



SE ZG568 / SS ZG568, Applied Machine Learning Lecture No. 15 [11- May-2025]



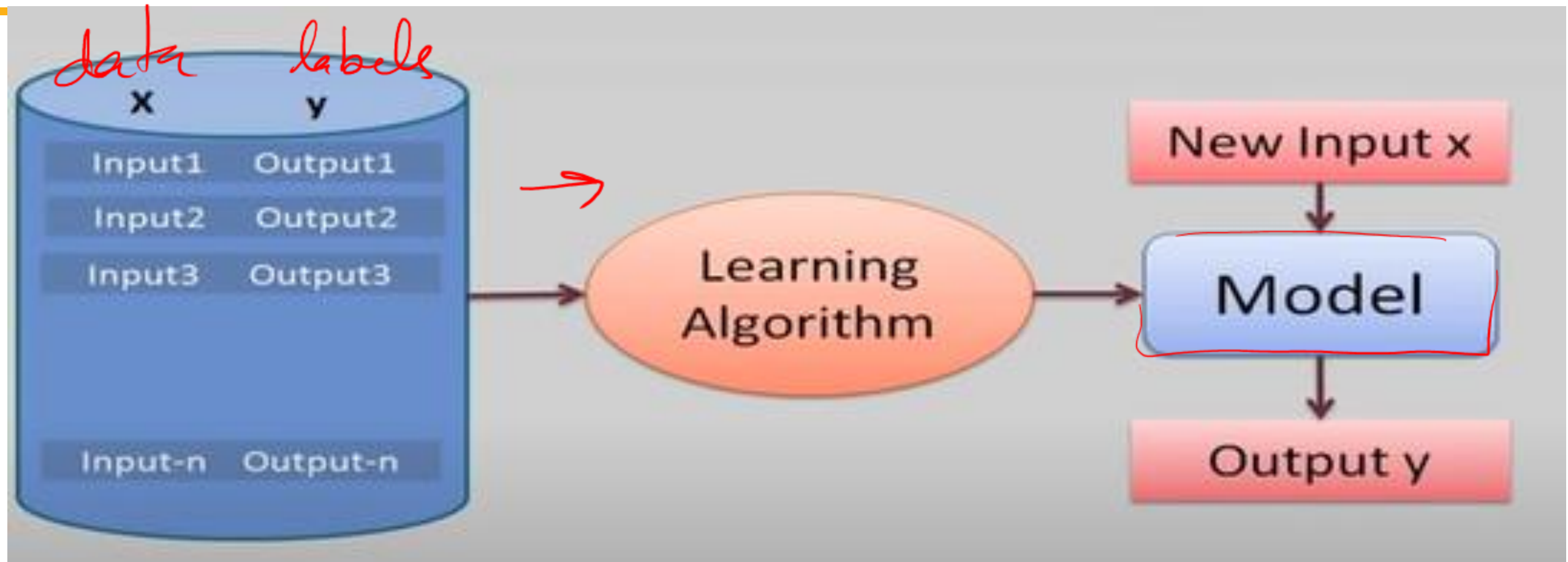
Topic of Discussion

Unsupervised Learning
K Means Clustering

Acknowledgement

Prof. Tamara Broderick, MIT Institute for Foundations of Data Science (MIFODS)

Supervised Learning



$$[f]: x \rightarrow y$$

Image Source: Prof. Sudeshna Sarkar's lecture

Unsupervised Learning

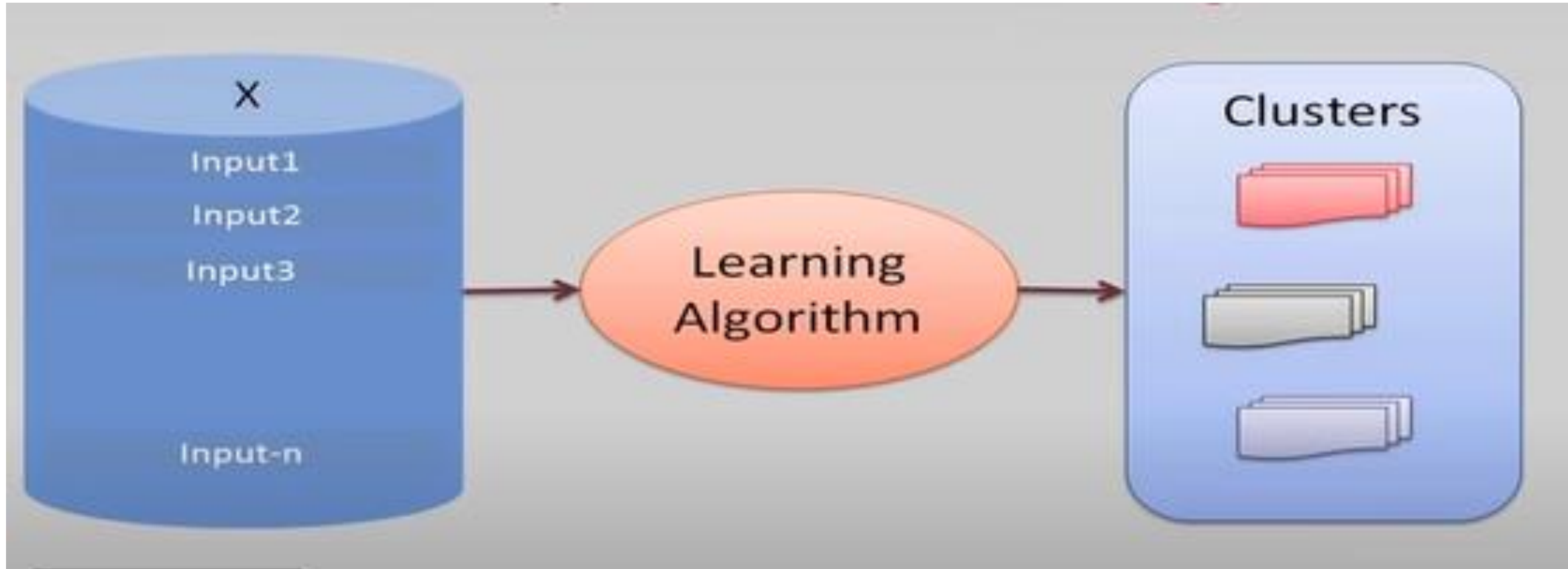
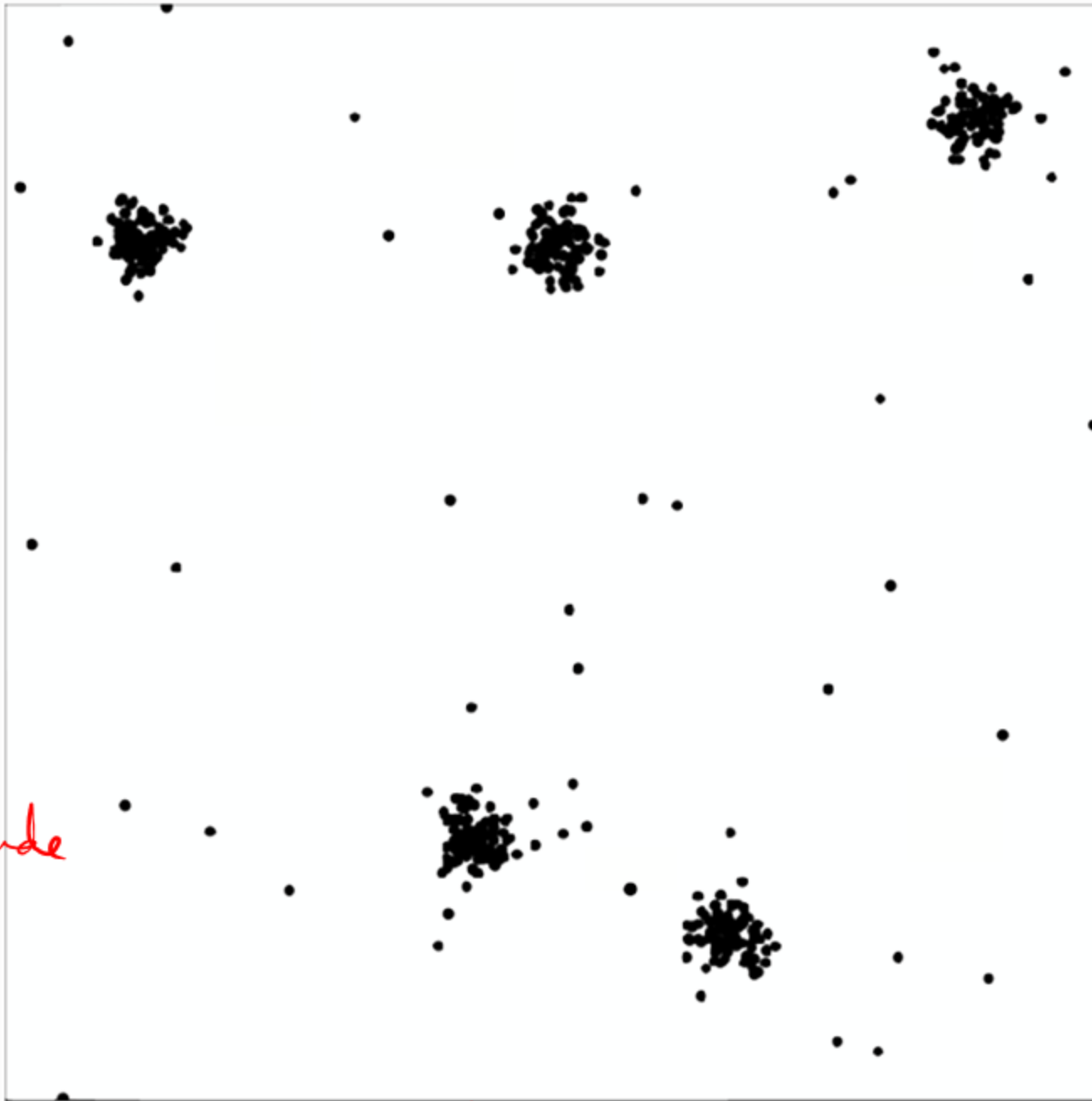


Image Source: Prof. Sudeshna Sarkar's lecture

Food distribution placement

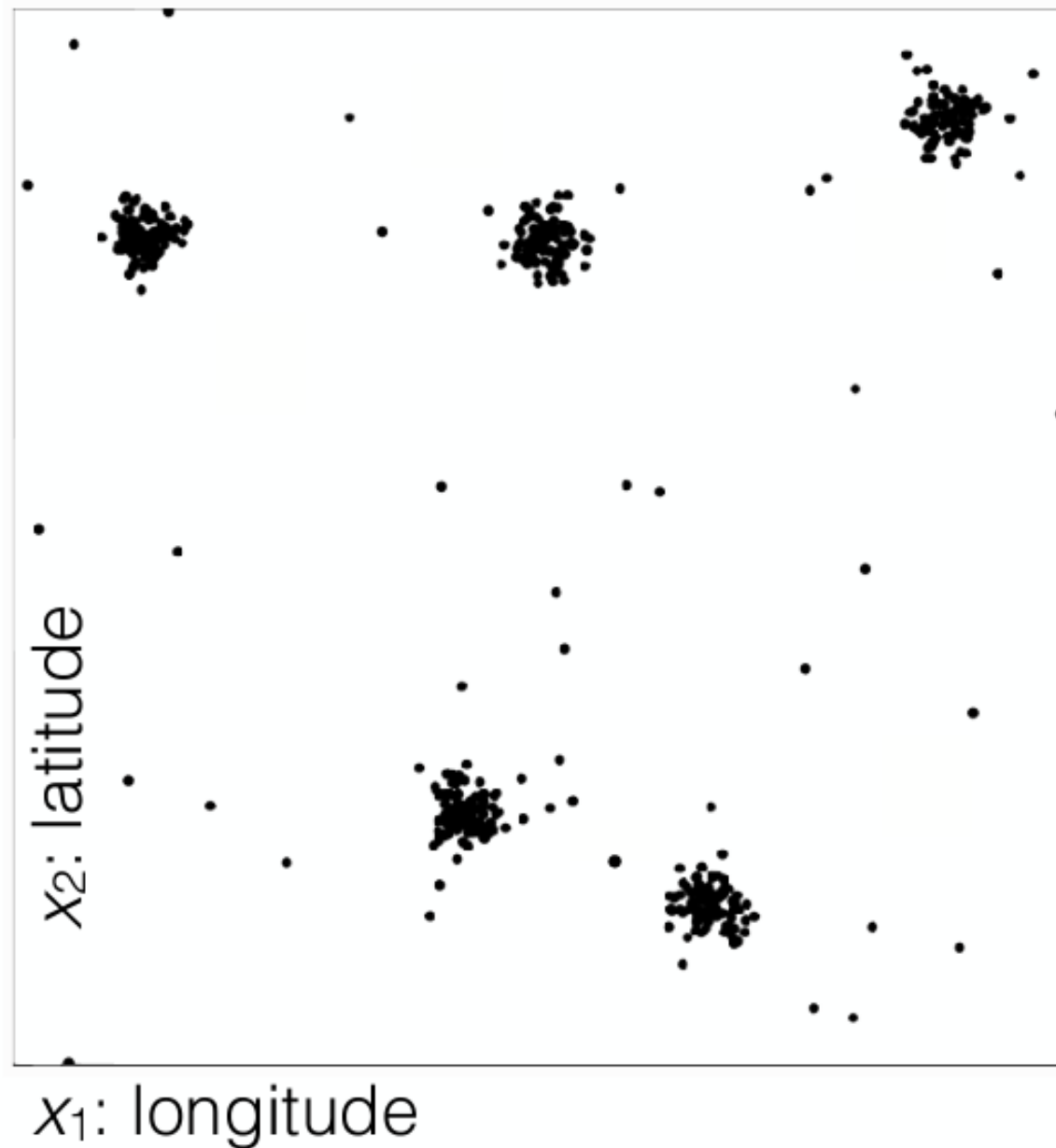
- Where should I have my k food trucks park?



latitude
 x_2

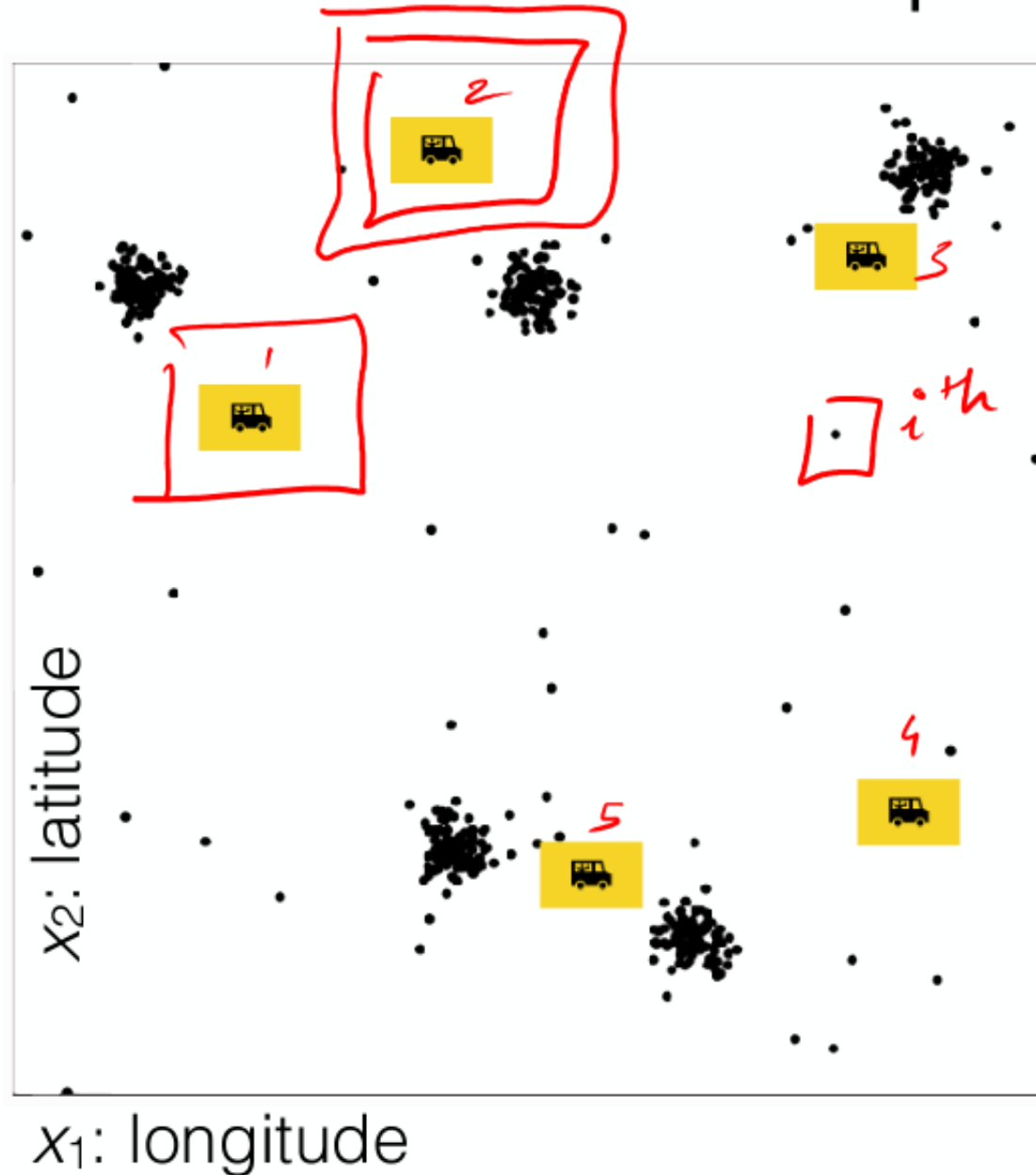
x_1 : longitude

Food distribution placement



- Where should I have my k food trucks park?
- Want to minimize the loss of people we serve

Food distribution placement



- Where should I have my k food trucks park?
- Want to minimize the loss of people we serve
- Person i location $x^{(i)}$
- Food truck j location $\mu^{(j)}$

$k=5 \rightarrow \text{people}$

$$x^{(i)} = \begin{bmatrix} x_1^{(i)} & x_2^{(i)} \end{bmatrix}$$

\downarrow longitude \downarrow latitude

$j = 1 \text{ to } k$

$$\mu^{(1)} = \begin{bmatrix} \mu_1^{(1)} & \mu_2^{(1)} \end{bmatrix}$$

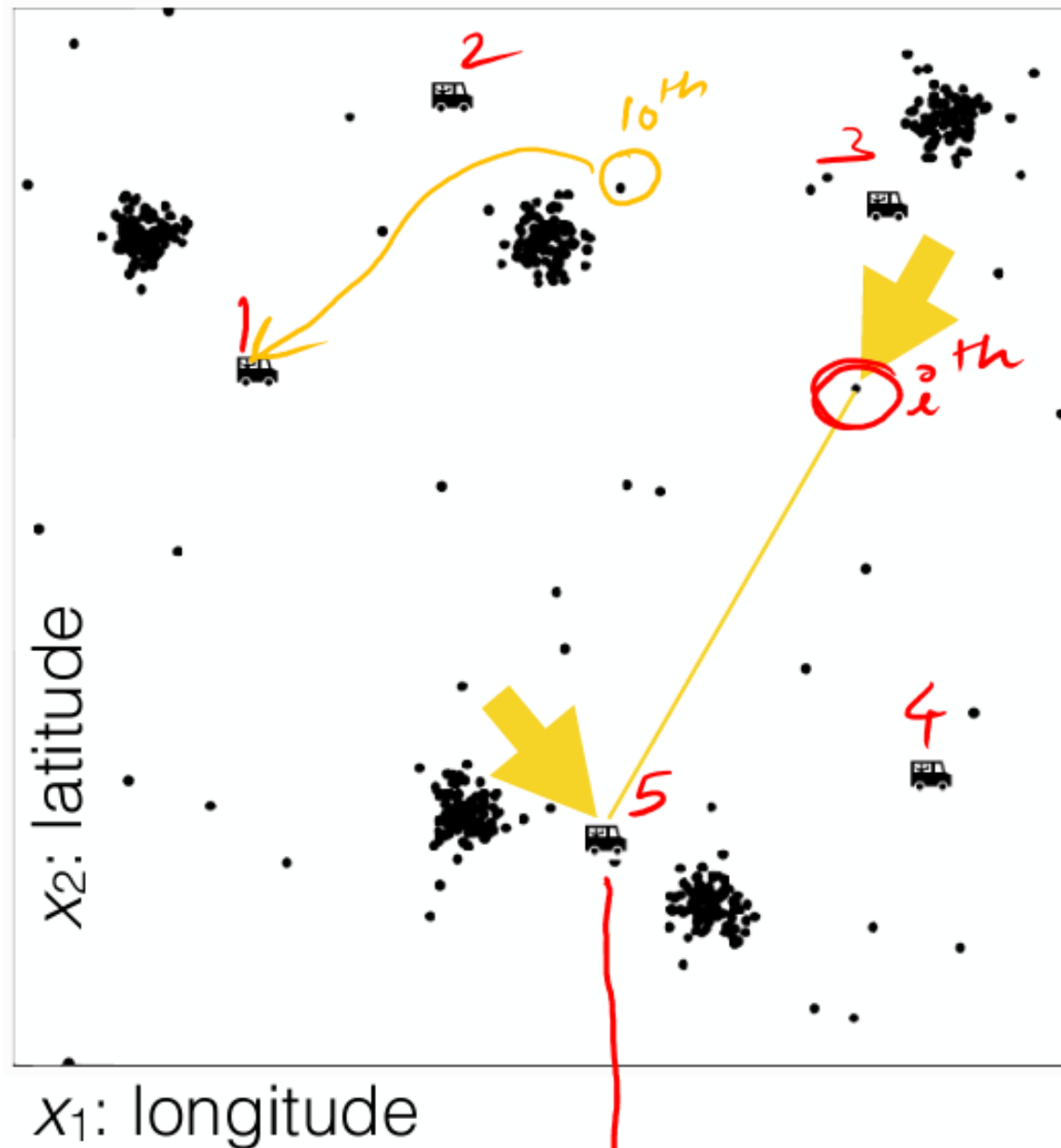
$$\mu^{(2)} = \begin{bmatrix} \mu_1^{(2)} & \mu_2^{(2)} \end{bmatrix}$$

} Truck position

$i = 1 \text{ to } n$

" n " people or " n " data instance

Food distribution placement



- Where should I have my k food trucks park?
- Want to minimize the loss of people we serve
- Person i location $x^{(i)}$
- Food truck j location $\mu^{(j)}$
- Index of truck where person i walks: $y^{(i)}$
- Loss if i walks to truck j :

$$\|x^{(i)} - \mu^{(j)}\|_2^2$$

$$x^{(j)} = \begin{bmatrix} x_1^{(j)} & x_2^{(j)} \end{bmatrix}$$

$$\mu^{(5)} = \begin{bmatrix} \mu_1^{(5)} & \mu_2^{(5)} \end{bmatrix}$$

$$\|x^{(j)} - \mu^{(5)}\|_2^2 = \left((x_1^{(j)} - \mu_1^{(5)})^2 + (x_2^{(j)} - \mu_2^{(5)})^2 \right)$$

k-means algorithm

`k-means(k,)`

k-means algorithm

no of food truck
max. ite

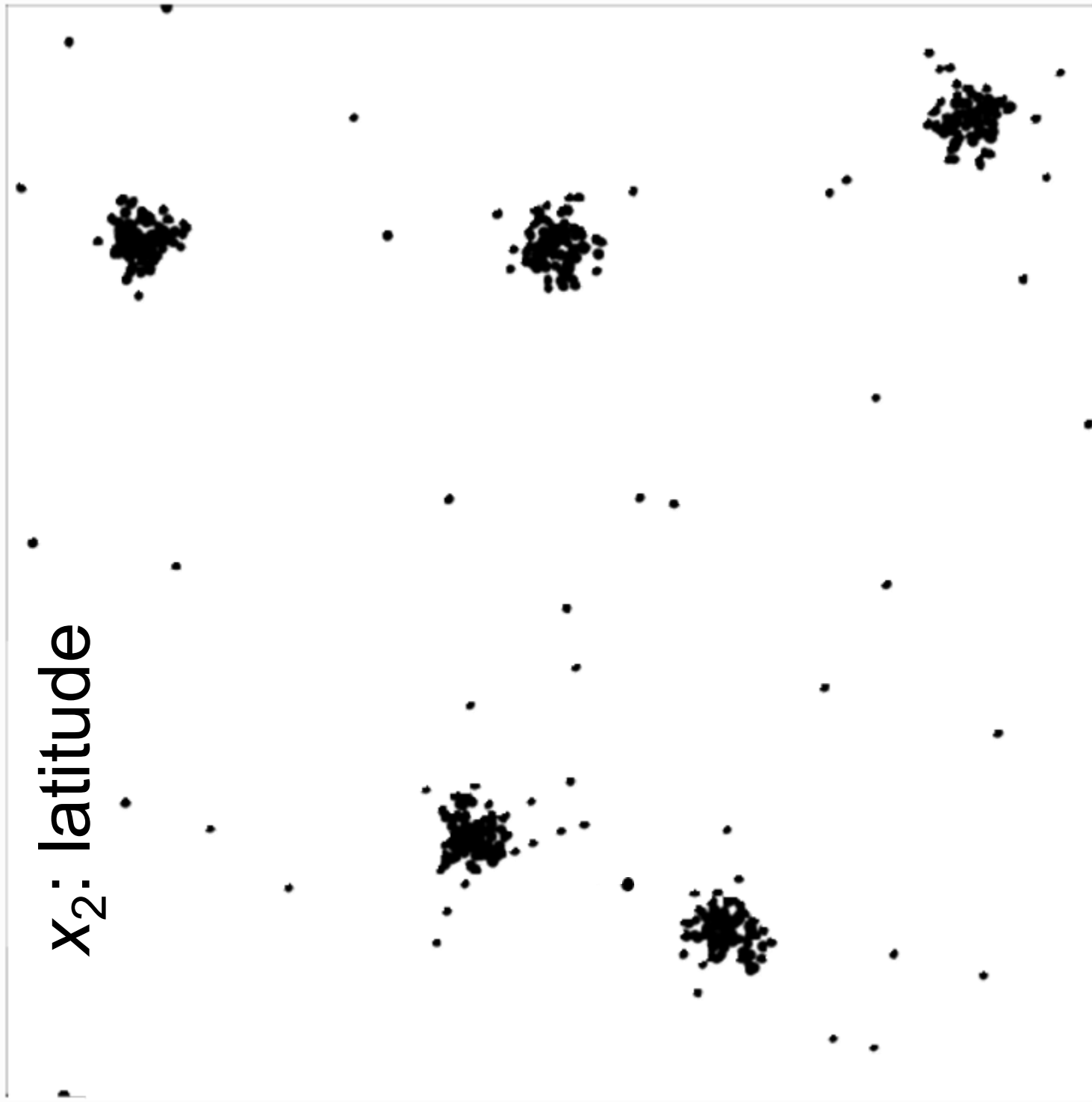
k-means (k , τ)

k-means algorithm

k-means (k, **τ**)

k-means algorithm

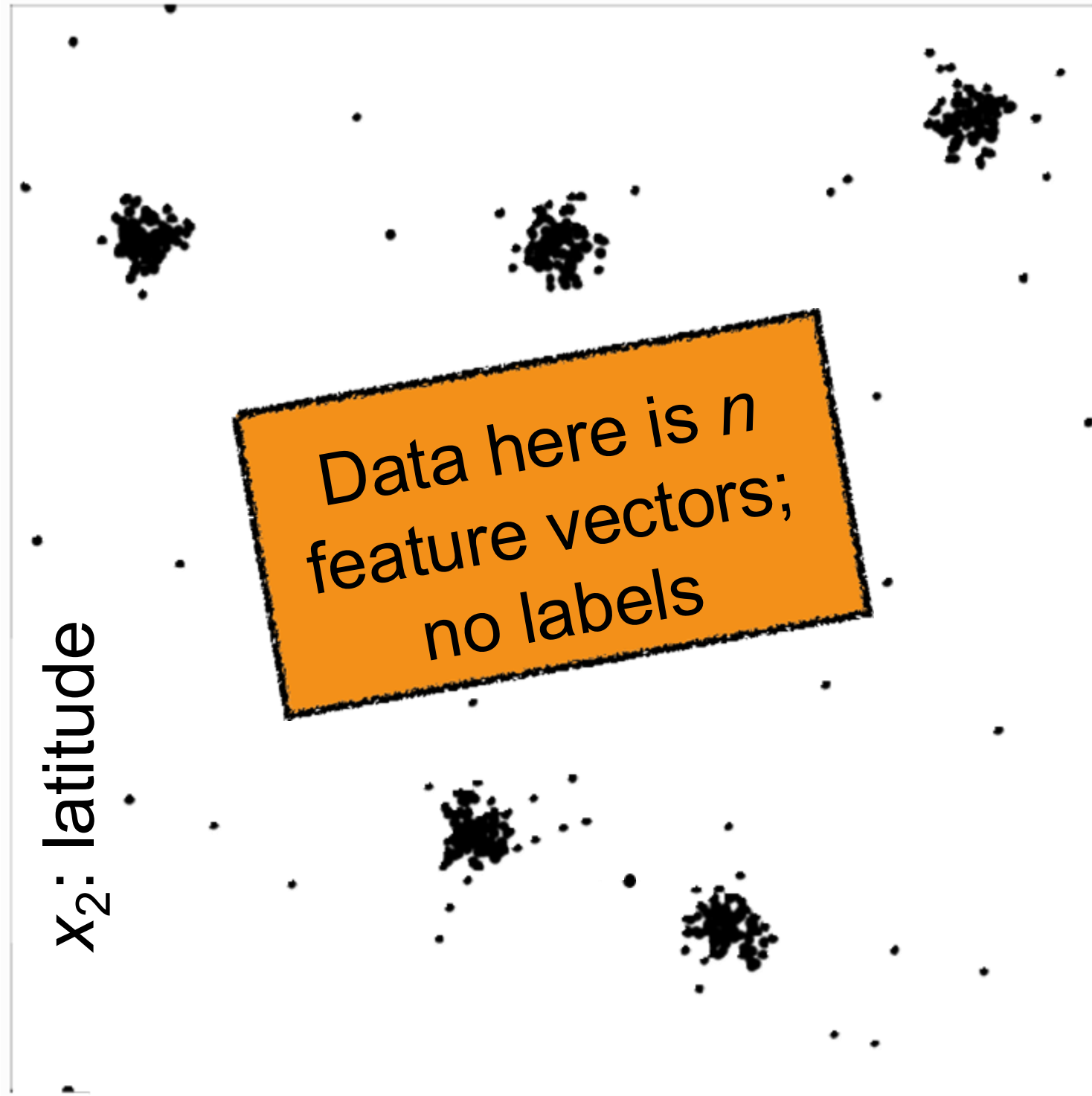
k-means (k, τ)



x_1 : longitude

k-means algorithm

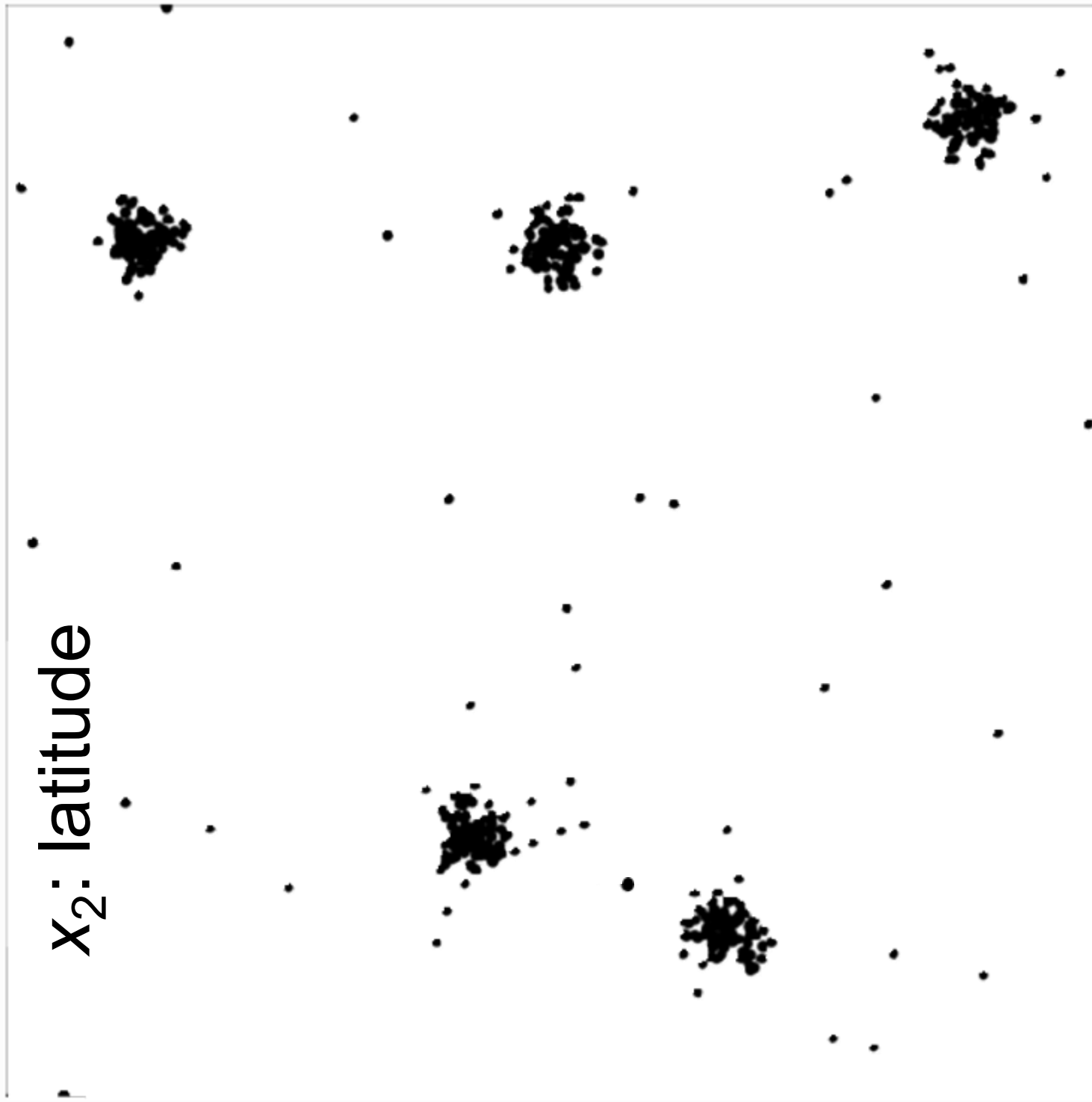
k-means (k, τ)



x_1 : longitude

k-means algorithm

k-means ($k, \boldsymbol{\tau}$)

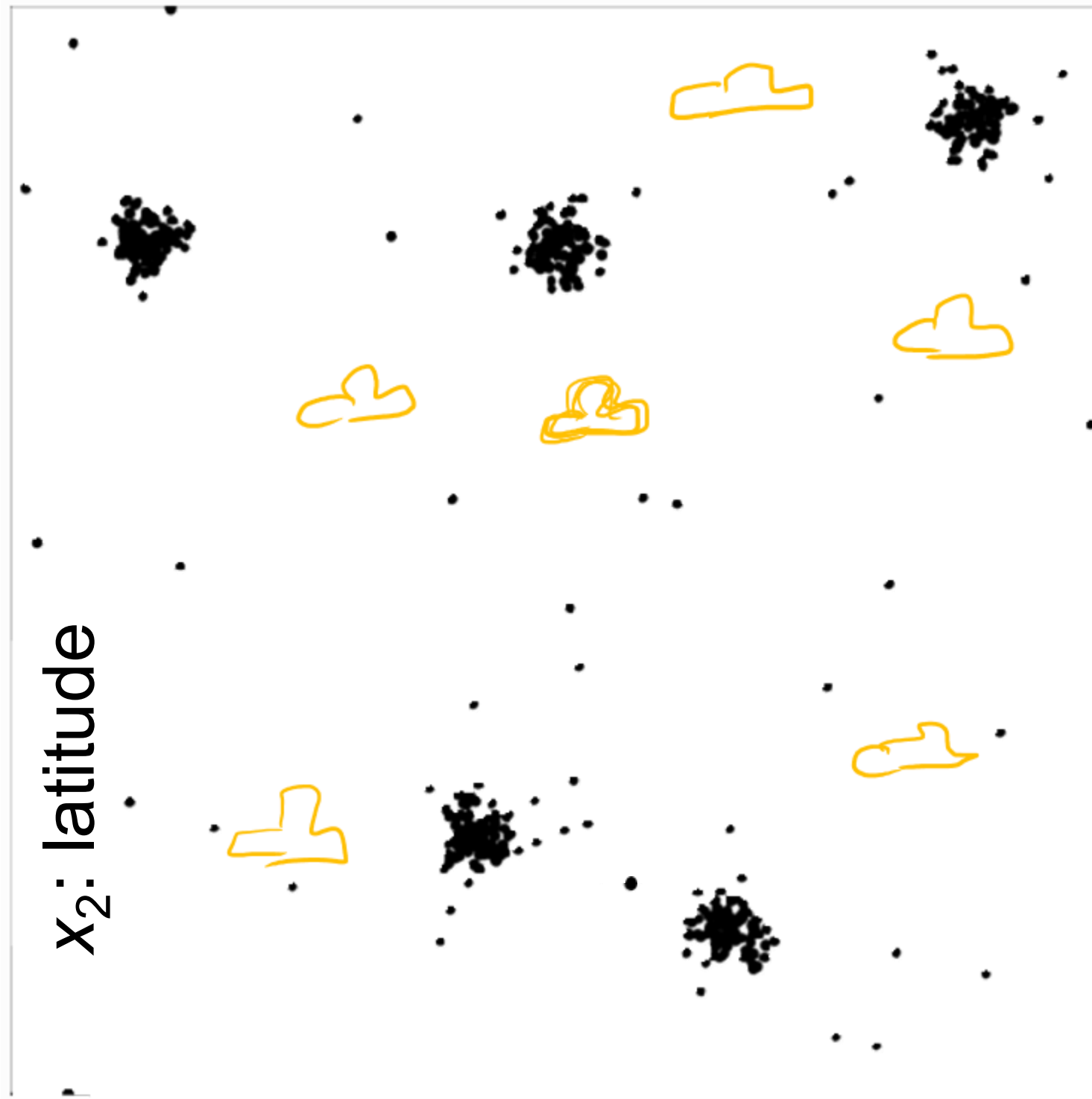


x_1 : longitude

k-means algorithm

k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$



x_1 : longitude

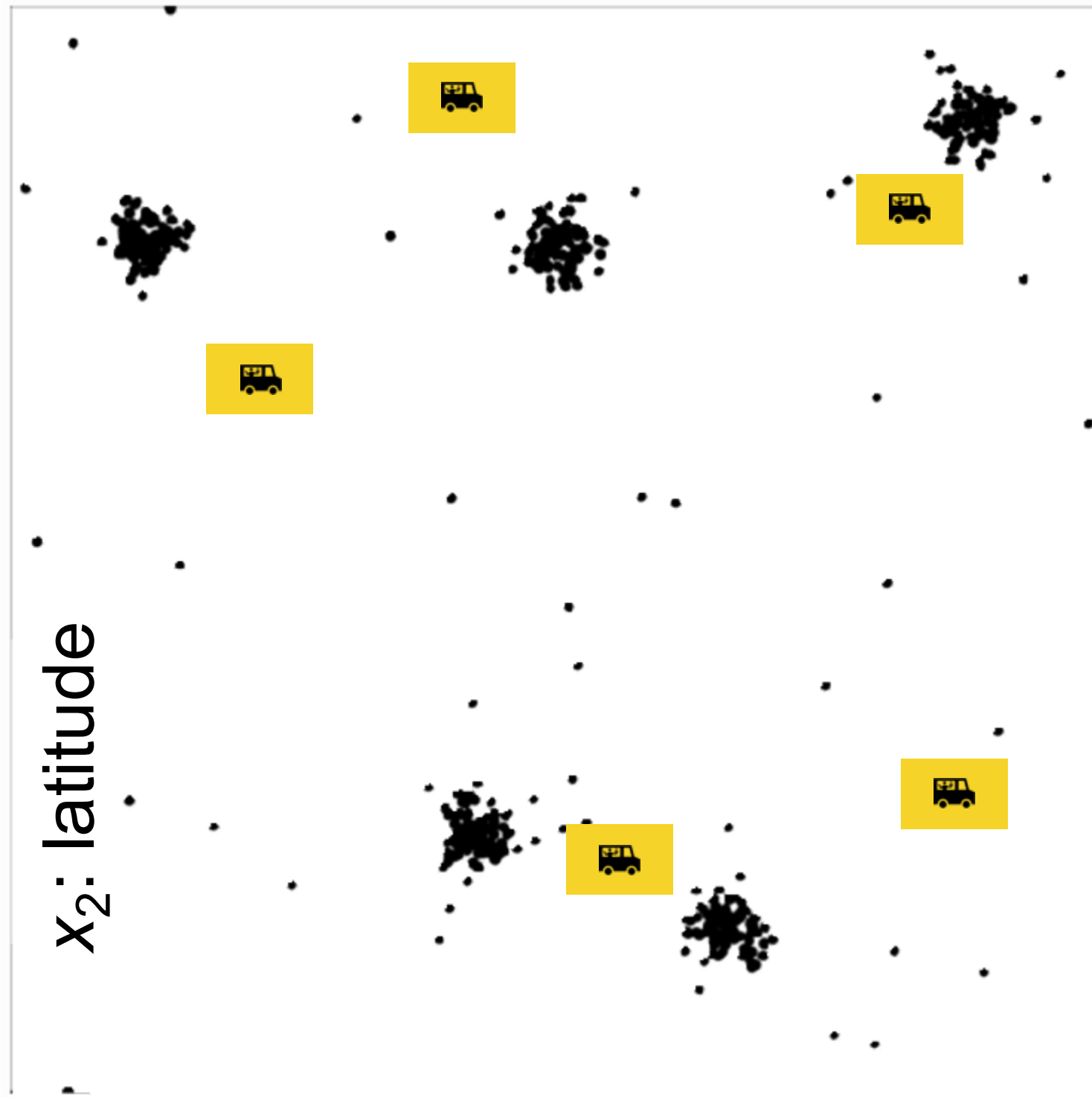
x_2 : latitude

SPB

k-means algorithm

k-means (k, τ)

