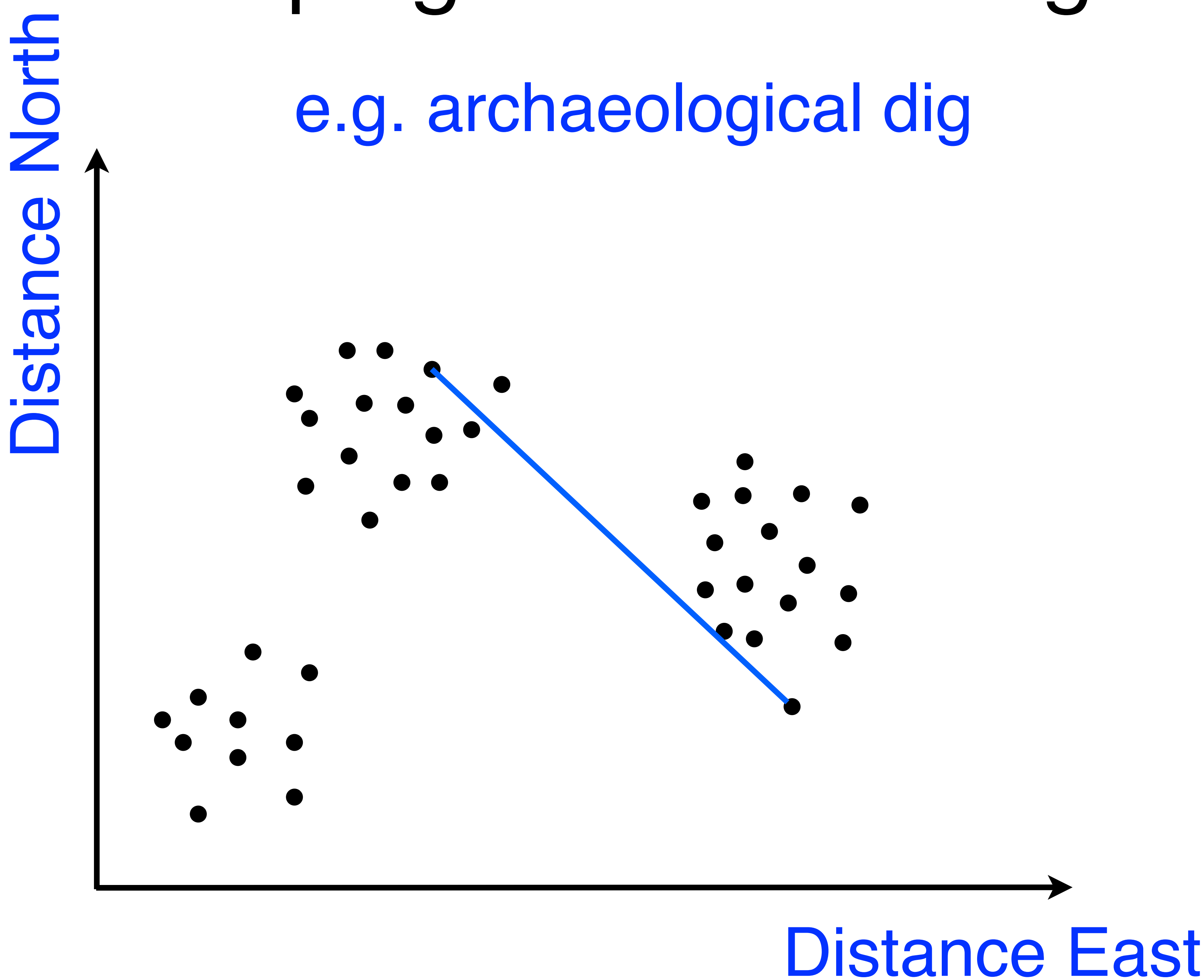

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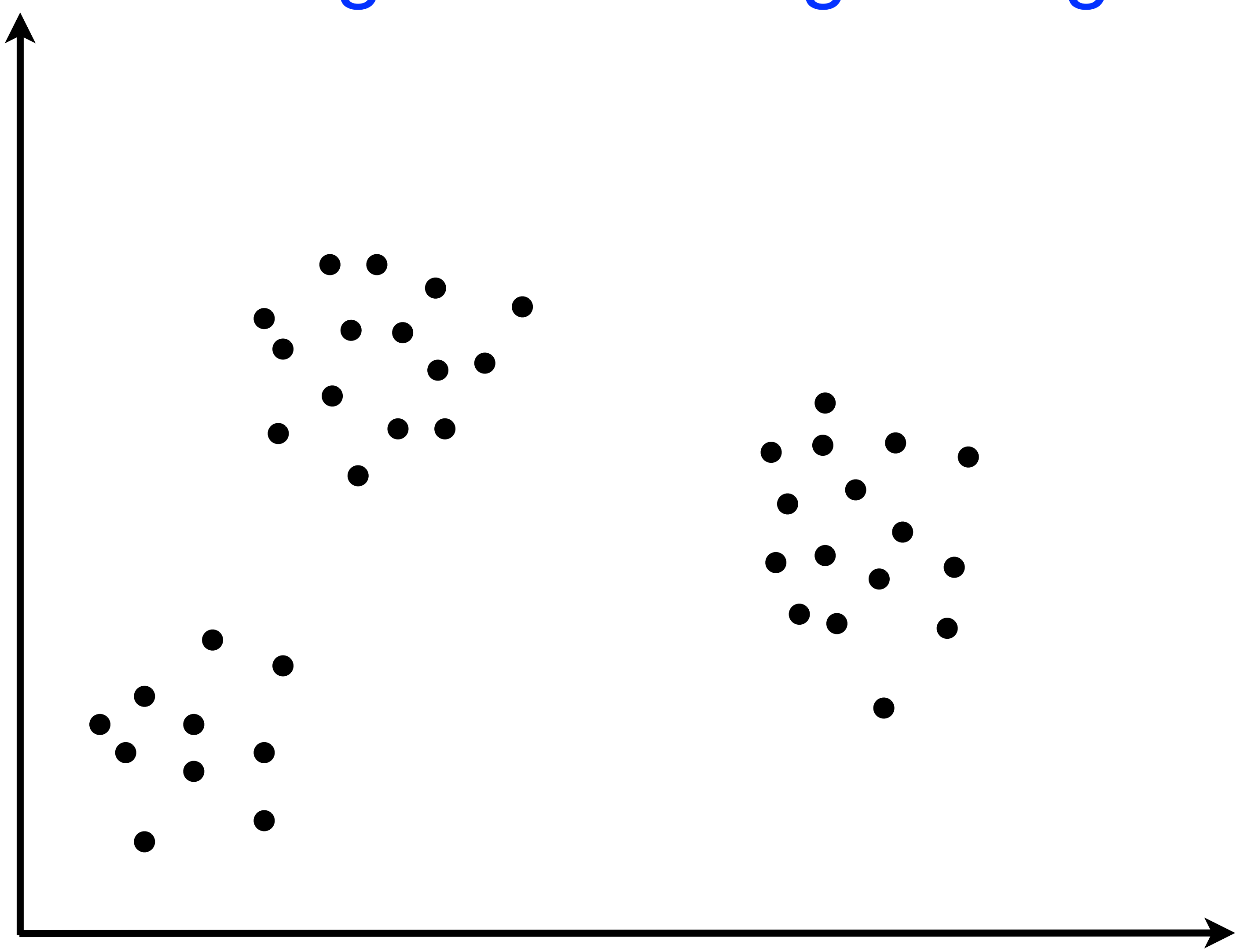
Clustering

- <u>Grouping</u> data according to similarity

e.g. archaeological dig

Distance North



Distance East

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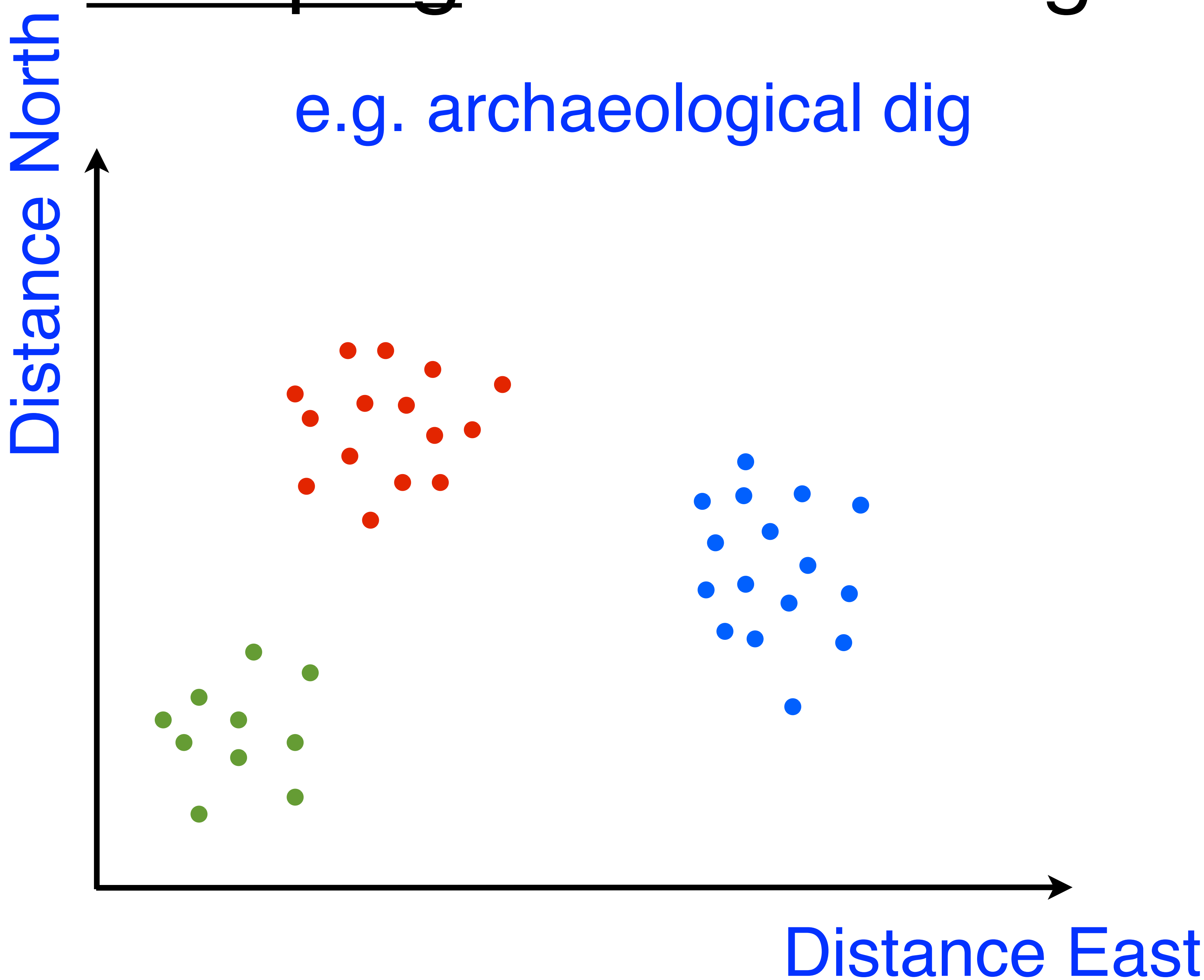
Clustering

- Grouping data according to similarity



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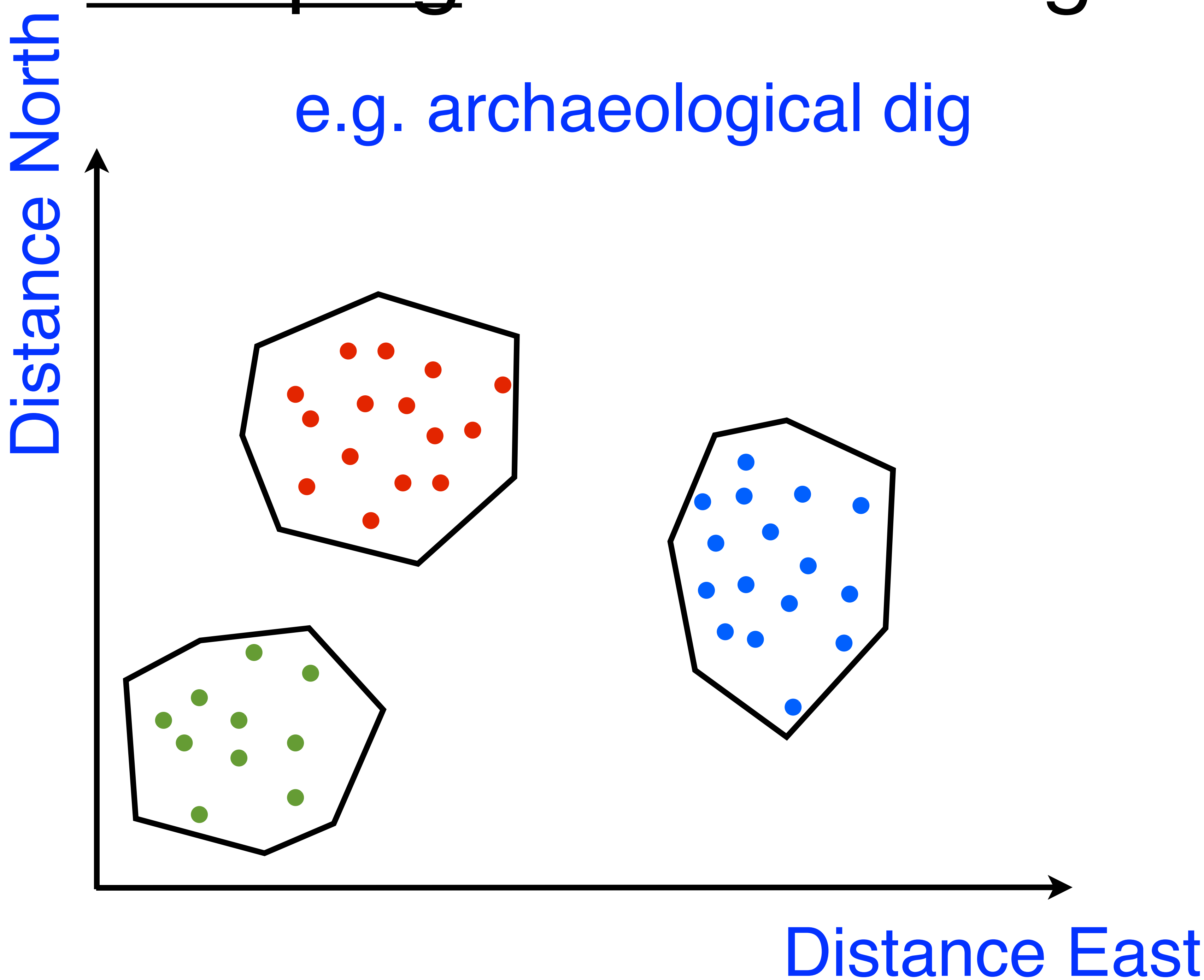
Clustering

- Grouping data according to similarity



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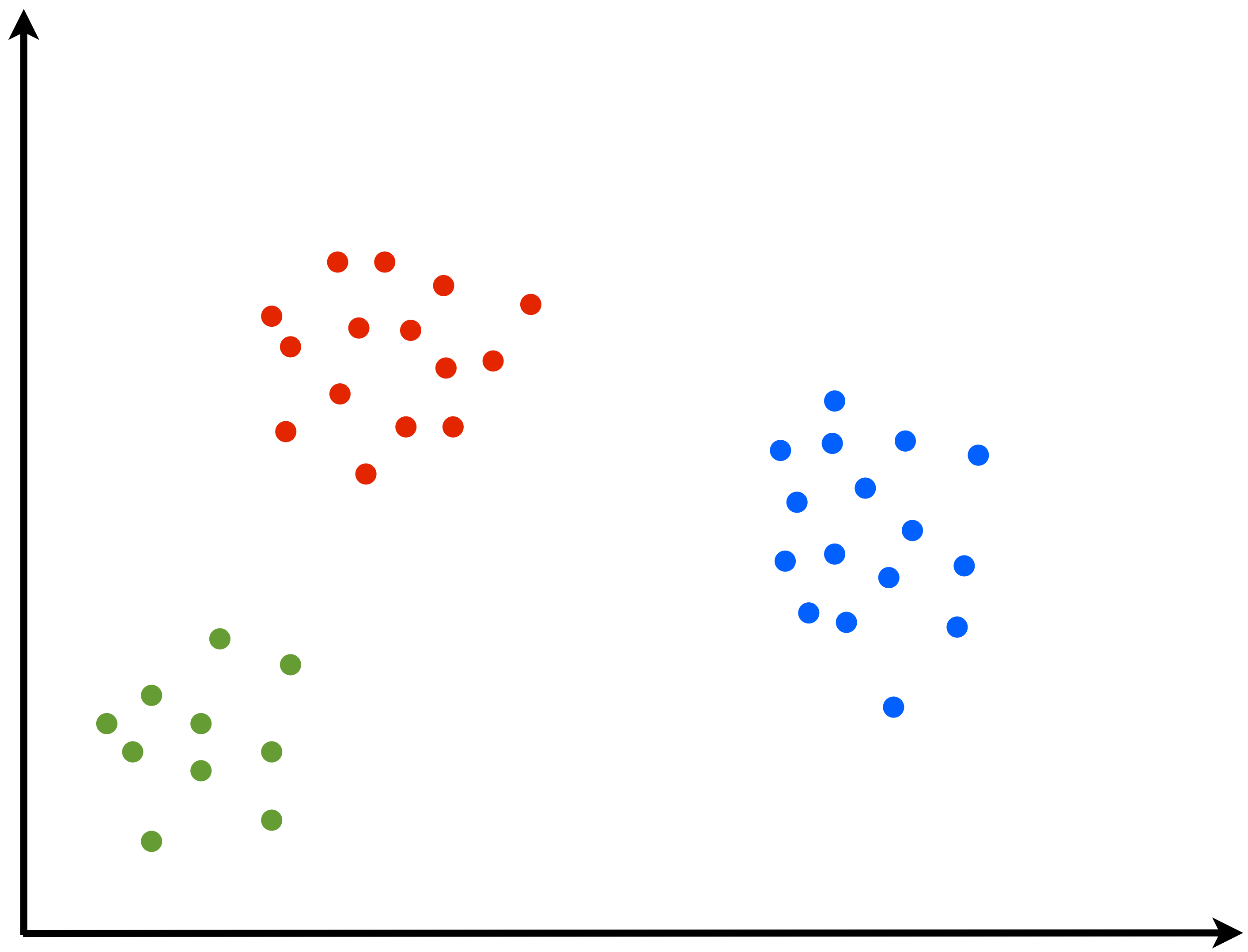
Clustering vs. Classification

- Grouping data according to similarity

  Predicting new labels from old labels



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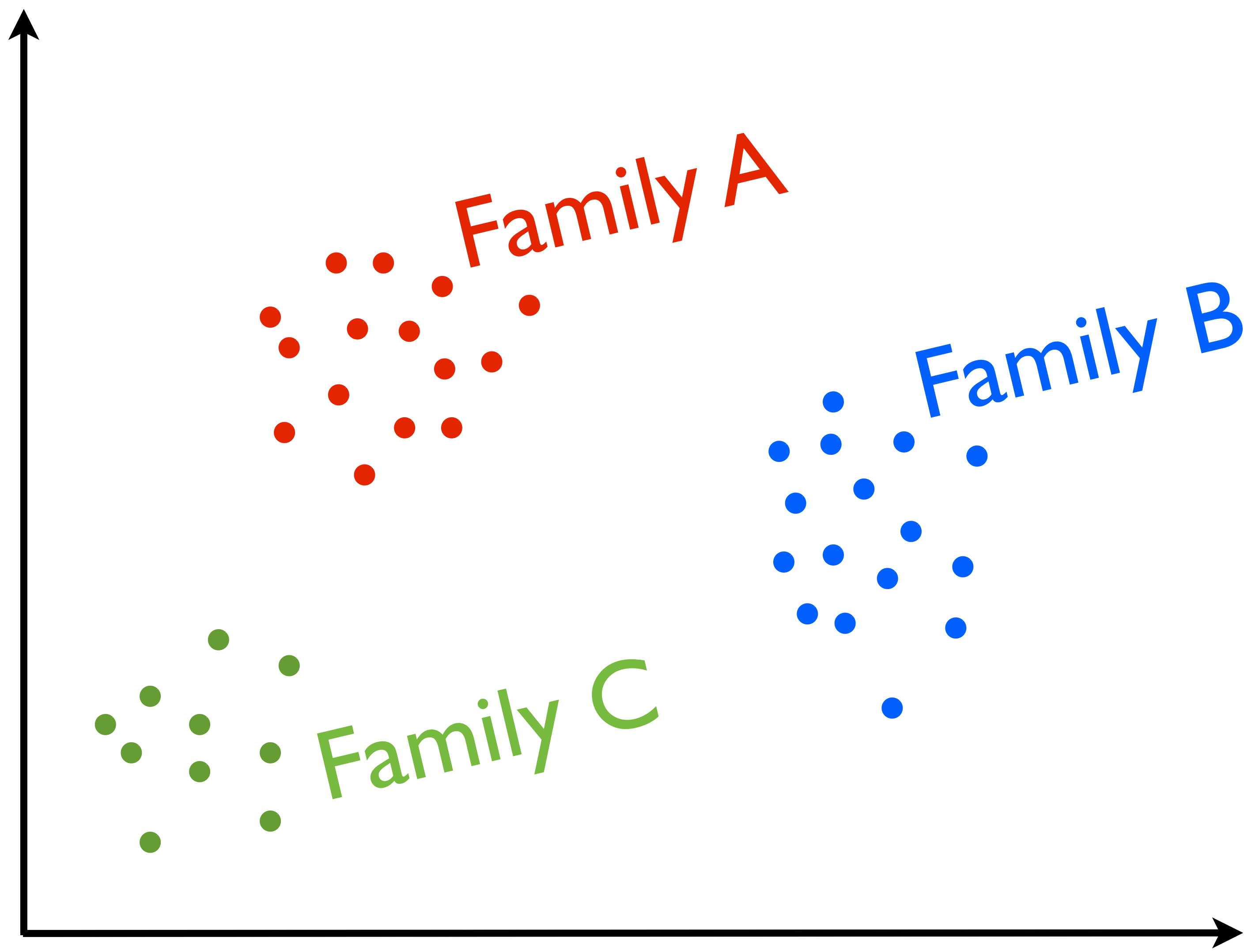
Clustering vs. Classification

- <u>Grouping</u> data according to similarity

<u>Predicting</u> new labels from old labels



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Clustering vs. Classification

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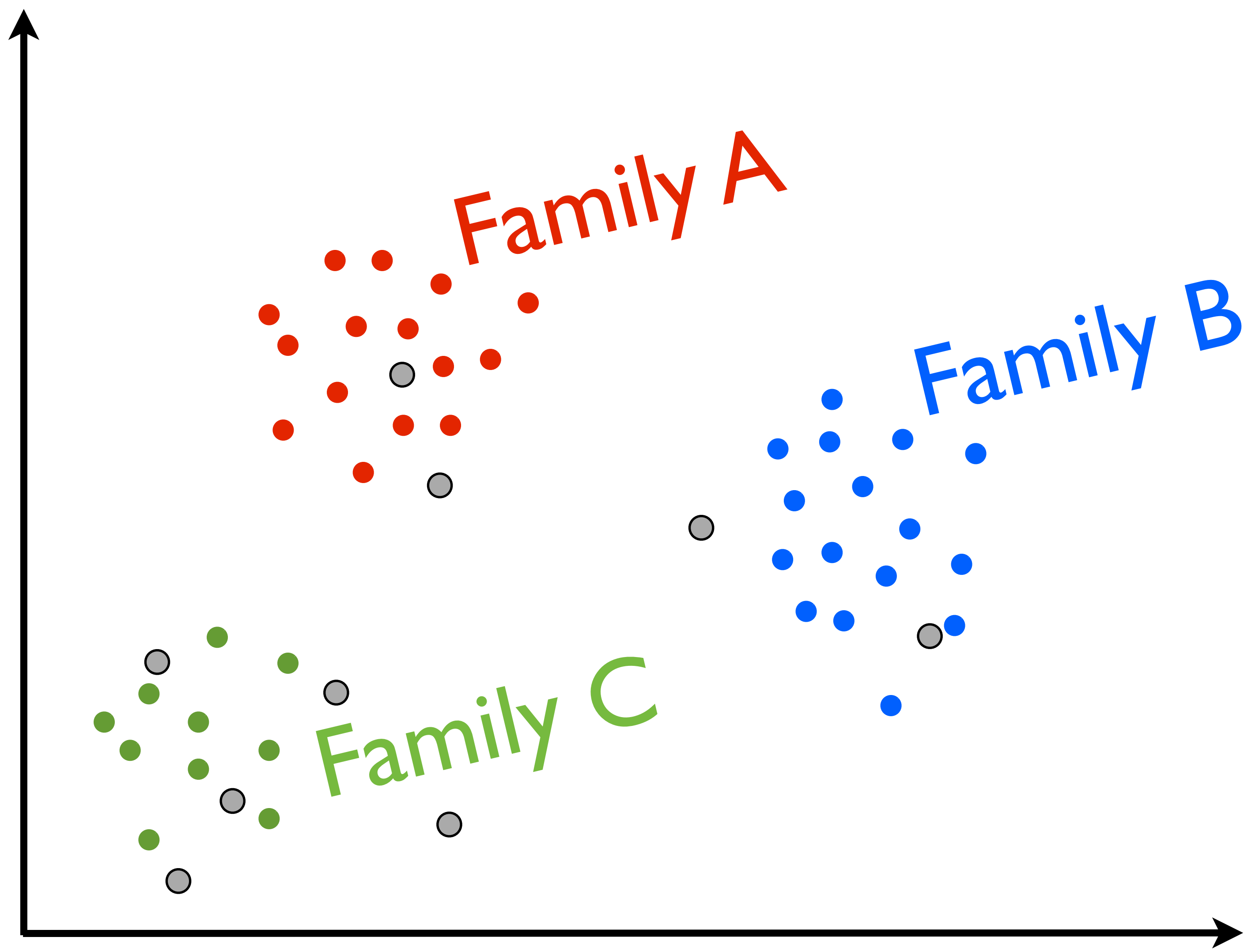

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Why use clustering… …instead of classification

- Exploratory data analysis

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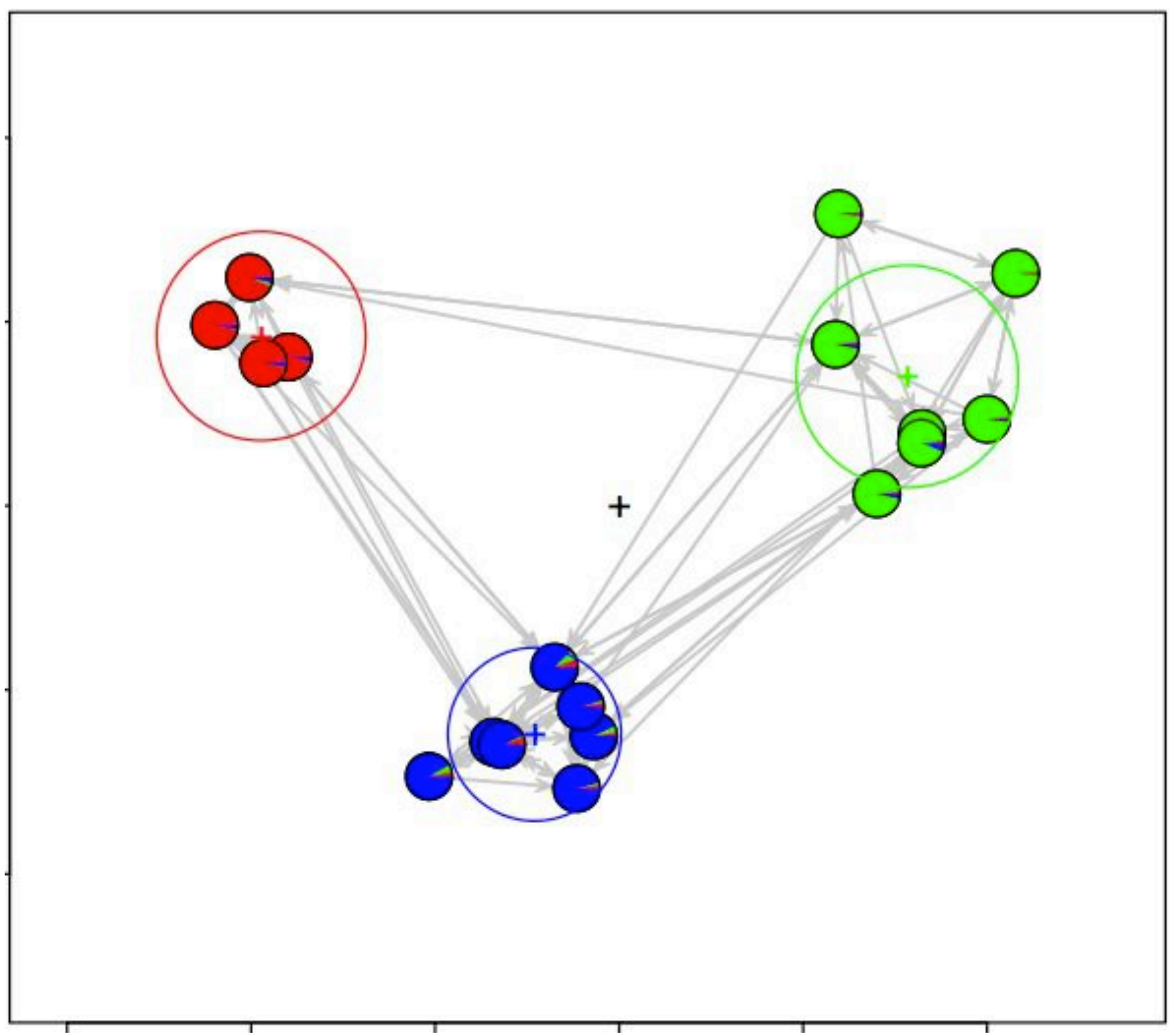

slide by Tamara Broderick

[Krivitsky Handcock 2008]

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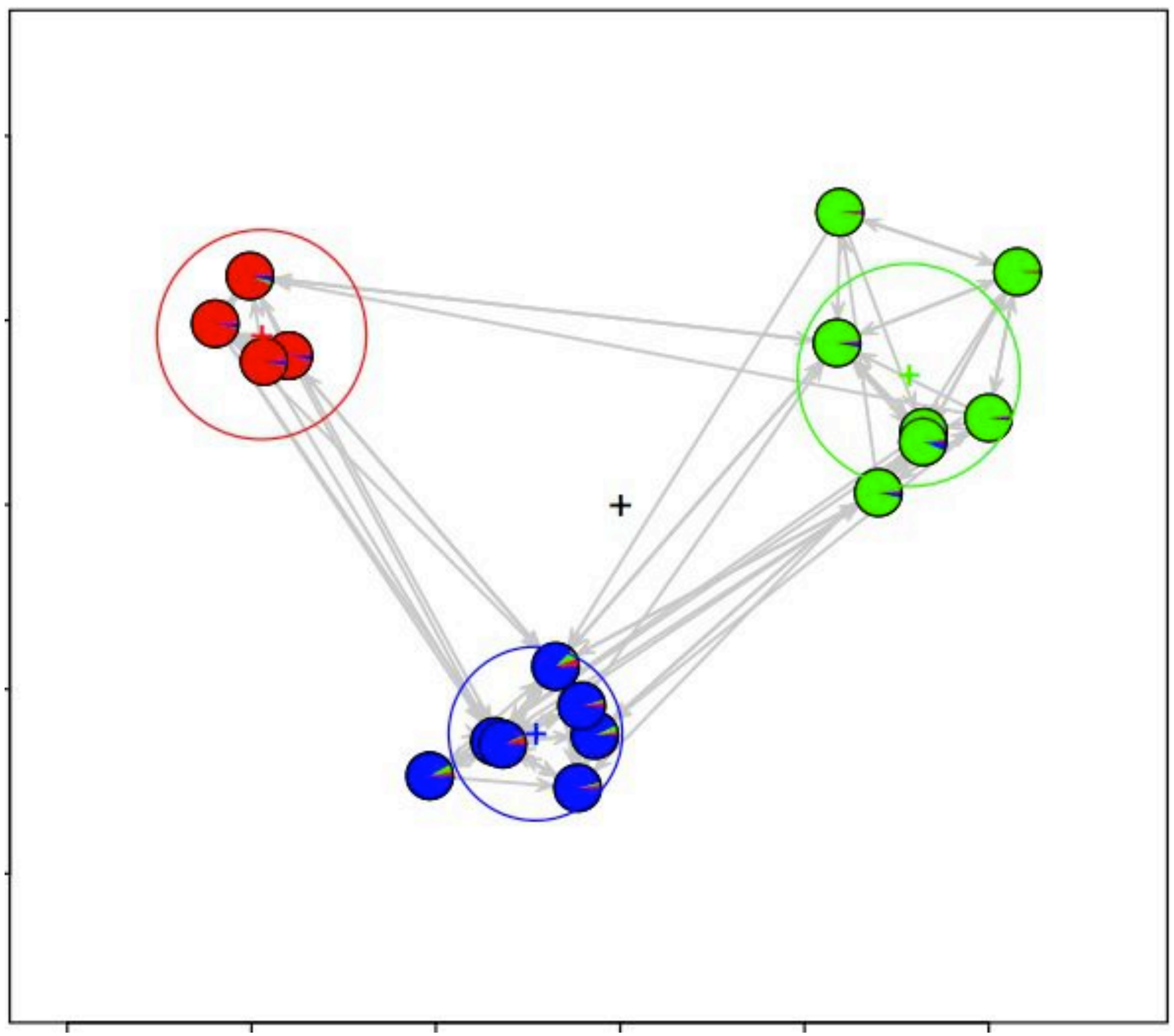

Datum: person

Similarity: the number of common interests of two people

slide by Tamara Broderick

[Krivitsky Handcock 2008]

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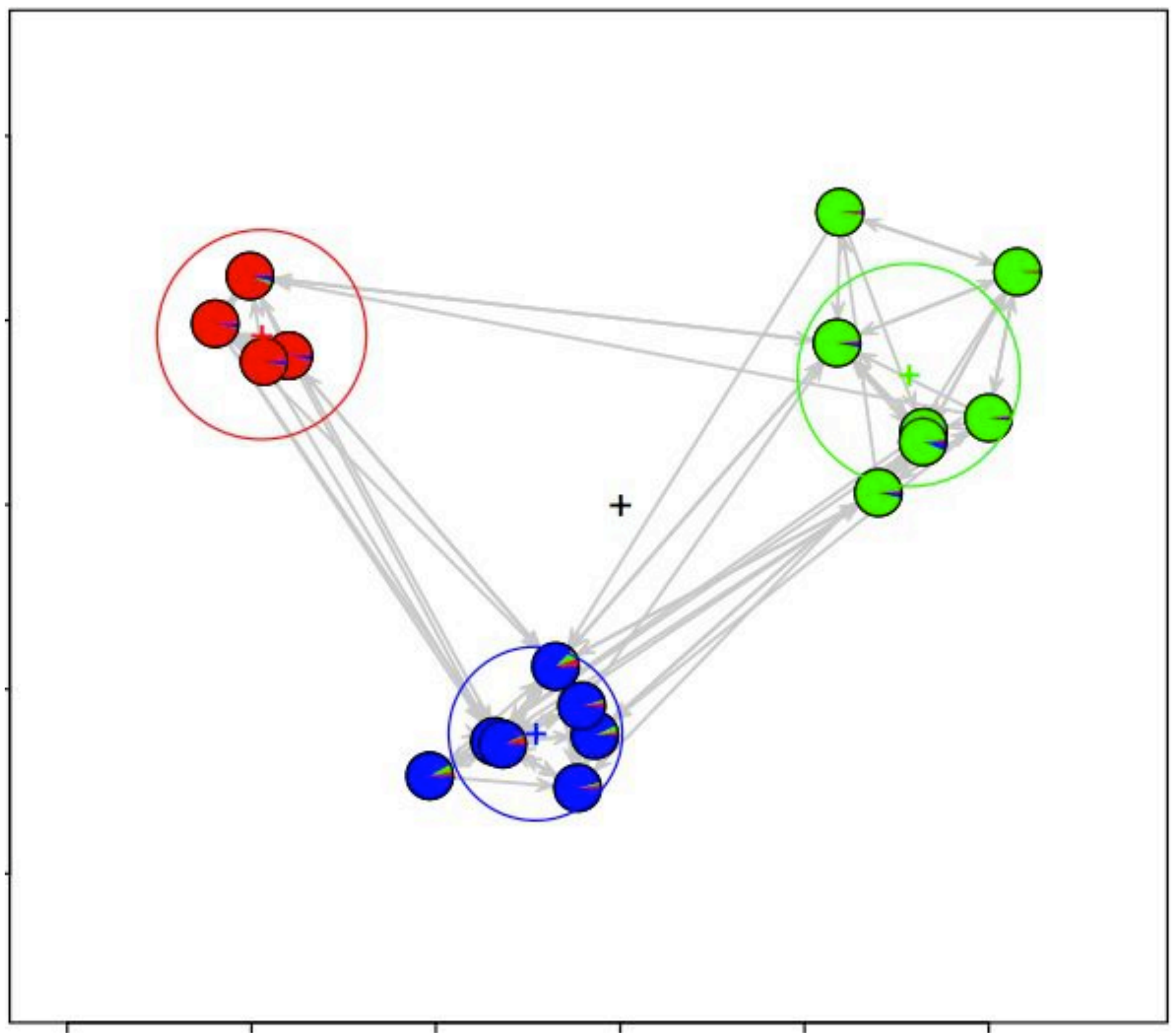

Datum: a binary vector specifying whether a person has each interest

Similarity: the number of common interests of two people

[Krivitsky Handcock 2008]

slide by Tamara Broderick

Why use clustering… …instead of classification

- Exploratory data analysis
- Classes are unspecified (unknown, changing too quickly, expensive to label data, etc)

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Topic Analysis

NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

earst Foundation will give $1.25 million to Lincoln Center, Metropoli-
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Hearst Foundation President Randolph A. Hearst said Monday in
Lincoln Center's share will be $200,000 for its new building, which
and provide new public facilities. The Metropolitan Opera Co. and
will receive $400,000 each. The Juilliard School, where music and
the performing arts are taught, will get $250,000. The Hearst Foundation, a leading supporter
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donation, too.

