6.036/6.862: Introduction to Machine Learning

Lecture: starts Tuesdays 9:35am (Boston time zone)

Course website: introml.odl.mit.edu

Who's talking? Prof. Tamara Broderick

Questions? discourse.odl.mit.edu ("Lecture 13" category)

Materials: Will all be available at course website

Last Time(s)

I. Supervised Learning
- Classification
- Regression

Today's Plan

I. Unsupervised learning

II. Clustering

III. k-means clustering

Food distribution placement

FEEDING AMERICA

MEALS on WHEELS AMERICA
TOGETHER, WE CAN DELIVER.

[https://commons.wikimedia.org/wiki/File:Food_Truck_-_The_Noun_Project.svg; https://www.feedingamerica.org/; https://www.mealsonwheelsamerica.org/]

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Food distribution placement

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- Where should I have my *k* food trucks park?

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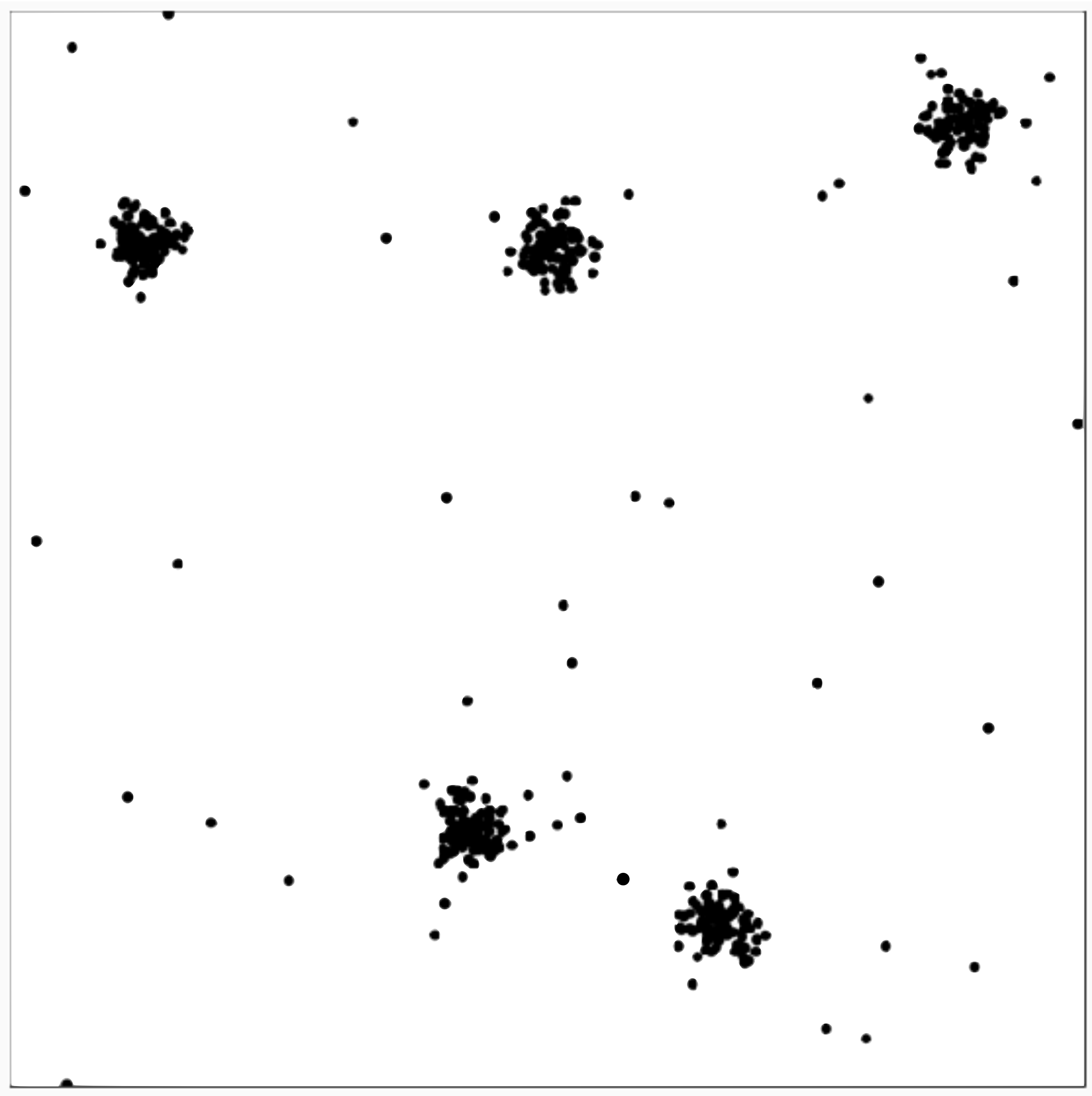

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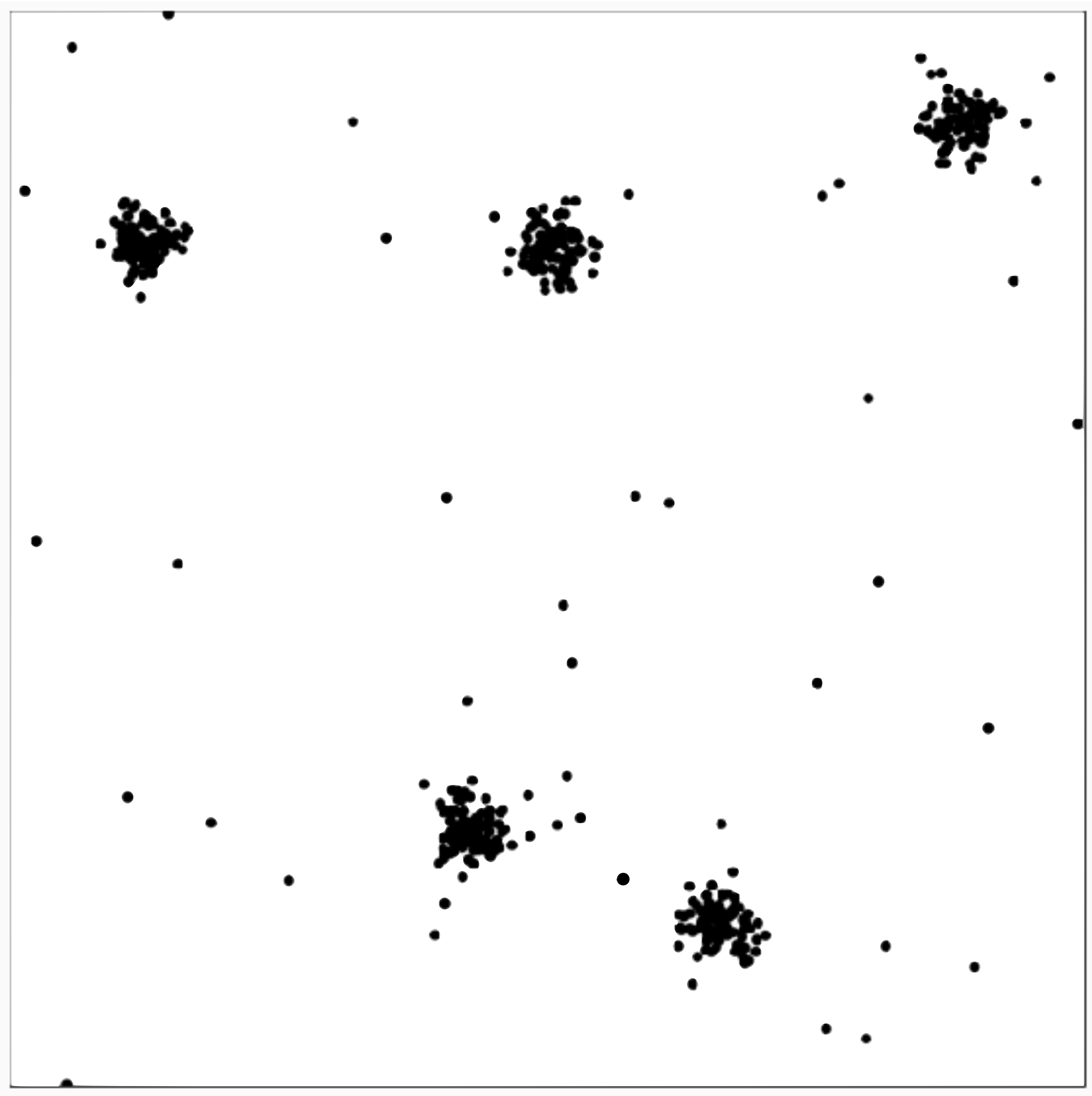

x_1: longitude

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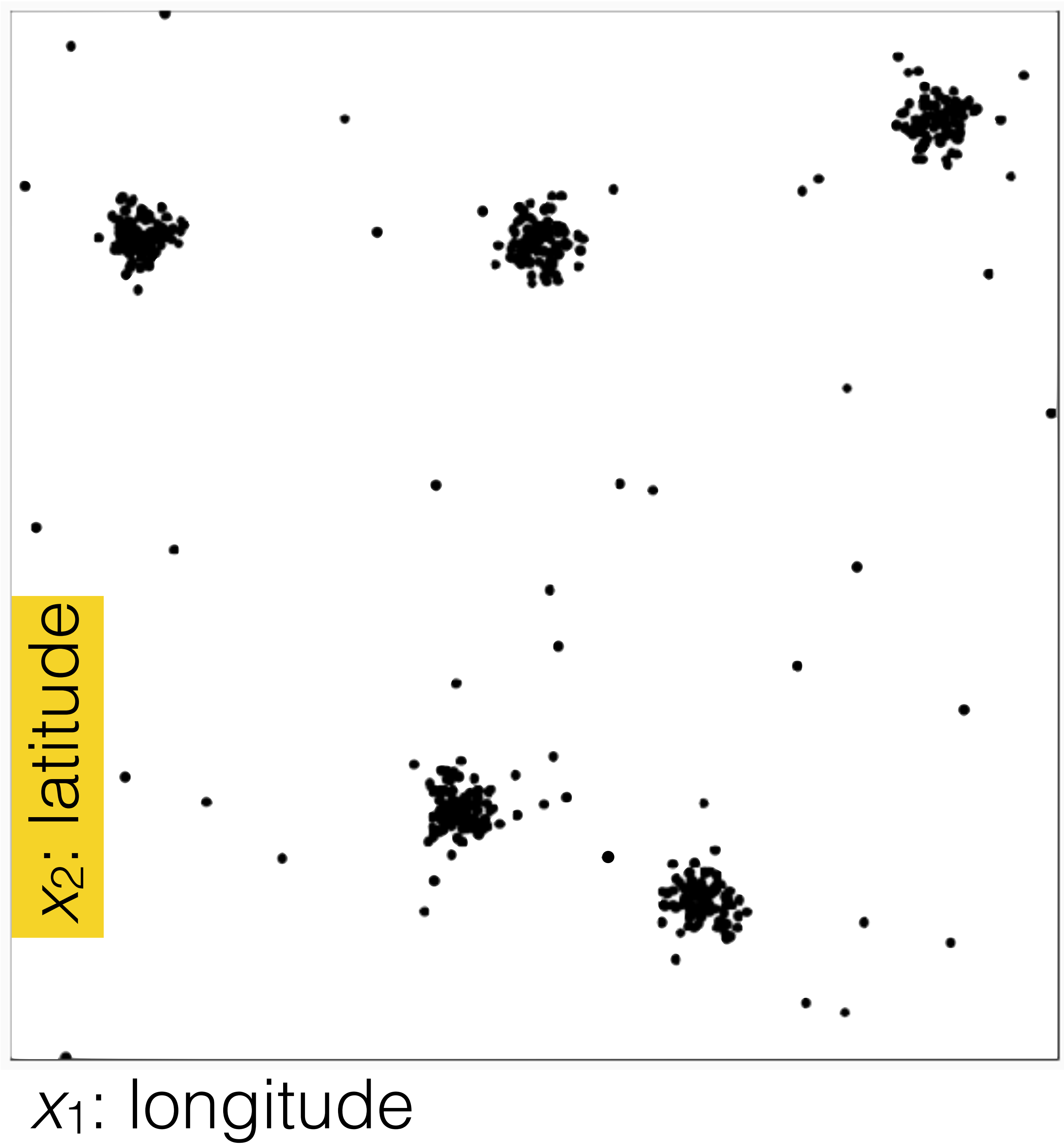

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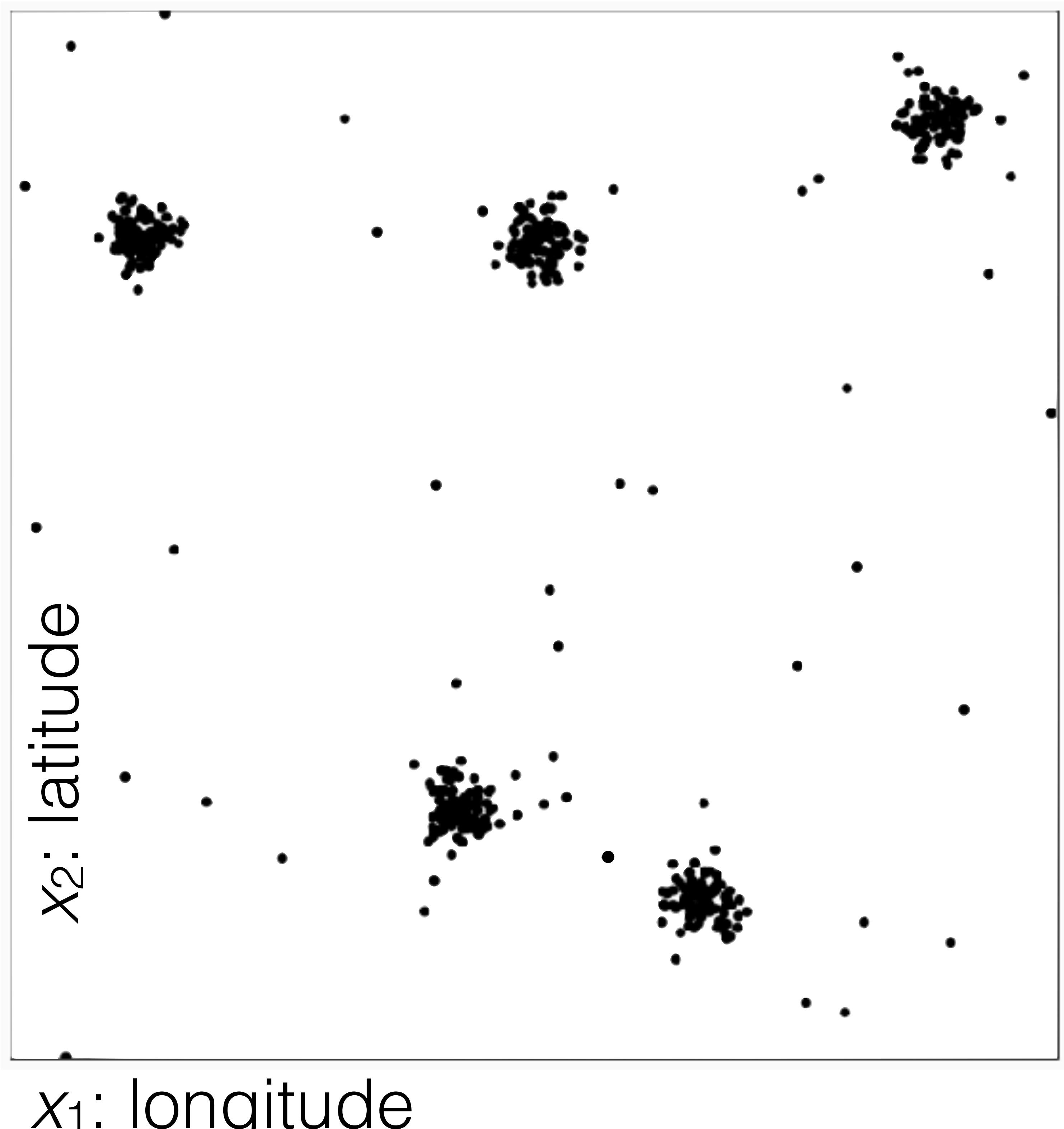

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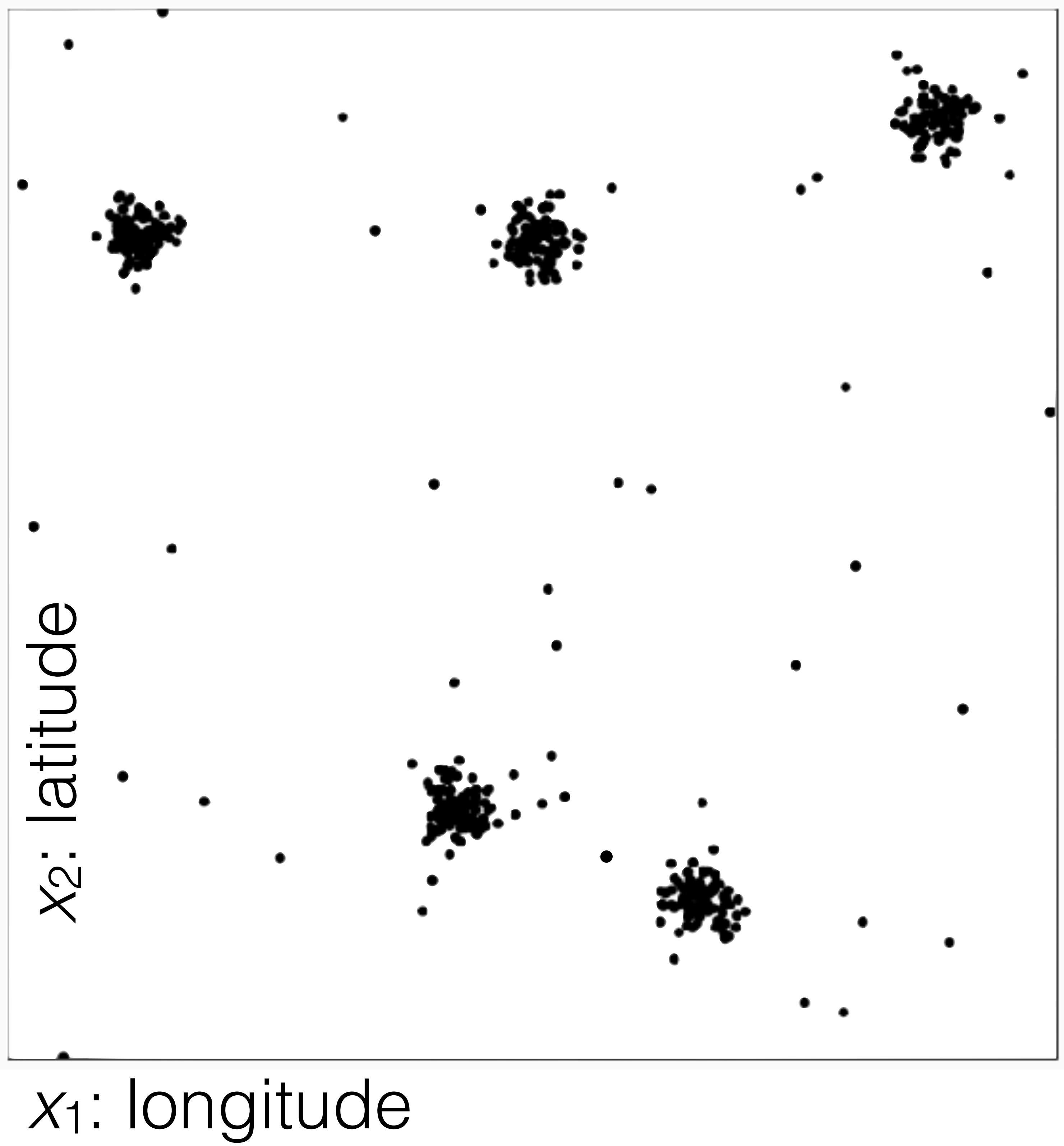

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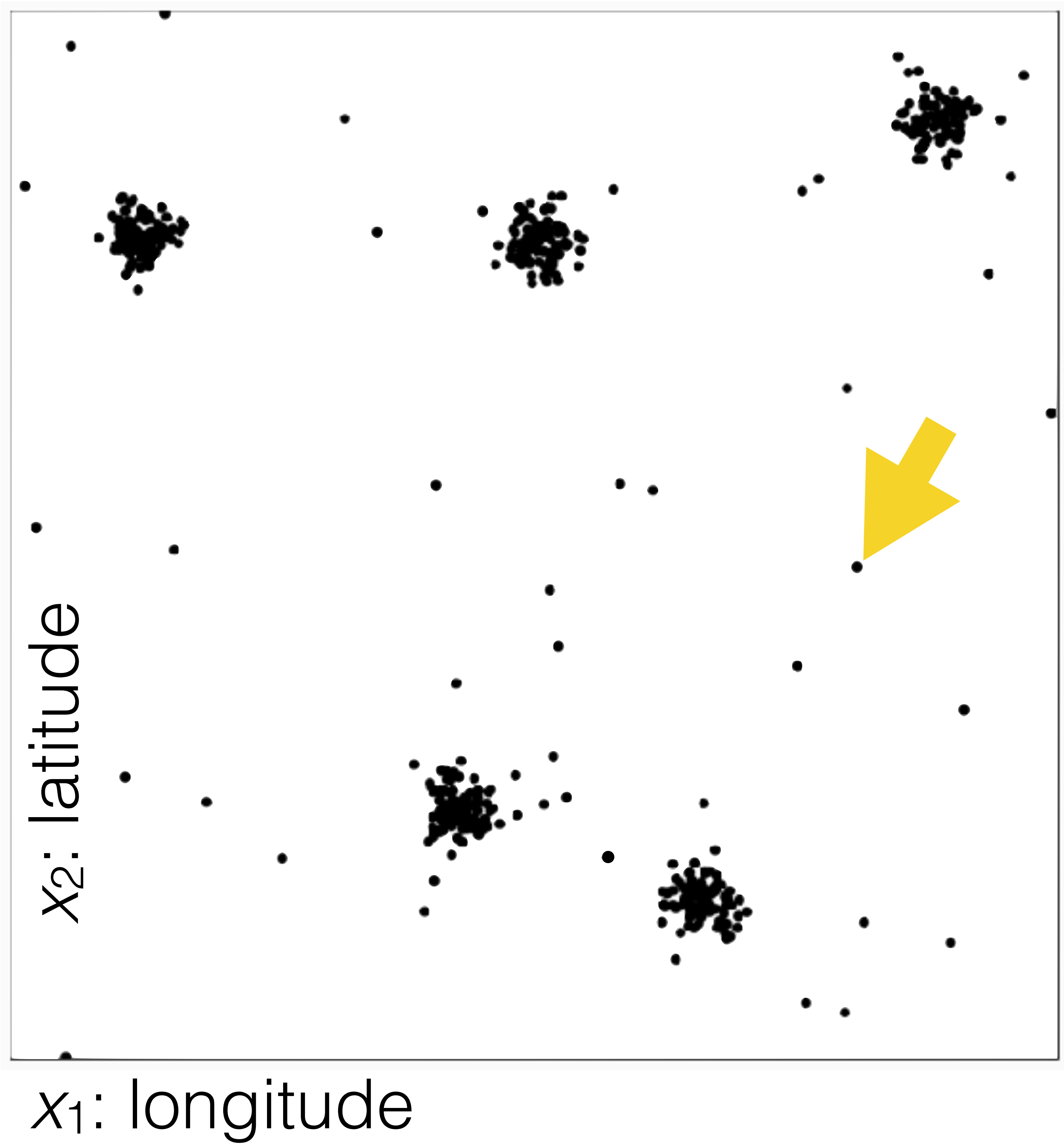

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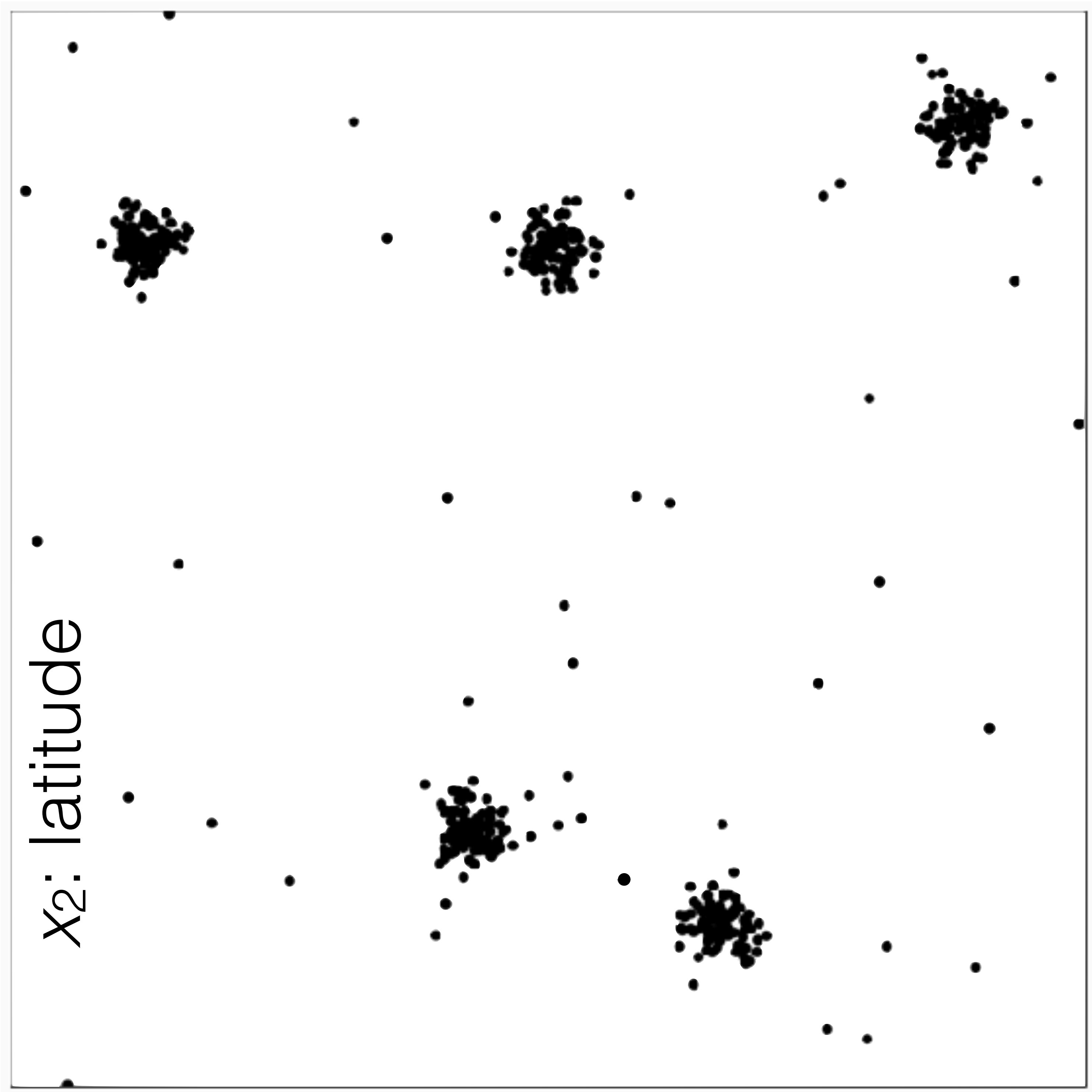

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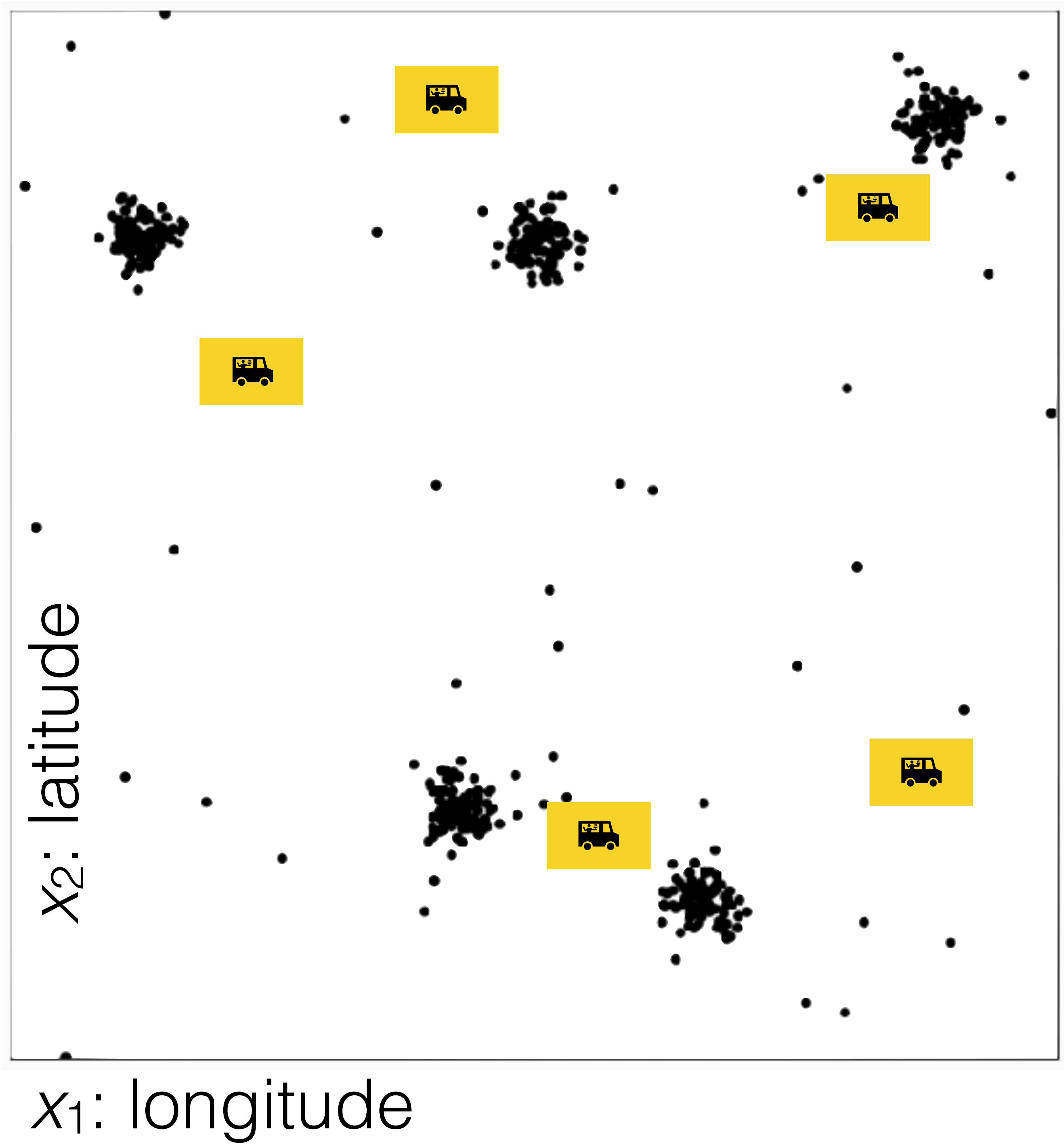

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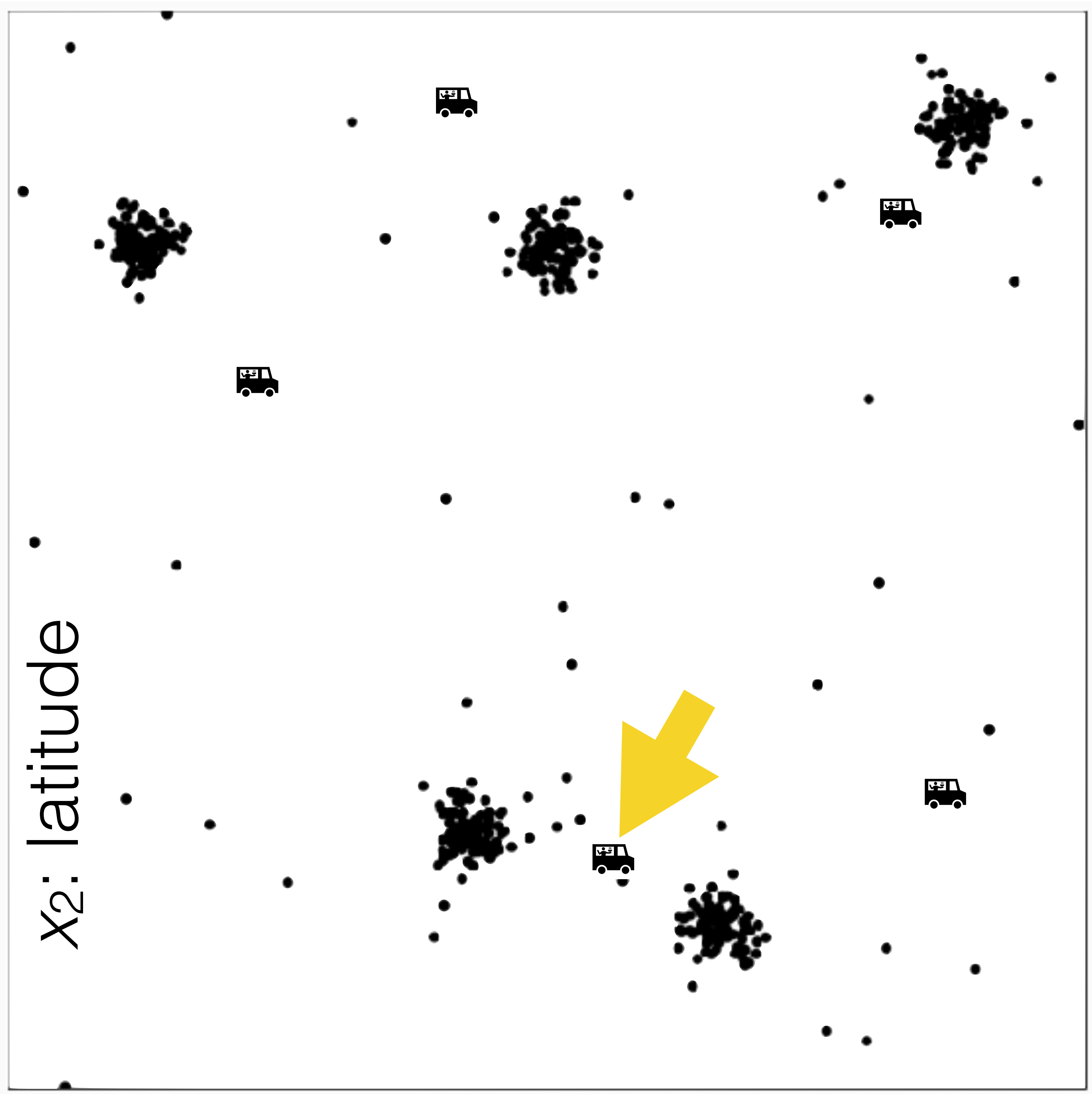

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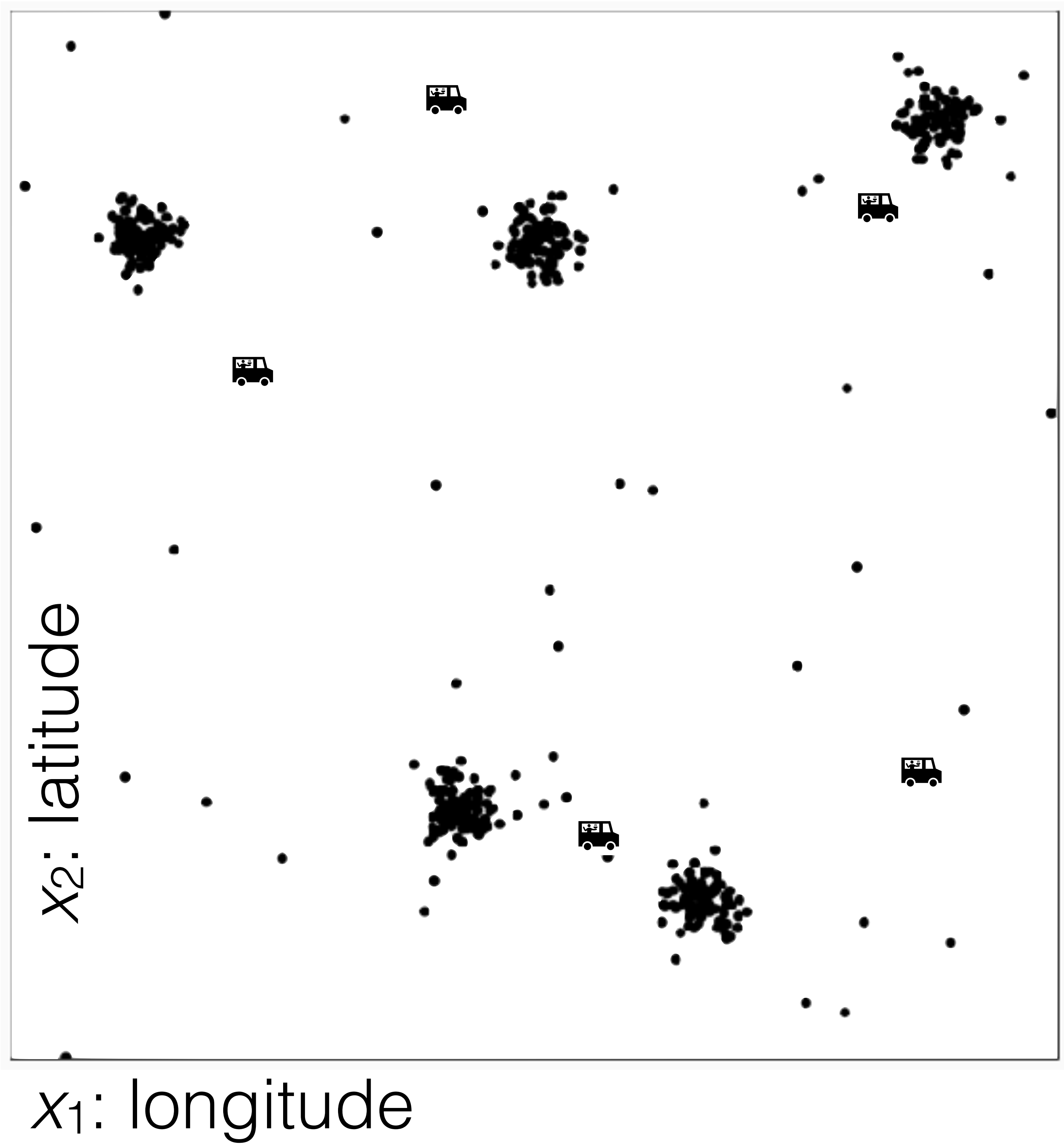