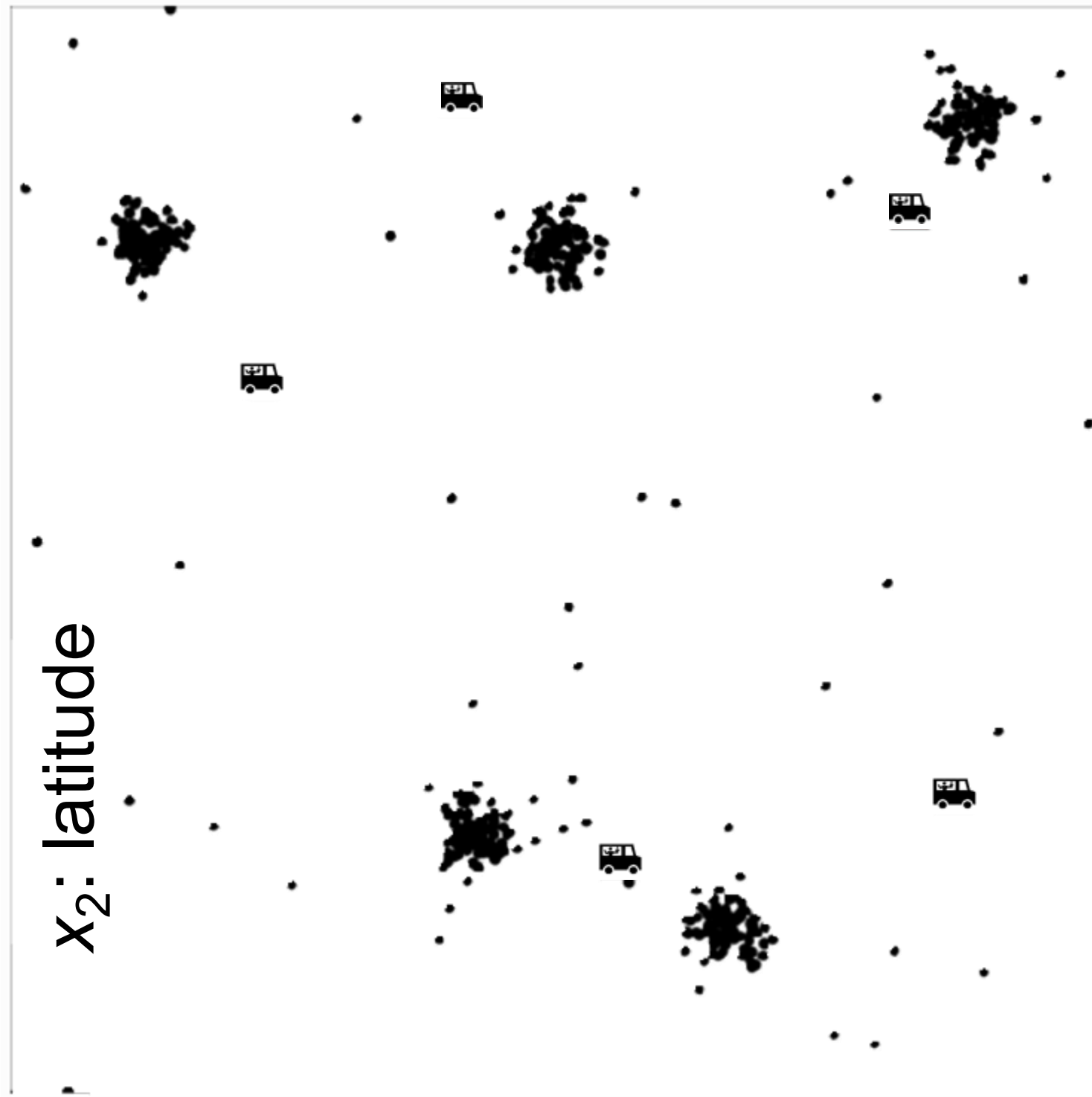
Init $\{\mu^{(j)}\}_{j=1}^k$



x_1 : longitude

x_2 : latitude

k-means algorithm



k-means (k, τ)

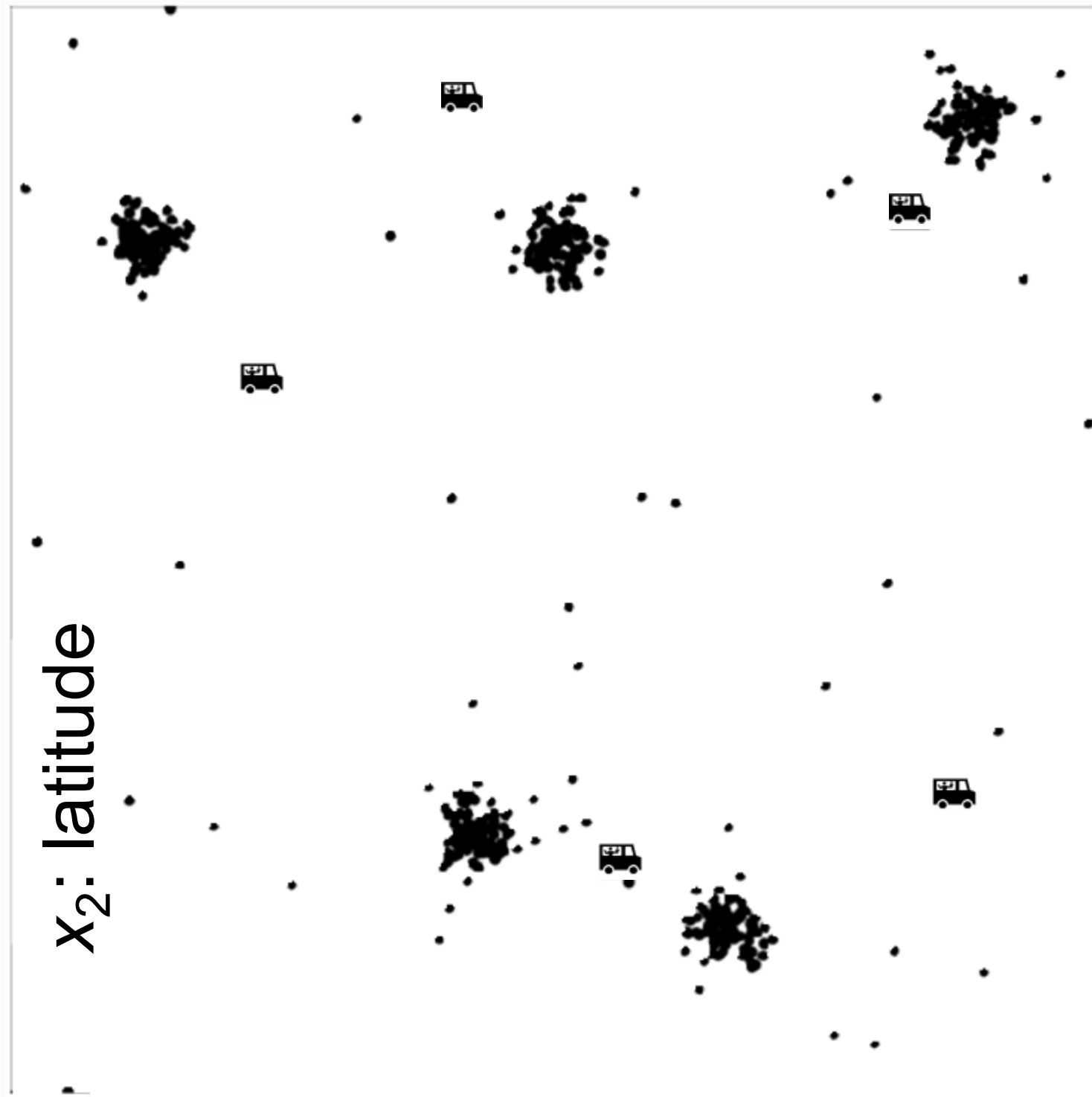
Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ **to** τ

maximal
↑
 τ

x_1 : longitude

k-means algorithm



x_1 : longitude

x_2 : latitude

k-means (k, τ)

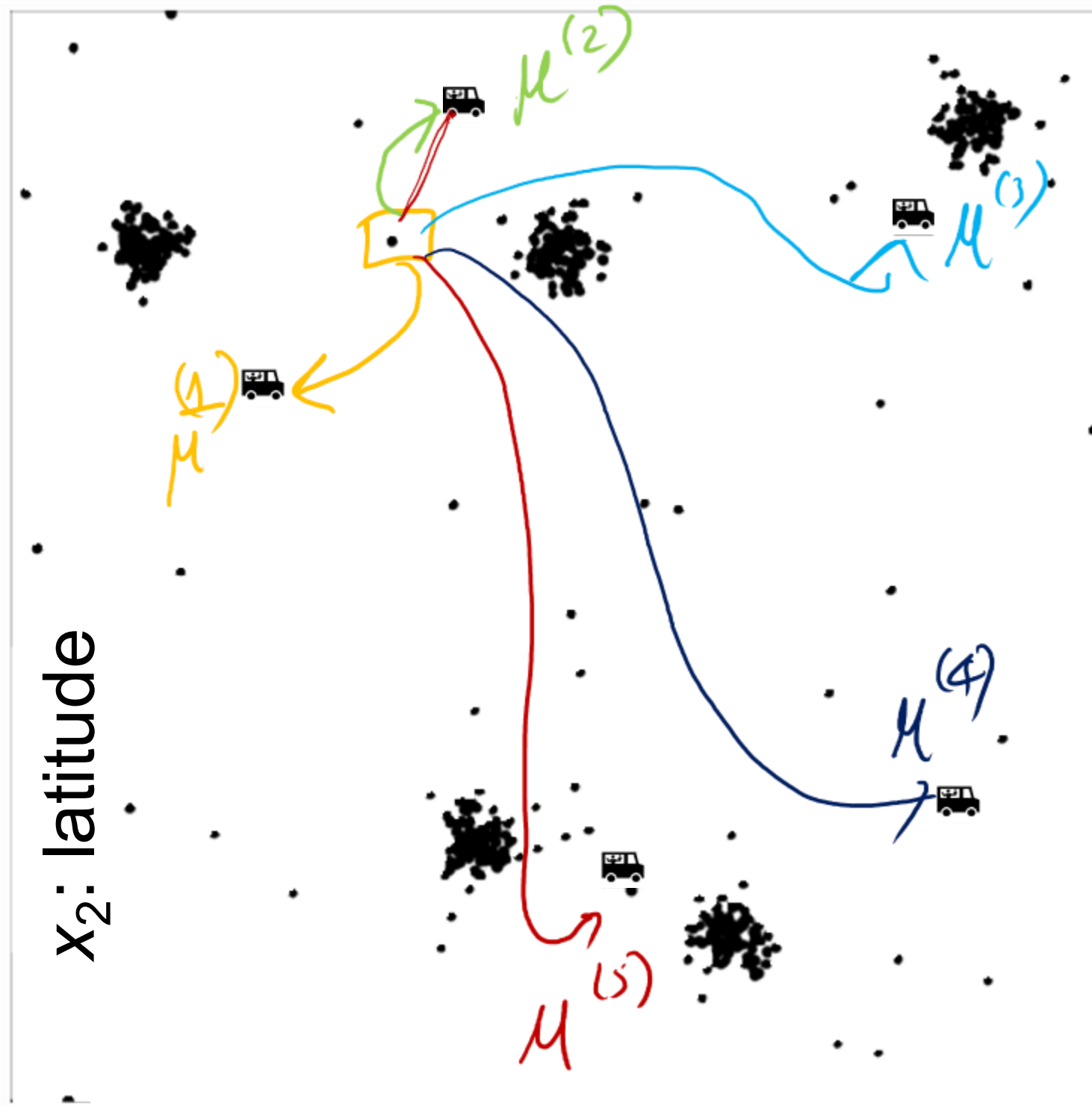
Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

max if
total no of people

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

$$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$$

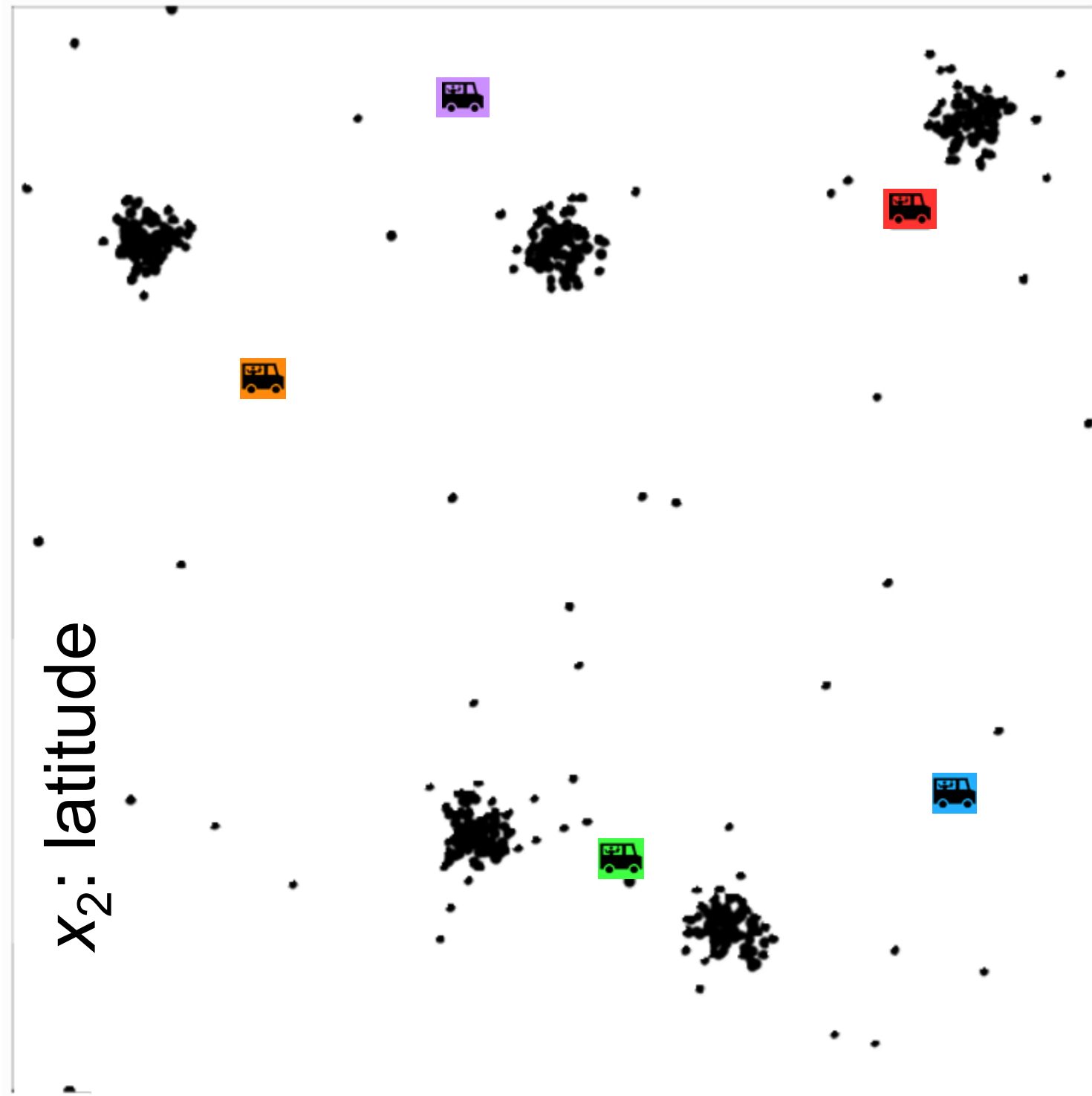
Assignment of $\text{bus } j$ to the i^{th} data instance

$y^{(i)} = 1 \text{ or } 2 \text{ or } 3 \text{ or } 4 \text{ or } 5$

$\min_x (x - s)^2$
 $\arg \min (x - s)^2$
 what is the val of x for which I get a min

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

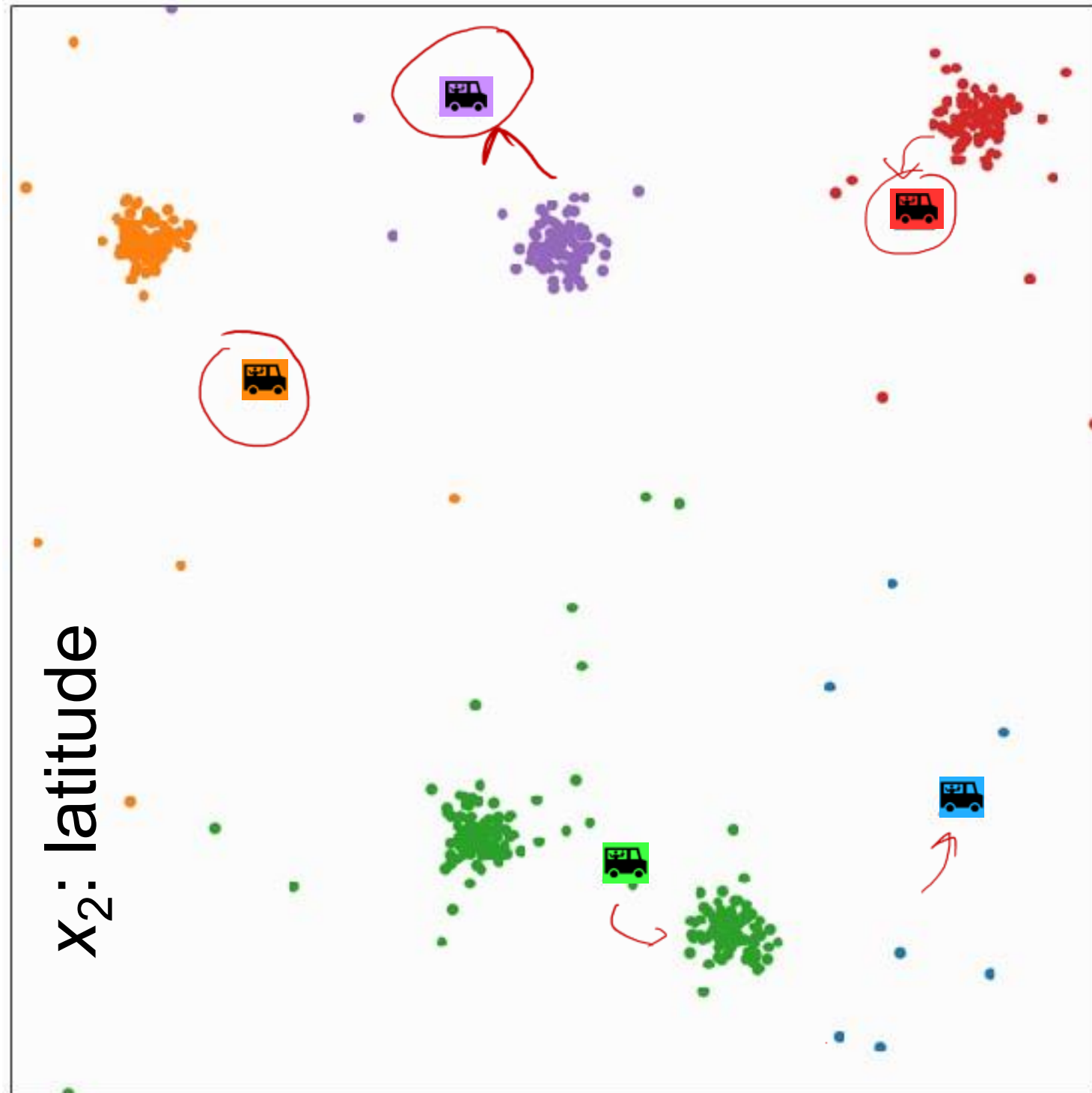
for $t = 1$ to τ

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

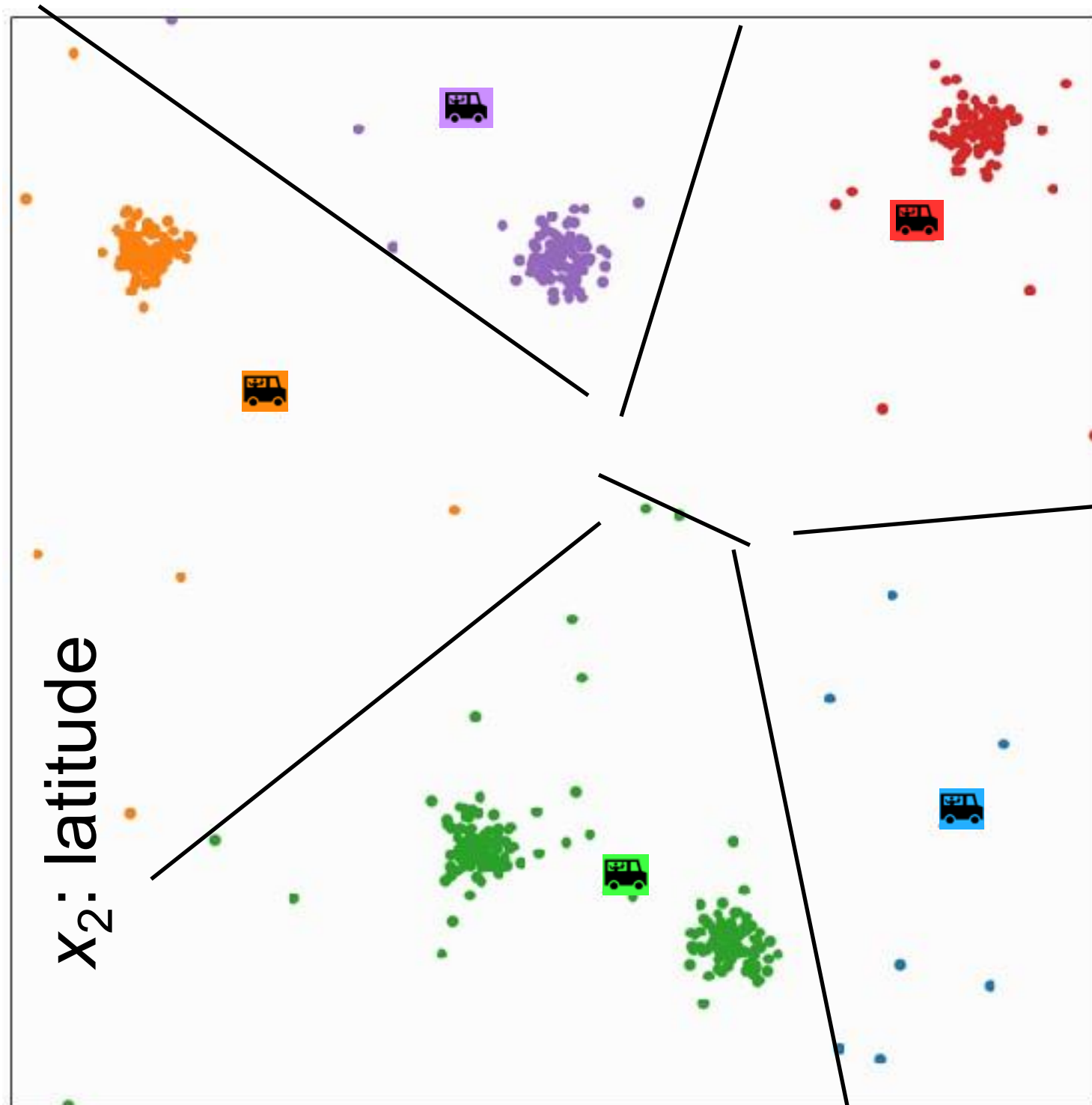
for $t = 1$ to τ

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

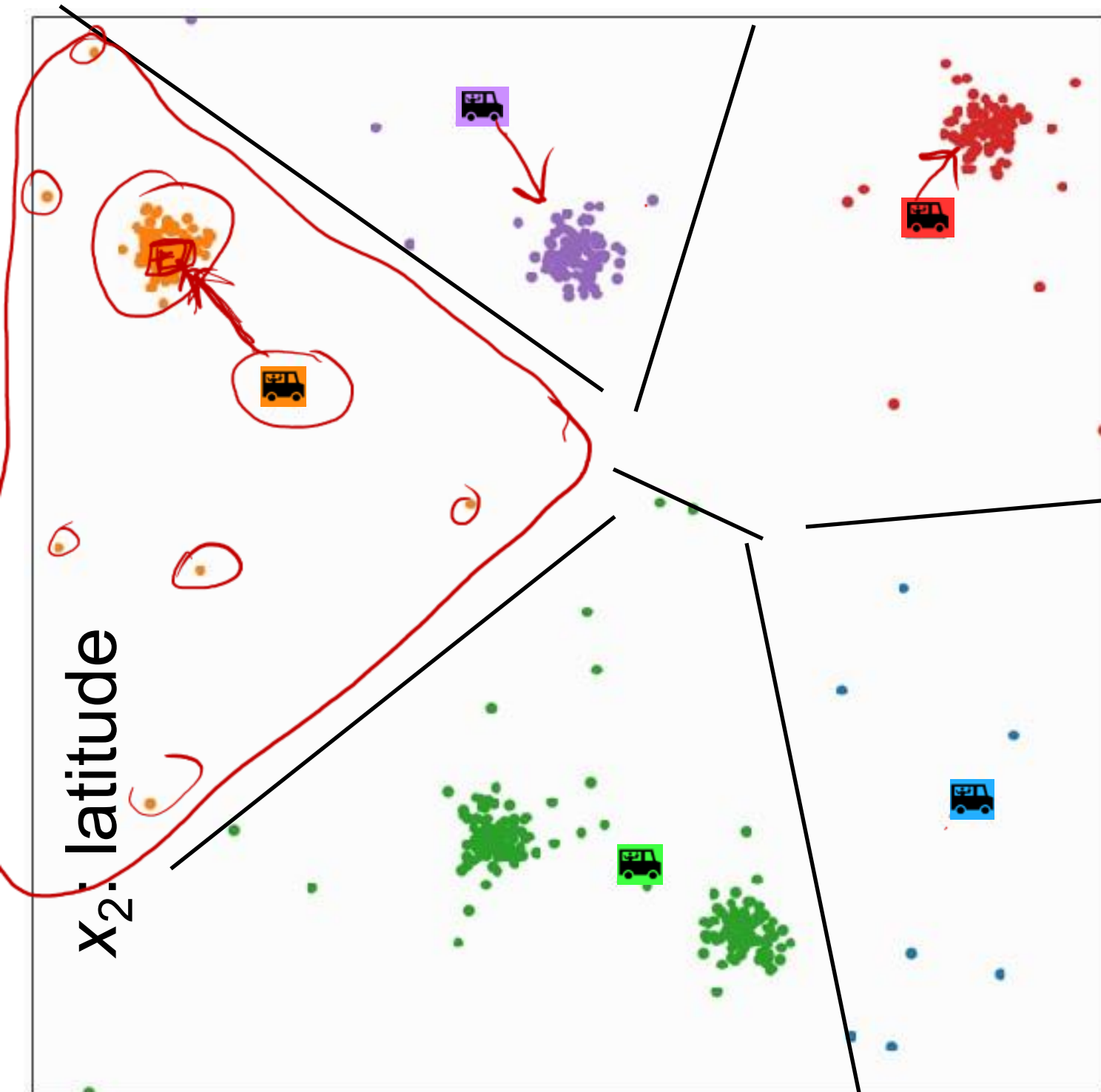
for $t = 1$ to τ

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

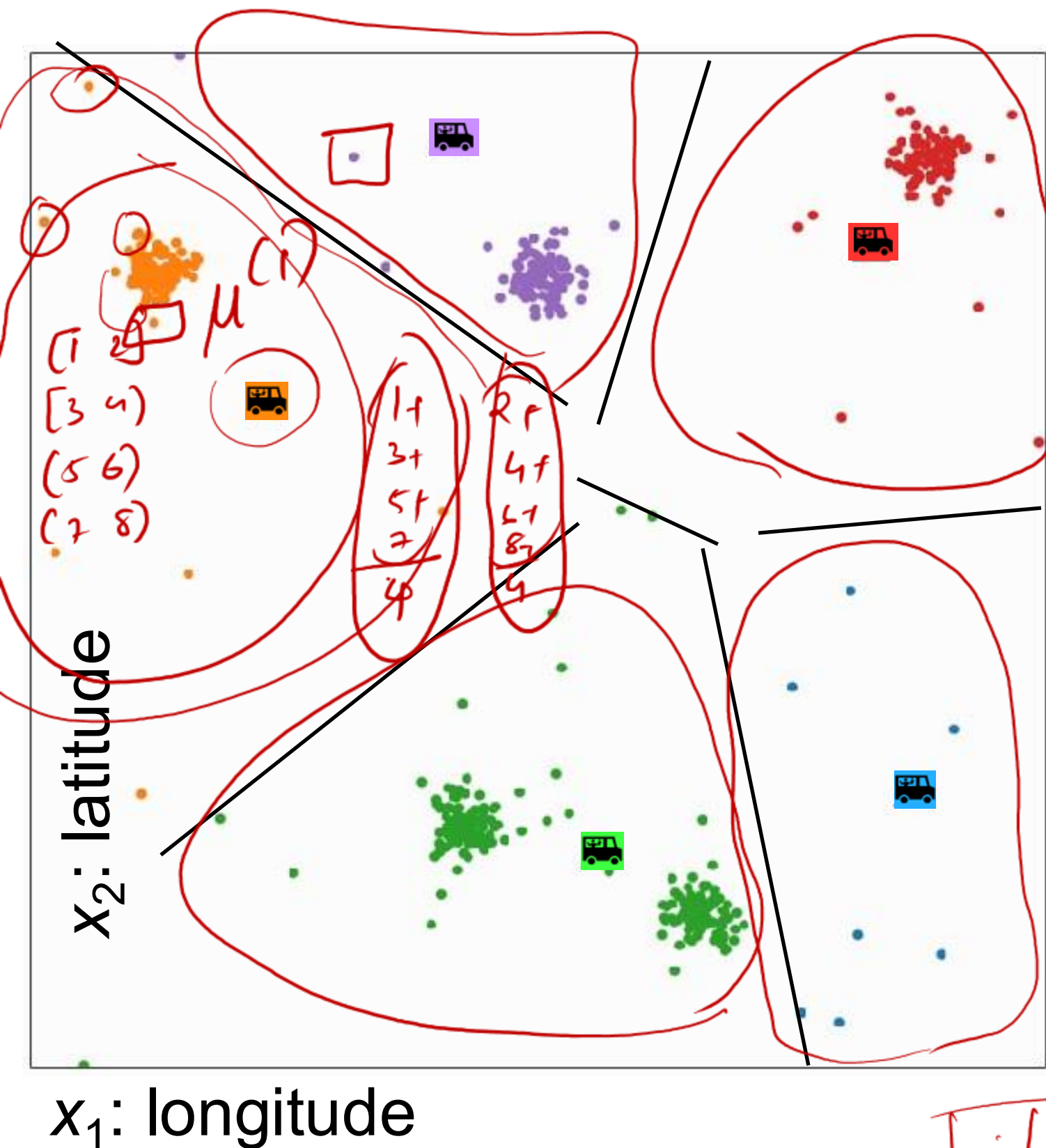
for $t = 1$ to τ

for $i = 1$ to n
assignment is done
 $y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

for $j = 1$ to k
update the position of centroids

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

for $j = 1$ to k

$$\mu^{(j)} = \frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

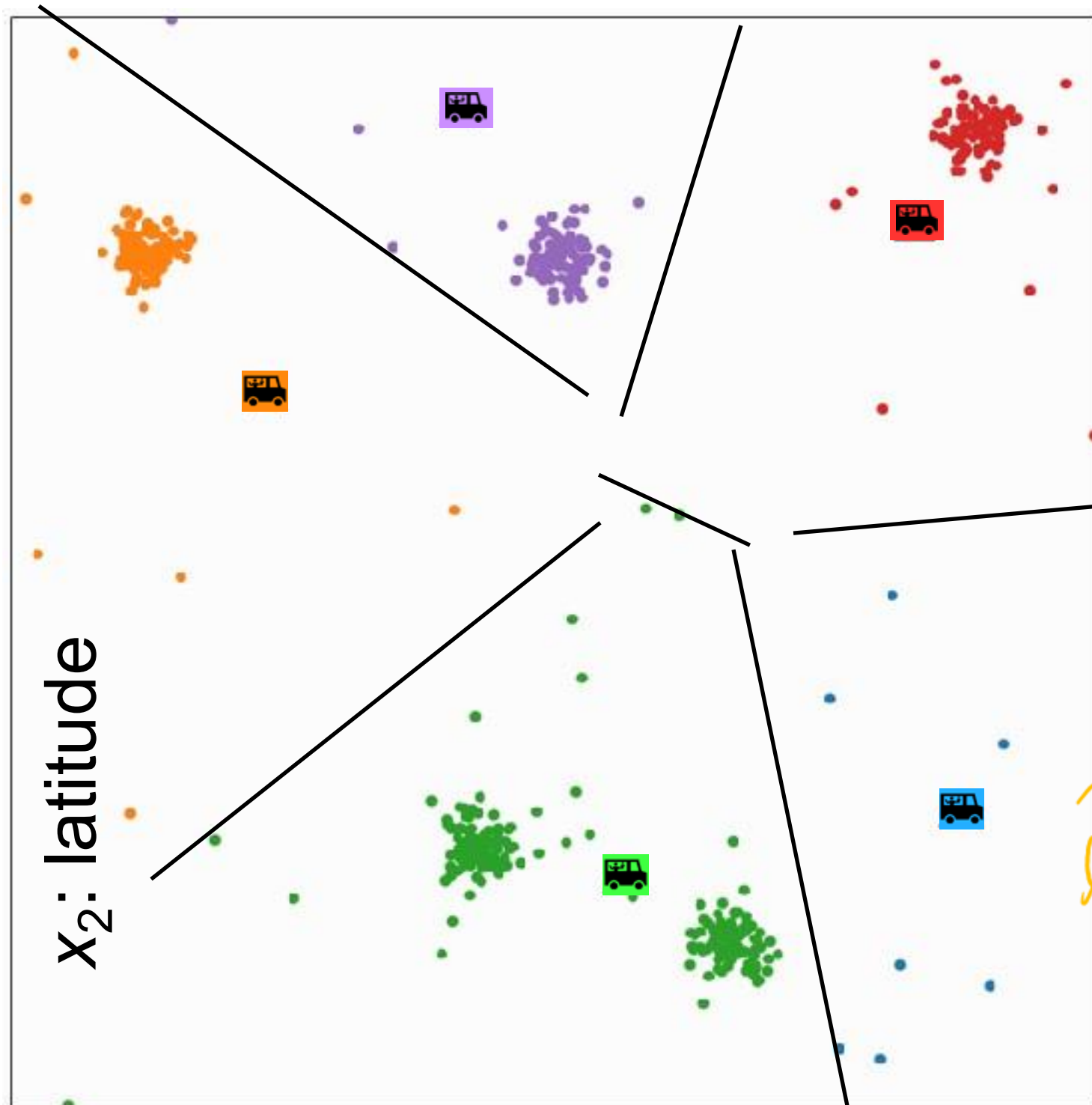
$$\mathbf{1}\{y^{(i)} = j\}$$

if $y^{(i)} = j$ then 1
else 0

3, 4, 5

$$\frac{3+4+5}{3}$$

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

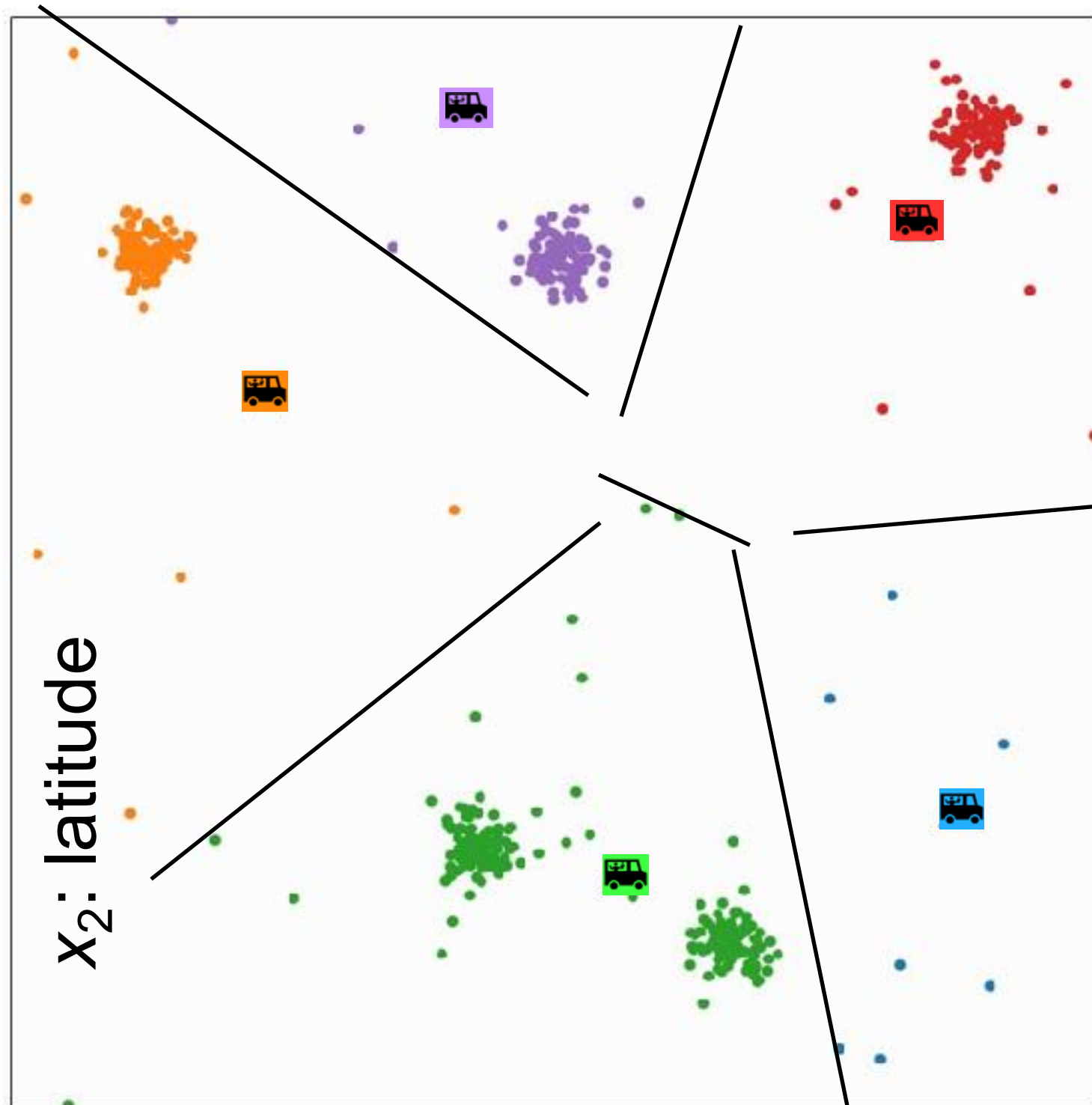
for $t = 1$ to τ

assignment update
for $i = 1$ to n
 $y^{(i)} =$
 $\arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

truck location update
for $j = 1$ to k
 $\mu^{(j)} =$
$$\frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