[Blei 2003]

slide by Tamara Broderick

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"Arts"	"Budgets"	"Children"	"Education"
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Topic Analysis

Datum: word

Similarity: how many documents exist where two words co-occur

Lincoln Center's share will be $200,000 for its new building, which and provide new public facilities. The Metropolitan Opera Co. and will receive $400,000 each. The Juilliard School, where music and the performing arts are taught, will get $250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual $100,000 donation, too.

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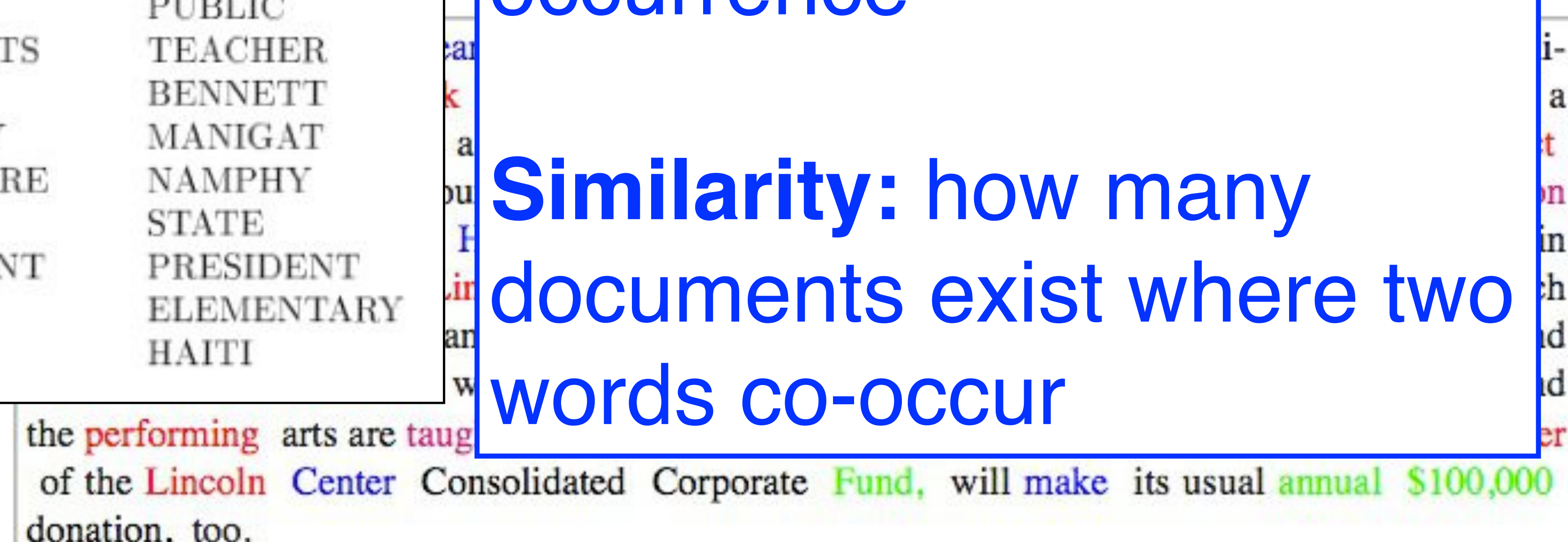
Topic Analysis

Datum: binary vector indicating document occurrence

Similarity: how many documents exist where two words co-occur



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Document clustering

[Carpineto et al. 2009]

slide by Tamara Broderick

Why use clustering…
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Document clustering

Datum: document

Dissimilarity: distance between topic distributions of two documents

[Carpineto et al. 2009]

slide by Tamara Broderick

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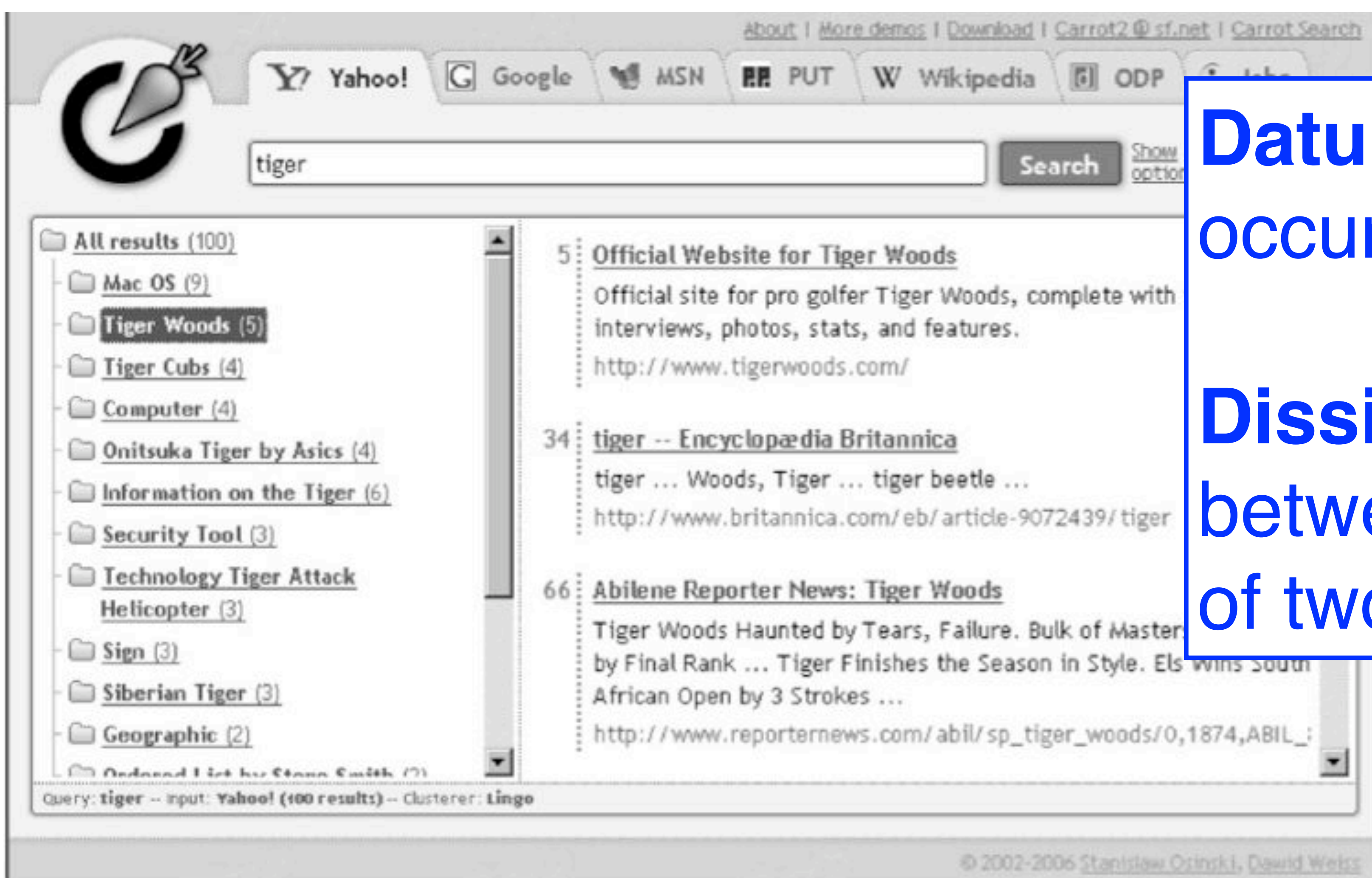

<u>Document clustering</u>

Datum: vector of topic occurrences

Dissimilarity: distance between topic distributions of two documents

slide by Tamara Broderick

[Carpineto et al. 2009]

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slide by Tamara Broderick

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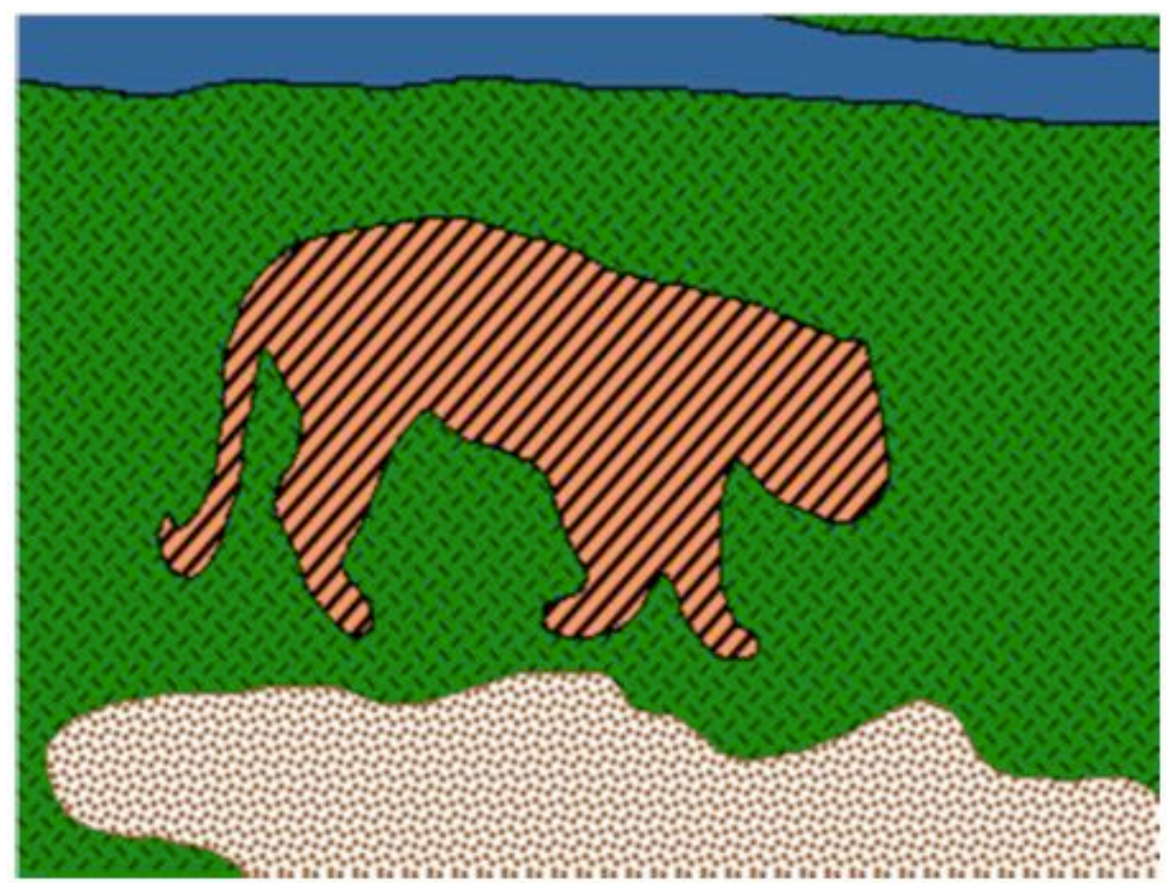
Image segmentation

[Fei-Fei 2011]

slide by Tamara Broderick

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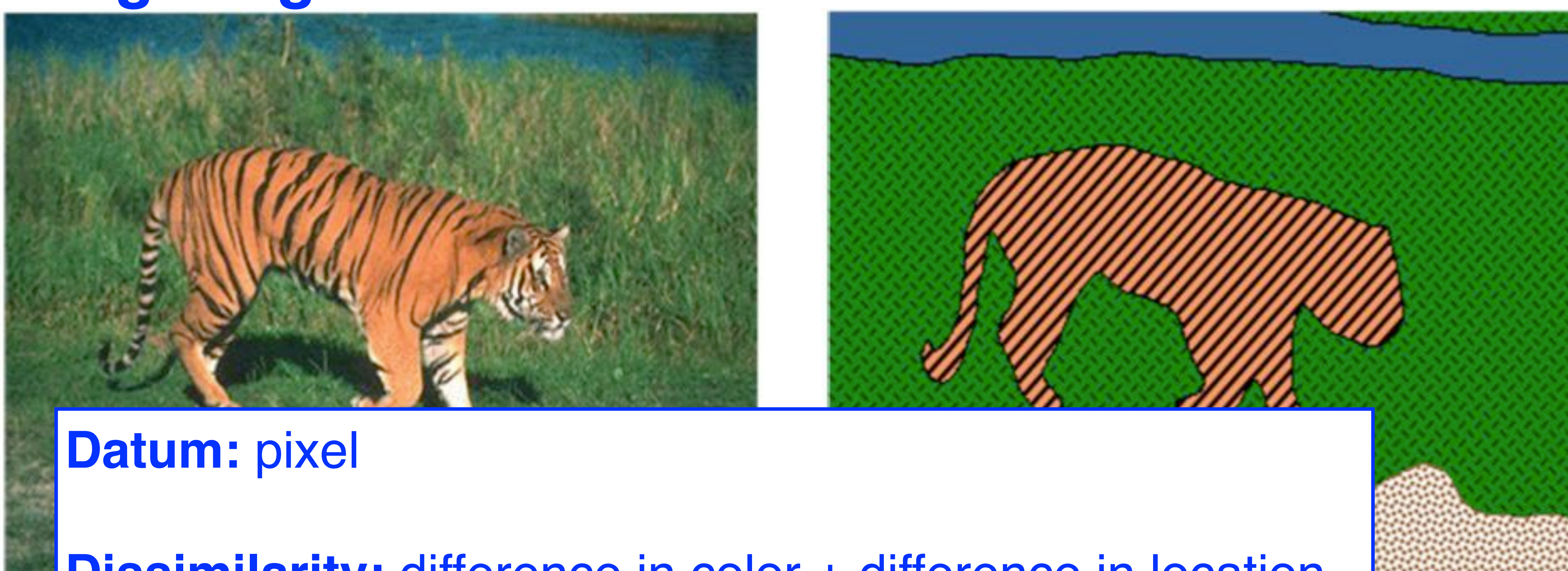

Datum: pixel

Dissimilarity: difference in color + difference in location

[Fei-Fei 2011]

slide by Tamara Broderick

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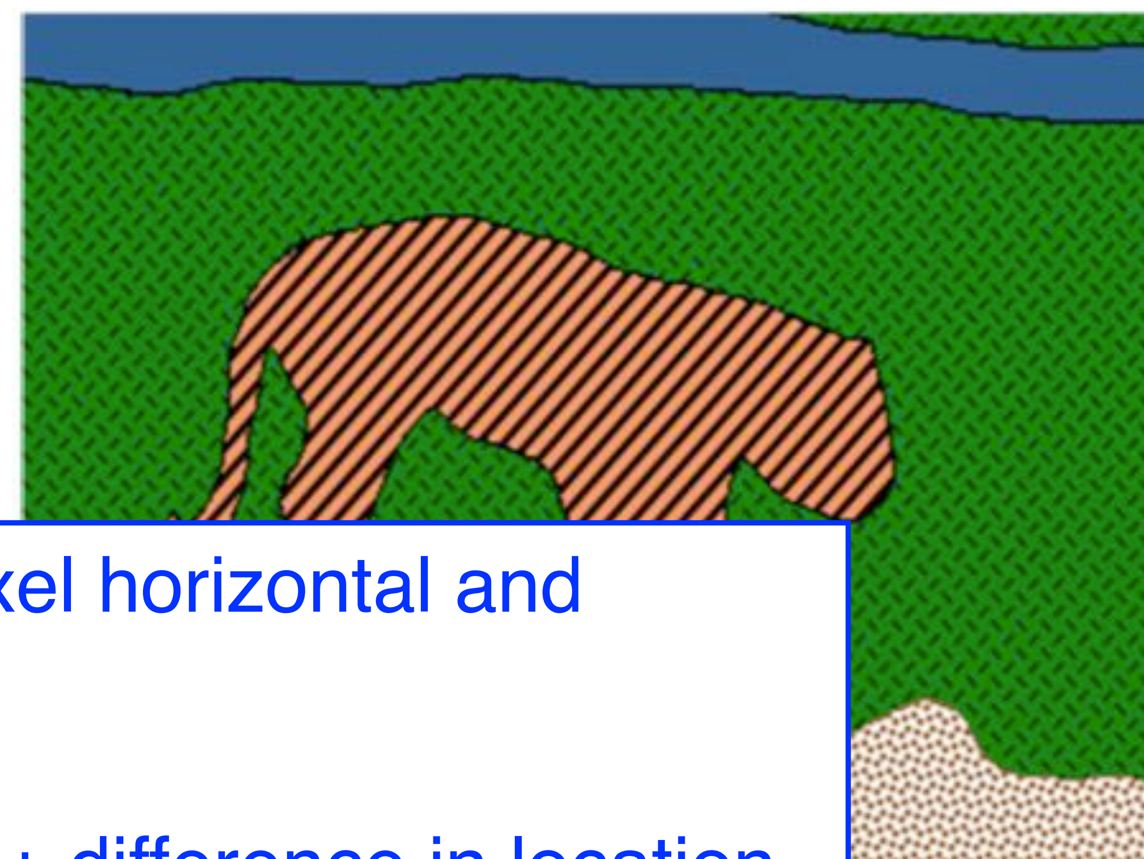

Datum: pixel RGB values and pixel horizontal and vertical locations

Dissimilarity: difference in color + difference in location

[Fei-Fei 2011]

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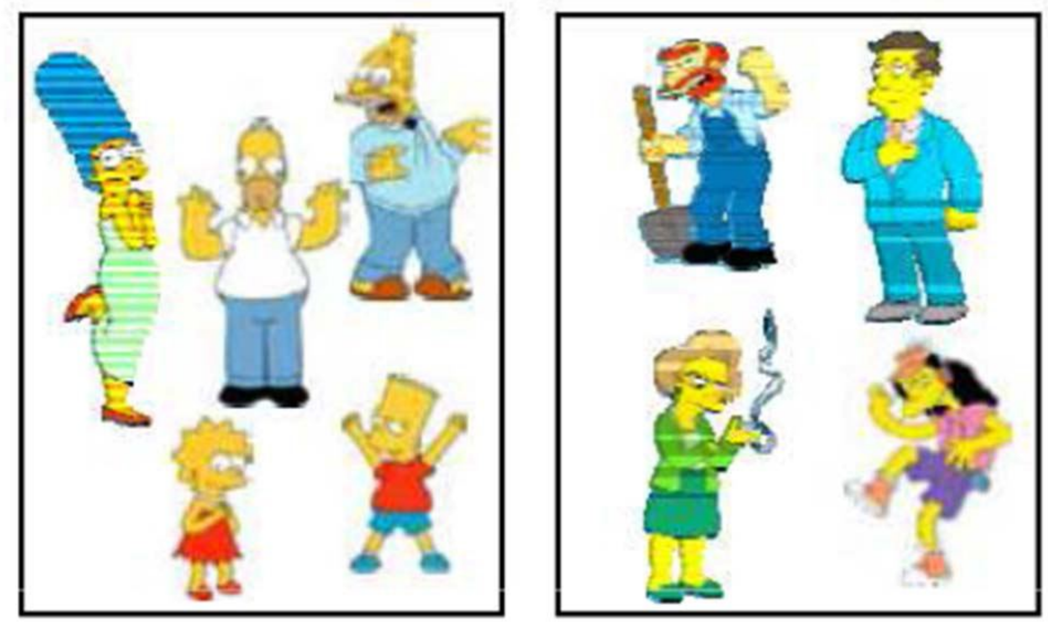
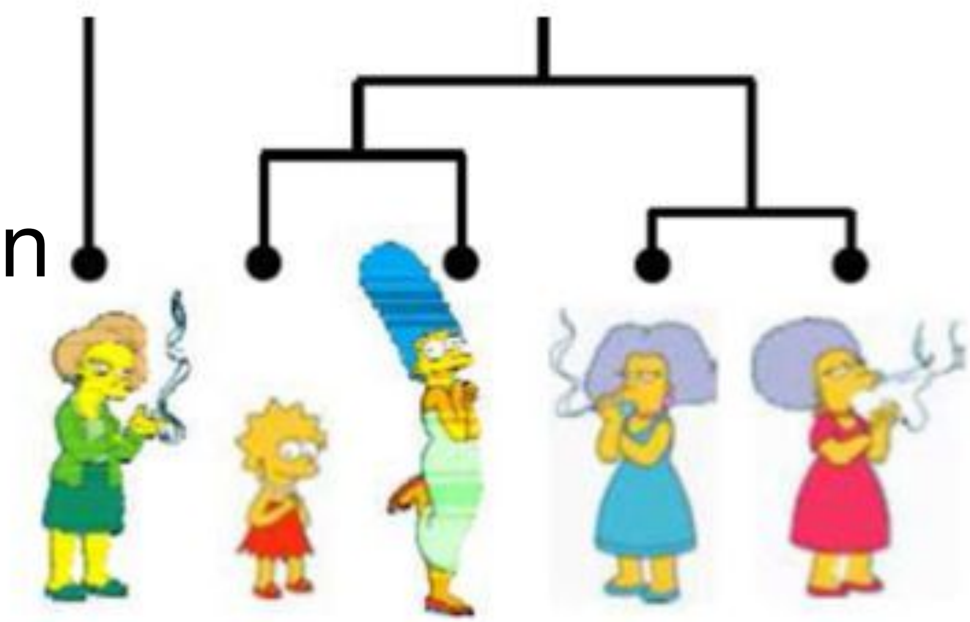
Clustering algorithms

- Partitioning algorithms
  - Construct various partitions and then evaluate them by some criterion
    - K-means
    - Mixture of Gaussians
    - Spectral Clustering



- Hierarchical algorithms
  - Create a hierarchical decomposition of the set of objects using some criterion
  - Bottom-up – agglomerative
  - Top-down – divisive



slide by Eric Xing

Desirable Properties of a Clustering Algorithm

- Scalability (in terms of both time and space)
- Ability to deal with different data types
- Minimal requirements for domain knowledge to determine input parameters
- Ability to deal with noisy data
- Interpretability and usability

- Optional
  - Incorporation of user-specified constraints

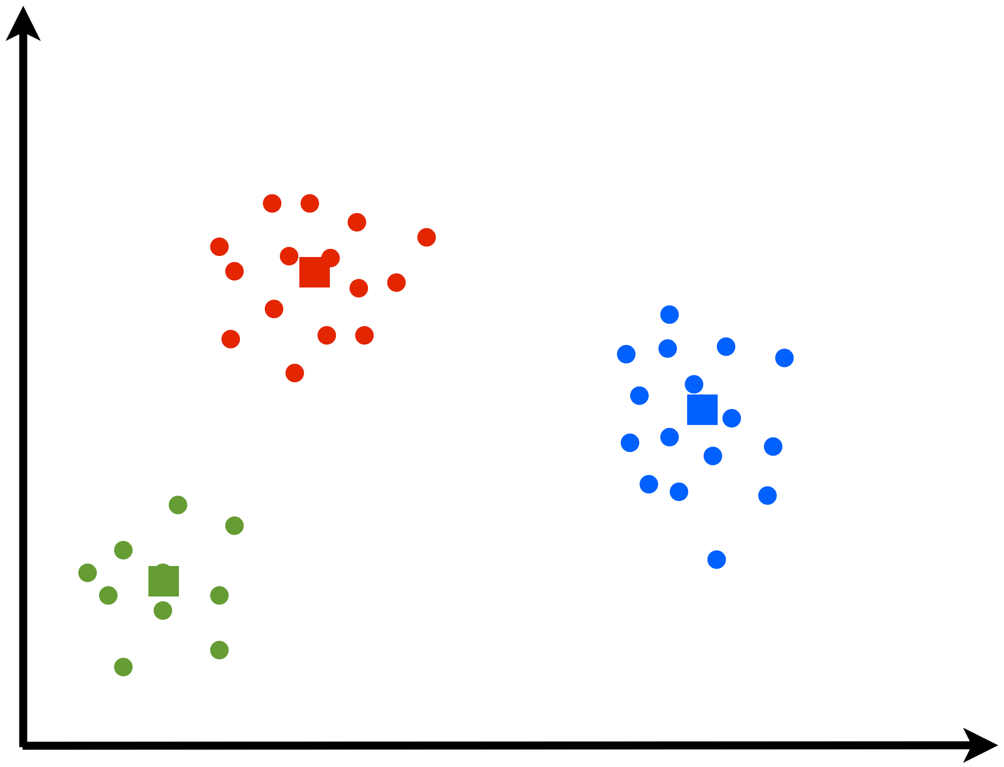
slide by Andrew Moore

K-Means Clustering

K-Means Clustering

Benefits

- Fast
- Conceptually straightforward
- Popular



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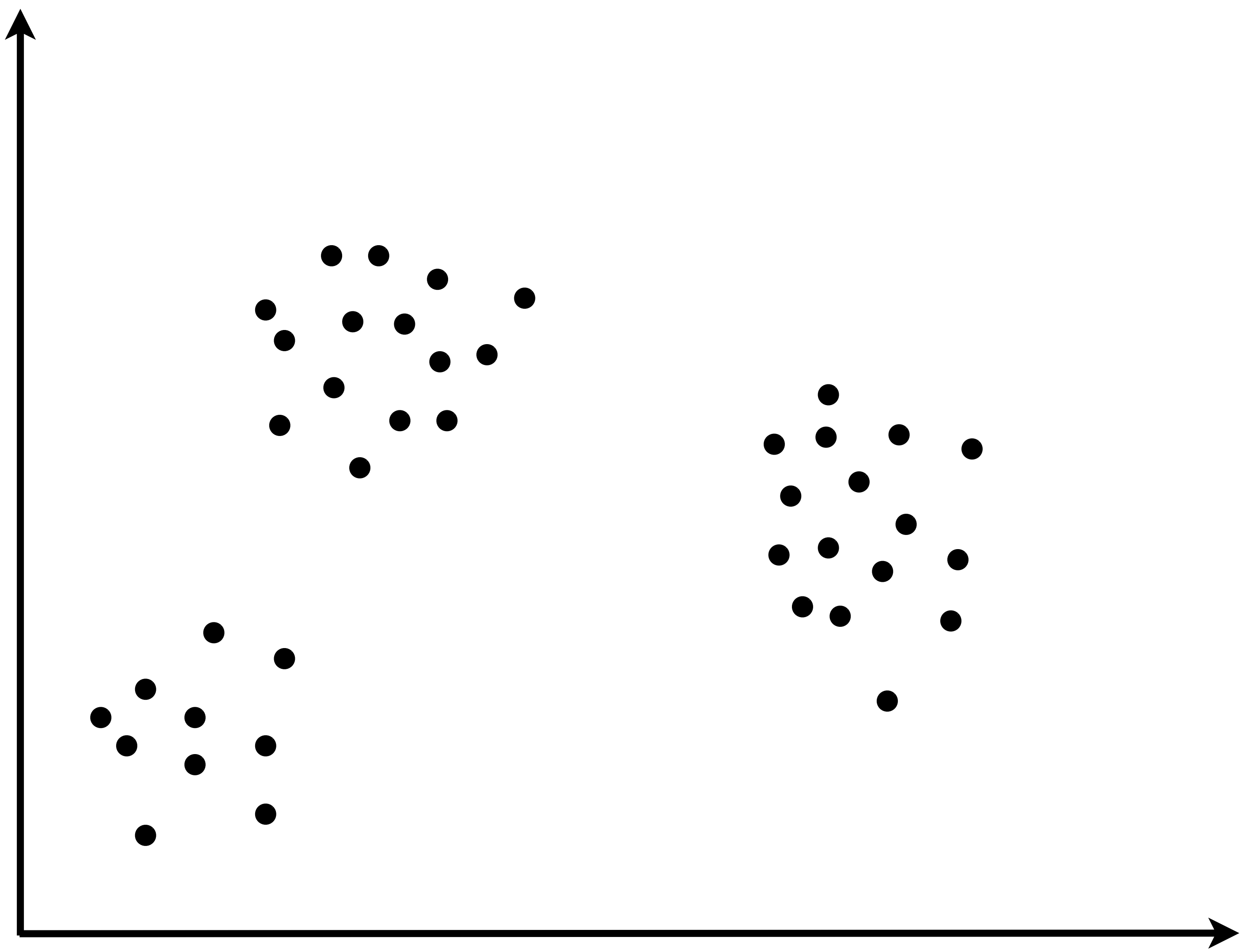
K-Means: Preliminaries



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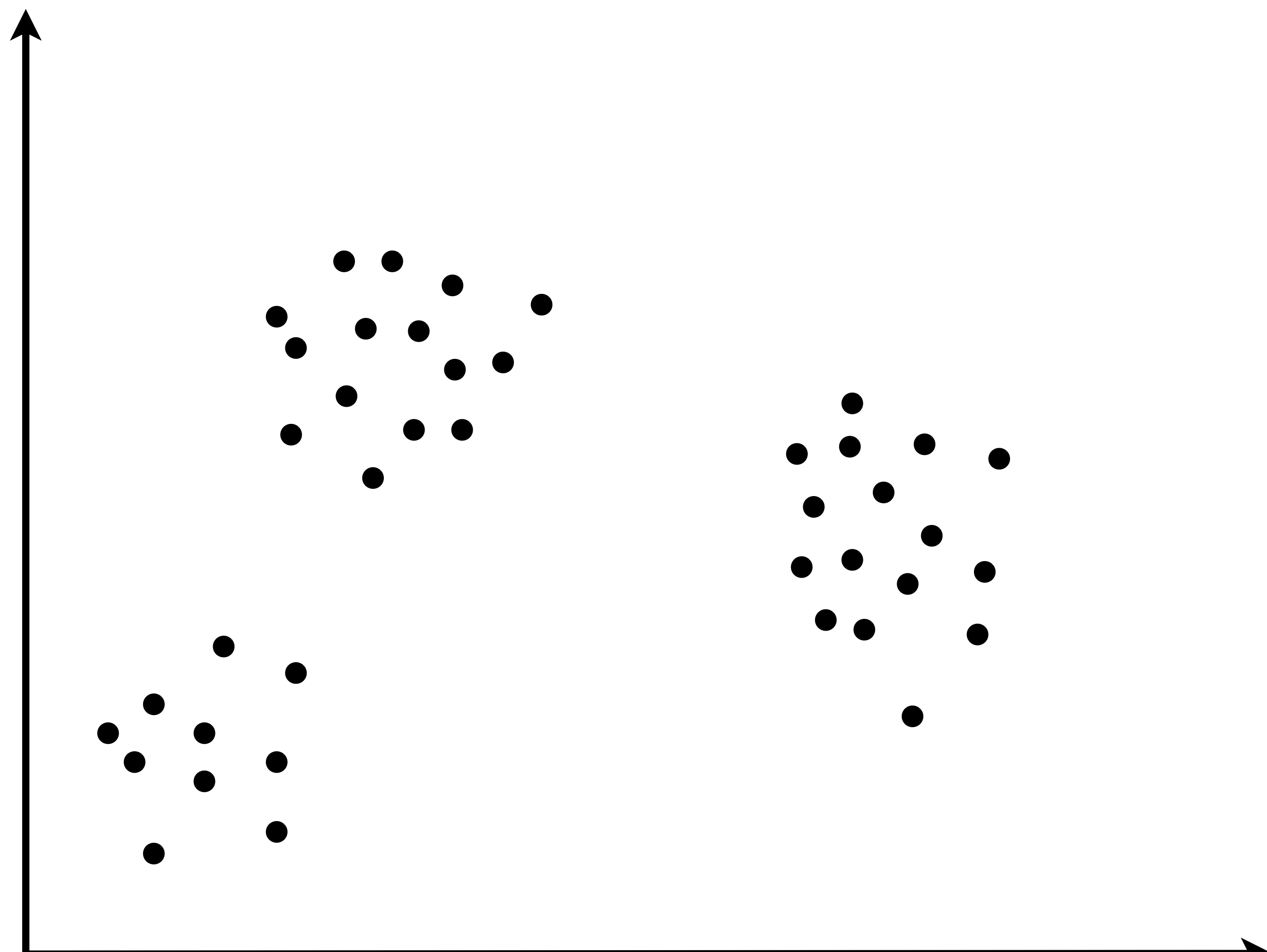
K-Means: Preliminaries

Datum: Vector of continuous values



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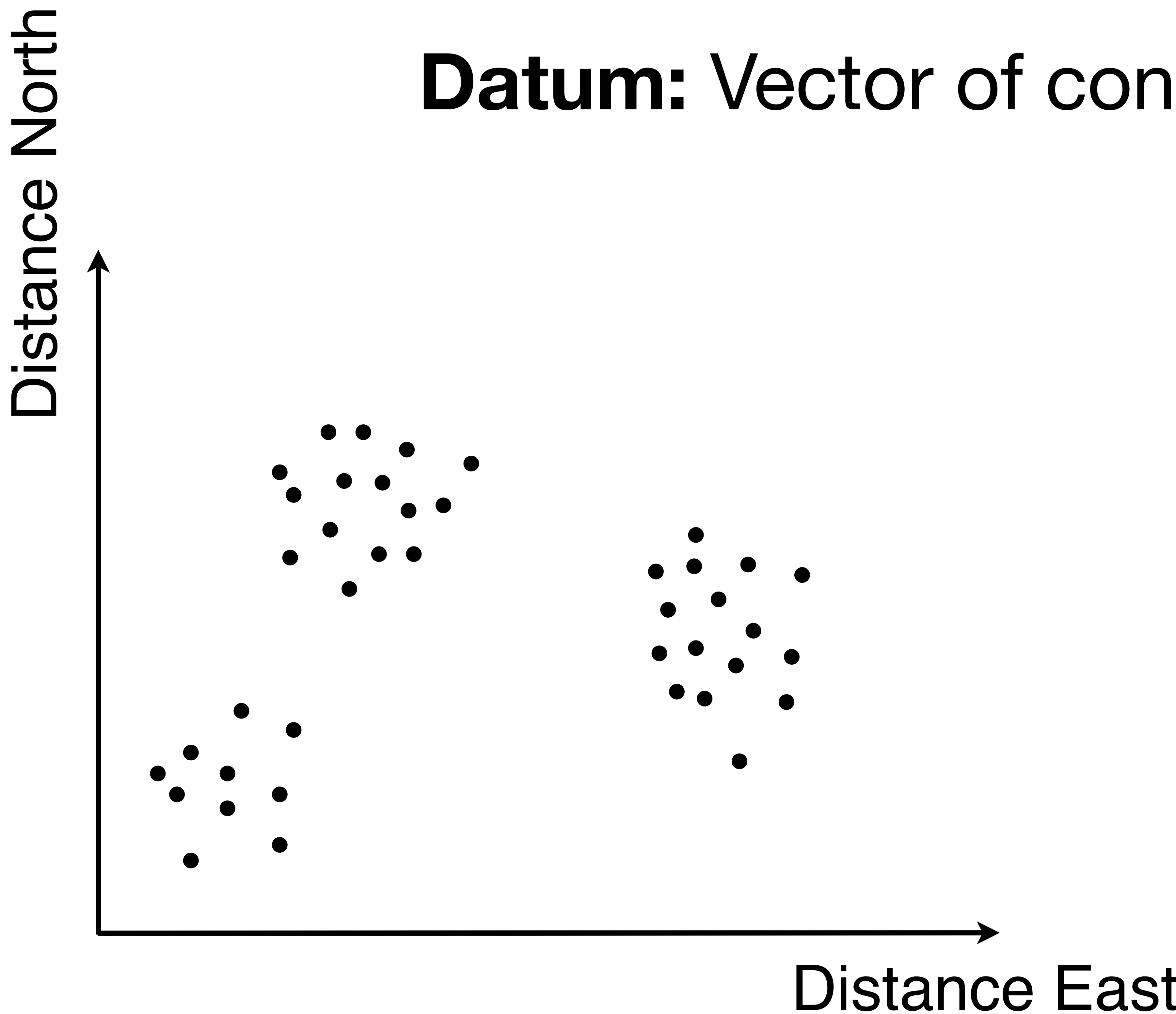