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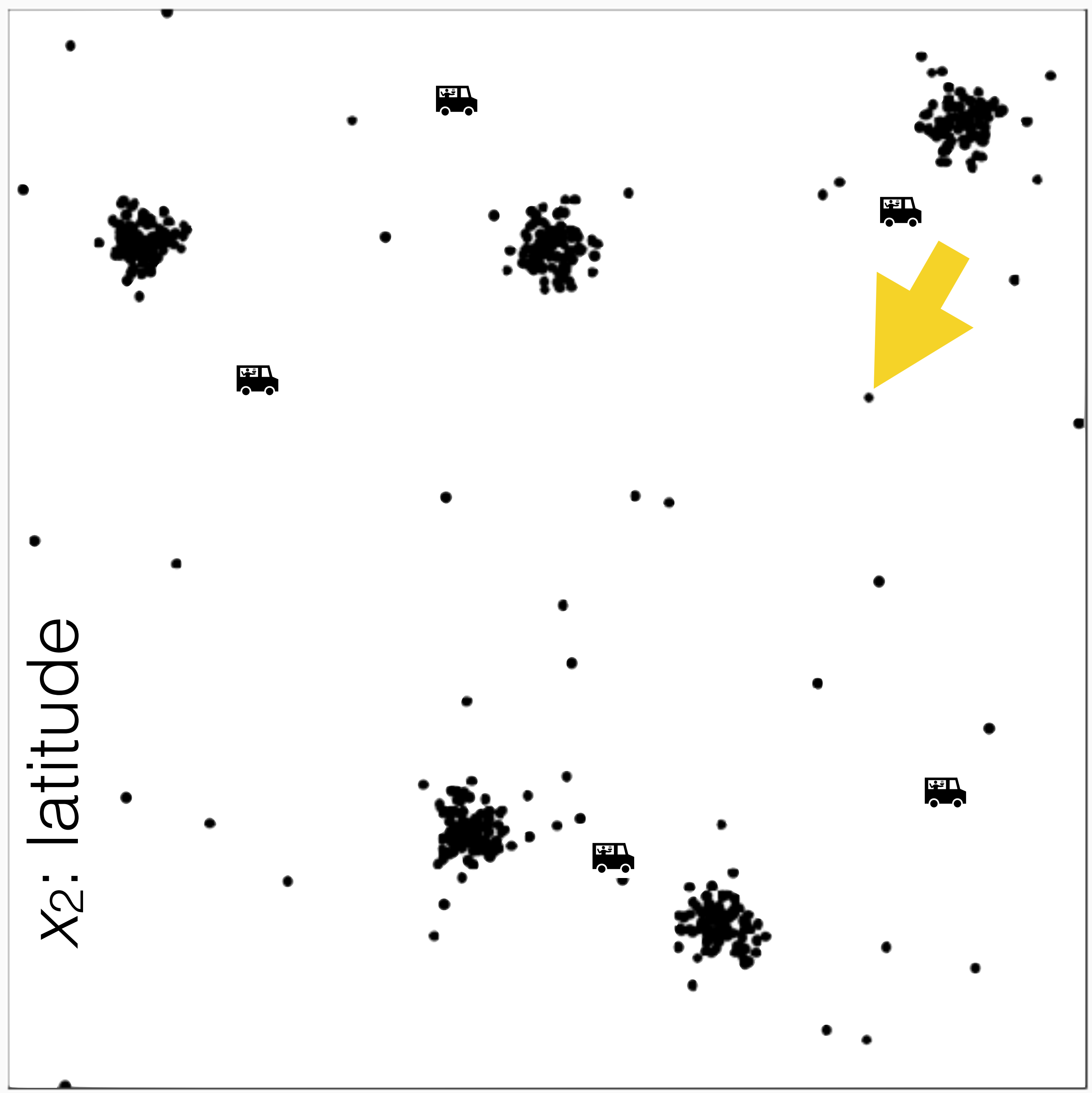

x_2: latitude

x_1: longitude

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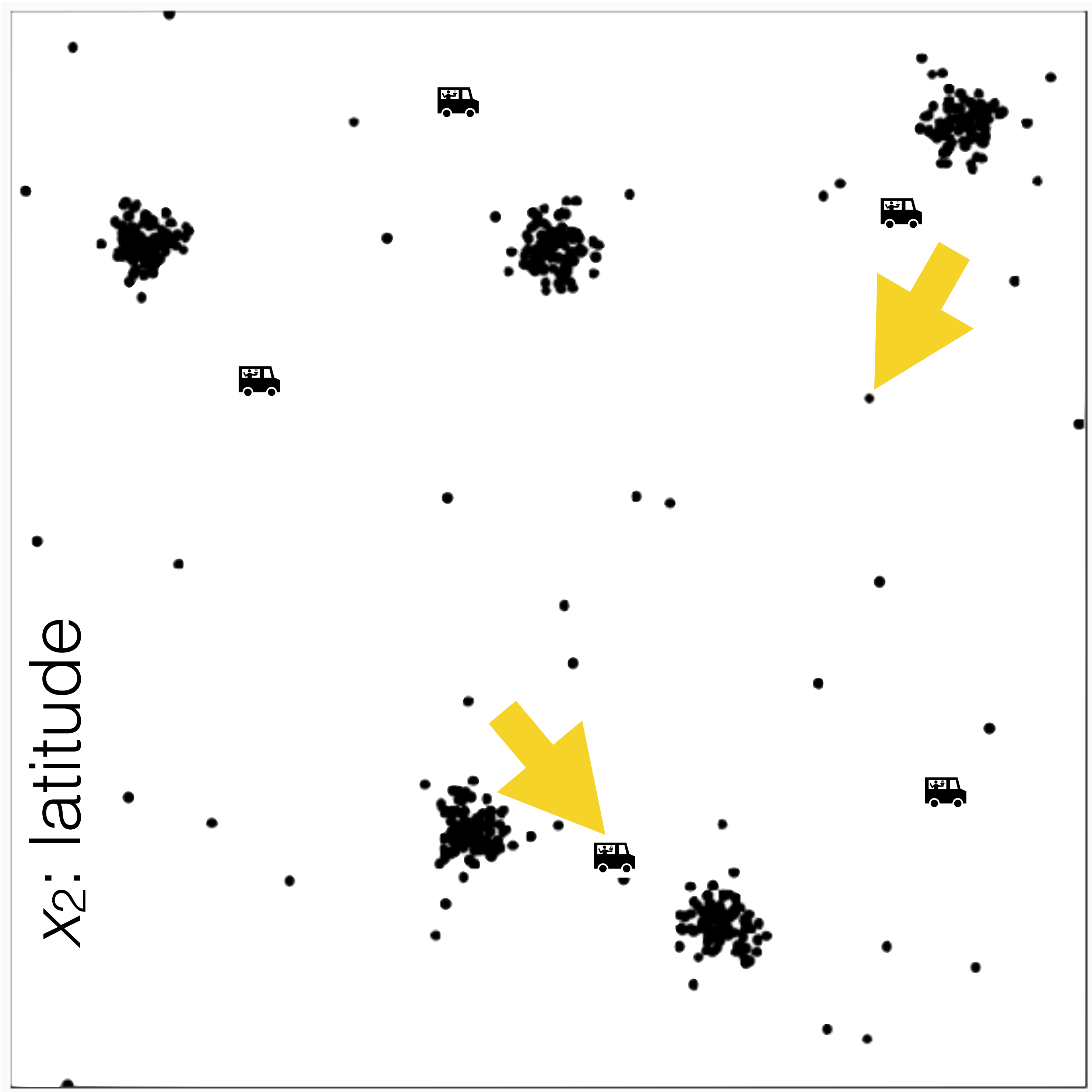

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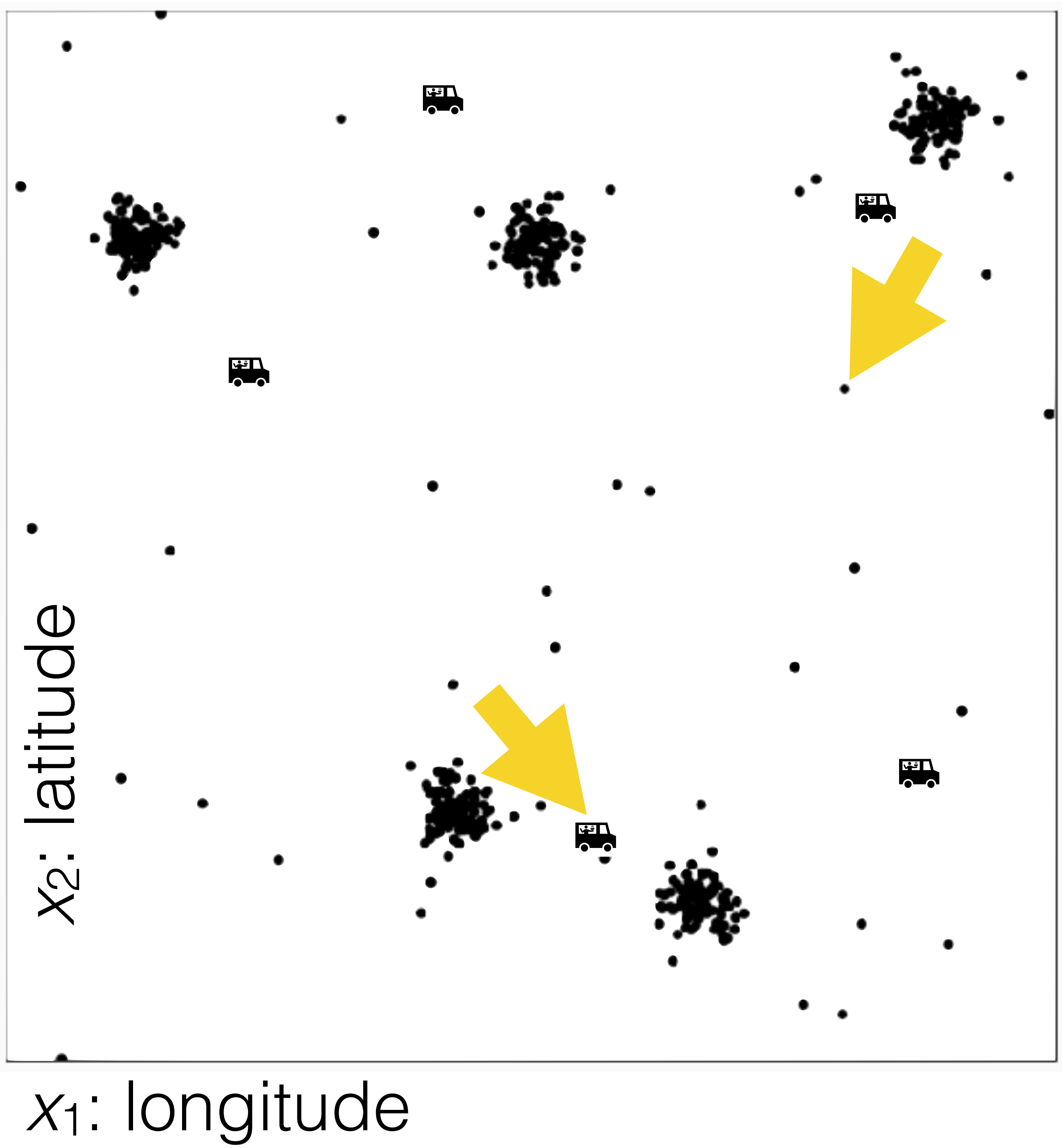

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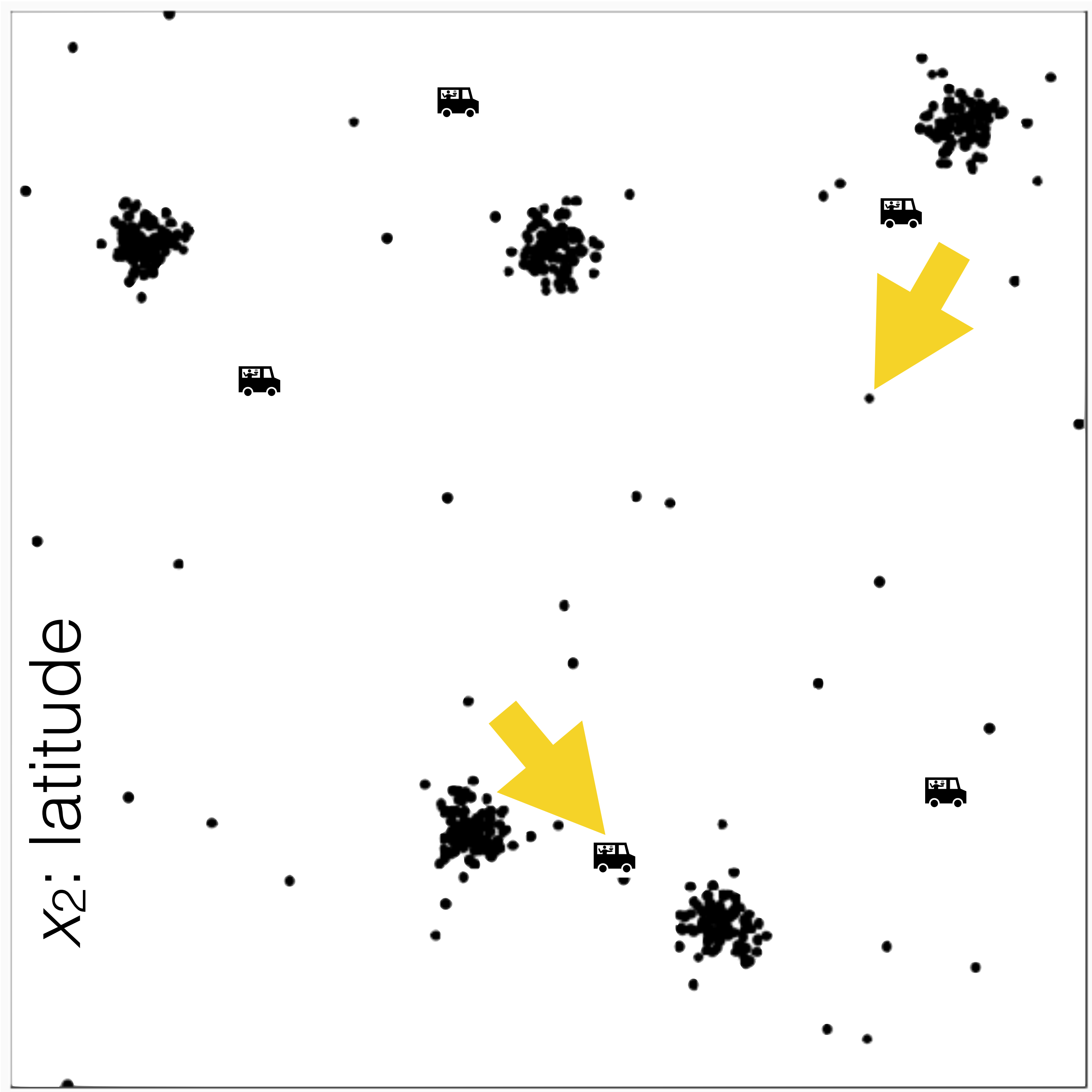

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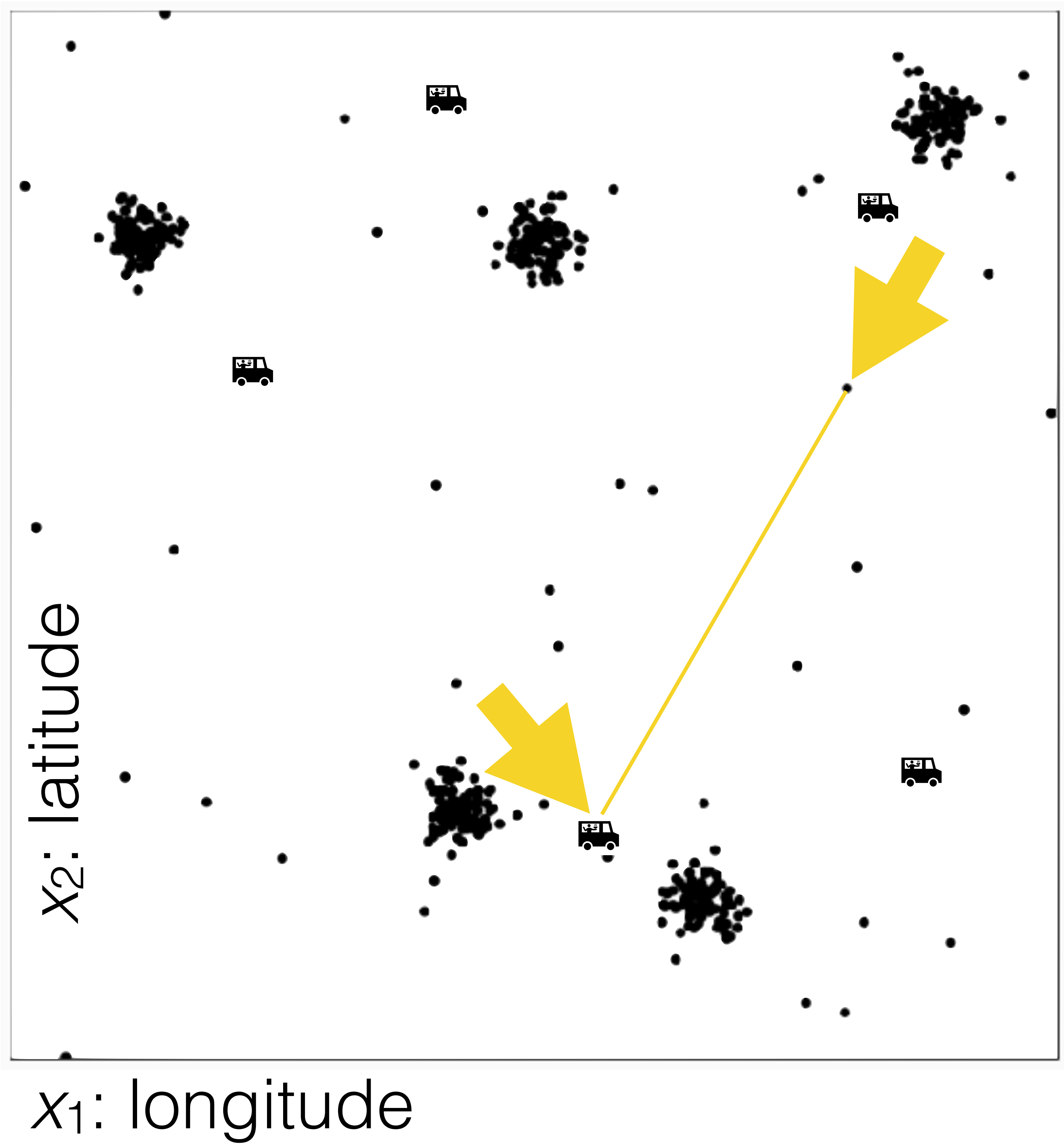

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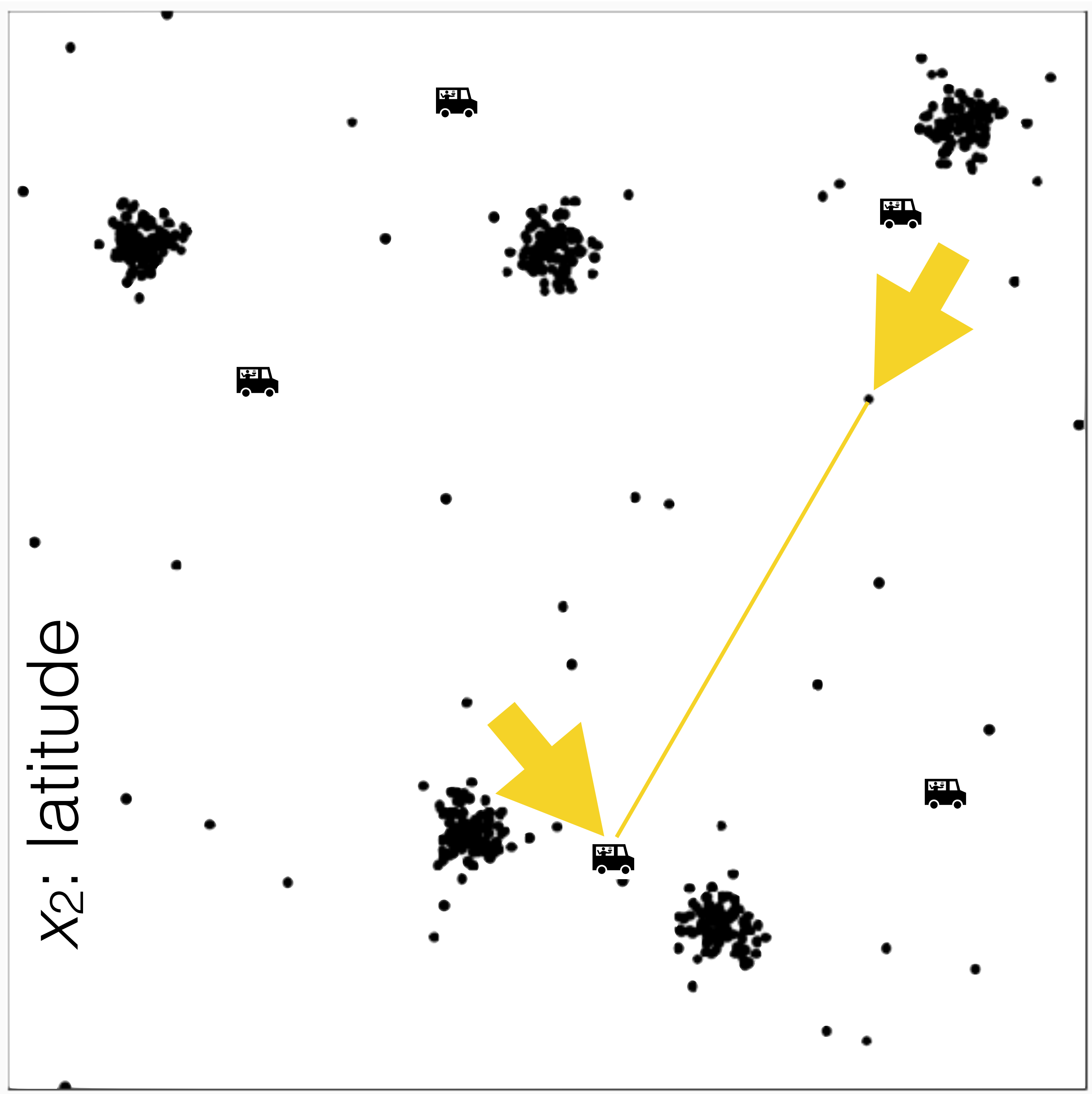

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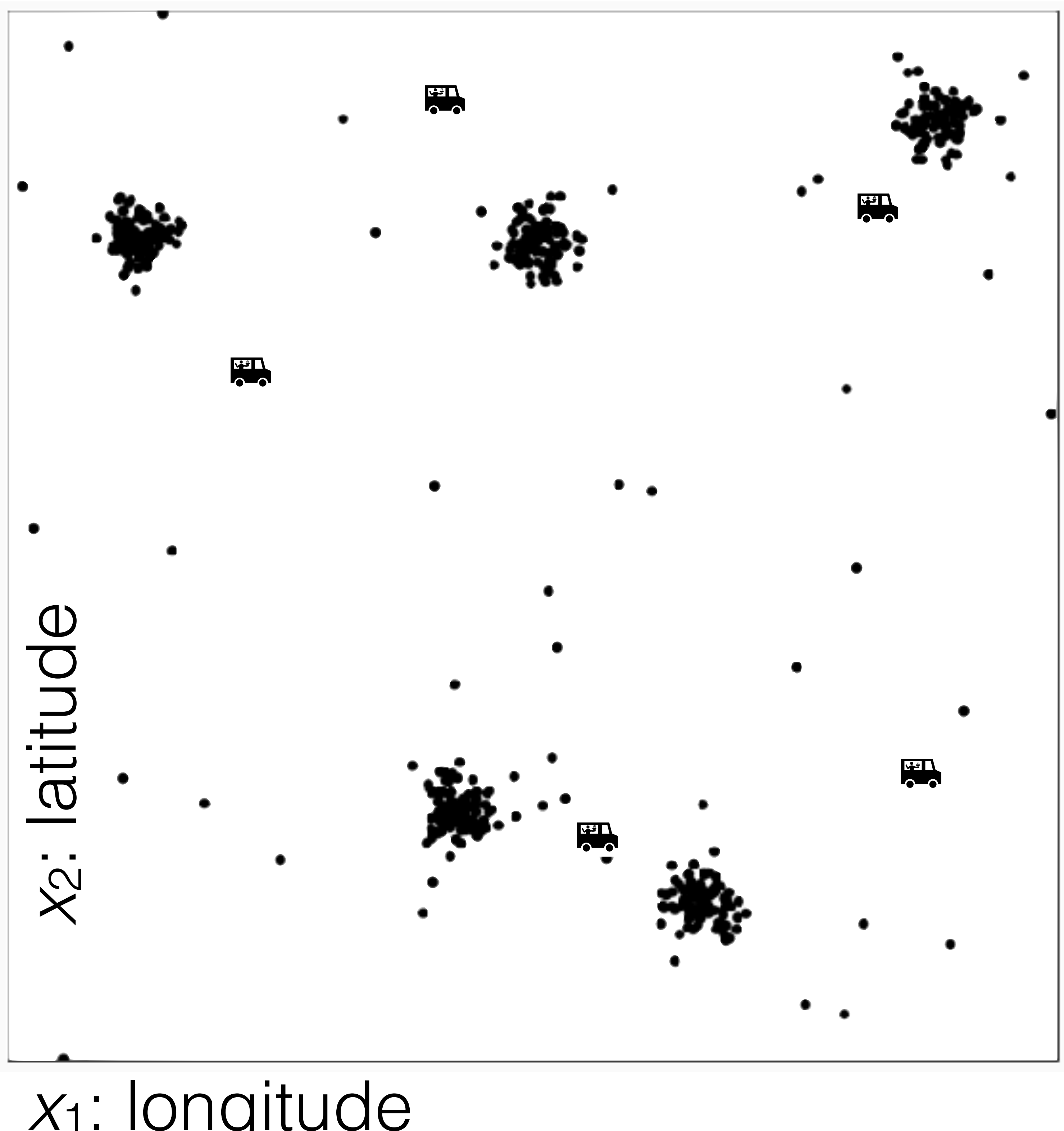

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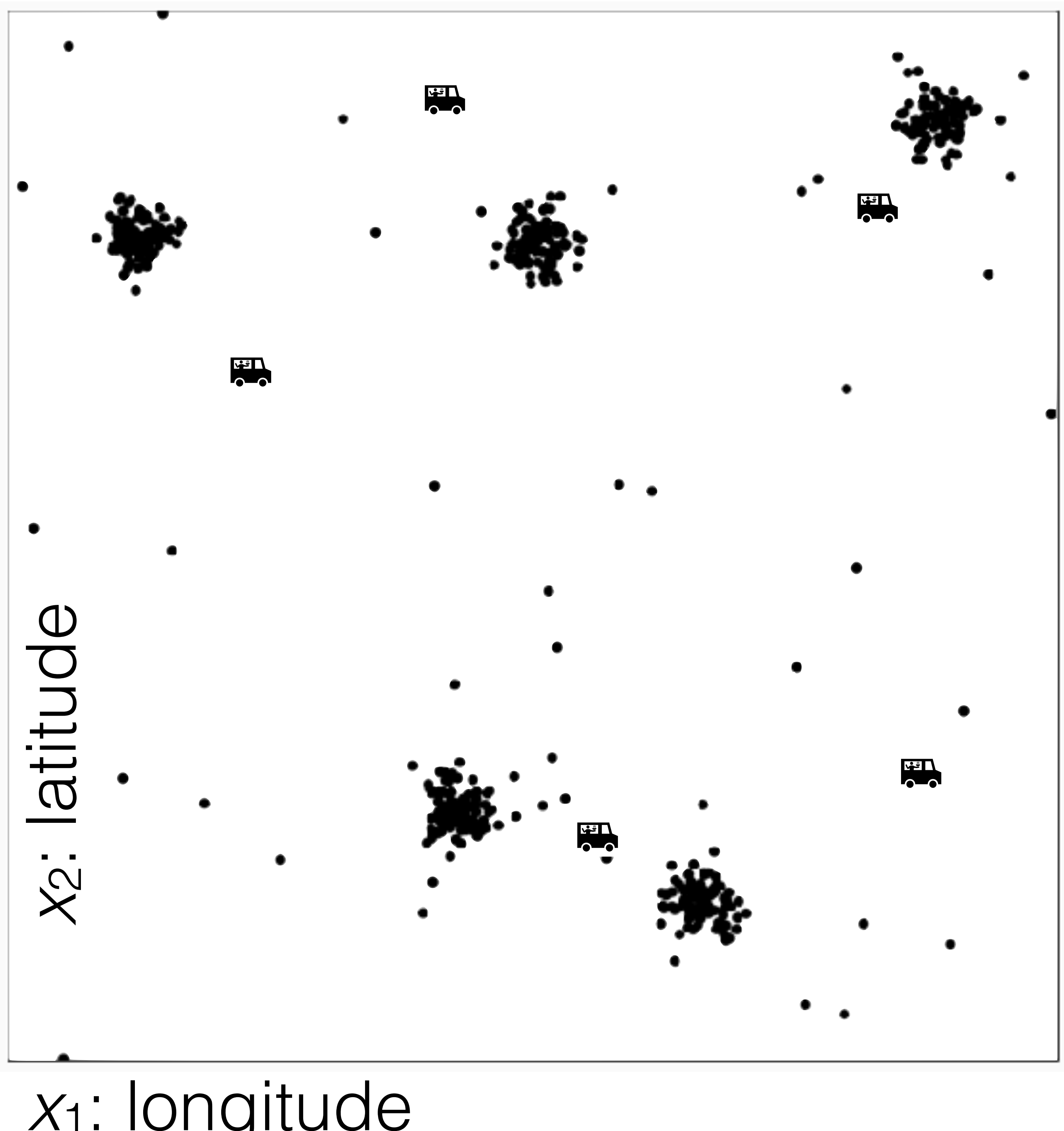

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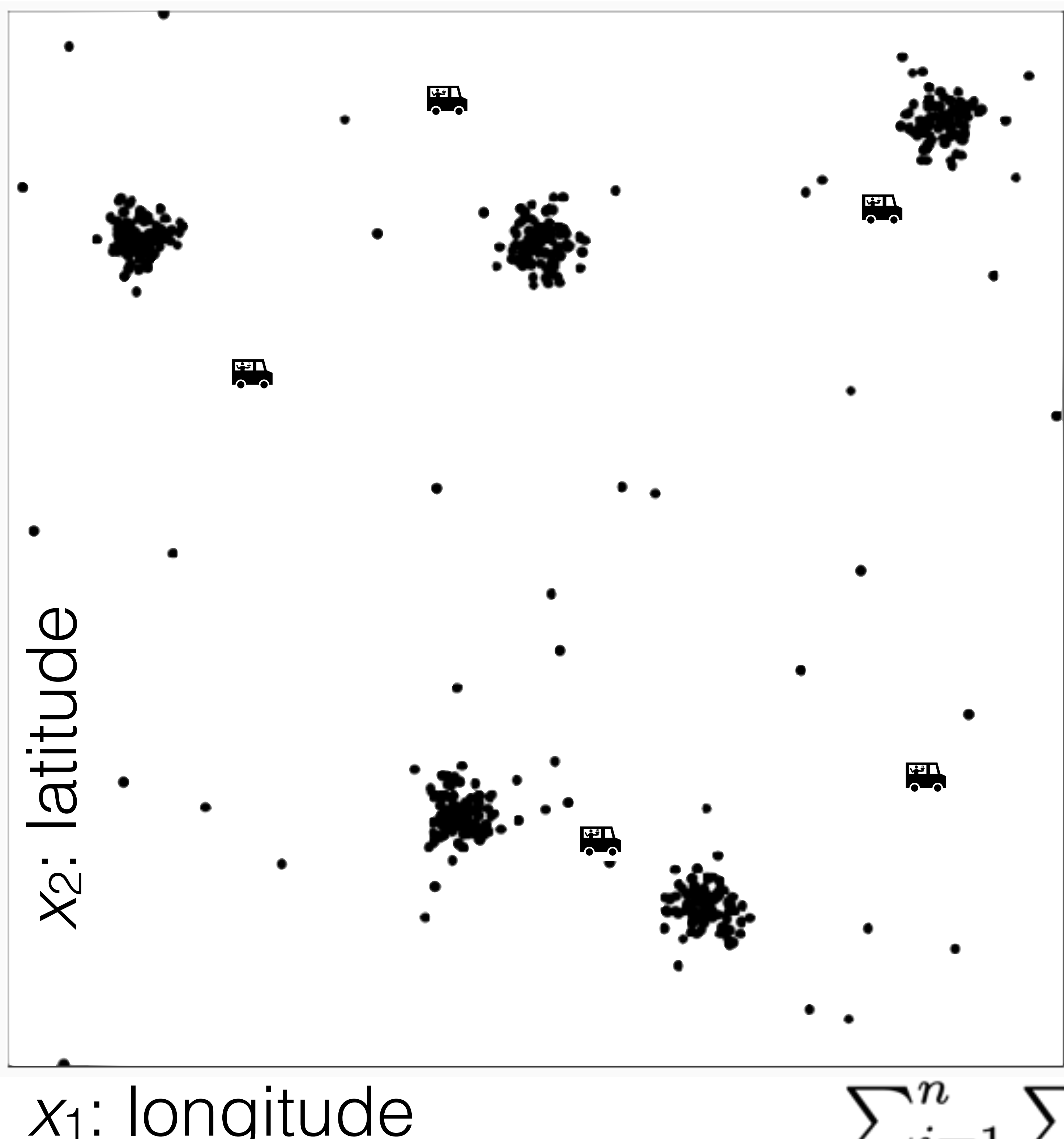

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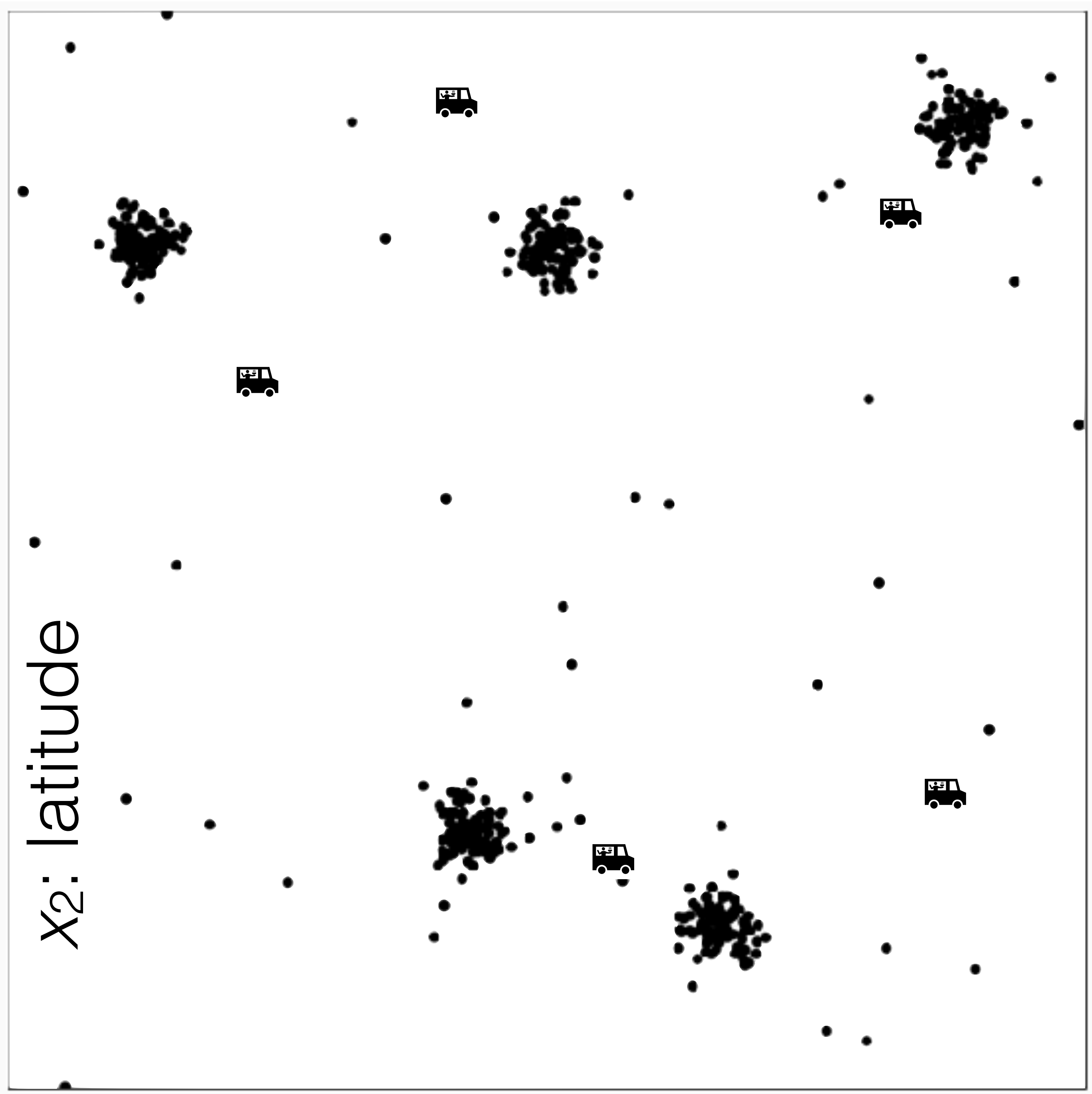

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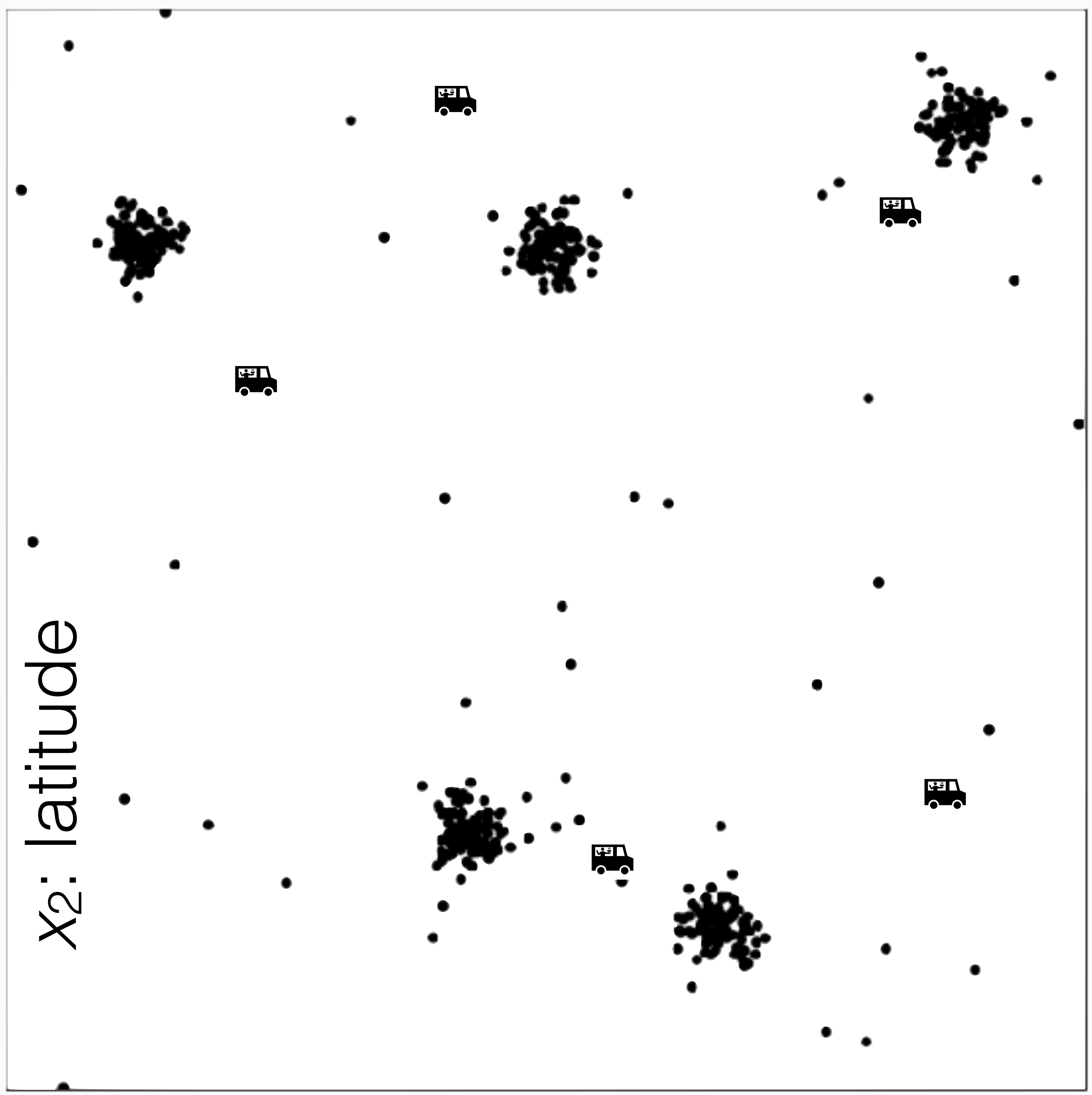