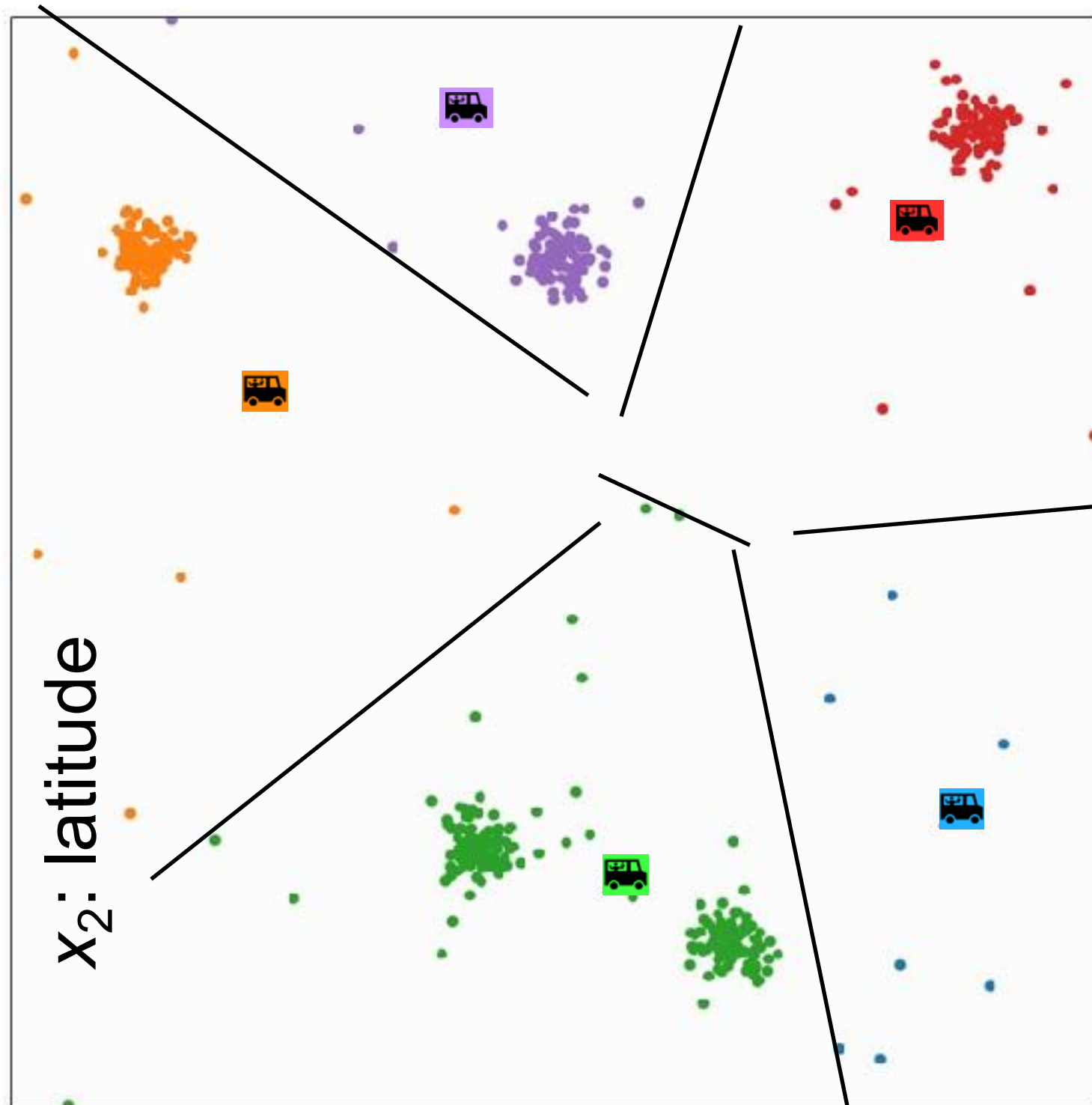
for $i = 1$ to n

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for $j = 1$ to k

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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

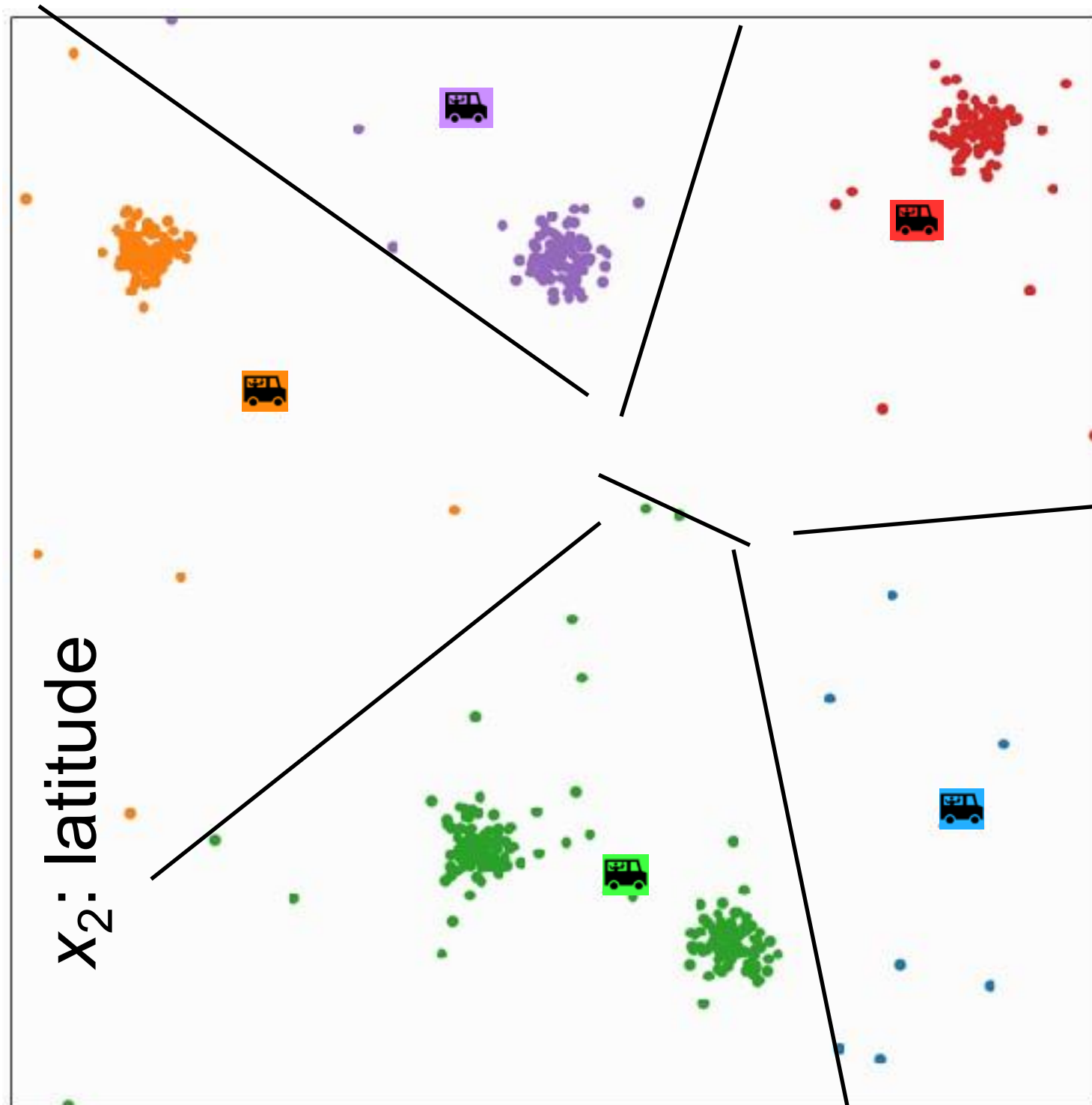
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

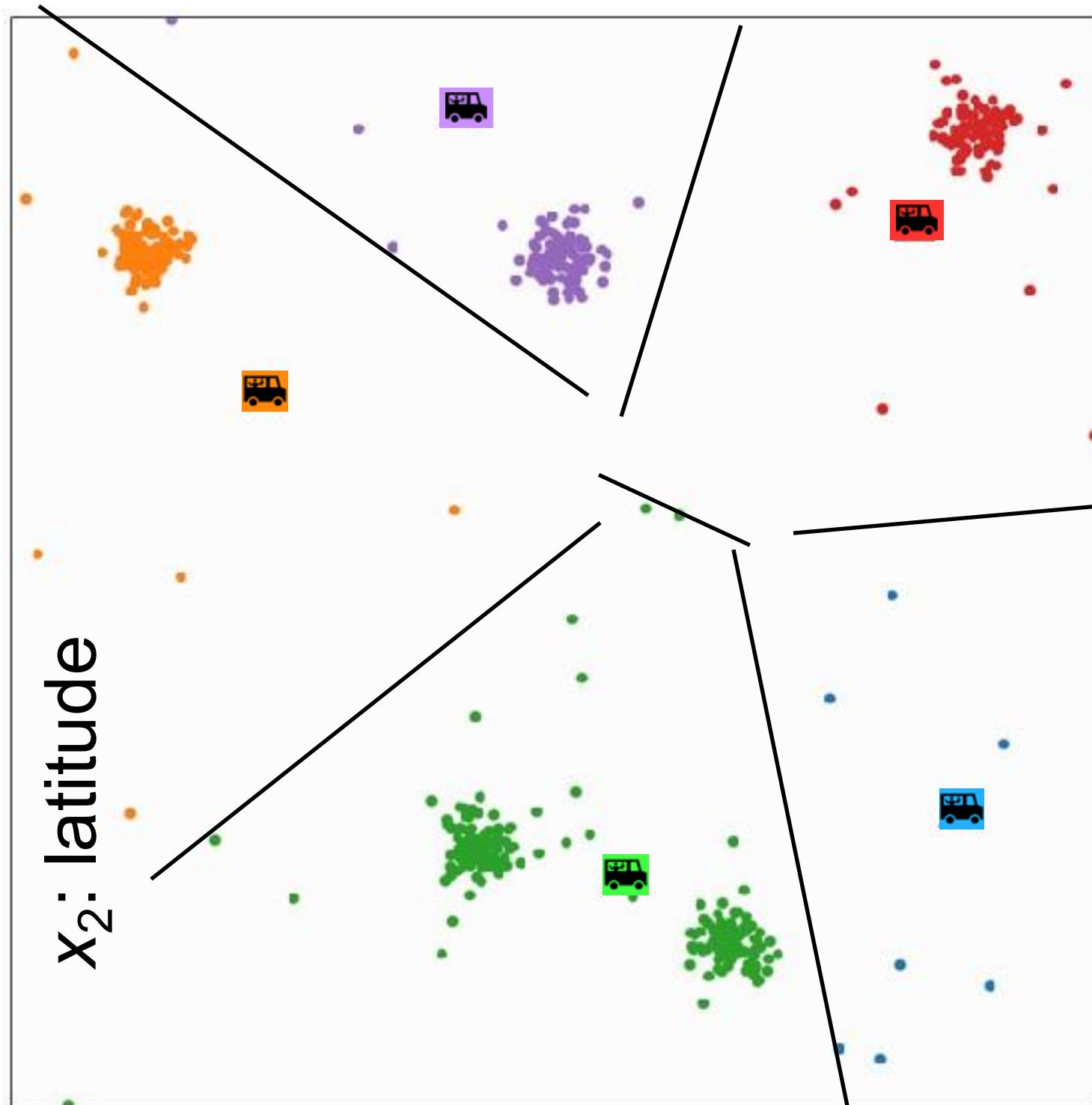
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

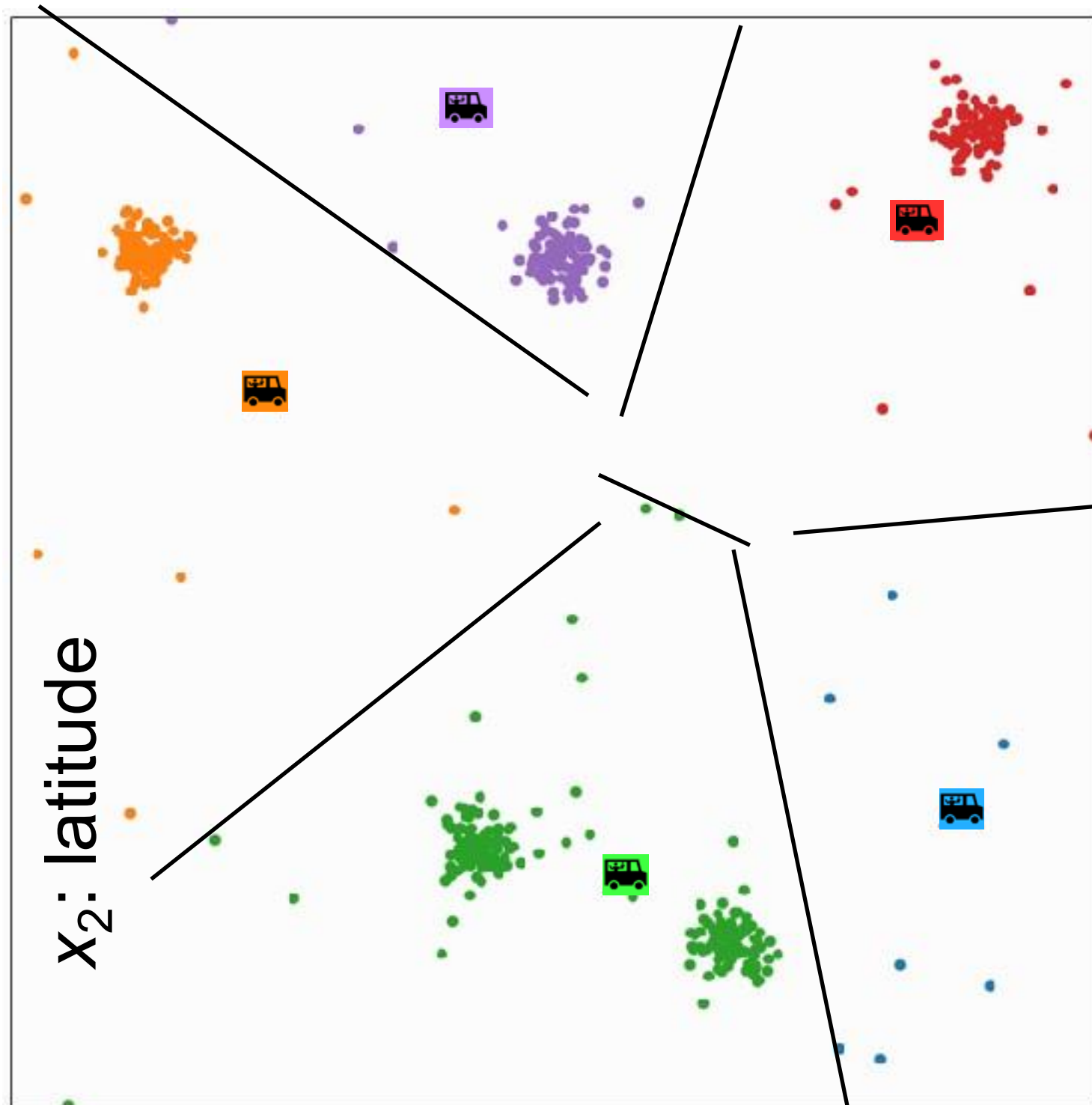
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

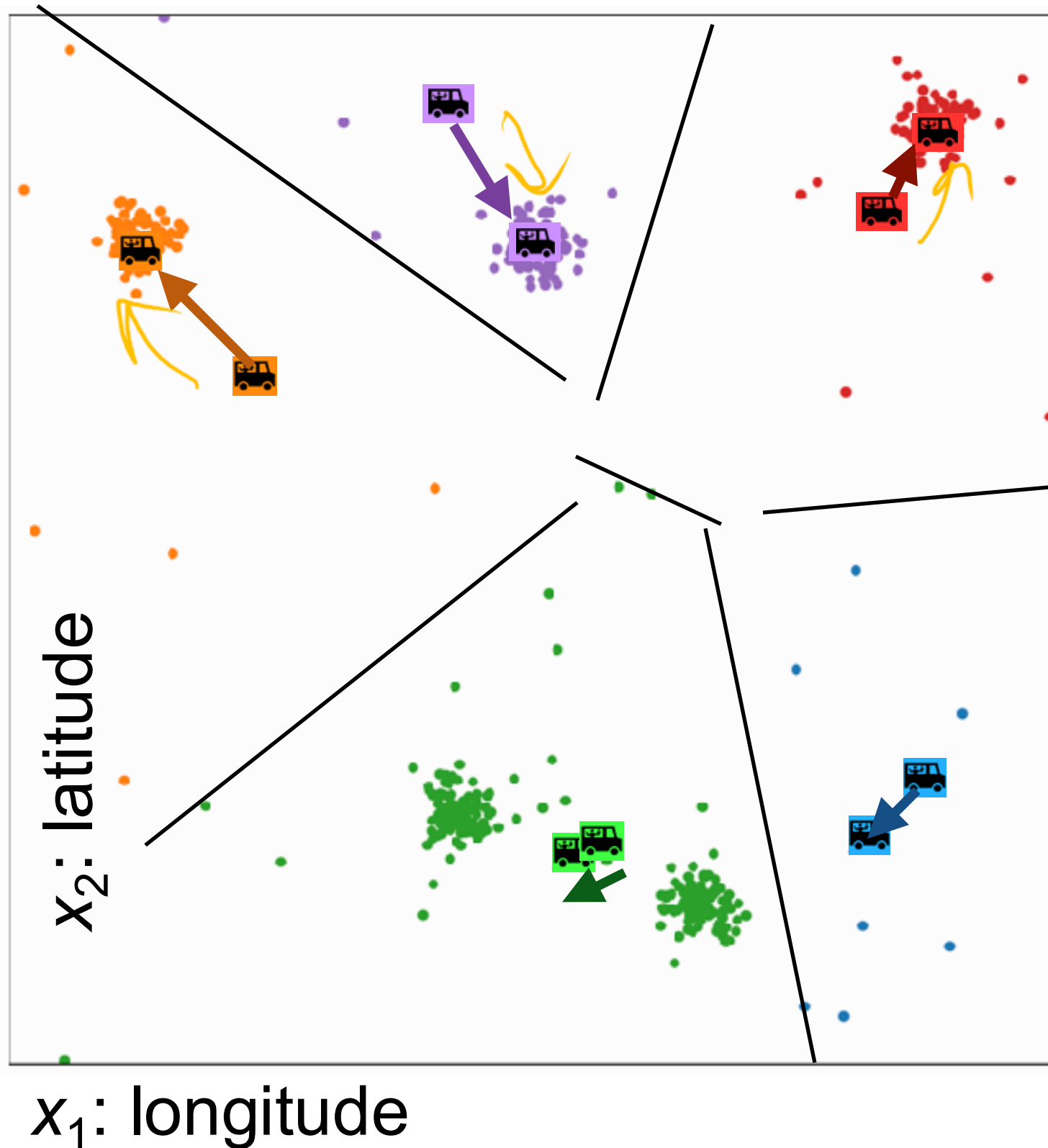
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

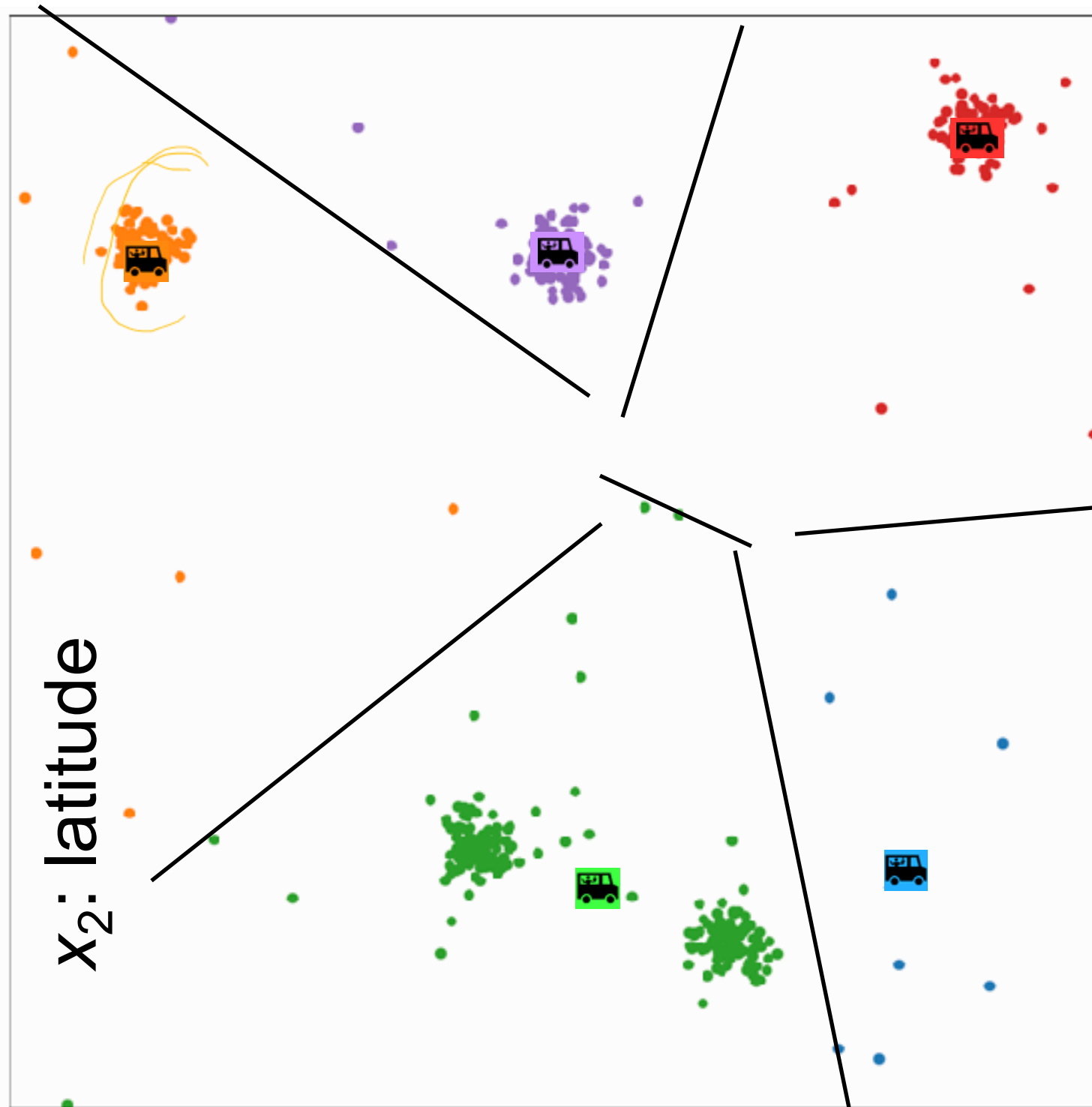
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for $j = 1$ to k

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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

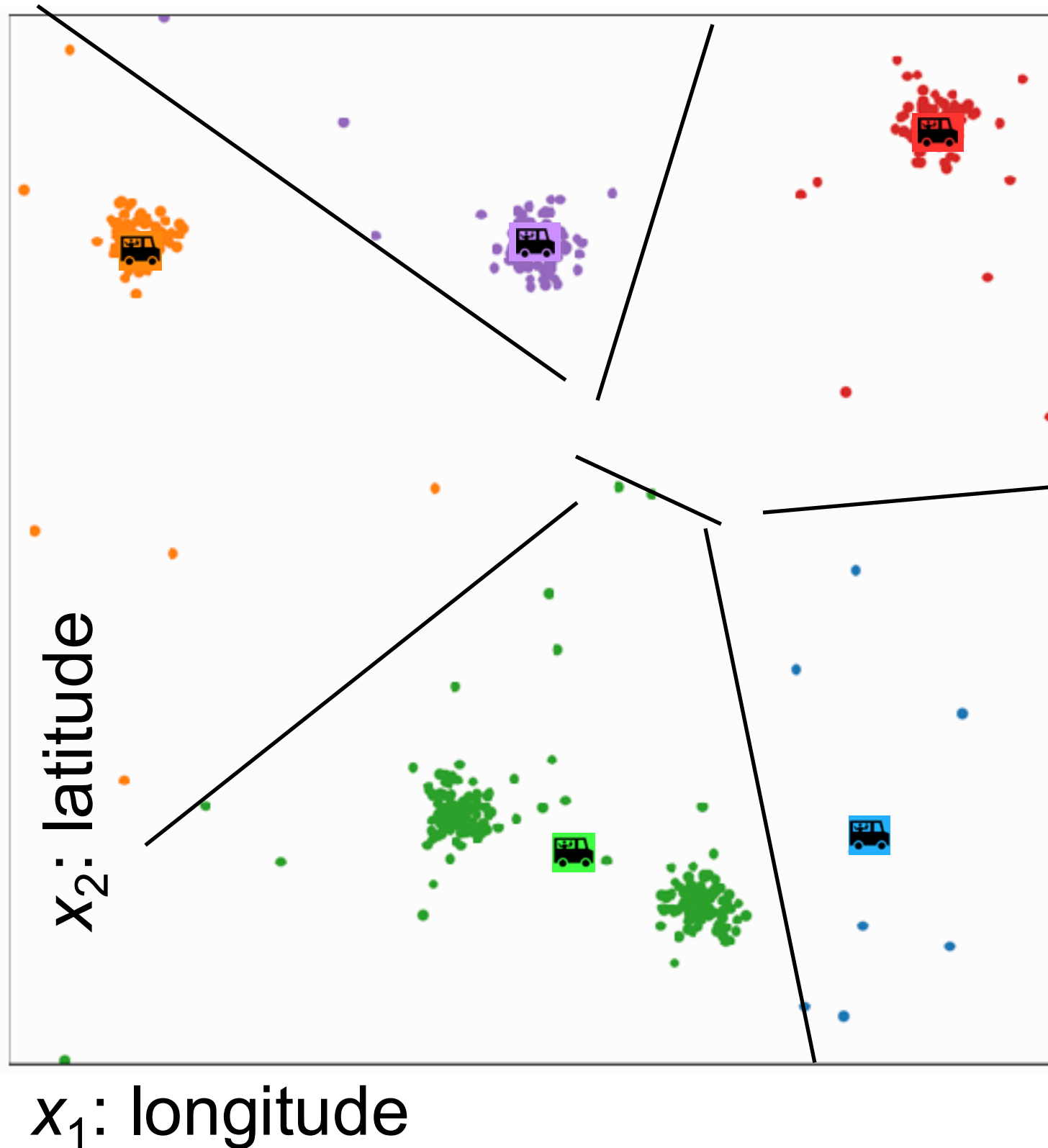
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for $j = 1$ to k

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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

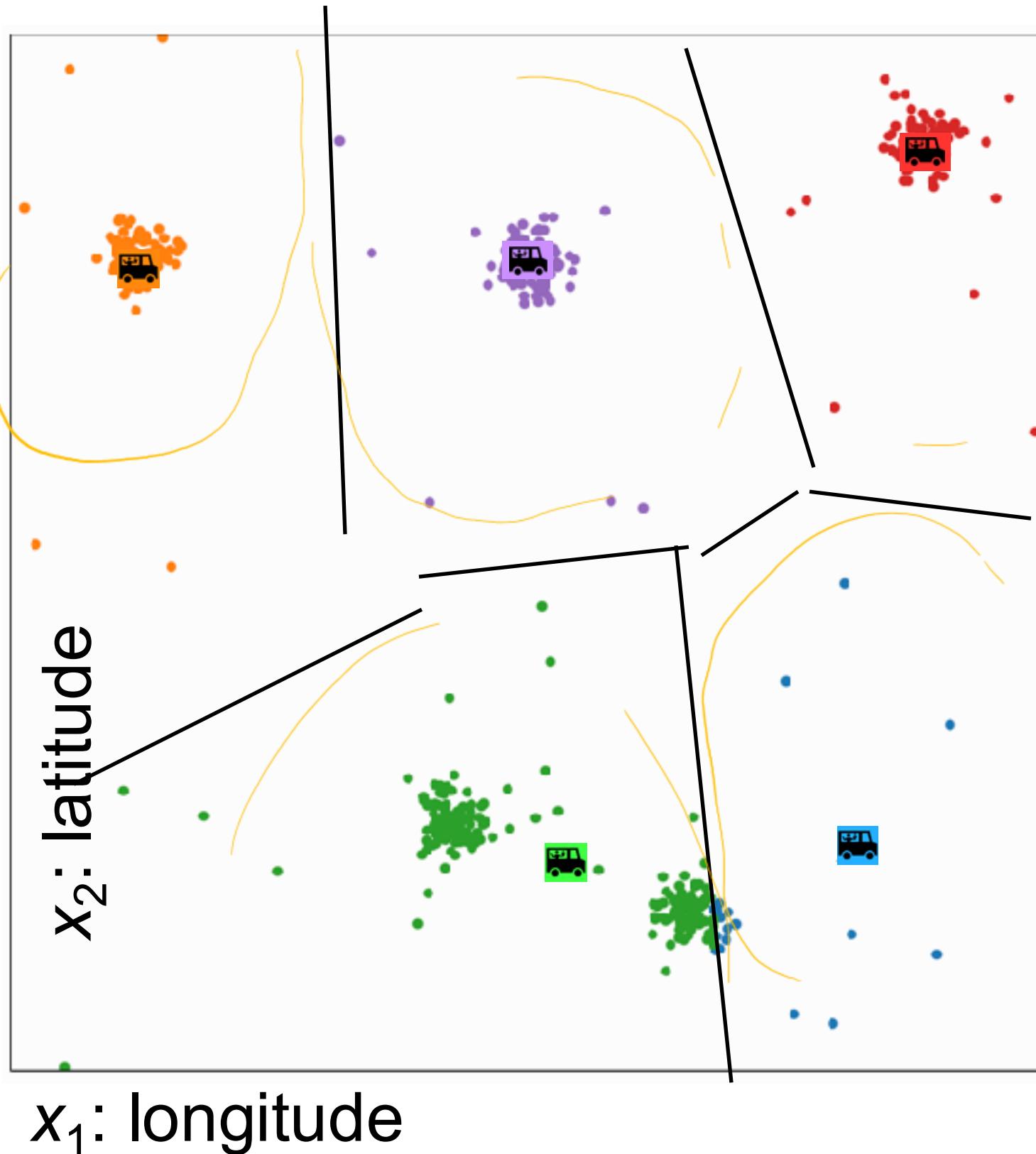
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for $j = 1$ to k

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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

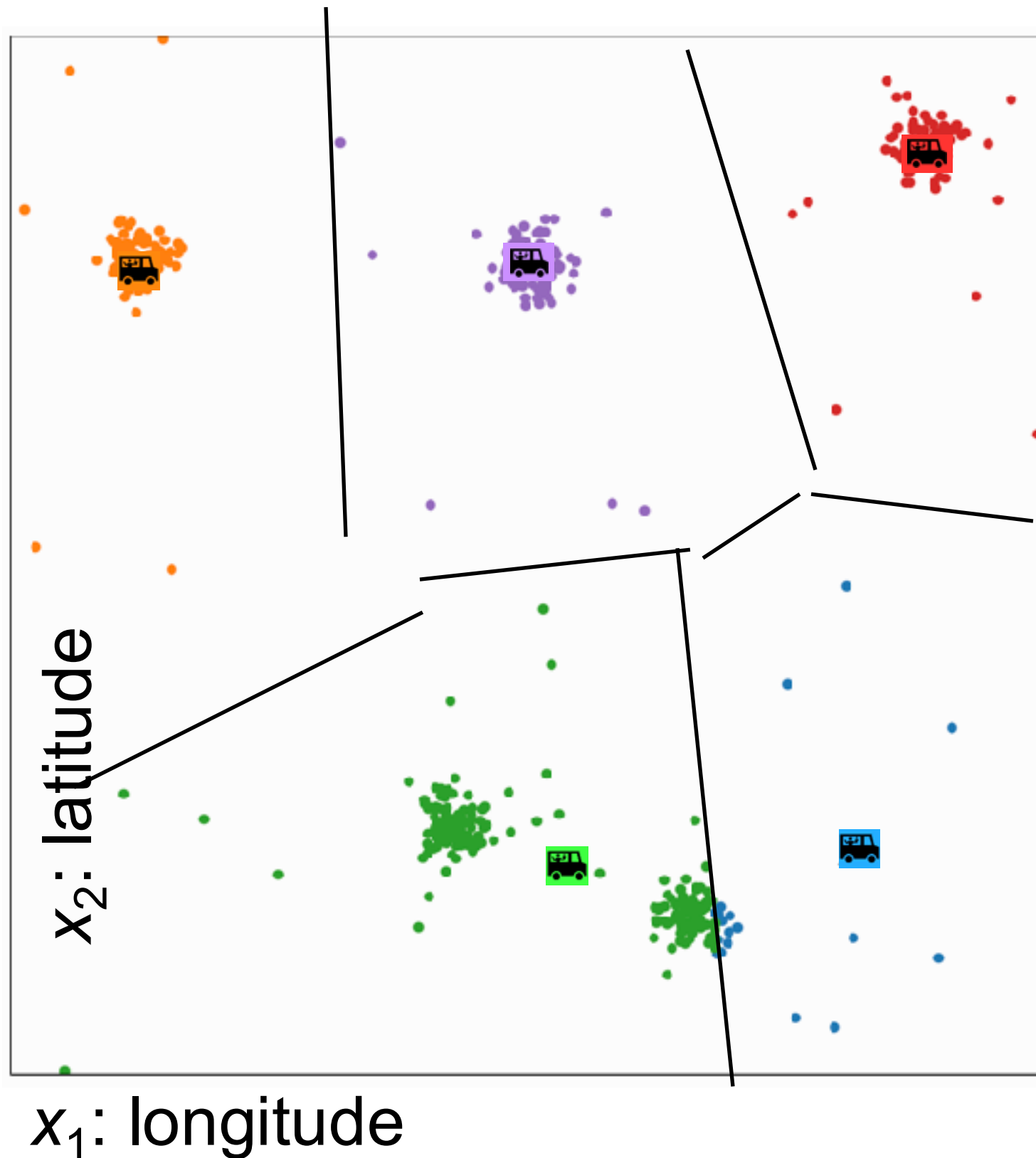
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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

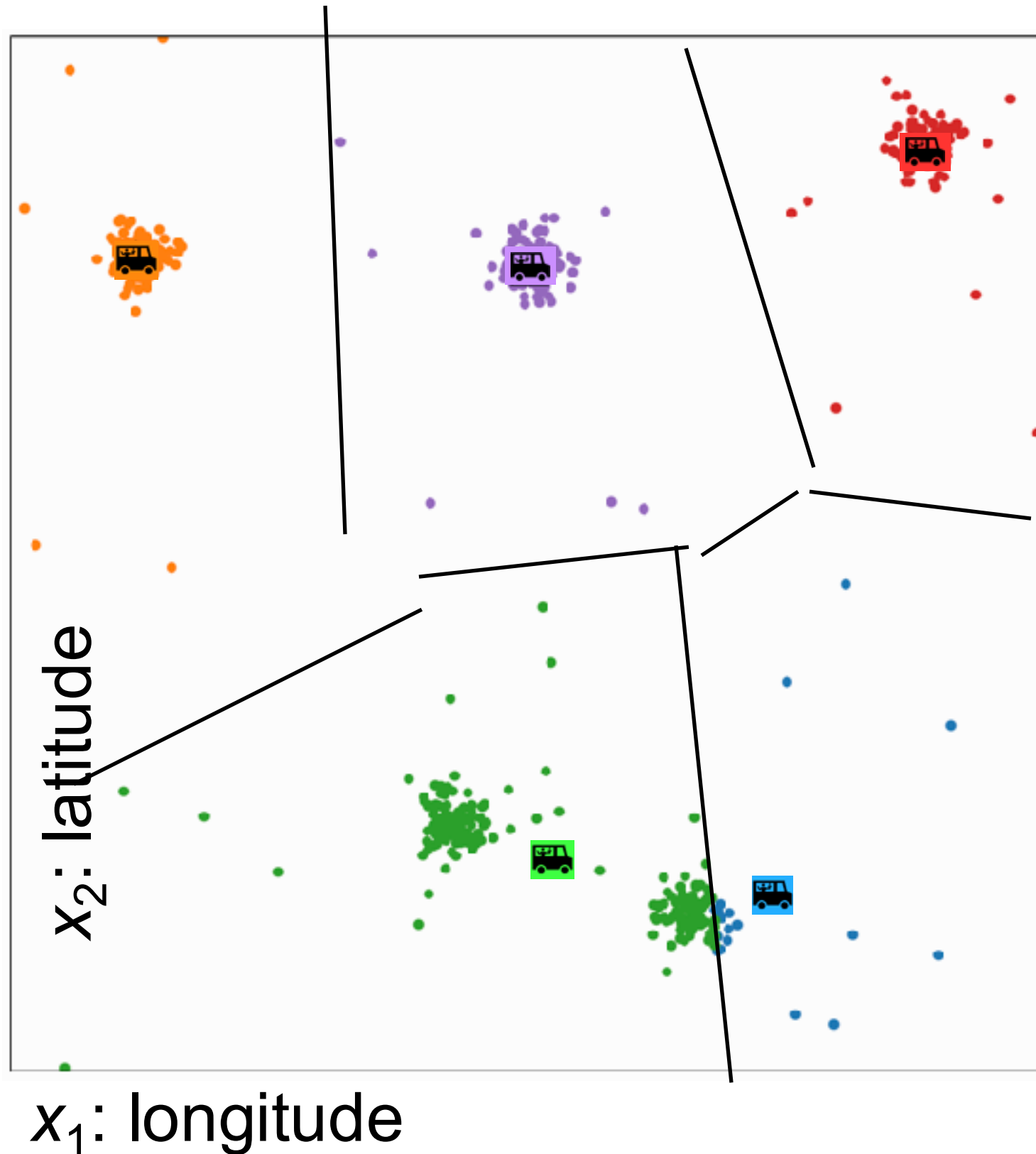
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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