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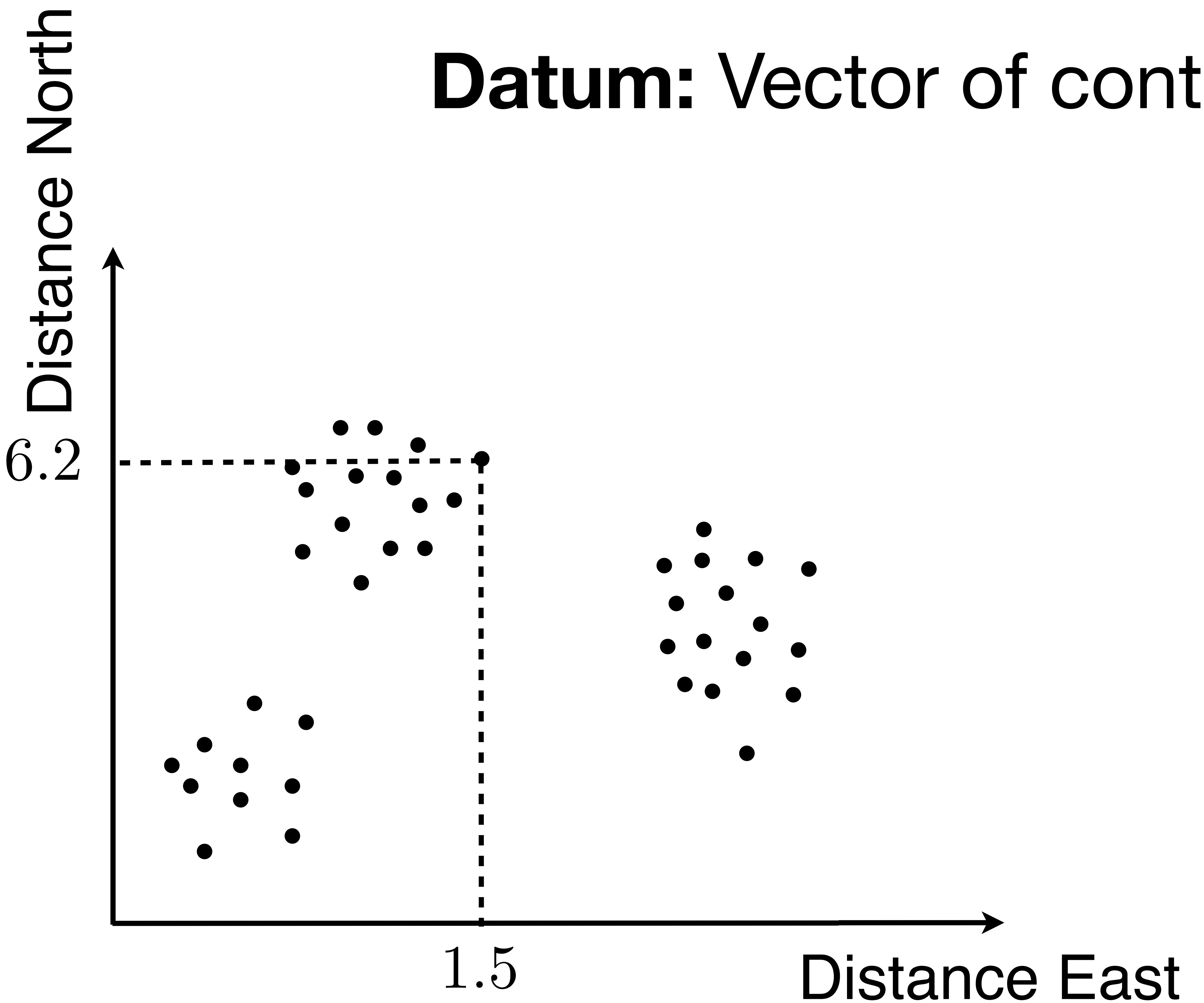

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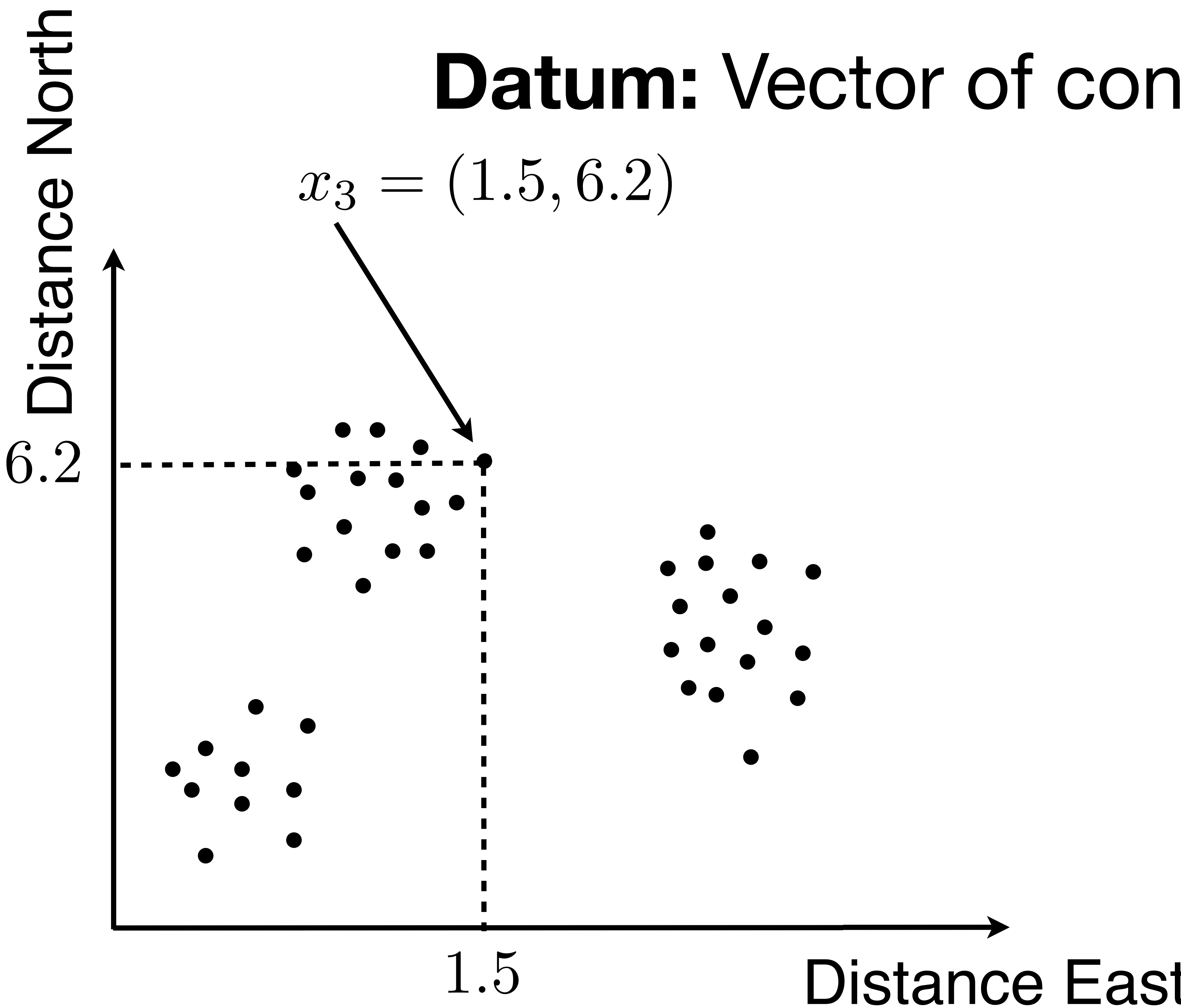
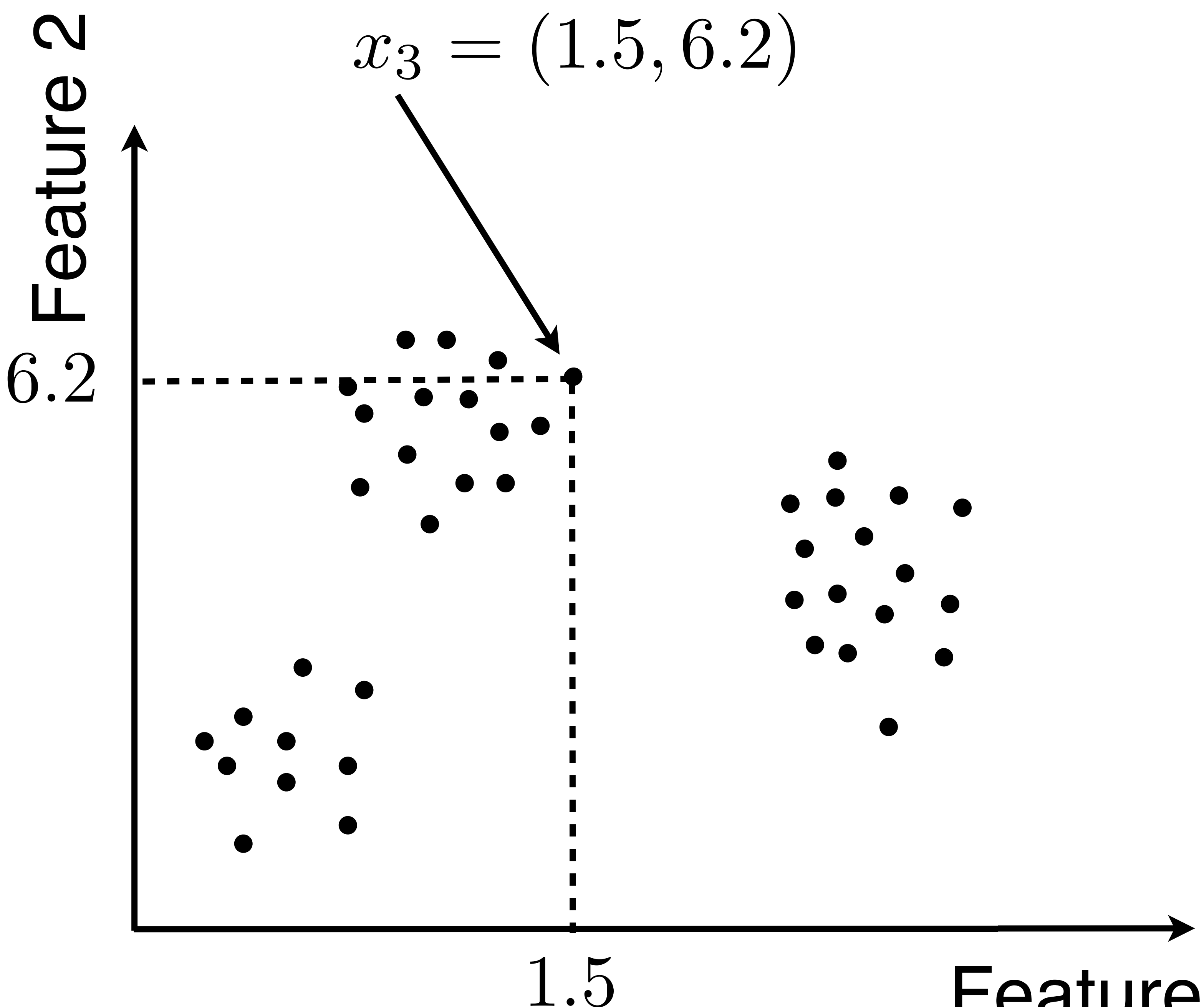


	North	East
x_1	1.2	5.9
x_2	4.3	2.1
x_3	1.5	6.3
$\vdots$		
x_N	4.1	2.3

slide by Tamara Broderick

K-Means: Preliminaries

Datum: Vector of continuous values

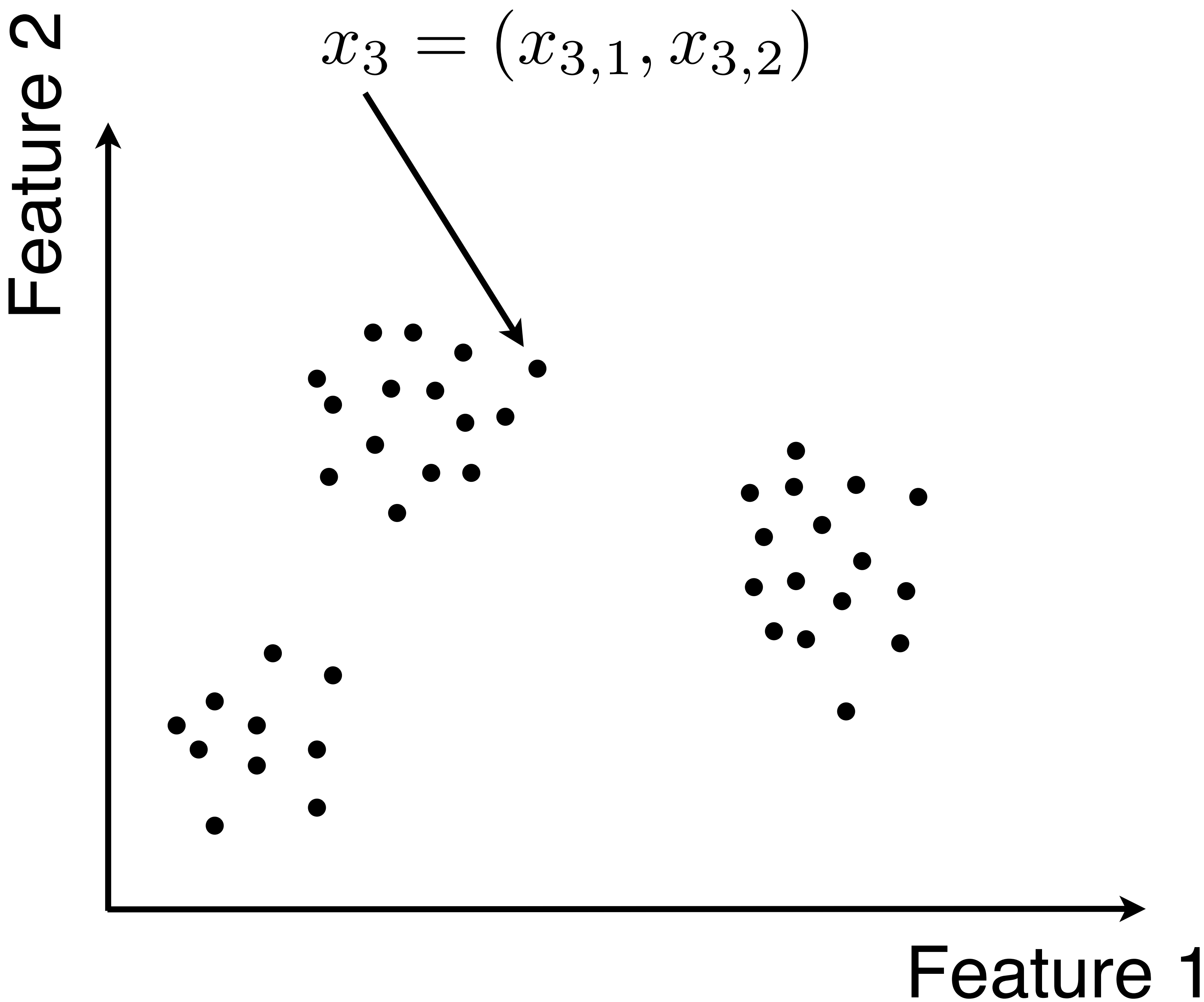


	Feature 1	Feature 2
x_1	1.2	5.9
x_2	4.3	2.1
x_3	1.5	6.3
$\vdots$		
x_N	4.1	2.3

slide by Tamara Broderick

K-Means: Preliminaries

Datum: Vector of continuous values

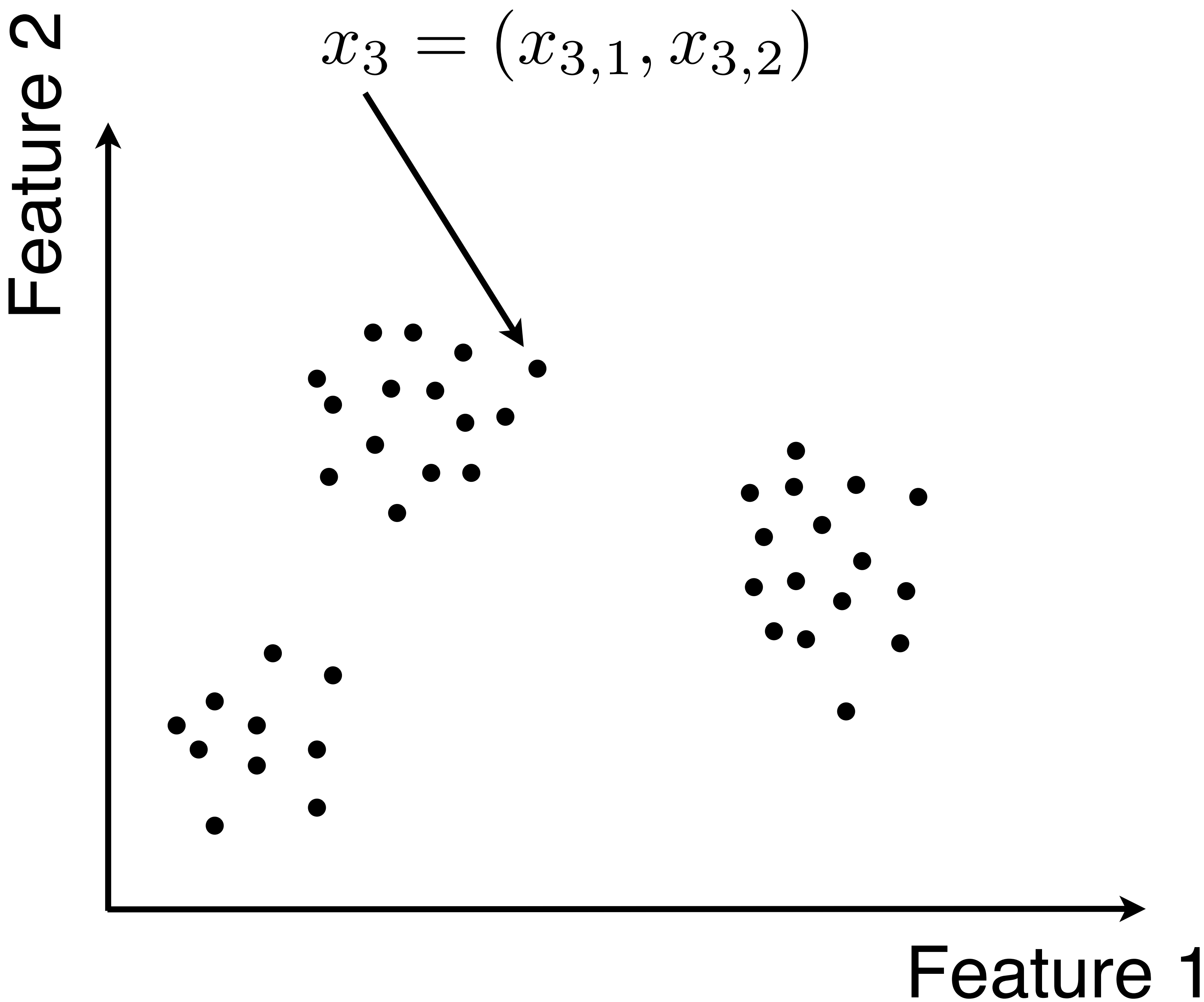


	Feature 1	Feature 2
x_1	$x_{1,1}$	$x_{1,2}$
x_2	$x_{2,1}$	$x_{2,2}$
x_3	$x_{3,1}$	$x_{3,2}$
$\vdots$		
x_N	$x_{N,1}$	$x_{N,2}$

slide by Tamara Broderick

K-Means: Preliminaries

Datum: Vector of D continuous values



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slide by Tamara Broderick

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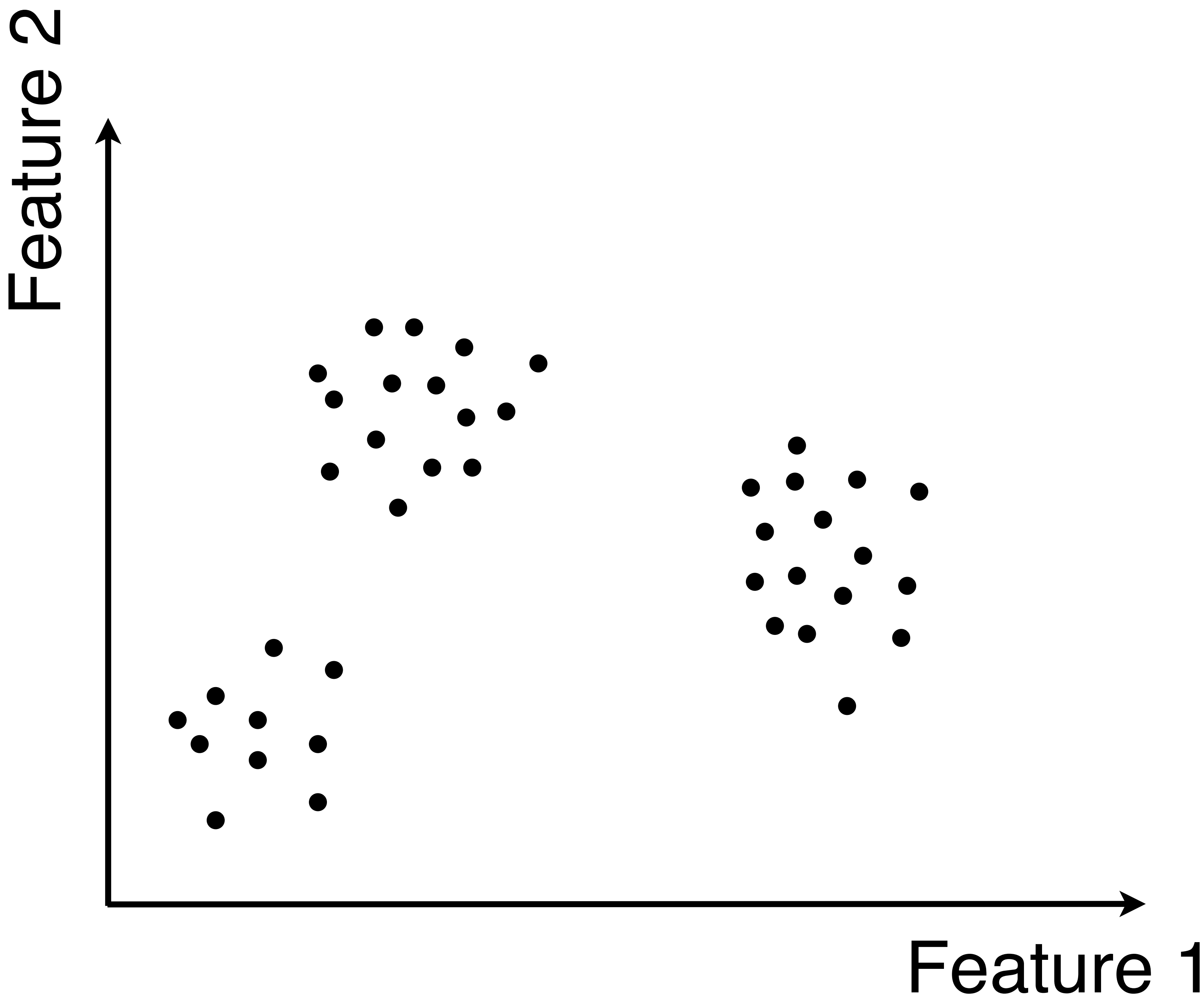

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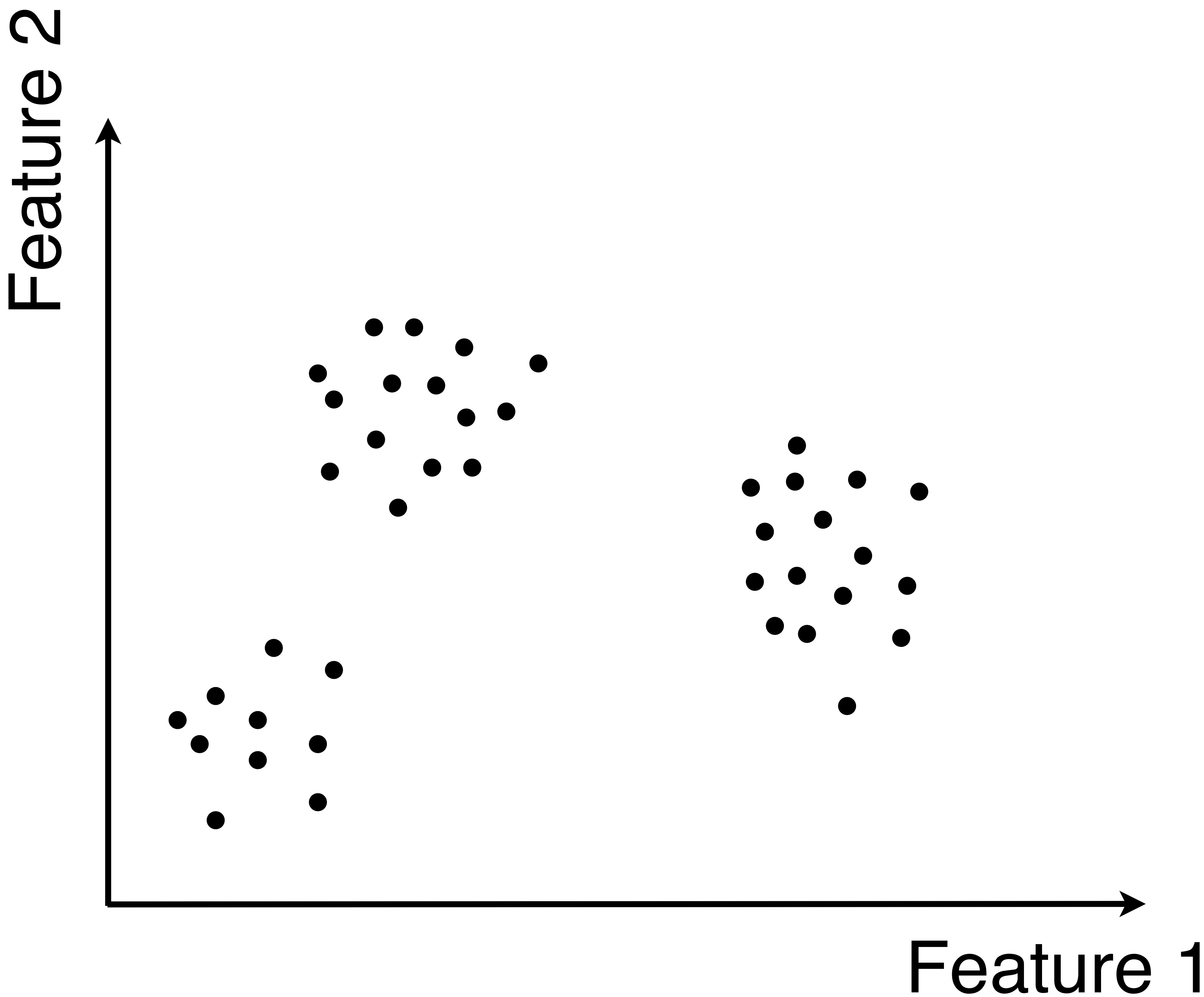
K-Means: Preliminaries

Dissimilarity: Distance as the crow flies



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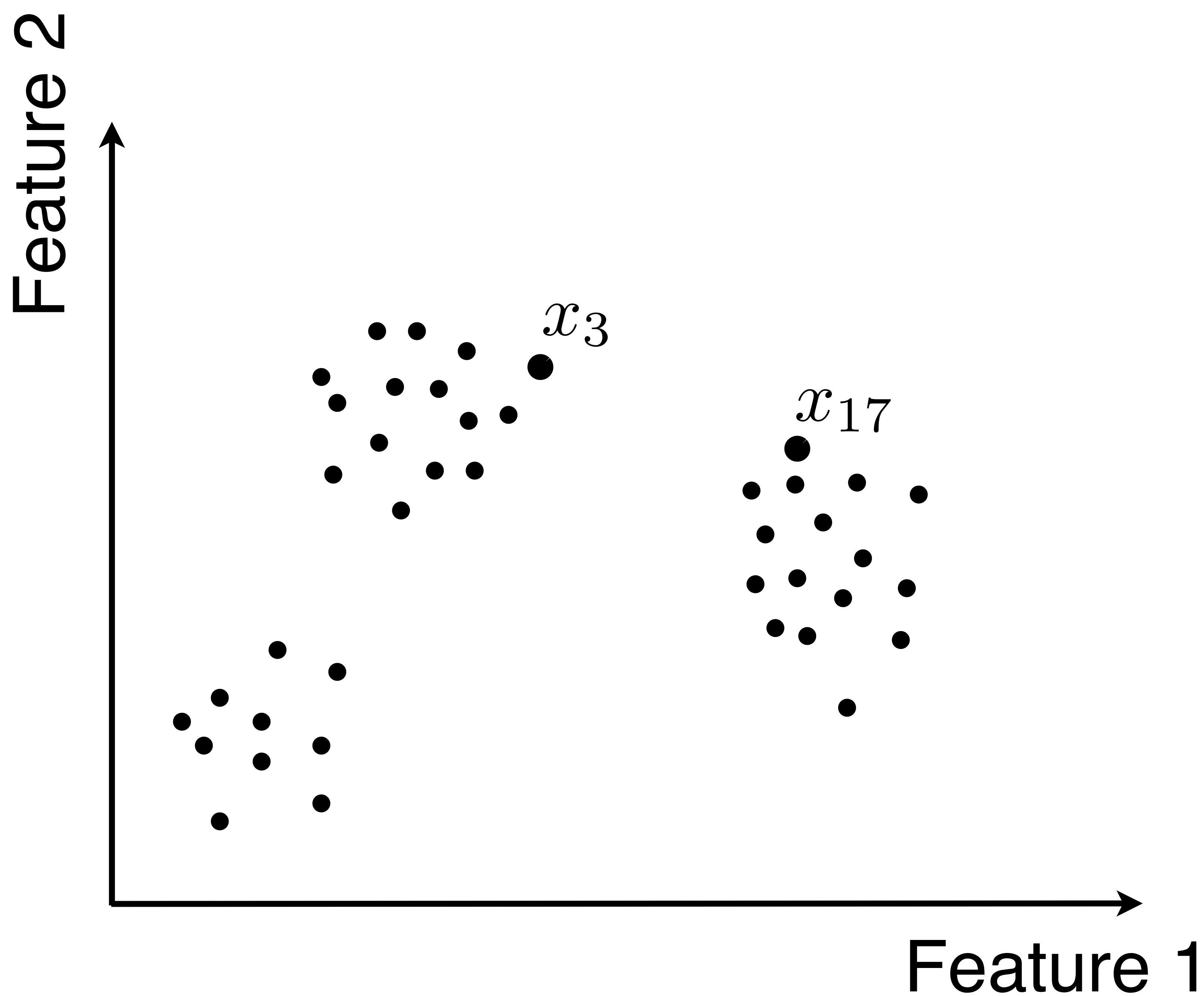

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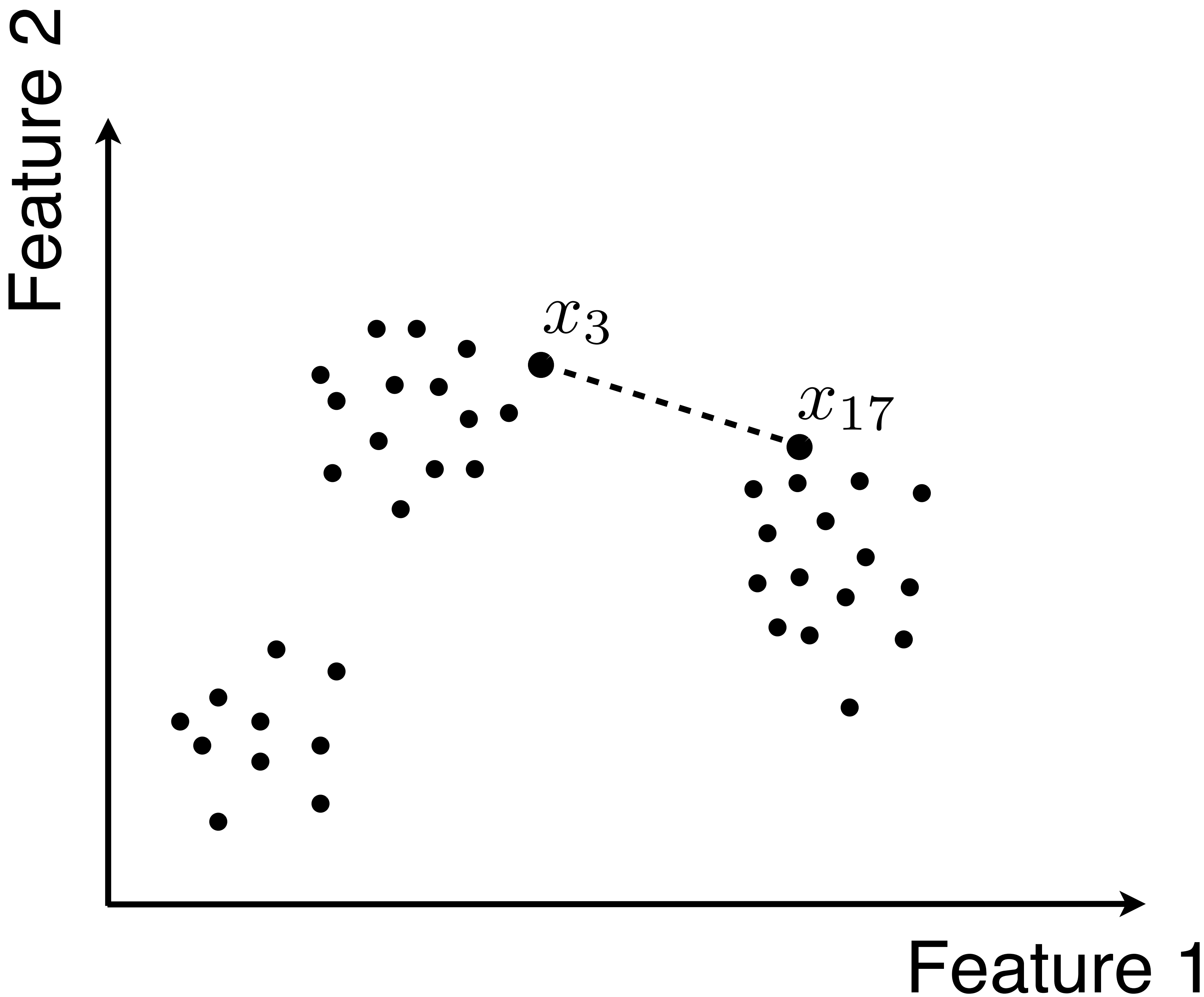
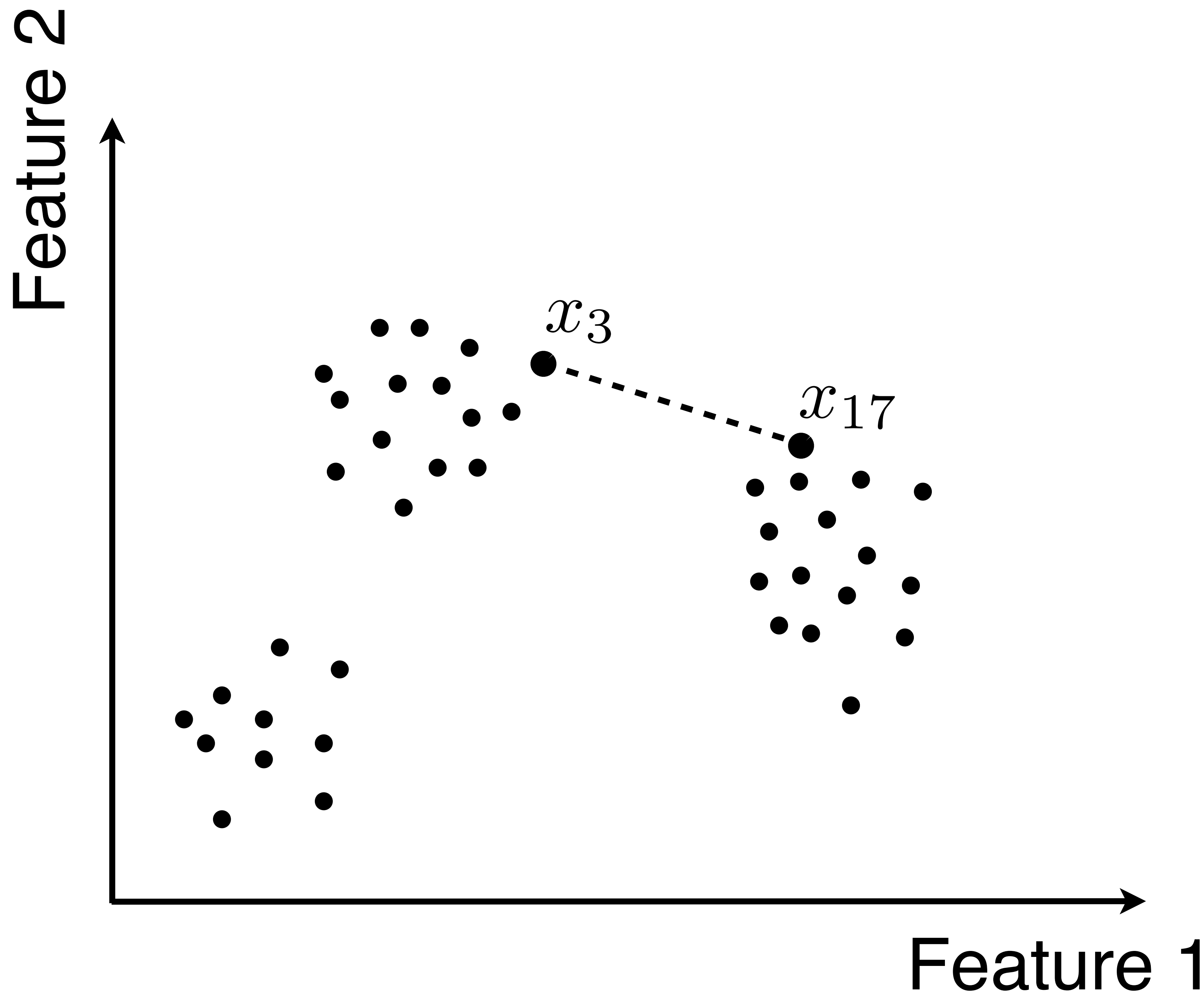


slide by Tamara Broderick

K-Means: Preliminaries

Dissimilarity: Euclidean distance



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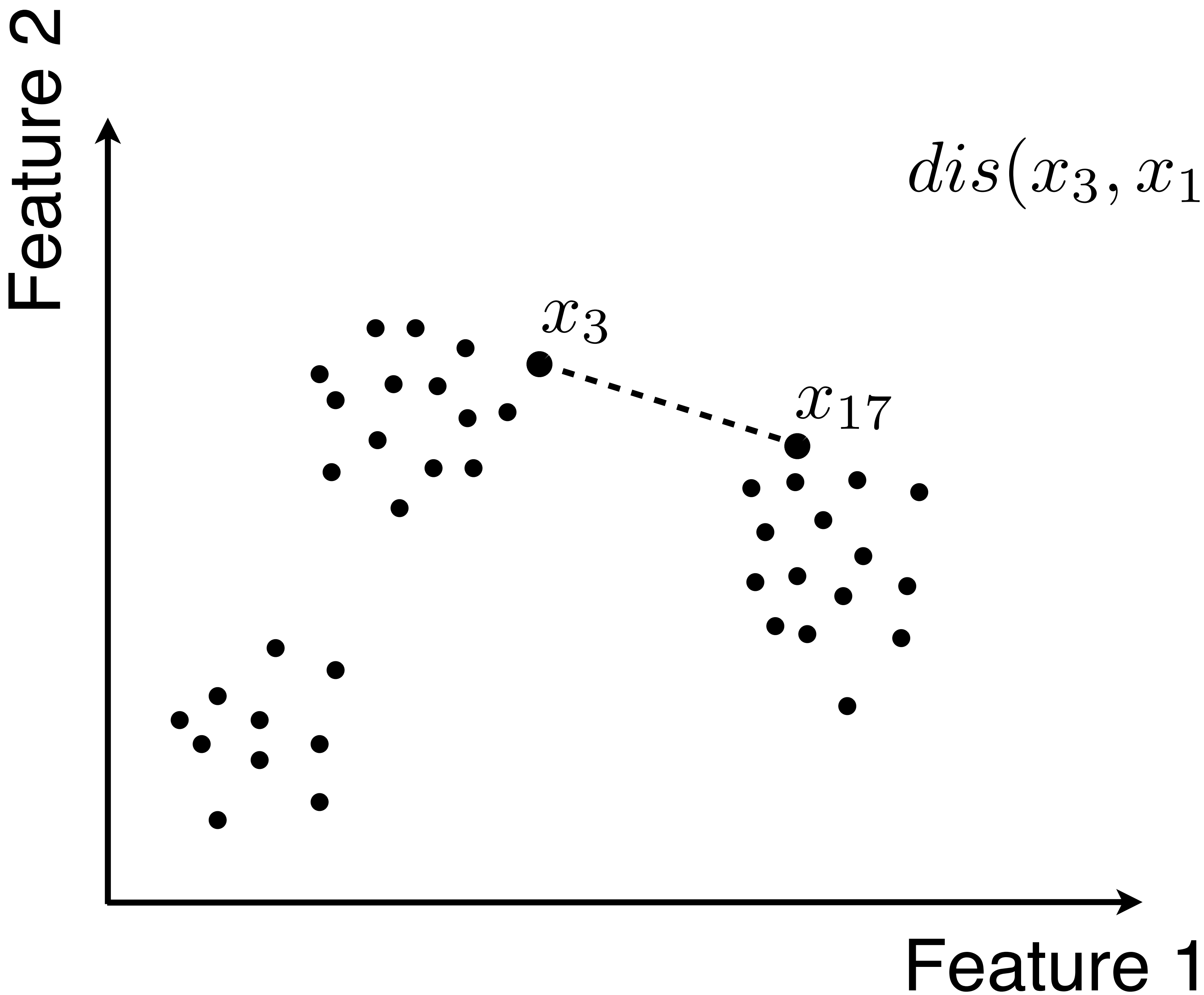
K-Means: Preliminaries