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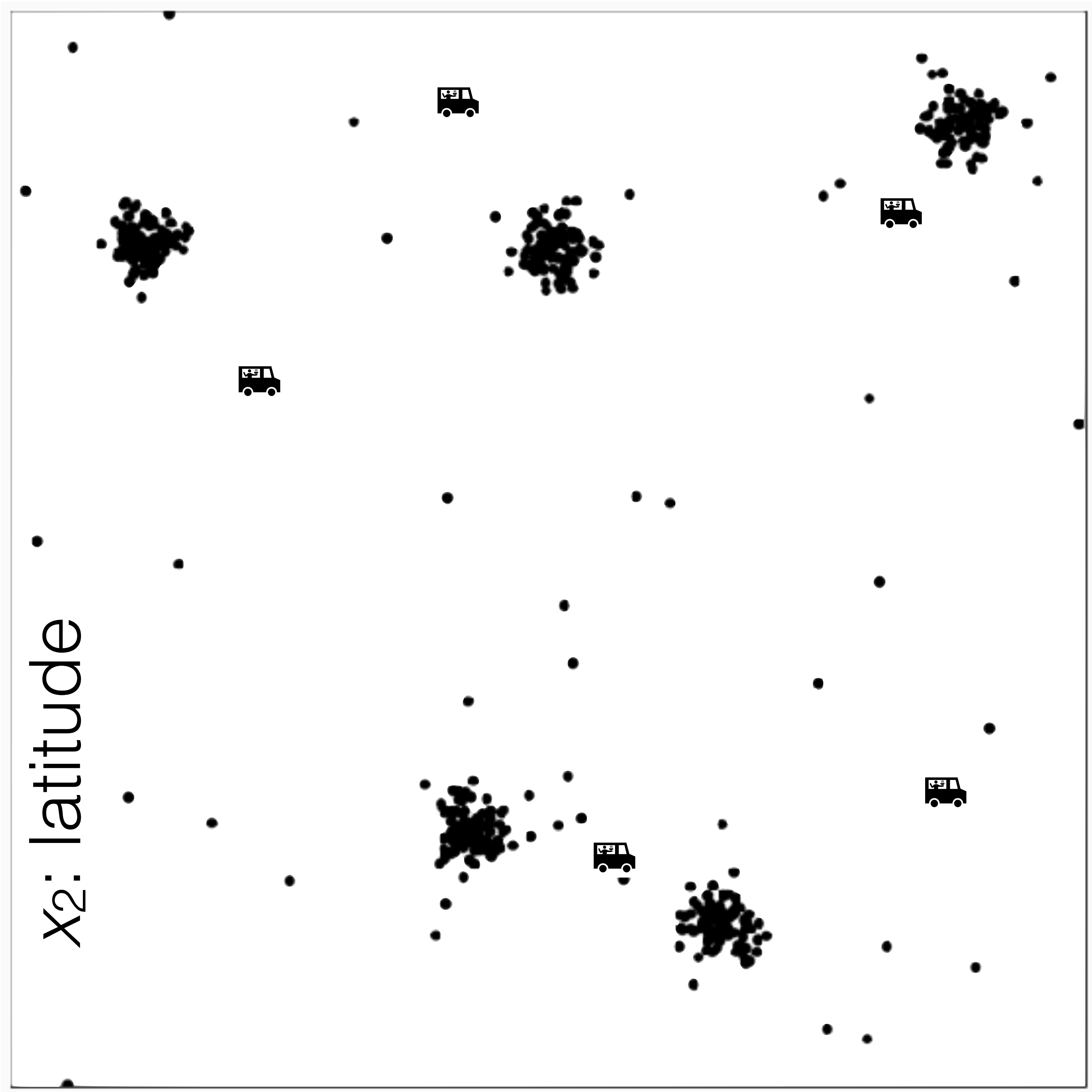

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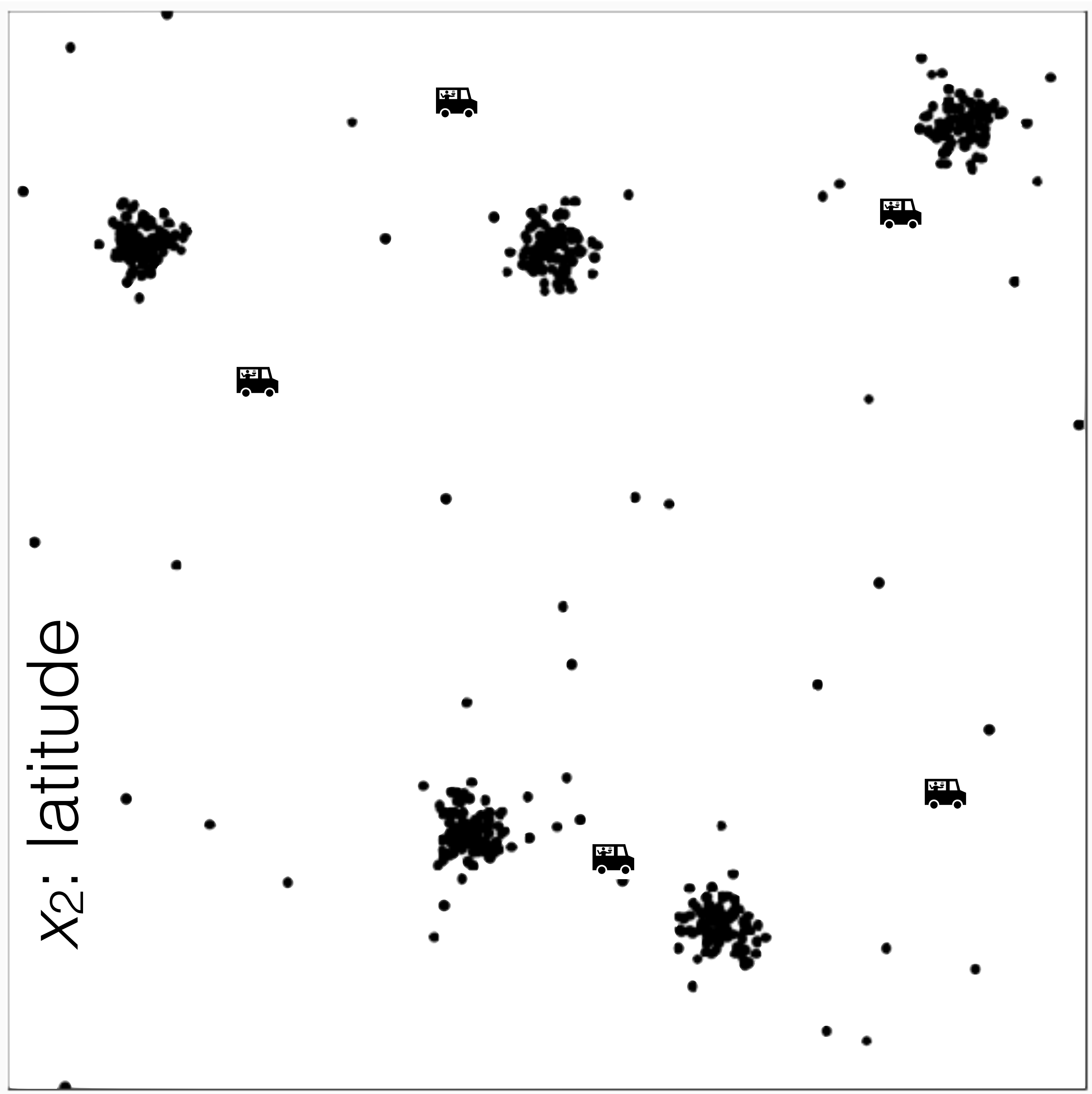

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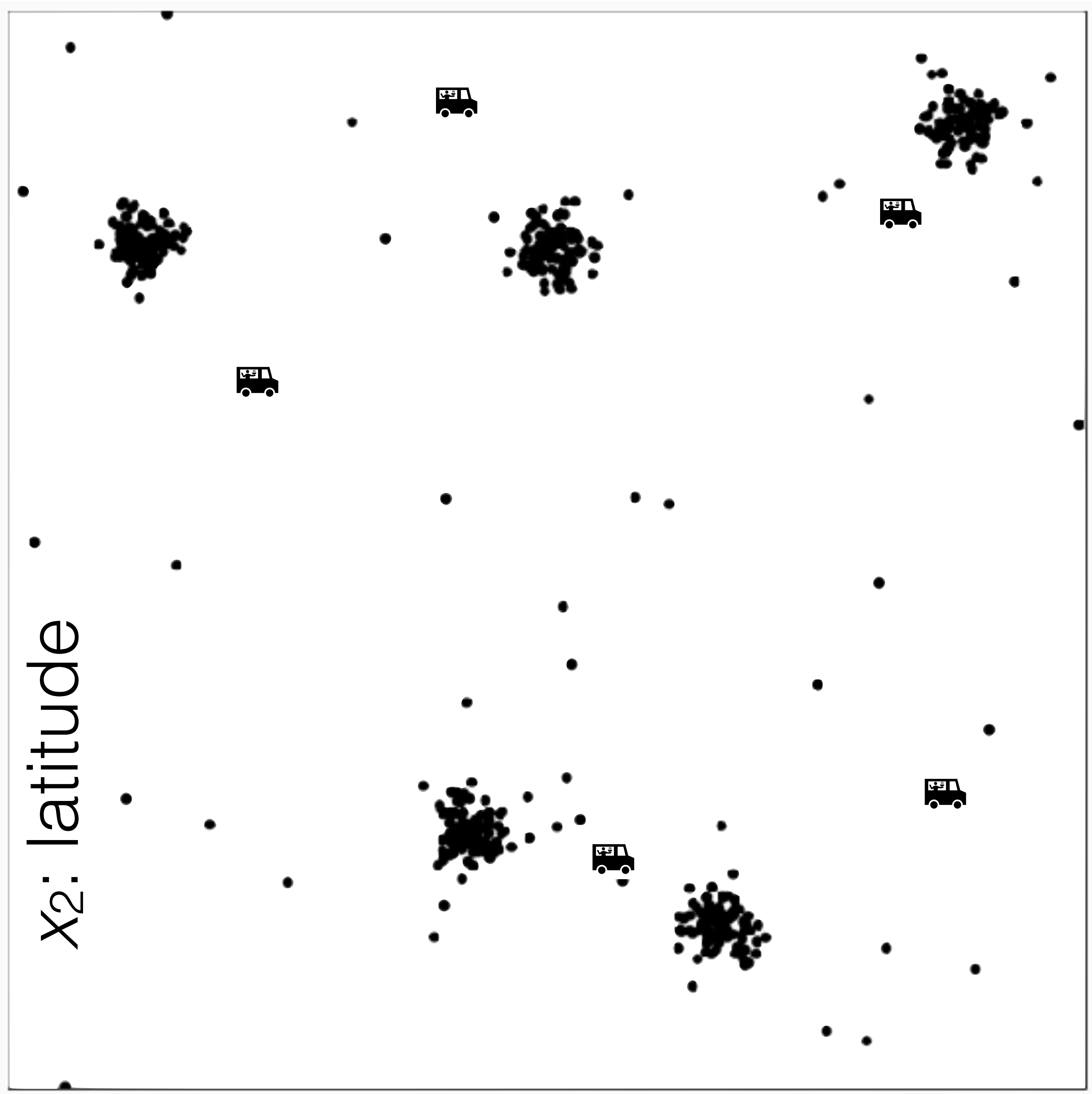

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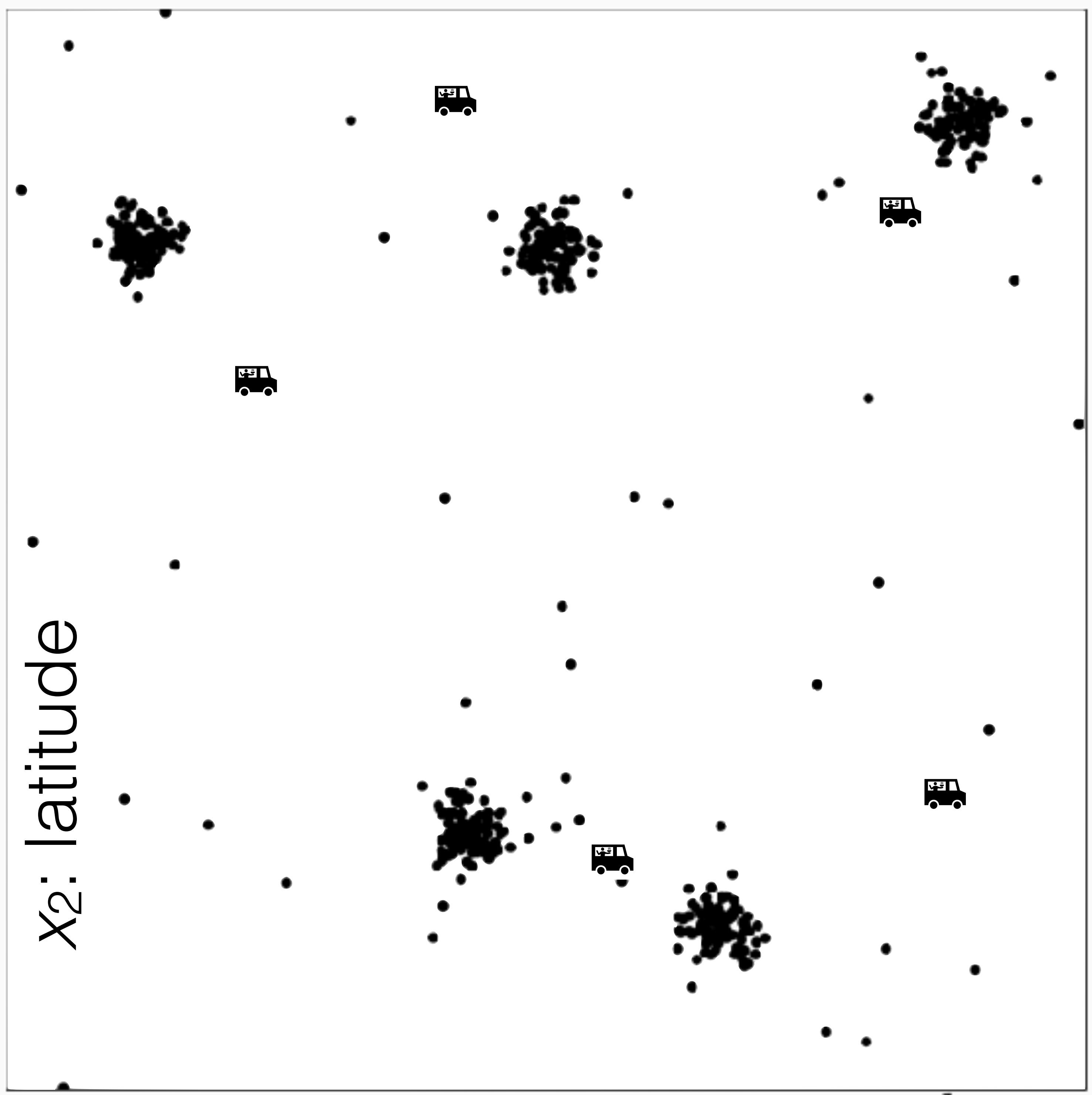

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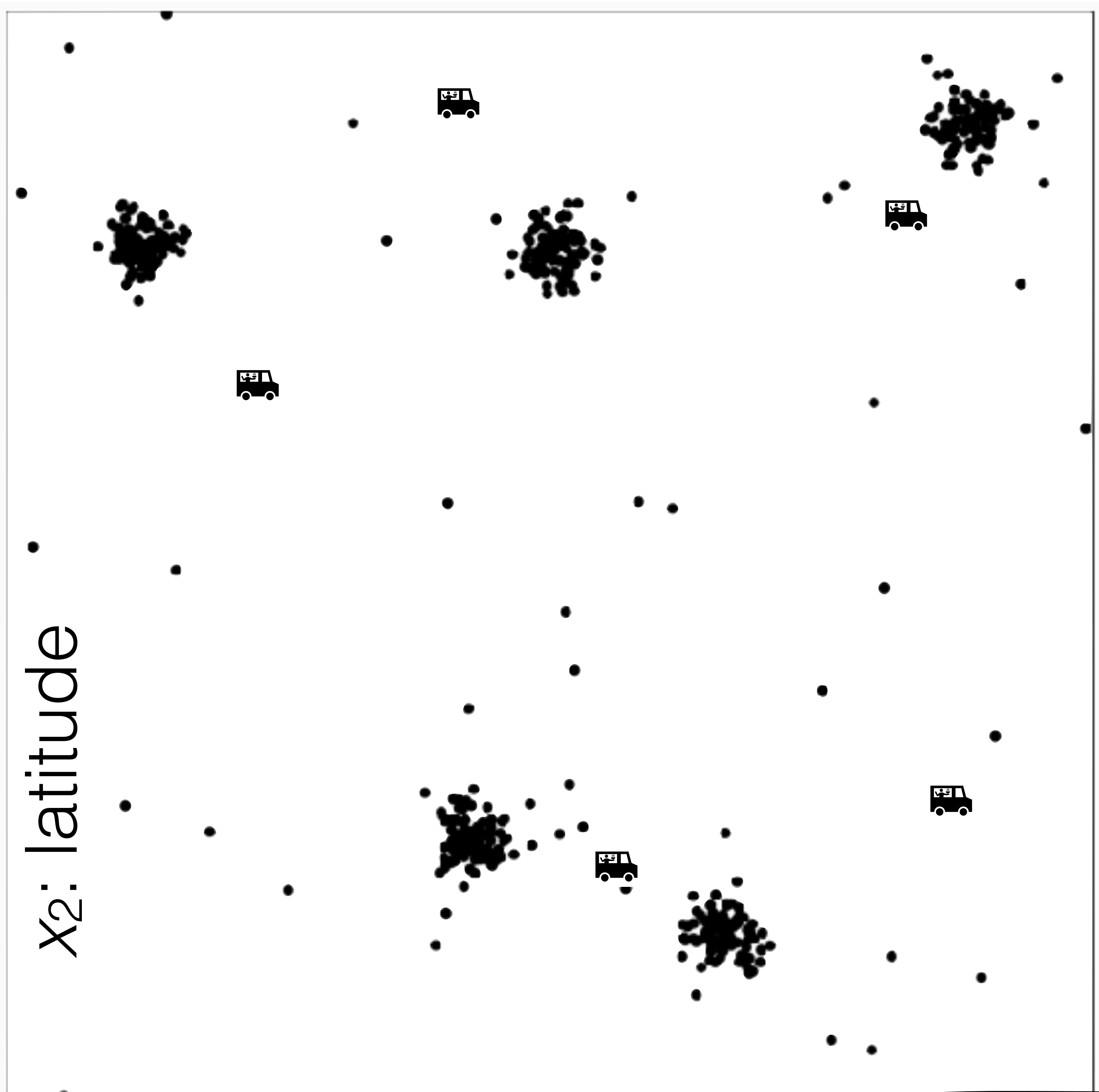

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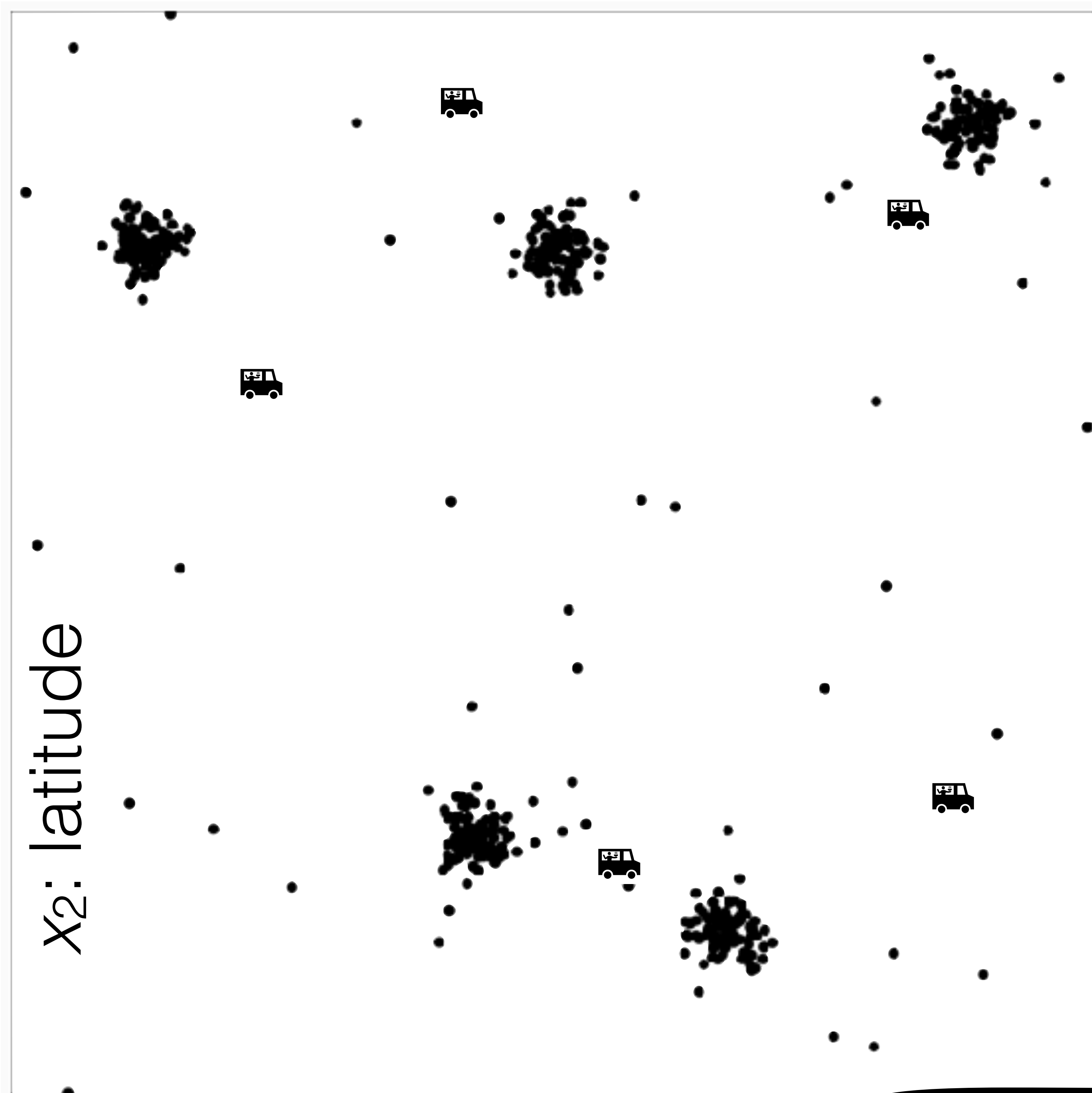

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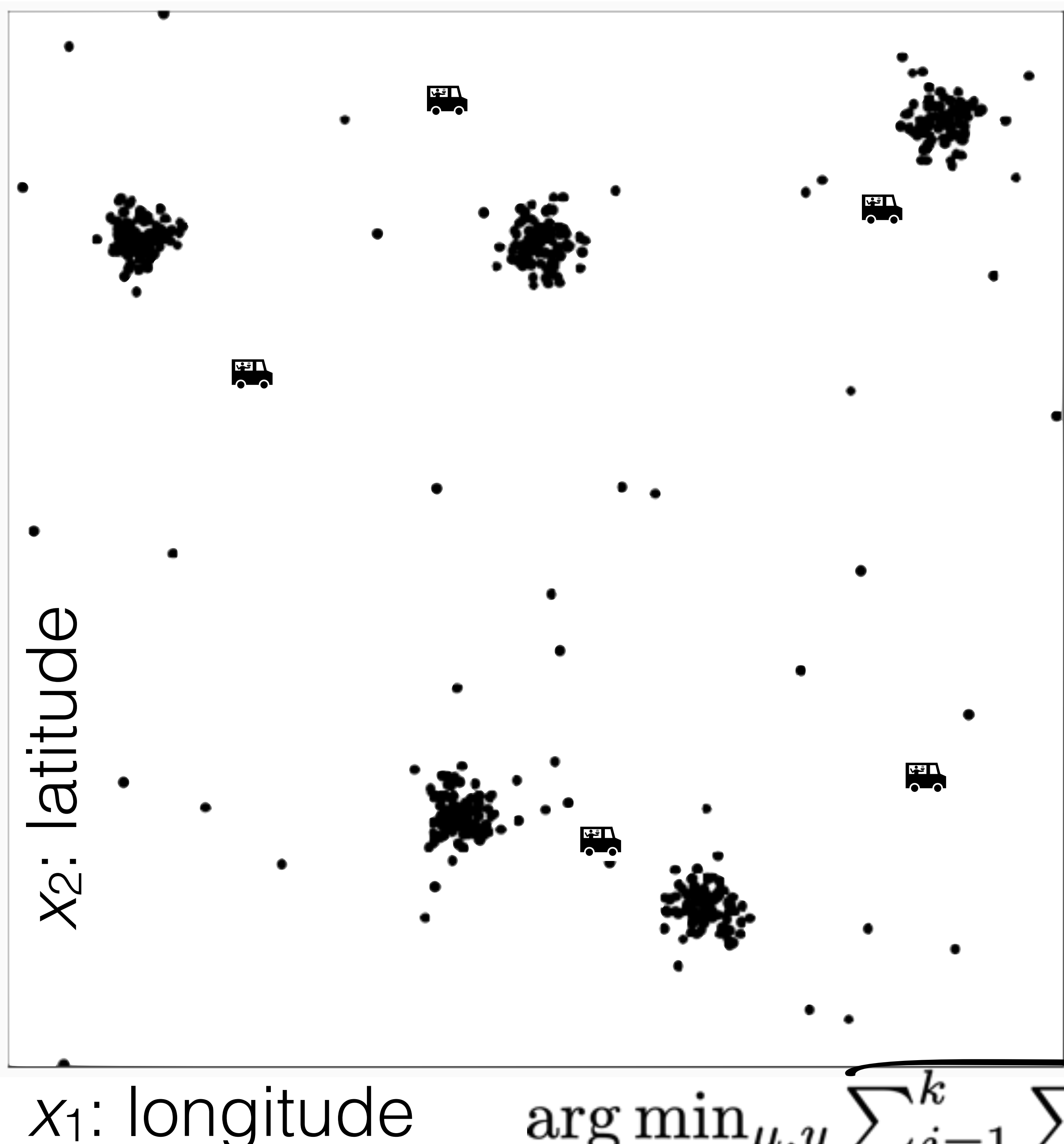

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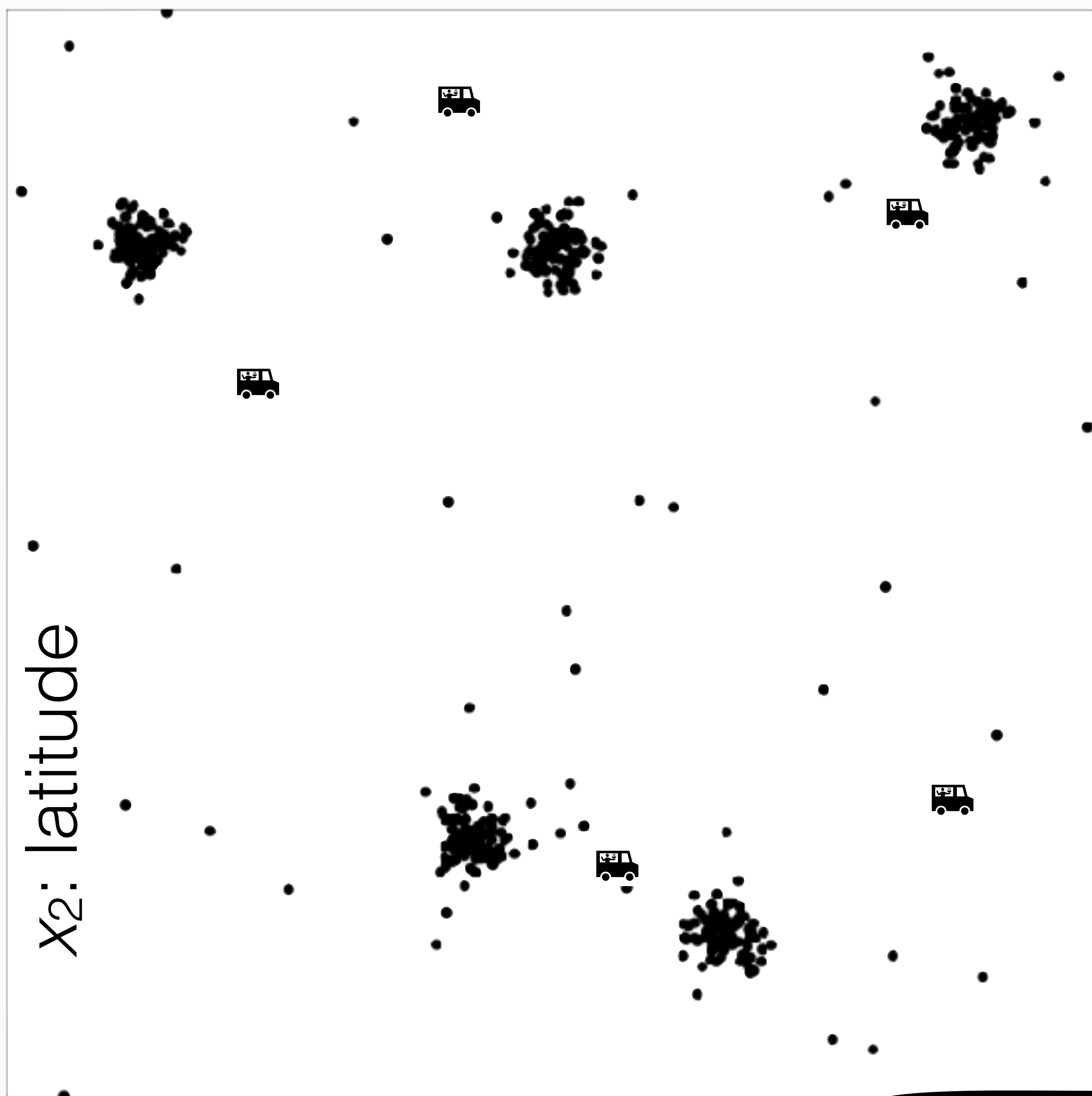

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k-means algorithm

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`k-means`

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`k-means(k,` τ`)`

k-means algorithm

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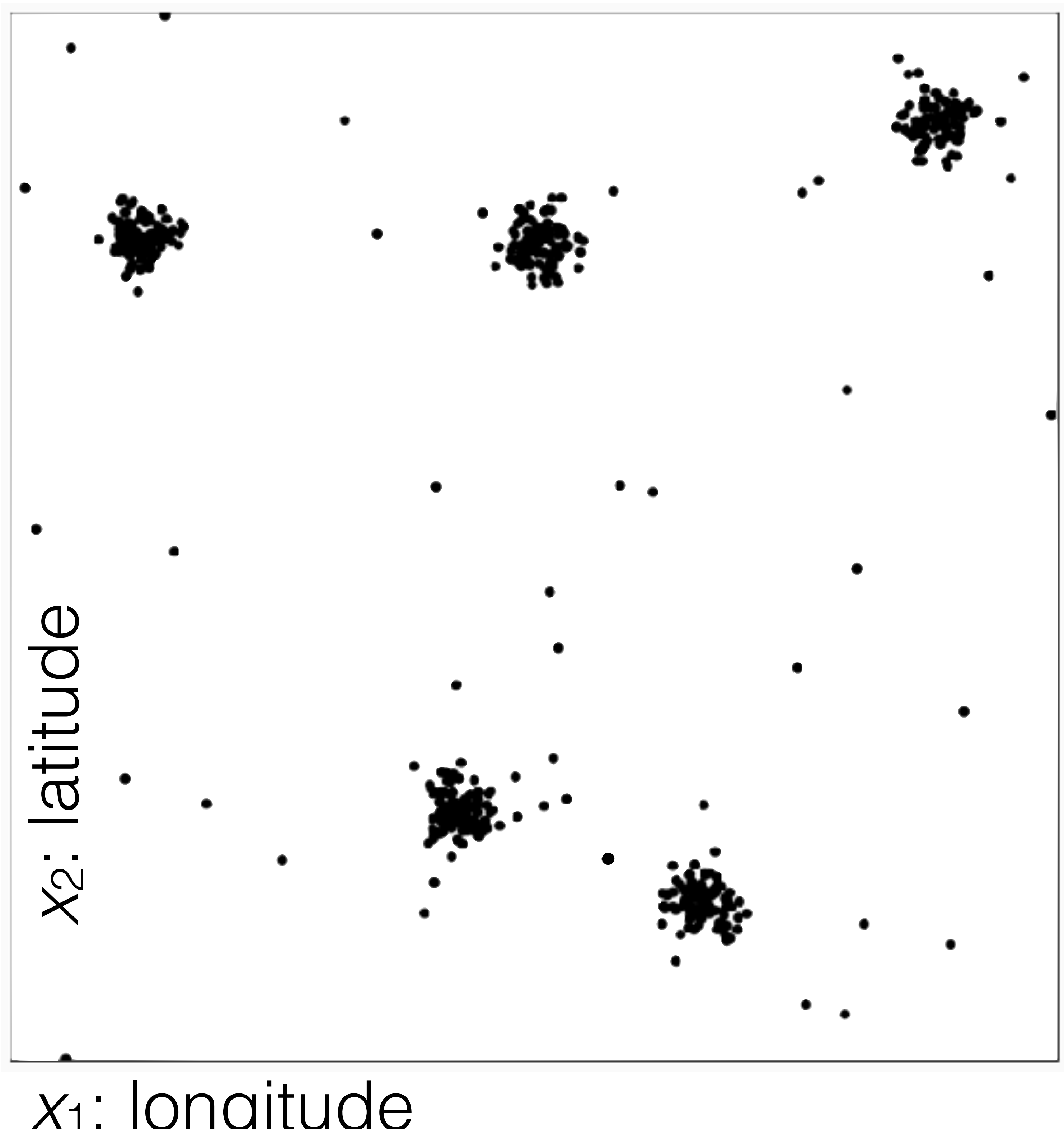
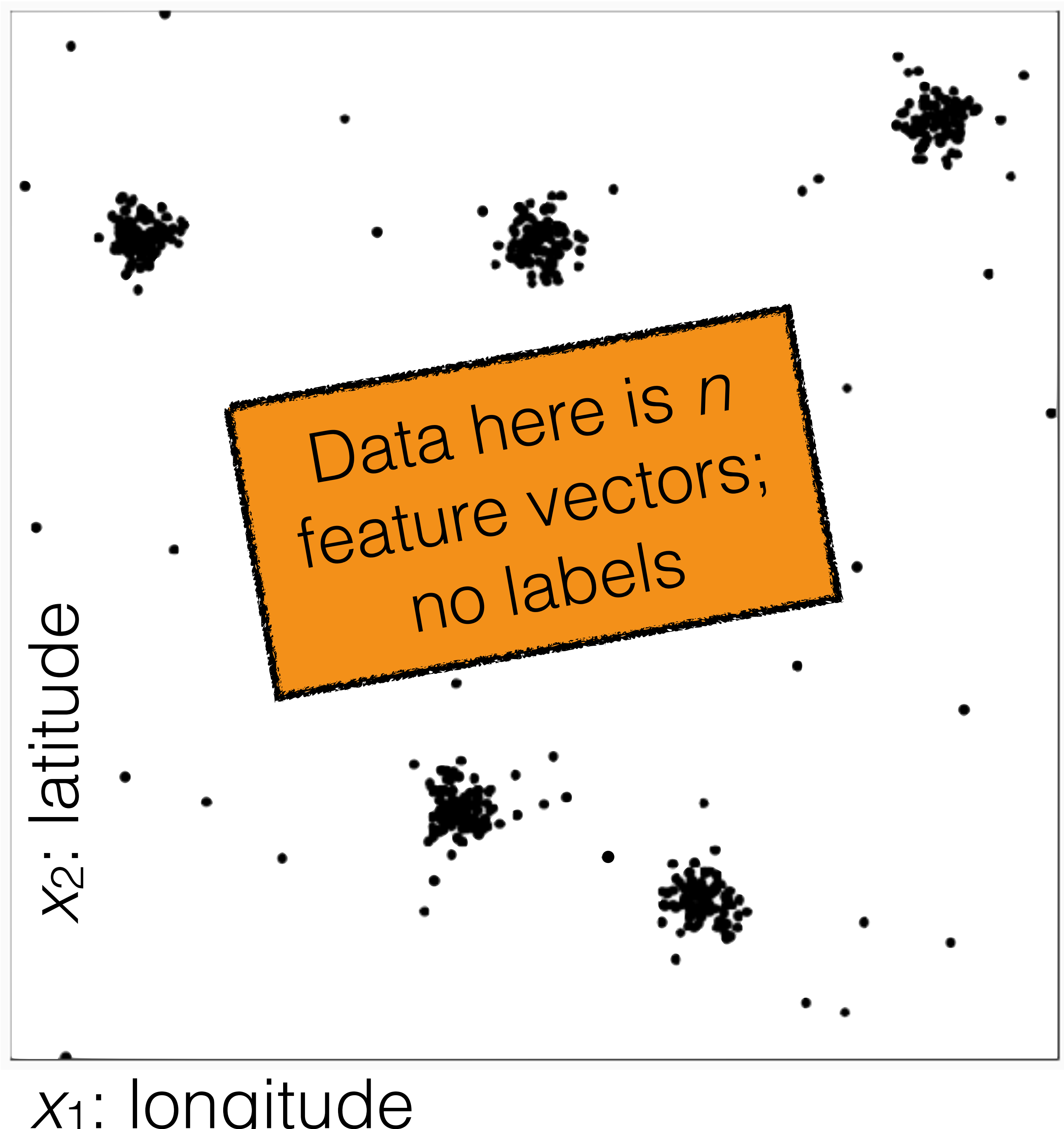