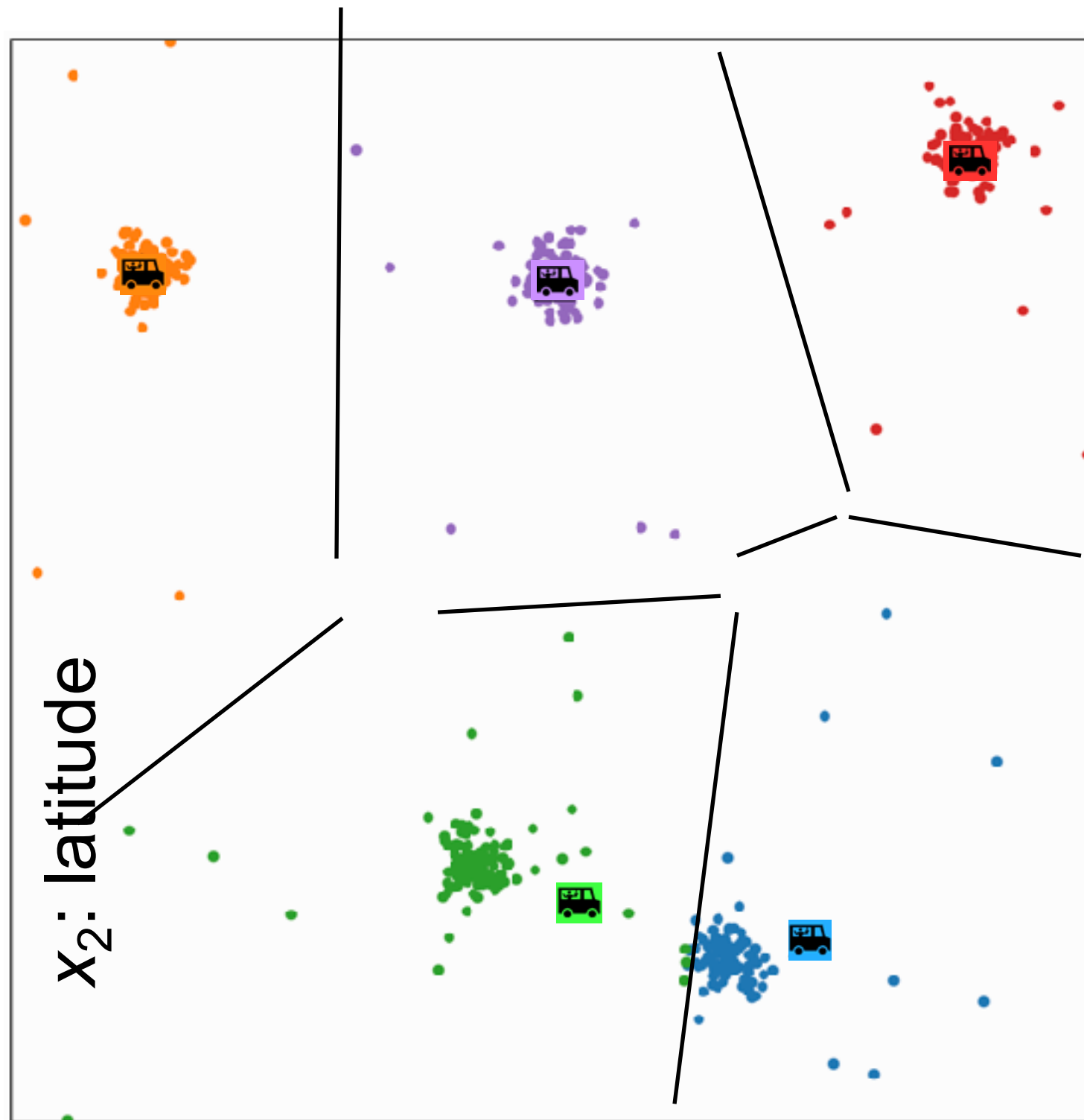
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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

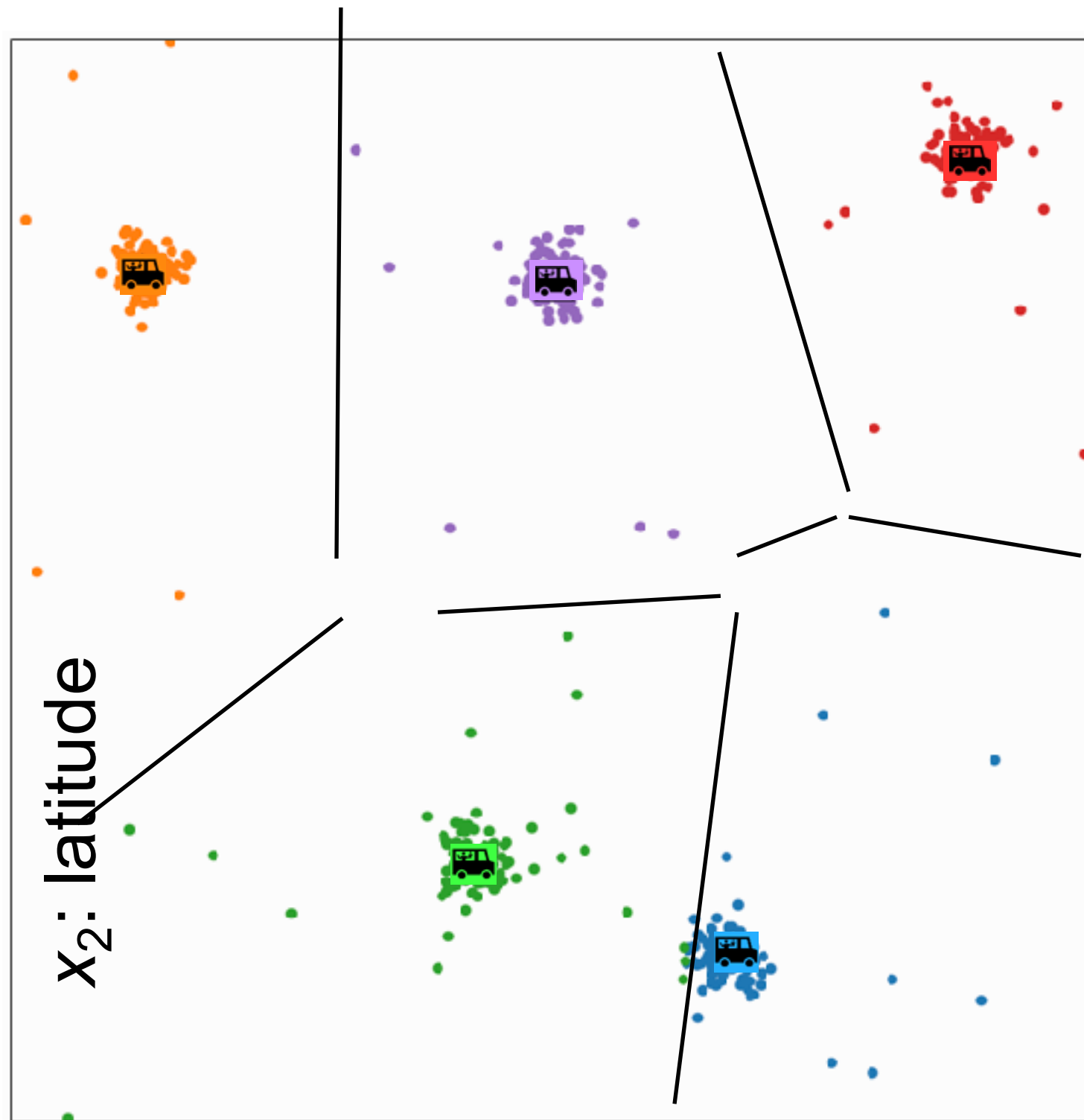
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x_1 : longitude

k-means algorithm



x_1 : longitude

k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

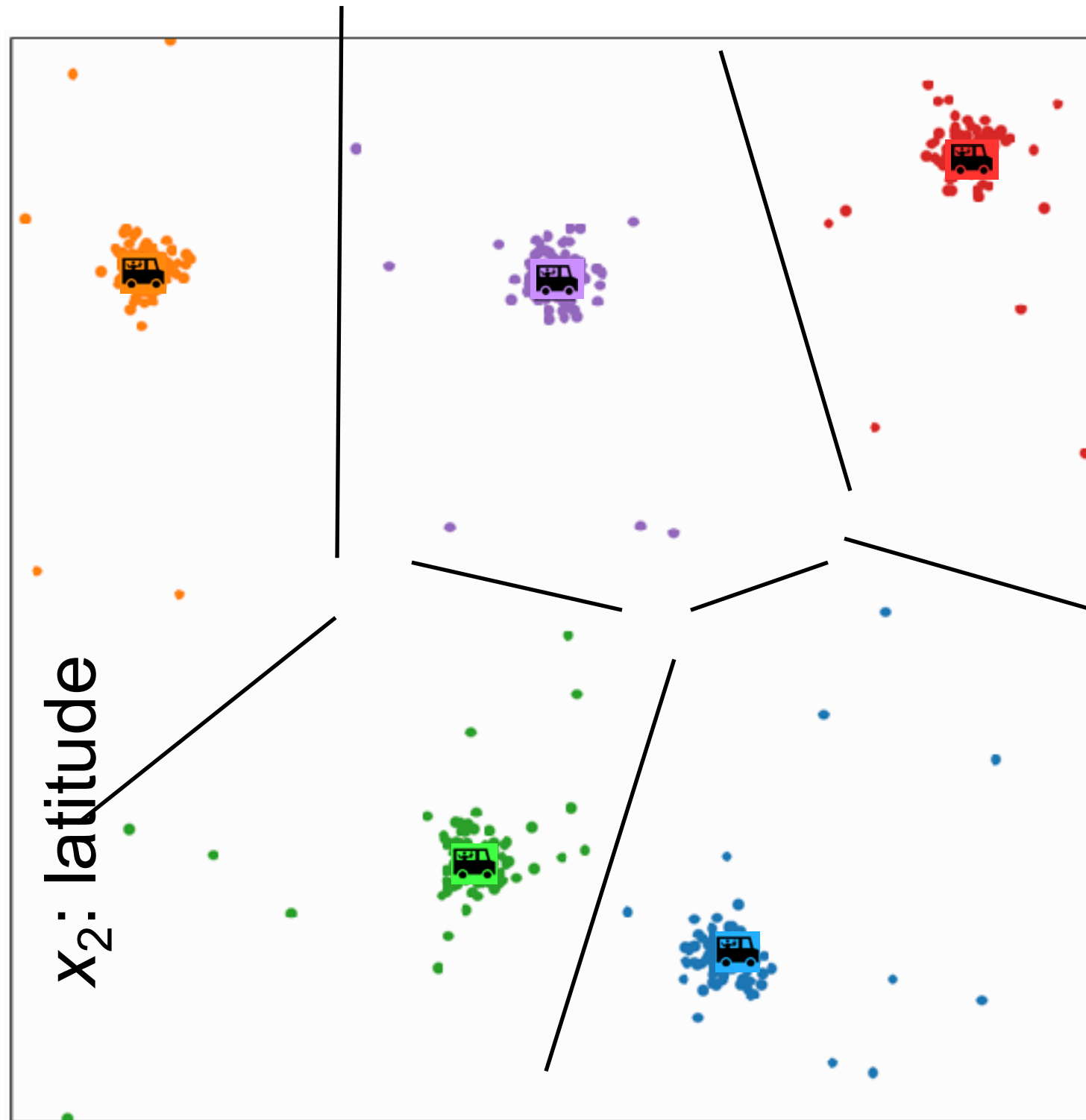
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k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

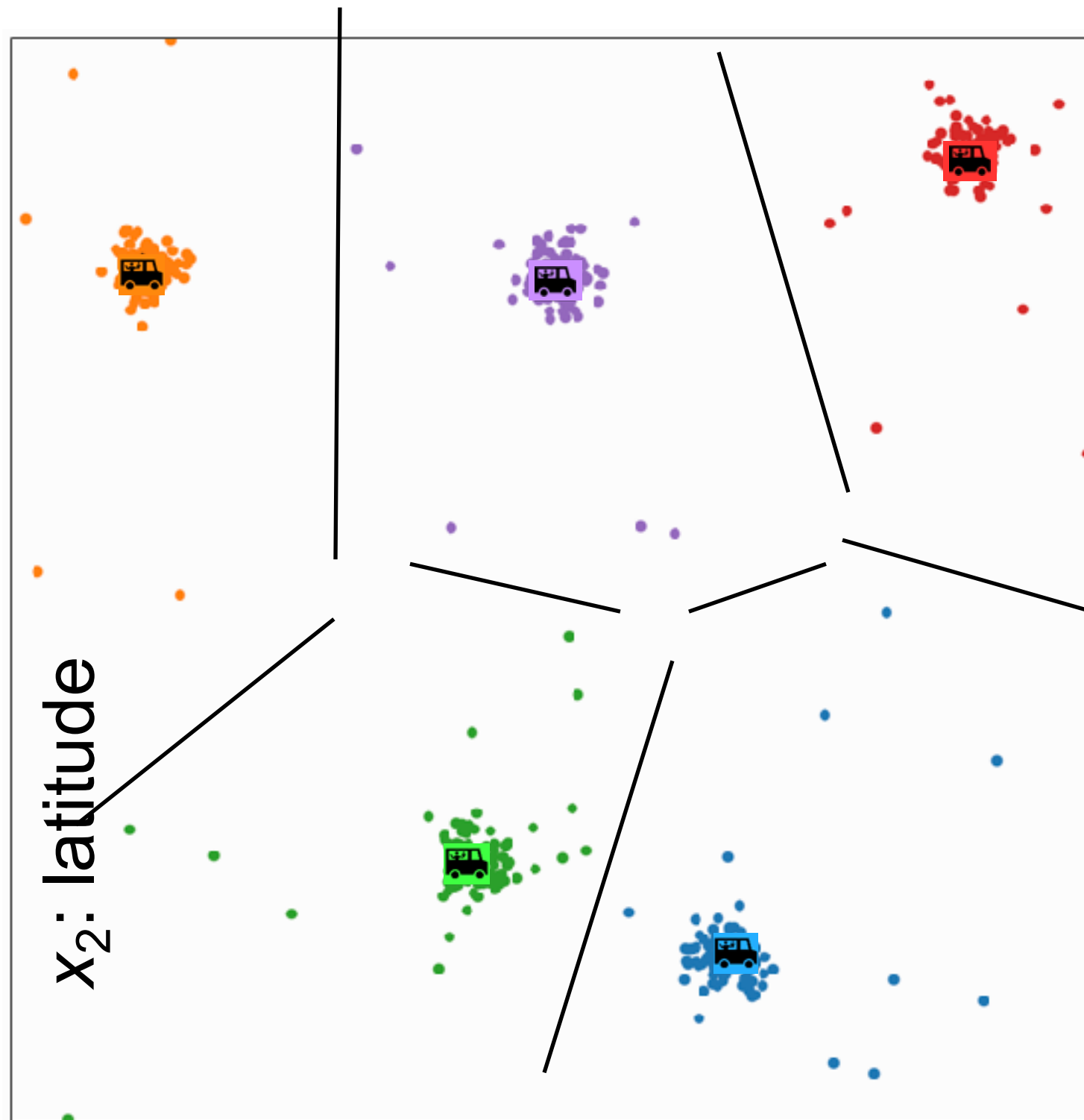
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

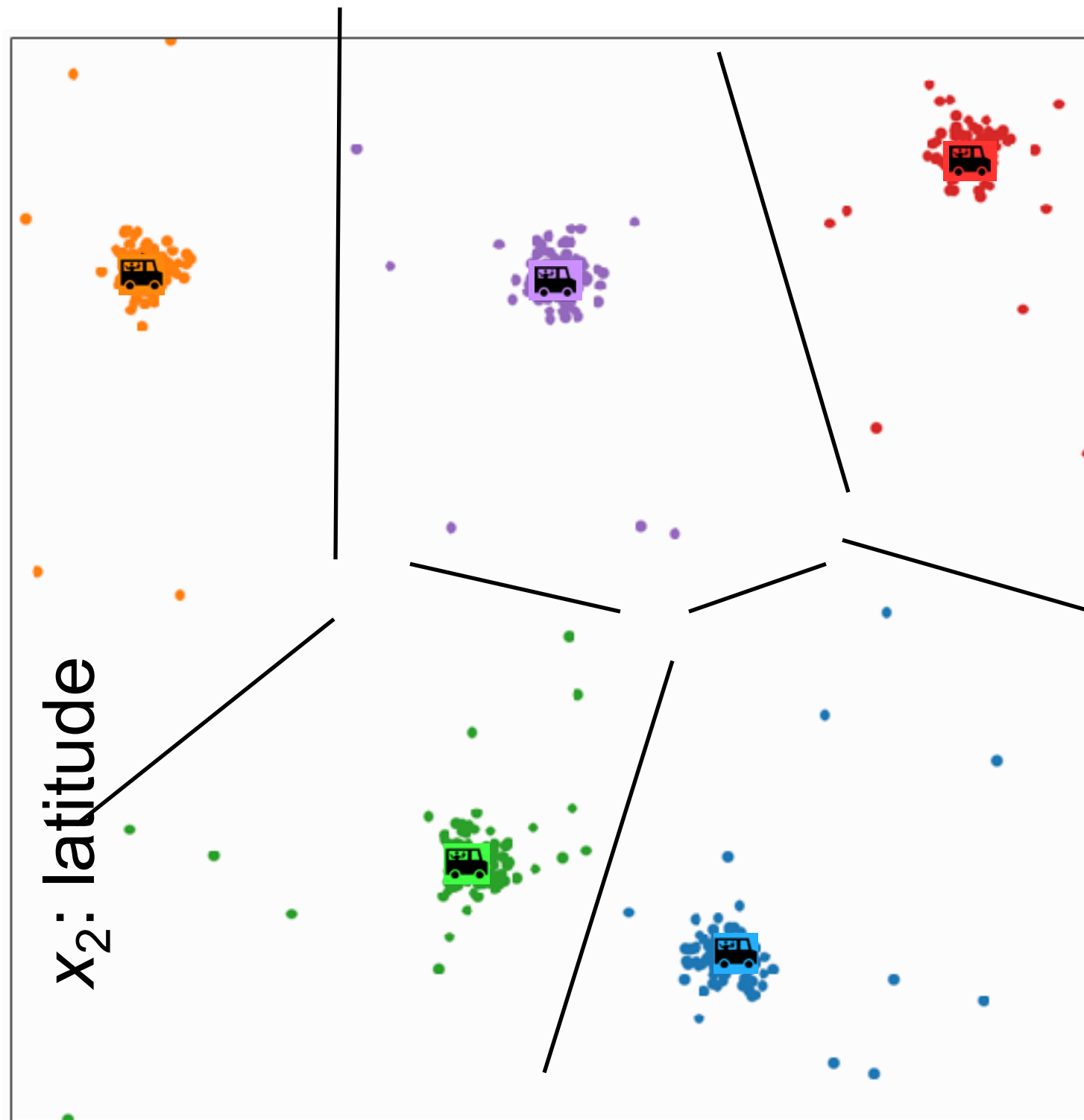
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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

for $i = 1$ to n

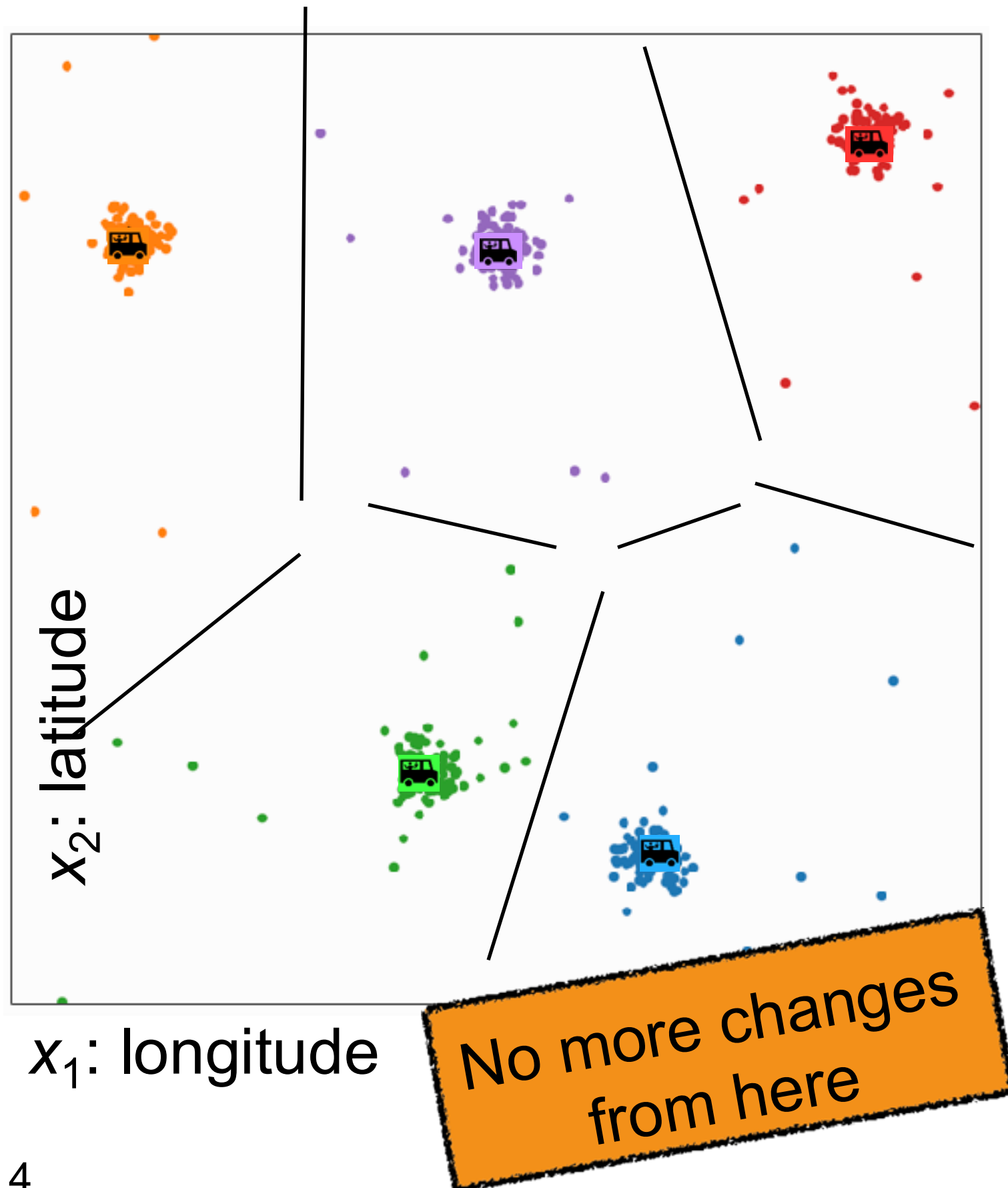
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for $j = 1$ to k

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x_1 : longitude

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

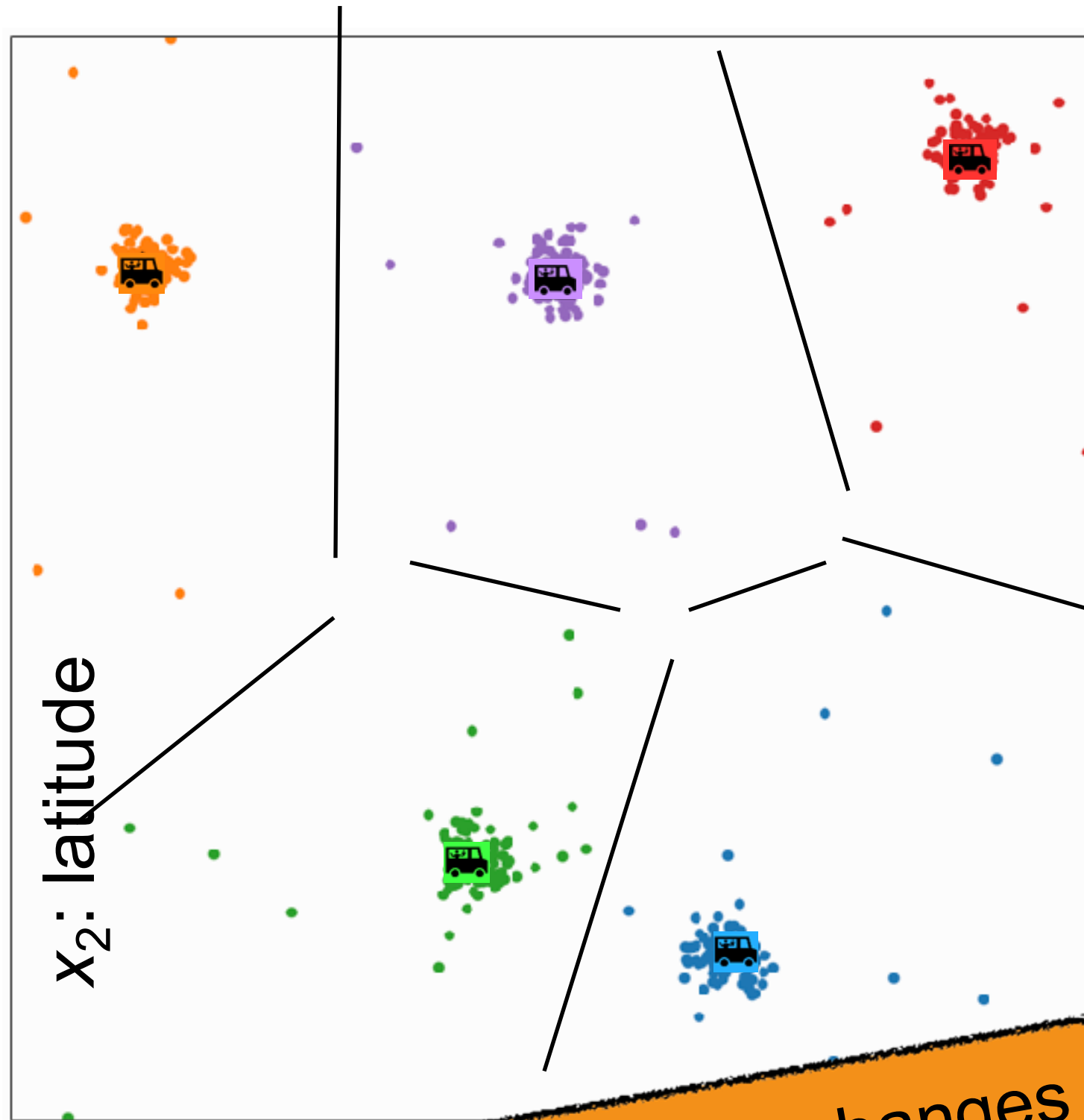
for $i = 1$ to n

$$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$$

for $j = 1$ to k

$$\mu^{(j)} = \frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

k-means algorithm



x_1 : longitude

x_2 : latitude

No more changes
from here

k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

3 onwards

for $t = 1$ to τ

for $i = 1$ to n

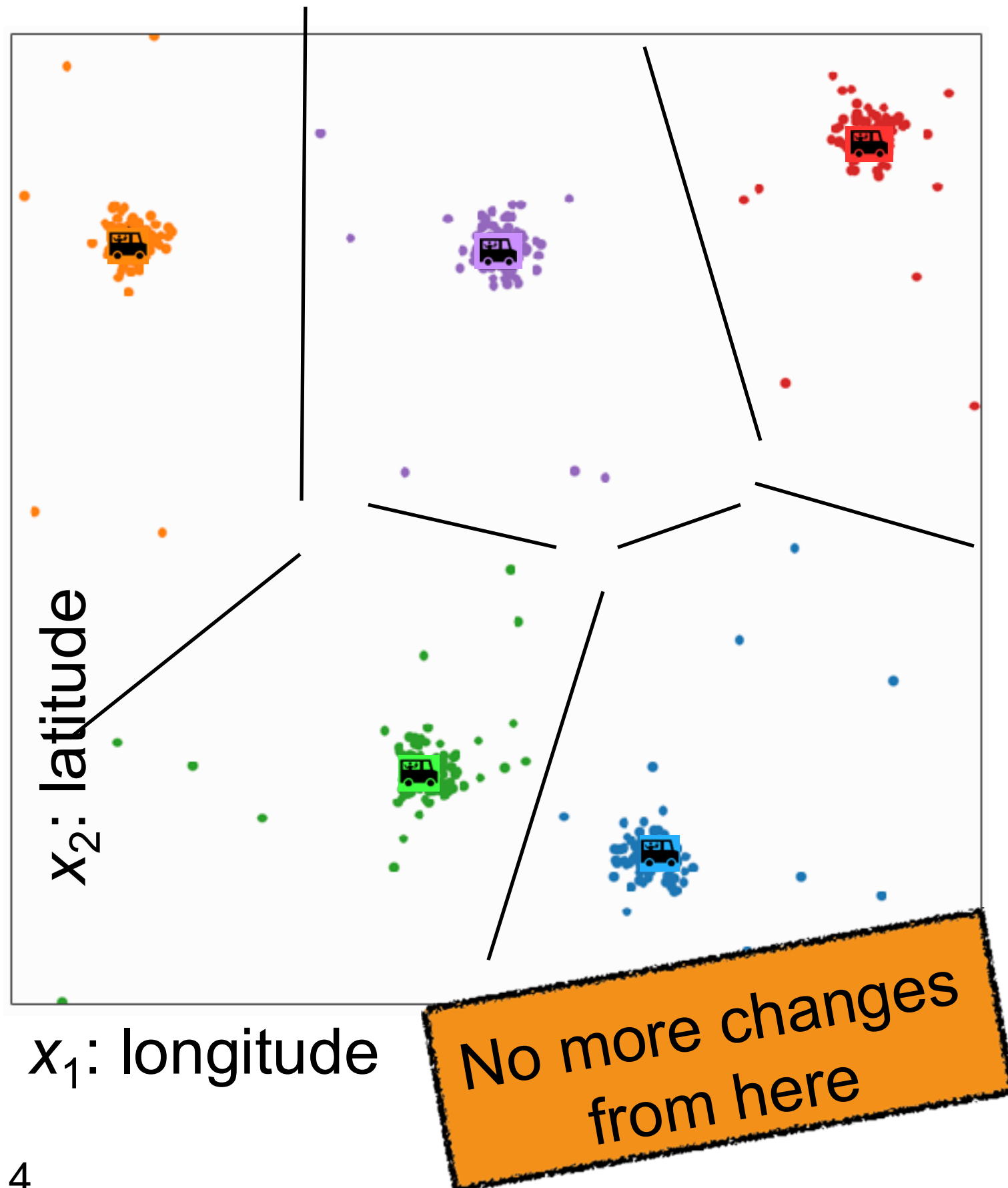
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How can I be so
sure?

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k$

for $t = 1$ to τ

$y_{\text{old}} = y$

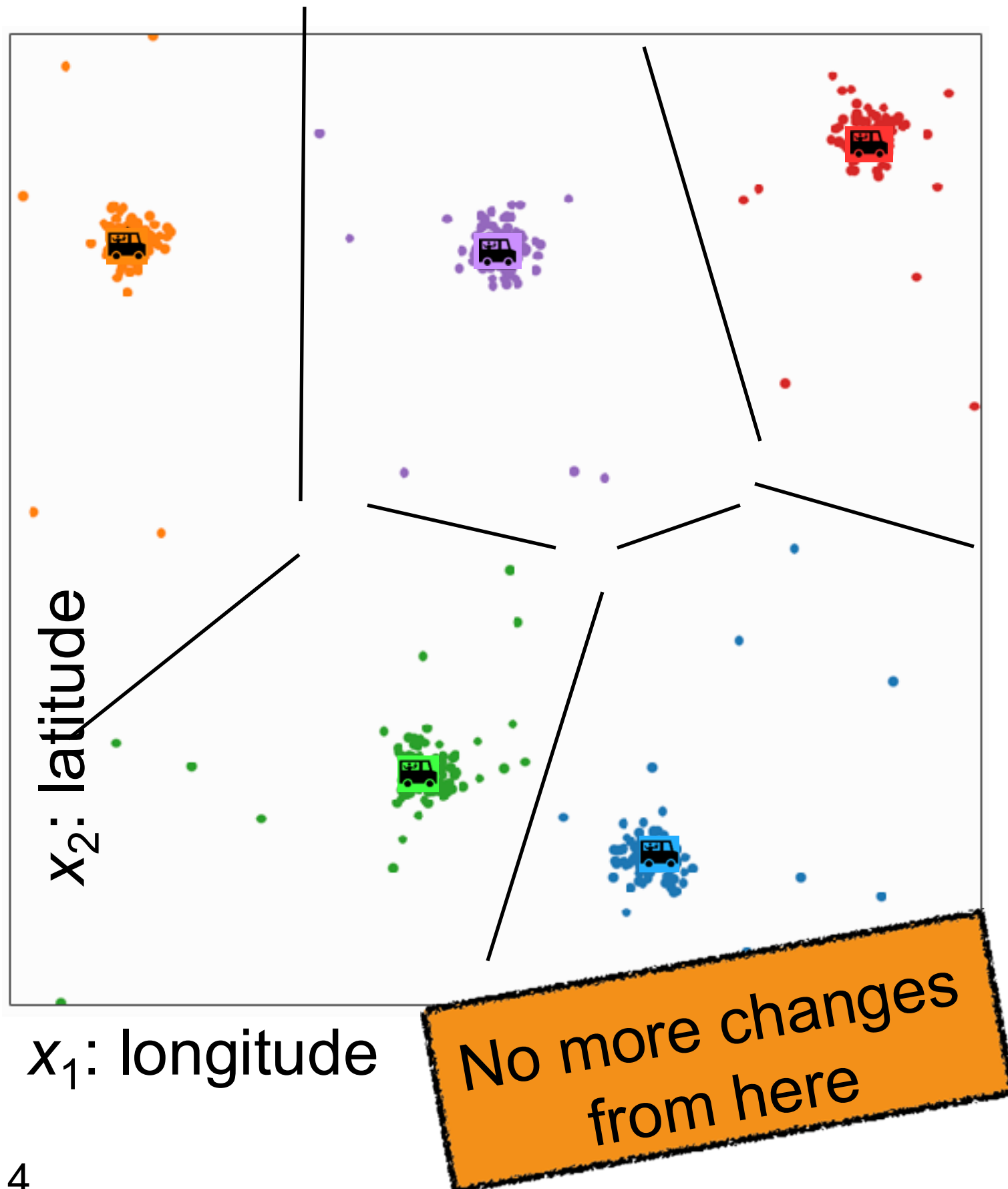
for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

for $j = 1$ to k

$$\mu^{(j)} = \frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k, \mathcal{Y}$

for $t = 1$ to τ

$y_{\text{old}} = y$

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

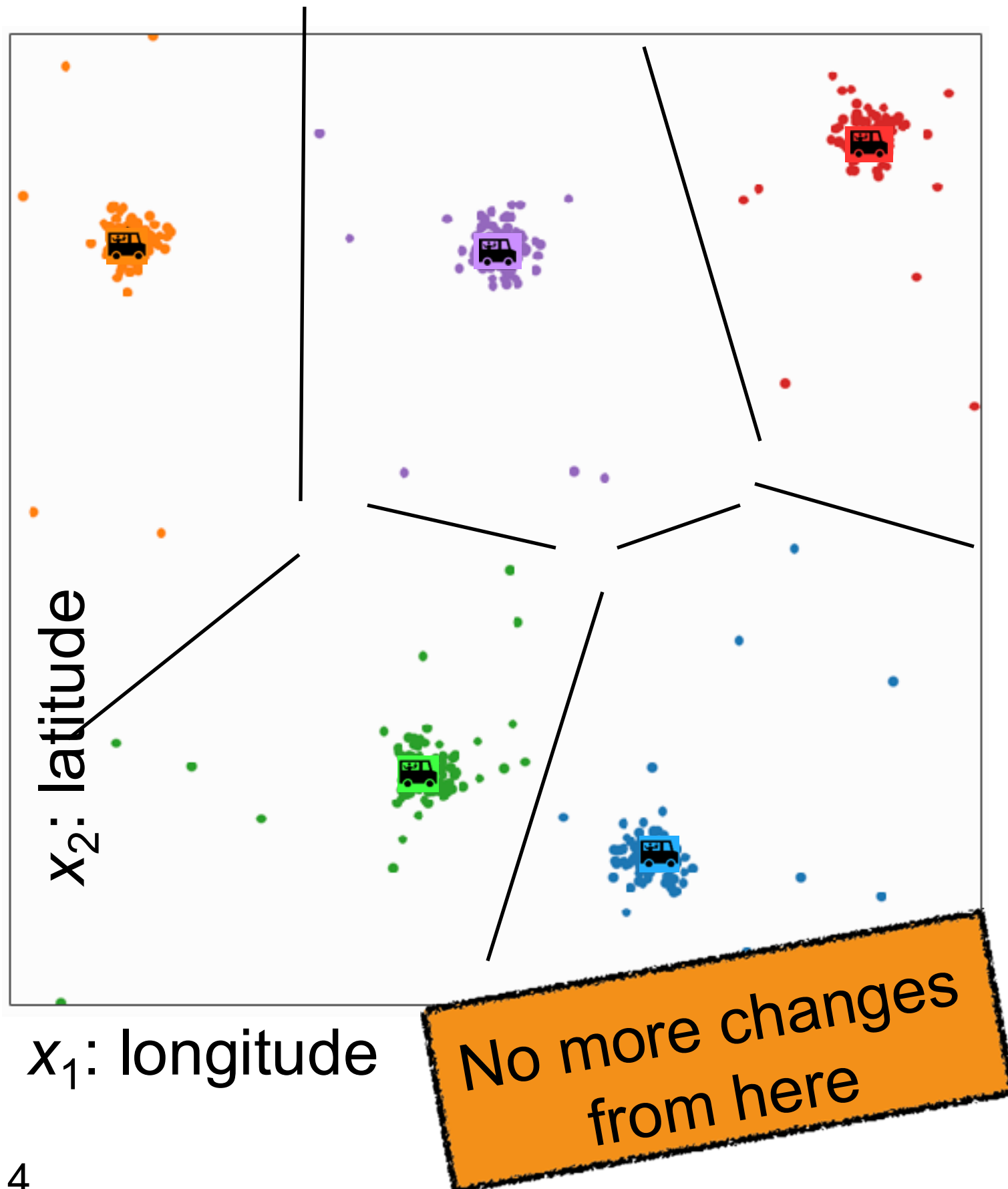
for $j = 1$ to k

$$\mu^{(j)} = \frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

if $y = y_{\text{old}}$

break

k-means algorithm



k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k, \{y^{(i)}\}_{i=1}^n$

for $t = 1$ to τ

$y_{\text{old}} = y$

for $i = 1$ to n

$y^{(i)} = \arg \min_j \|x^{(i)} - \mu^{(j)}\|_2^2$

for $j = 1$ to k

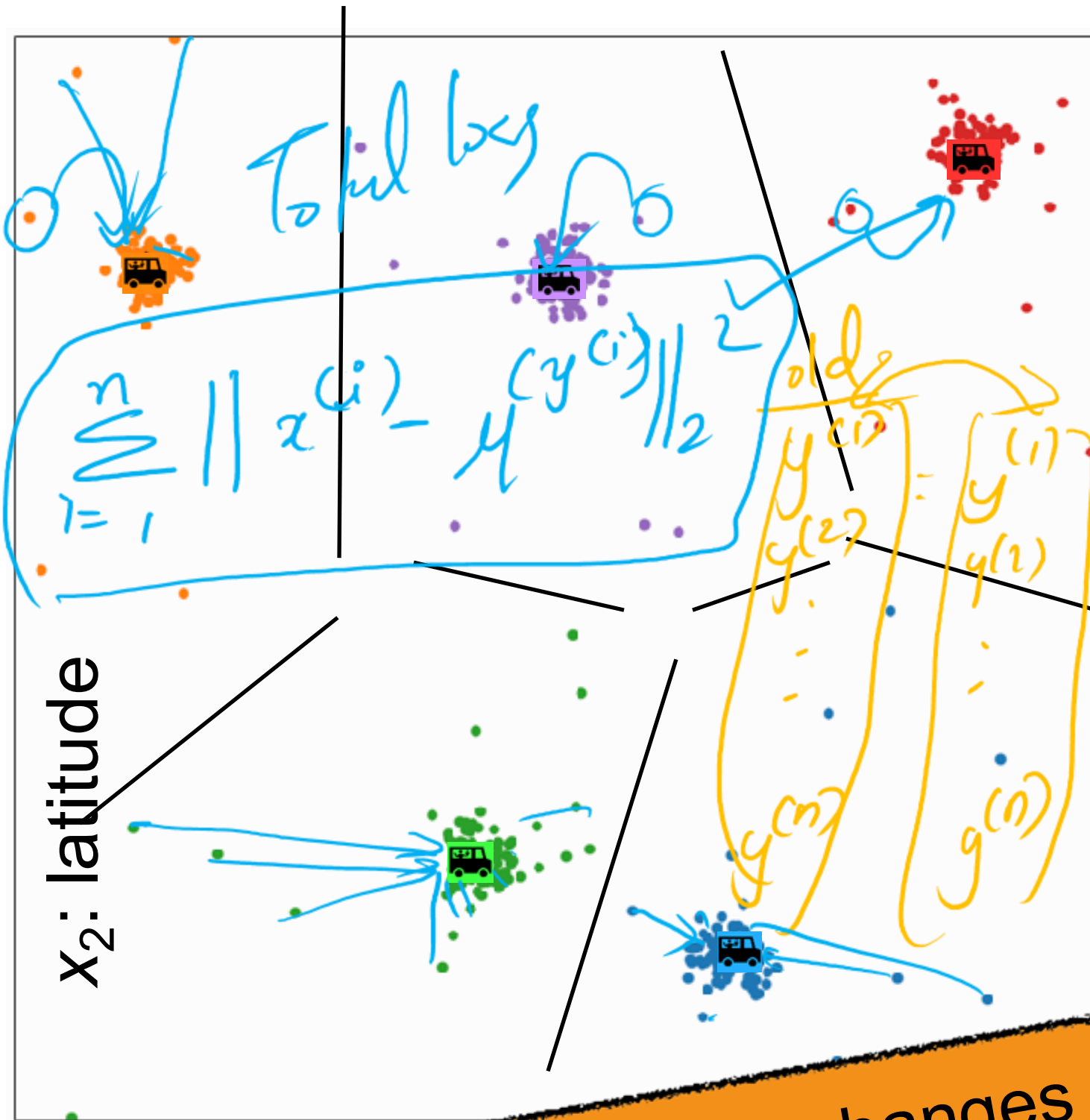
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if $y = y_{\text{old}}$

break

k-means algorithm

10



No more changes from here

k-means (k, τ)