Dissimilarity: Squared Euclidean distance



$$dis(x_3, x_{17}) = (x_{3,1} - x_{17,1})^2 + (x_{3,2} - x_{17,2})^2$$

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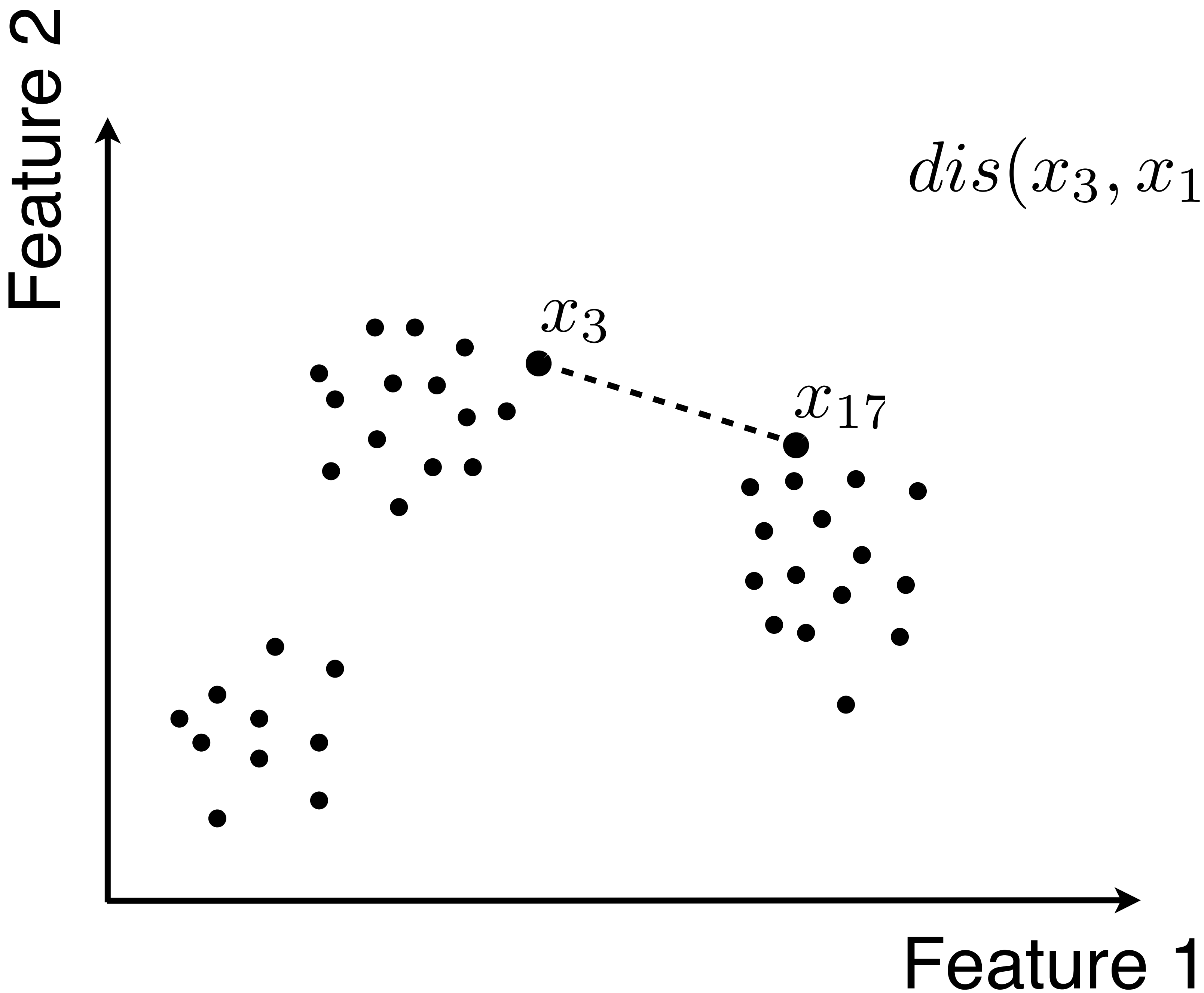
K-Means: Preliminaries

Dissimilarity: Squared Euclidean distance



$$dis(x_3, x_{17}) = \sum_{d=1}^{D} (x_{3,d} - x_{17,d})^2$$

For each feature

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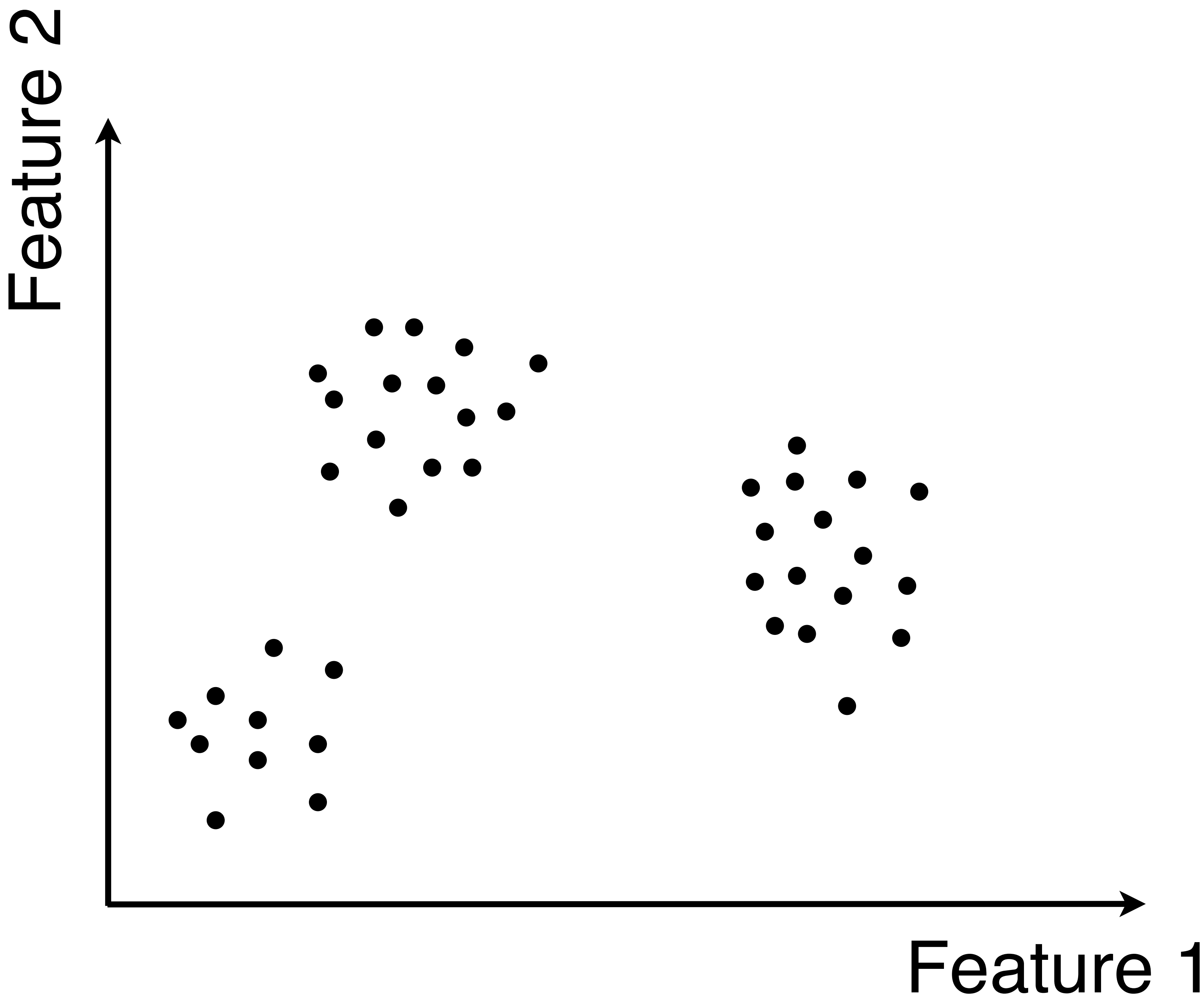
K-Means: Preliminaries

Dissimilarity



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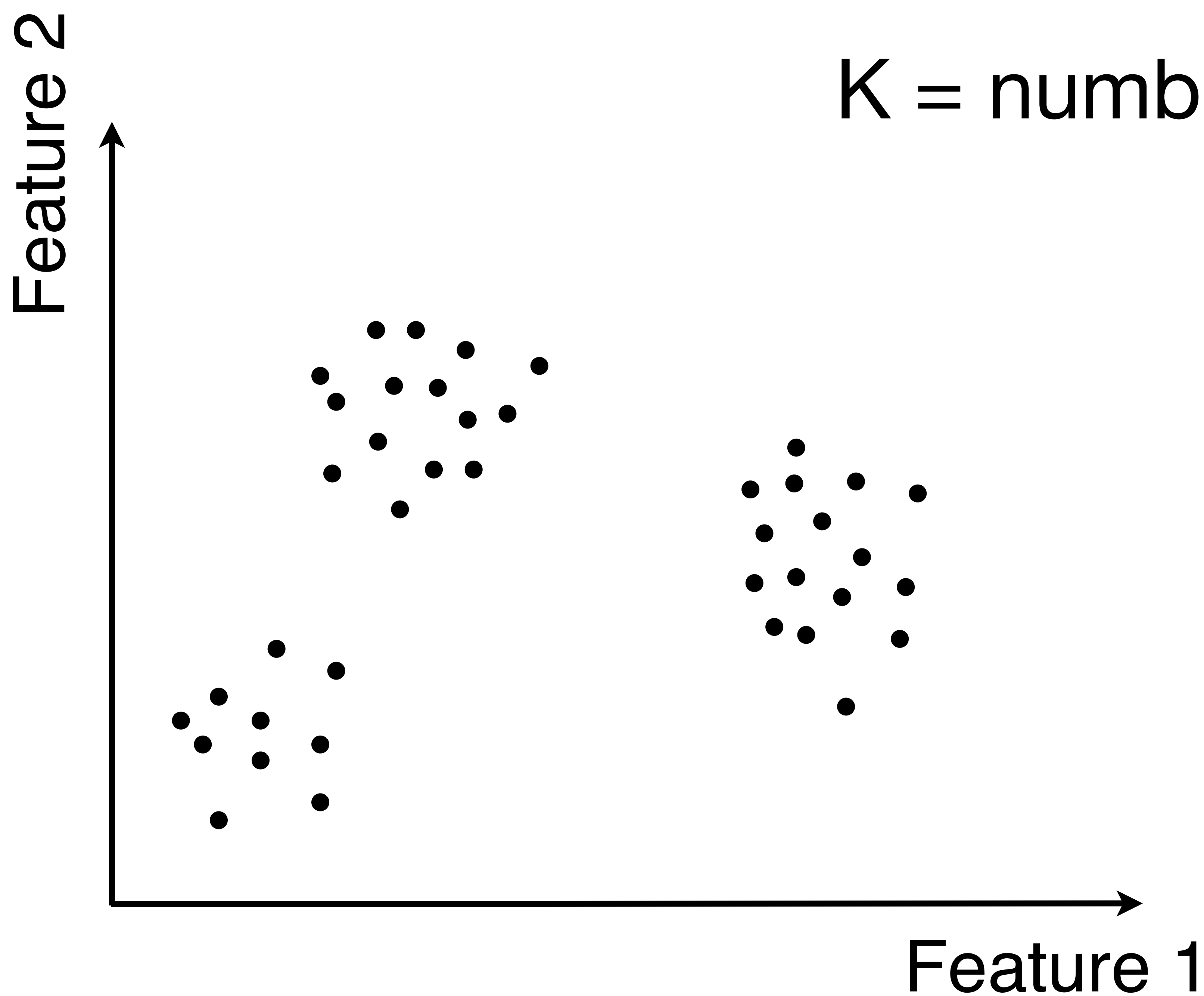
K-Means: Preliminaries

Cluster summary

K = number of clusters



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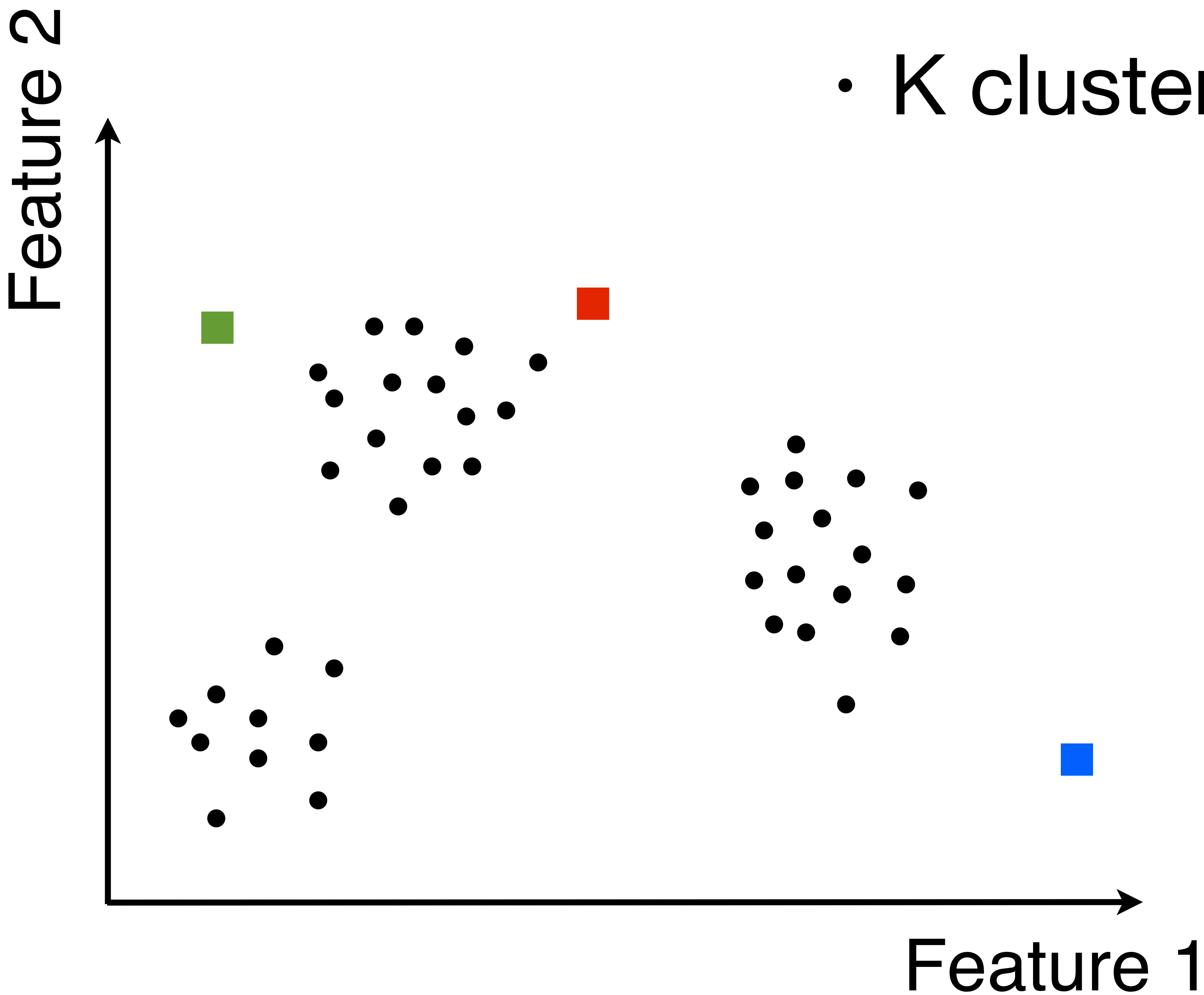
K-Means: Preliminaries

Cluster summary

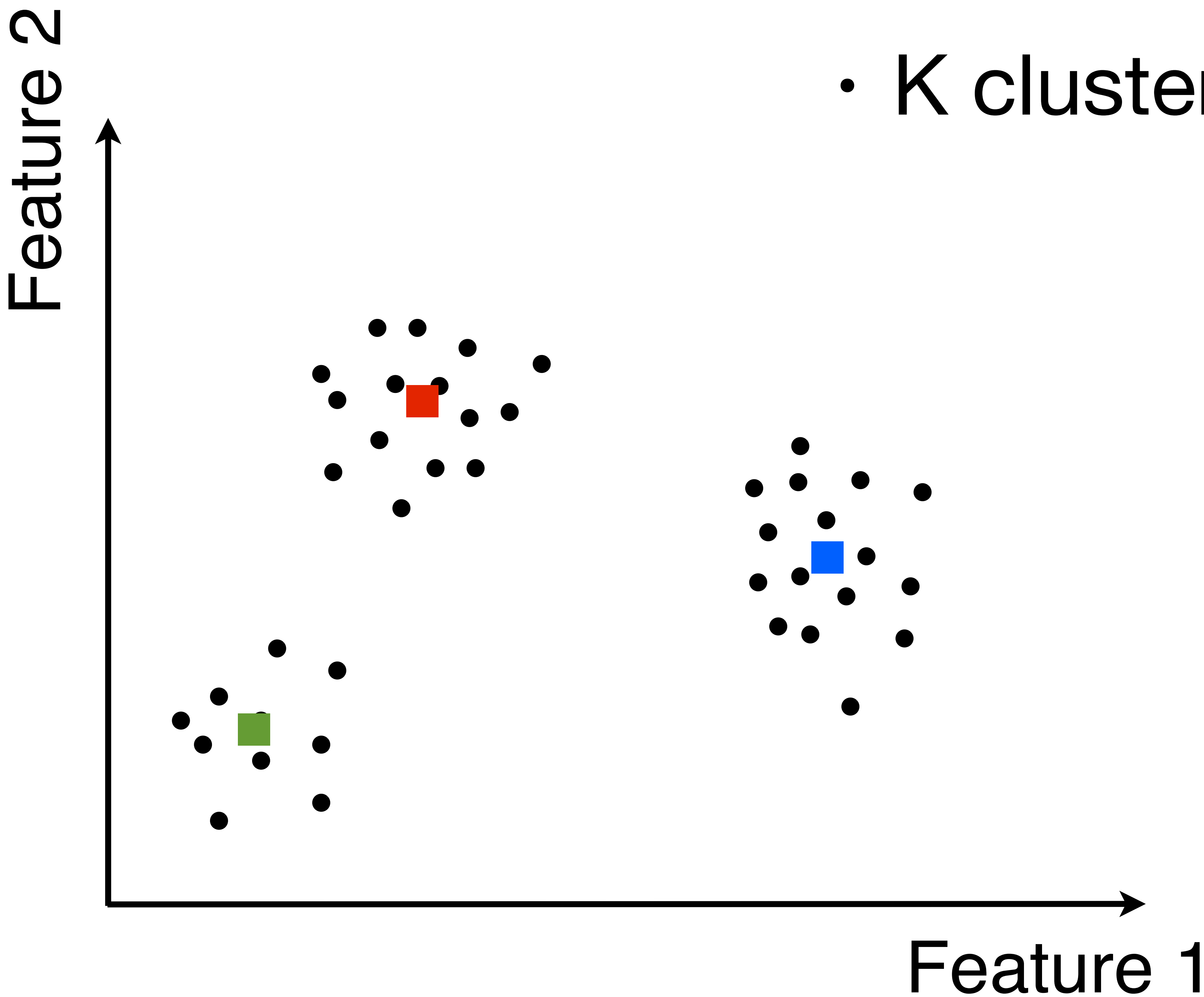
- K cluster centers



K-Means: Preliminaries

Cluster summary

- K cluster centers



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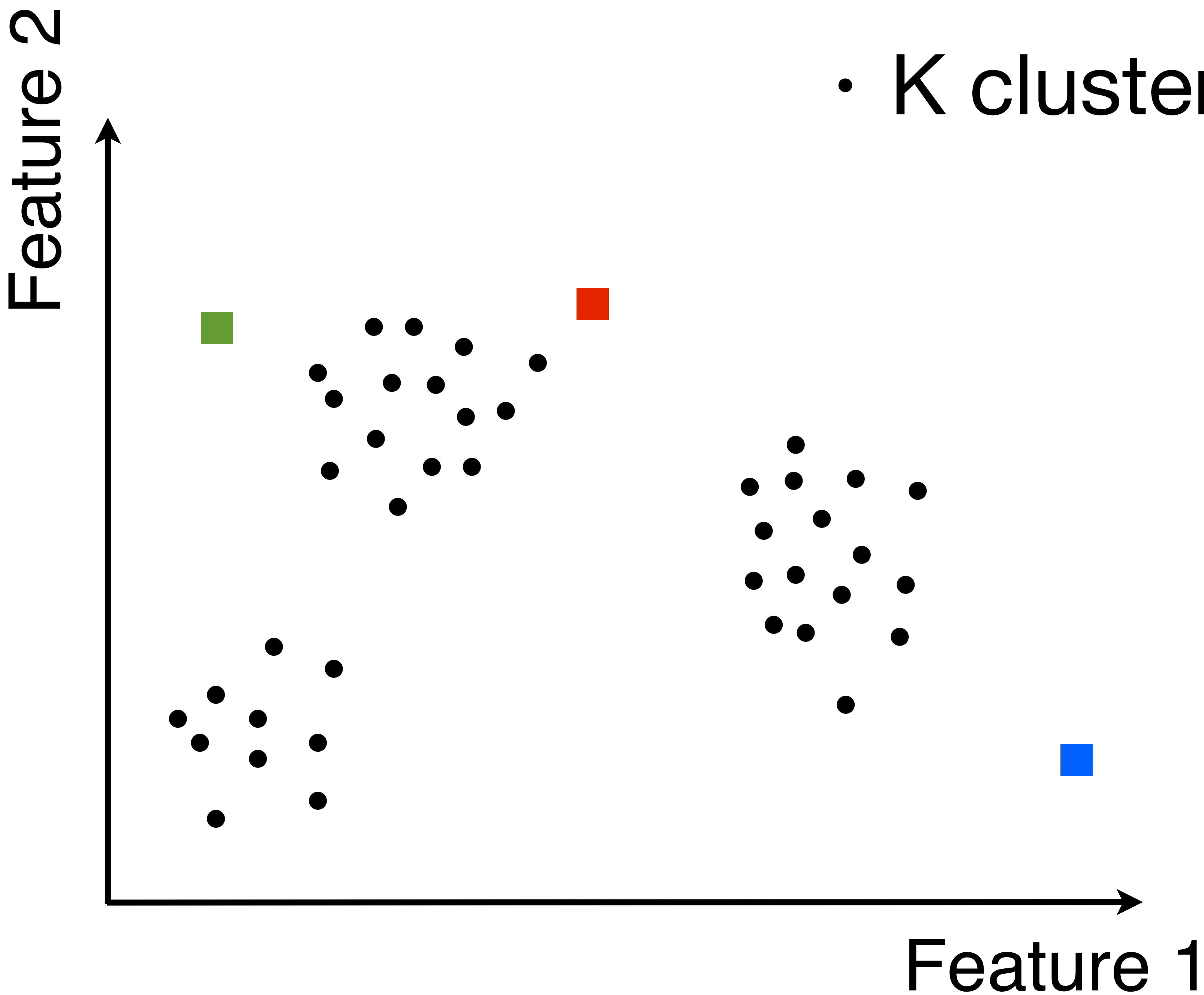
K-Means: Preliminaries

Cluster summary

- K cluster centers



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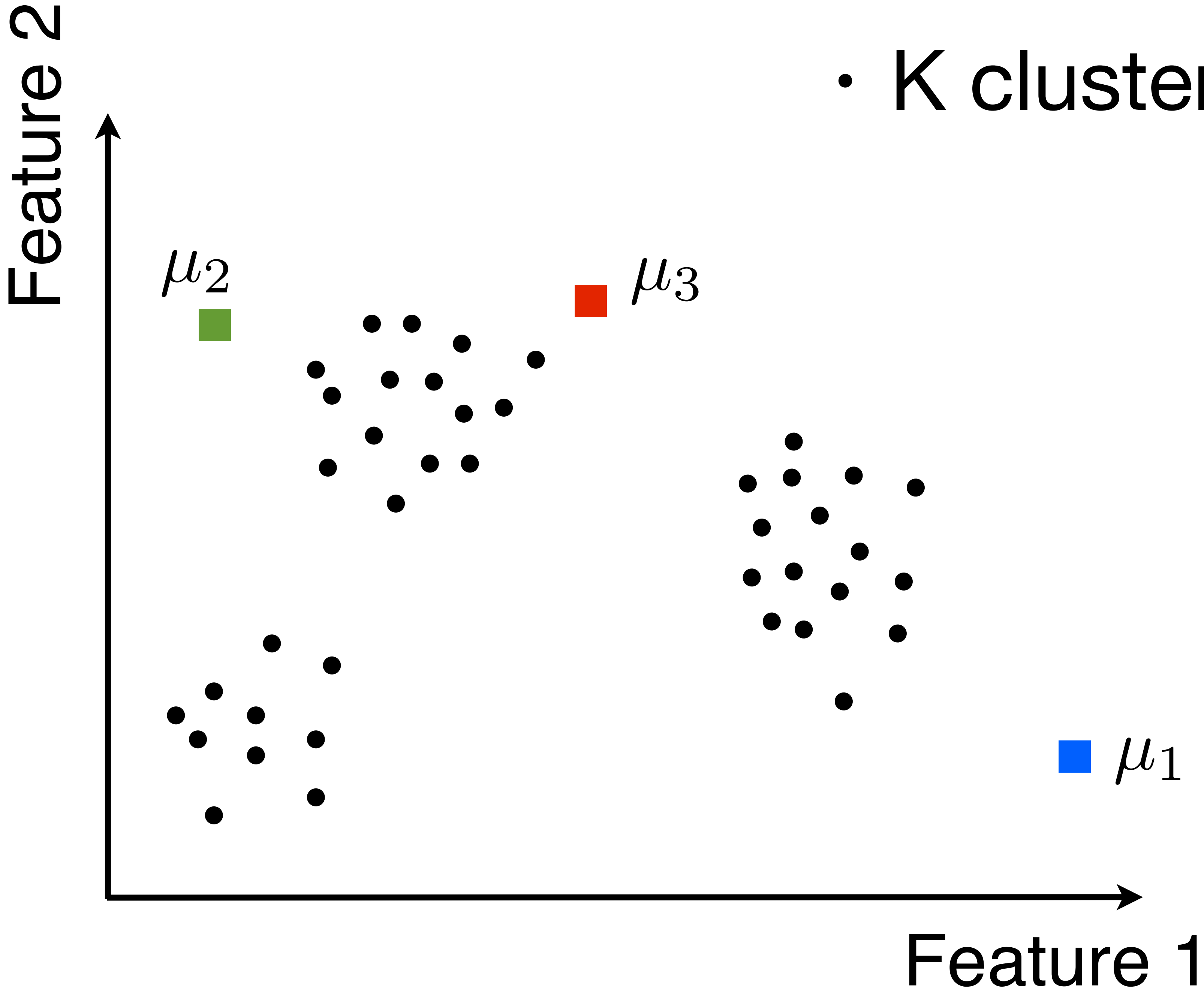
K-Means: Preliminaries

Cluster summary

- K cluster centers



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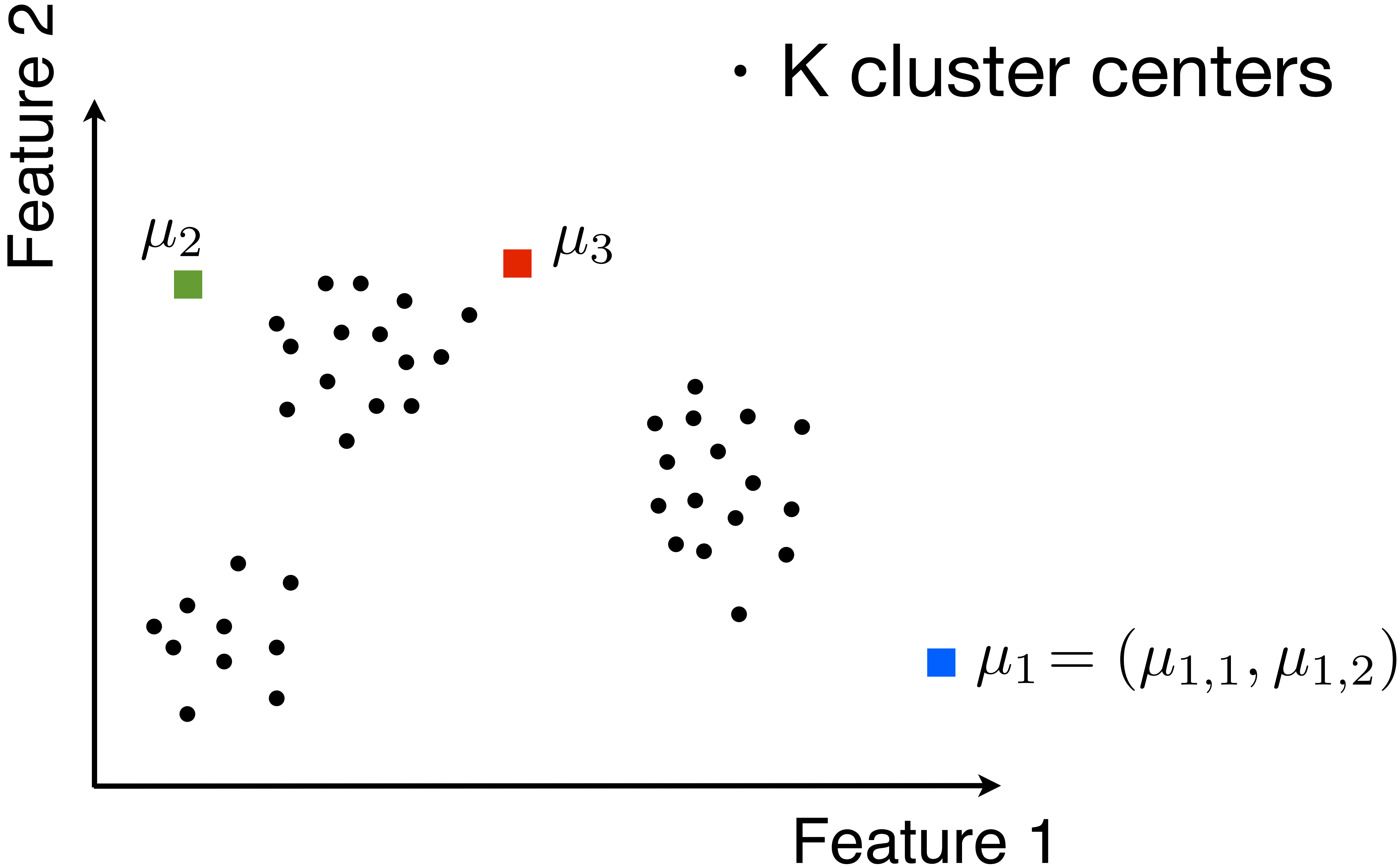
K-Means: Preliminaries

Cluster summary

- K cluster centers



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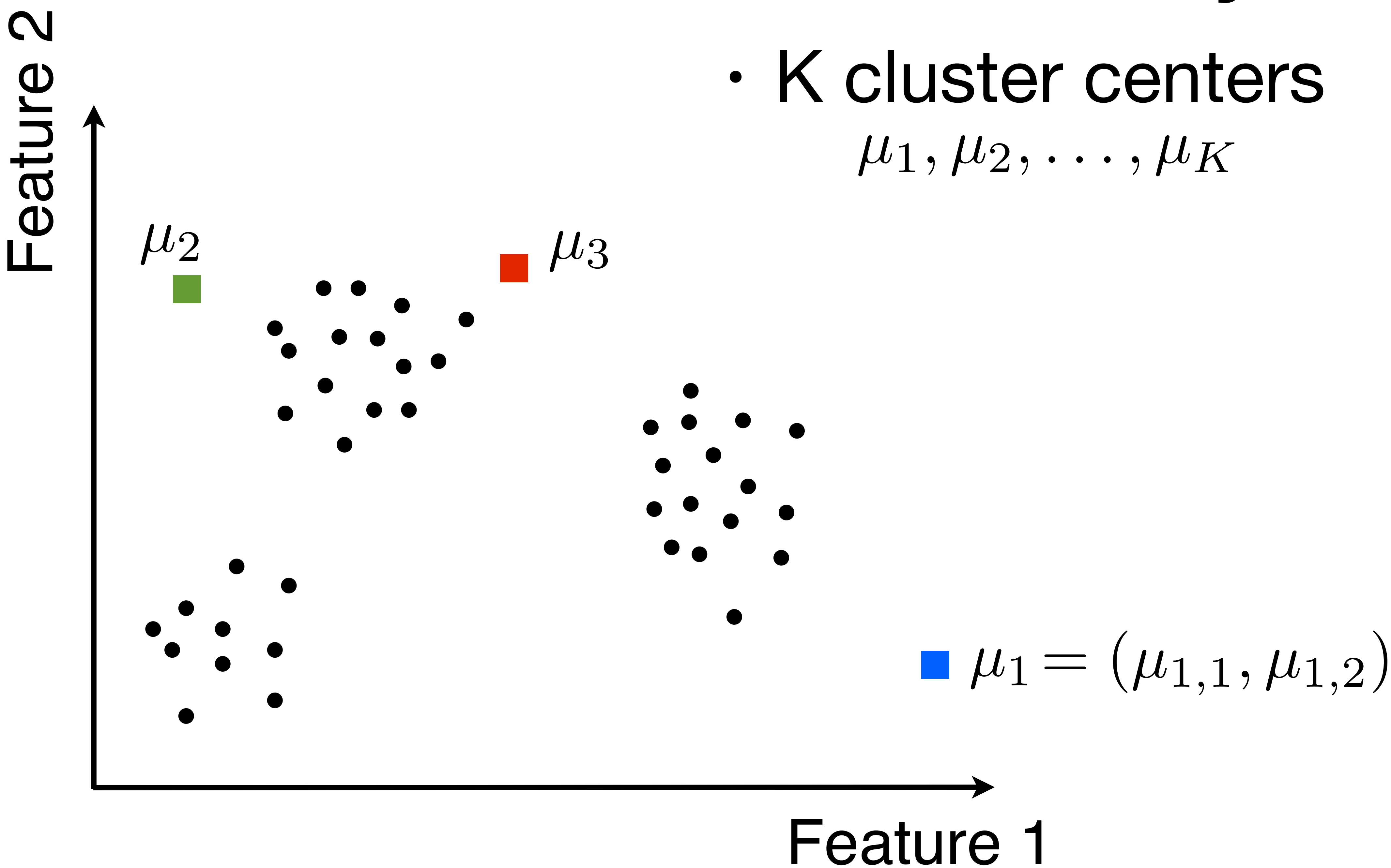
K-Means: Preliminaries