`k-means(k,` τ`)`

k-means algorithm



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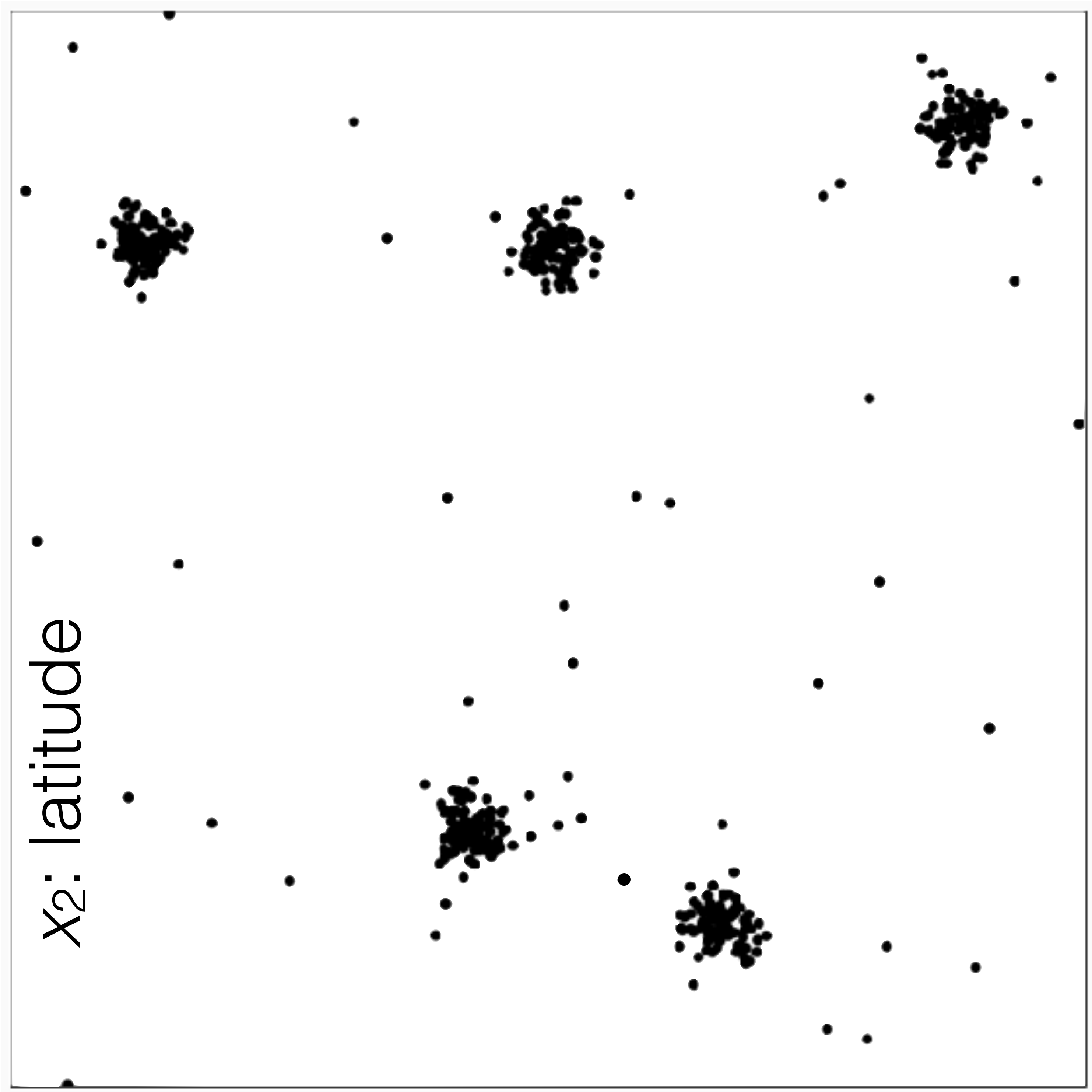

`k-means(k, τ)`

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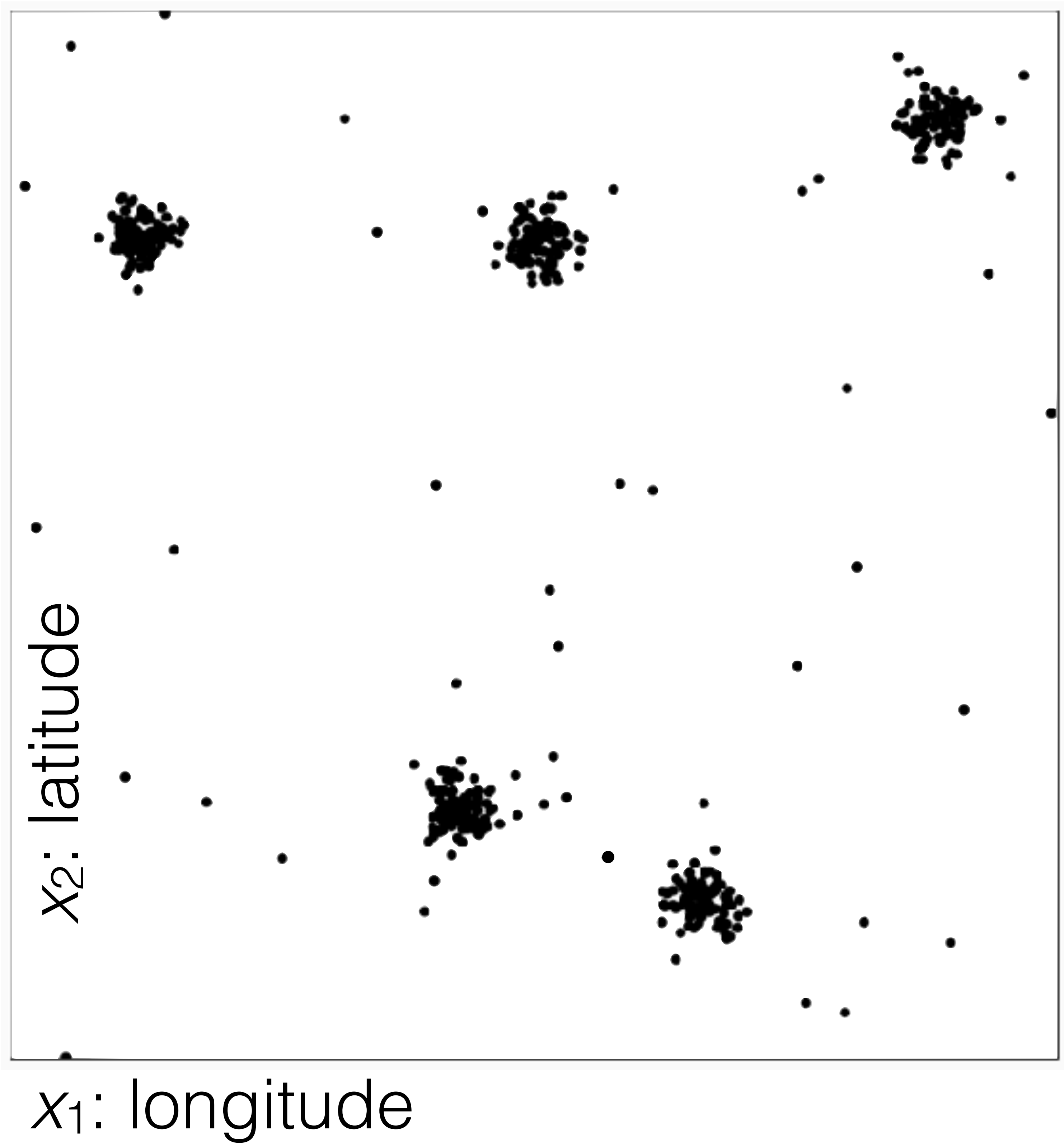

`k-means(k,` τ`)`

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

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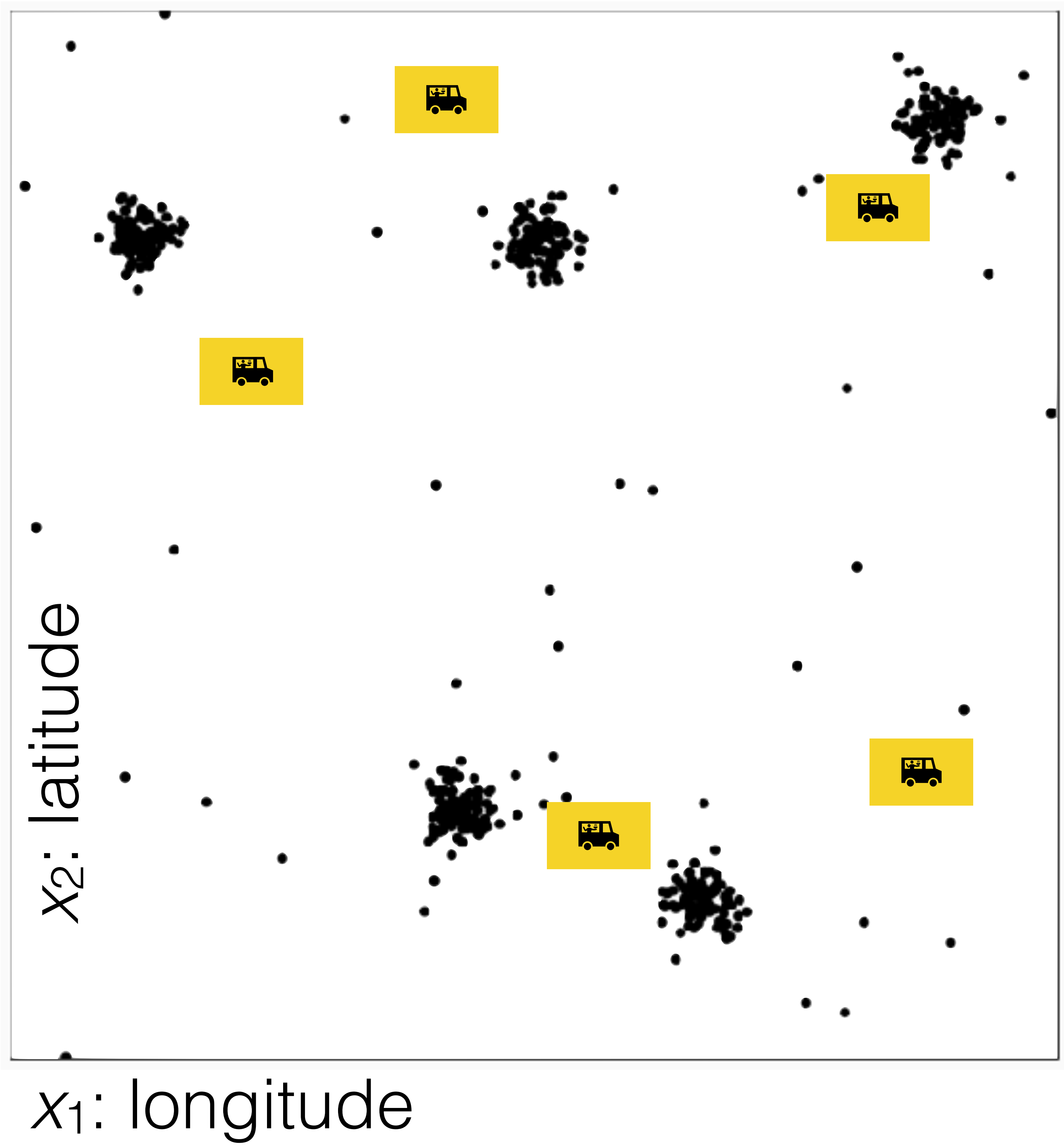

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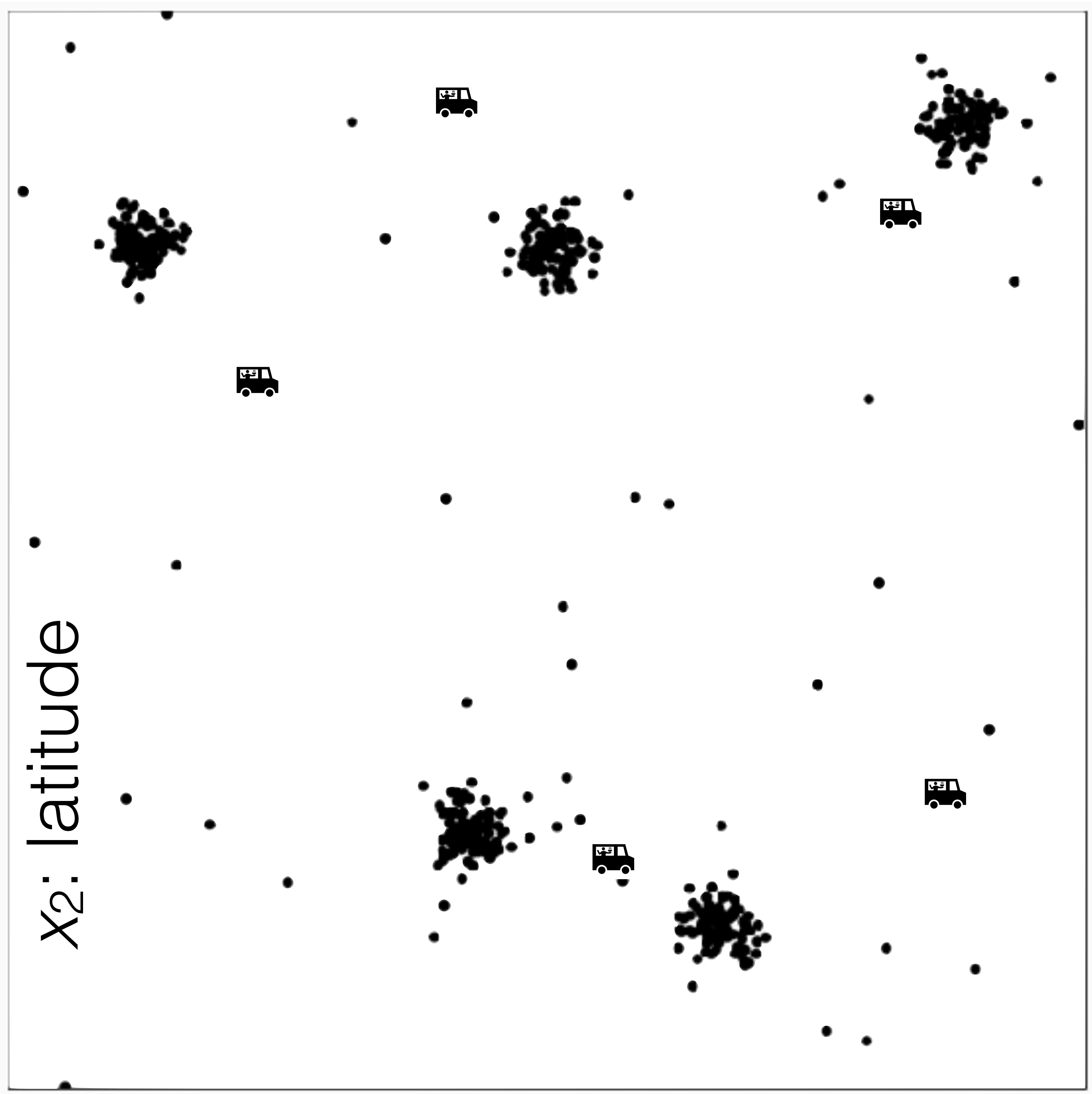

x_1: longitude

x_2: latitude

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k-means(k, τ)
 Init {μ^(j)}_{j=1}^k
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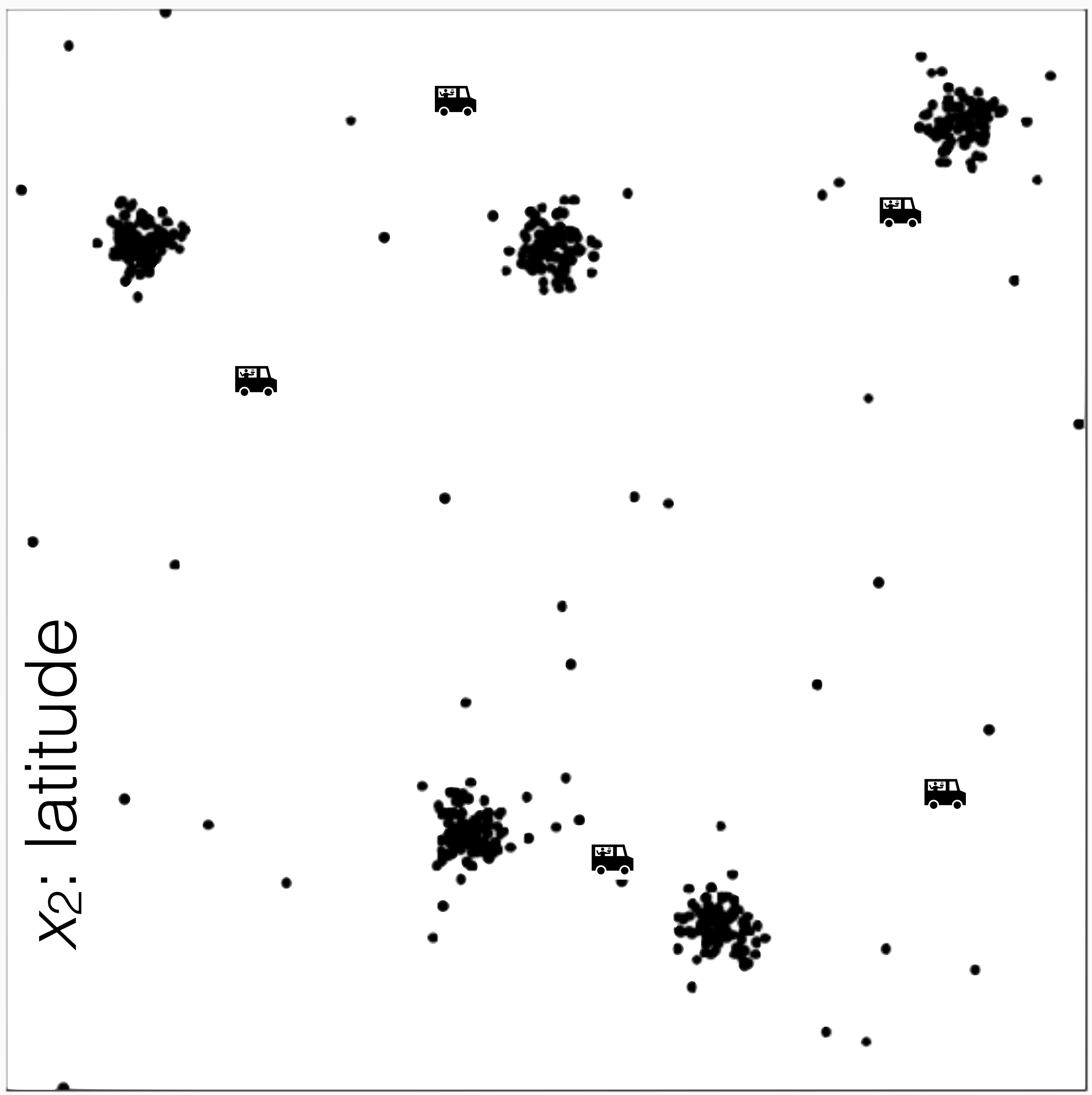
k-means algorithm

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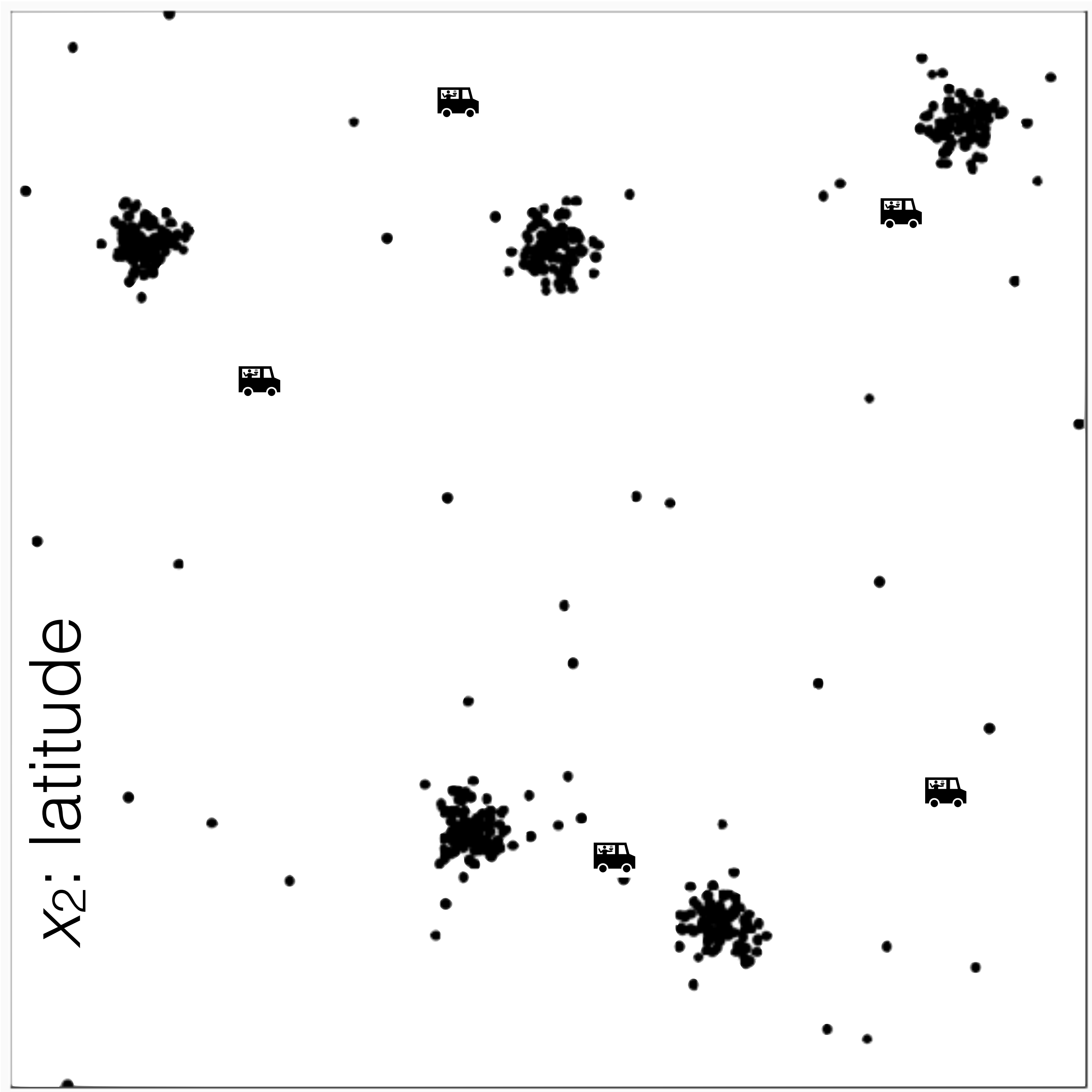
$$\text{Init } \{\mu^{(j)}\}_{j=1}^{k}$$

k-means algorithm

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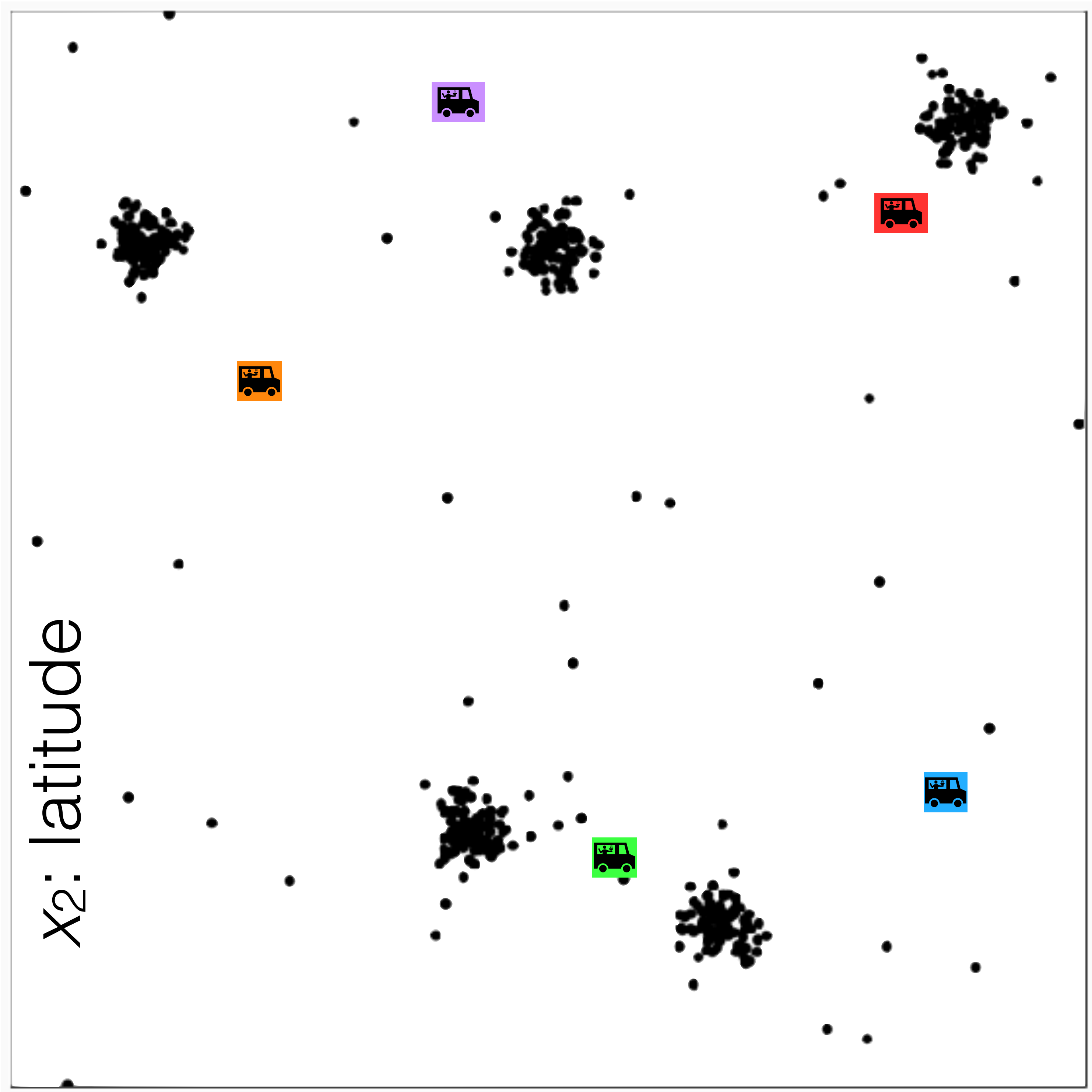
k-means algorithm

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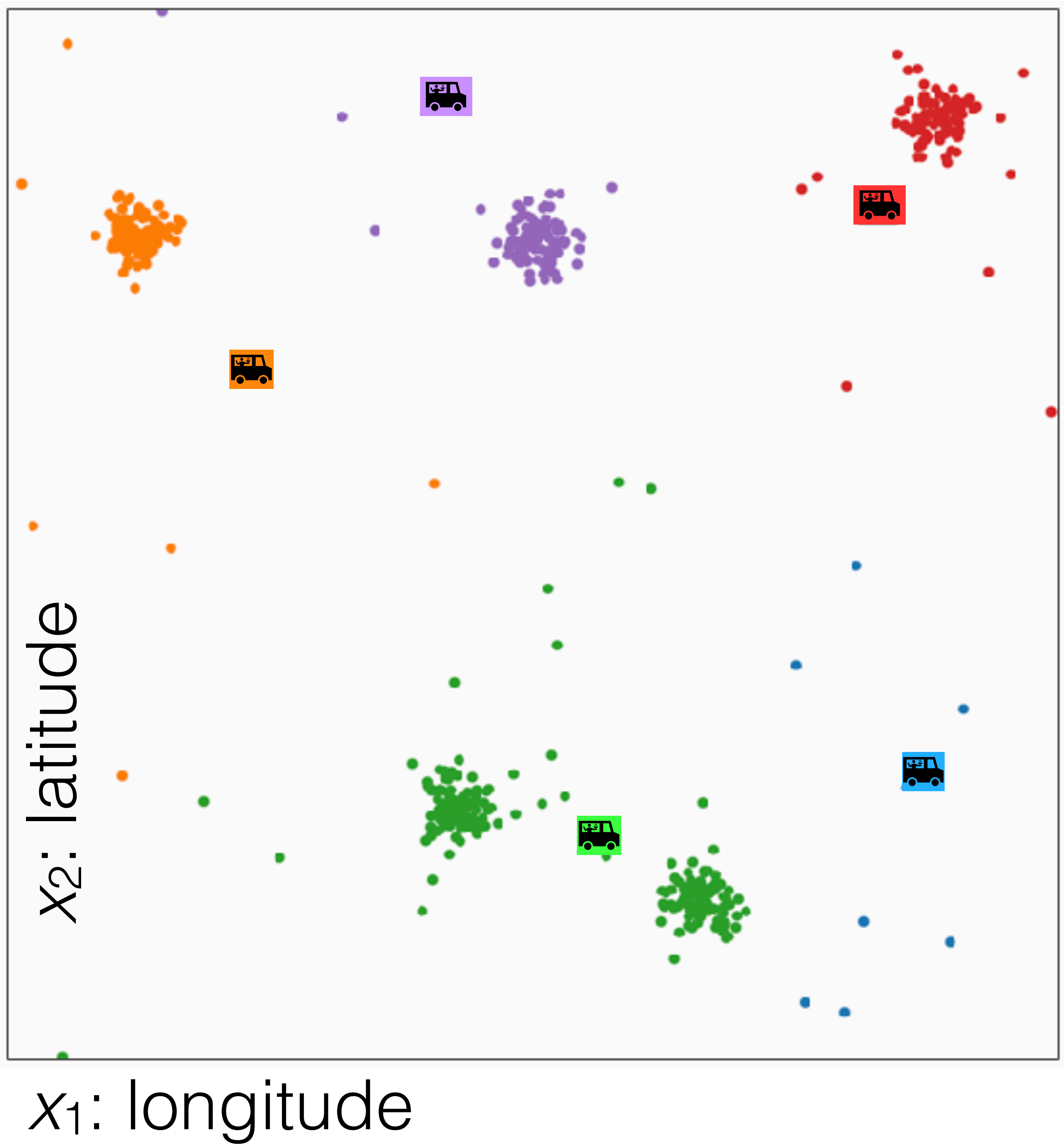


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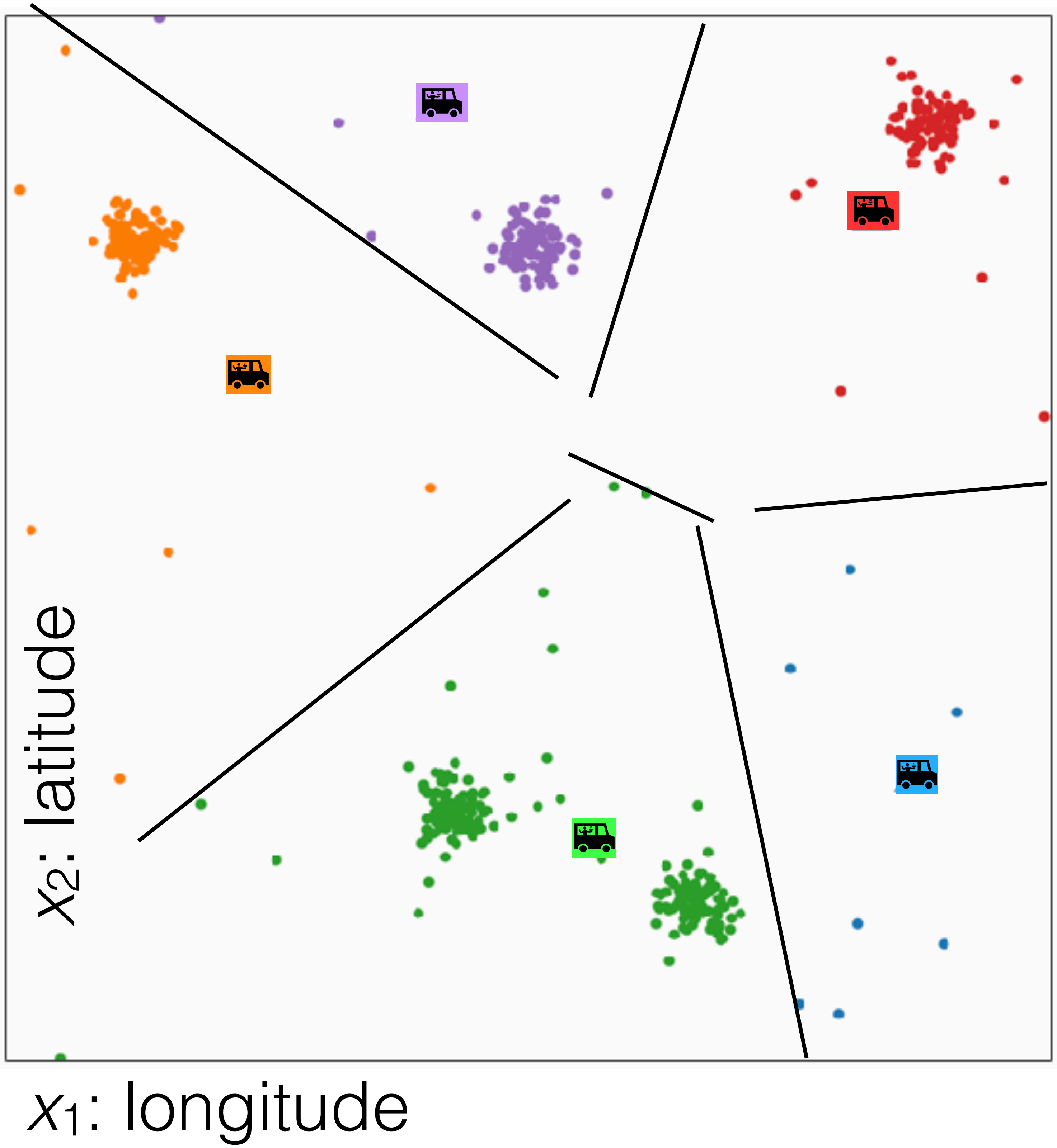


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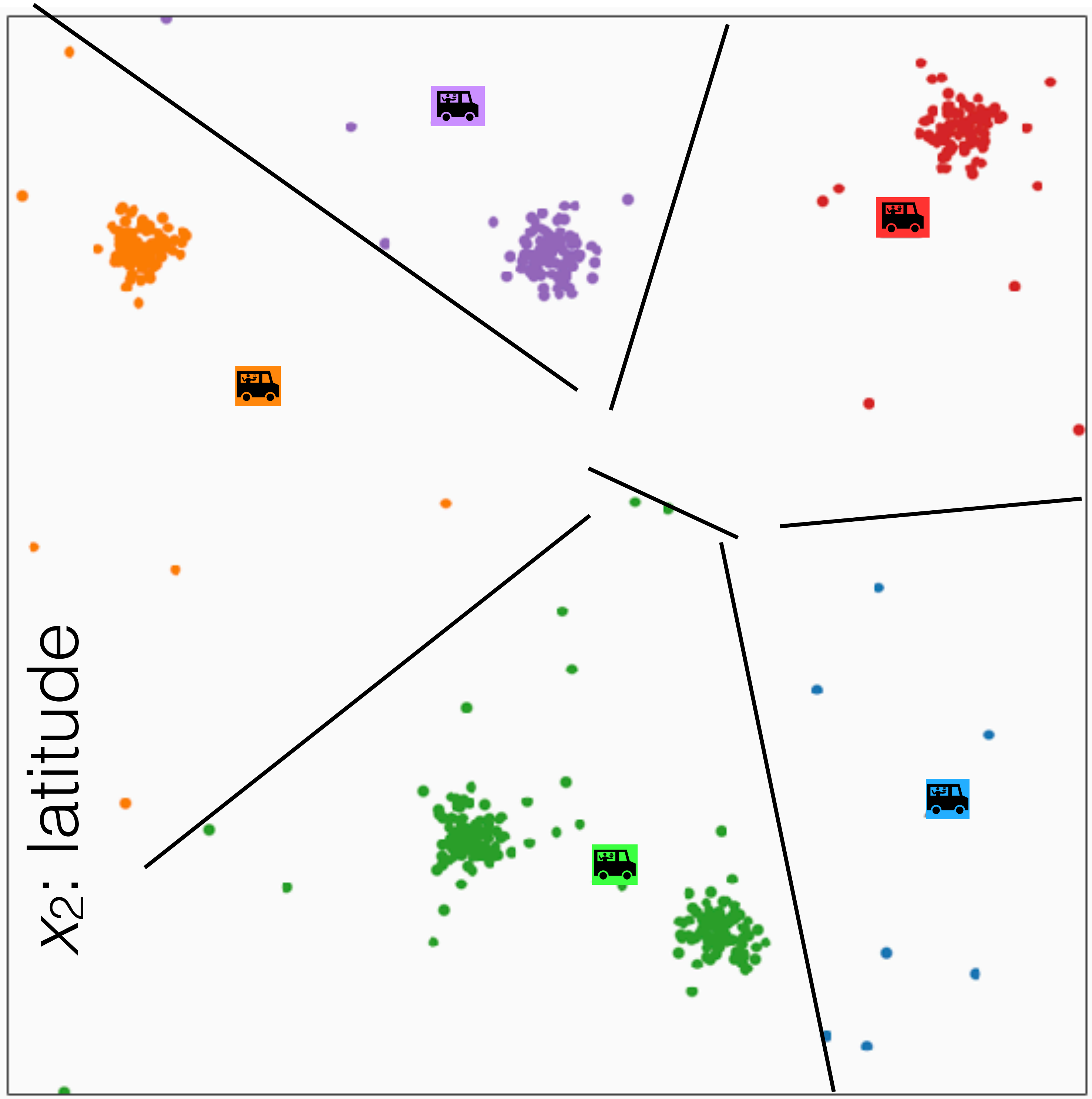