Init $\{\mu^{(j)}\}_{j=1}^k, \{y^{(i)}\}_{i=1}^n$

for $t = 1$ to τ

$y_{\text{old}} = y$

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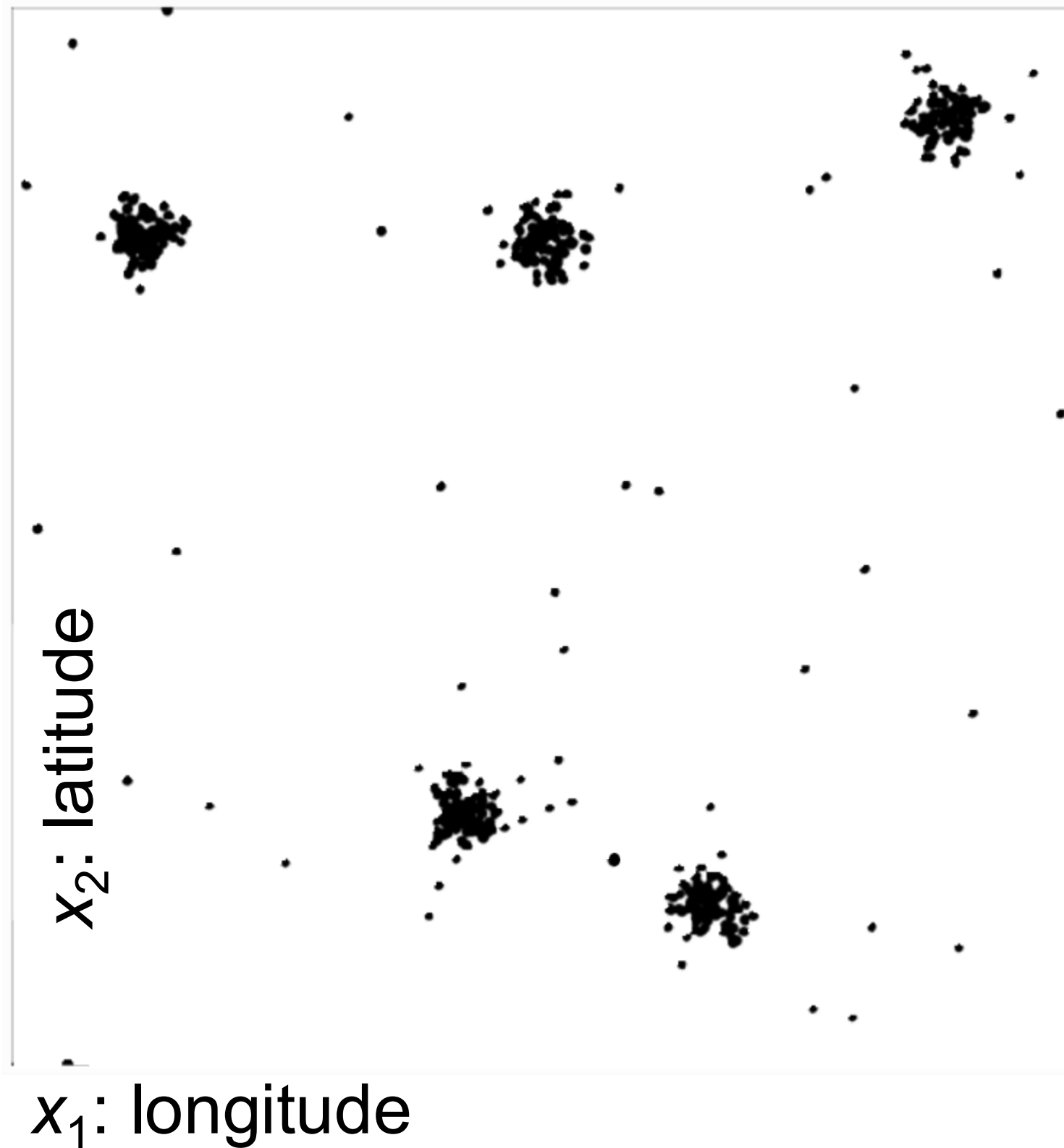
for $j = 1$ to k

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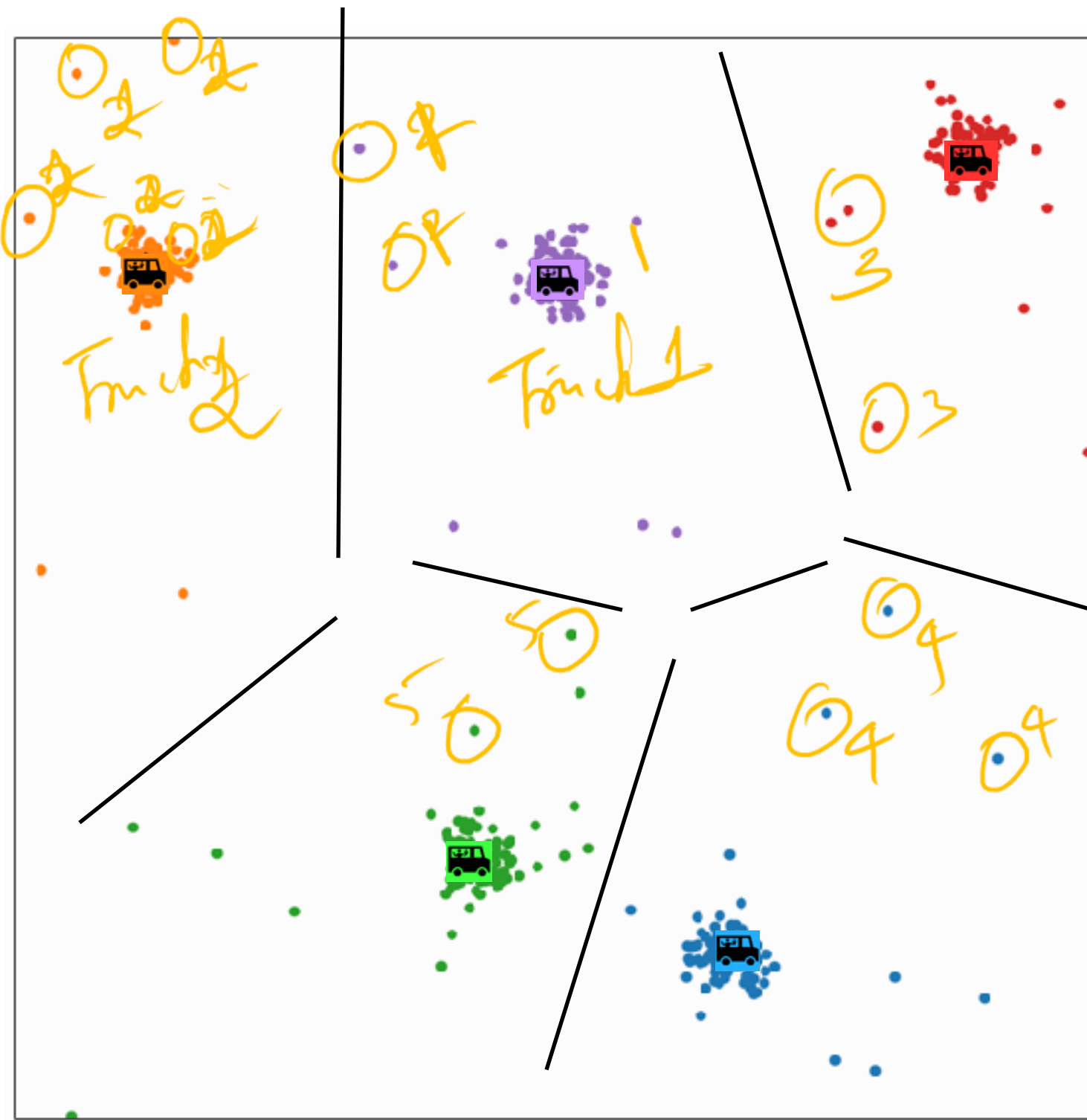
if $y = y_{\text{old}}$ *vector*

break

return $\{\mu^{(j)}\}_{j=1}^k, \{y^{(i)}\}_{i=1}^n$

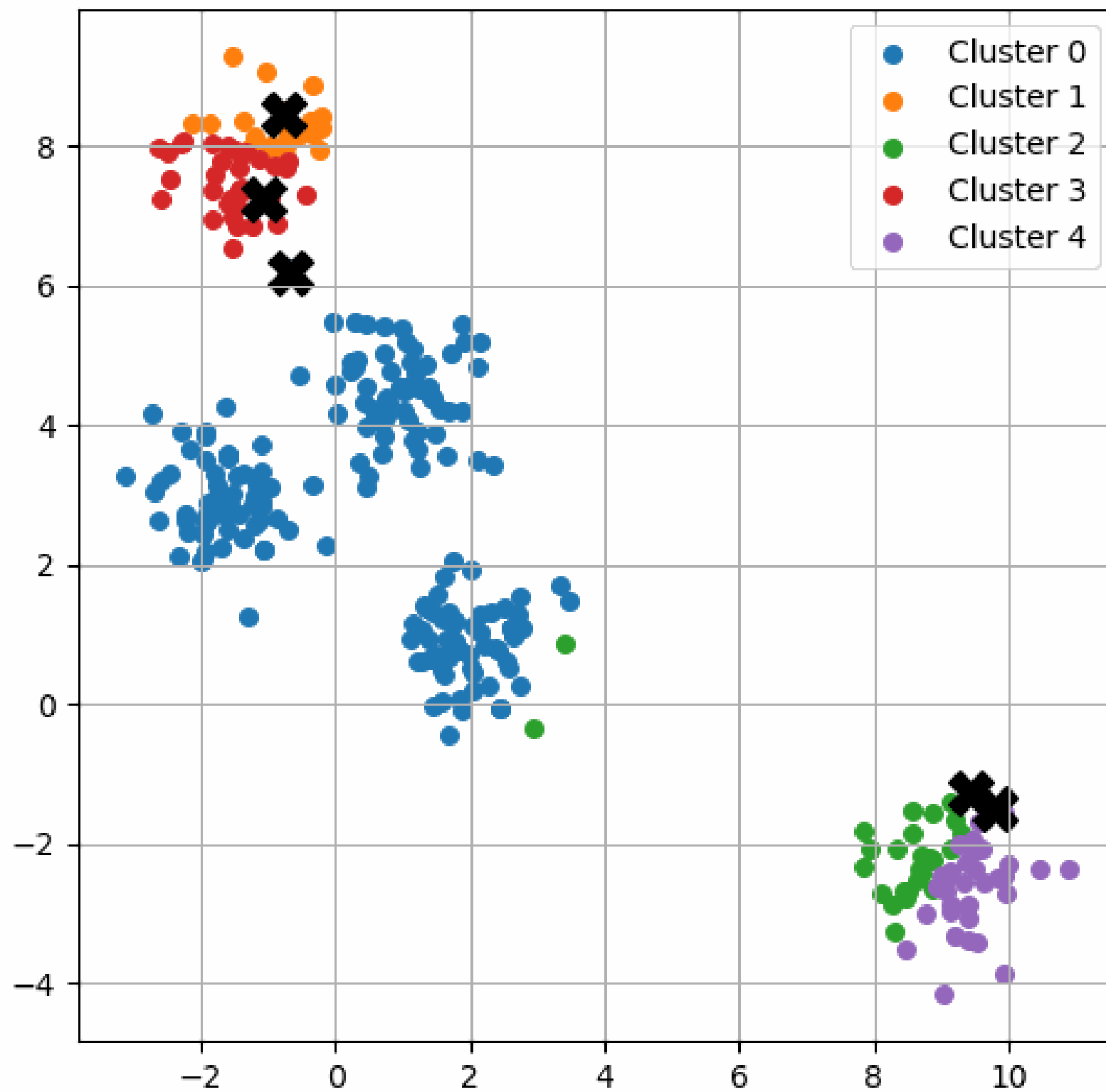


- So what did we do?
- We *clustered* the data: we grouped the **data** by similarity

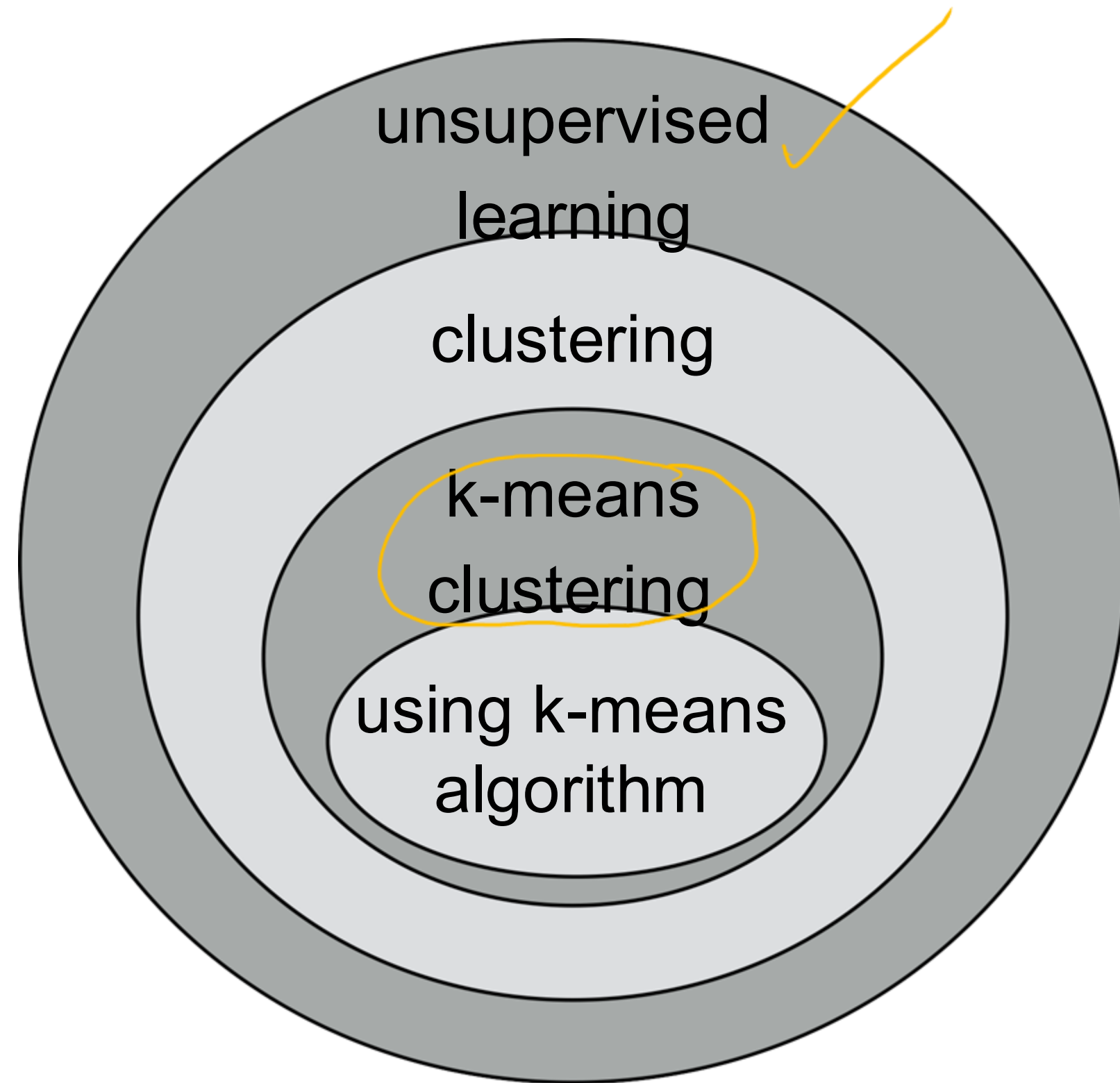


- So what did we do?
- We *clustered* the data: we **grouped** the data by similarity

K-Means Iteration 0

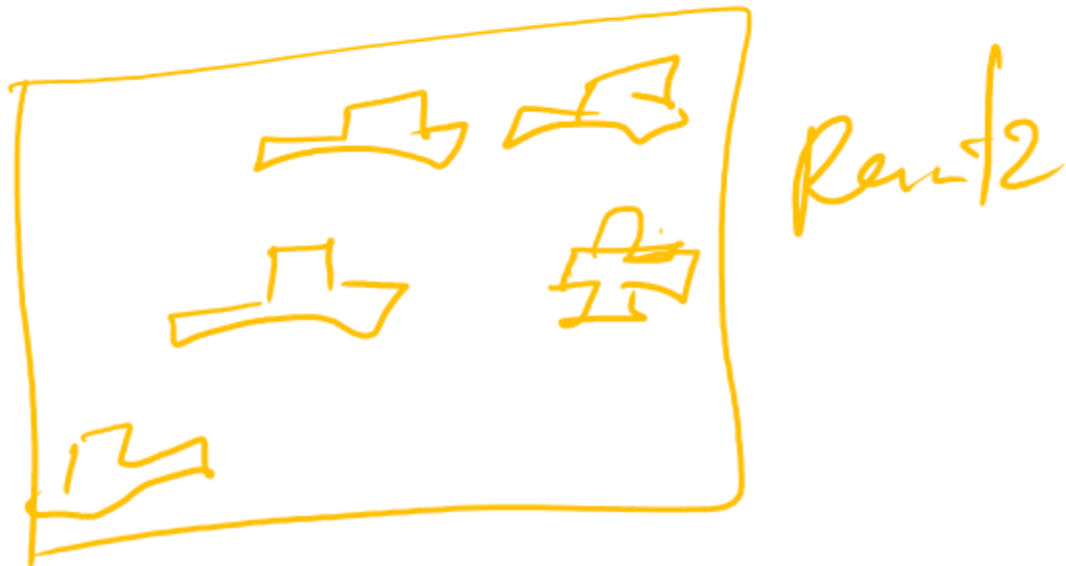
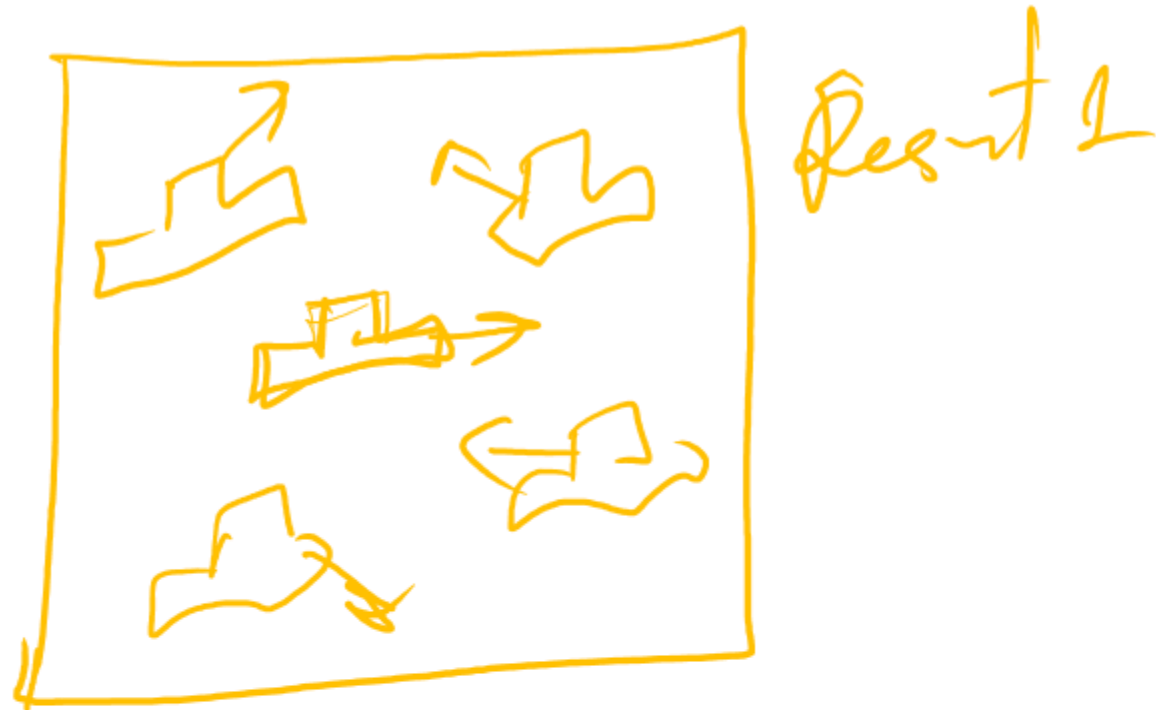


Clustering & related



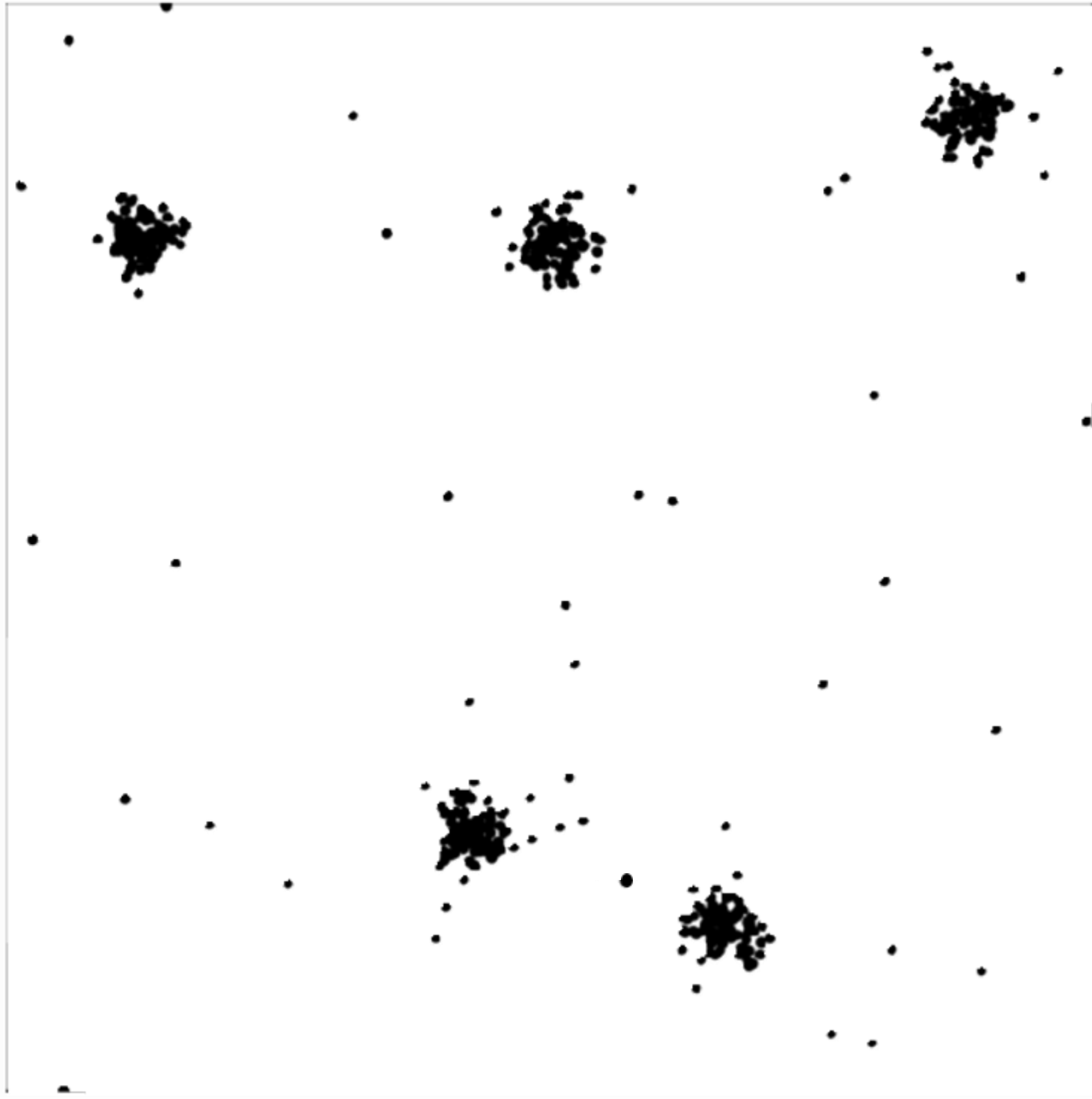
k-means algorithm: initialization

k-means algorithm: initialization



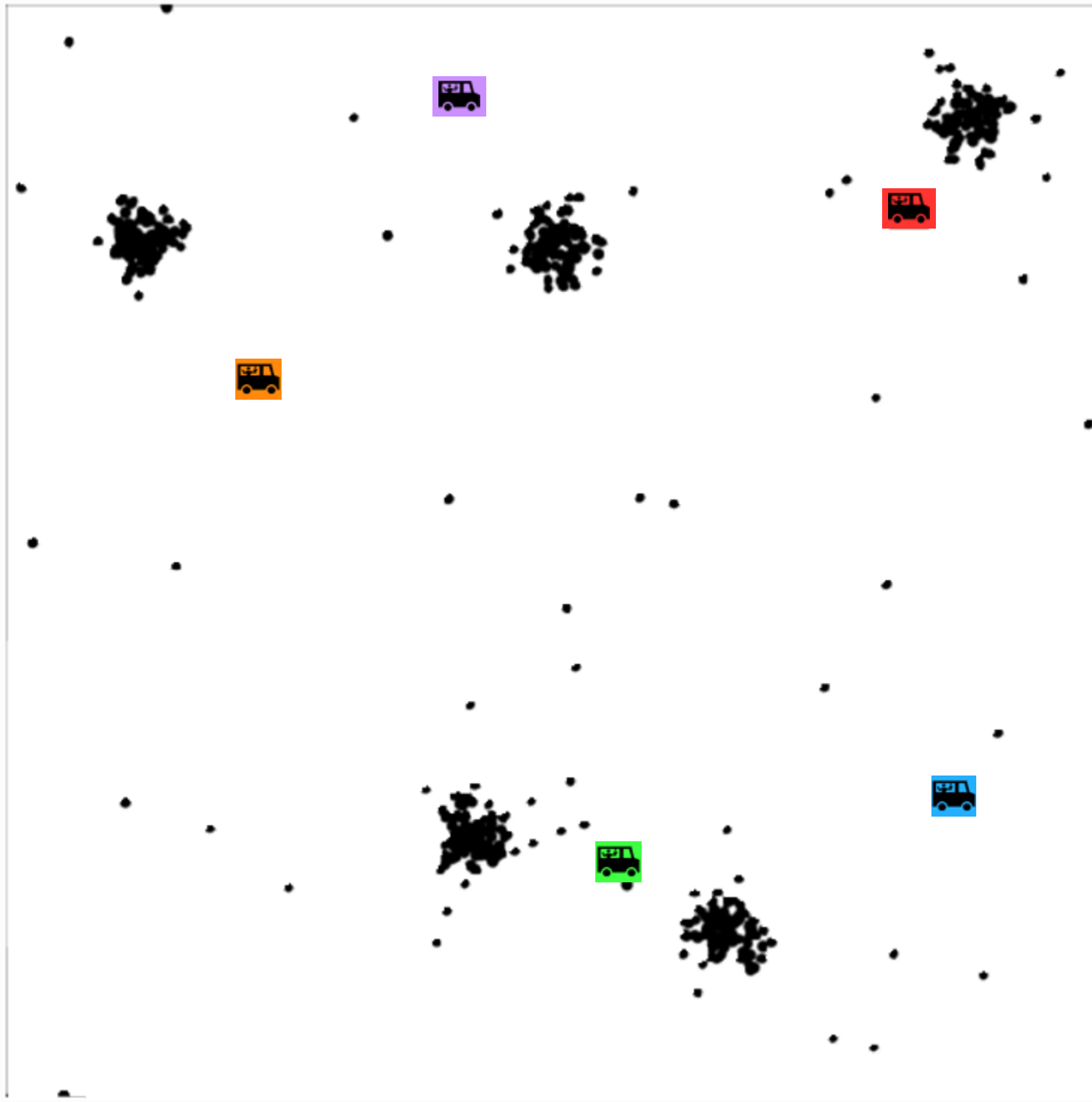
- **Theorem.** If run for enough outer iterations, the k-means algorithm will converge to a local minimum of the k-means objective

k-means algorithm: initialization



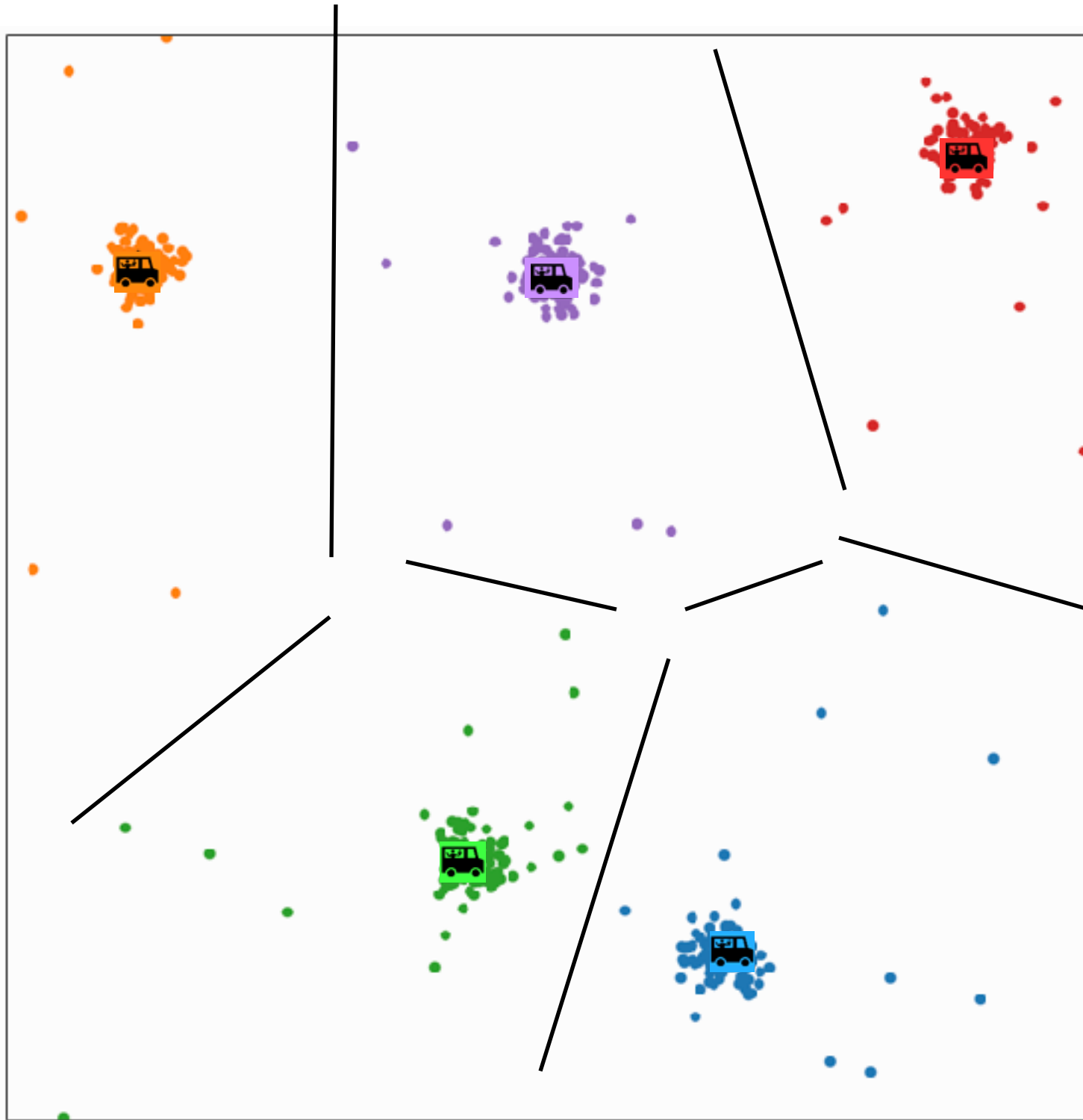
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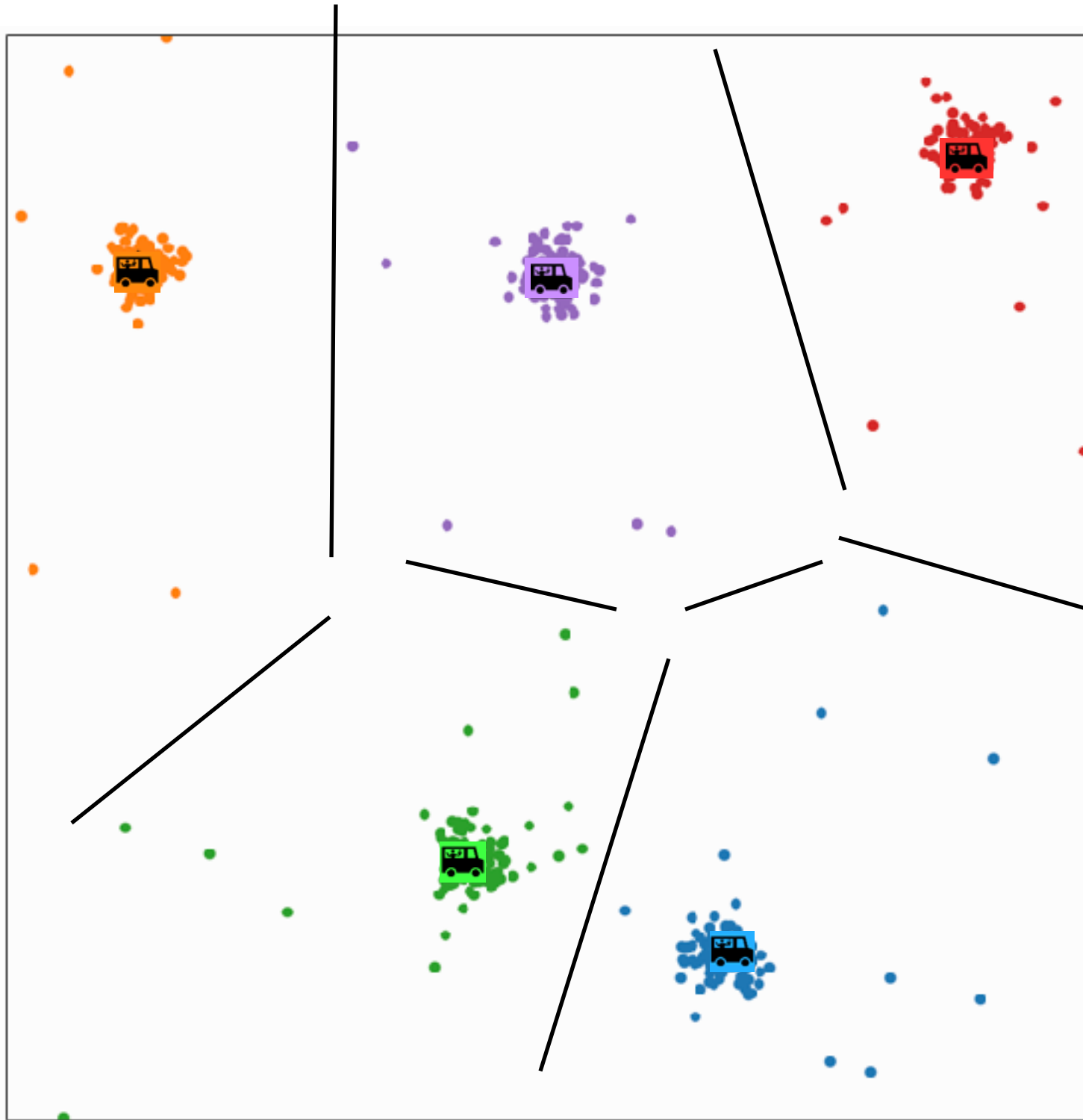
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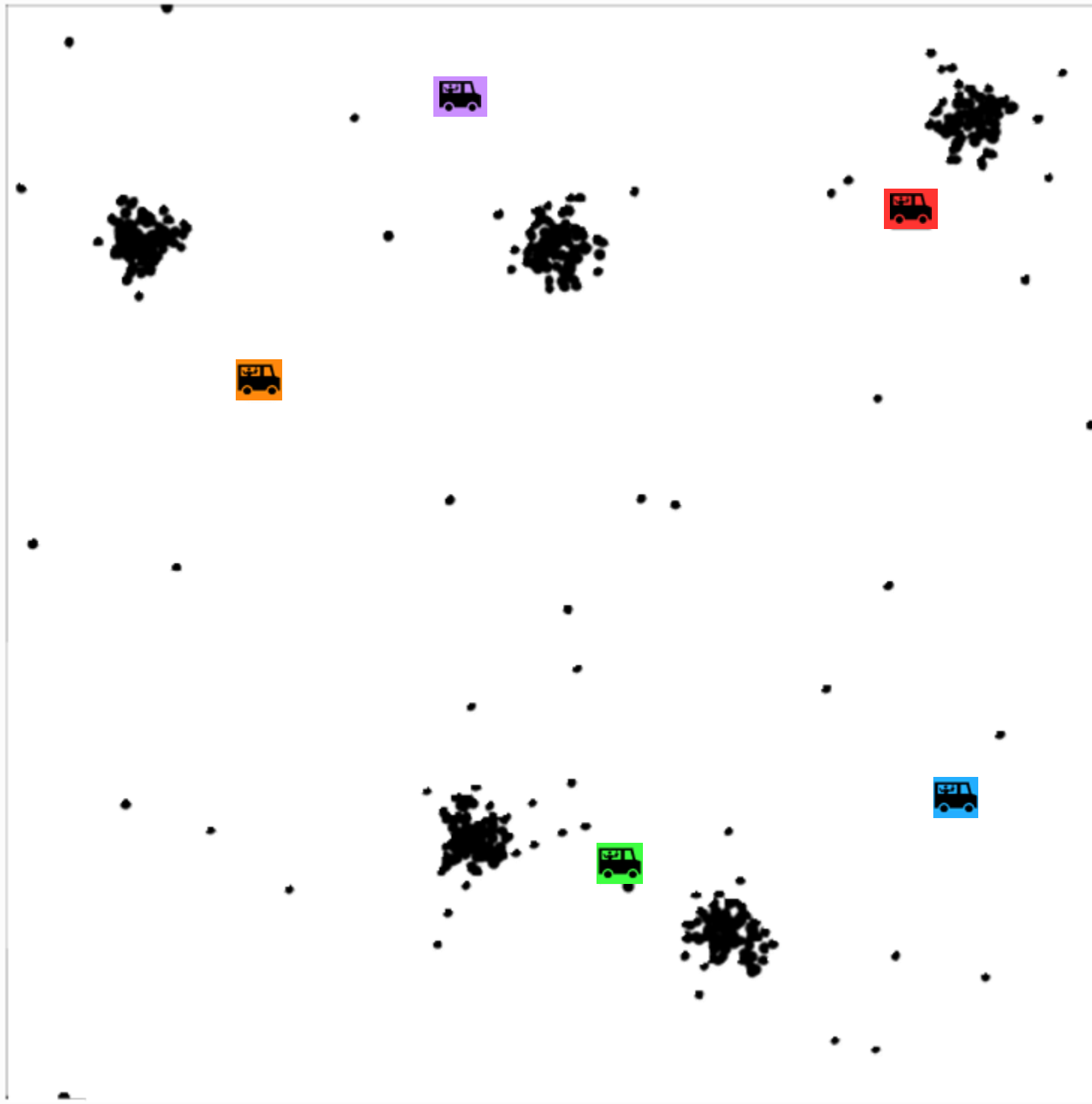
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k-means algorithm: initialization