Cluster summary

- K cluster centers

$\mu_1, \mu_2, \ldots, \mu_K$



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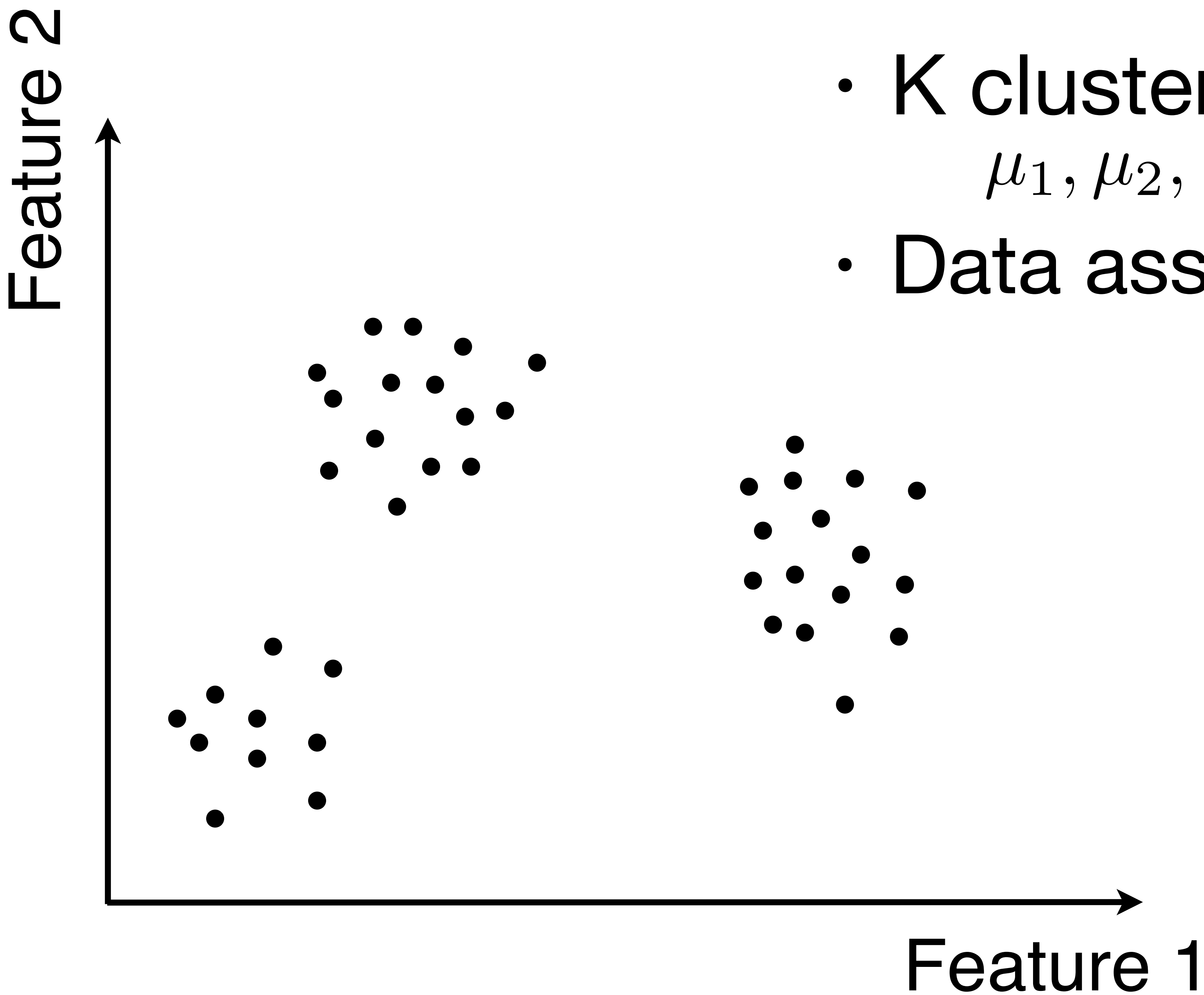
K-Means: Preliminaries



Cluster summary

- K cluster centers
  $\mu_1, \mu_2, \ldots, \mu_K$
- Data assignments to clusters

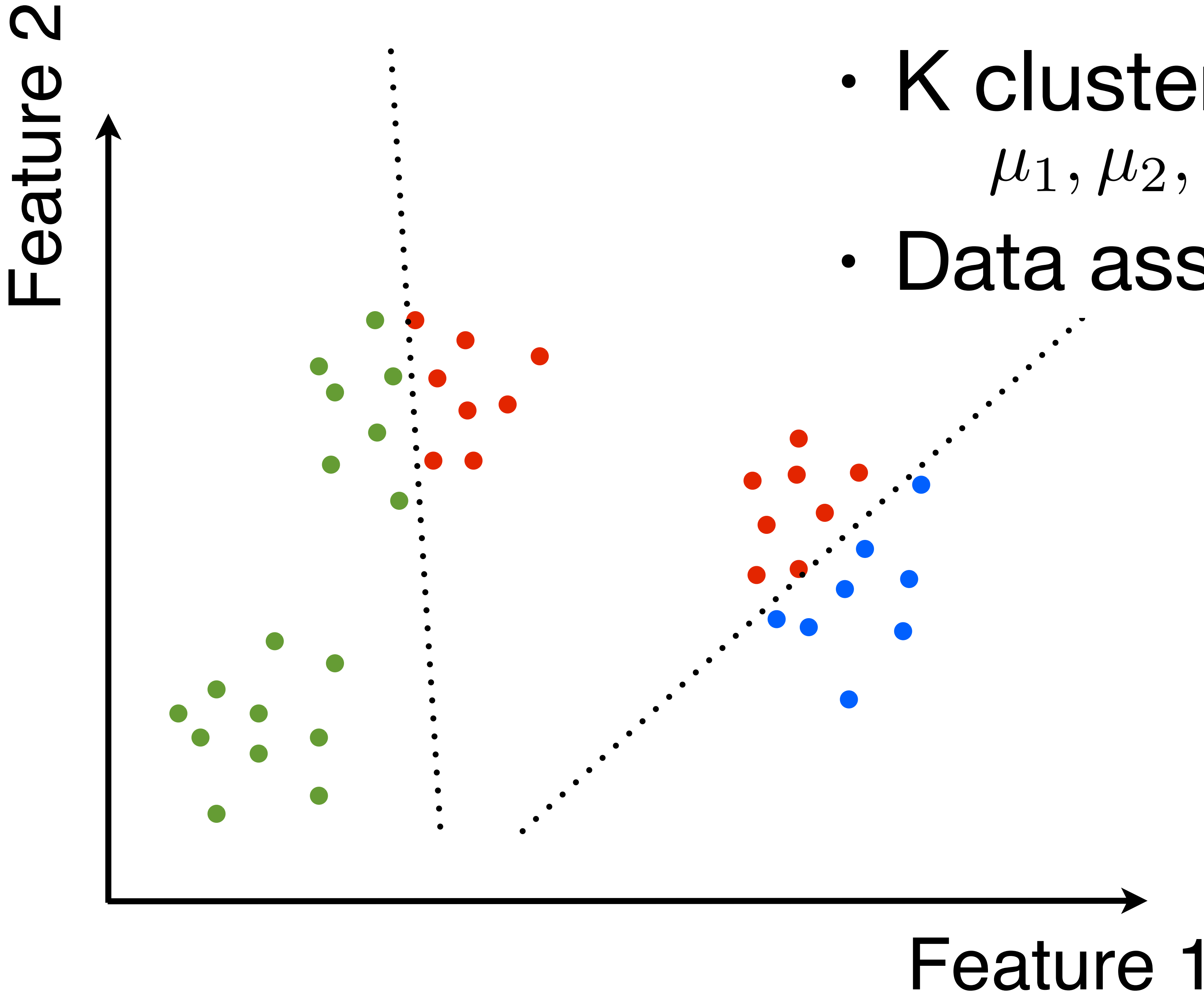
K-Means: Preliminaries

Cluster summary

- K cluster centers

  $\mu_1, \mu_2, \ldots, \mu_K$

- Data assignments to clusters



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K-Means: Preliminaries

Cluster summary

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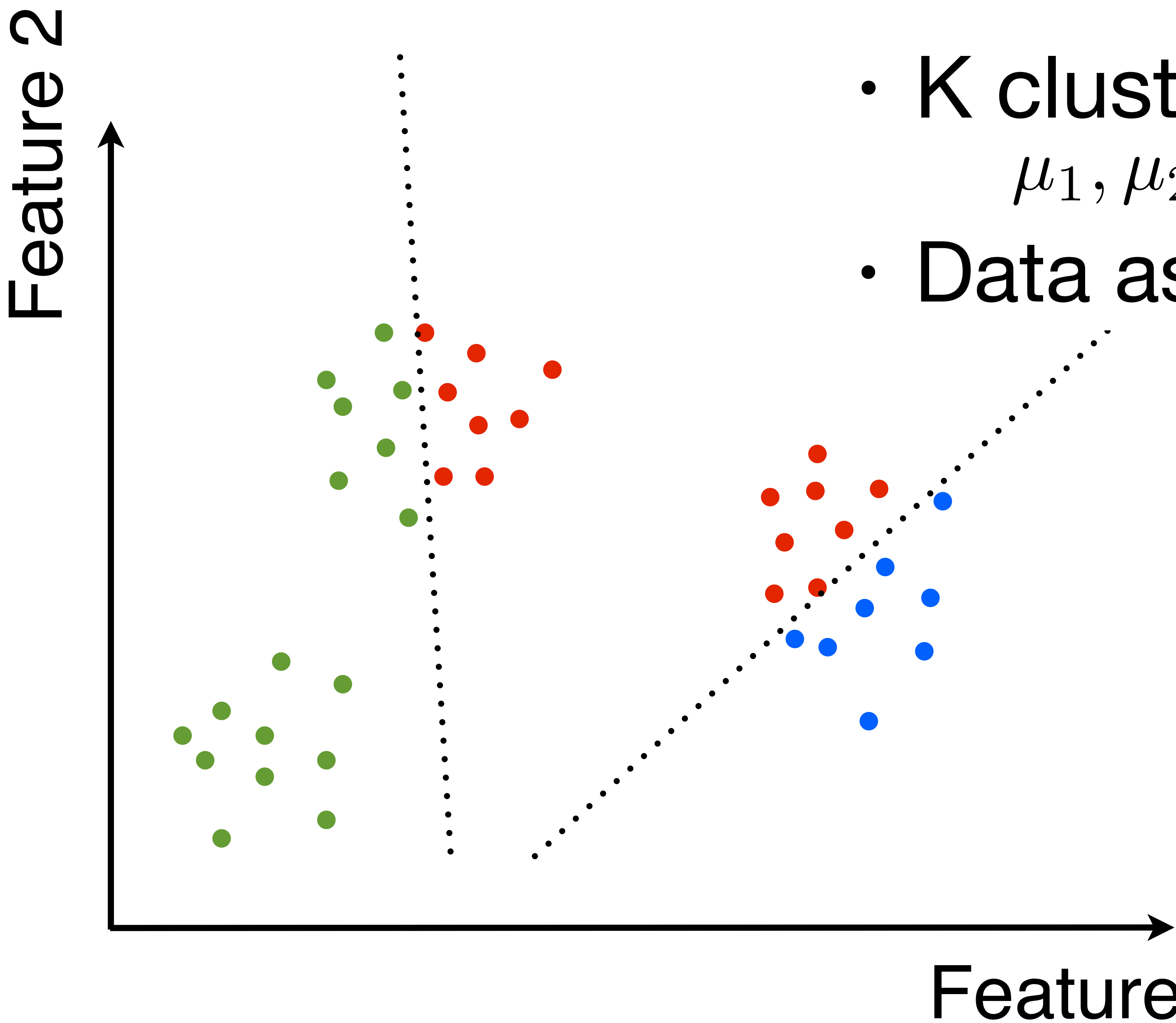
- Data assignments to clusters



S_k = set of points in cluster k

K-Means: Preliminaries

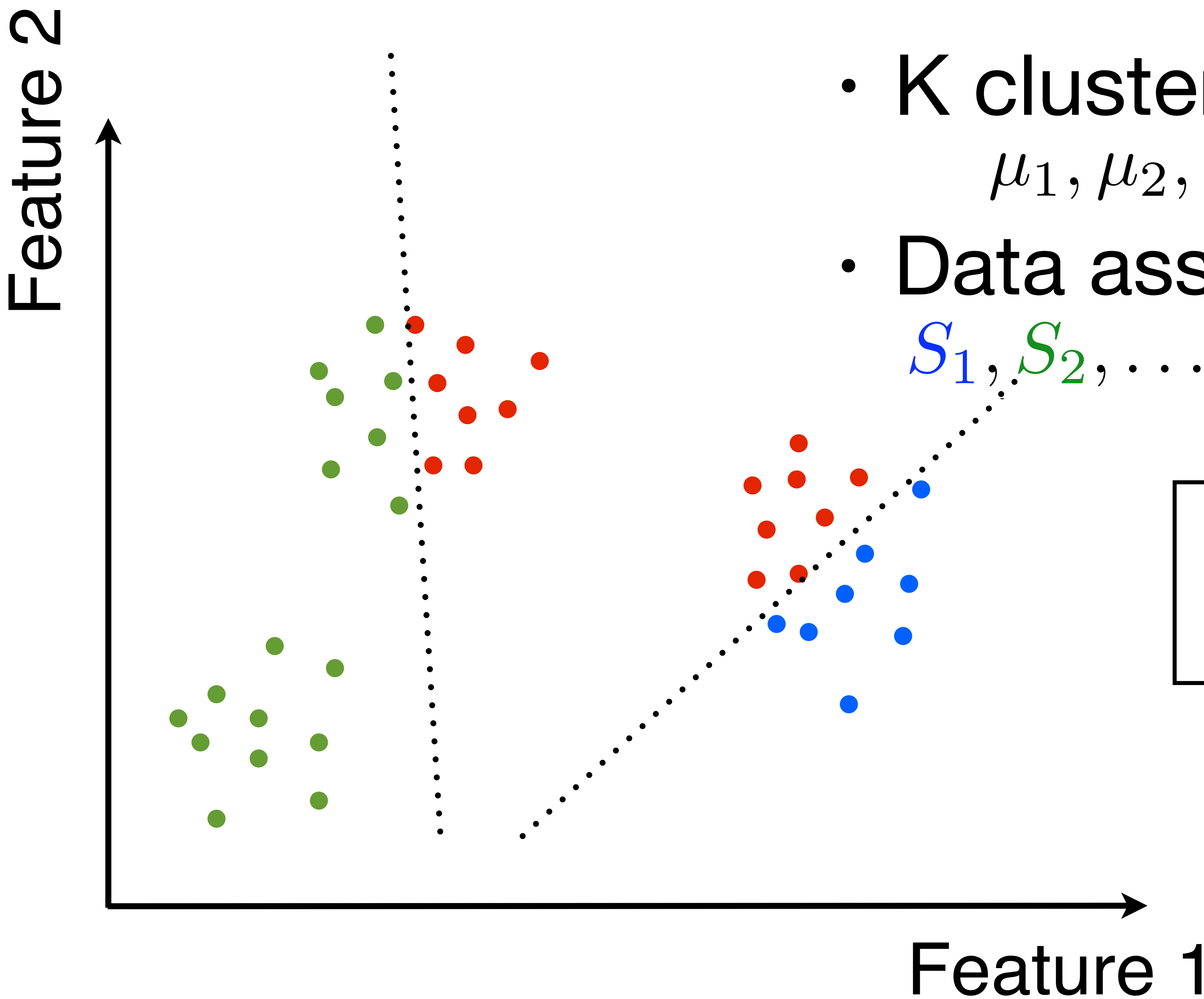
Cluster summary

- K cluster centers

  $\mu_1, \mu_2, \ldots, \mu_K$

- Data assignments to clusters

  $S_1, S_2, \ldots, S_K$



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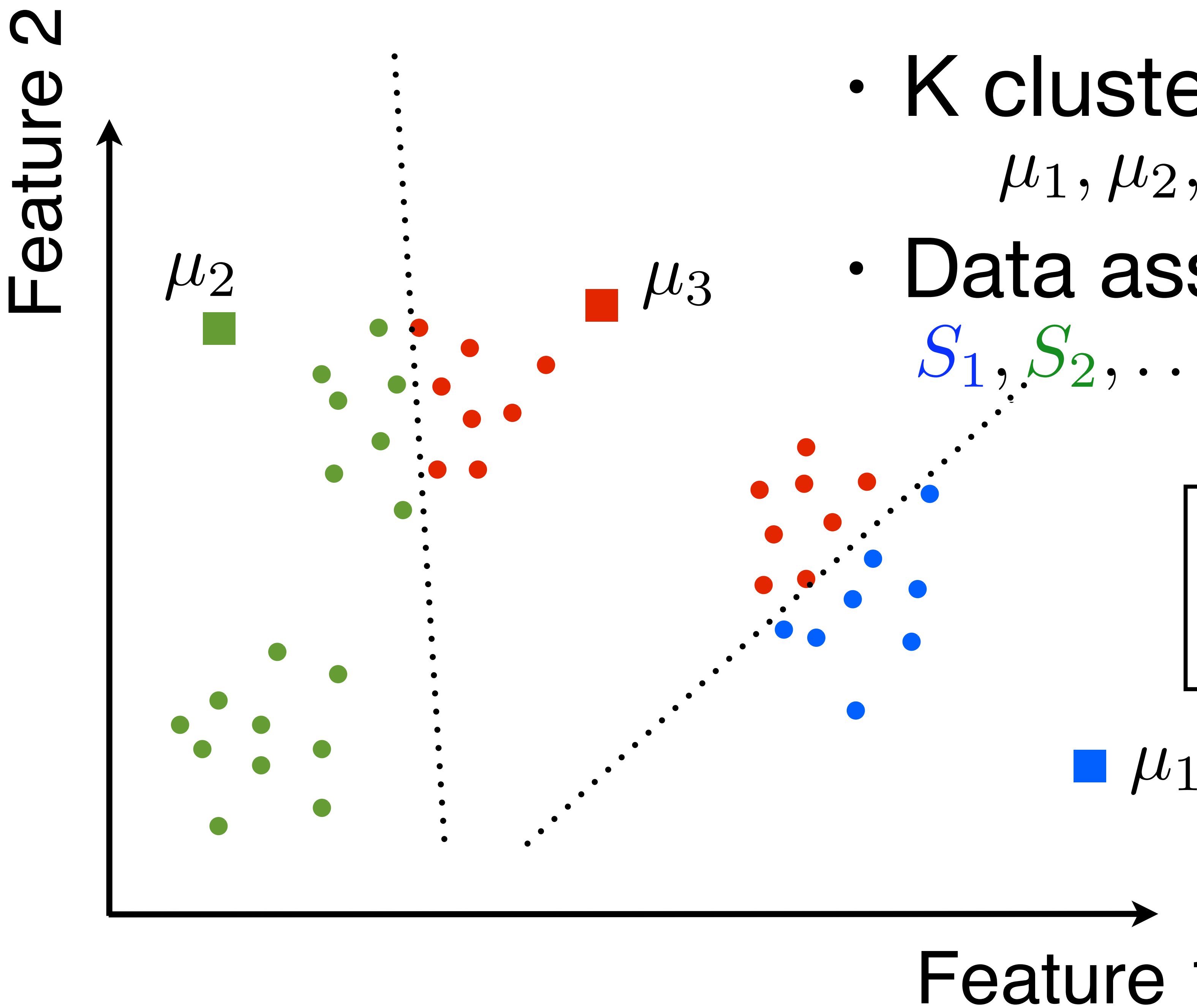
K-Means: Preliminaries



Cluster summary

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- Data assignments to clusters

  $S_1, S_2, \ldots, S_K$

S_k = set of points in cluster k

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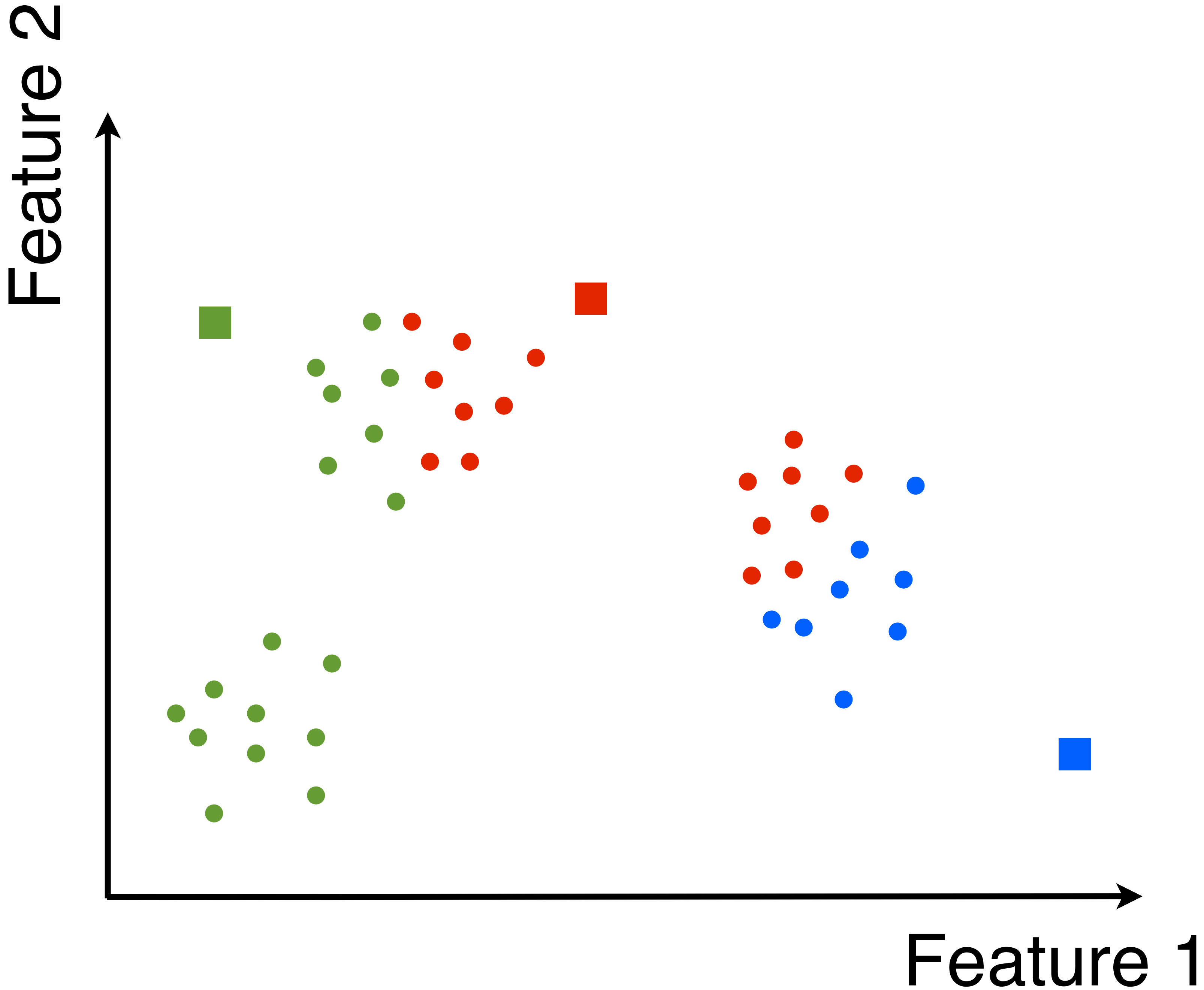
K-Means: Preliminaries

Dissimilarity



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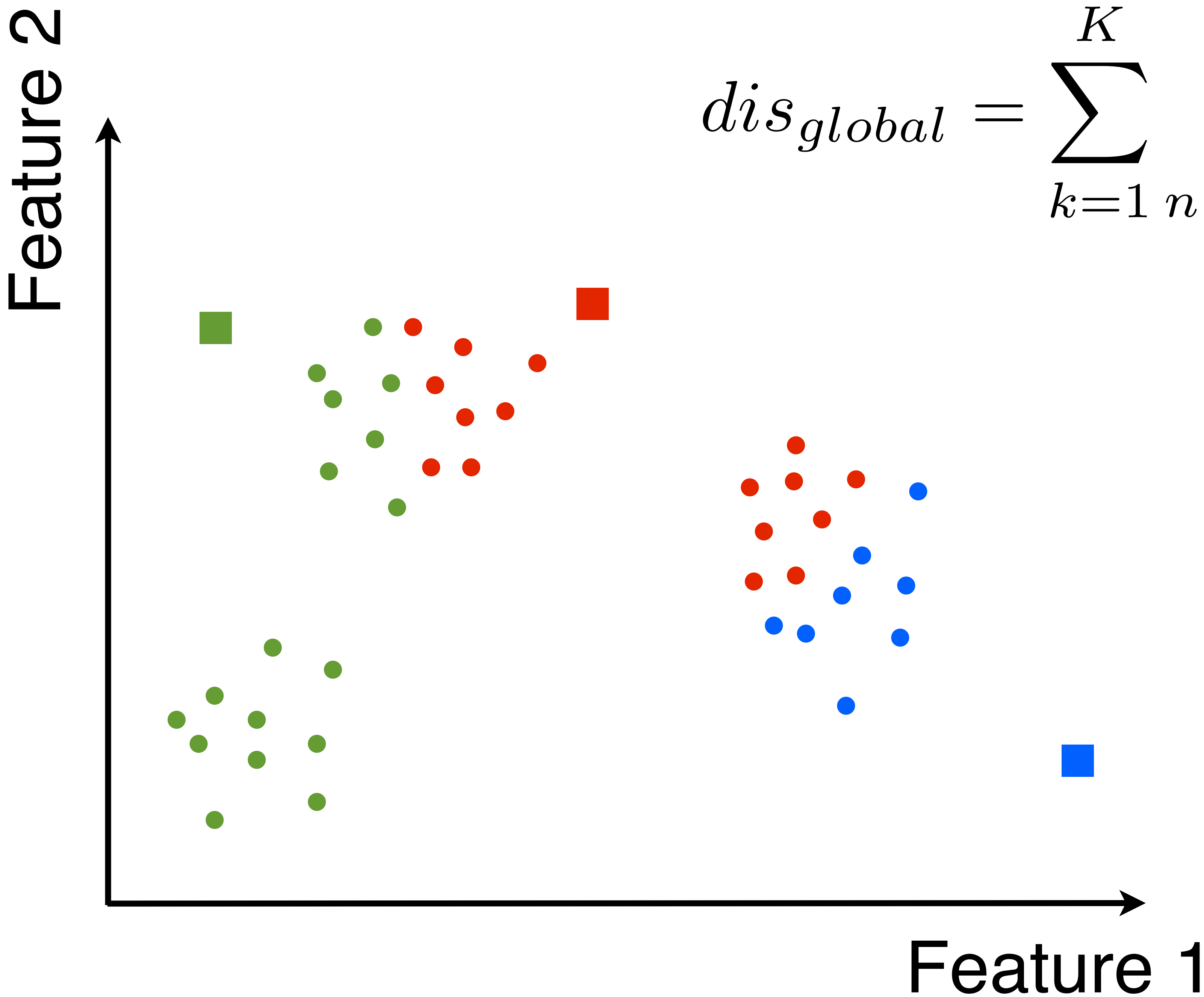
K-Means: Preliminaries

Dissimilarity (global)

$$dis_{global} = \sum_{k=1}^{K} \sum_{n: x_n \in S_k} \sum_{d=1}^{D} (x_{n,d} - \mu_{k,d})^2$$



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K-Means: Preliminaries

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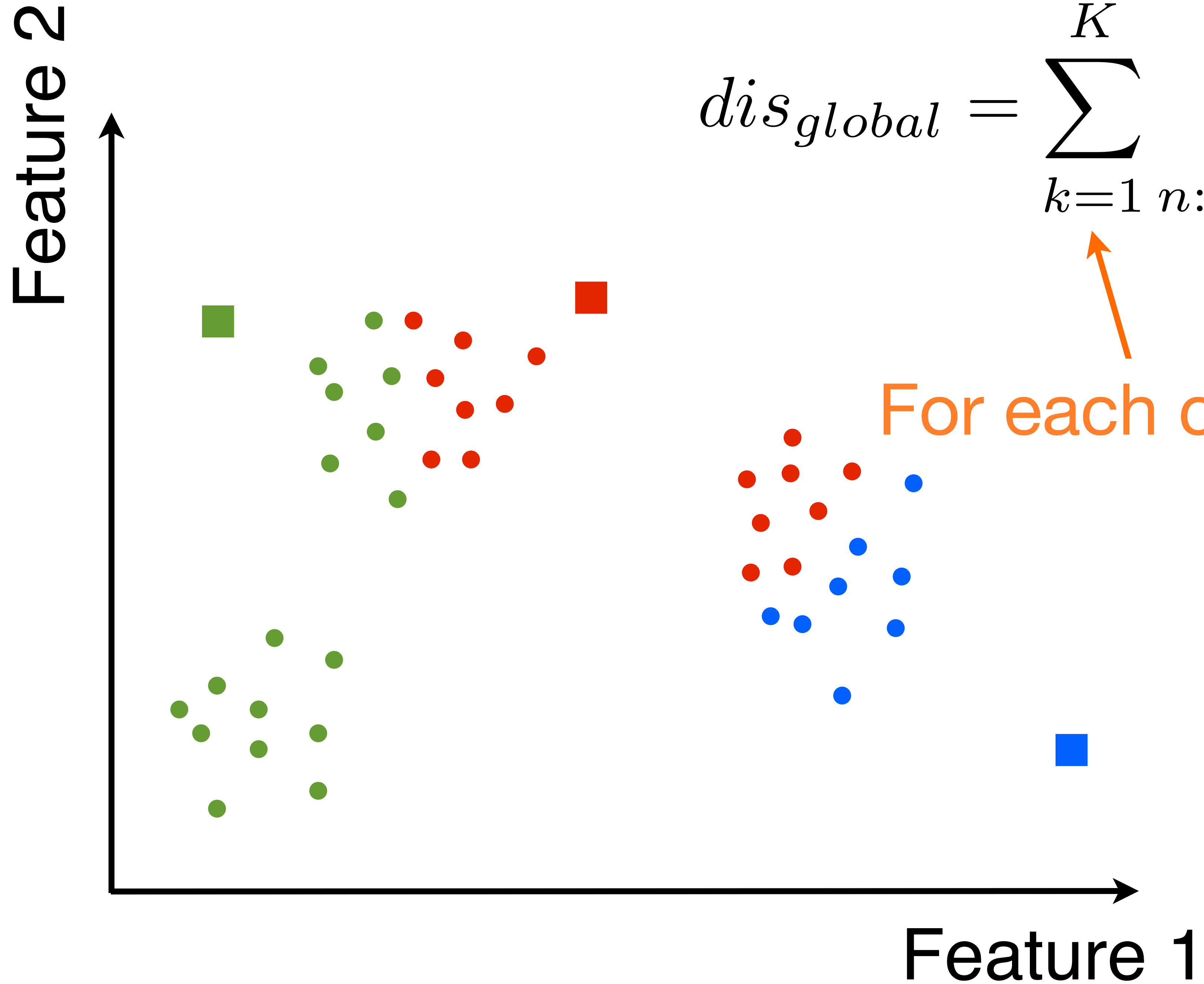
For each cluster



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K-Means: Preliminaries

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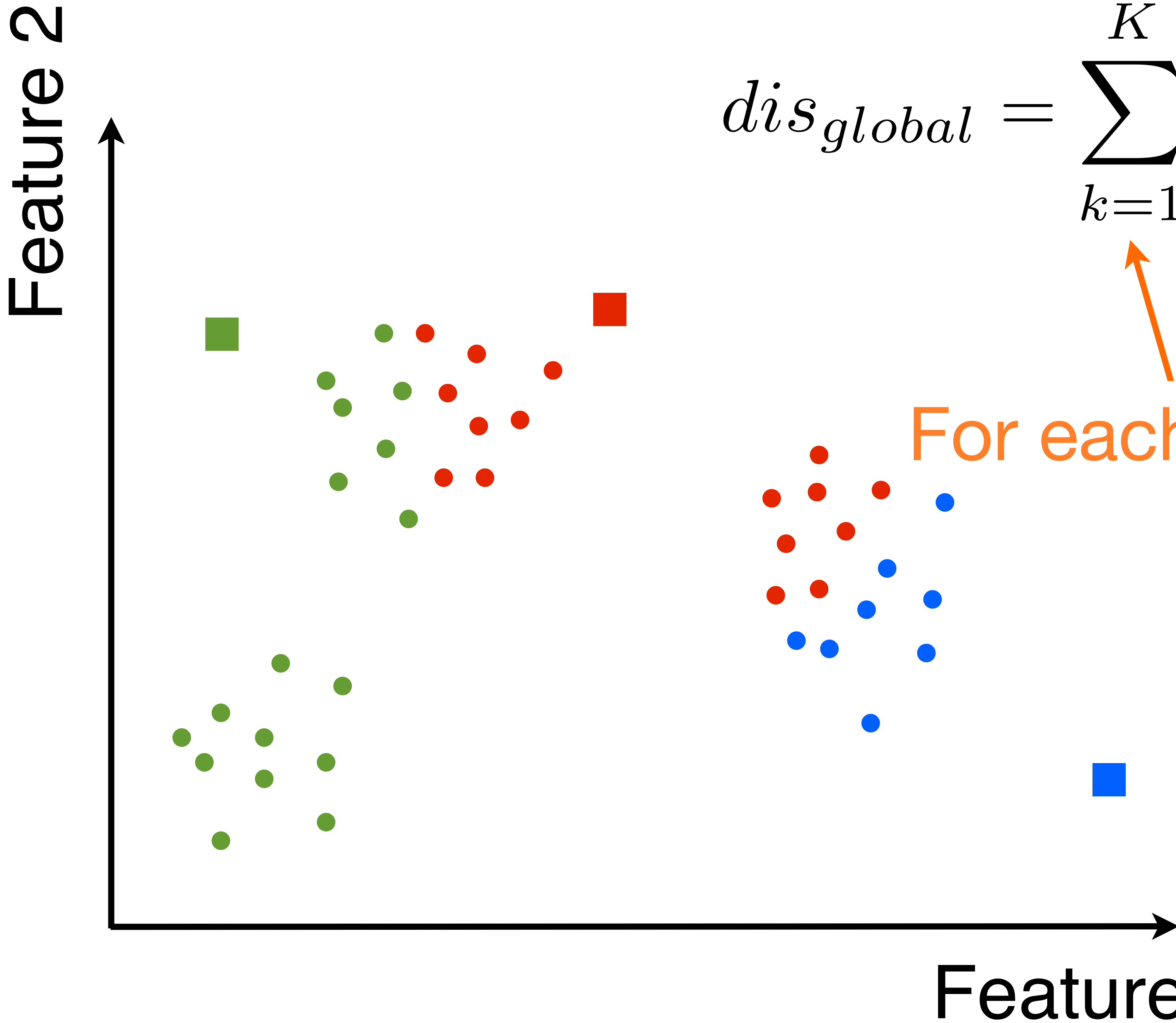
$$dis_{global} = \sum_{k=1}^{K} \sum_{n: x_n \in S_k} \sum_{d=1}^{D} (x_{n,d} - \mu_{k,d})^2$$

For each cluster

For each data point in the kth cluster



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K-Means: Preliminaries

Dissimilarity (global)