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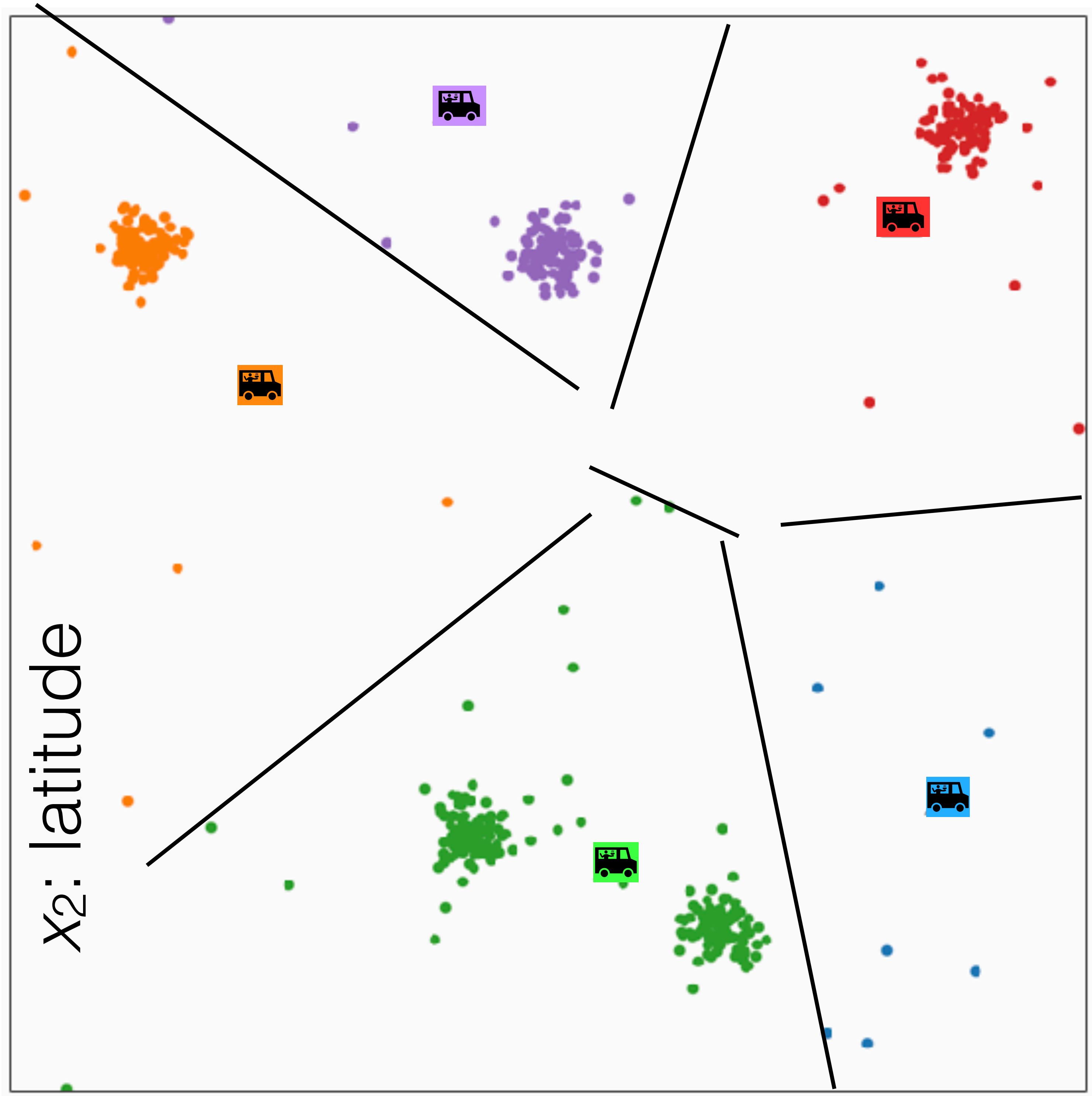
k-means algorithm