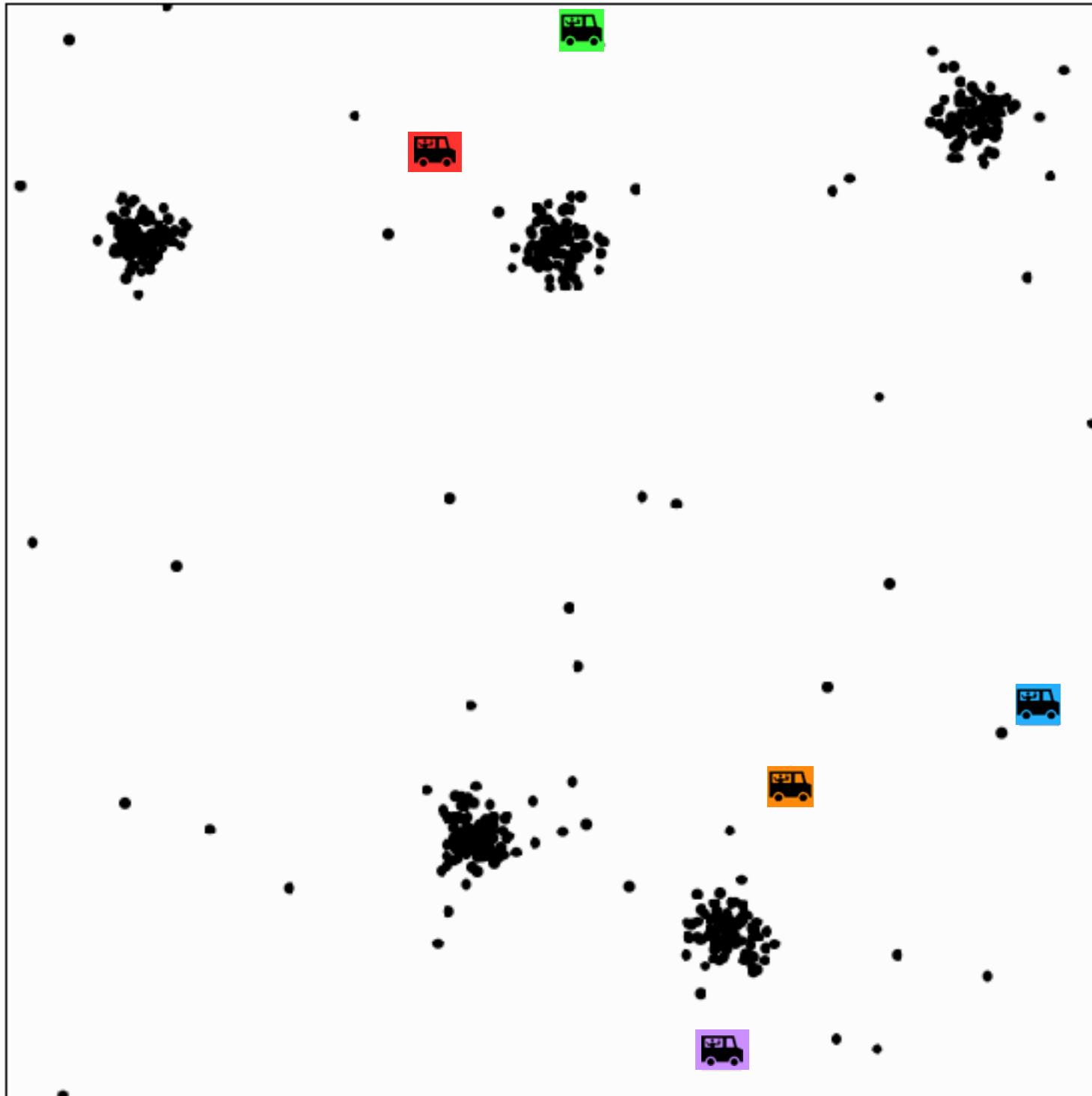
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- That local minimum could be bad!

k-means algorithm: initialization



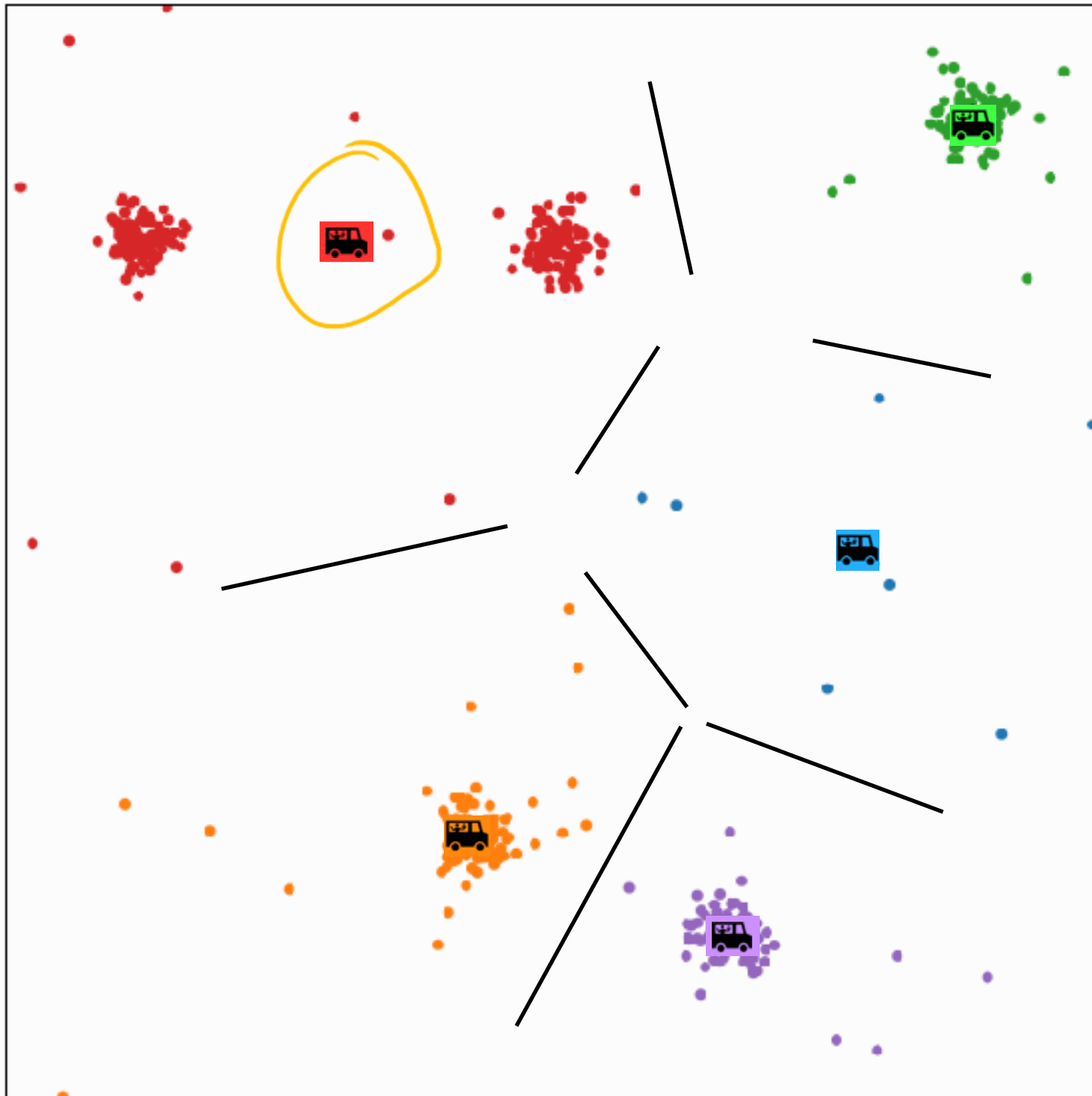
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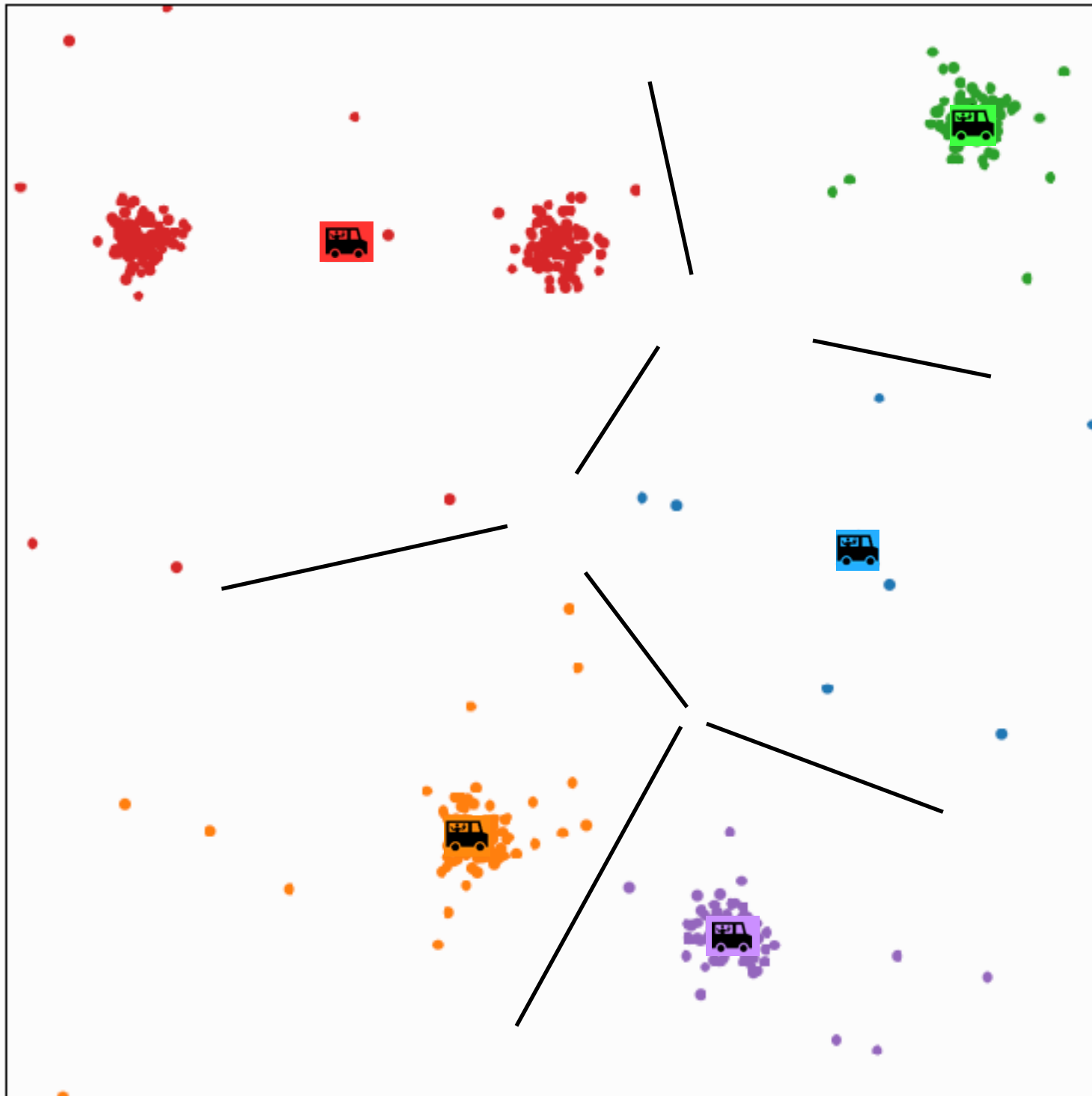
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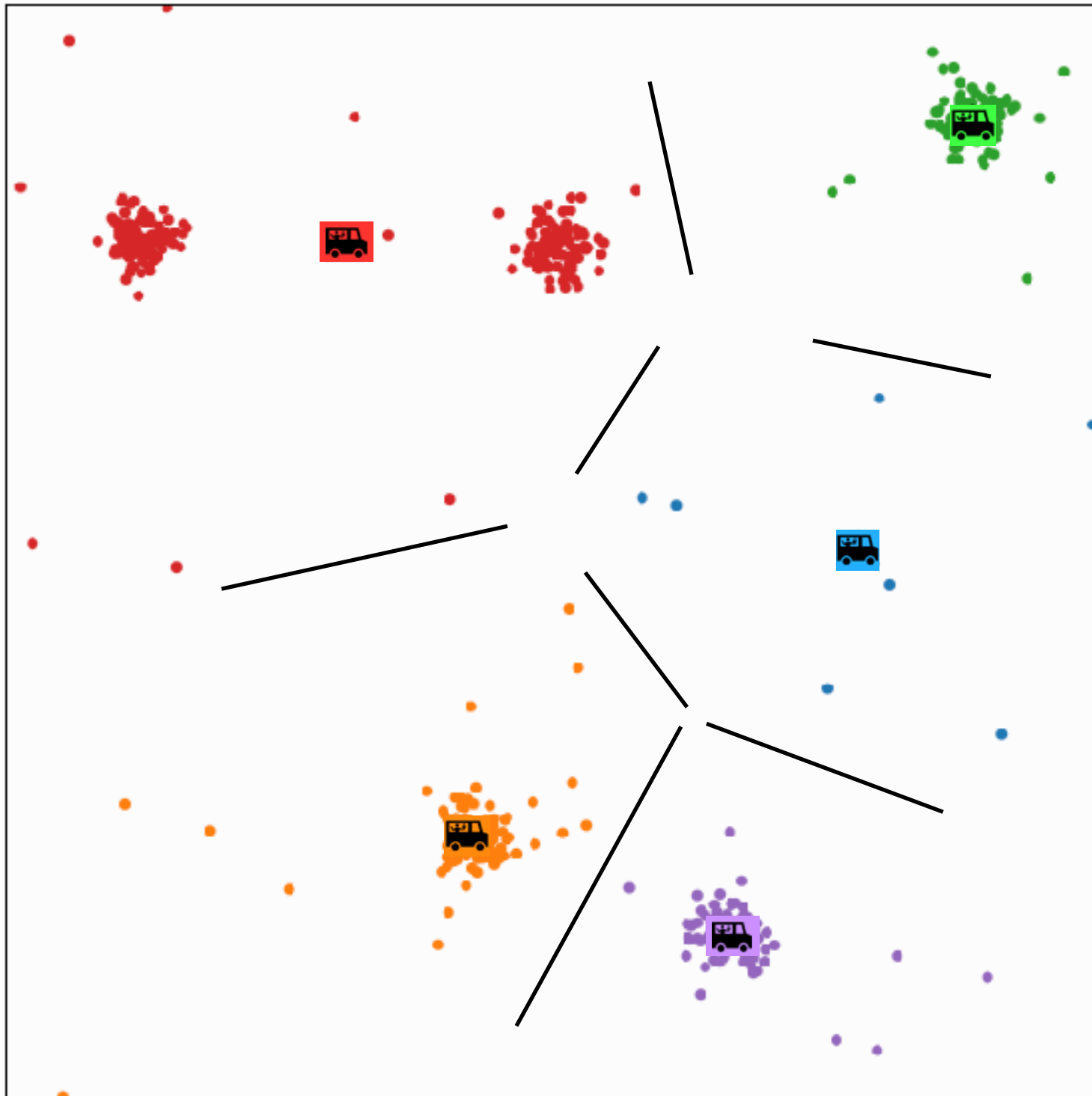


- **Theorem.** If run for enough outer iterations, the k-means algorithm will converge to a local minimum of the k-means objective
- means objective

That local minimum could be

Is this clustering worse than the one we found before?

k-means algorithm: initialization



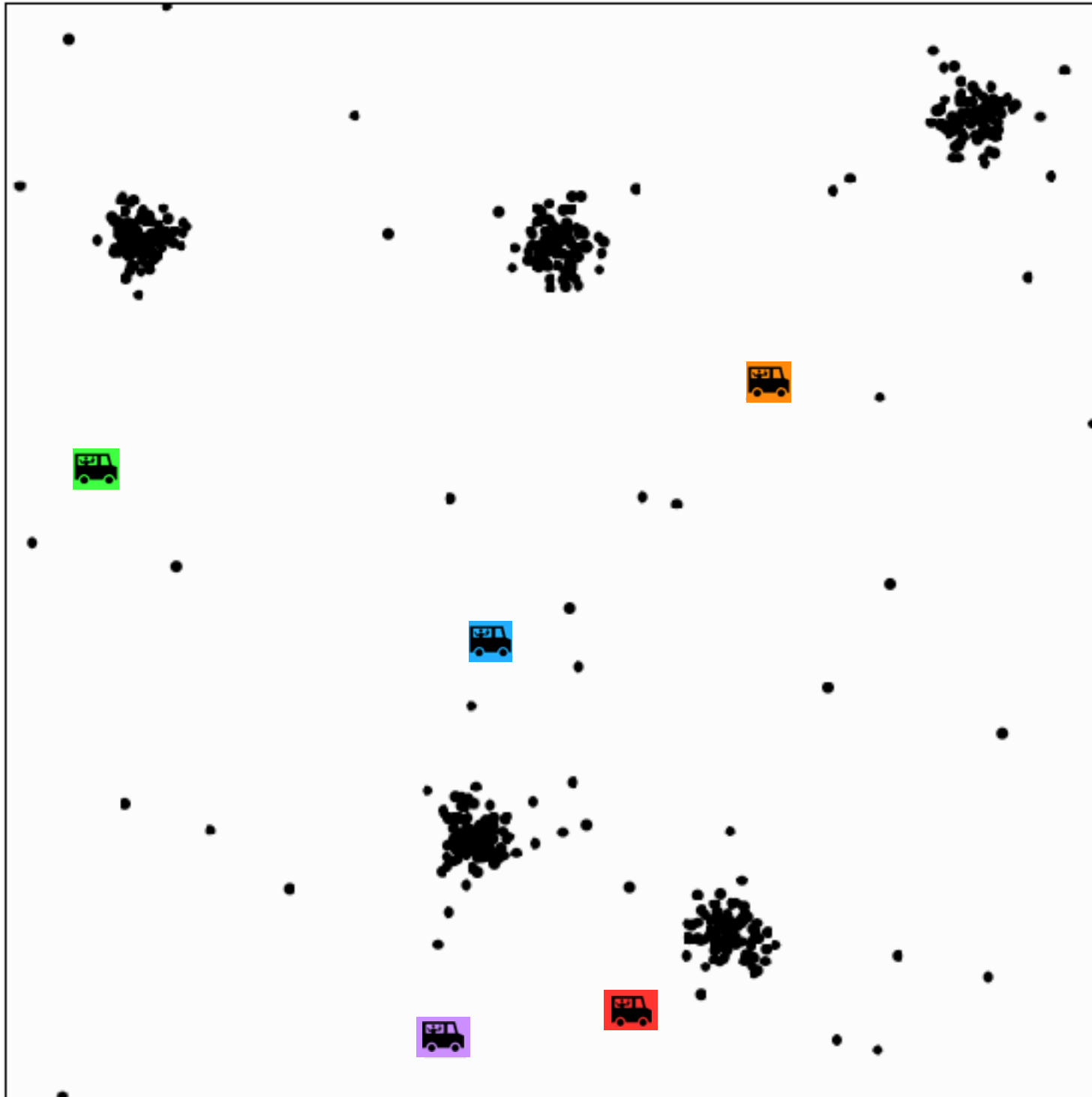
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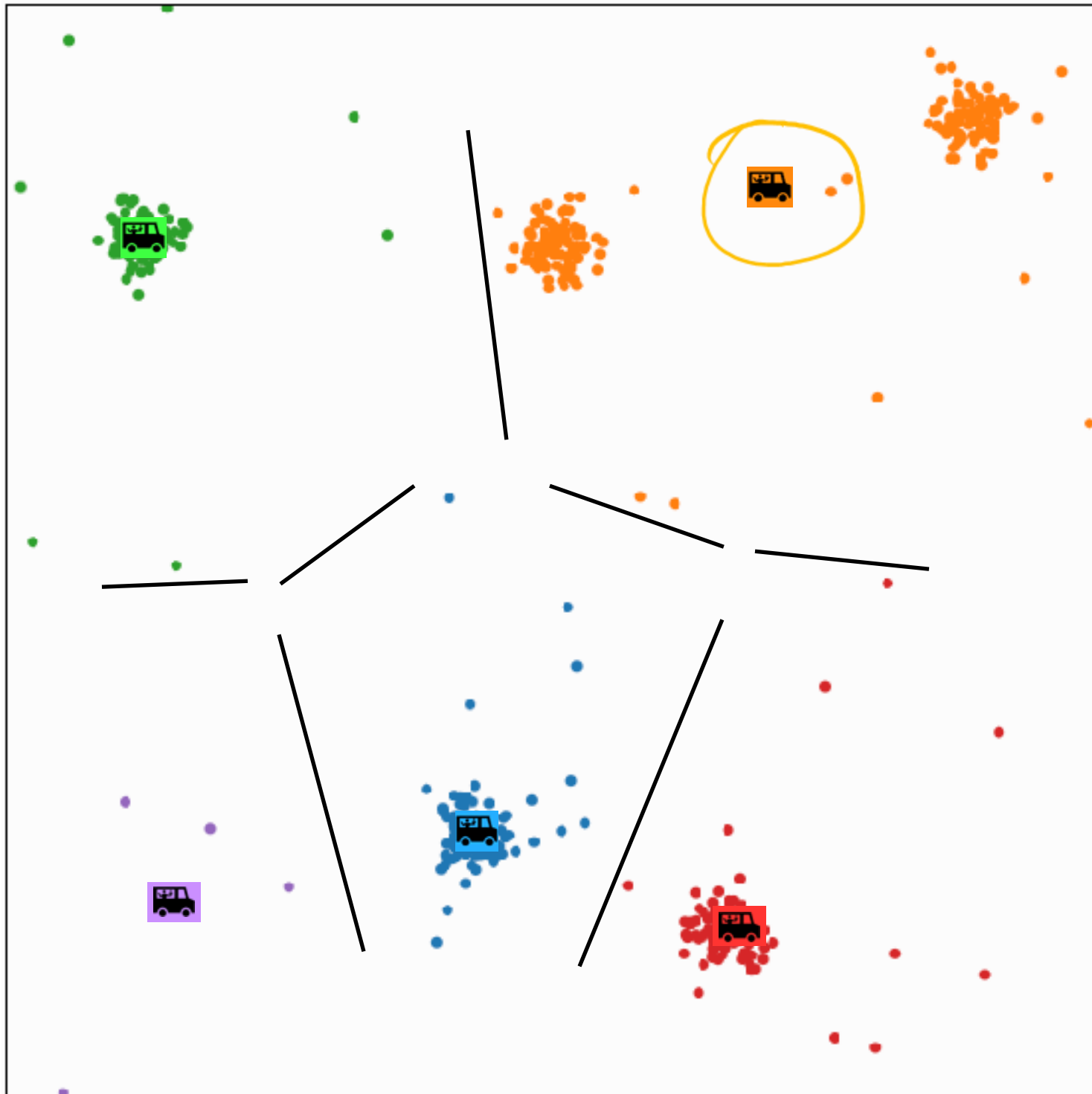
Why or why not?

k-means algorithm: initialization



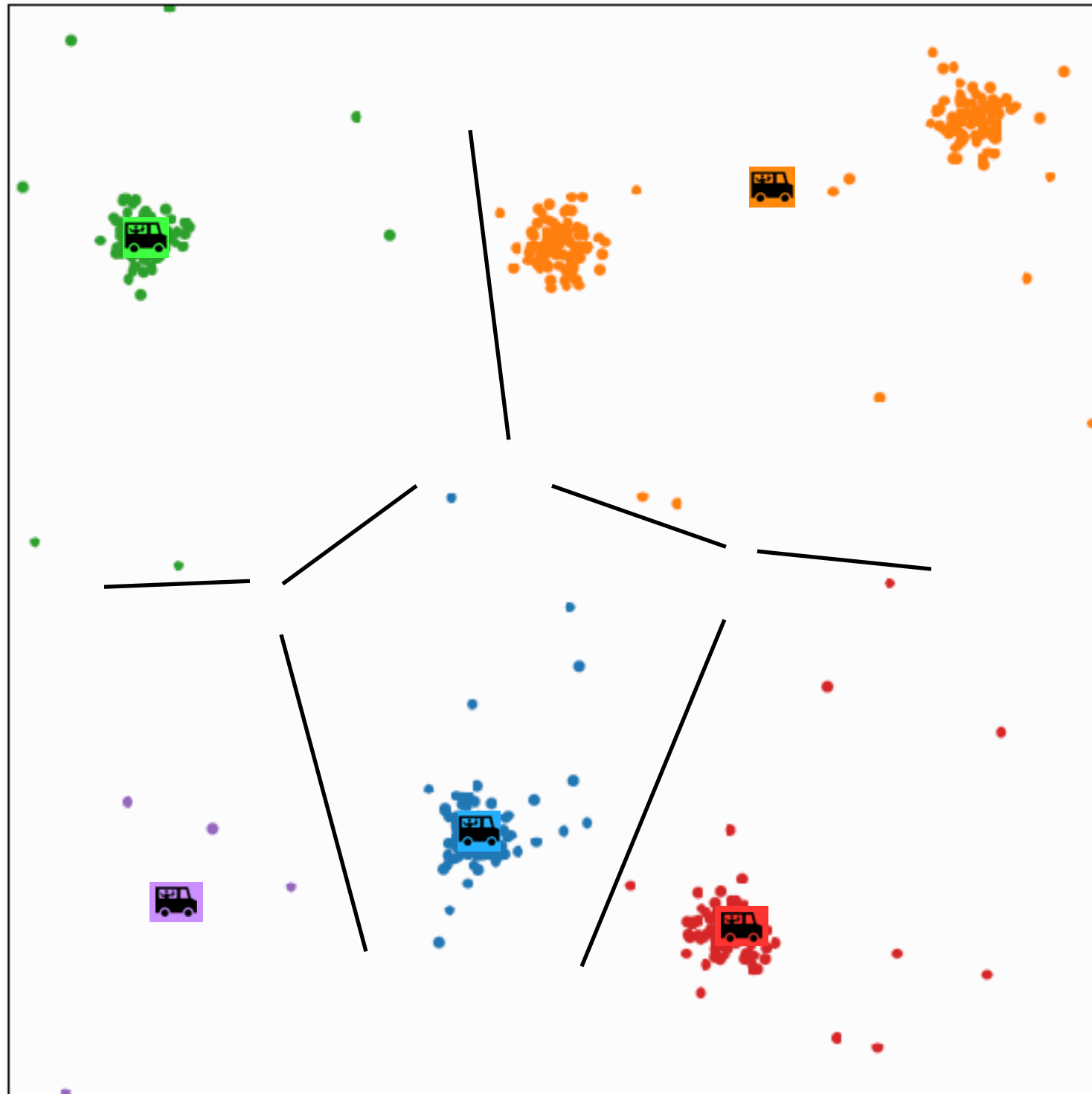
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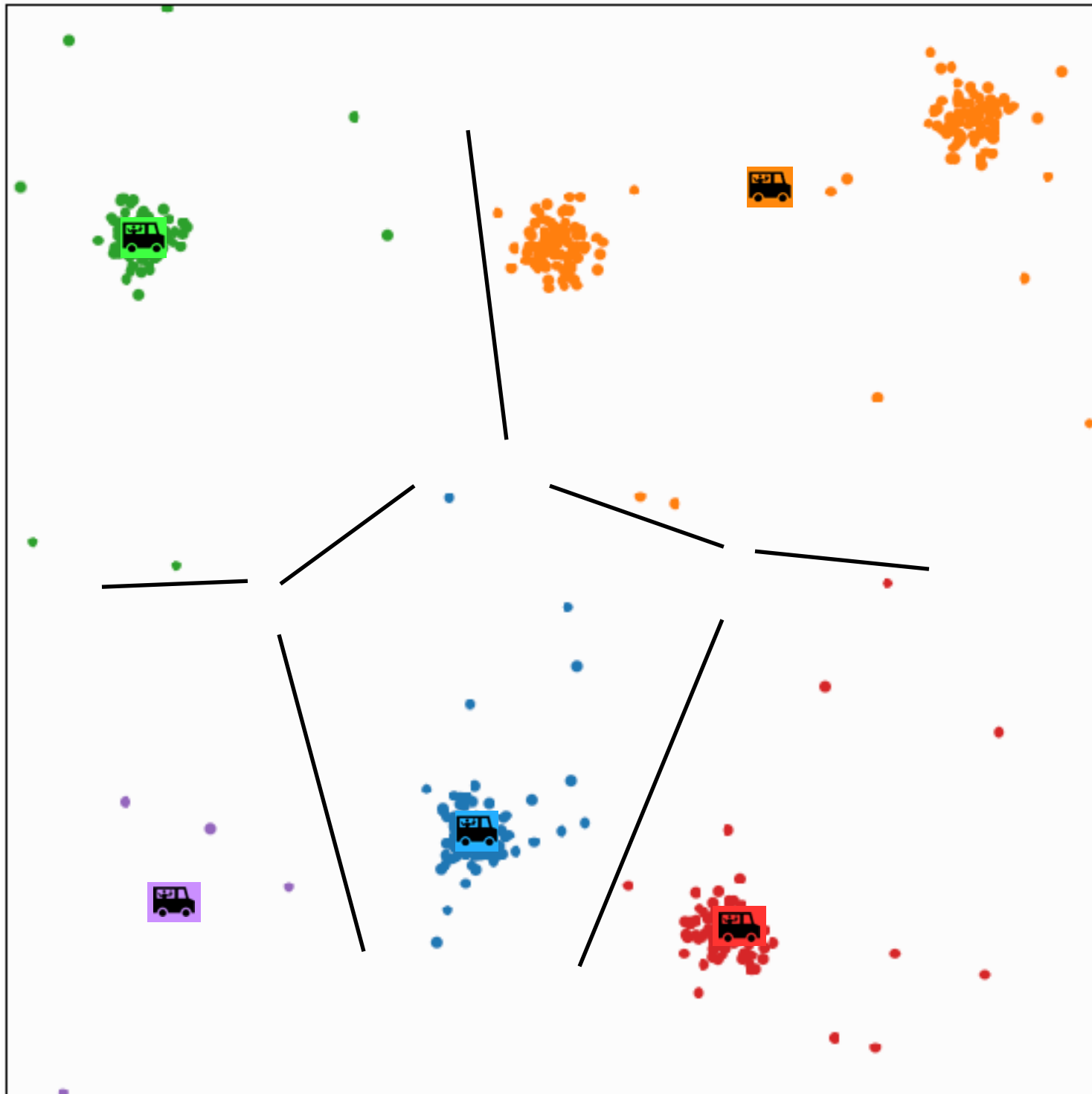
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k-means algorithm: initialization



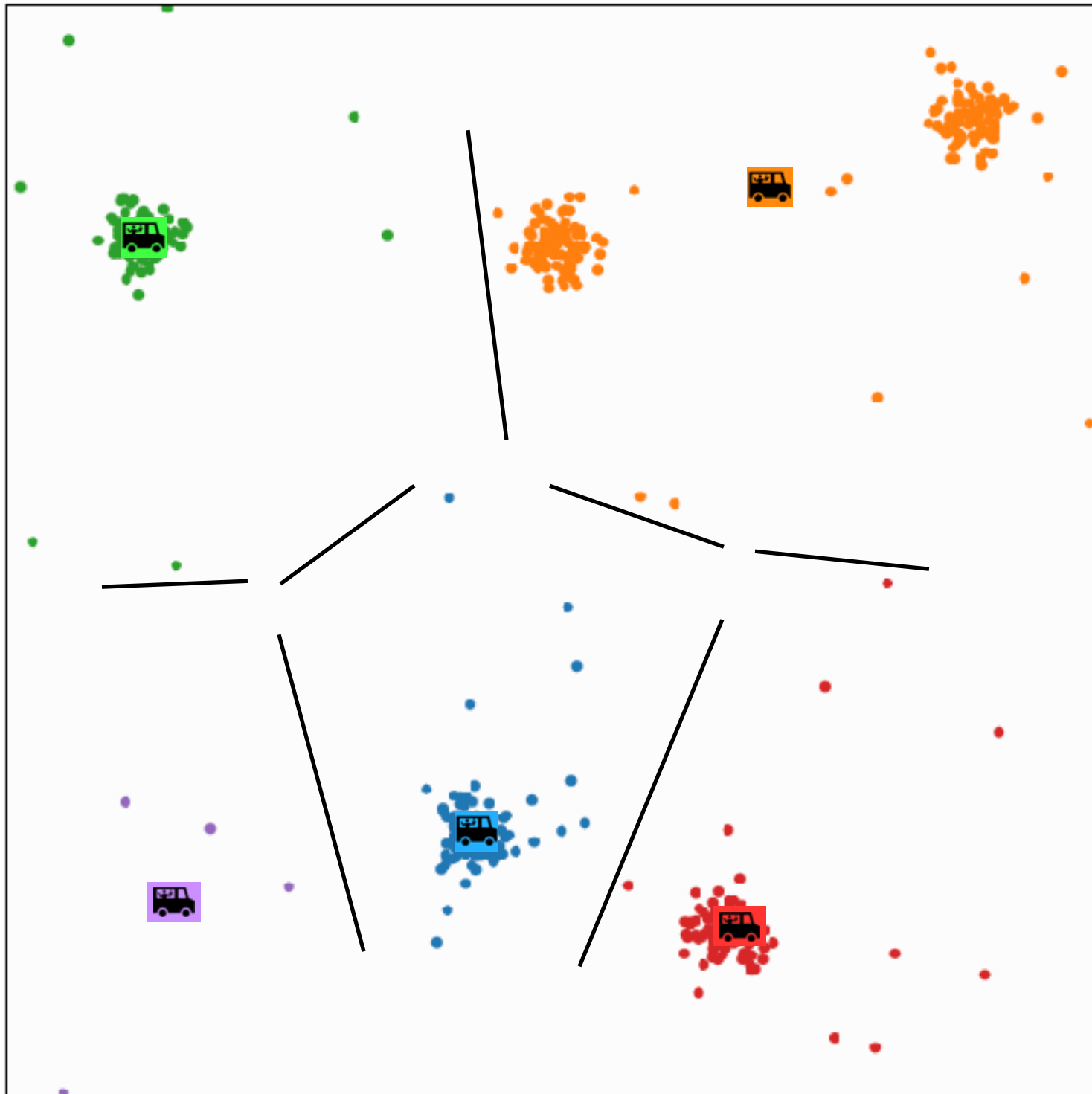
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k-means algorithm: initialization



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k-means algorithm: initialization



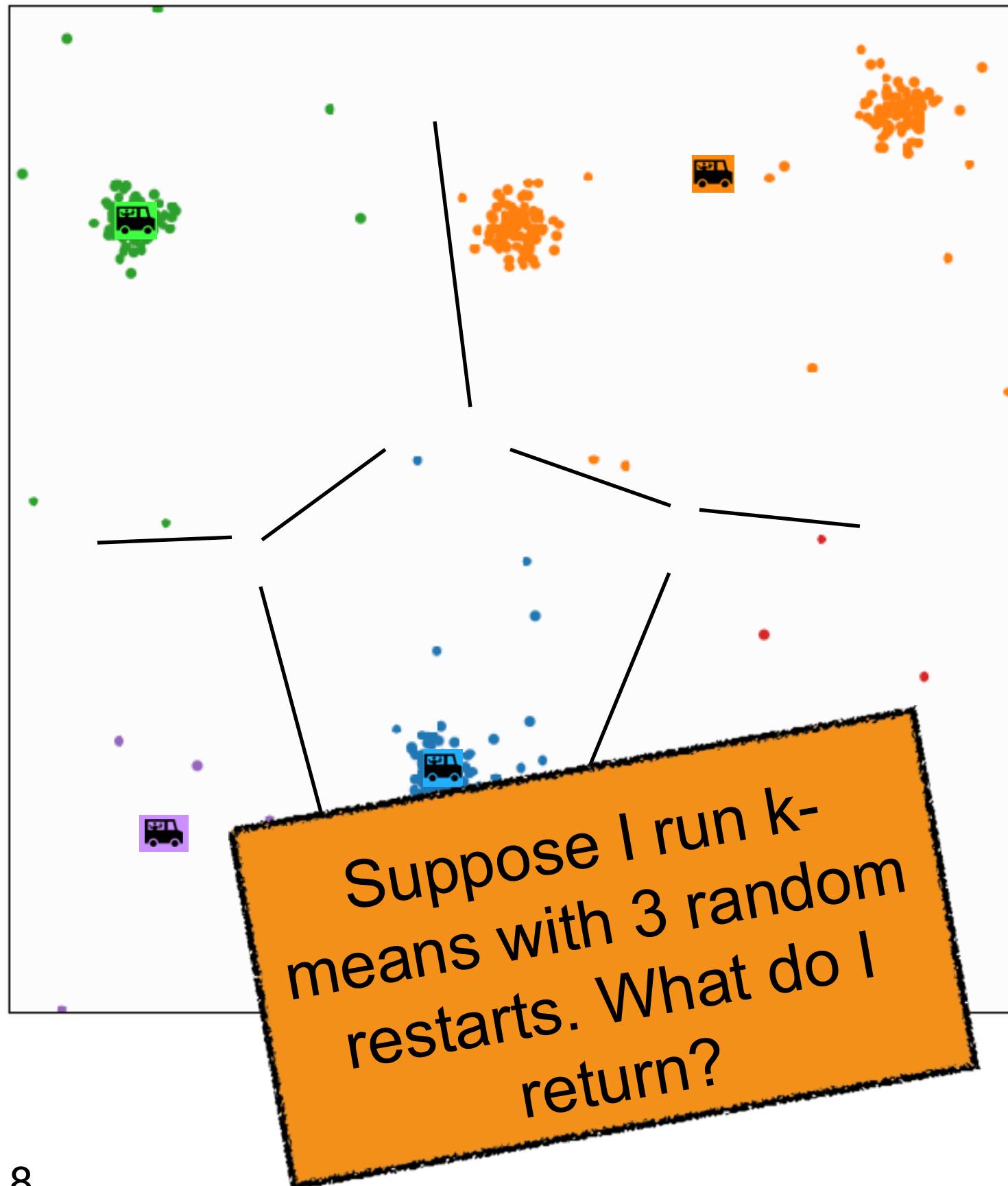
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k-means algorithm: initialization