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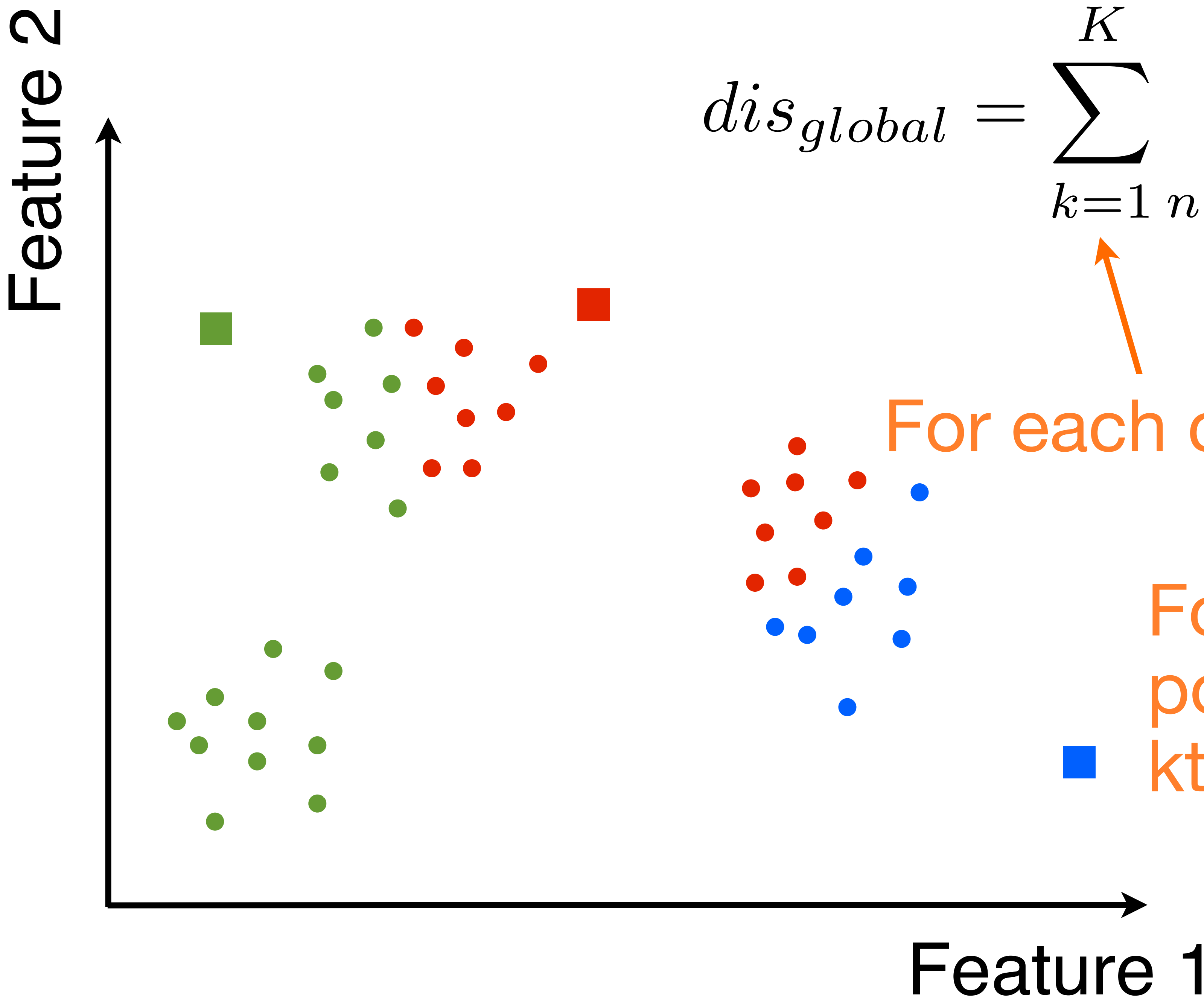
For each cluster

For each data point in the kth cluster

For each feature



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K-Means: Preliminaries

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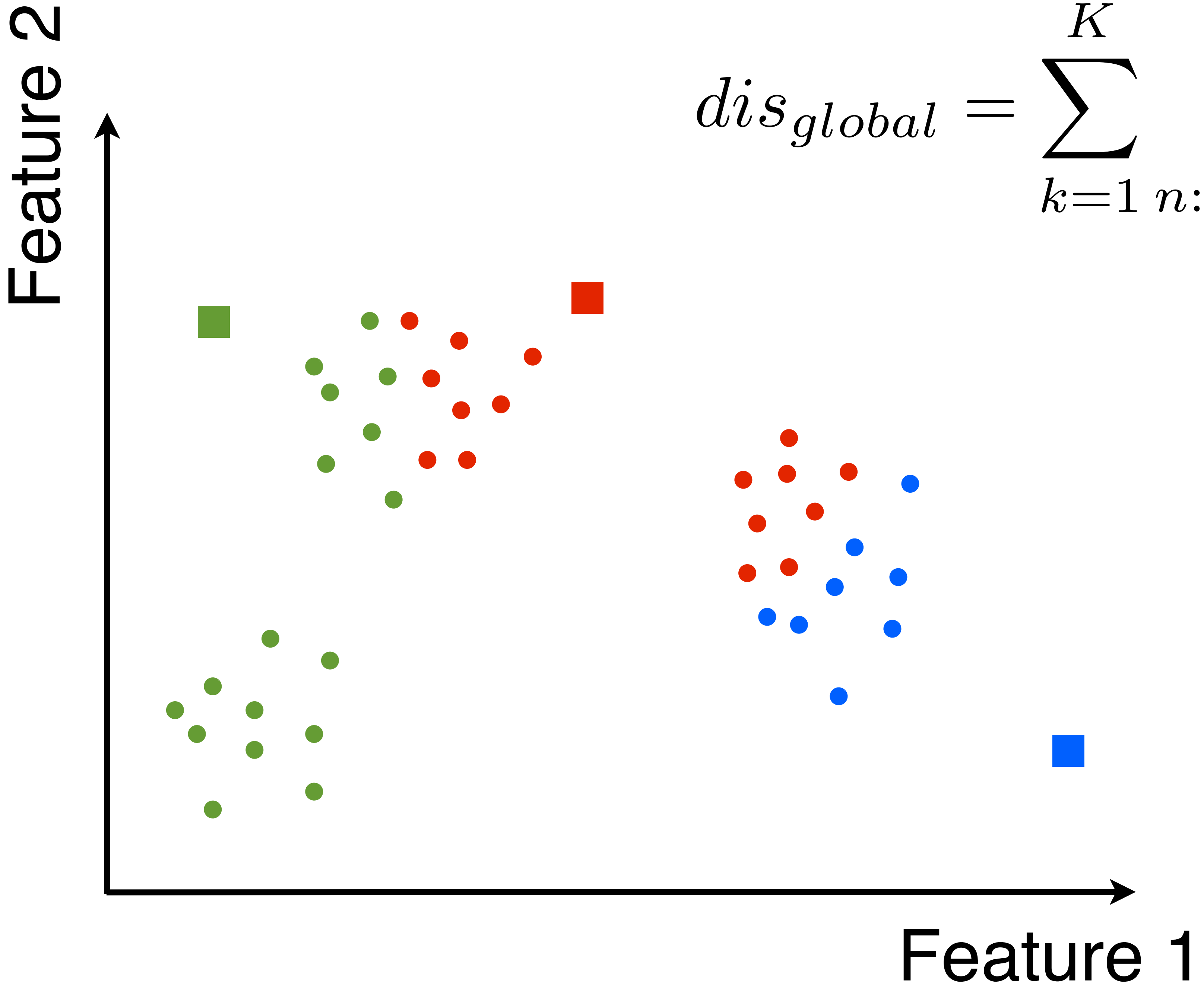

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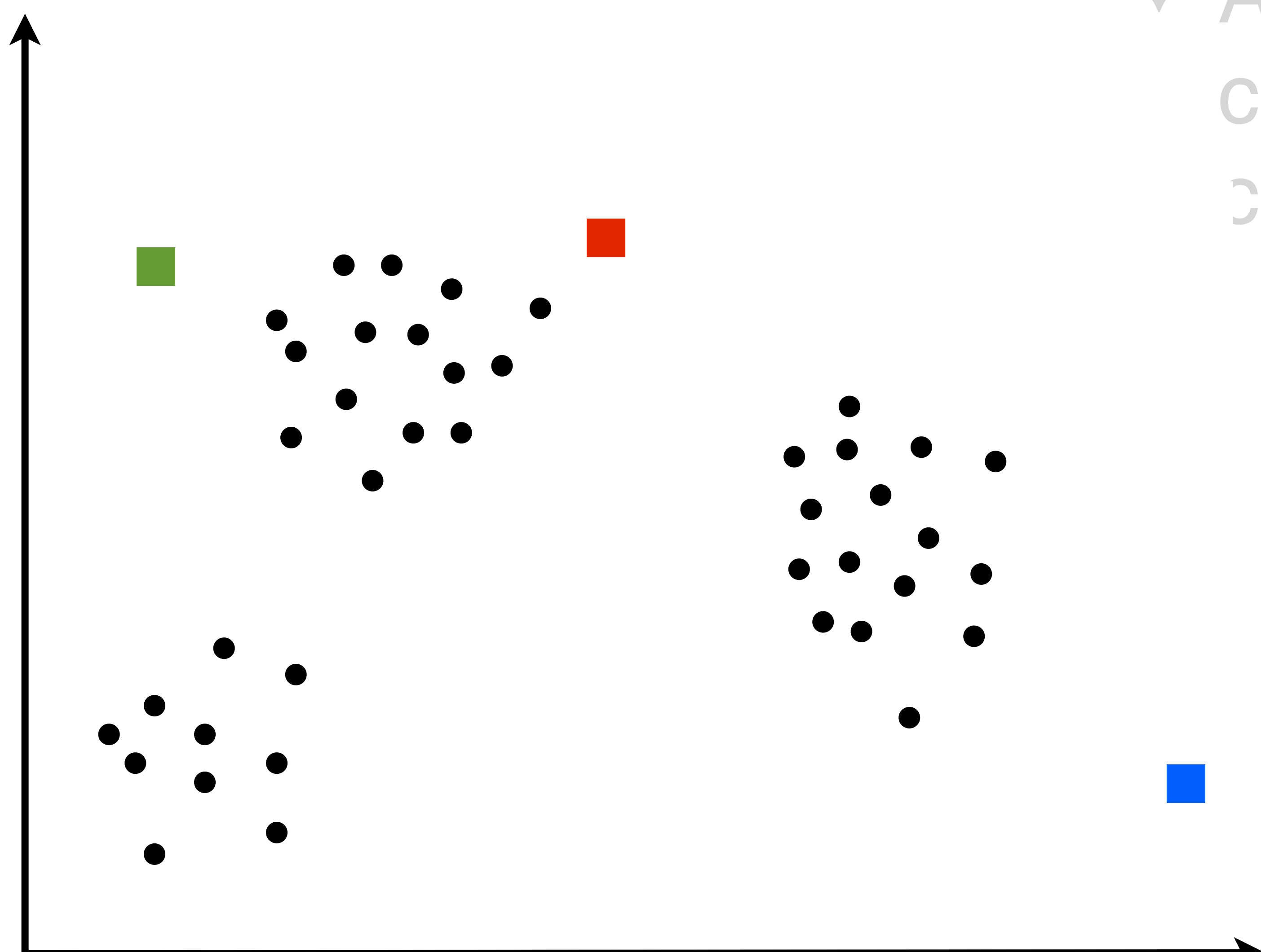
K-Means Algorithm

- Initialize K cluster centers
- Repeat until convergence:
  - ✦ Assign each data point to the cluster with the closest center.
  - ✦ Assign each cluster center to be the mean of its cluster's data points



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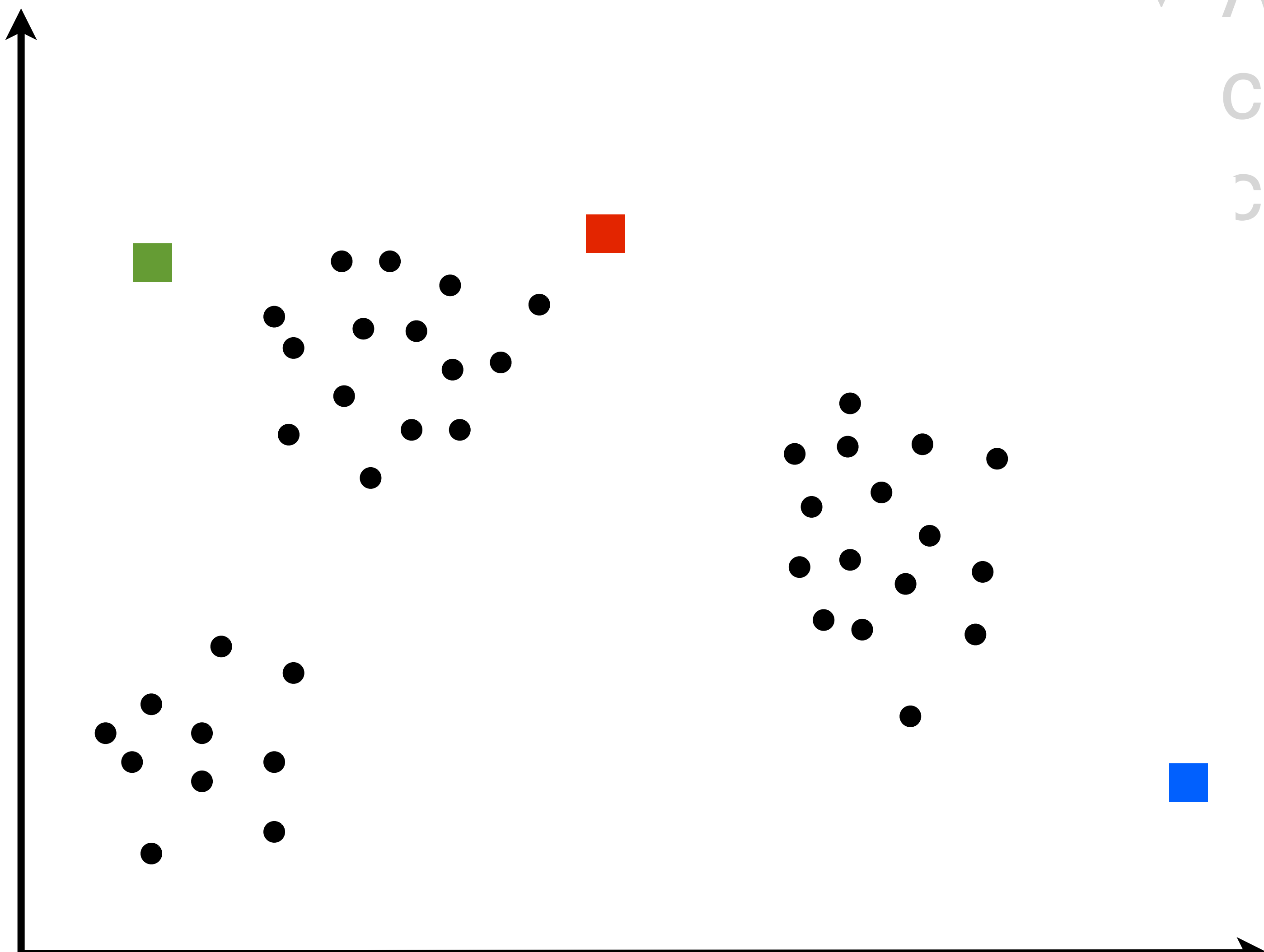

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K-Means Algorithm

- For k = 1,…, K
  - ✦ Randomly draw n from 1,…,N without replacement
  - ✦ $\mu_k \leftarrow x_n$
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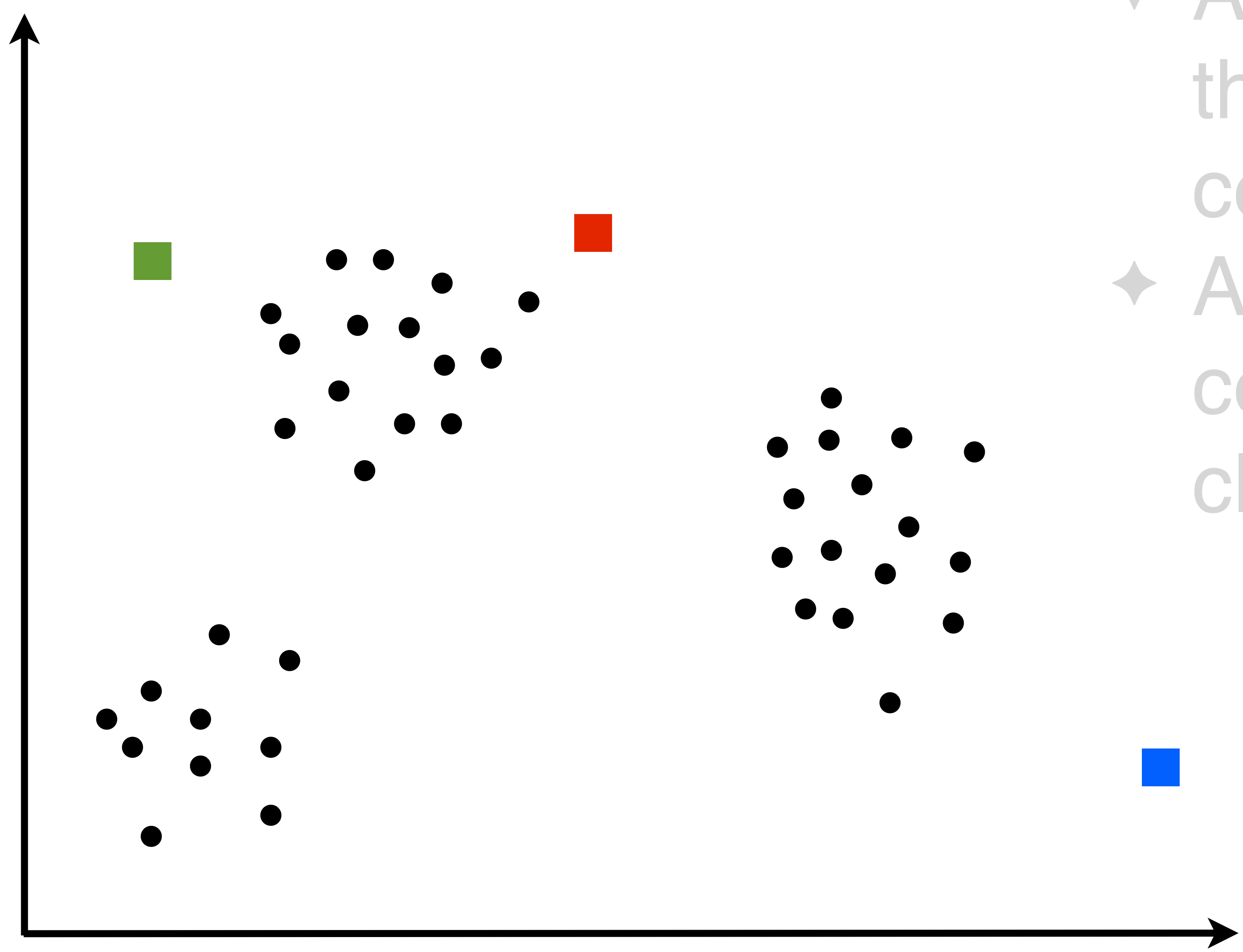

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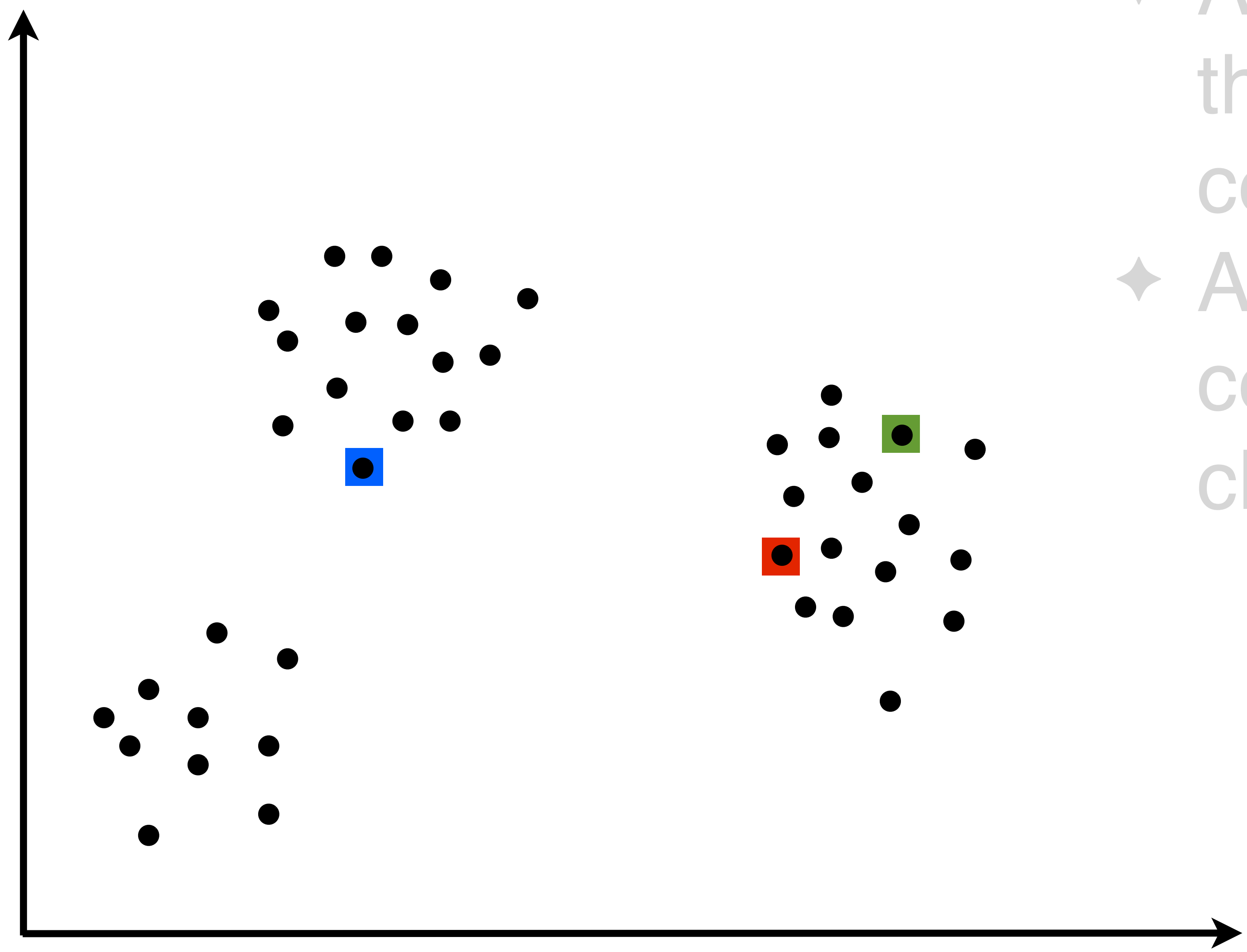

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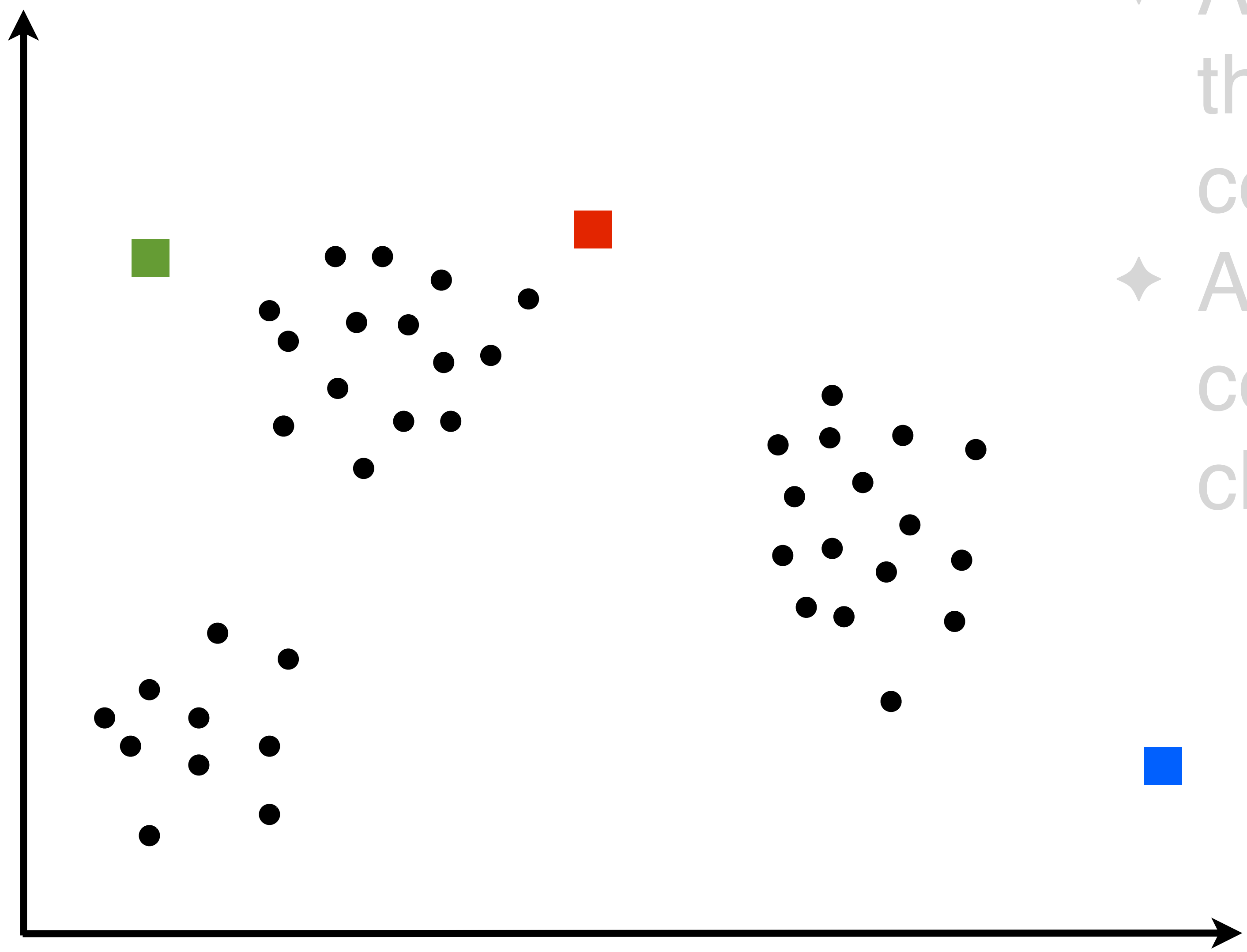

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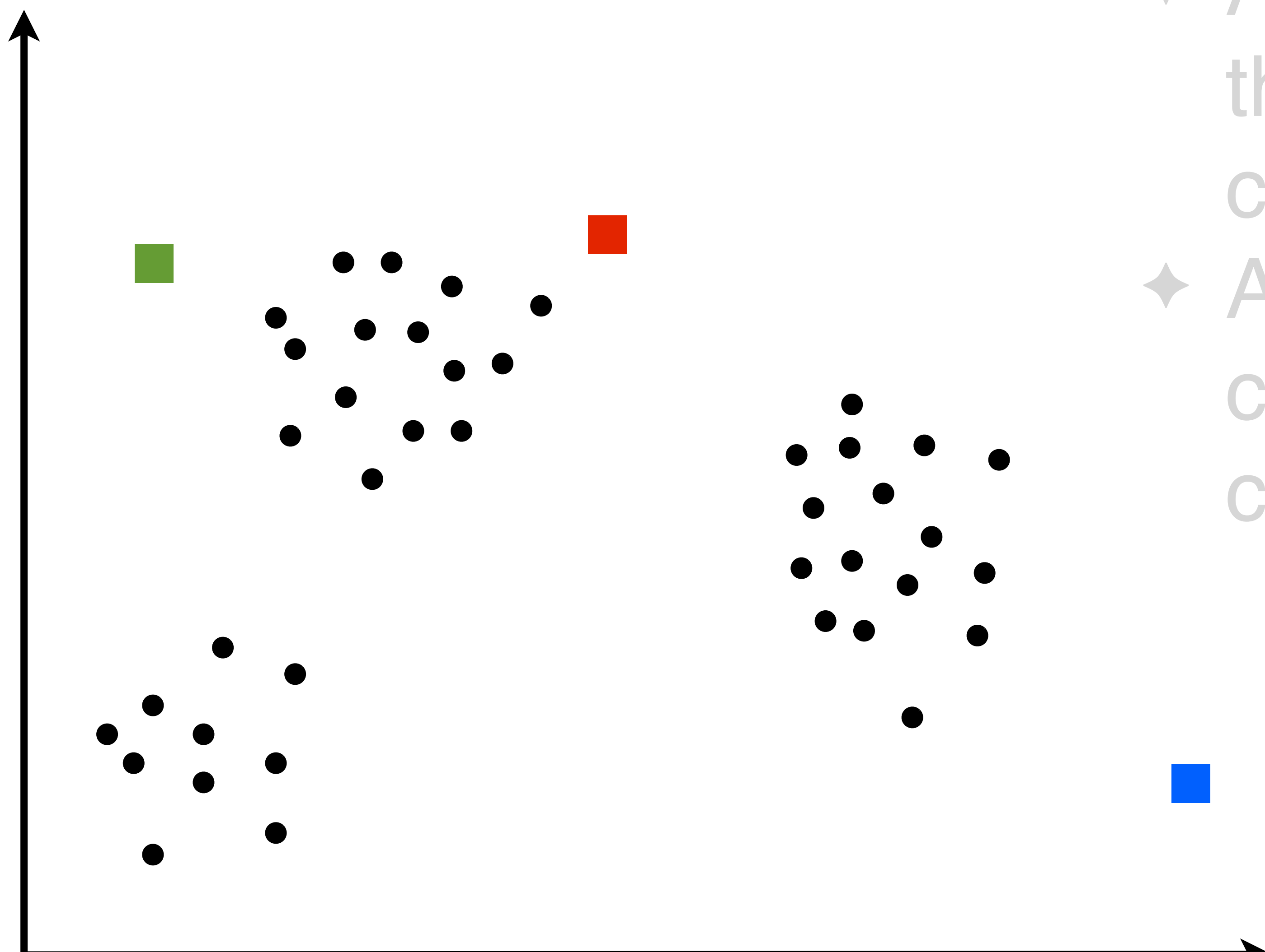

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K-Means Algorithm

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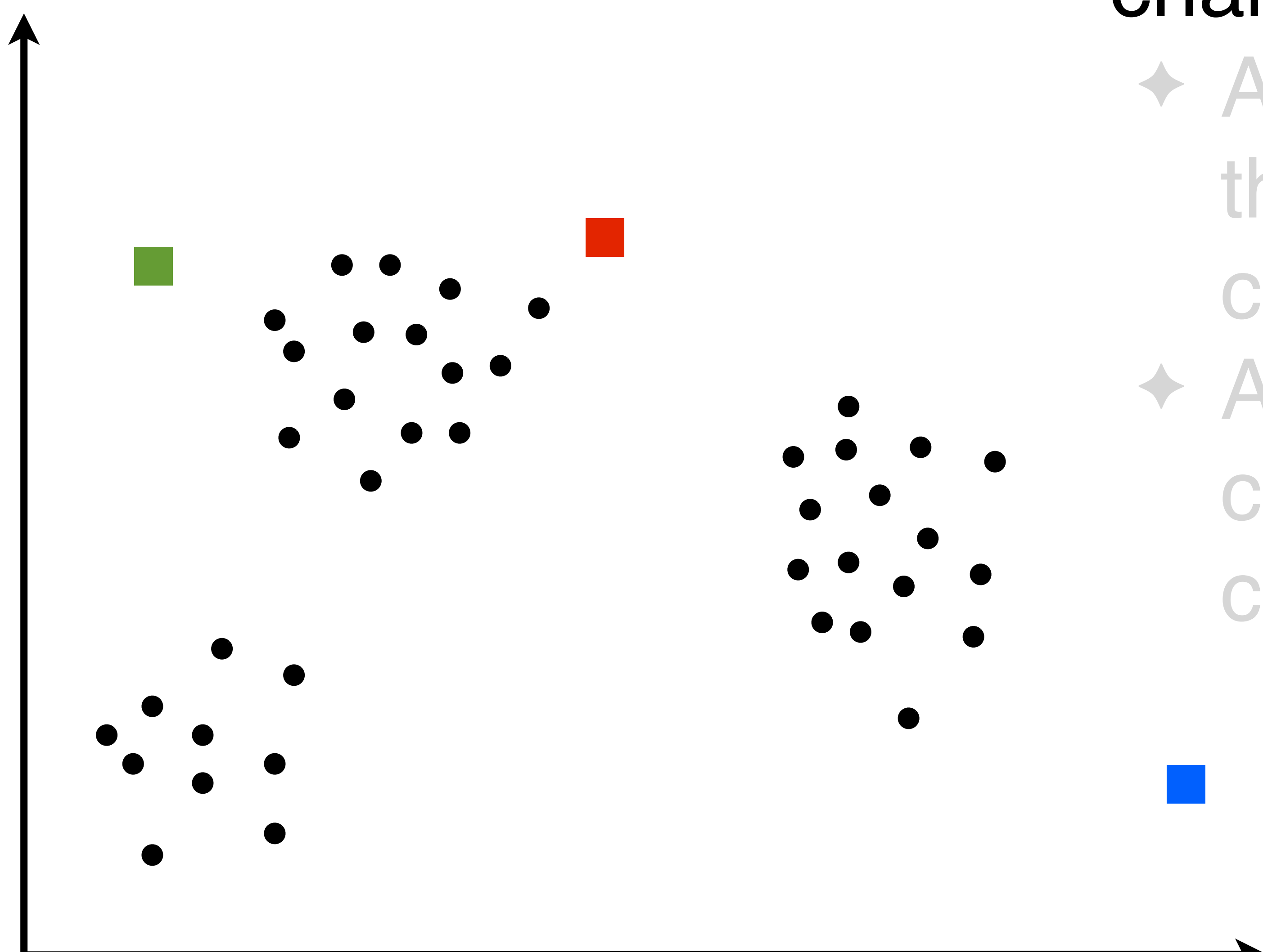

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K-Means Algorithm

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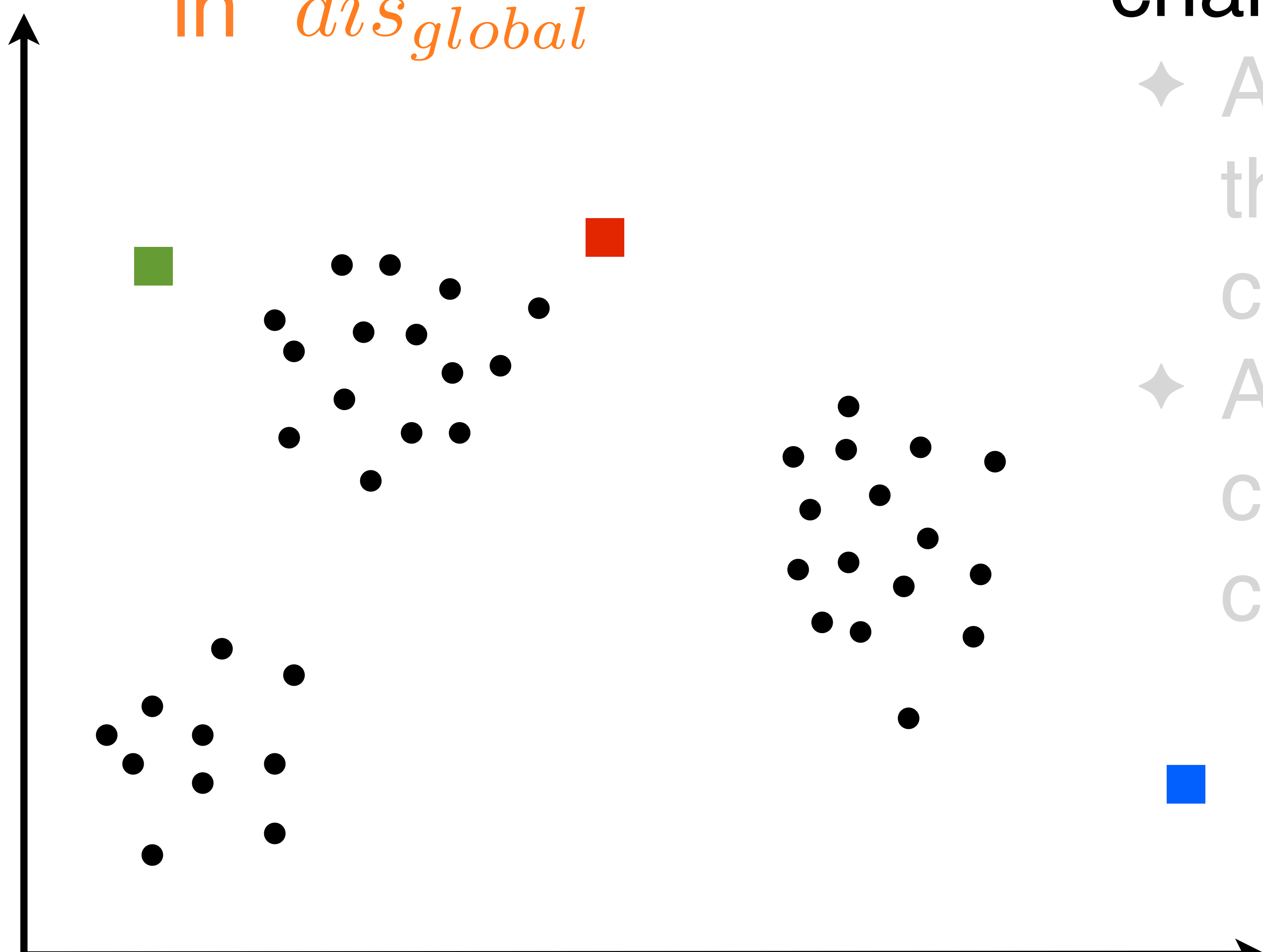
Or no change in dis_{global}