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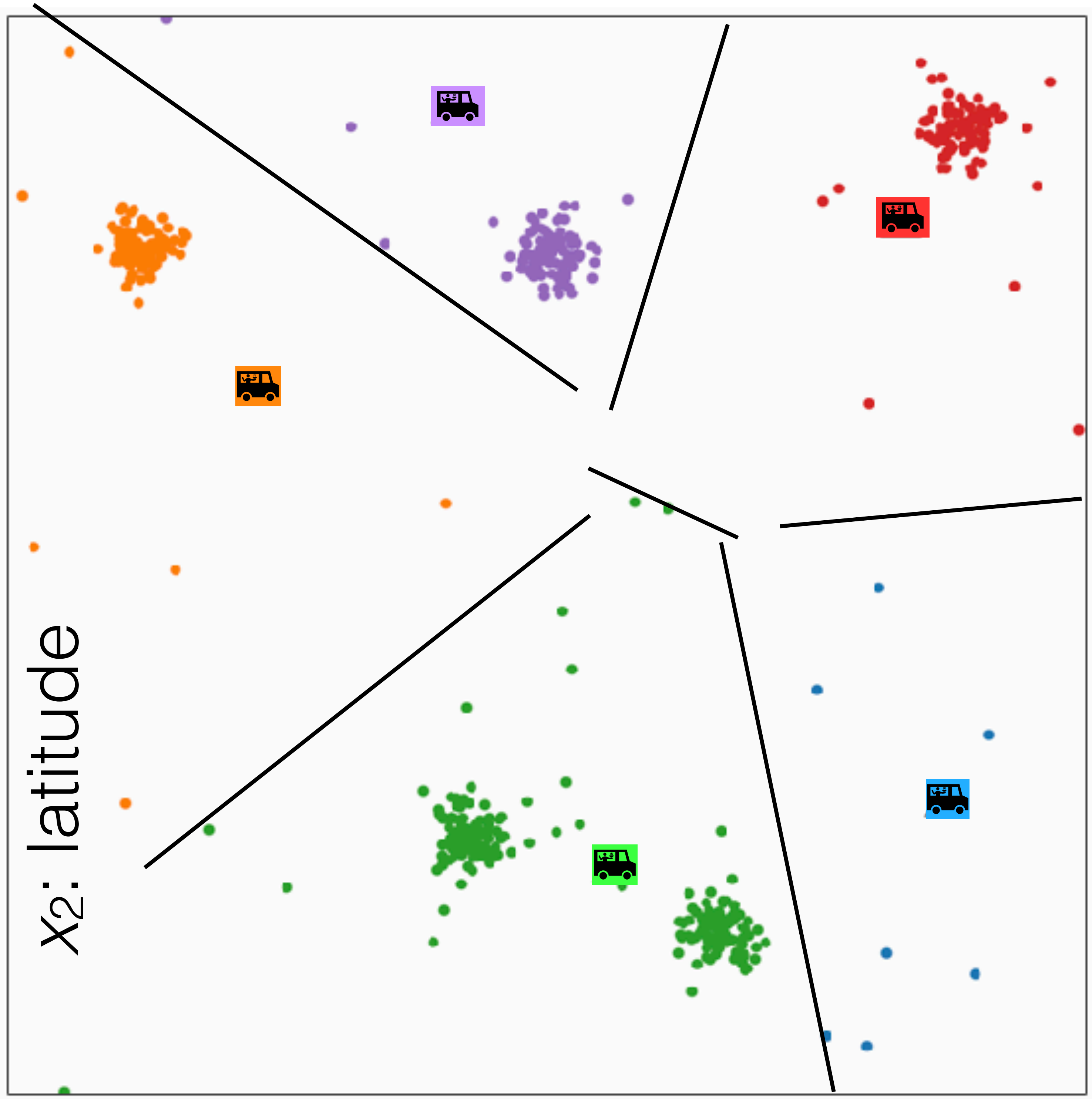
```

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

k-means algorithm

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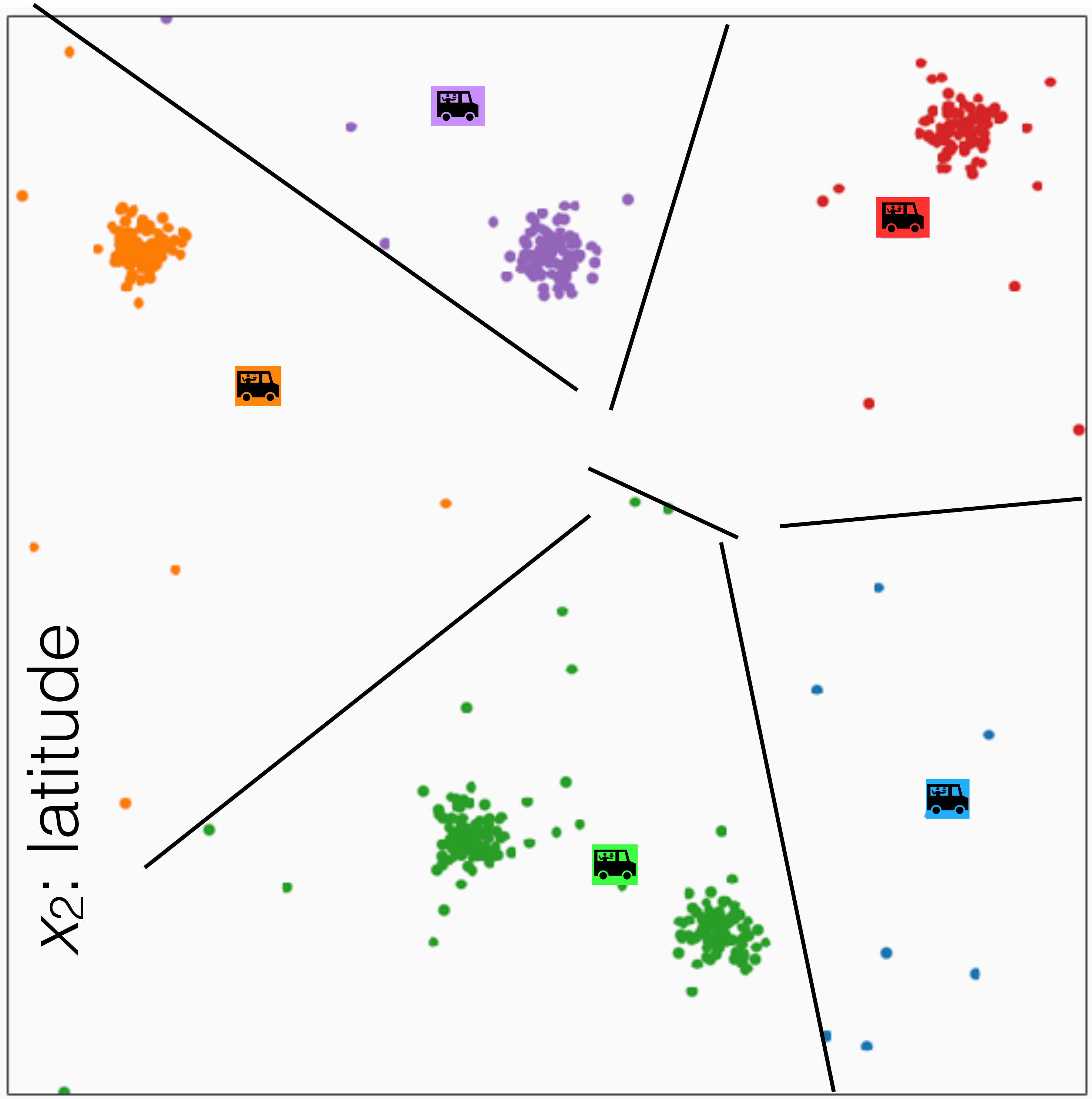


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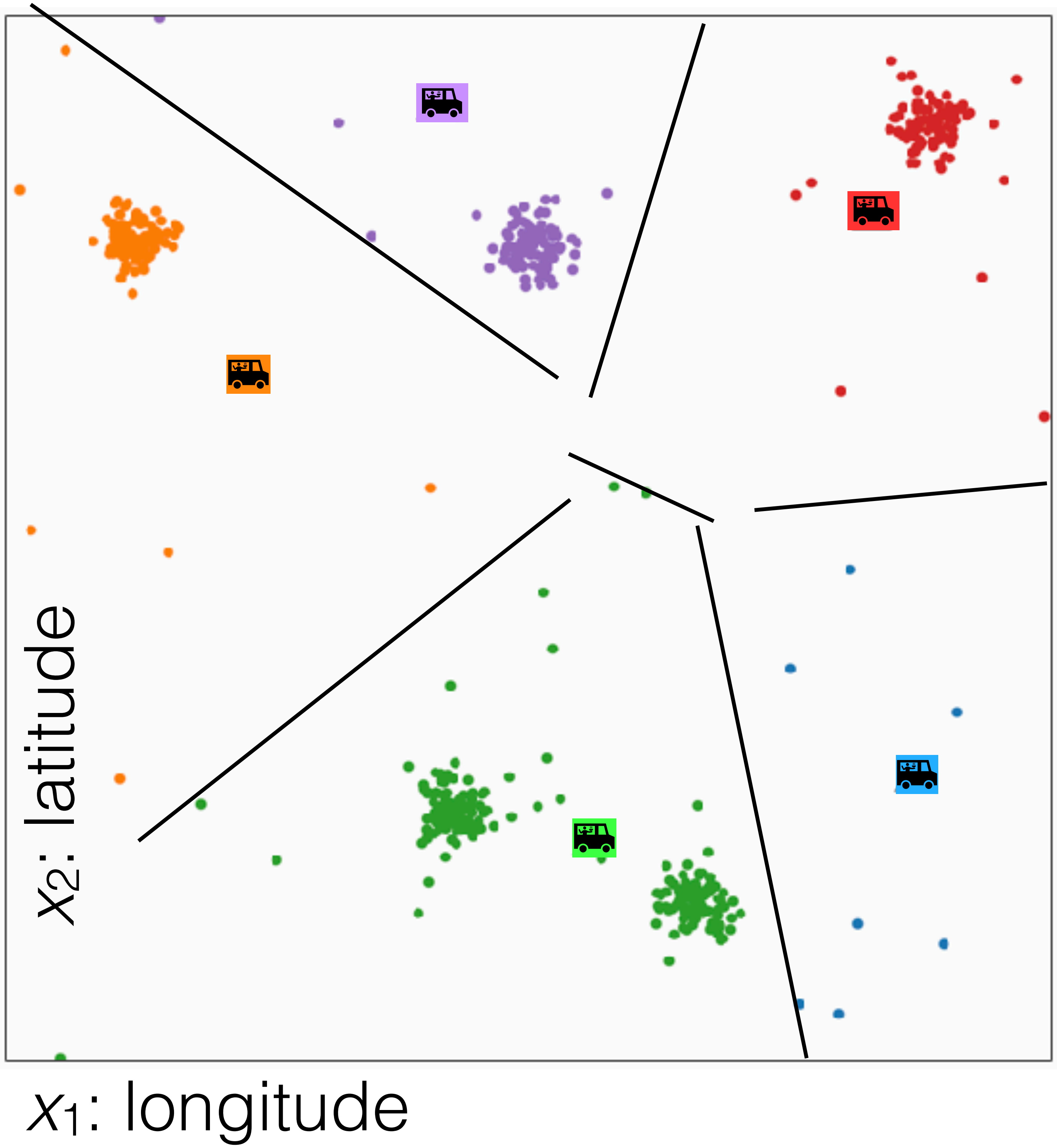

k-means(k, τ)

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

for t = 1 to τ

for i = 1 to n

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

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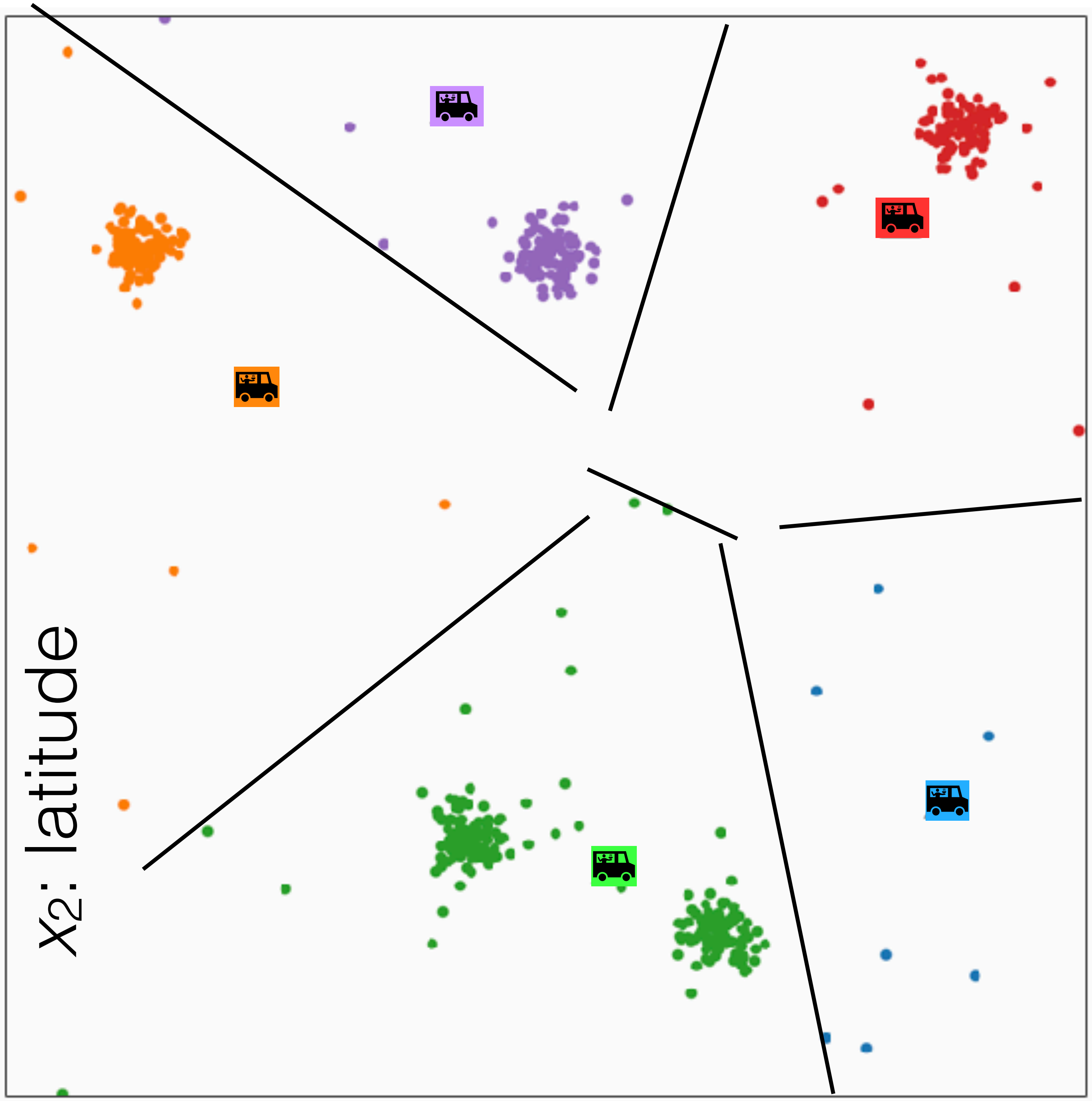


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$$\text{k-means}(k, \tau)$$
$$\text{Init } \{\mu^{(j)}\}_{j=1}^{k}$$
$$\textbf{for } t = 1 \text{ to } \tau$$
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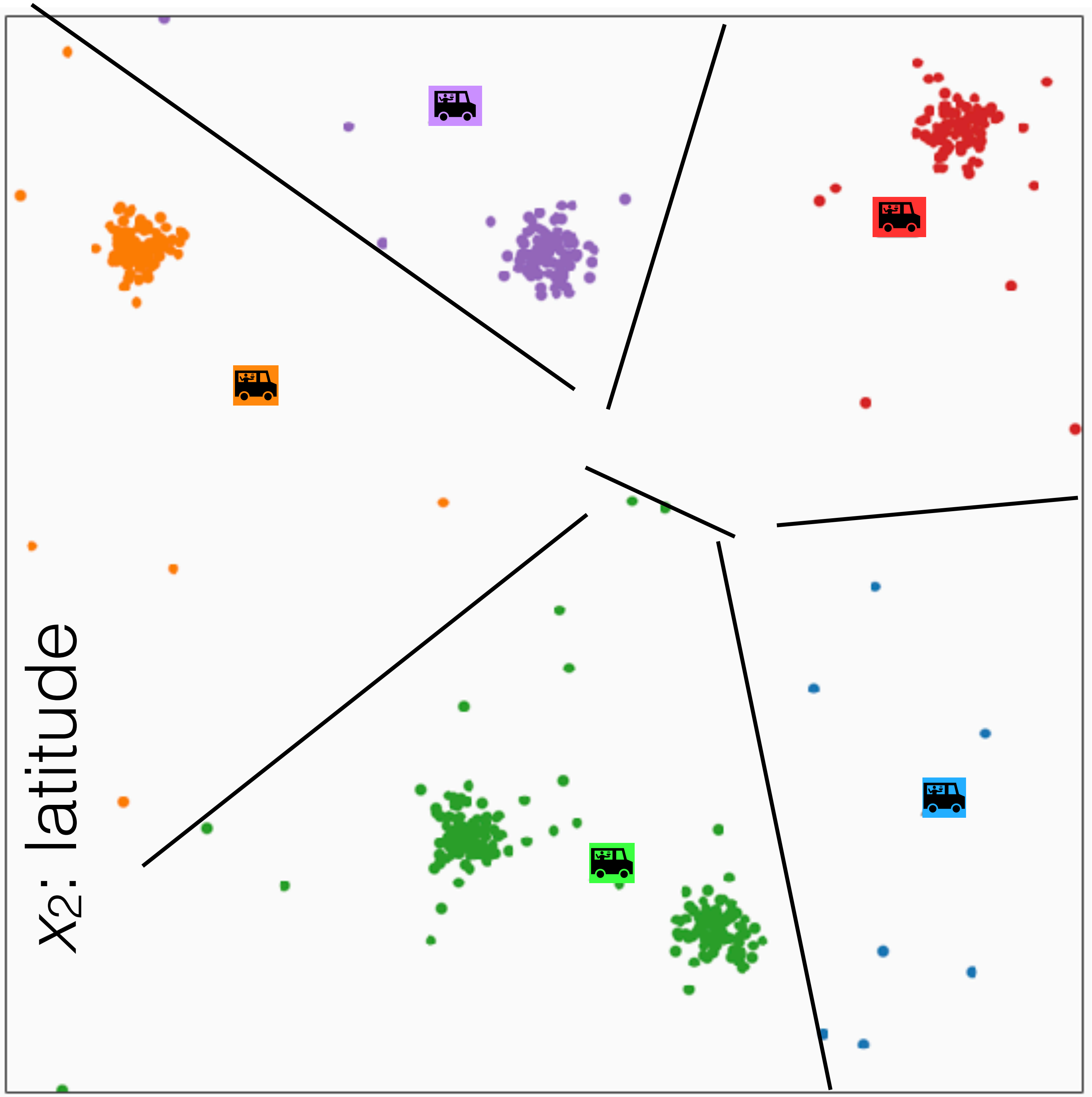


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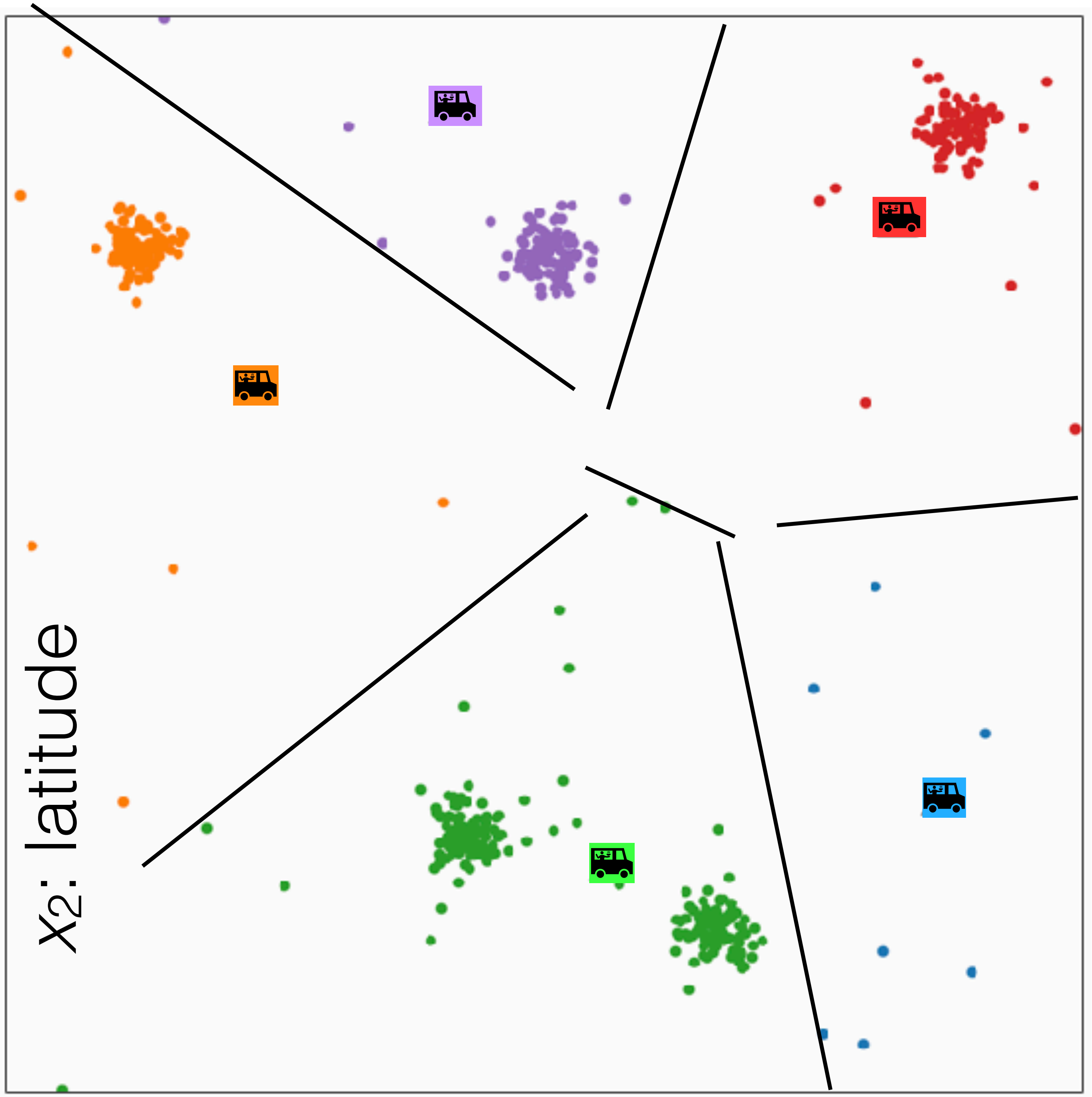


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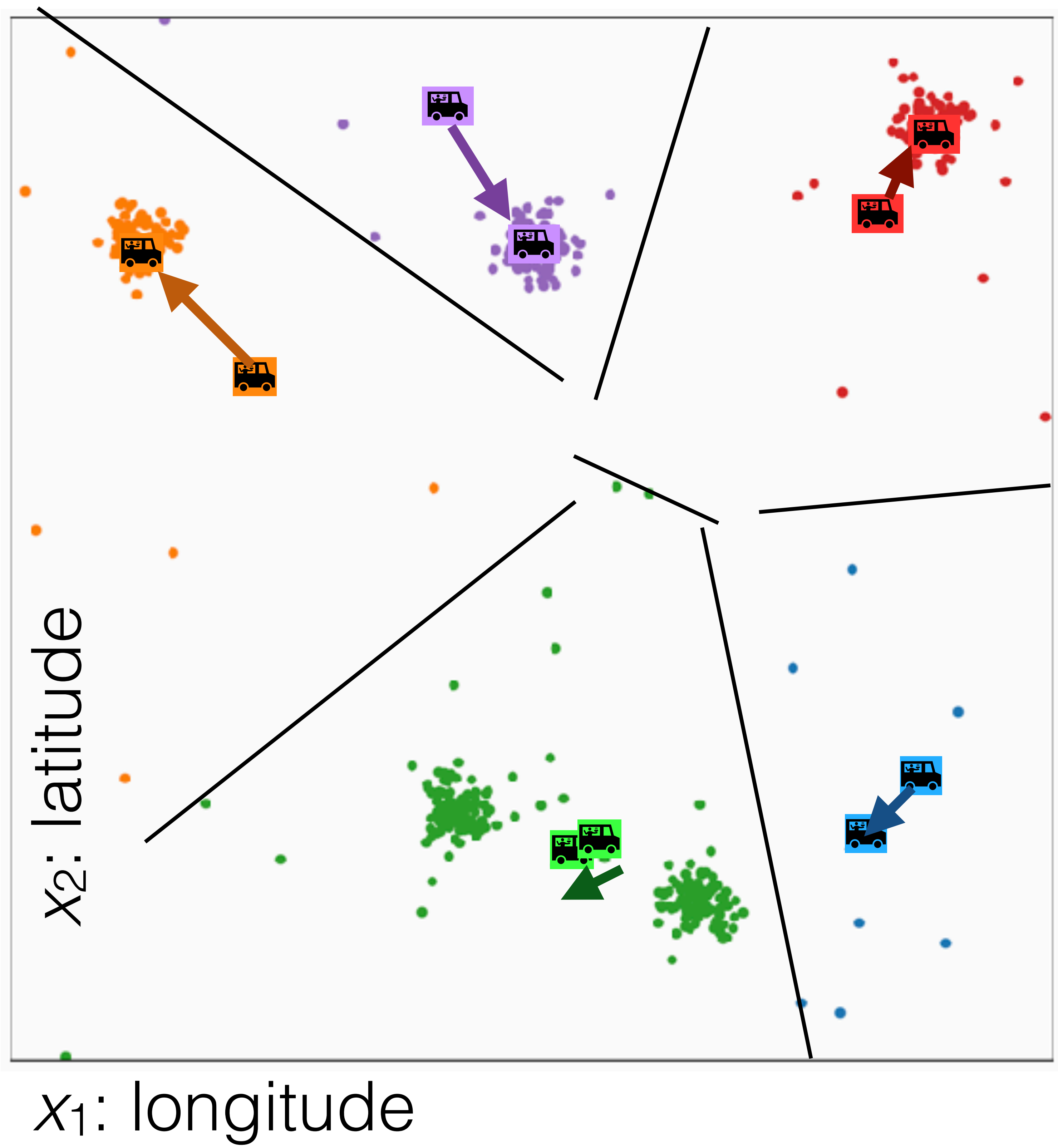


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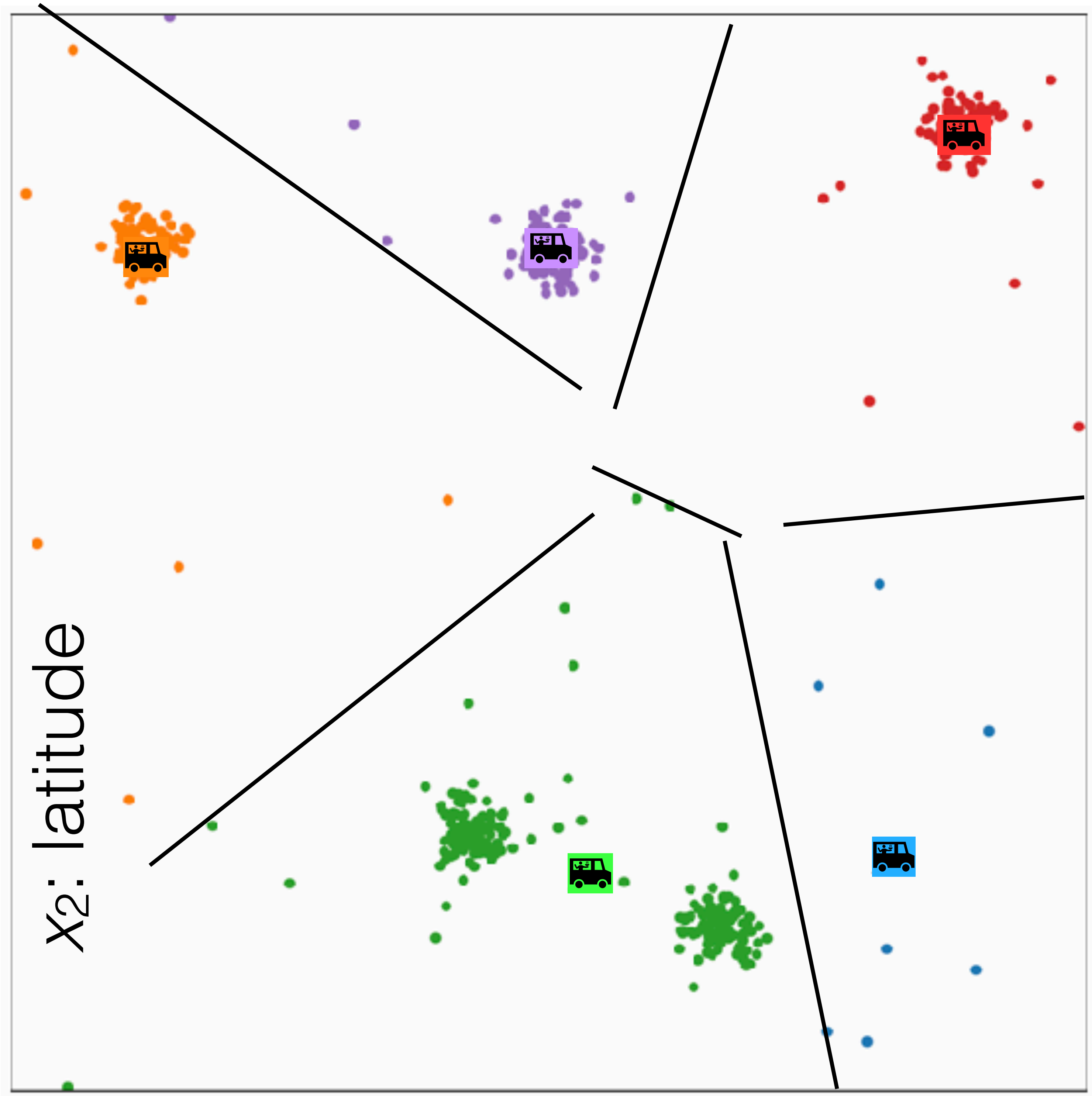
k-means algorithm

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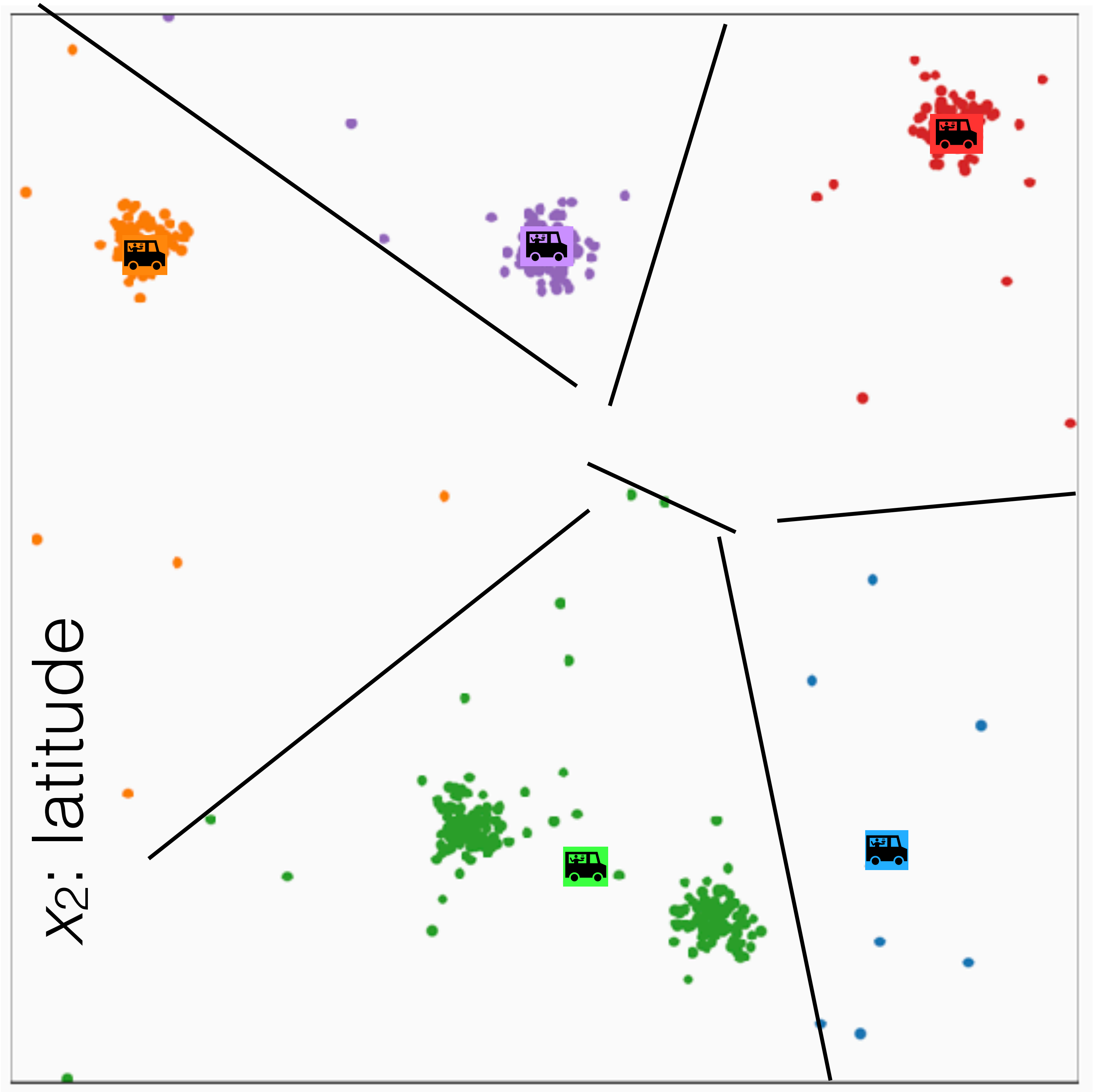


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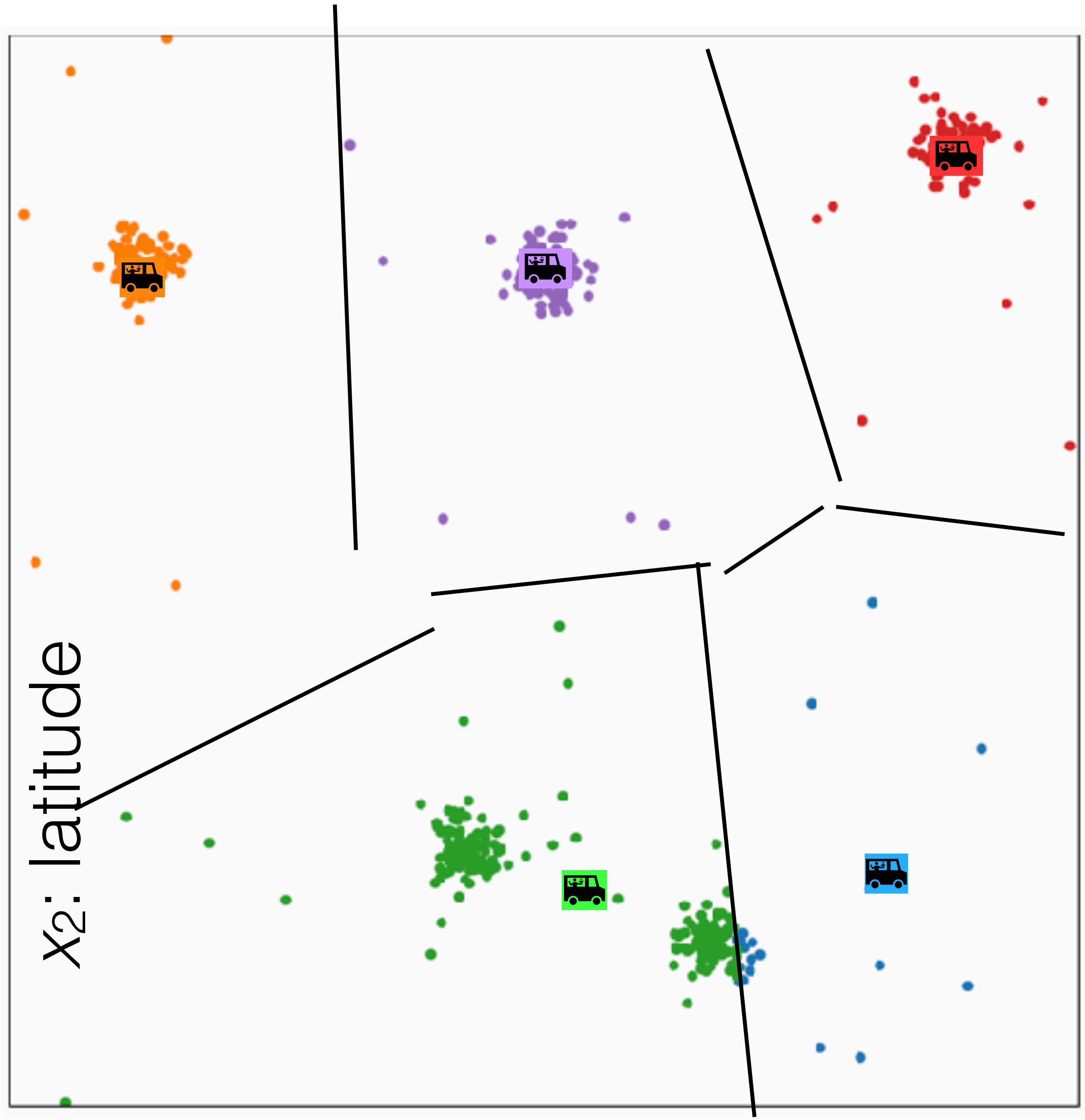


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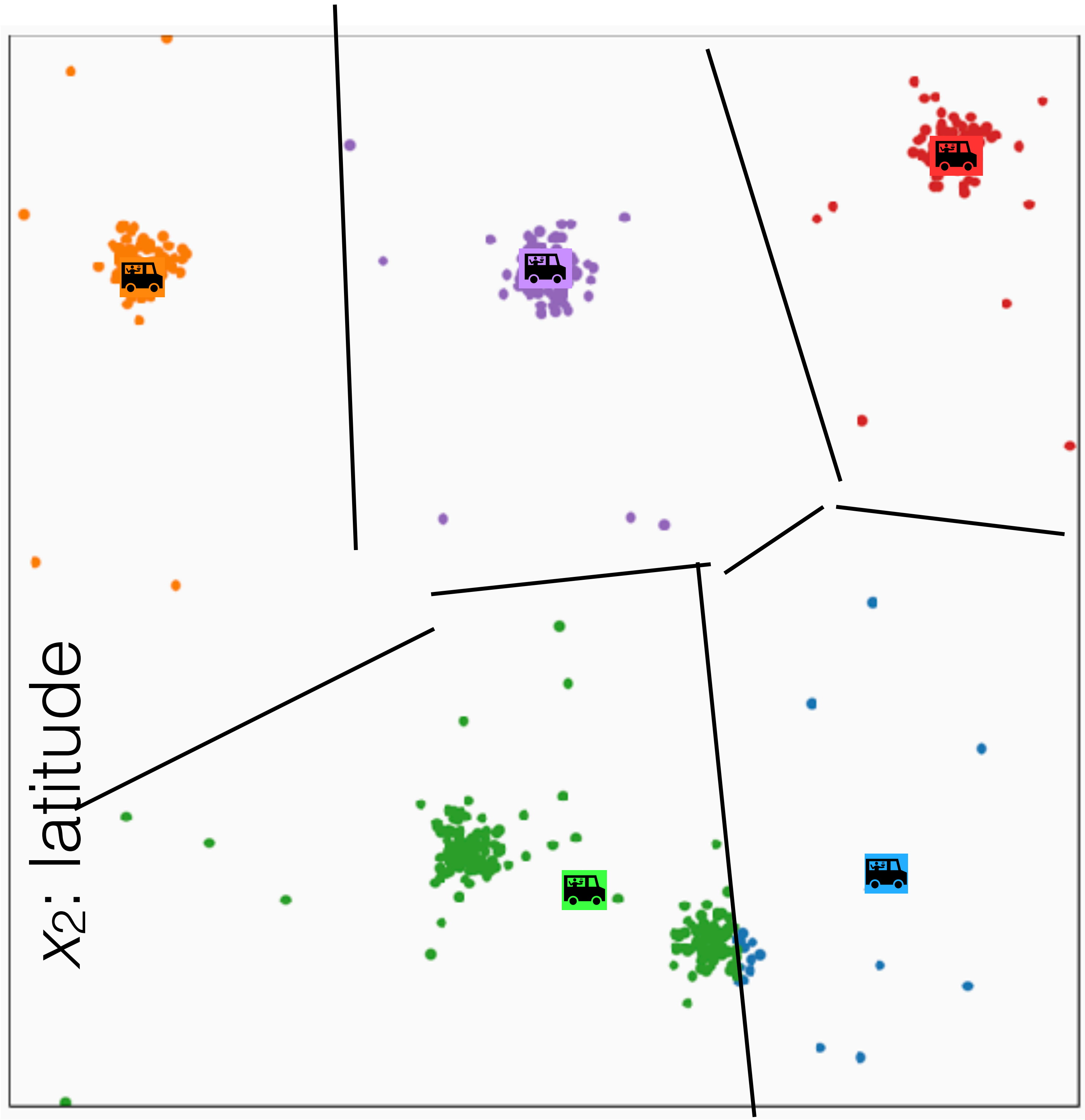


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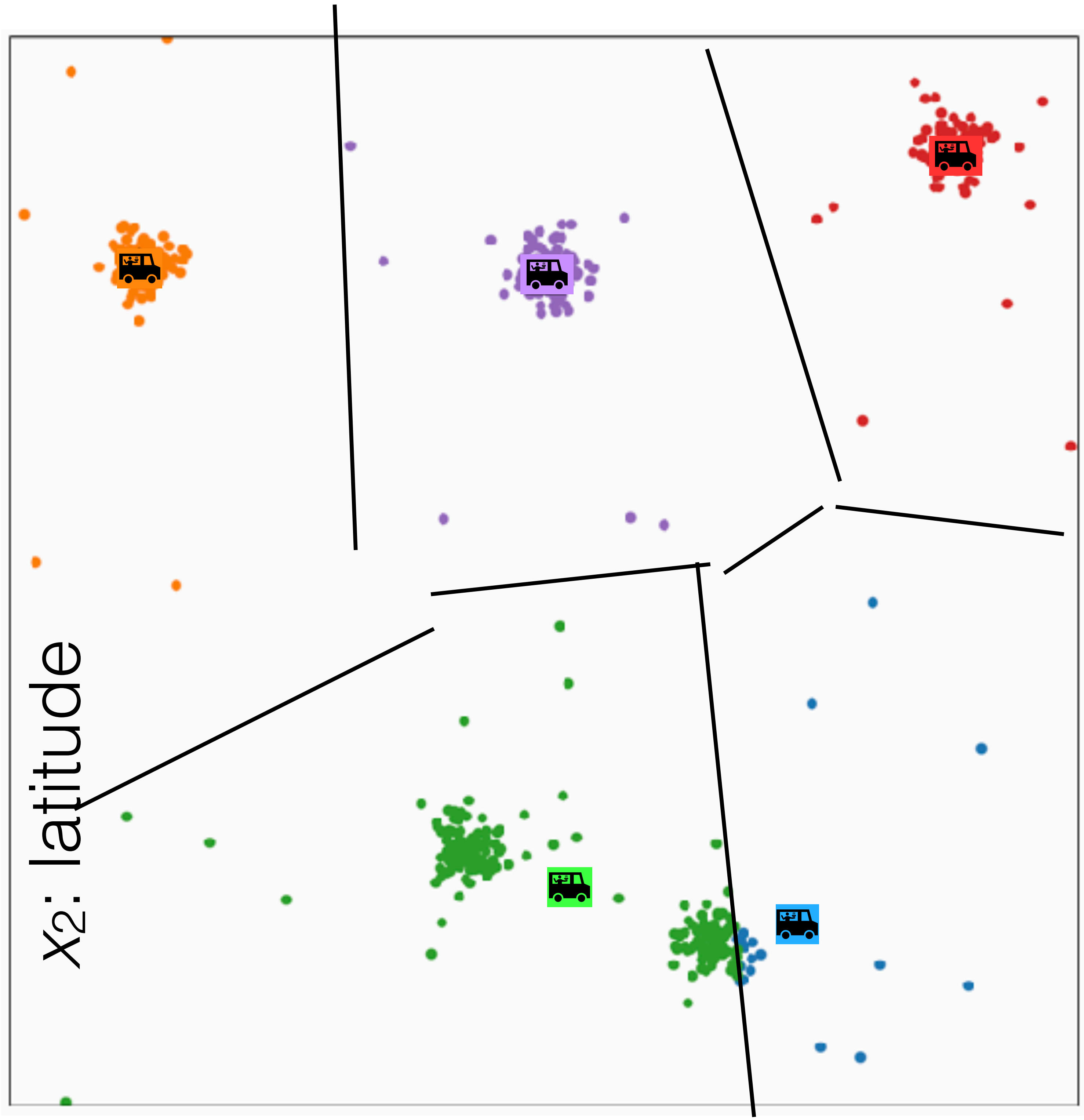

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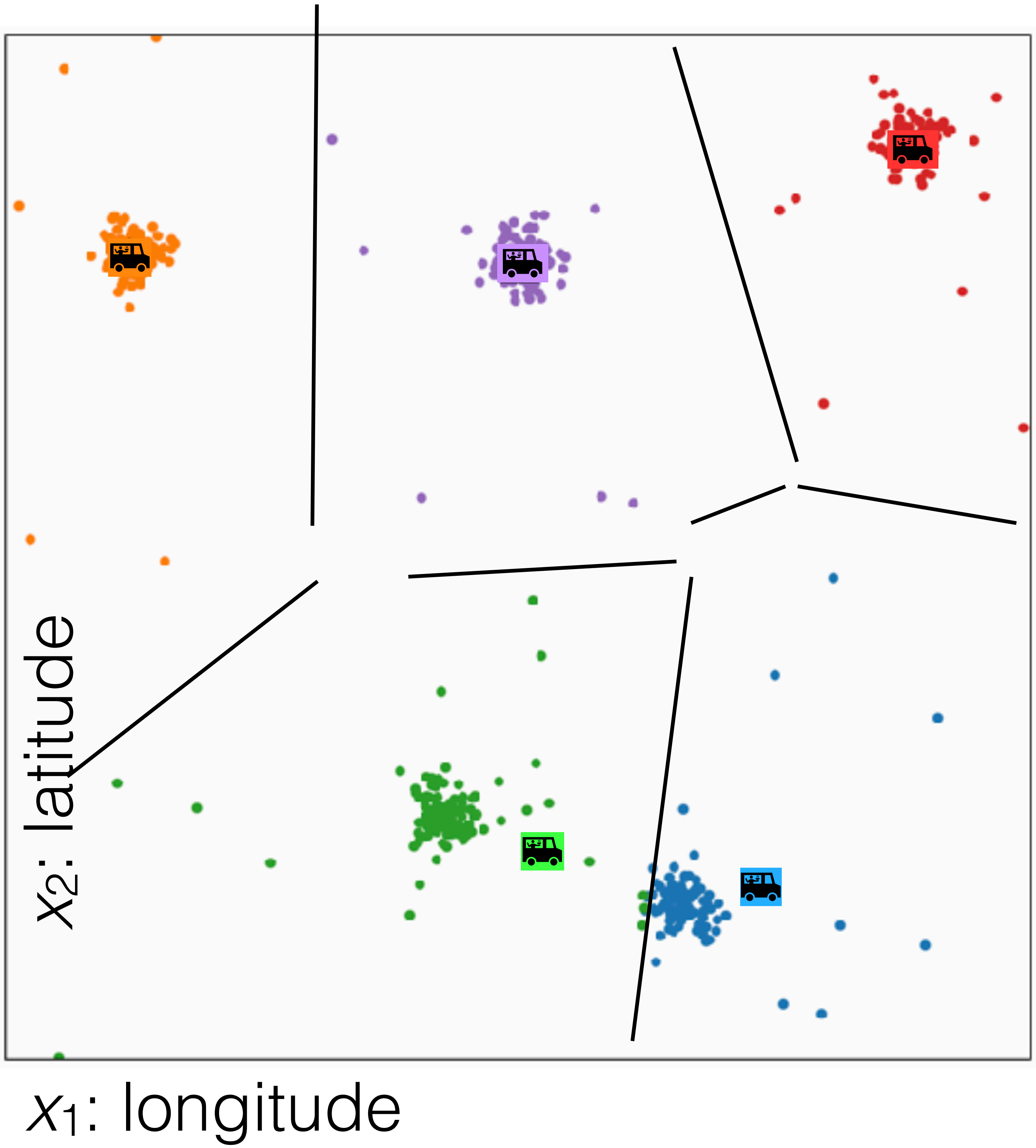


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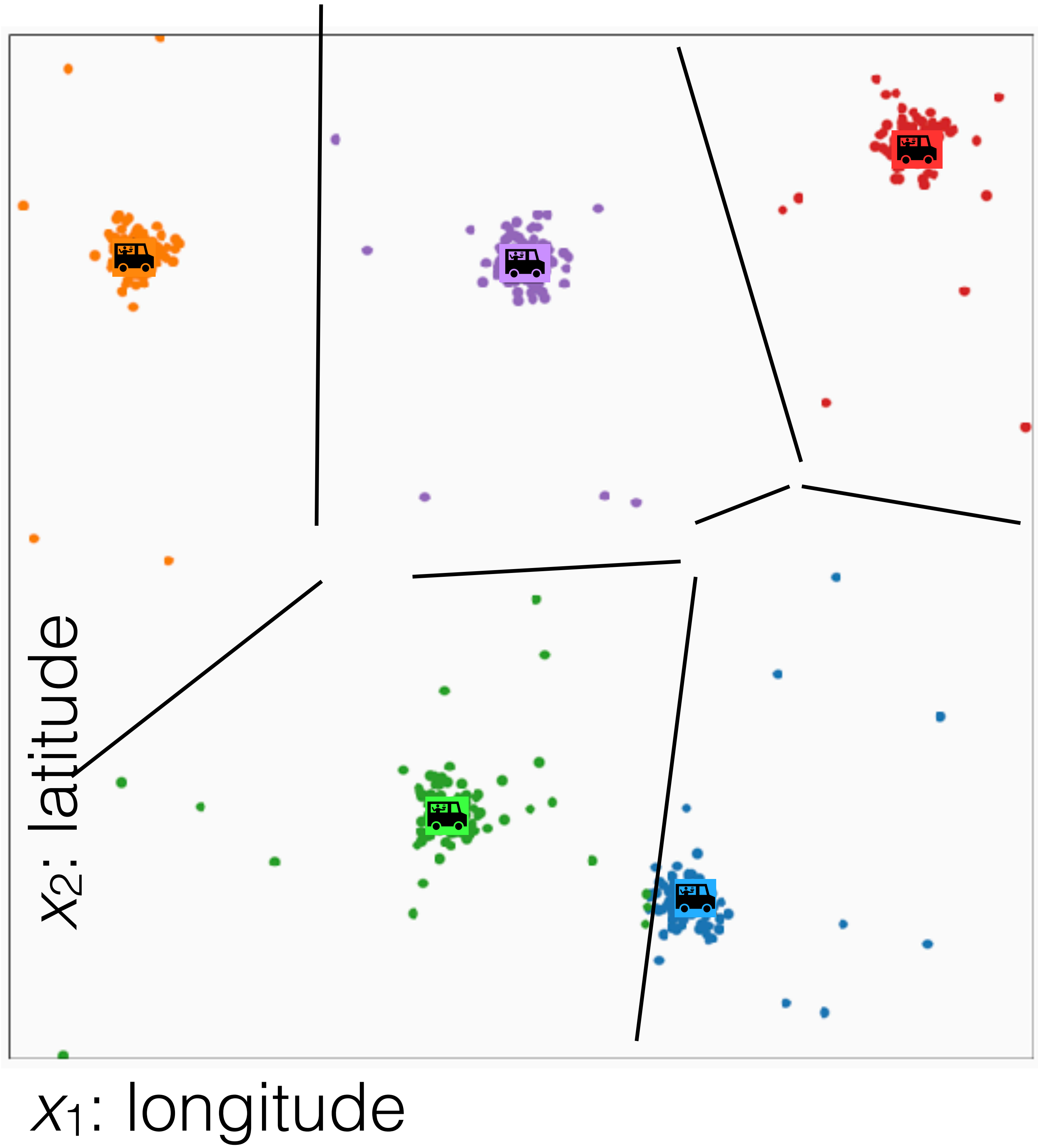