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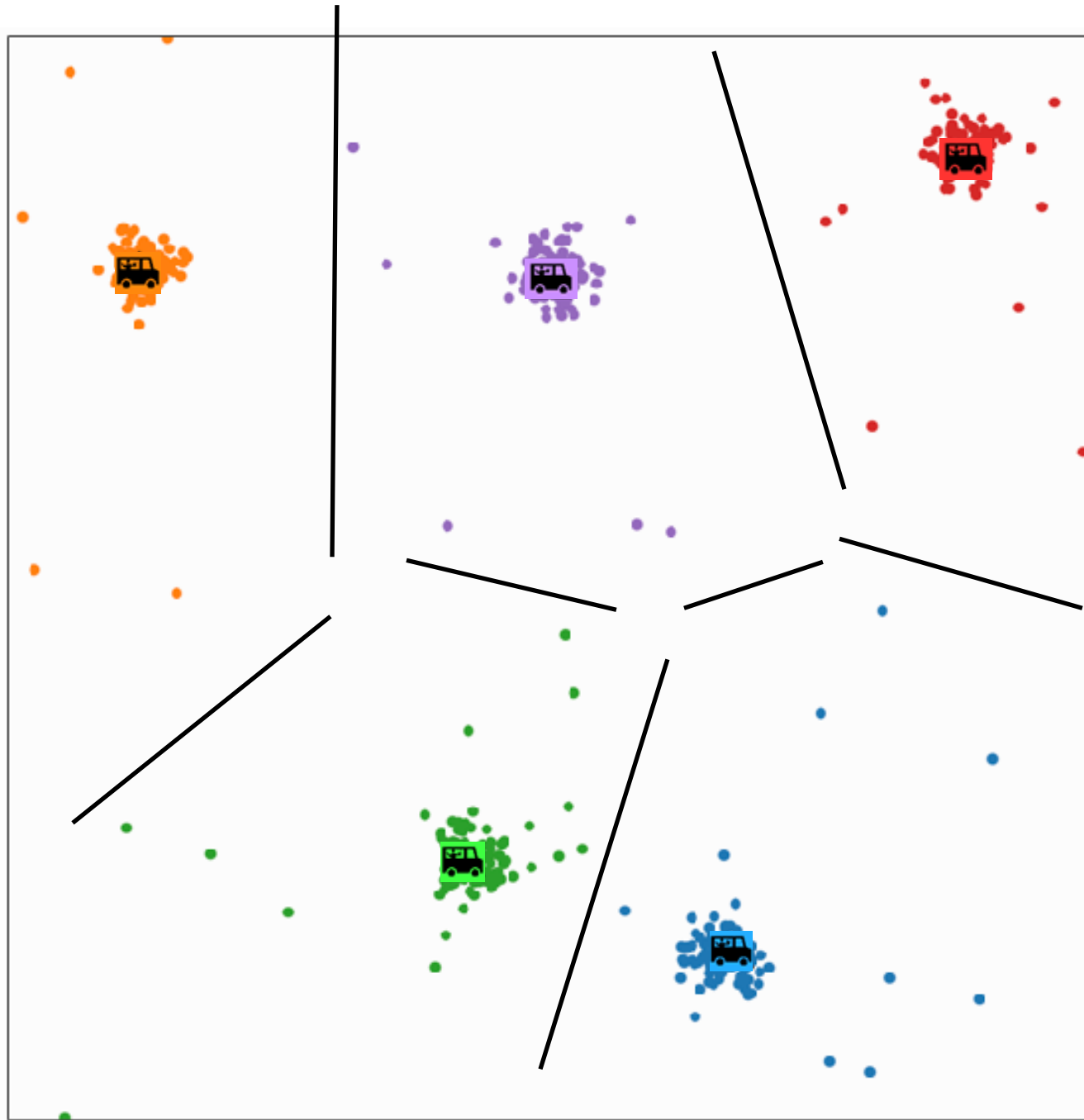
k-means algorithm: initialization



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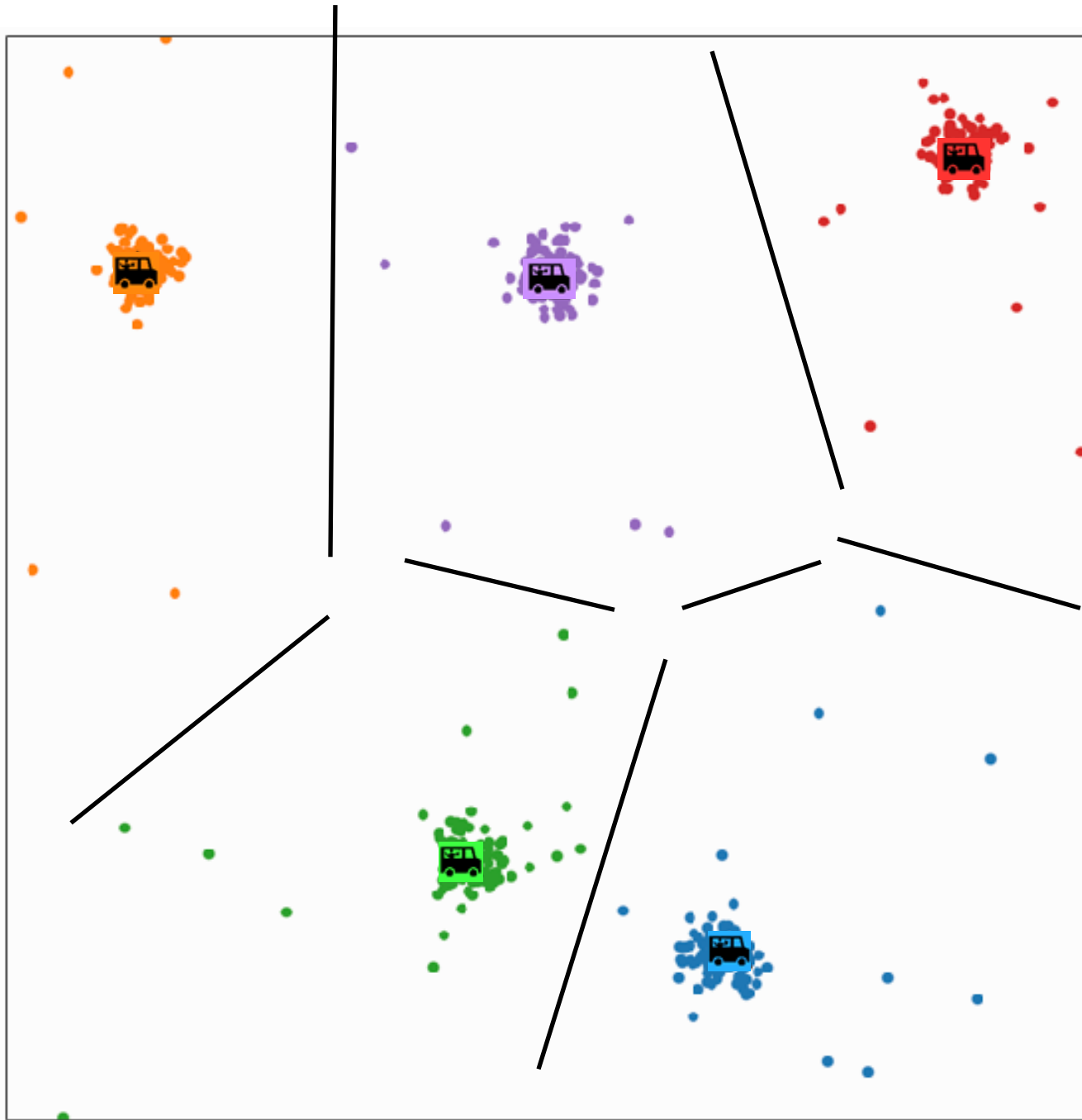
k-means algorithm: effect of k

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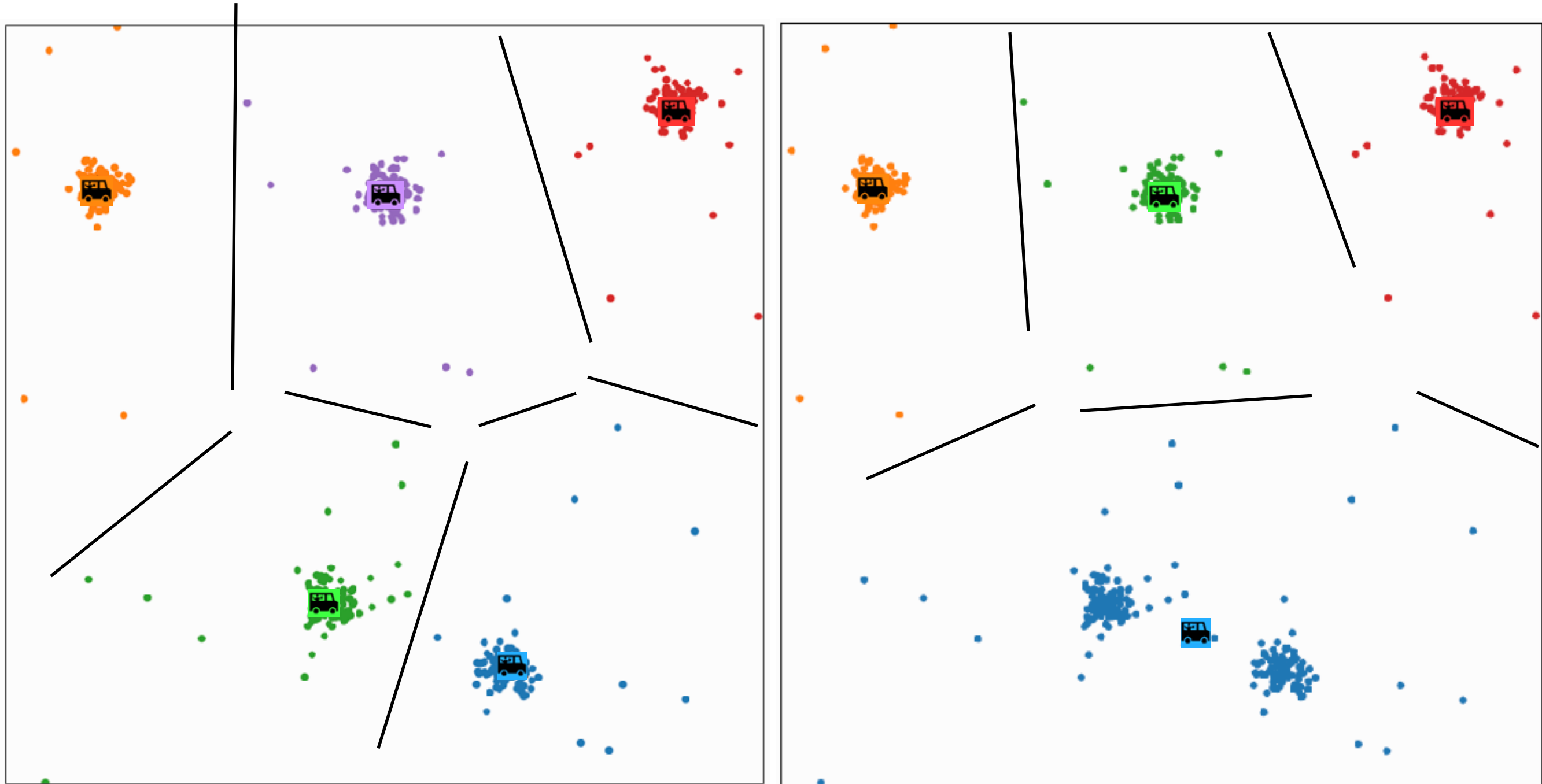
k-means algorithm: effect of k

- Different k will give us different results



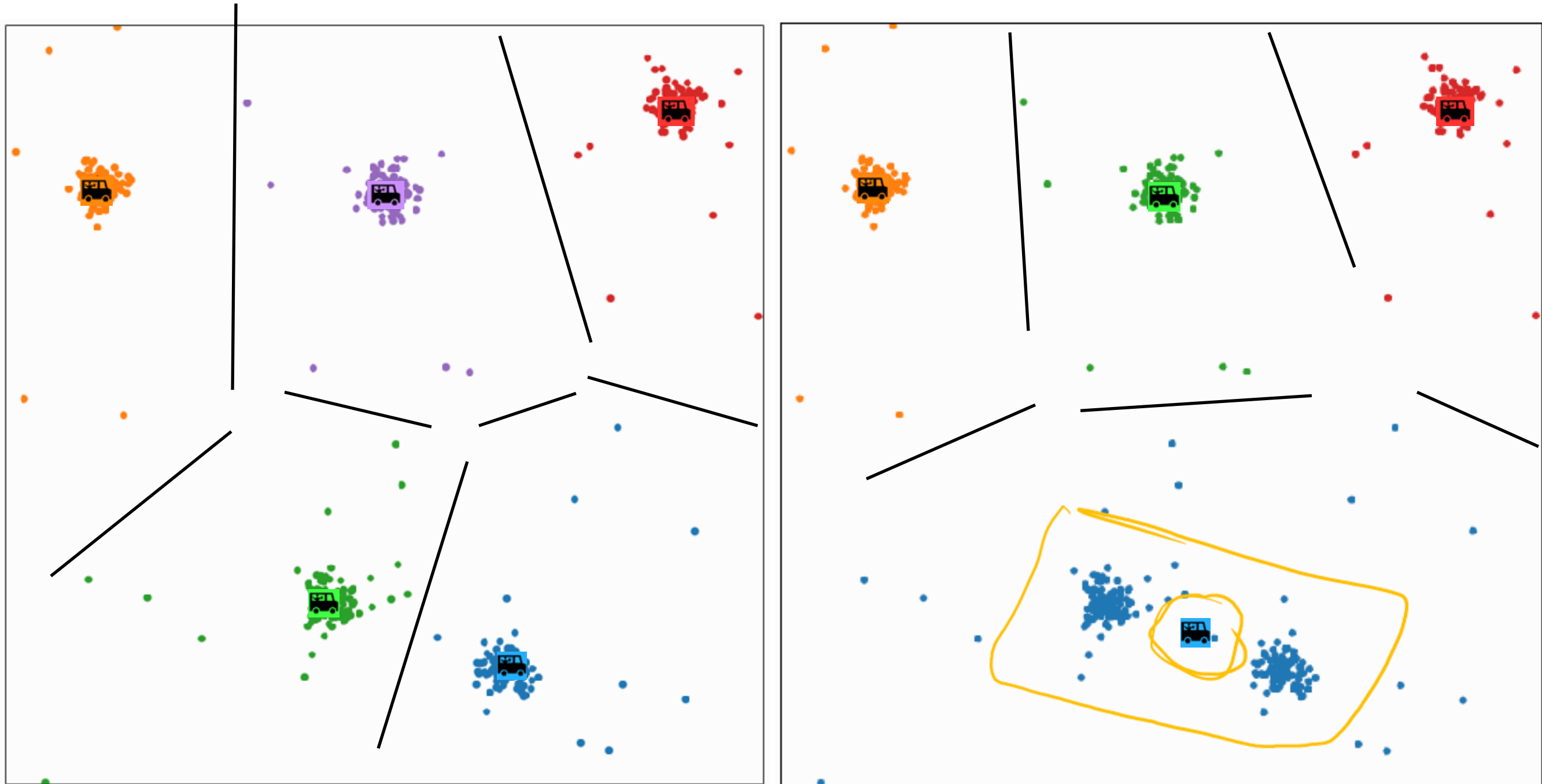
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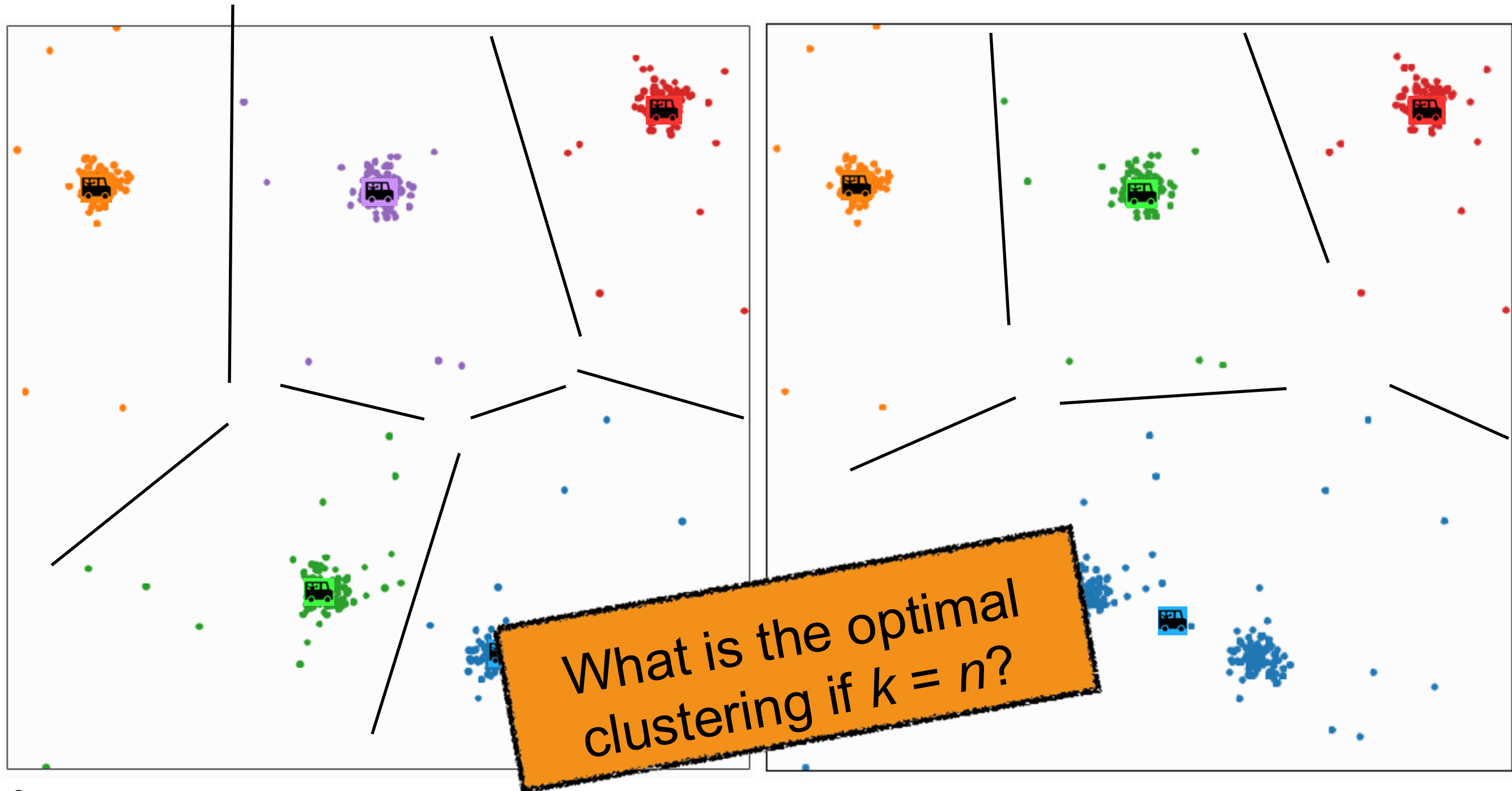
k-means algorithm: effect of k

- Different k will give us different results
- Larger k gets trucks closer to people



k-means algorithm: effect of k

- Different k will give us different results
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k-means algorithm: choosing k

k-means algorithm: choosing k

- Sometimes we know k

k-means algorithm: choosing k

- Sometimes we know



k-means algorithm: choosing k

- Sometimes we know



k-means algorithm: choosing k

- Sometimes we know



k-means algorithm: choosing k

- Sometimes we know



k-means algorithm: choosing k

- Sometimes we know



k-means algorithm: choosing k

- Sometimes we know



- Sometimes we'd like to choose/learn k

k-means algorithm: choosing k

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- Sometimes we'd like to choose/learn k
 - Can't just minimize the k-means objective over k too

k-means algorithm: choosing k

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$$\sum_{j=1}^k \sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2$$

k-means algorithm: choosing k

- Sometimes we know



- Sometimes we'd like to choose/learn k
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$$\arg \min_{y, \mu} \sum_{j=1}^k \sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2$$

loss function

$$\arg \min_{y, \mu} \left(\sum_{i=1}^n \sum_{j=1}^k \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2 \right)$$

k-means algorithm: choosing k

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$$\arg \min_{y, \mu, k} \sum_{j=1}^k \sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2$$

k-means algorithm: choosing k

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Why not?

k-means algorithm: choosing k

- Sometimes we know



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- How to choose k depends on what you'd like to do

k-means algorithm: choosing k

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- How to choose k depends on what you'd like to do
 - E.g. cost-benefit trade-off

k-means algorithm: choosing k

- Sometimes we know



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$$\arg \min_{y, \mu, k} \sum_{j=1}^k \sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2 + \text{cost}(k)$$

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k-means algorithm: choosing k

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$$\arg \min_{y, \mu, k} \sum_{j=1}^k \sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} \|x^{(i)} - \mu^{(j)}\|_2^2 + \text{cost}(k)$$

- How to choose k depends on what you'd like to do
 - E.g. cost-benefit trade-off
 - Often no single "right answer"

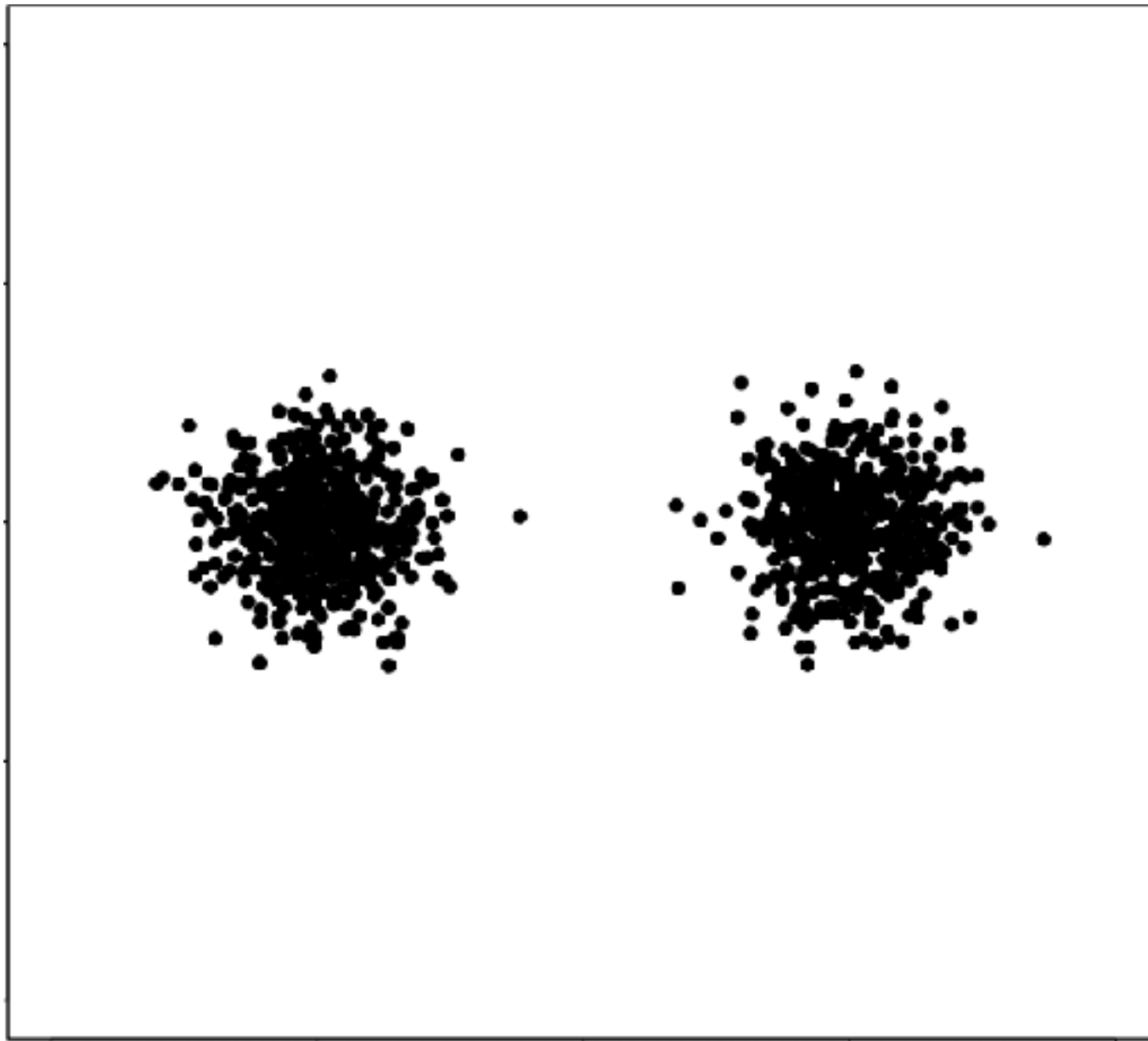
from k

Cluster shape

Cluster shape

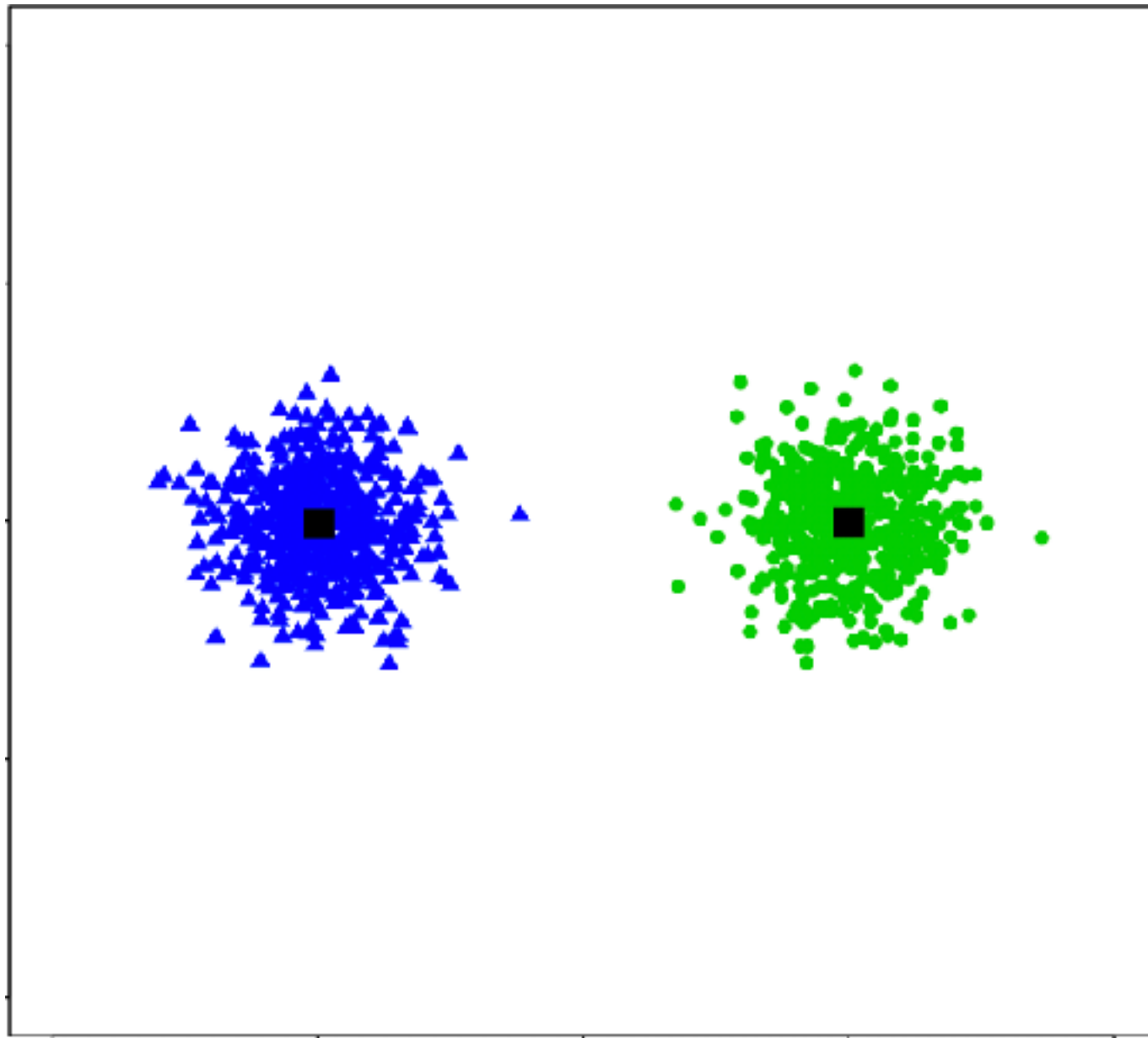
- k-means works well for well-separated circular clusters of the same size