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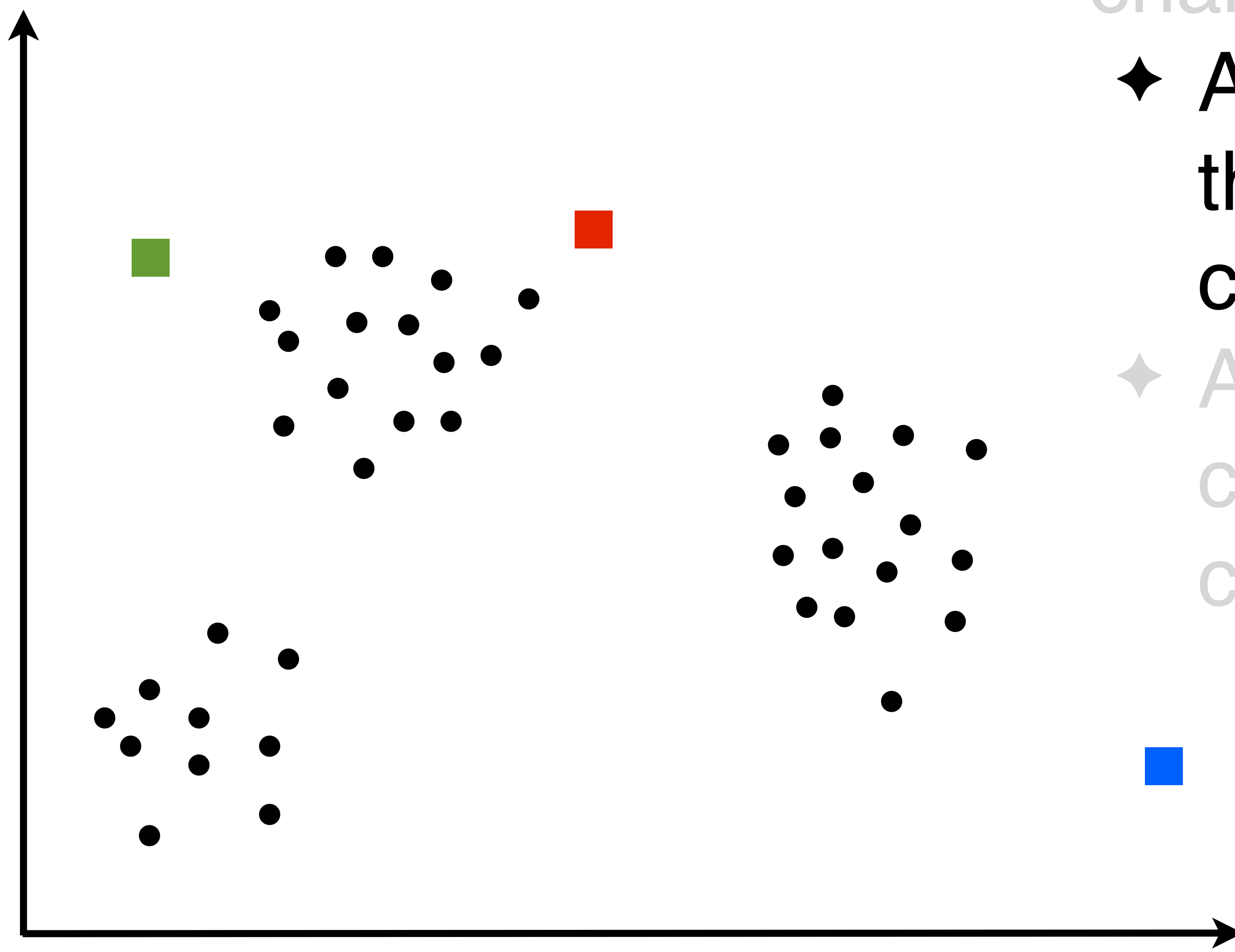
K-Means Algorithm



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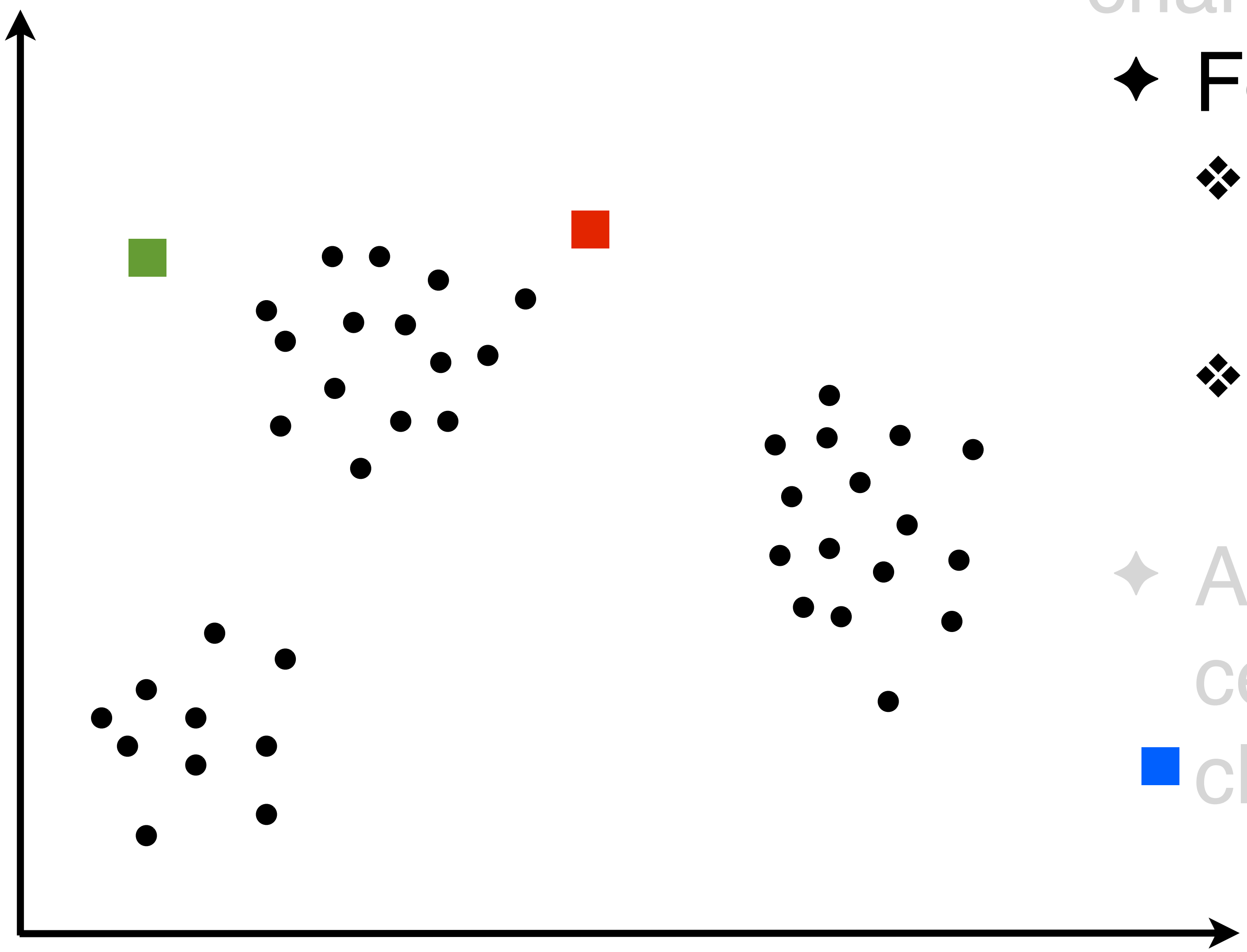

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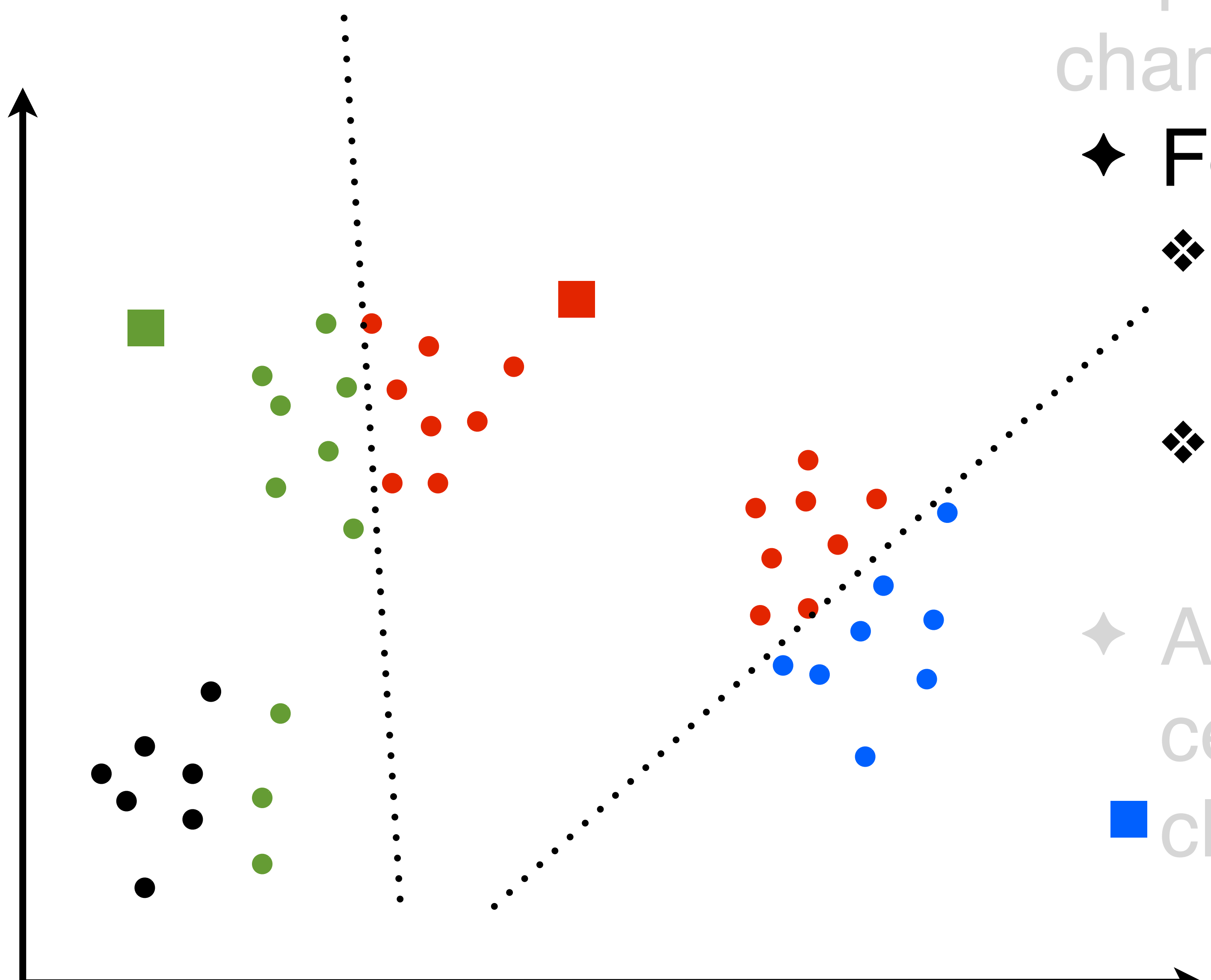
K-Means Algorithm



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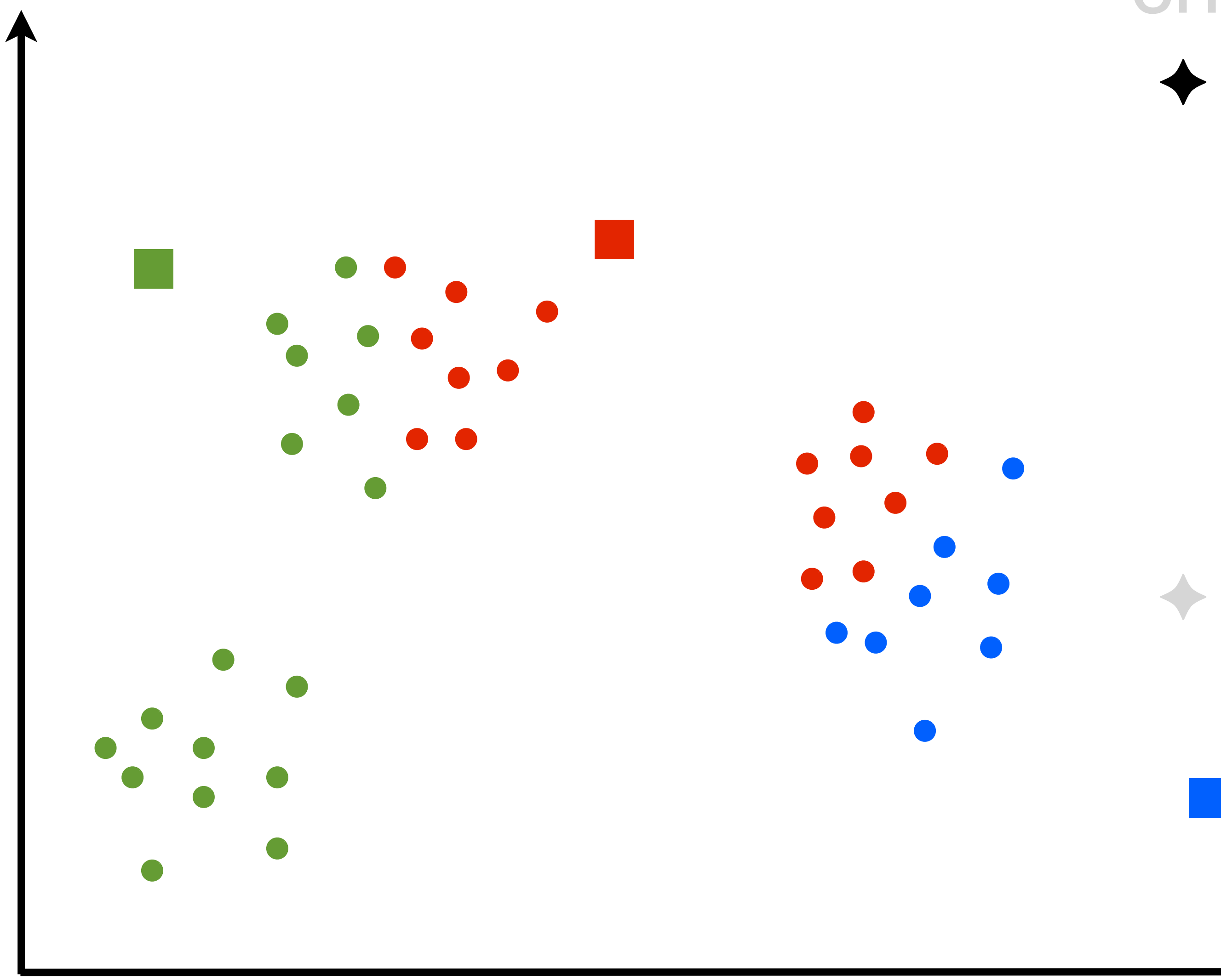
K-Means Algorithm



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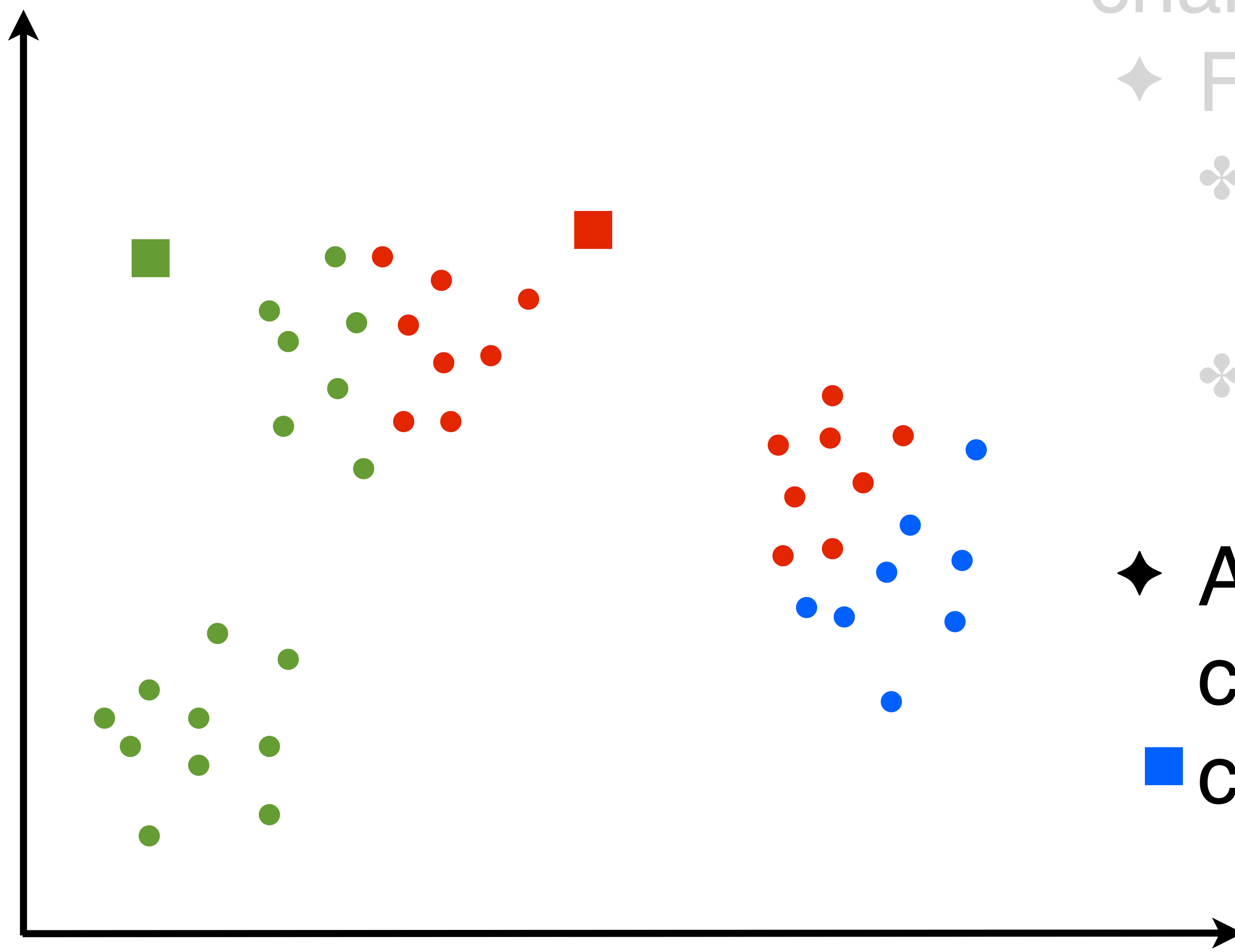
K-Means Algorithm



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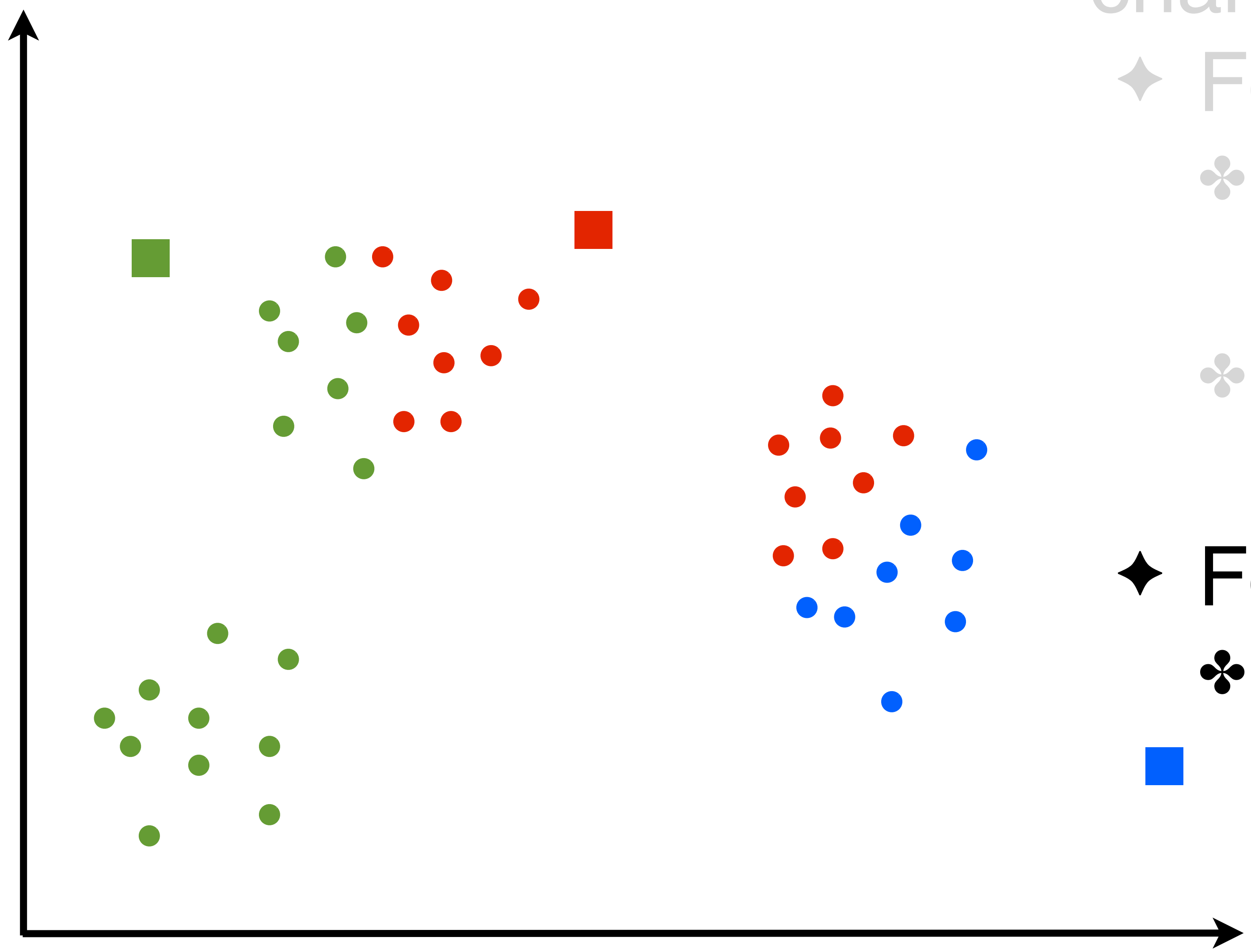
K-Means Algorithm



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K-Means Algorithm

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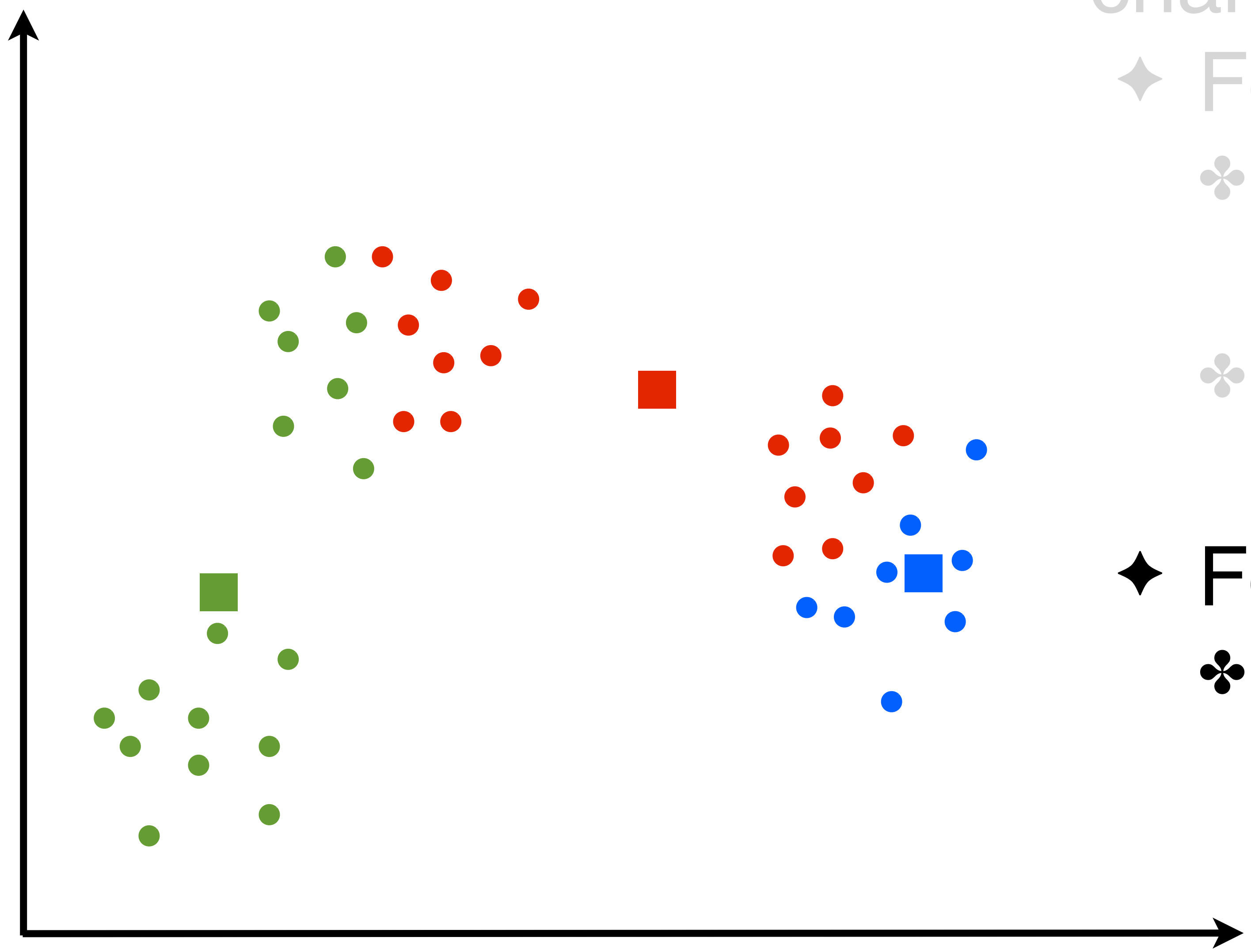

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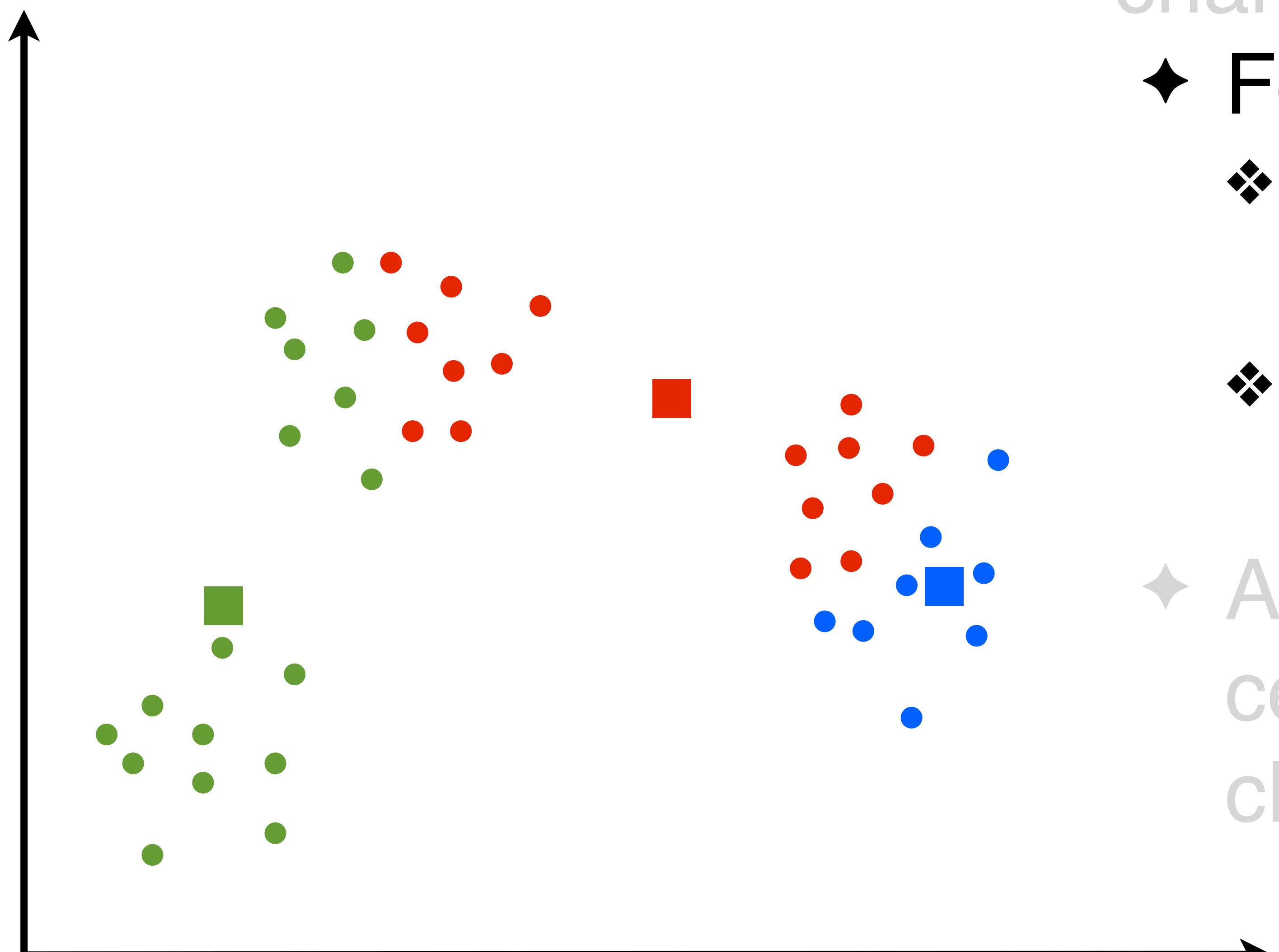
K-Means Algorithm



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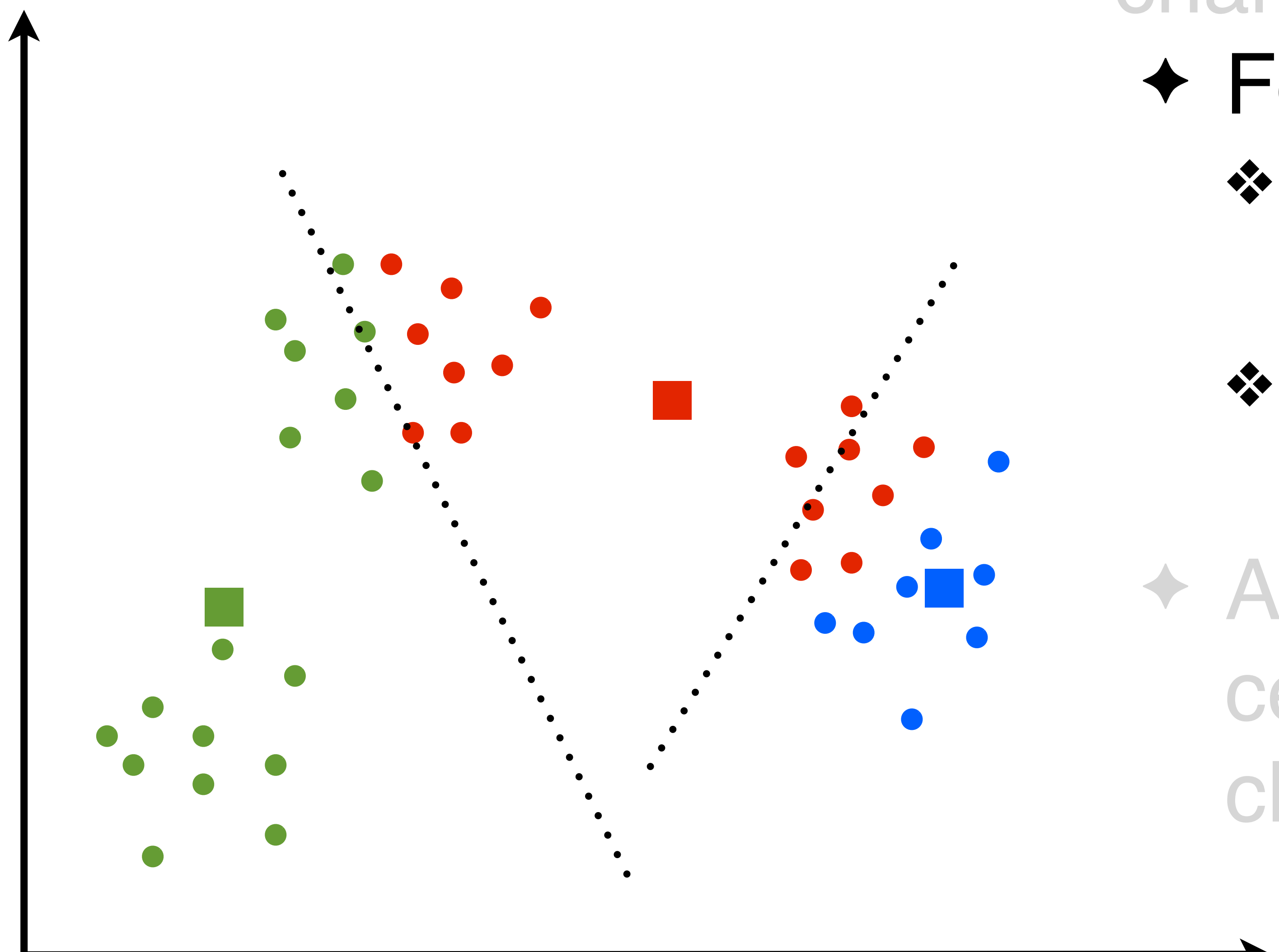

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K-Means Algorithm

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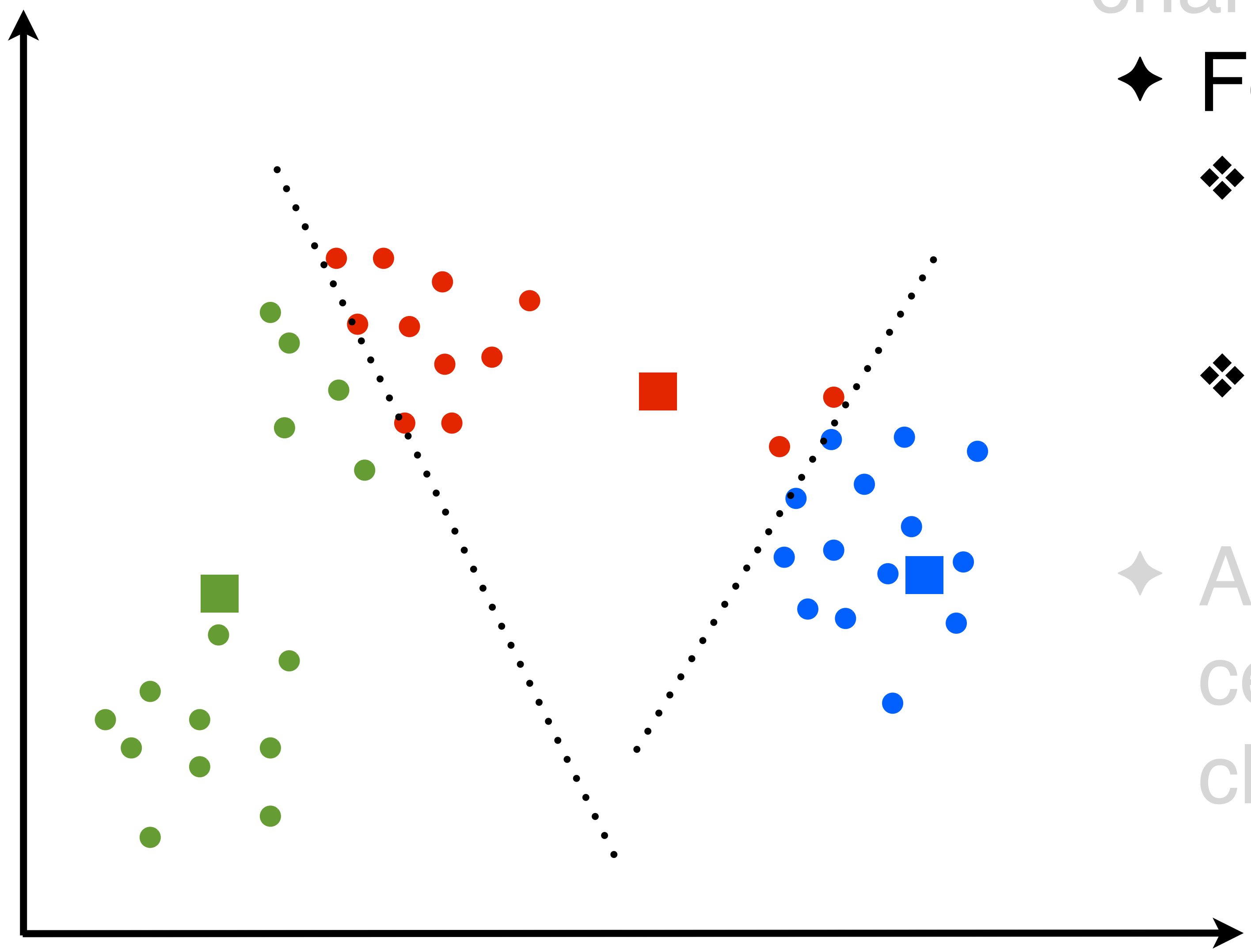