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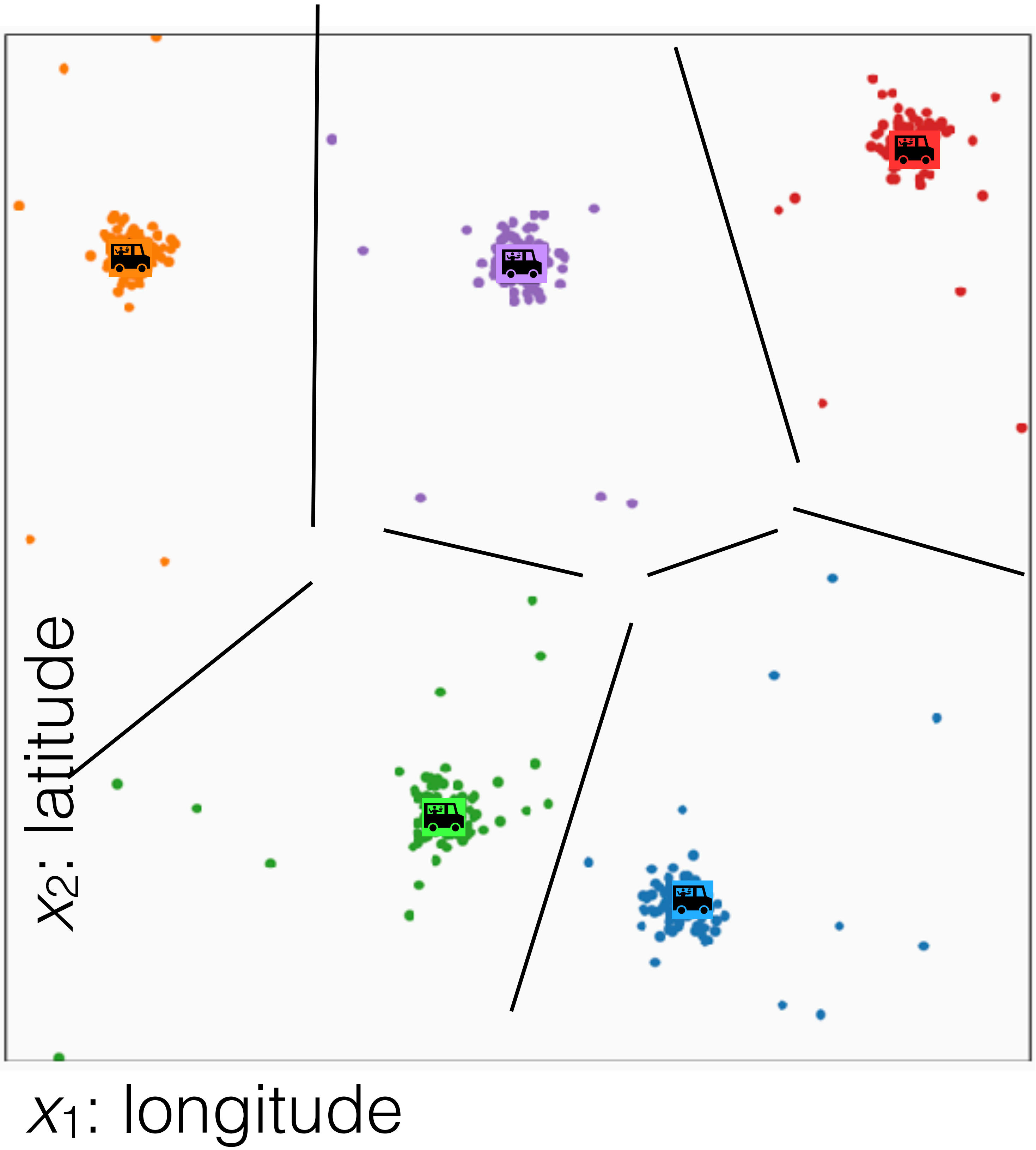

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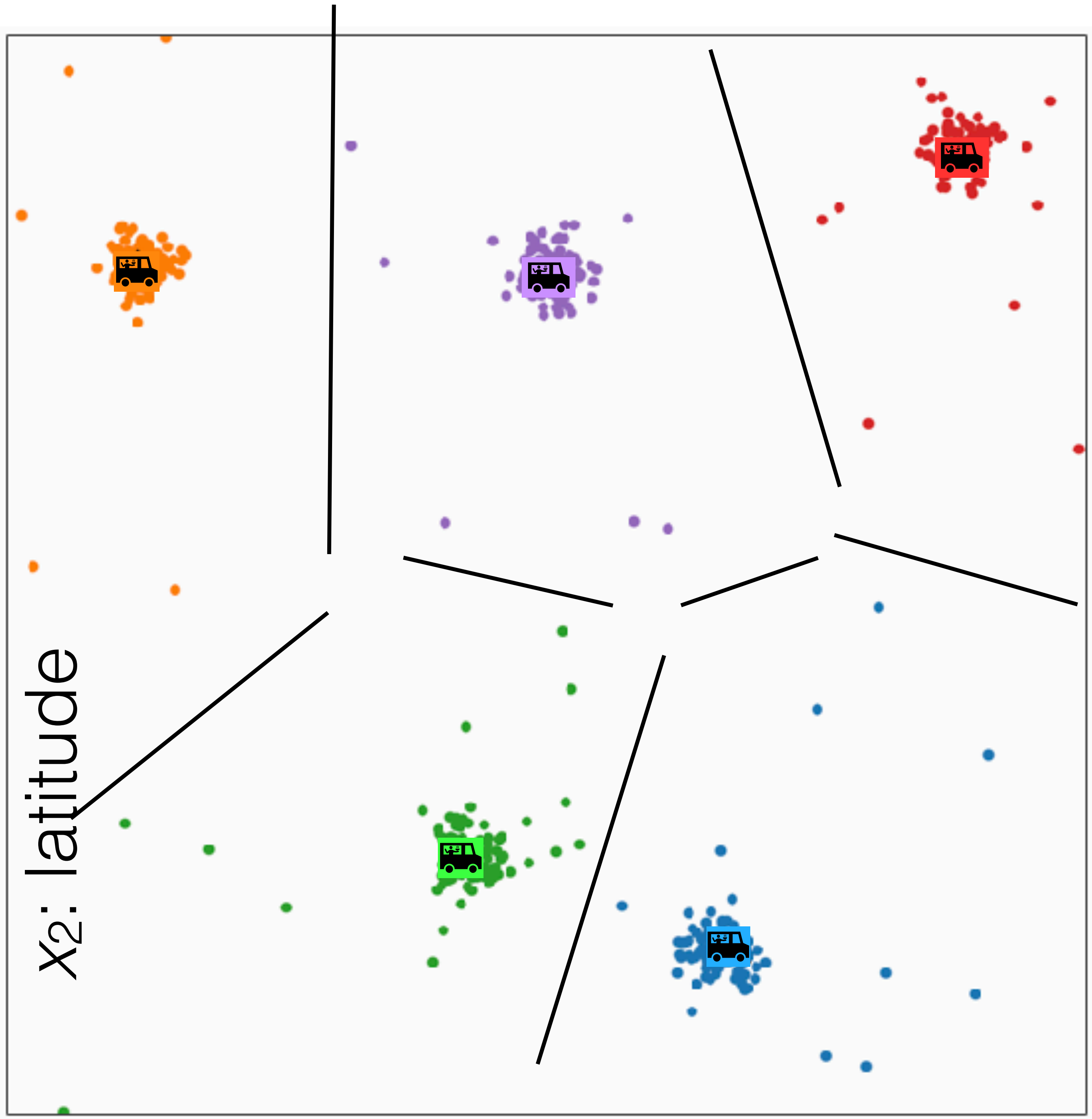


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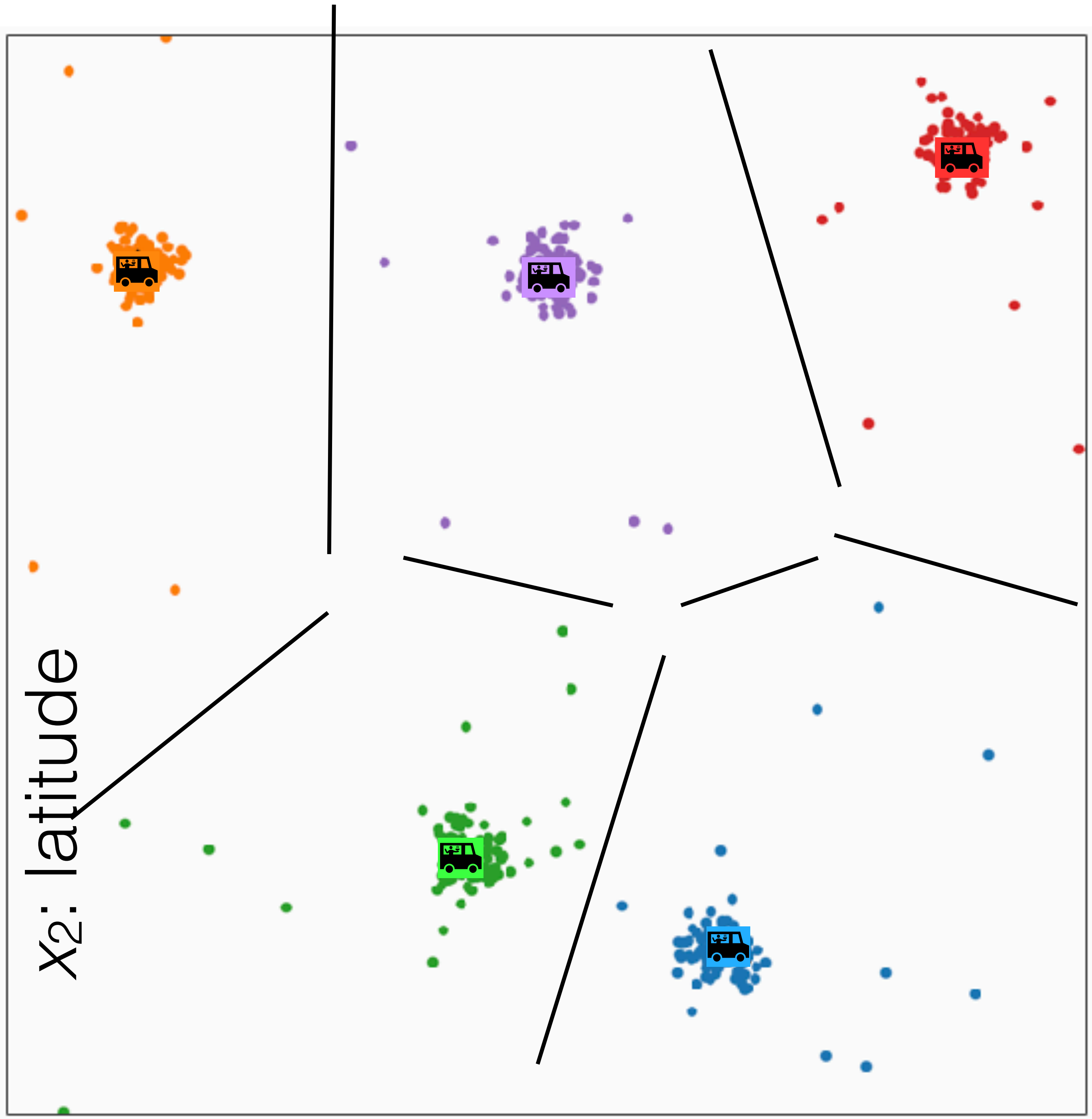

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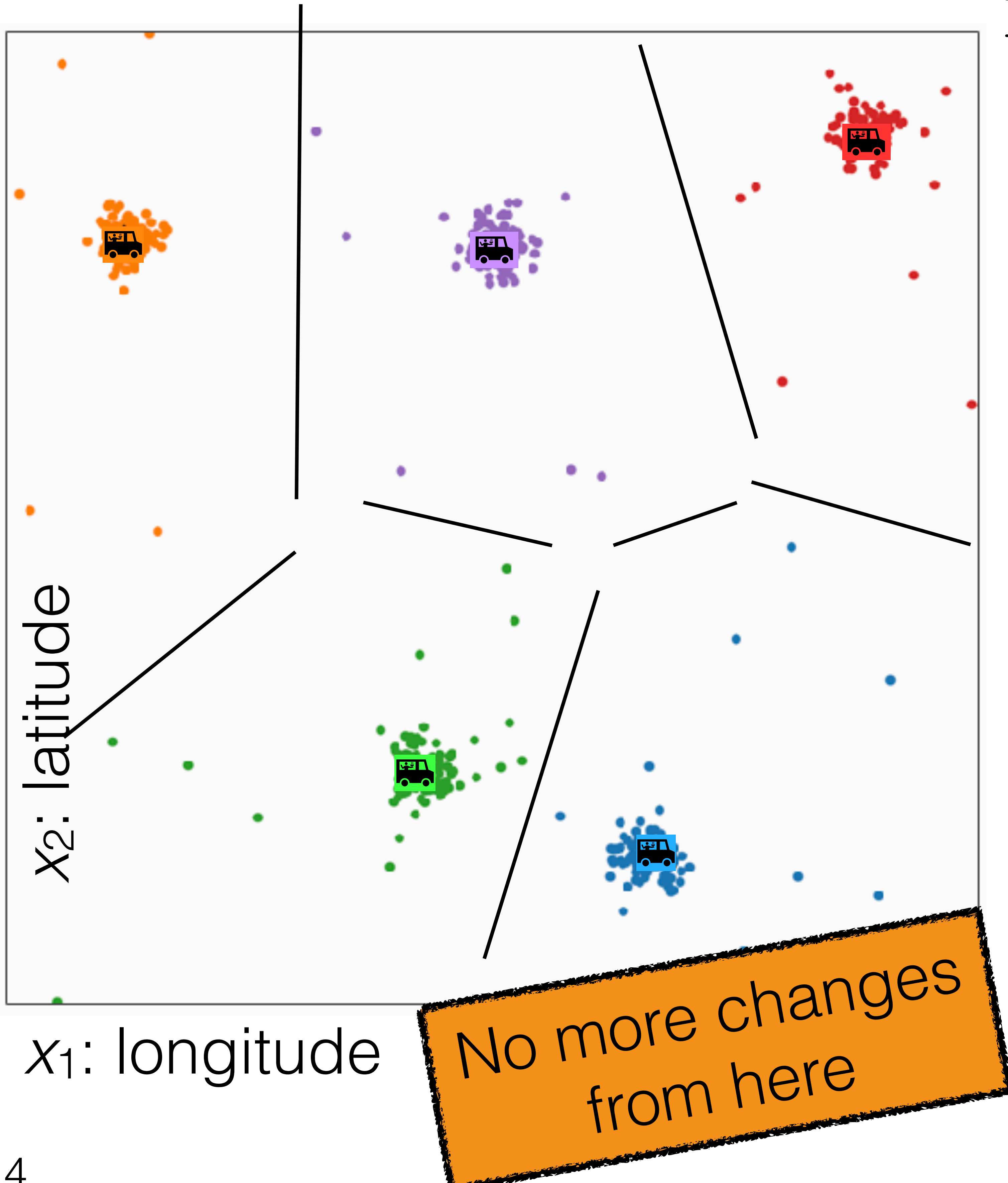


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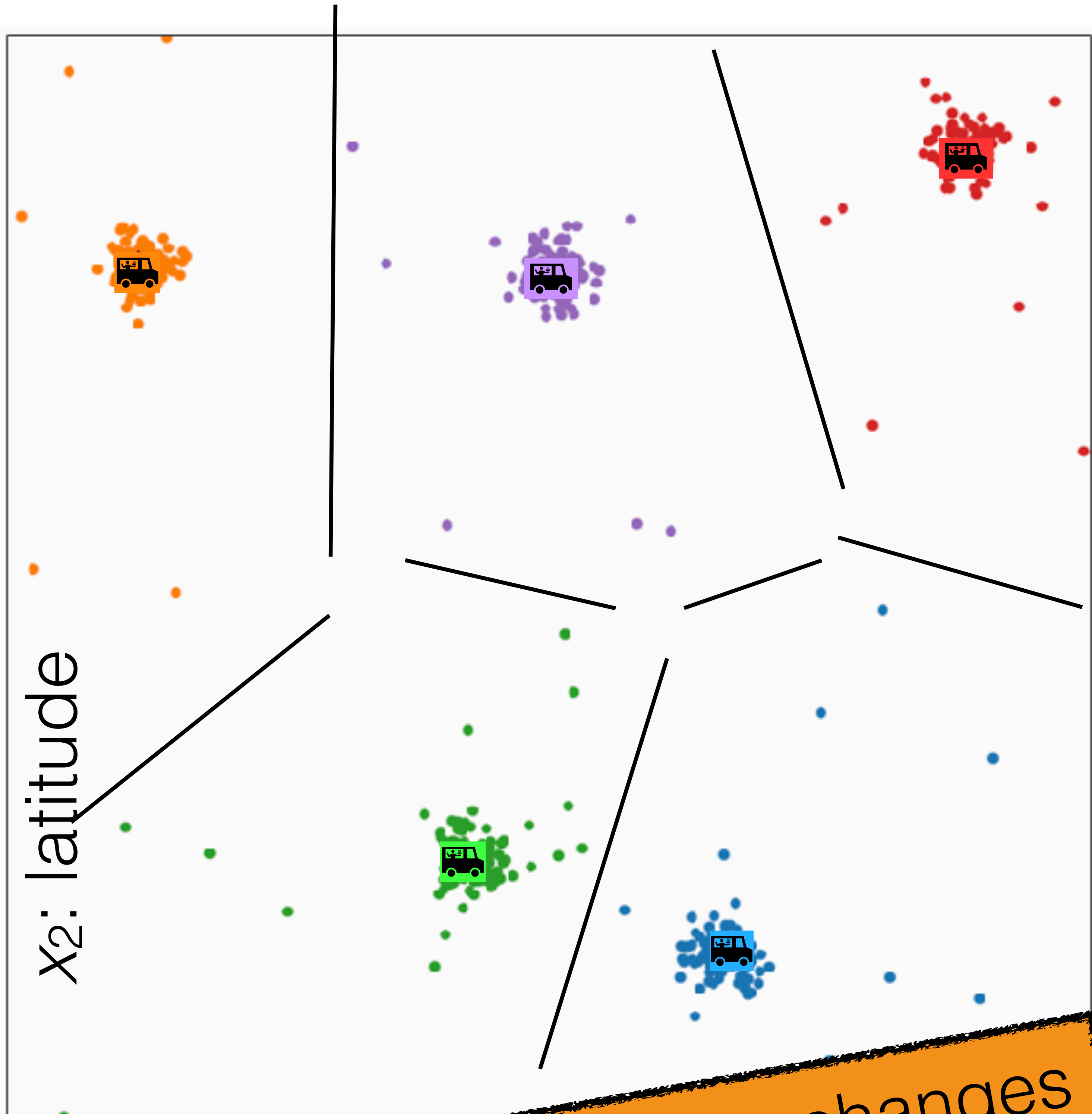


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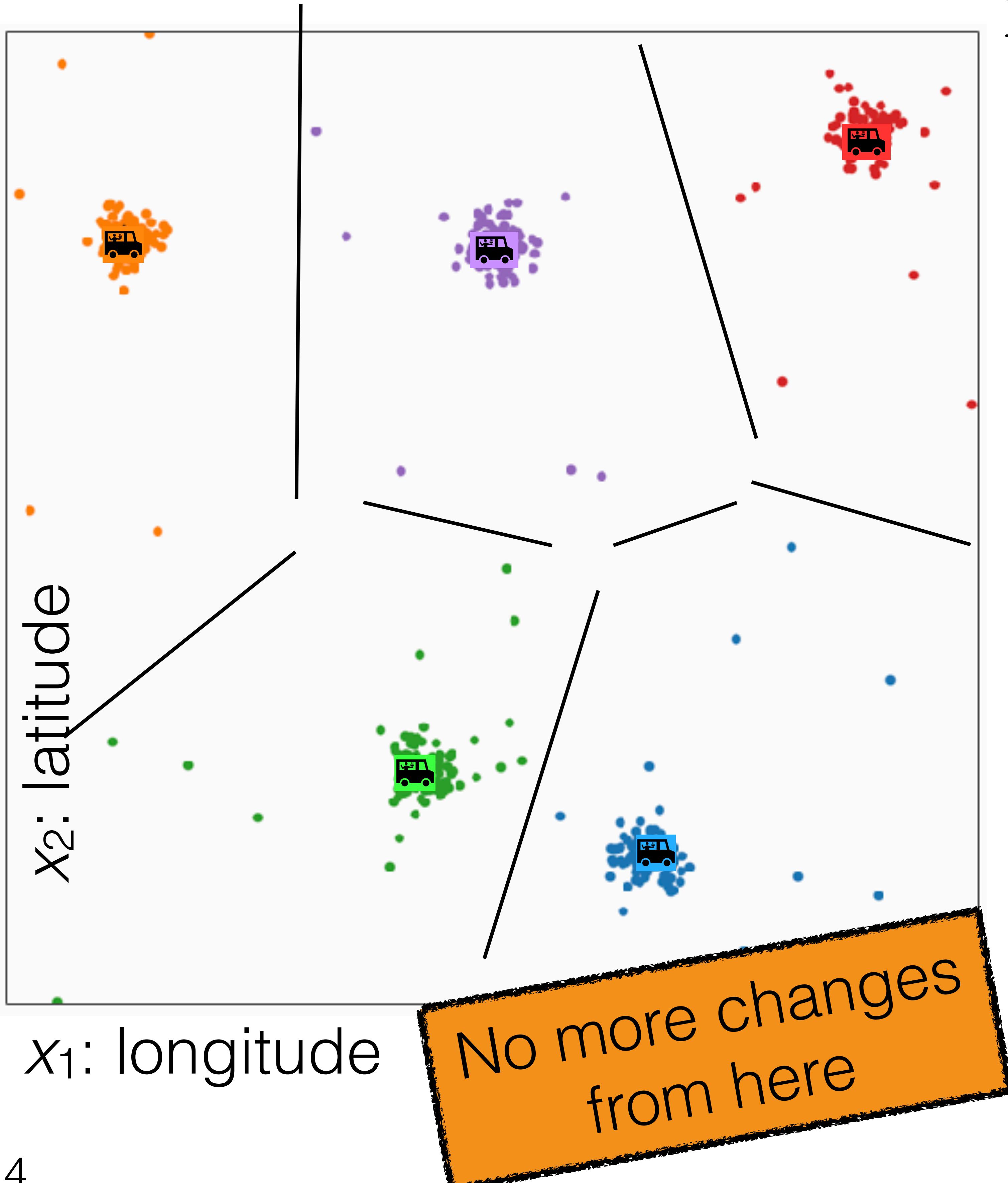
No more changes from here

How can I be so sure?

k-means algorithm

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

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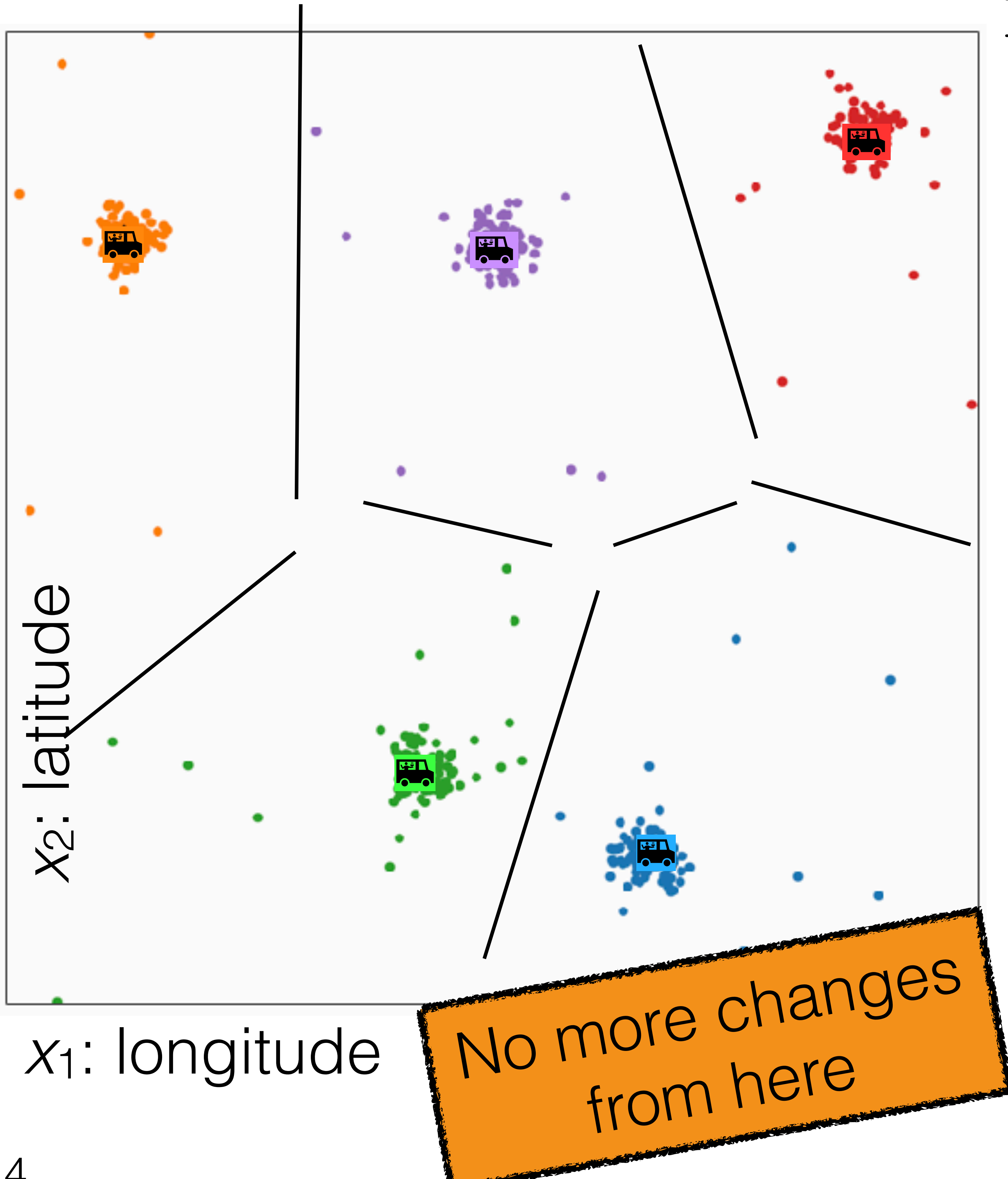
k-means algorithm

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    if y = y_old
      break
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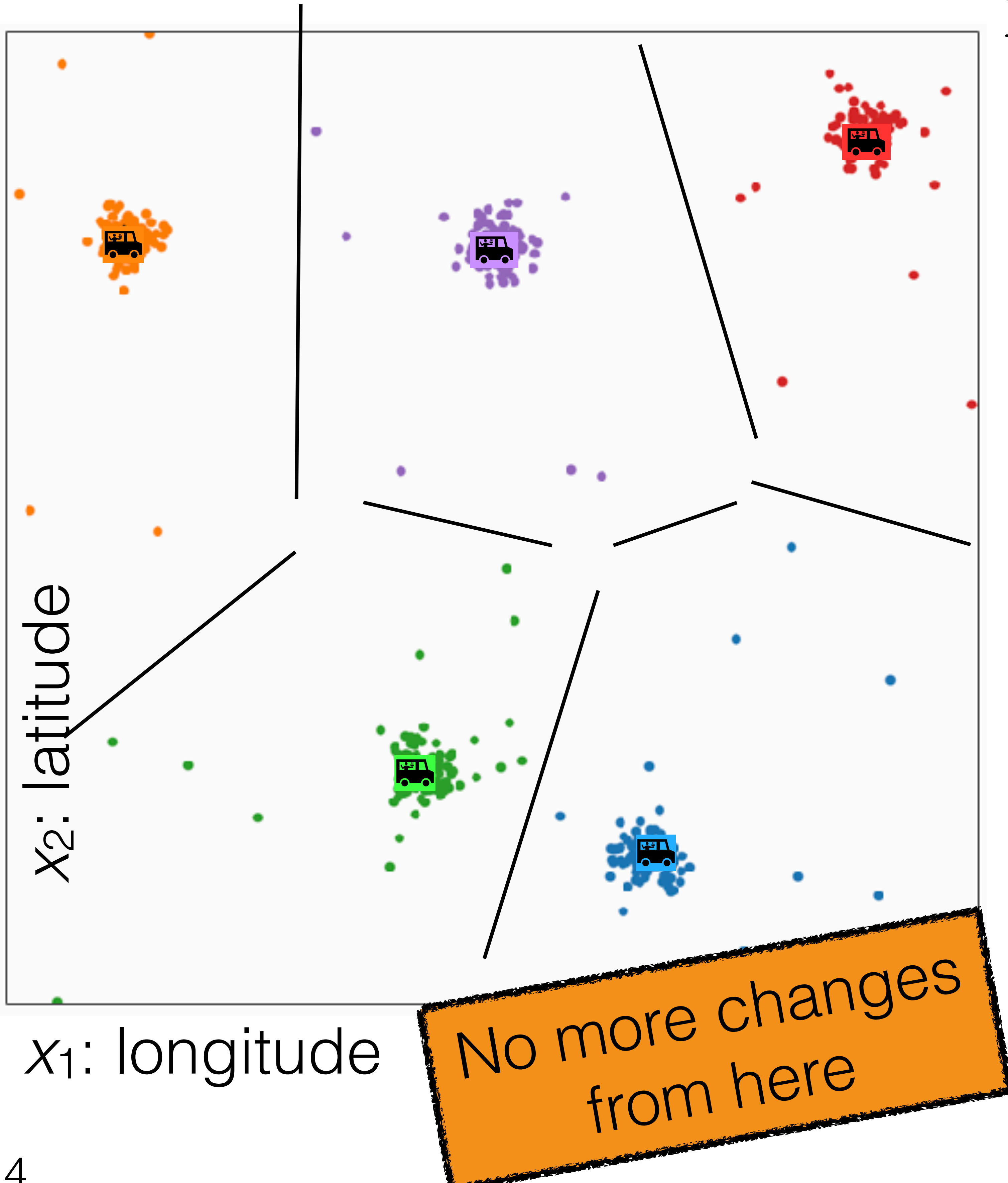
k-means algorithm



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

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

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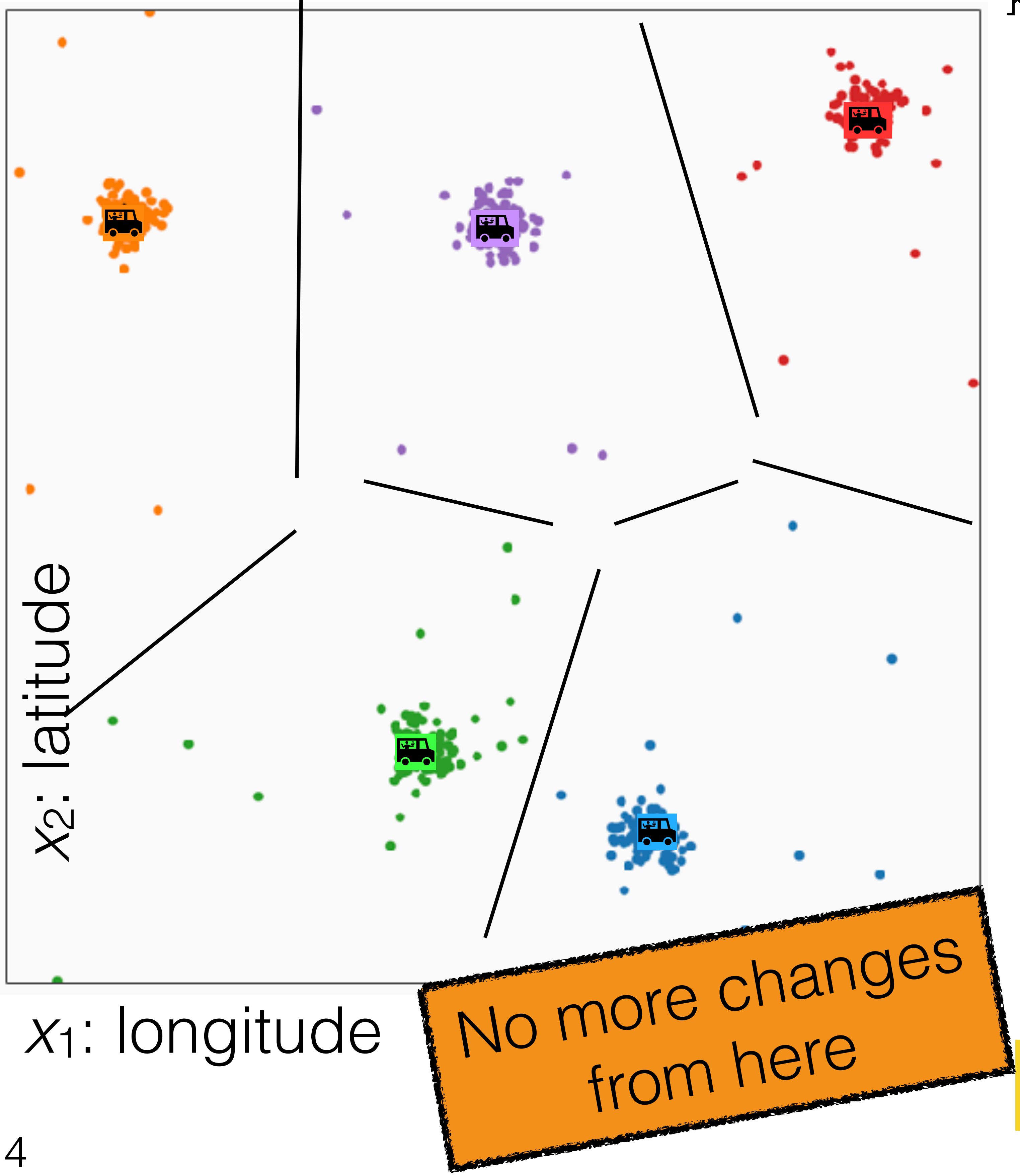
$$\mu^{(j)} = \frac{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = j\}}$$

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

break

k-means algorithm

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    for j = 1 to k
      μ^(j) = Σ_{i=1}^n 1{y^(i) = j} x^(i) / Σ_{i=1}^n 1{y^(i) = j}
    if y = y_old
      break
  return {μ^(j)}_{j=1}^k, {y^(i)}_{i=1}^n
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$$y^{(i)} = \arg\min_j \|x^{(i)} - \mu^{(j)}\|_2^2$$