Cluster shape



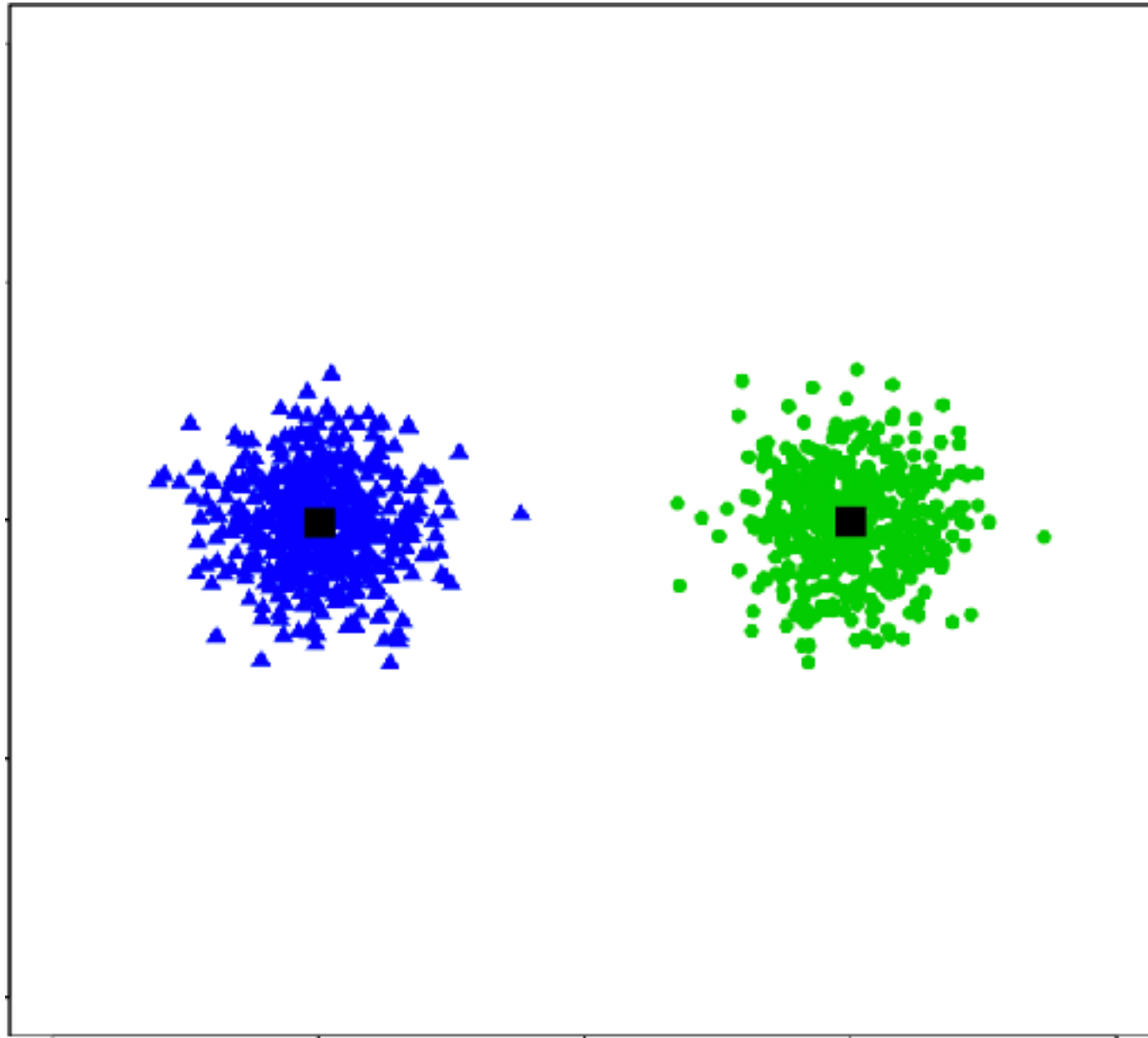
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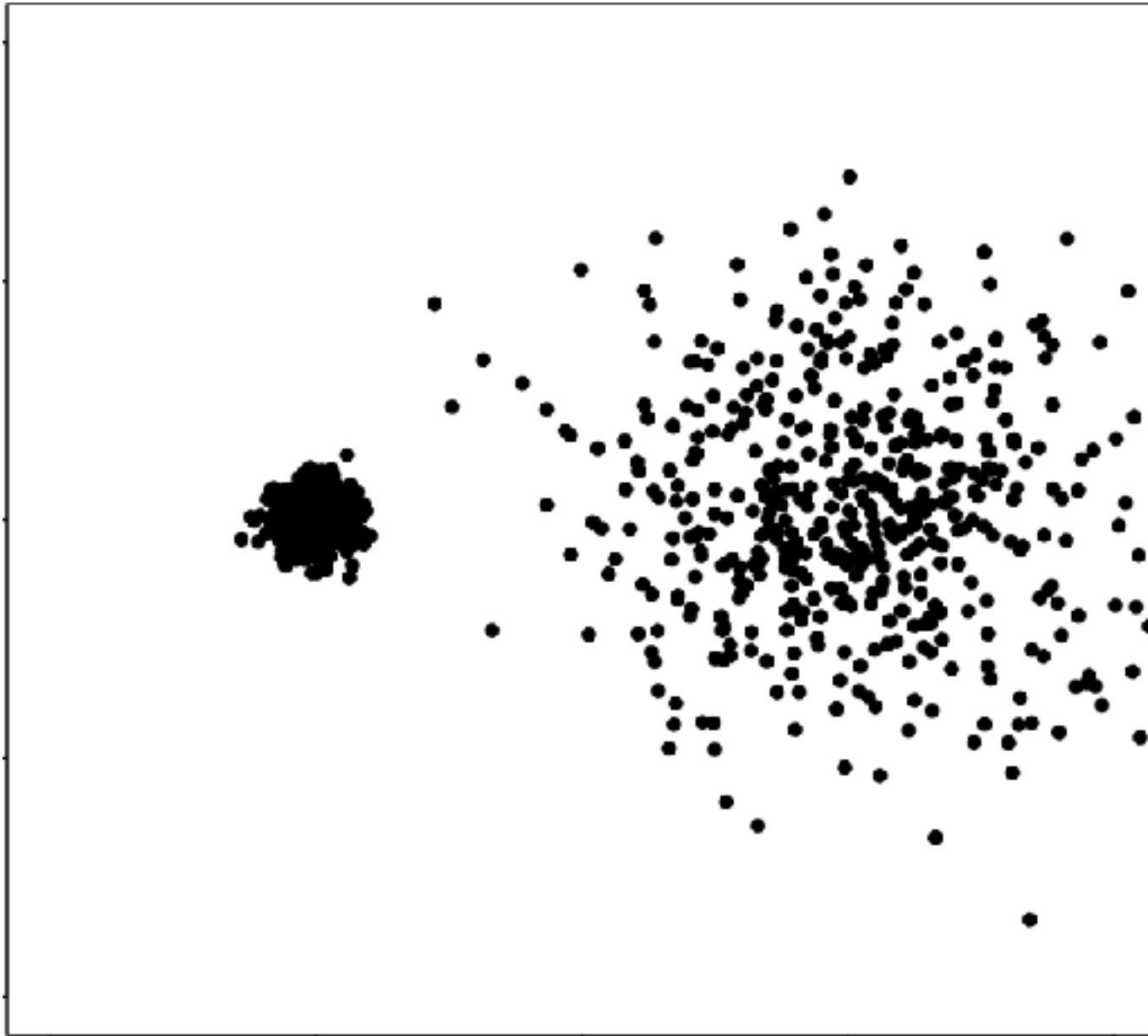
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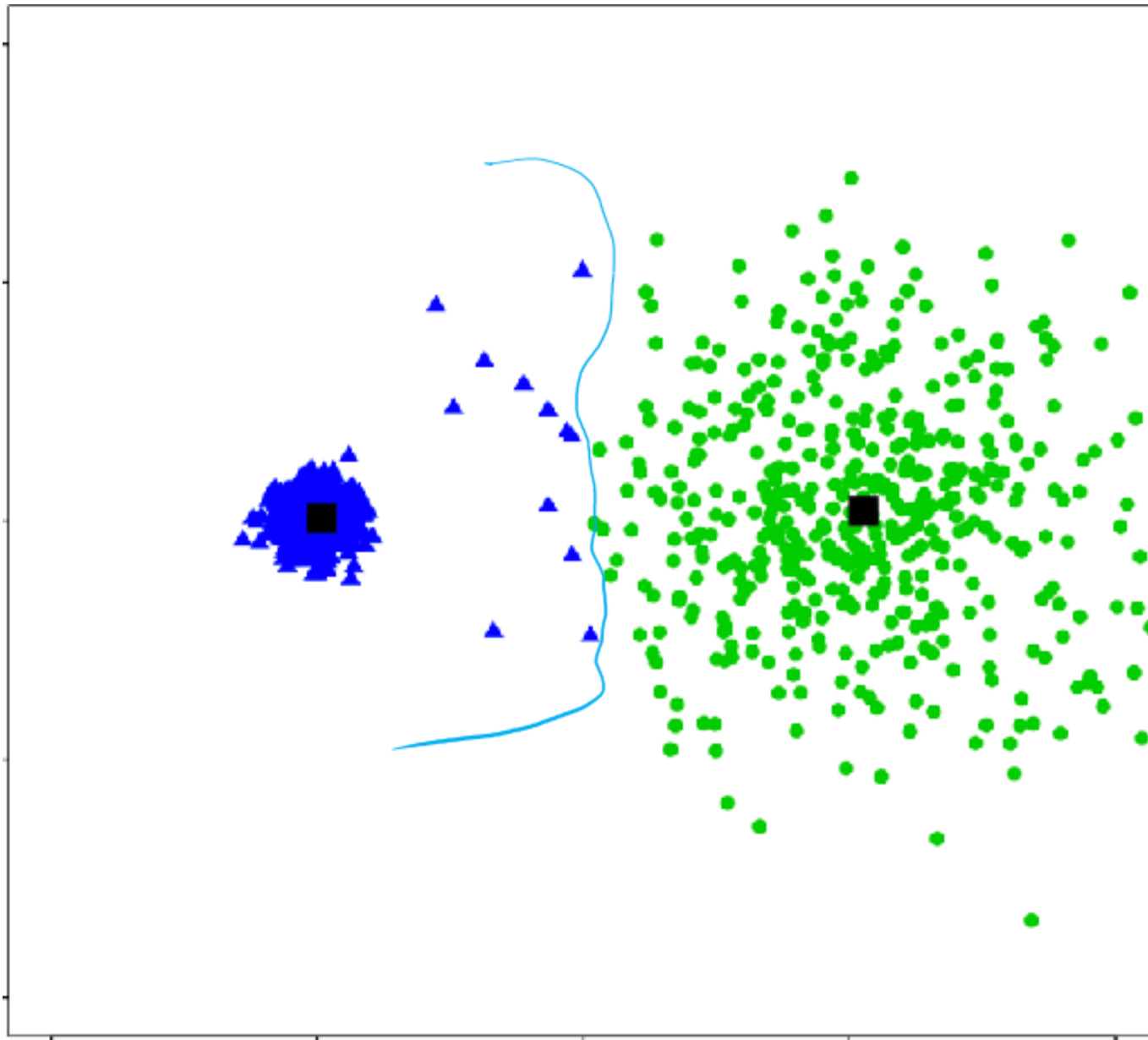
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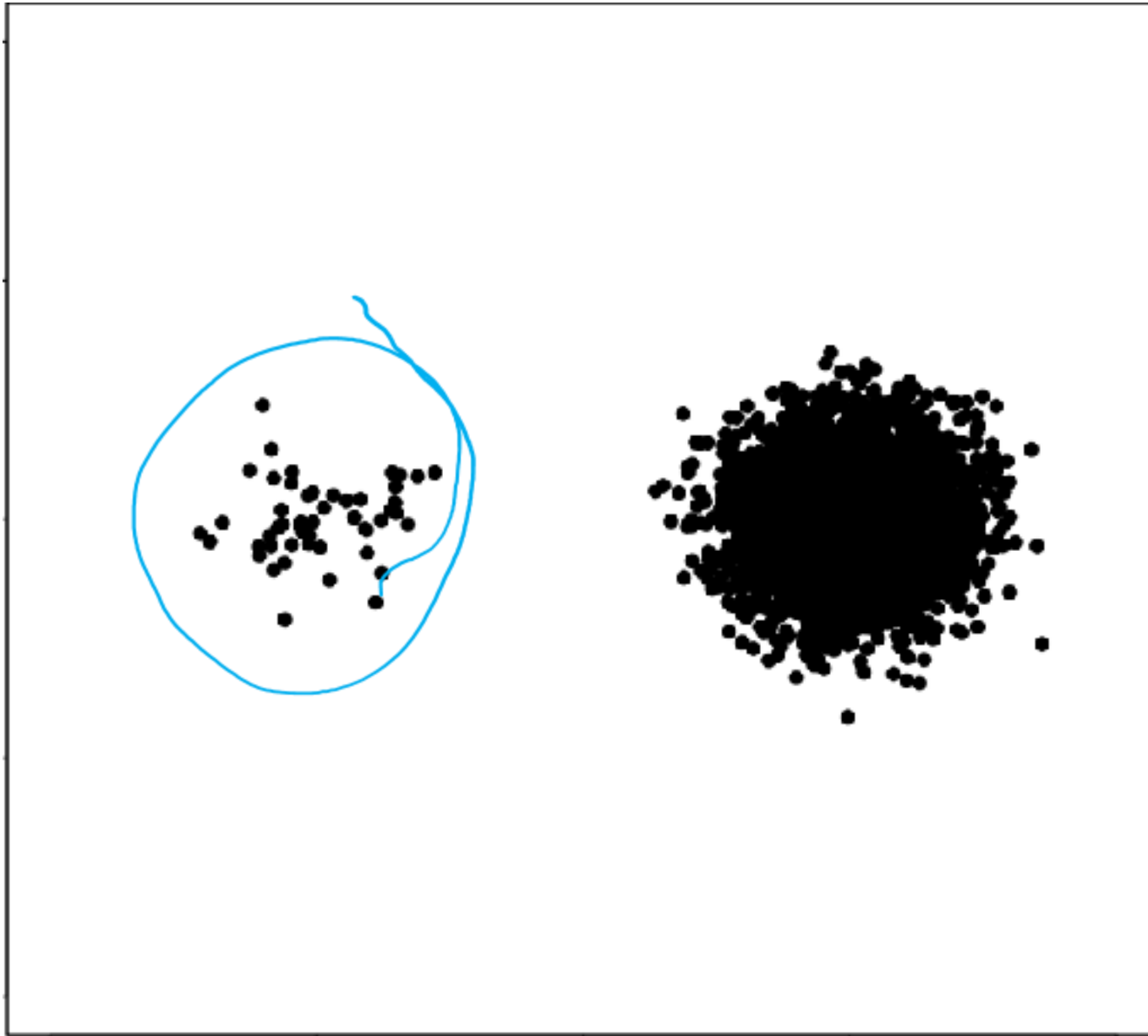
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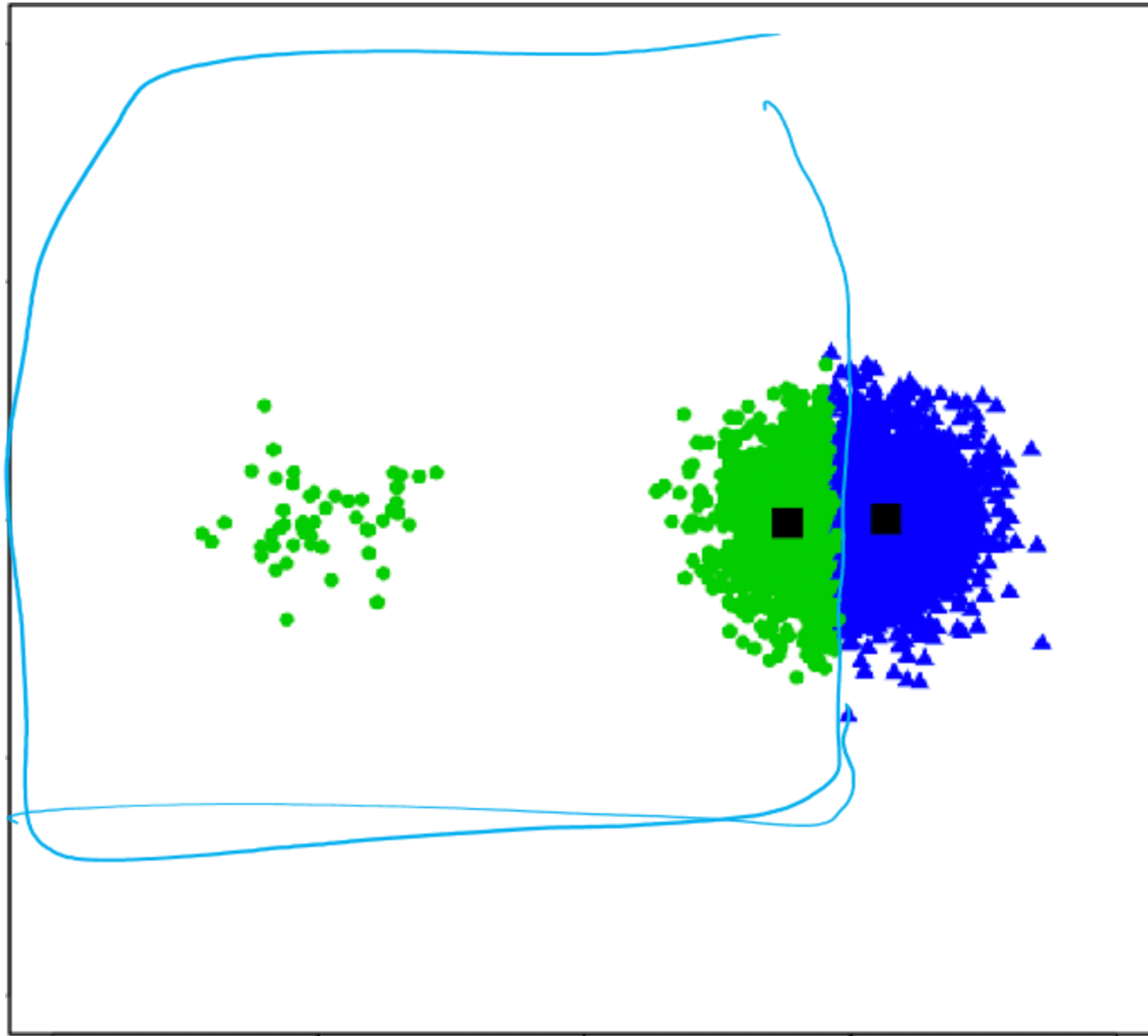
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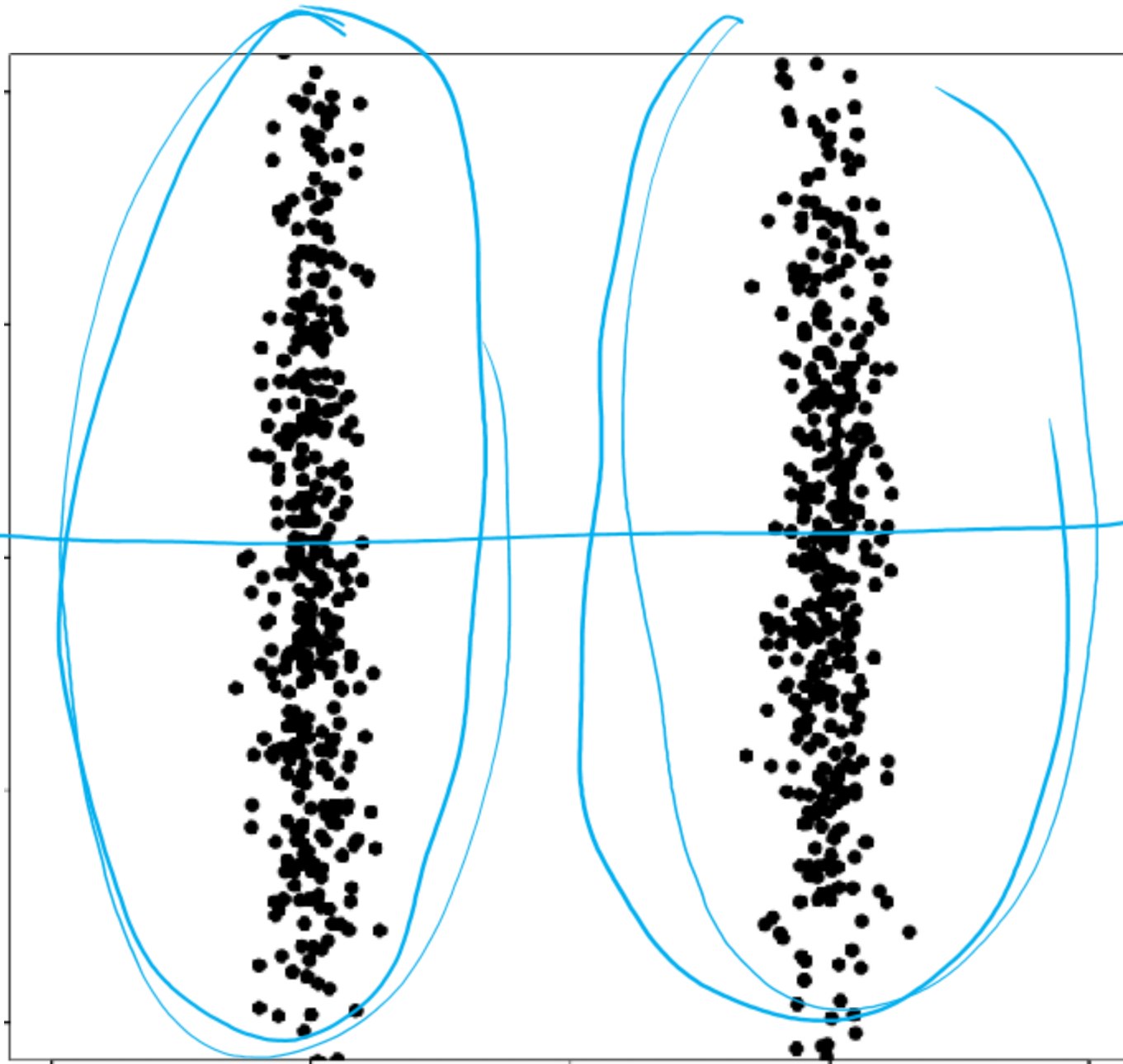
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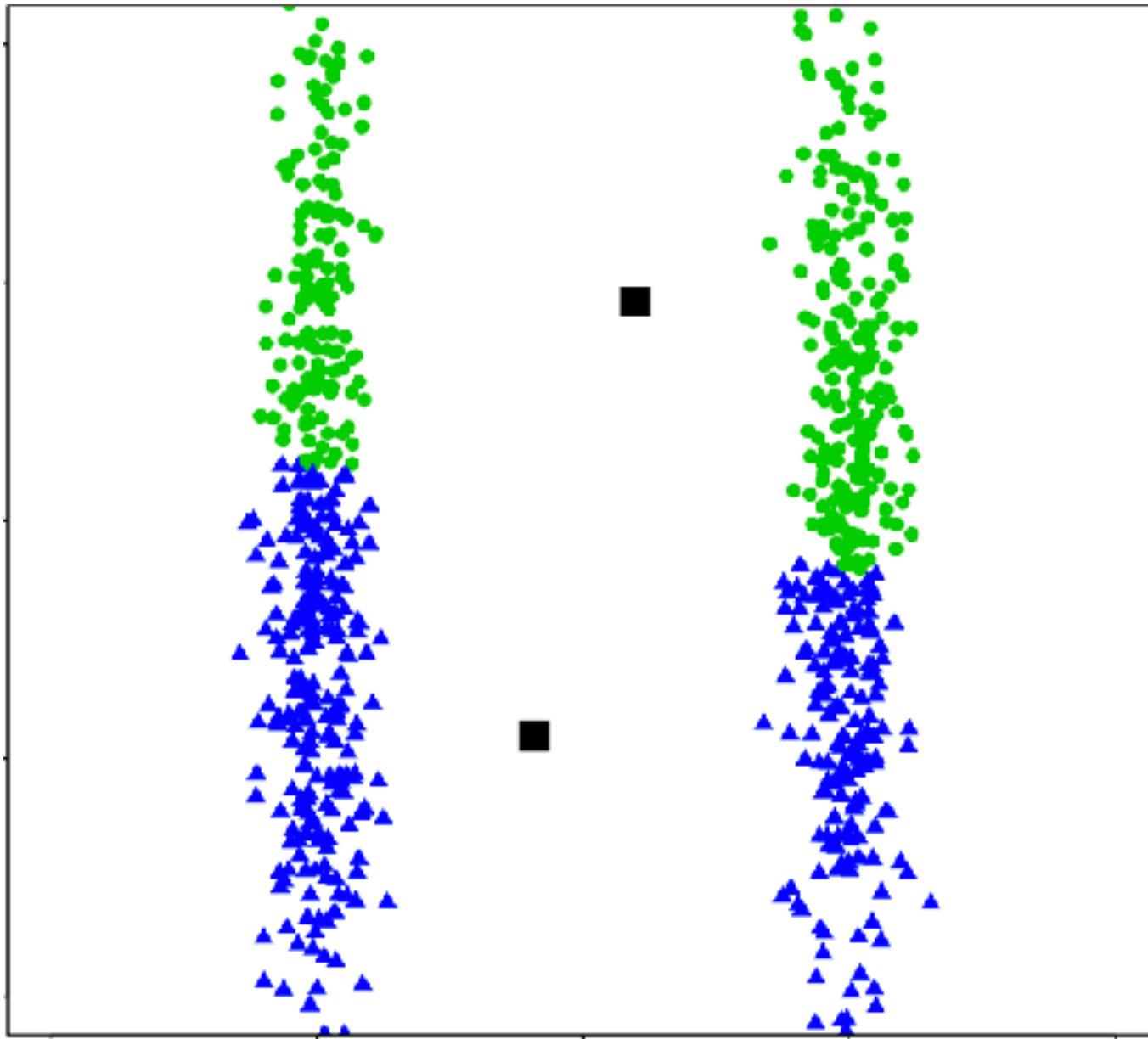
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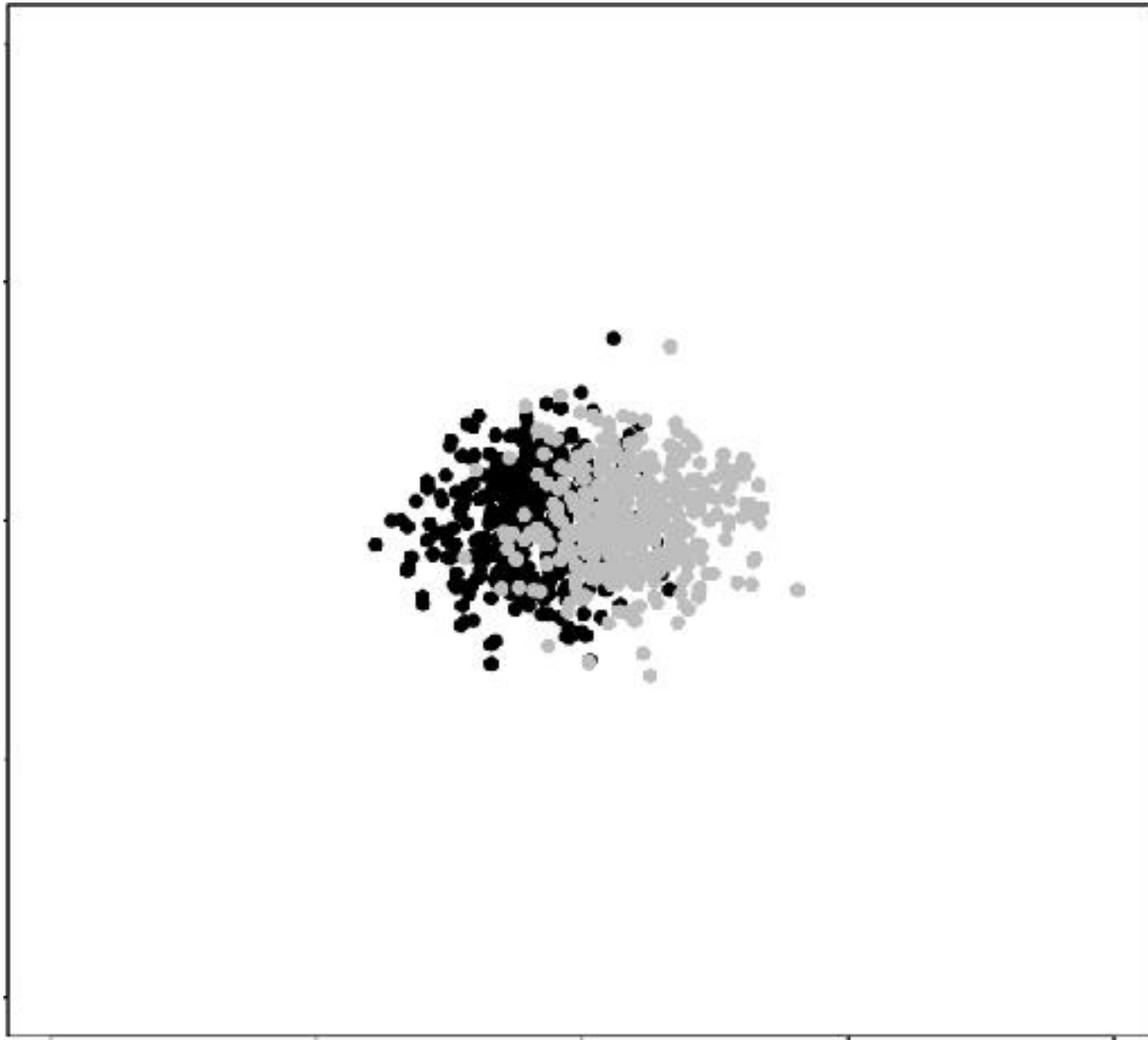
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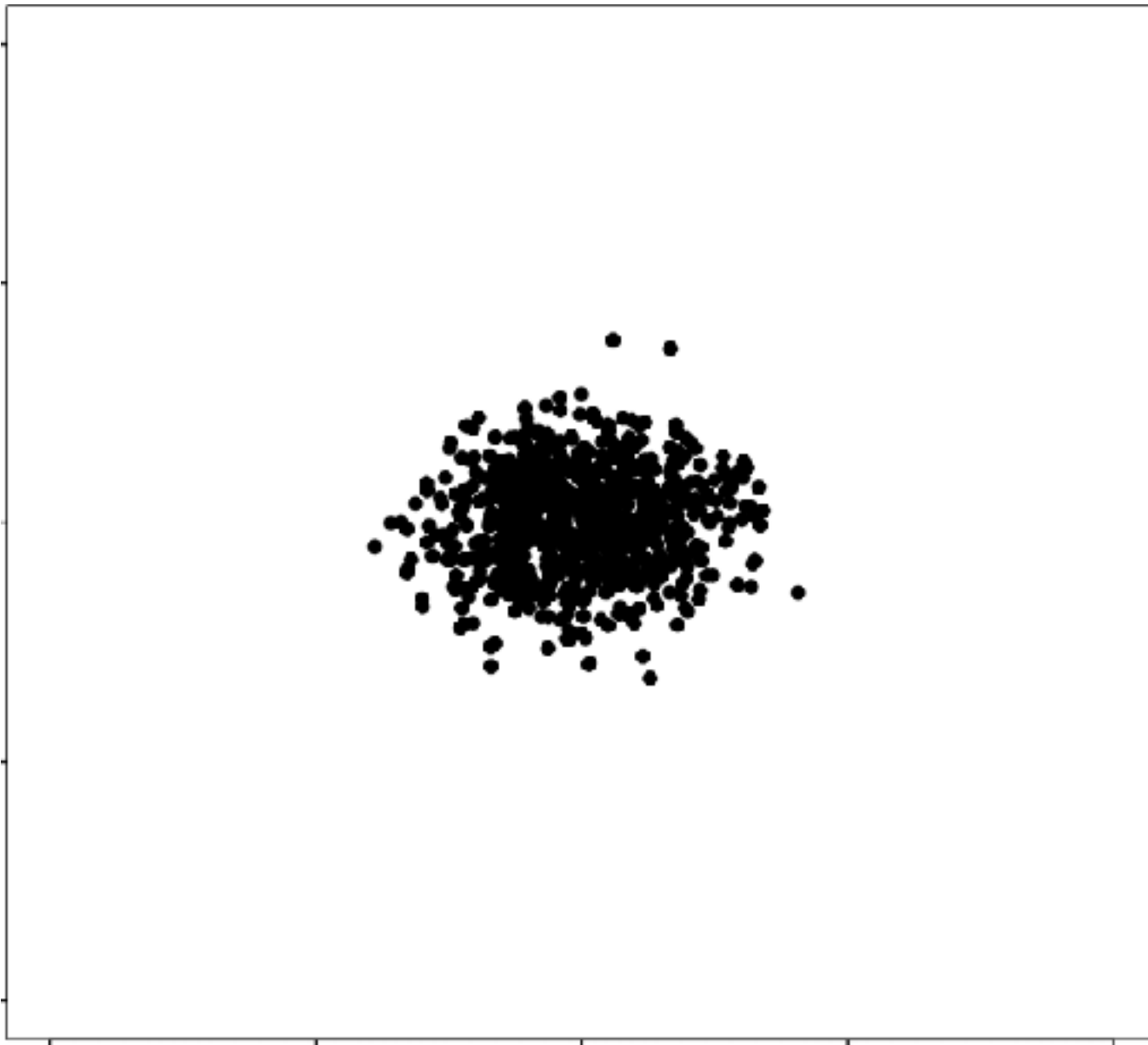
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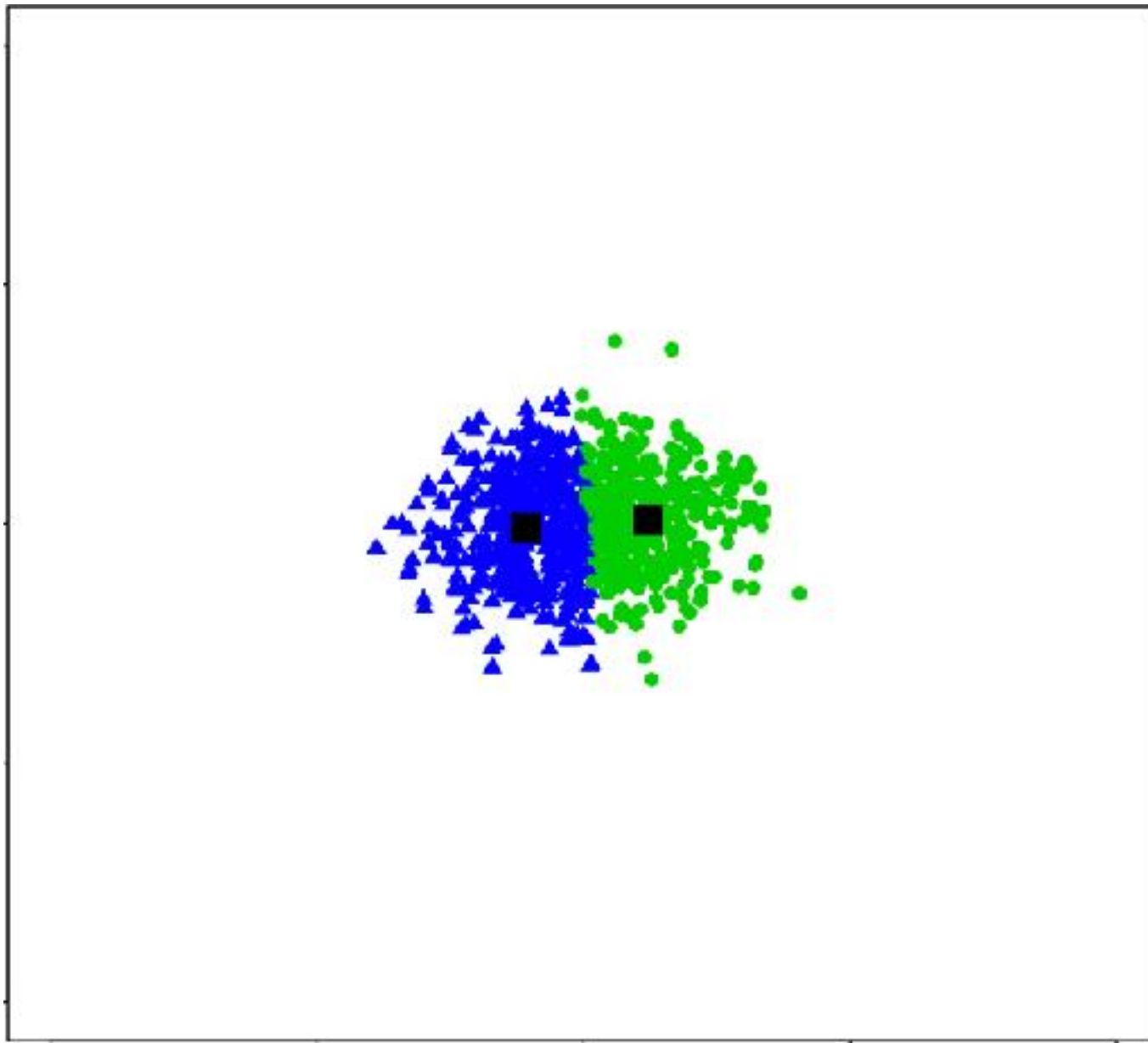
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Cluster shape



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Cluster shape



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Machine learning (ML): why & what

k Nearest Neighbors
Linear Regression & Ridge Regression
Decision Tree, Random Forest
(Bagging)

Logistic Regression

Naive Bayes

SVM

Perceptrons

Bias & Variance Trade off

K means Clustering

PCA, Linear Algebra
Principal Component
Analysis

Basics of Info. Theory

Accuracy, Precision, Recall,
F1 Score, Confusion matrix

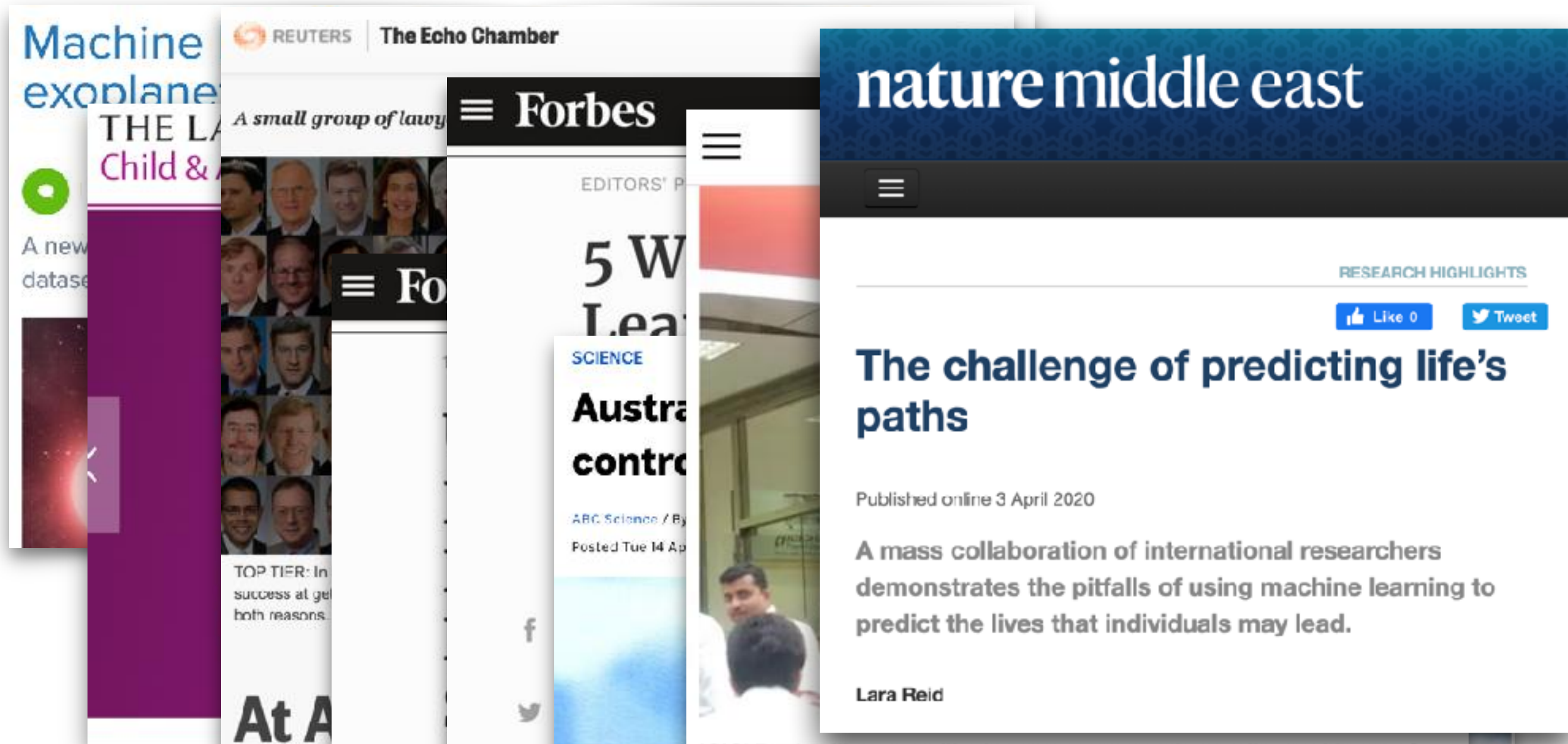
Class Imbalance

Encoding schemes

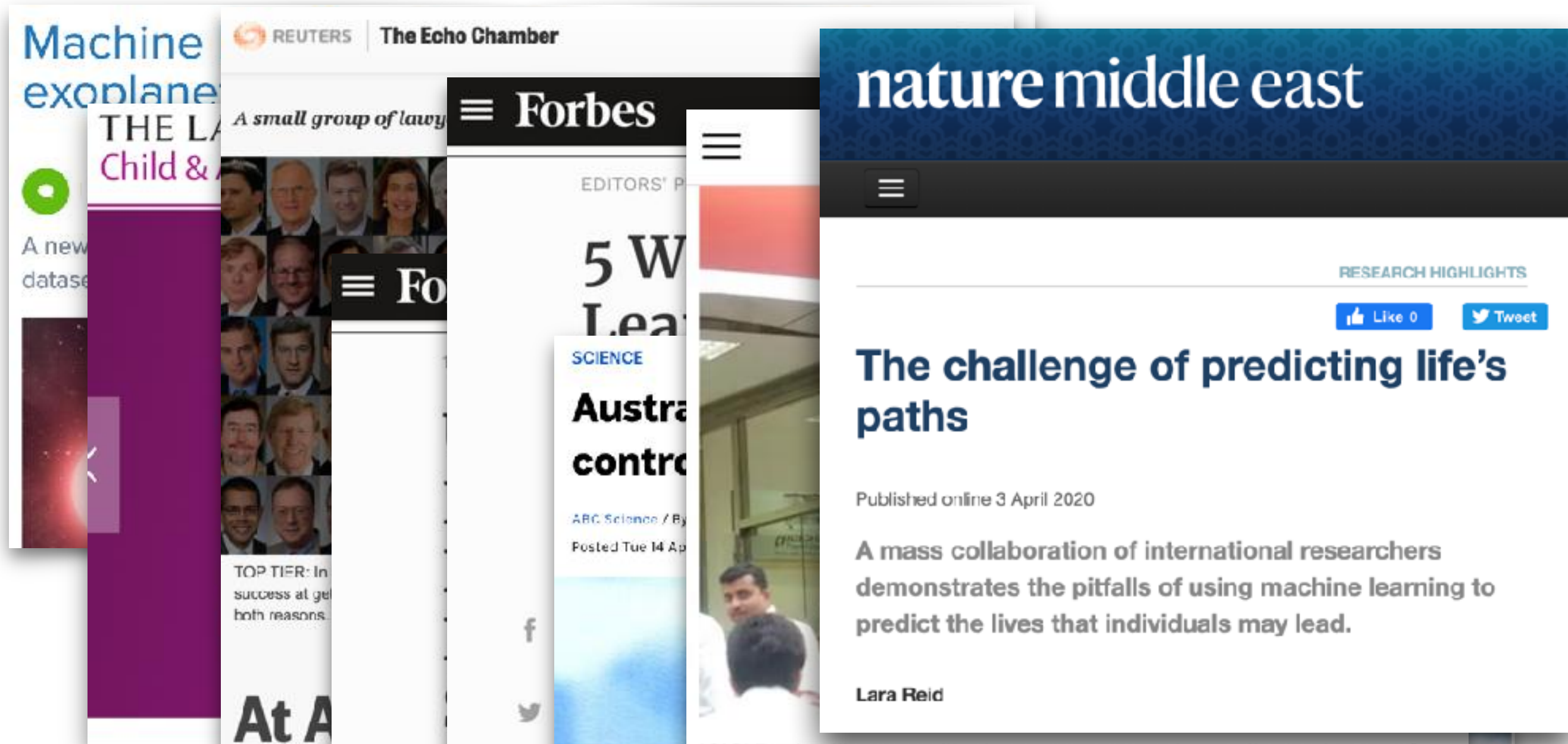
loss

$f: X \rightarrow Y$

Machine learning (ML): why & what

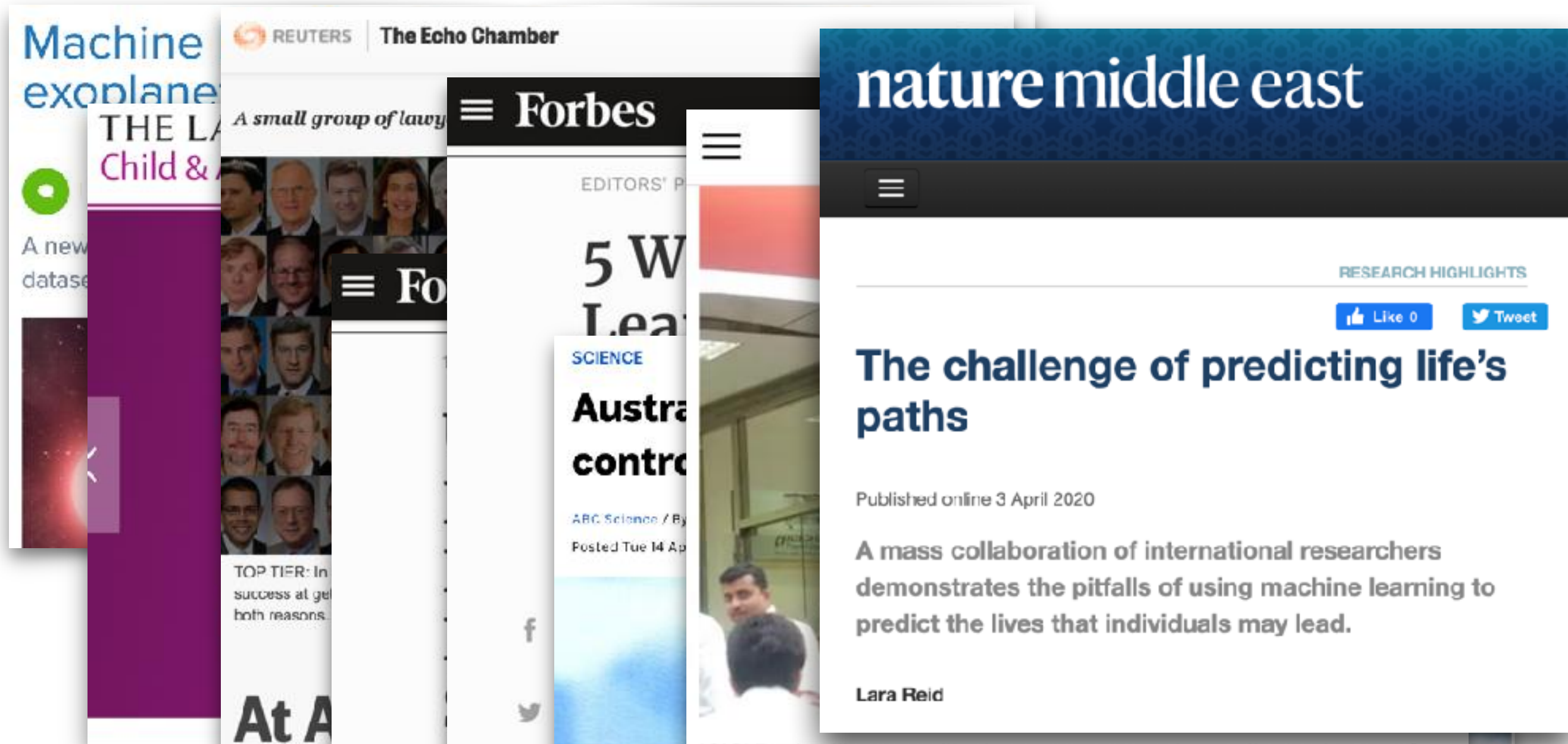


Machine learning (ML): why & what



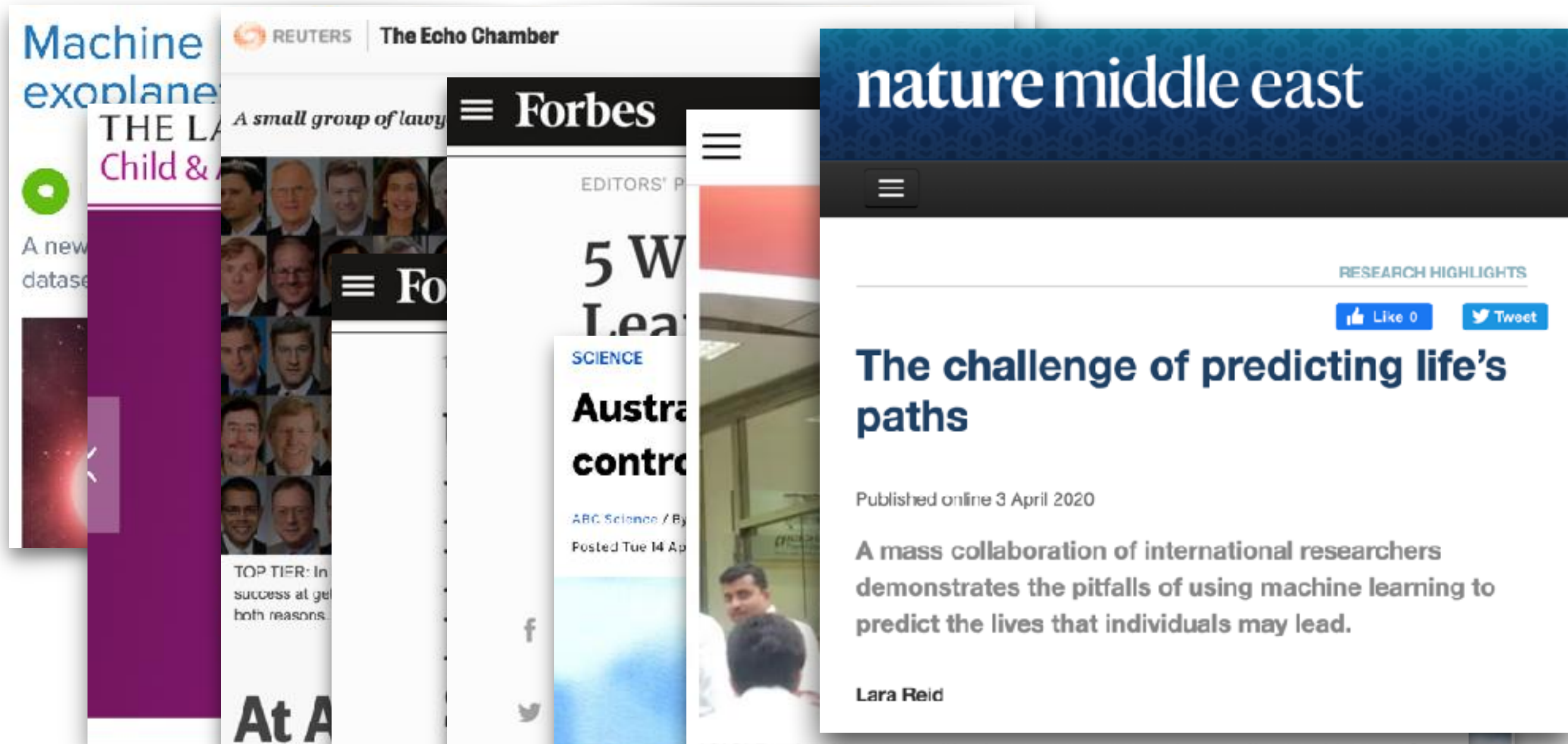
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Machine learning (ML): why & what



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Machine learning (ML): why & what



- **What is ML?** A set of methods for making decisions from data. (See the rest of the course!)
- **Why study ML?** To apply; to understand; to evaluate
- **Notes:** ML is not magic. ML is built on math.