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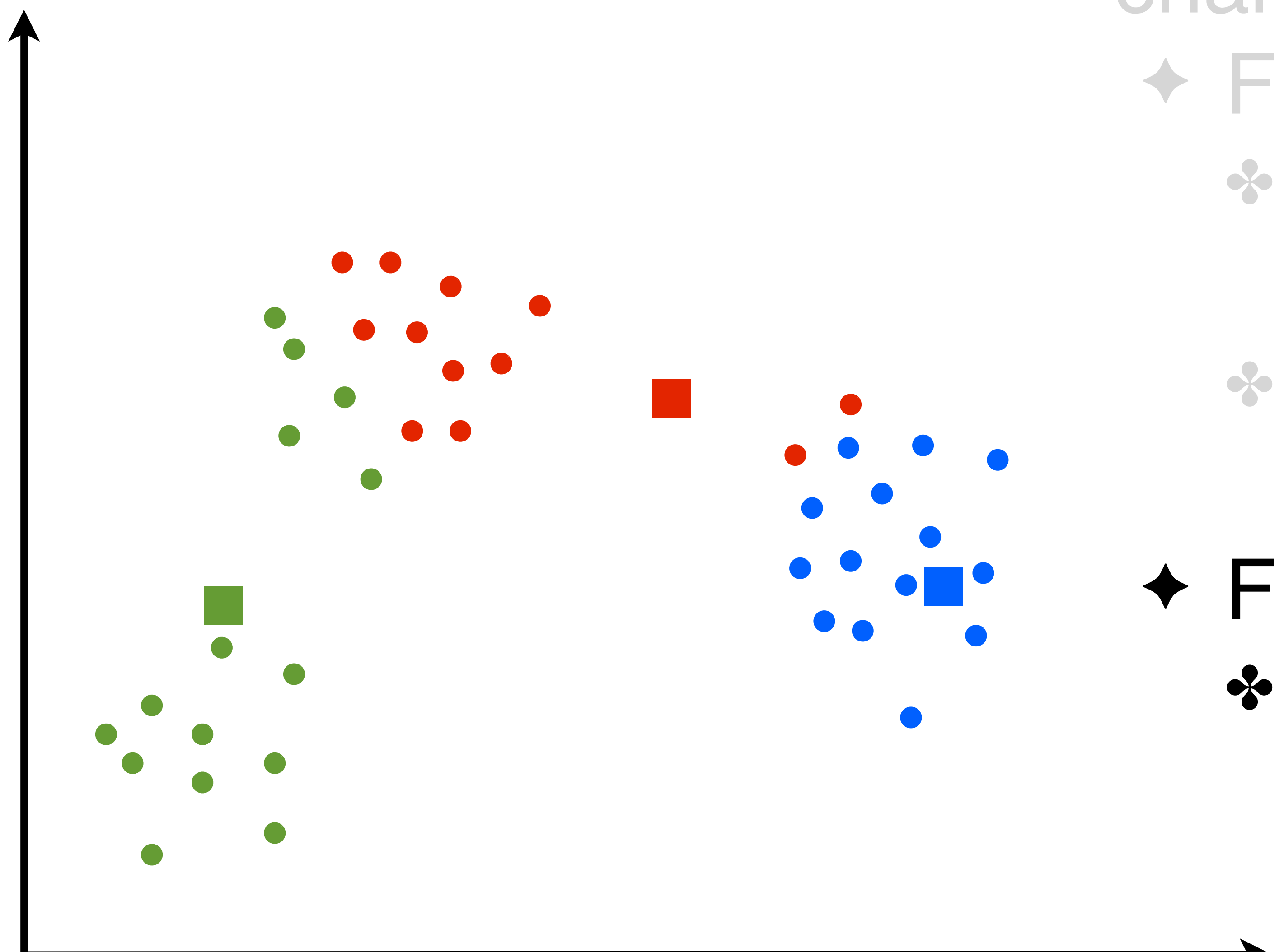
K-Means Algorithm



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slide by Tamara Broderick

K-Means Algorithm

- For k = 1,…, K
  - ✦ Randomly draw n from 1,…,N without replacement
  - ✦ $\mu_k \leftarrow x_n$
- Repeat until $S_1,\ldots,S_K$ don't change:
  - ✦ For n = 1,…N
    - ✤ Find k with smallest $dis(x_n, \mu_k)$
    - ✤ Put $x_n \in S_k$ (and no other S_j)
  - ✦ For k = 1,…,K
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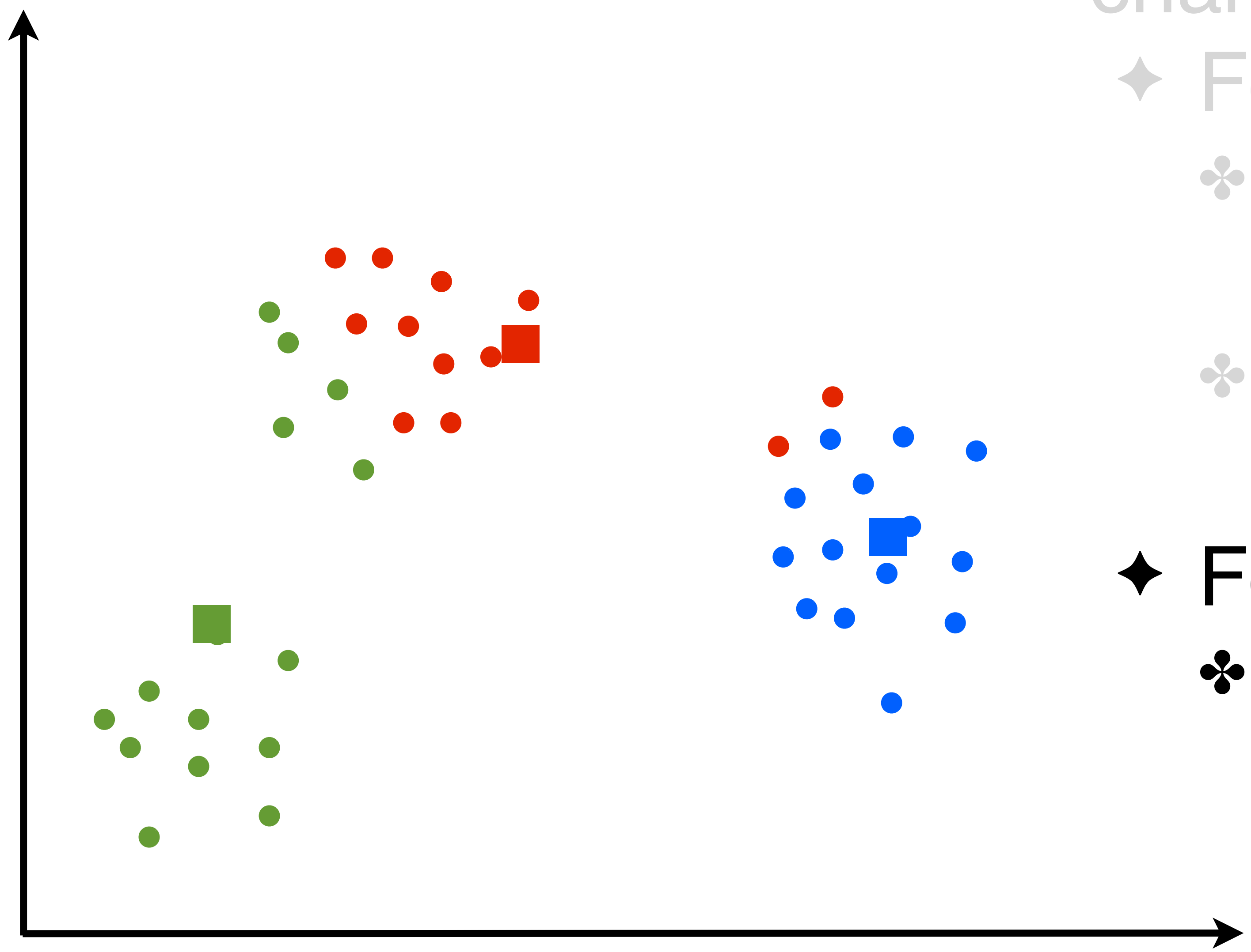

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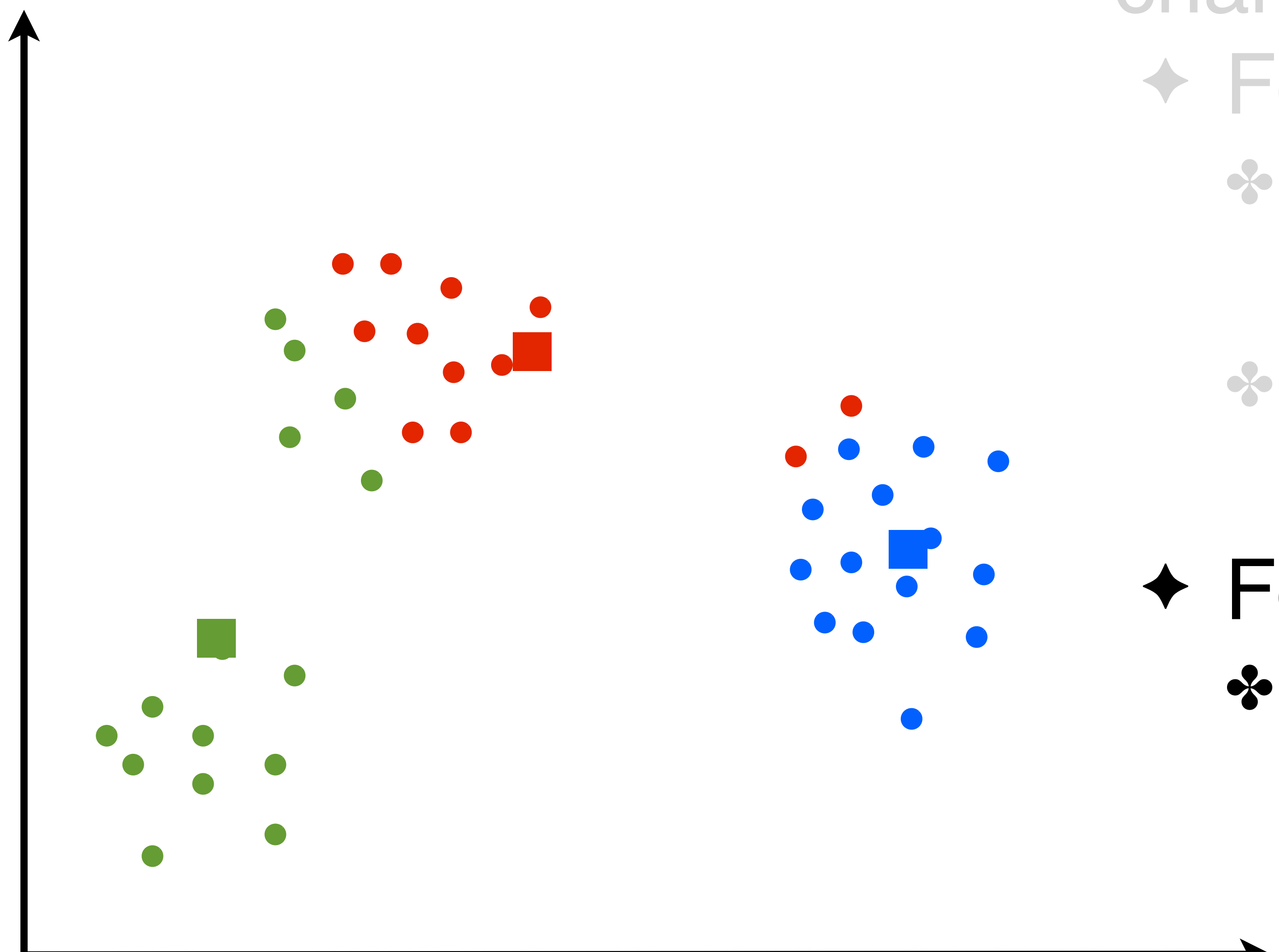

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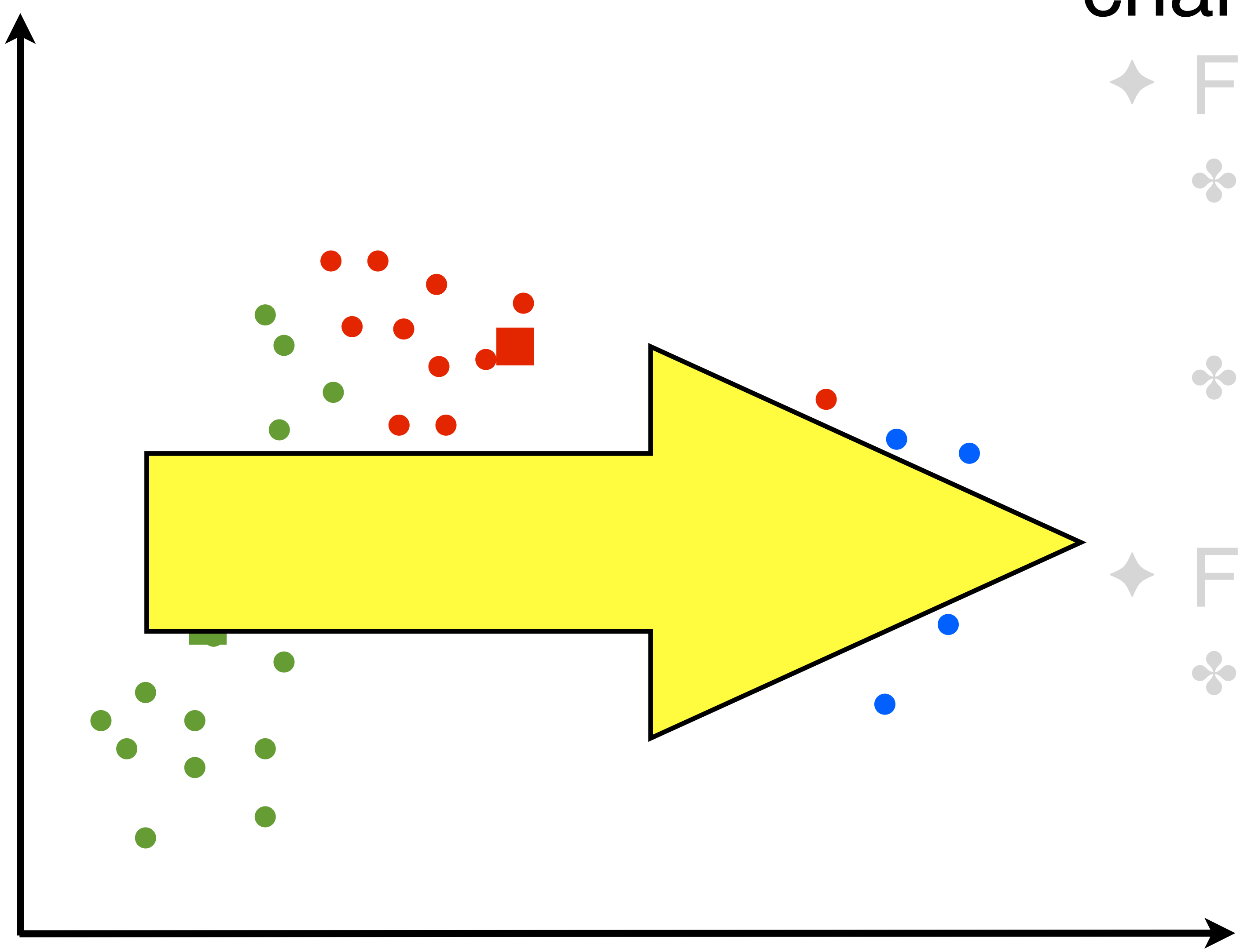

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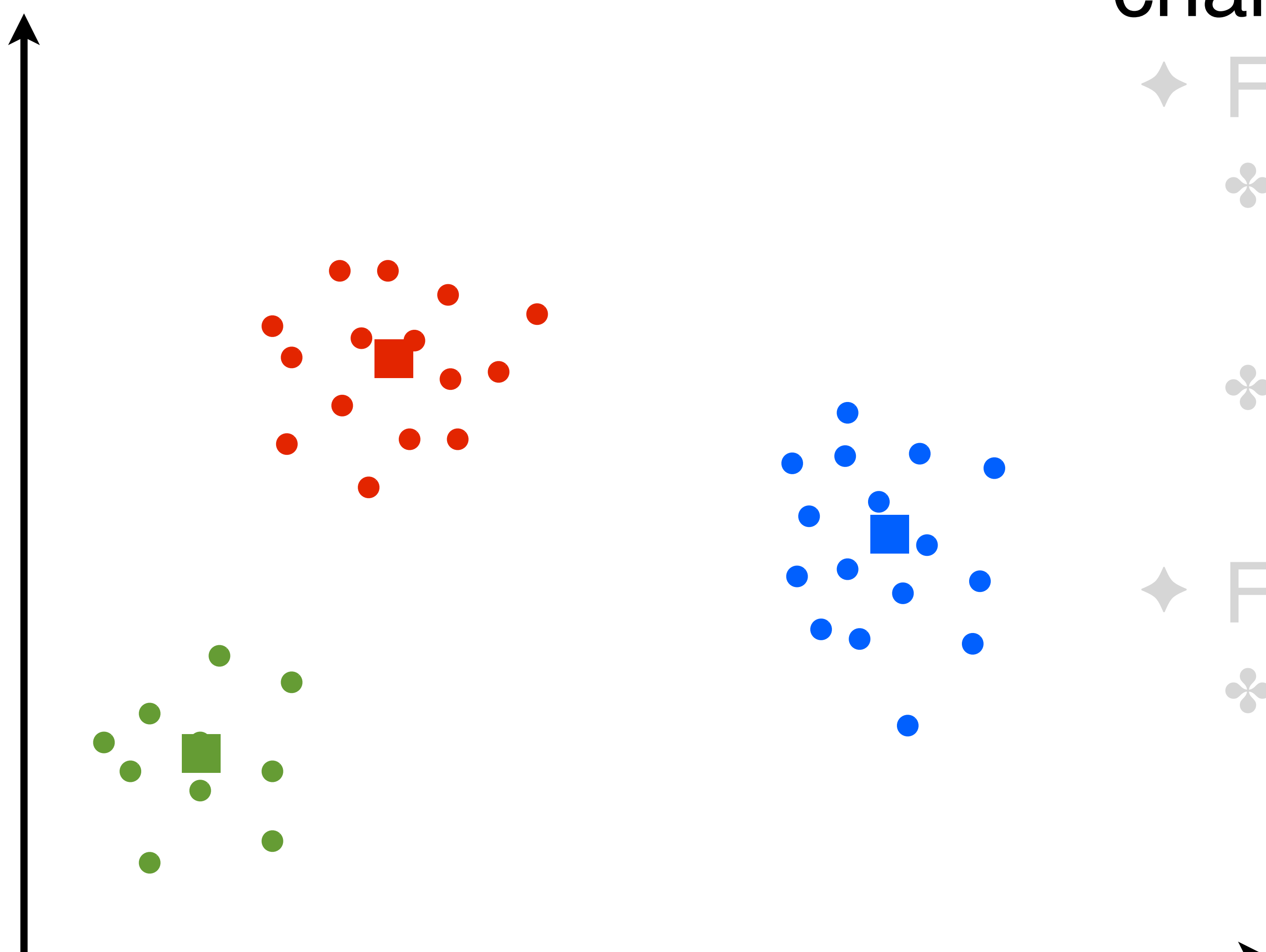

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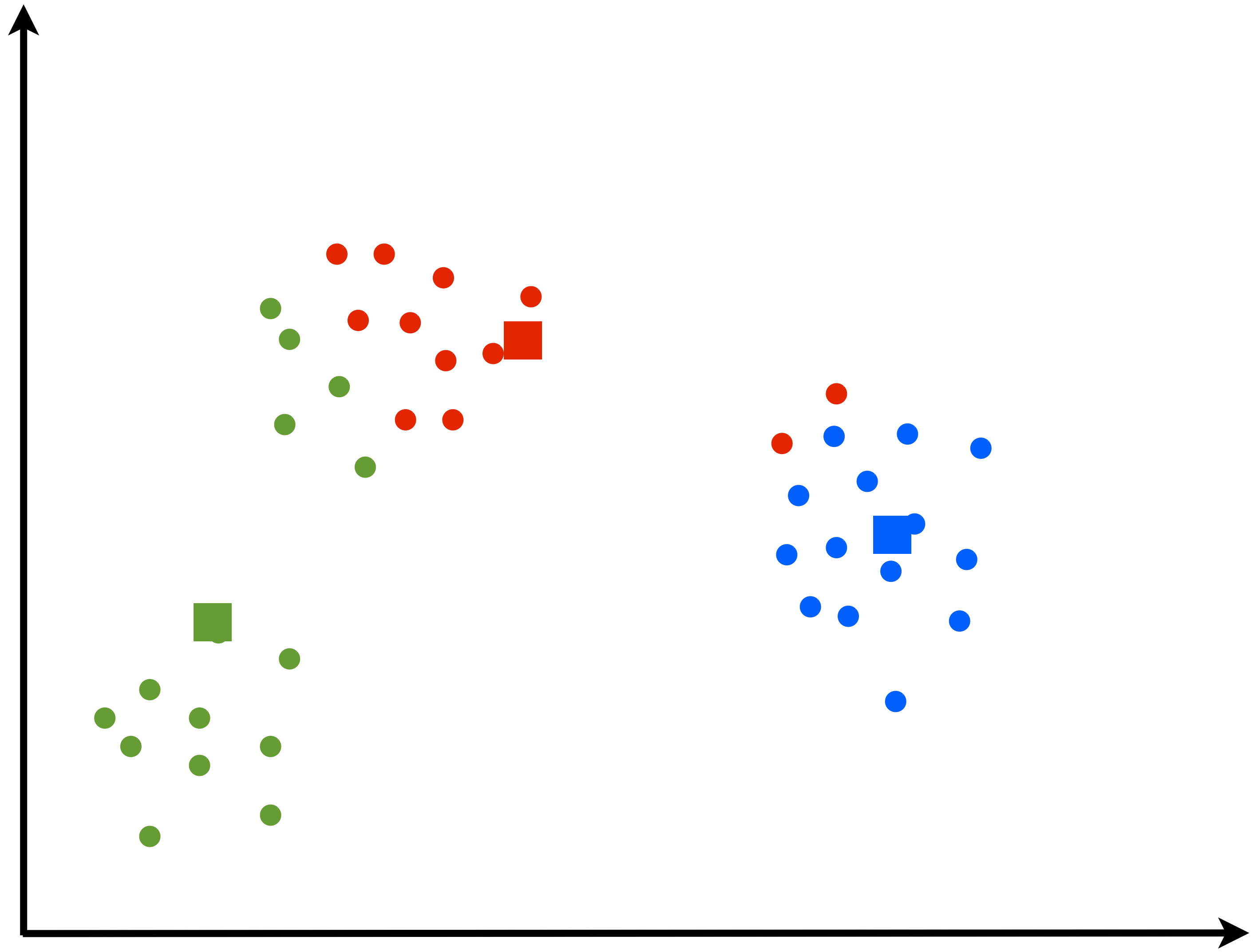
K-Means: Evaluation



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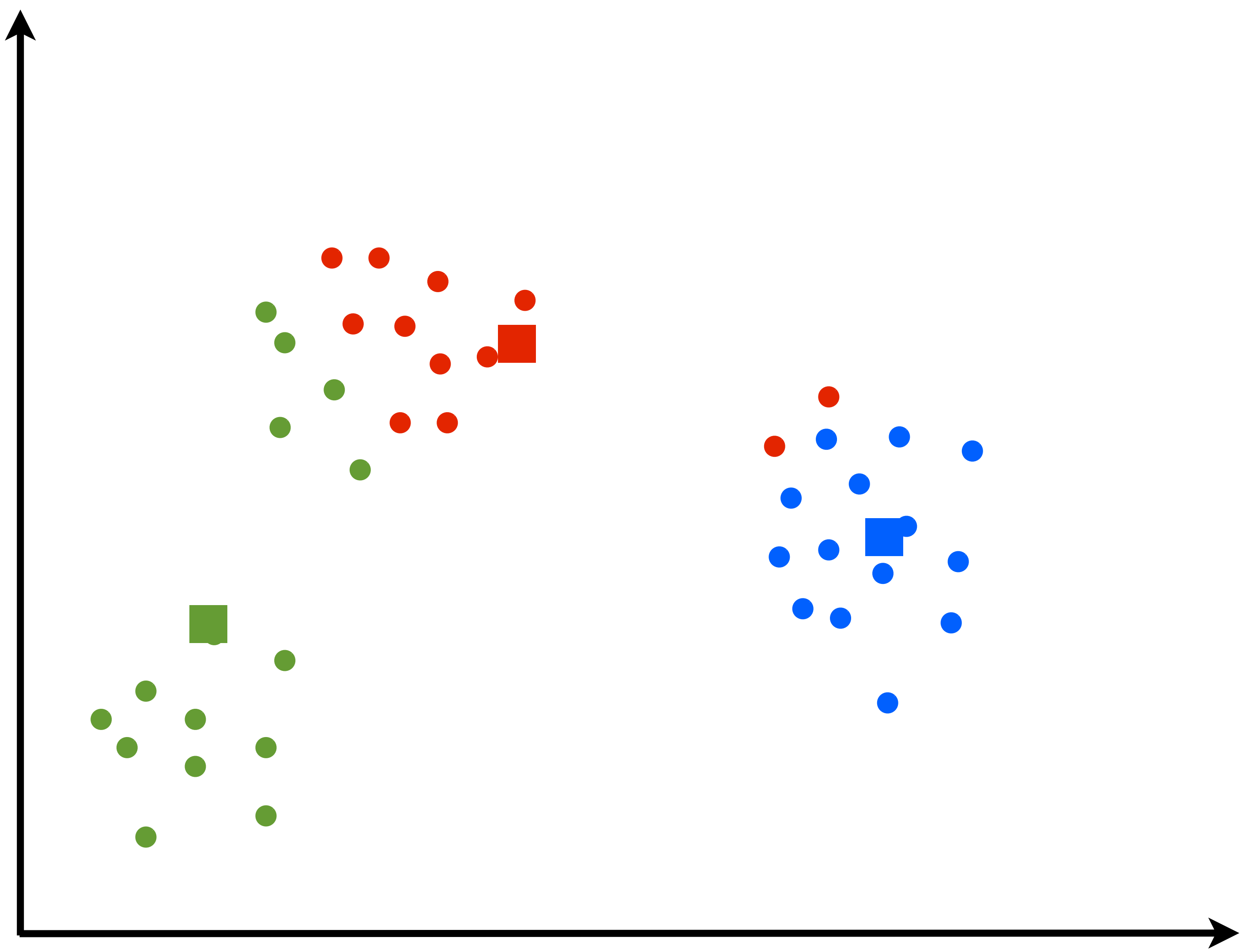
K-Means: Evaluation

- Will it terminate?
  Yes. Always.



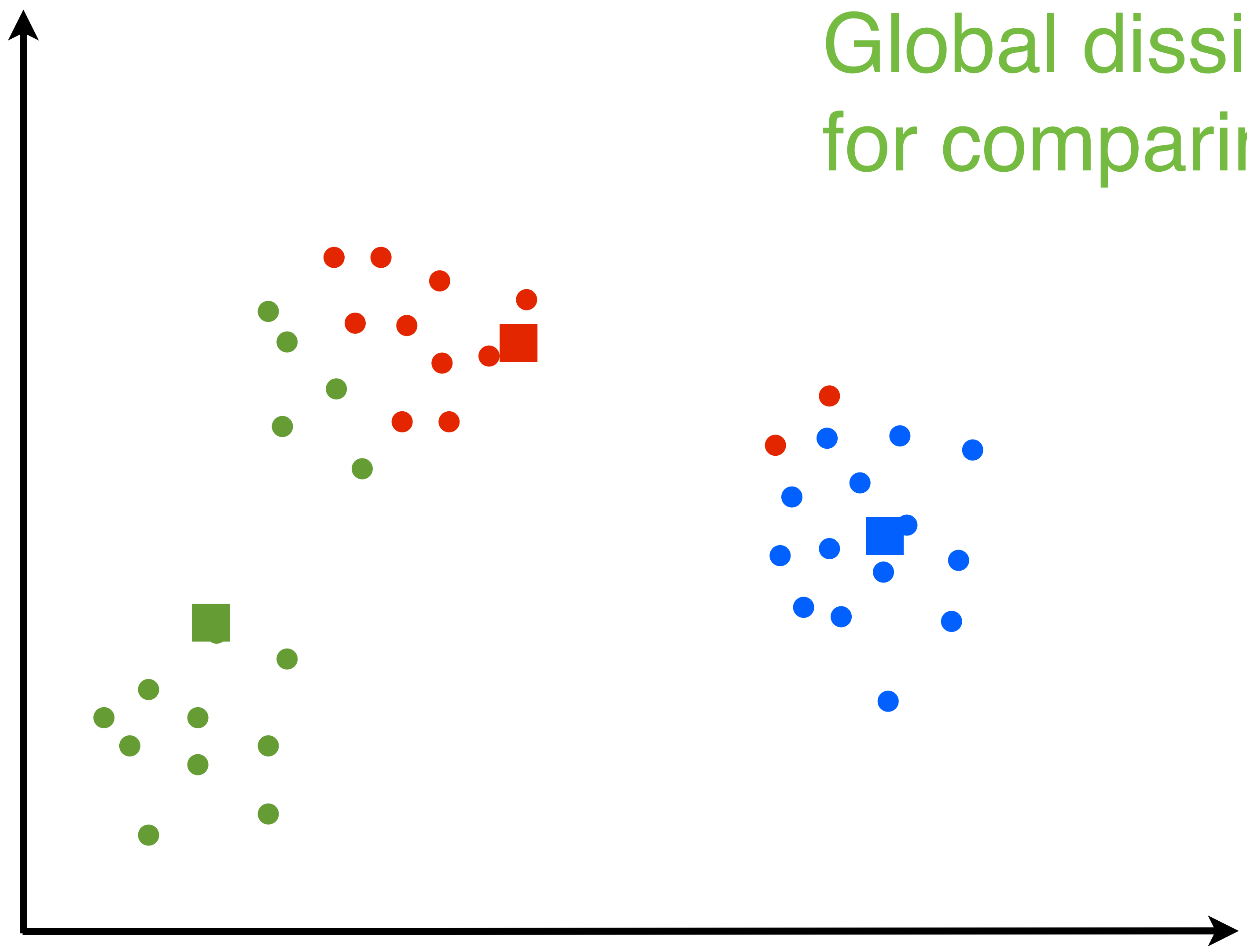
K-Means: Evaluation

- Will it terminate?

  Yes. Always.

- Is the clustering any good?

  Global dissimilarity only useful for comparing clusterings.



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K-Means: Evaluation

- Guaranteed to converge in a finite number of iterations

- Running time per iteration:
  1. Assign data points to closest cluster center
     O(KN) time
  2. Change the cluster center to the average of its assigned points
     O(N) time

slide by David Sontag

K-Means: Evaluation

Objective $$\min_{\mu} \min_{C} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2$$

1. Fix μ, optimize C:

$$\min_{C} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2 = \min_{c} \sum_{i}^{n} \left|x_i - \mu_{x_i}\right|^2$$

$\boxed{\textit{Step 1 of kmeans}}$

2. Fix C, optimize μ:

$$\min_{\mu} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2$$

– Take partial derivative of μ_i and set to zero, we have

$$\mu_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$$

$\boxed{\textit{Step 2 of kmeans}}$

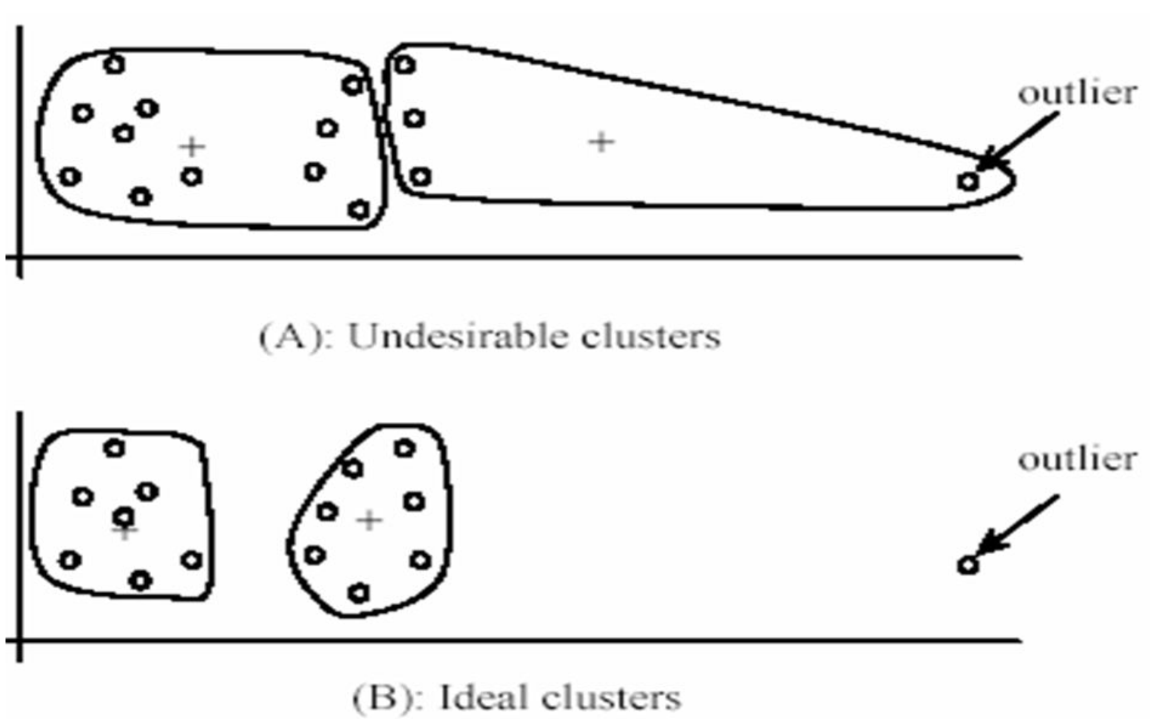
K-Means takes an alternating optimization approach, each step is guaranteed to decrease the objective – thus guaranteed to converge

slide by Alan Fern

Demo time…

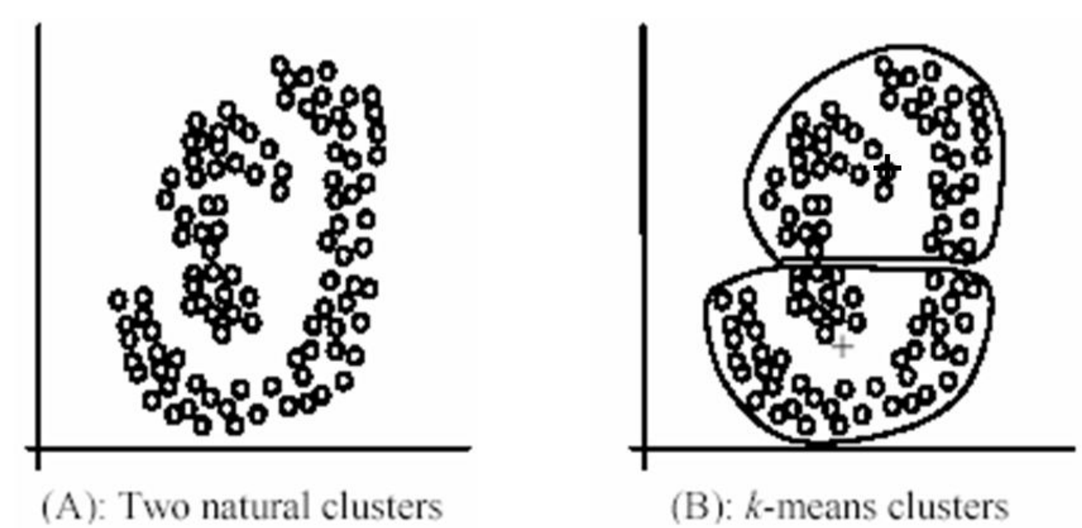
K-Means Algorithm: Some Issues

- How to set k?
- Sensitive to initial centers
  - Multiple initializations
- Sensitive to outliers
- Detects spherical clusters
- Assuming means can be computed
  - It requires continuous, numerical features



(A): Undesirable clusters

(B): Ideal clusters



(A): Two natural clusters

(B): *k*-means clusters

slide by Kristen Grauman

Next Lecture:

K-Means Applications,
Spectral clustering,
Hierarchical clustering and
What is a good clustering?