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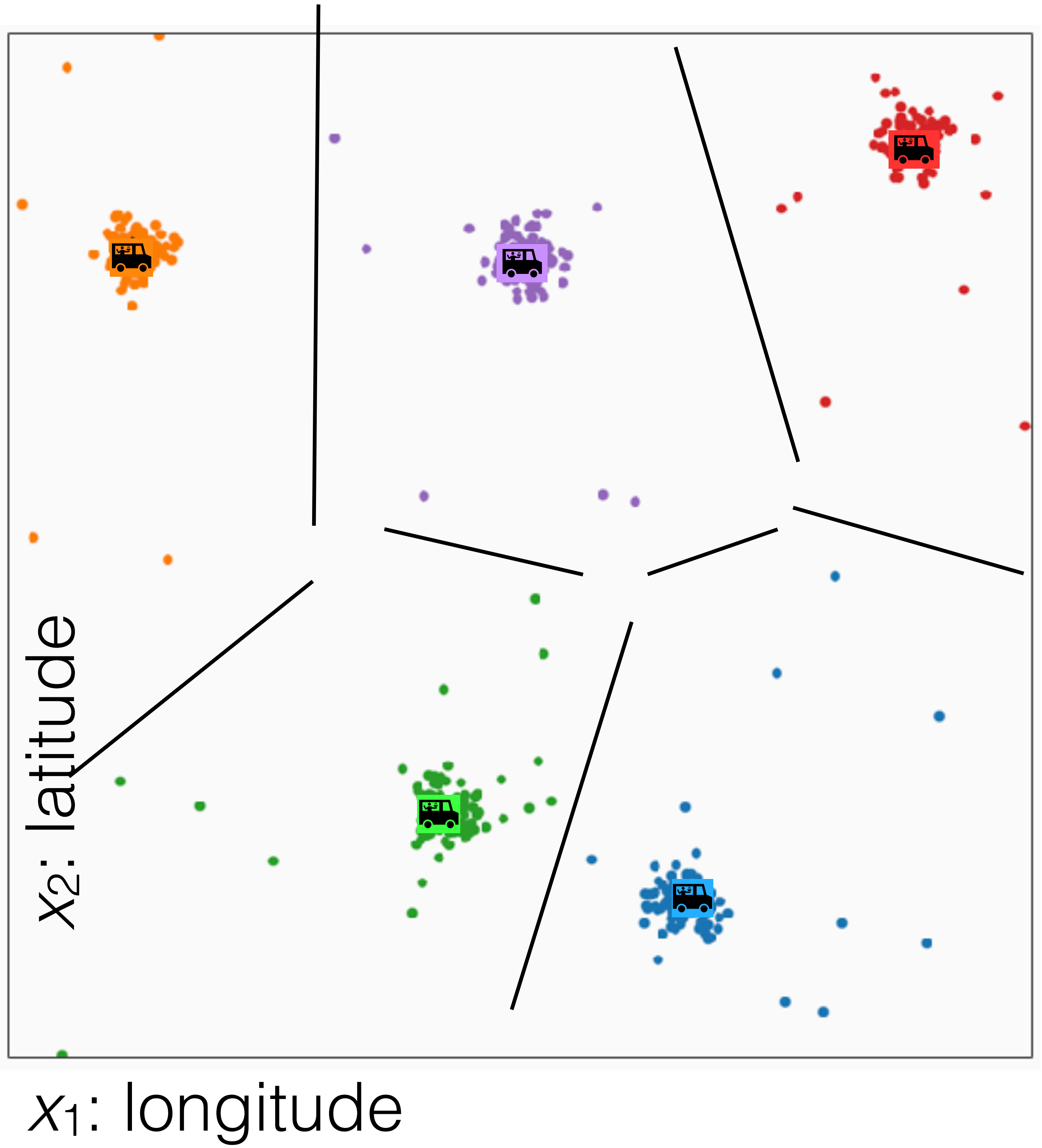
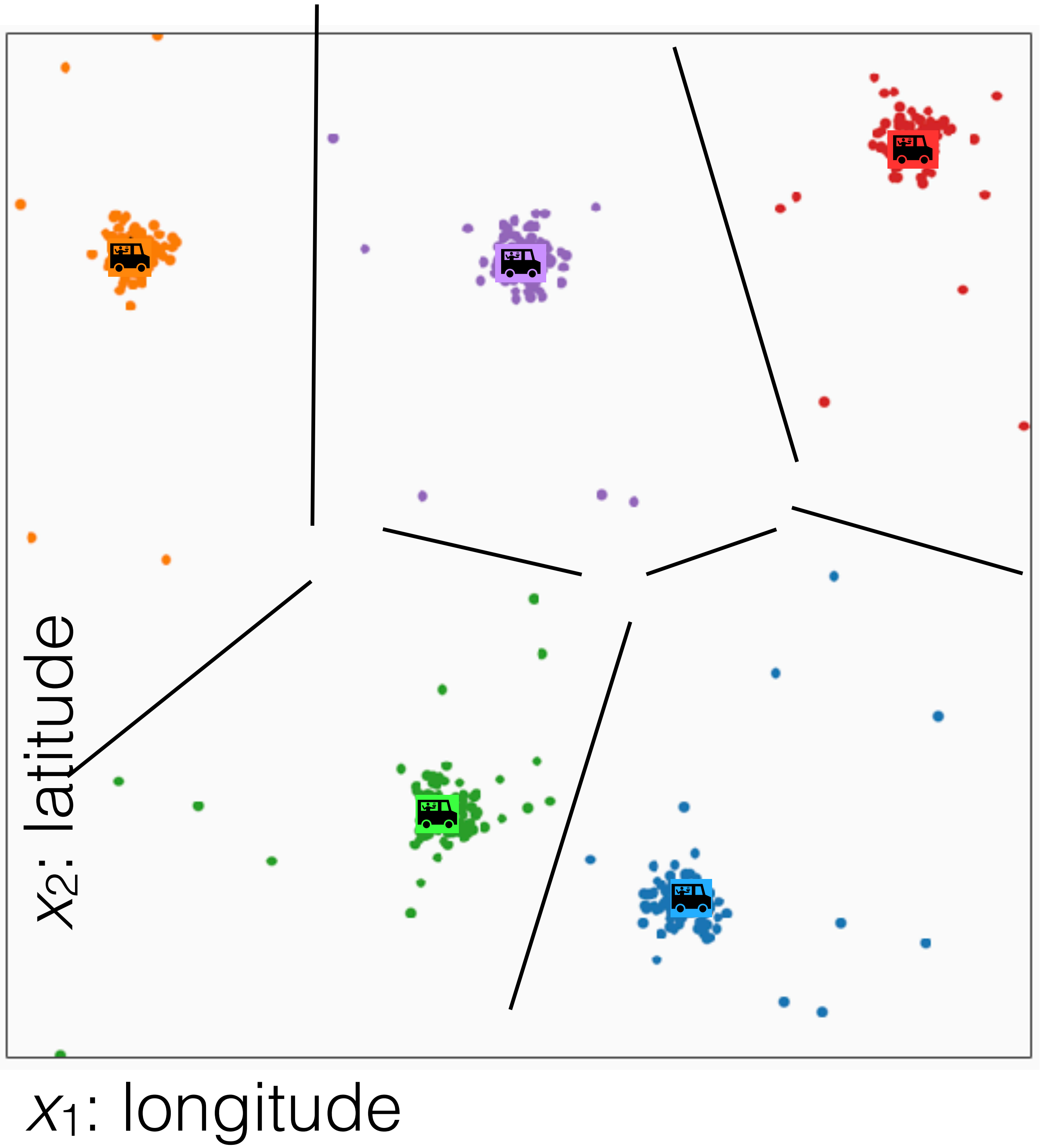
Compare to classification



Compare to classification



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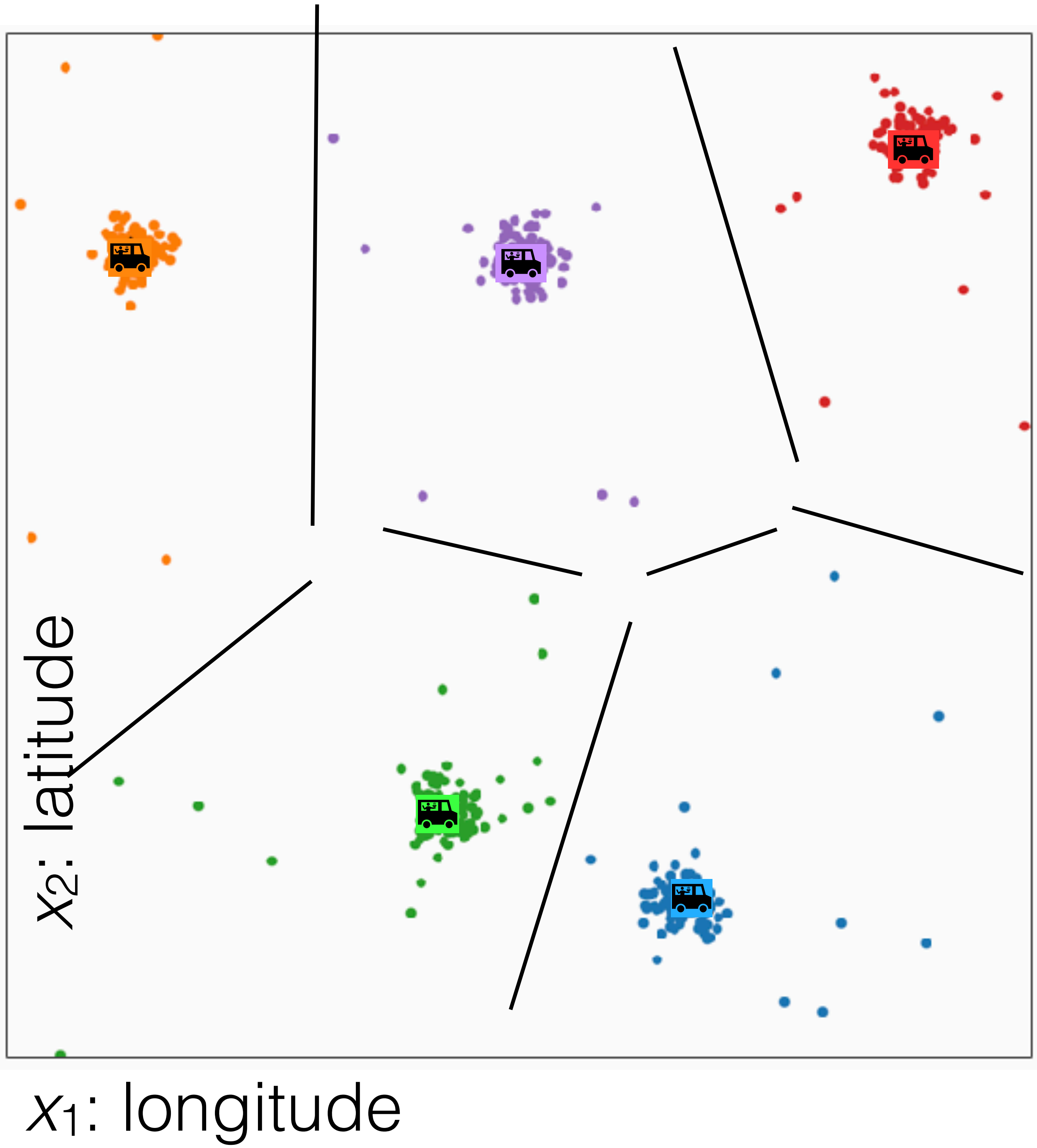

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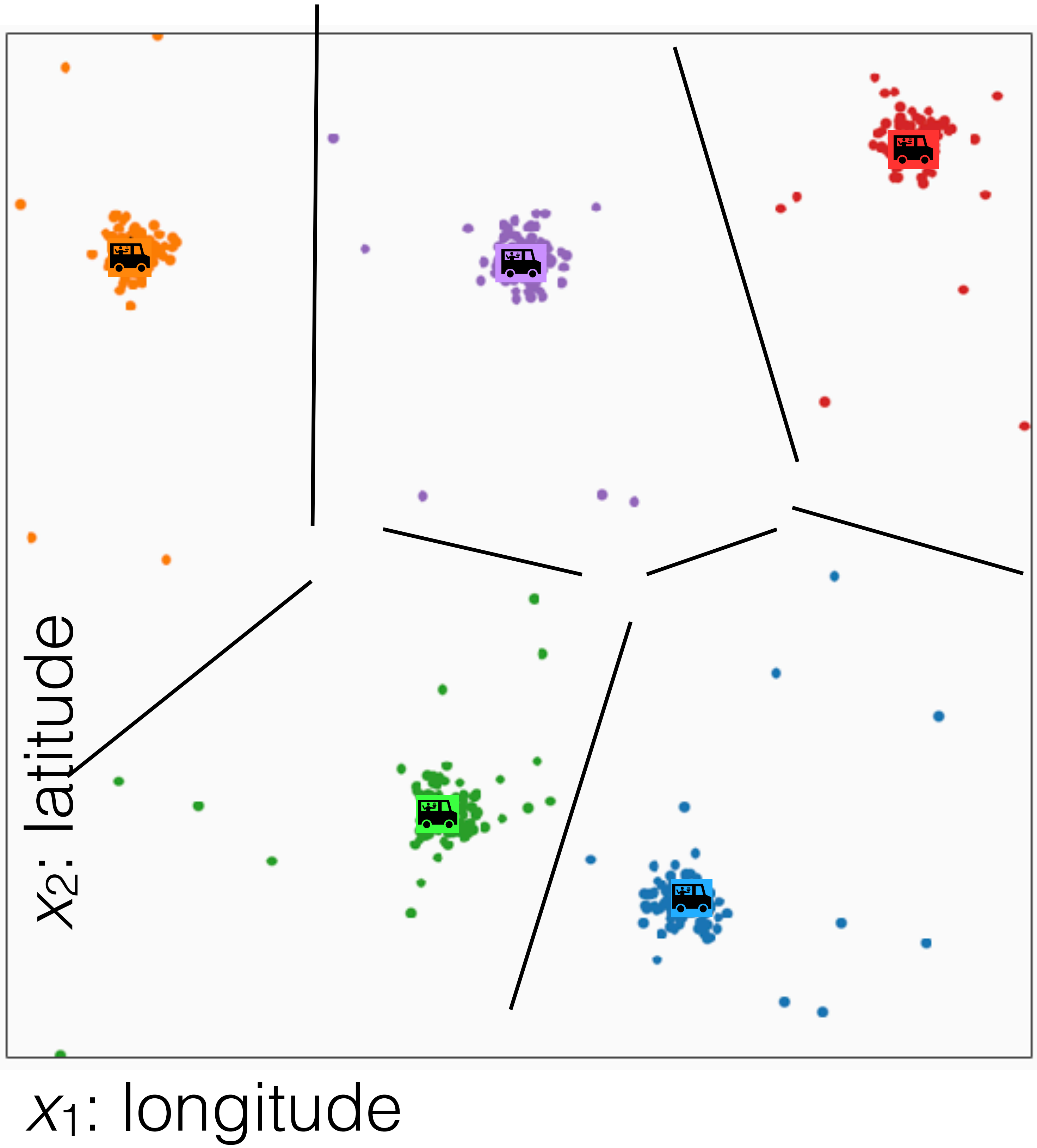

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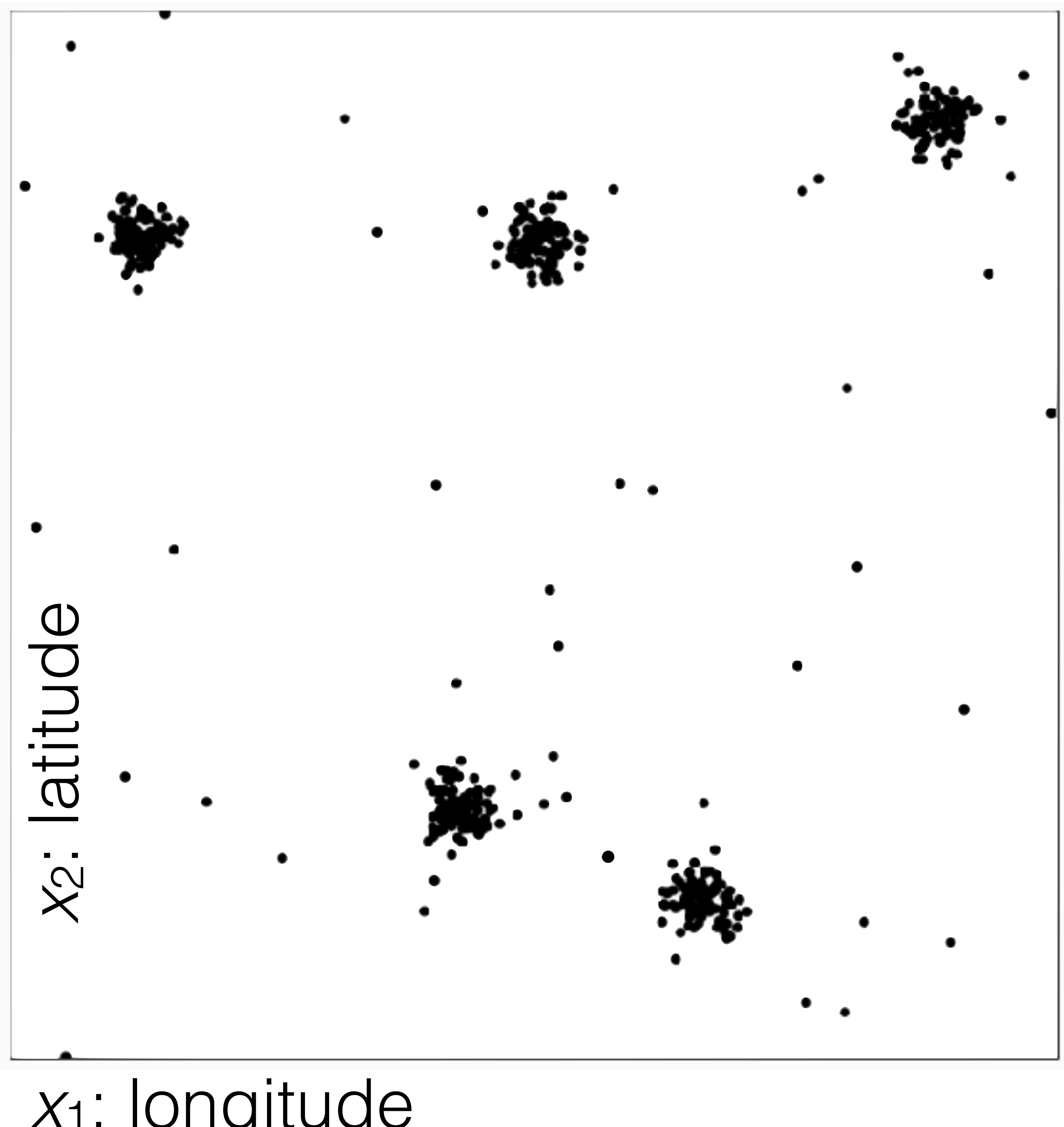

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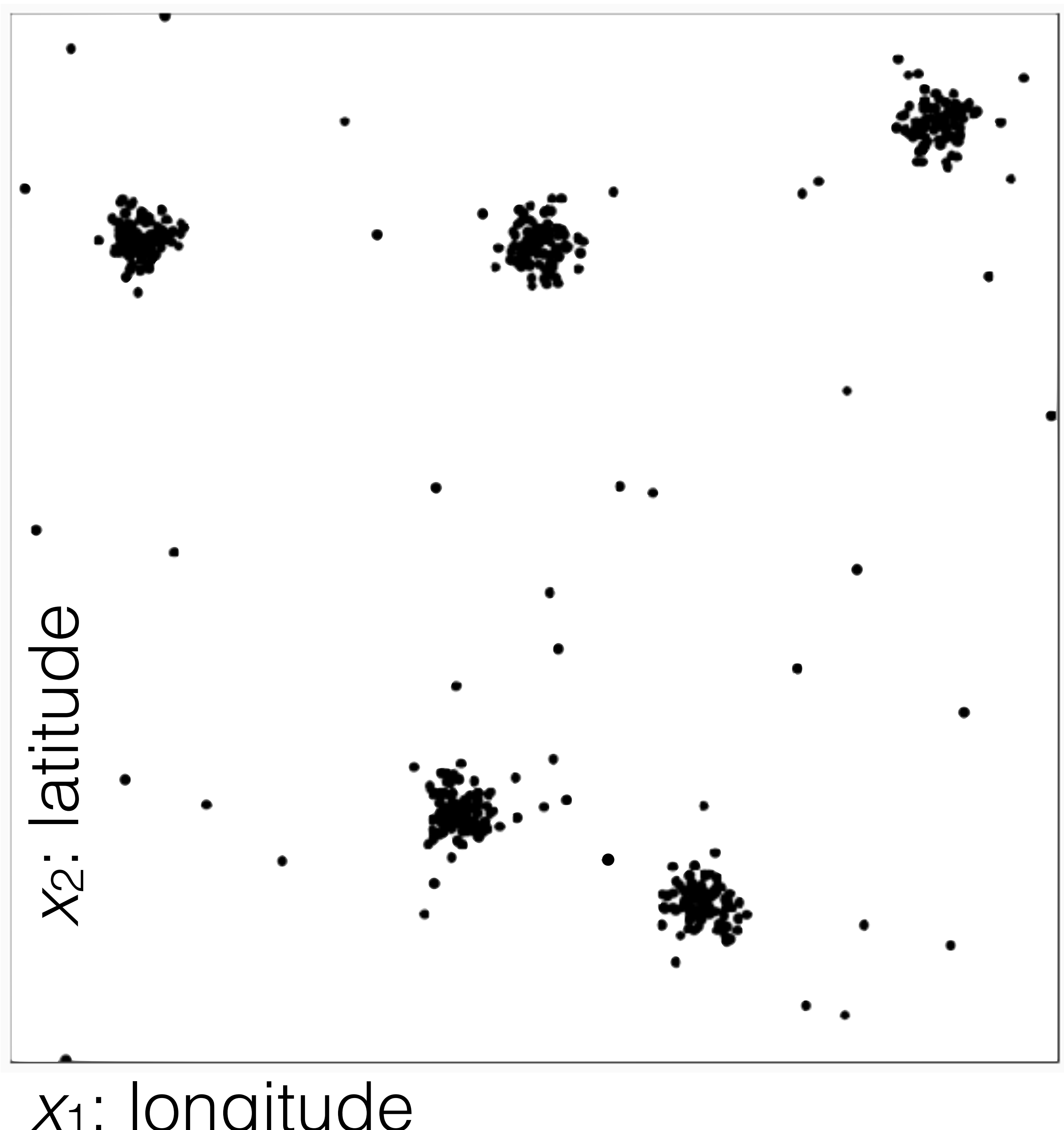

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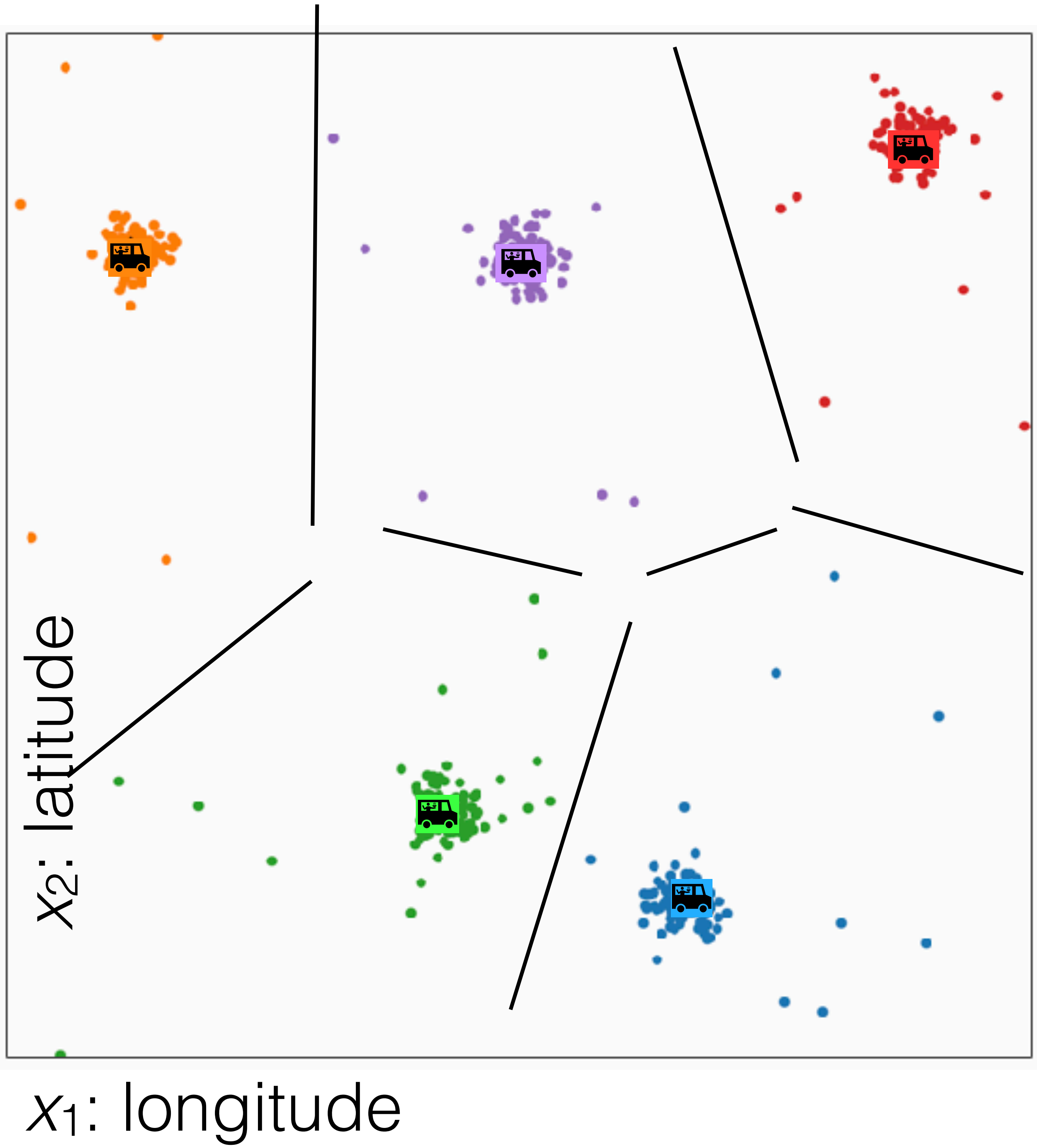

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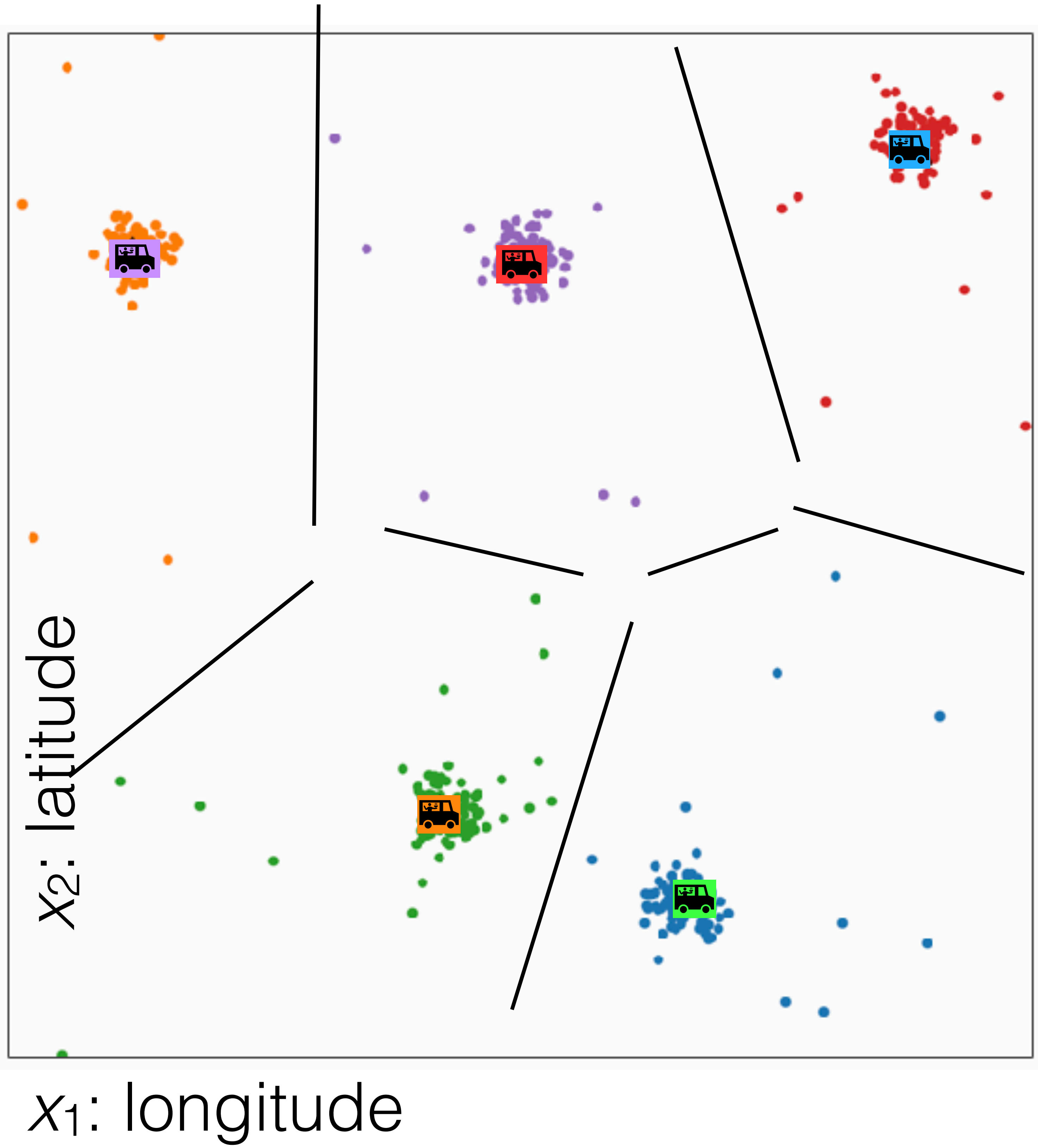

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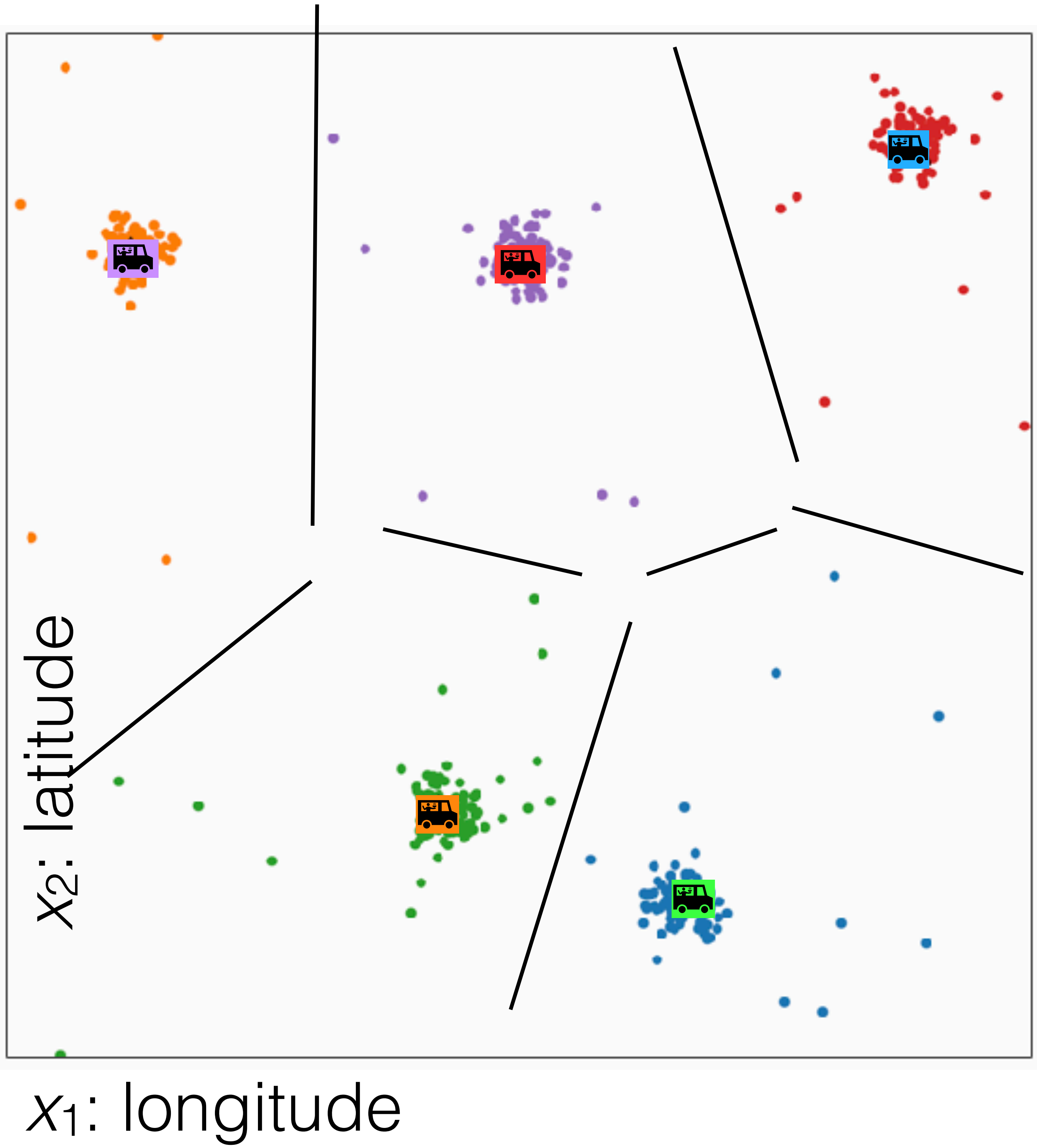

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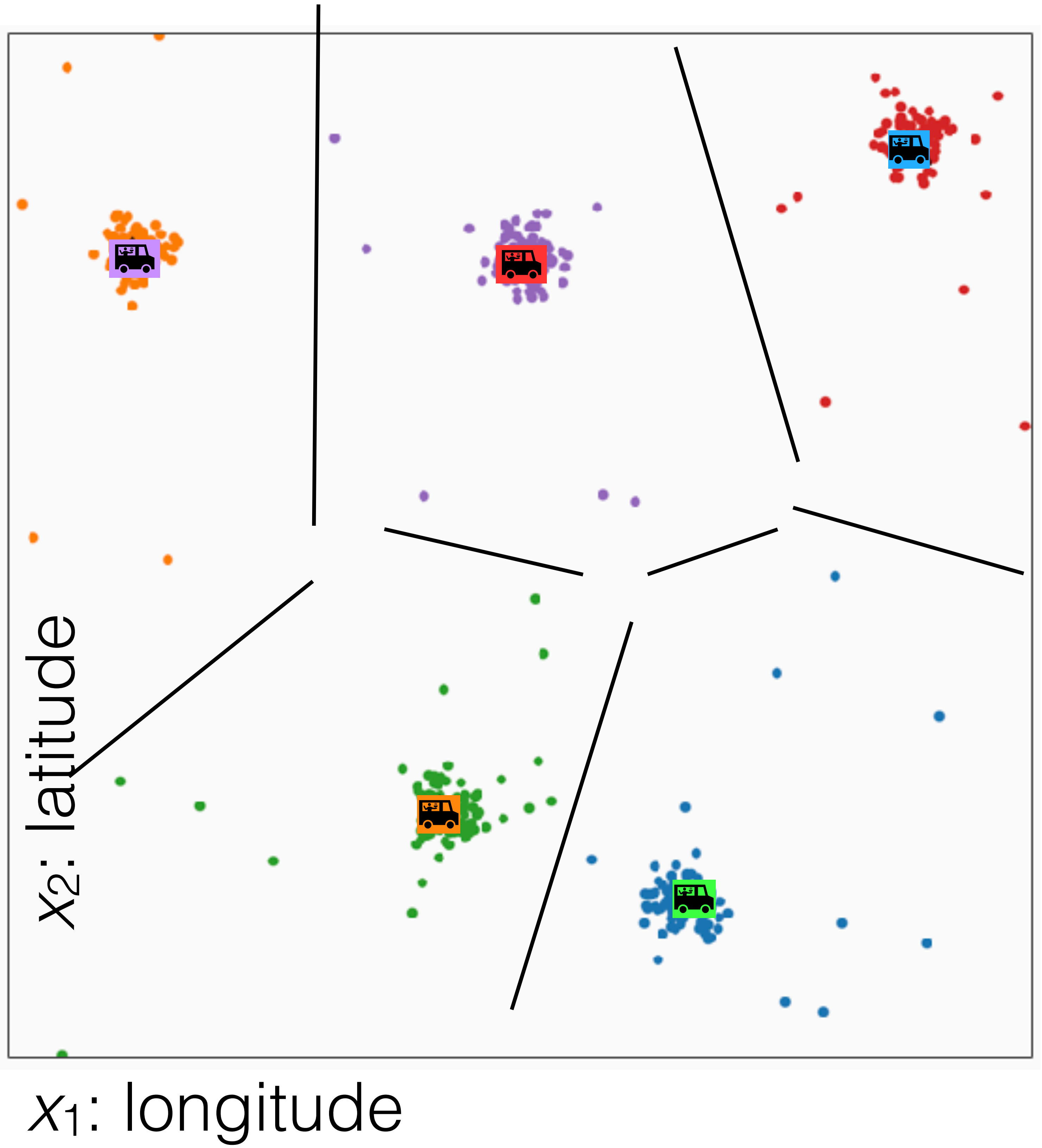
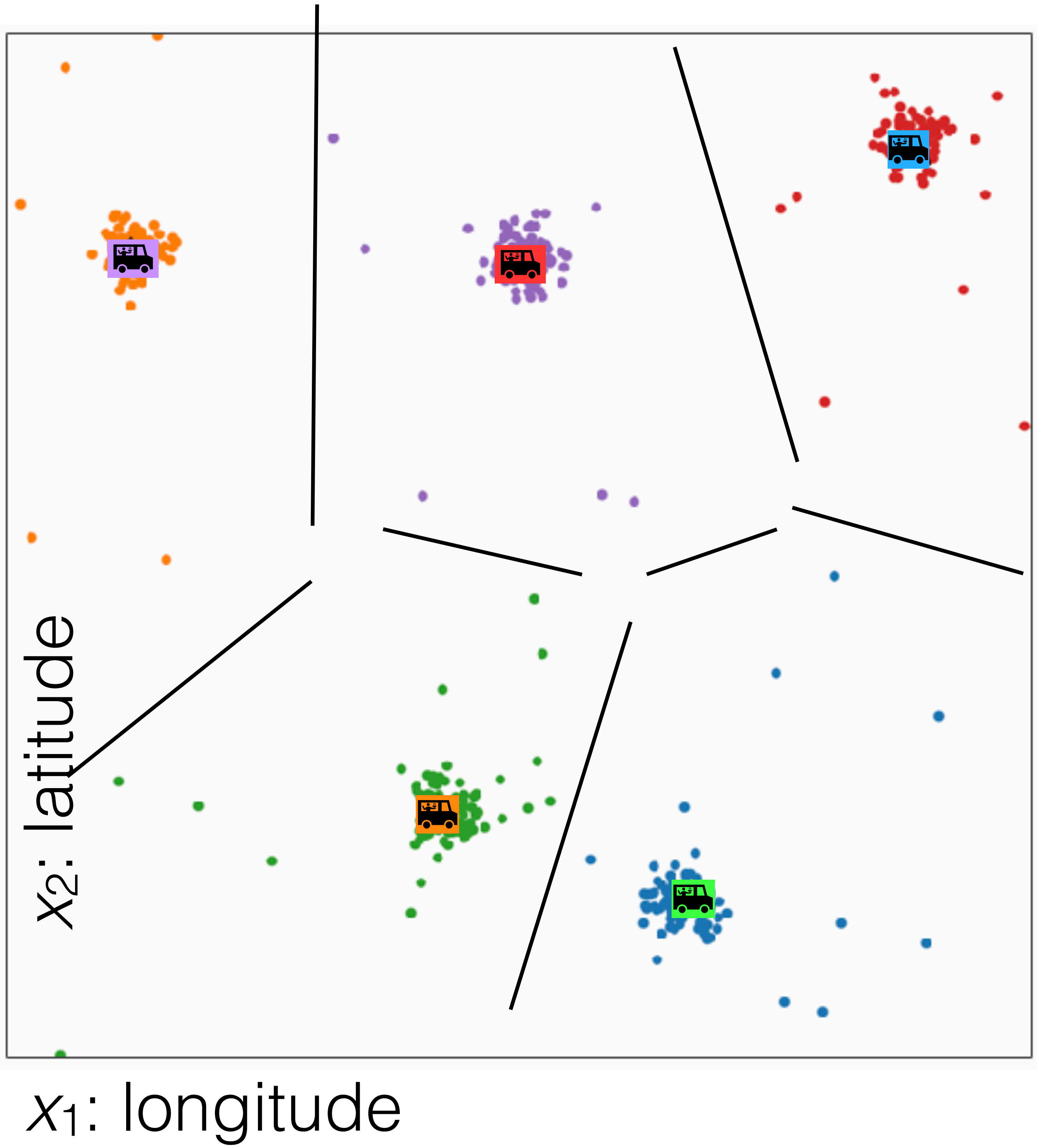
- Output is really a *partition* of the data



x_2: latitude
x_1: longitude



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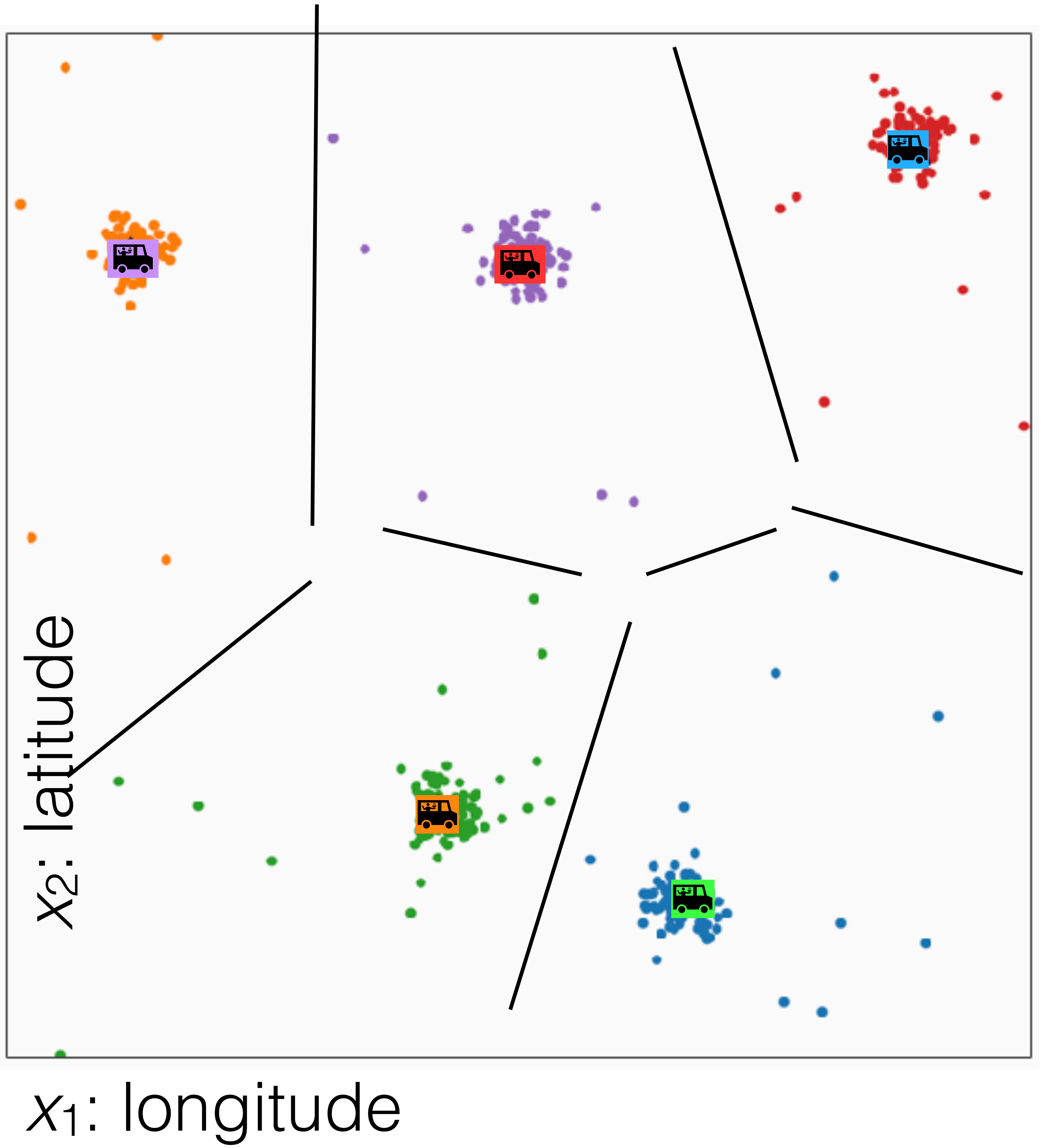

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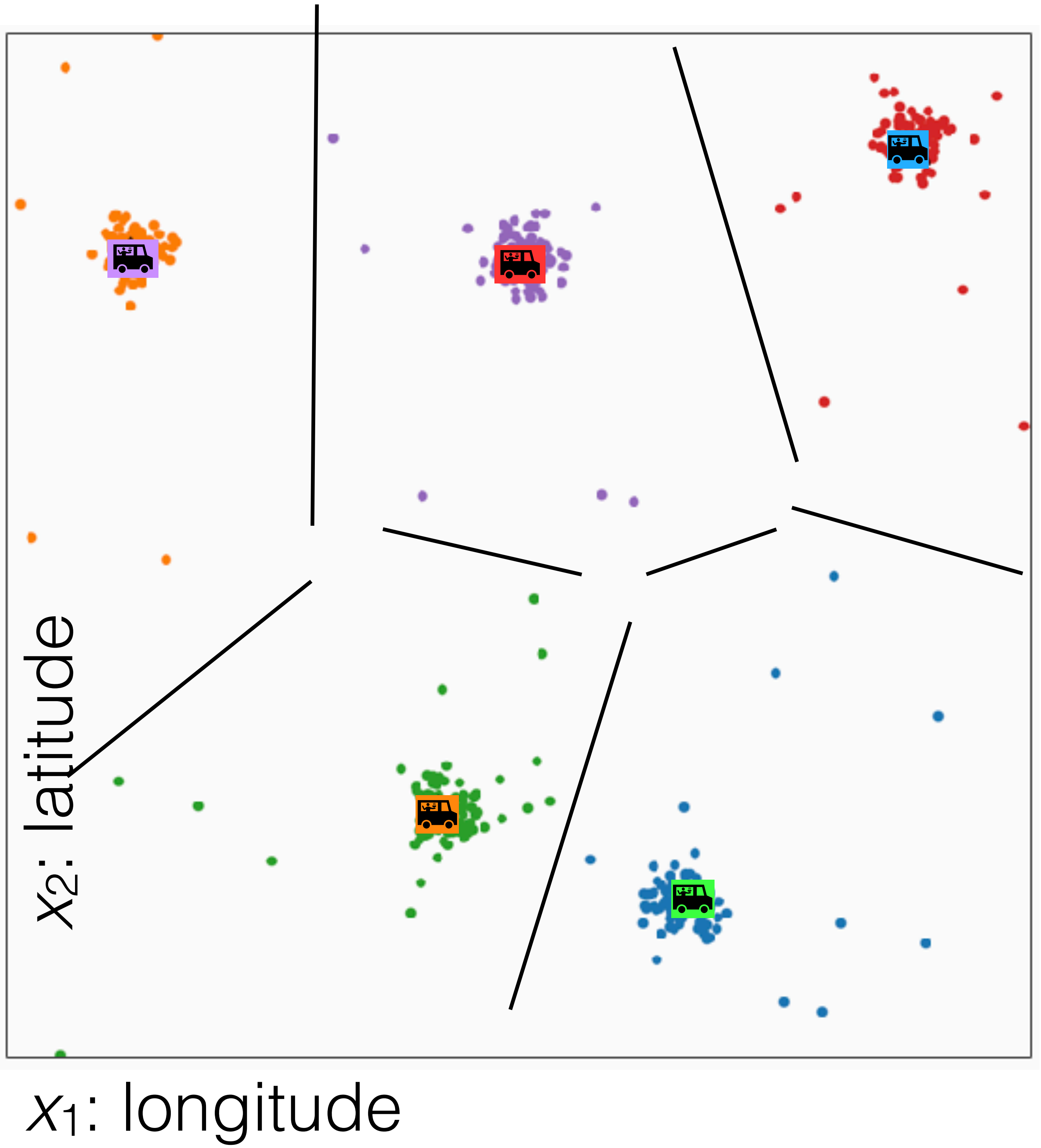

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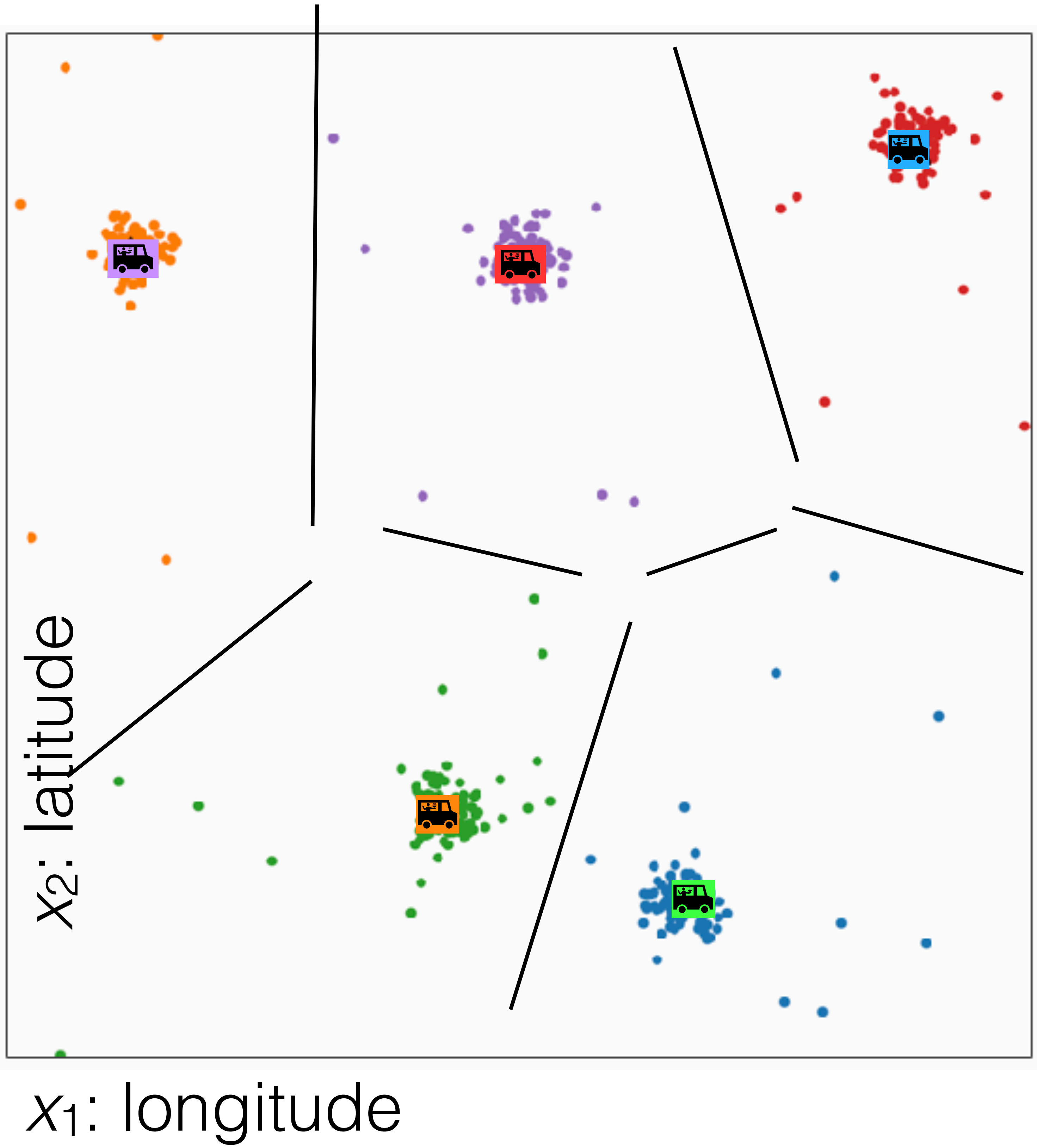

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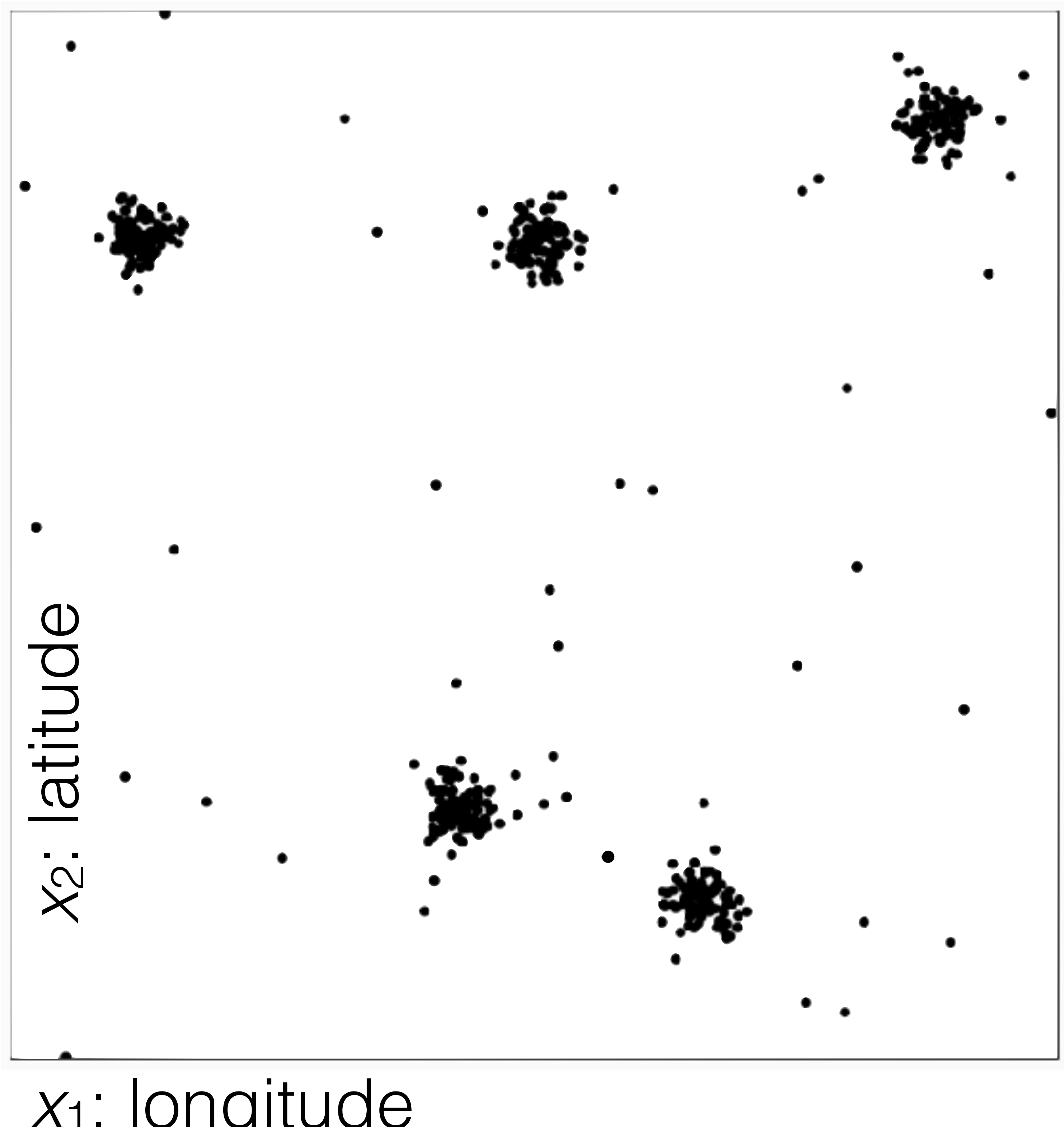

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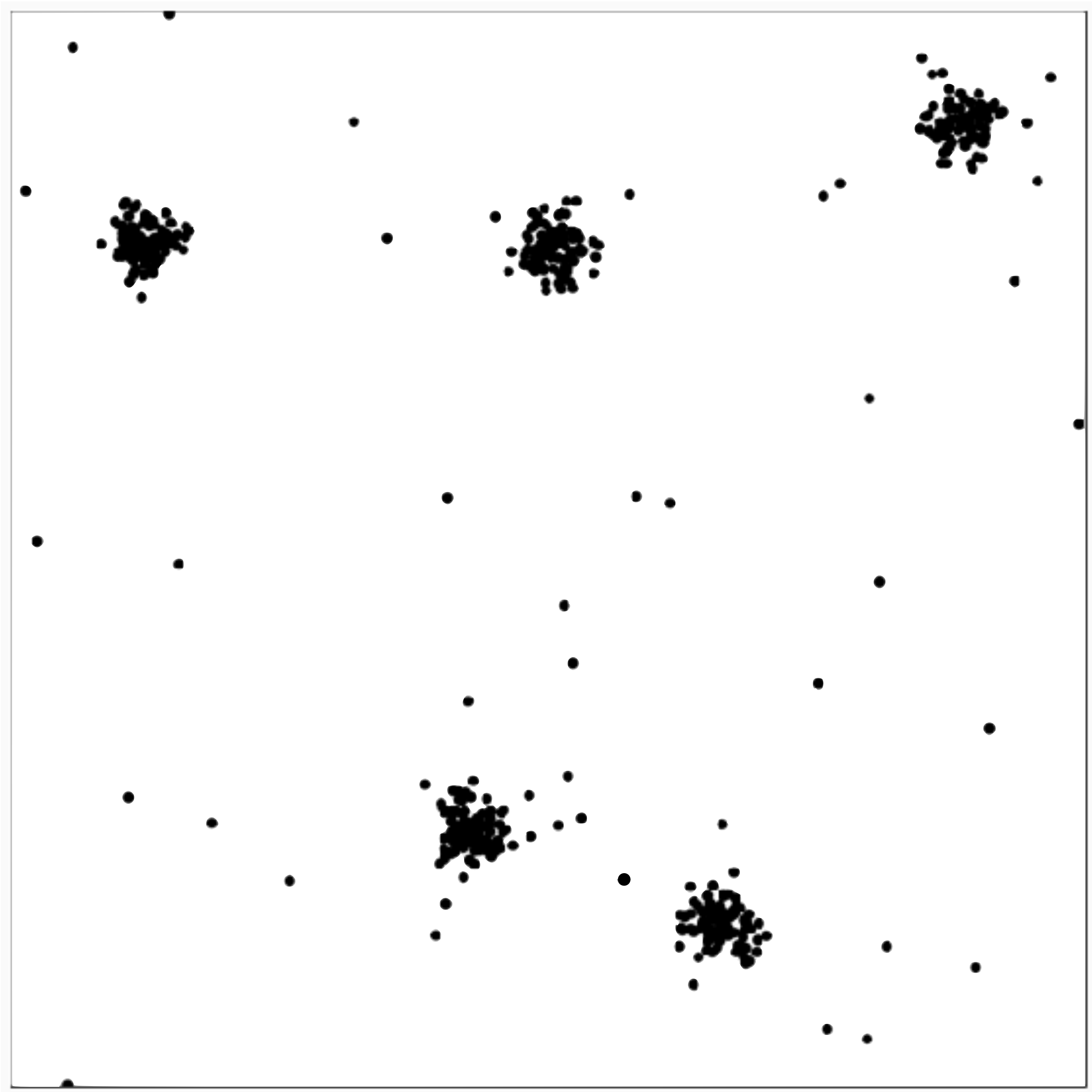

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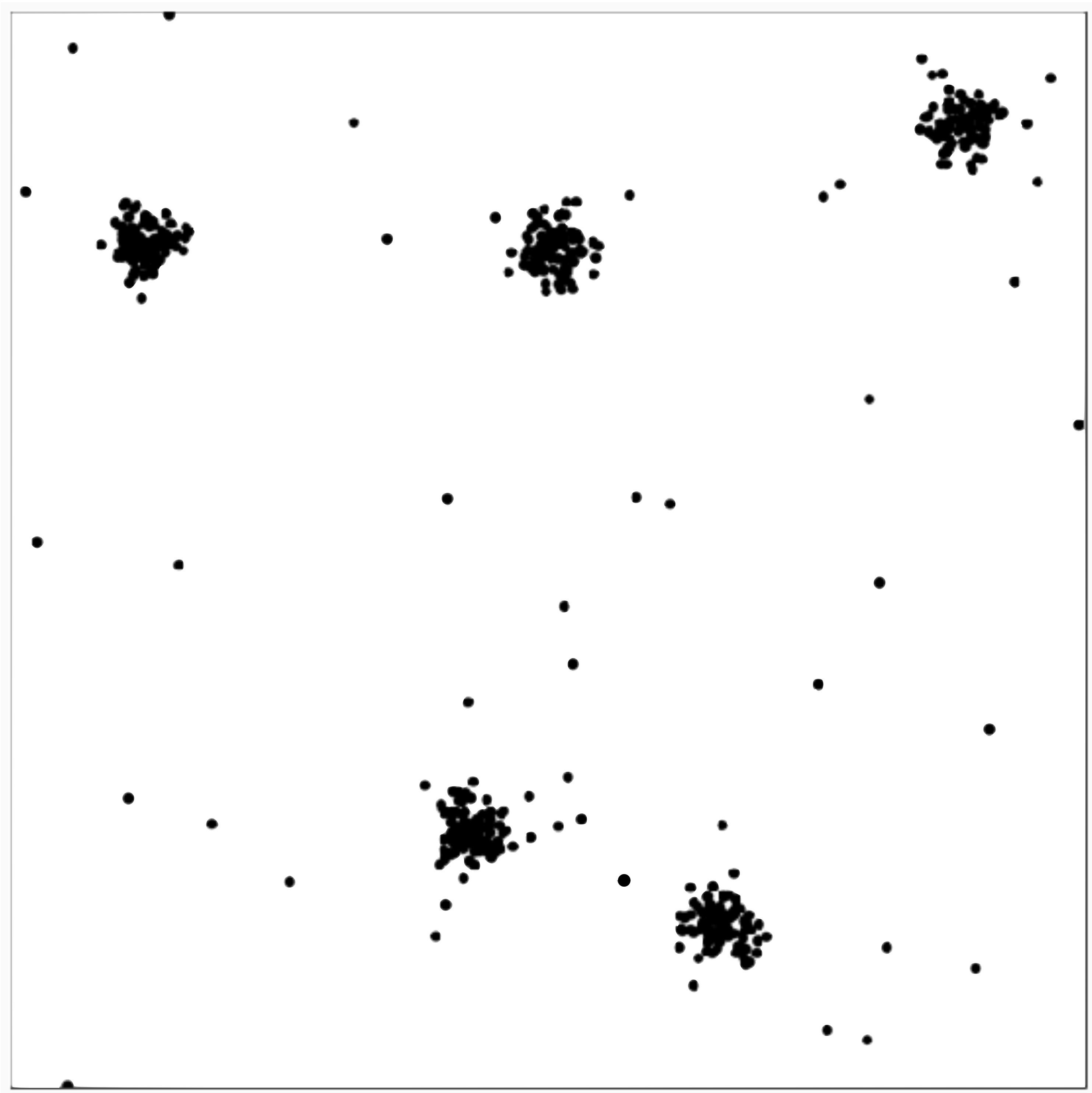

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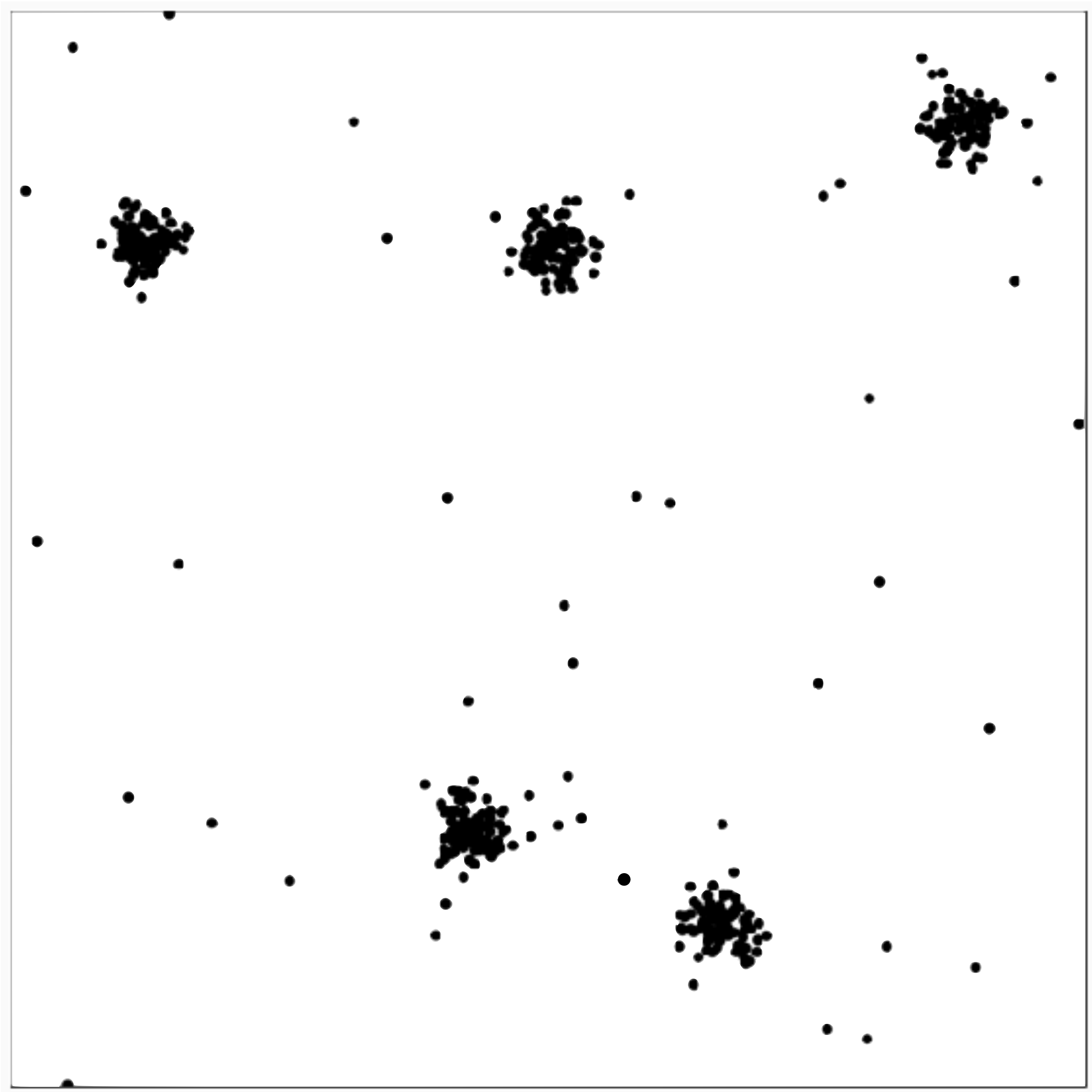

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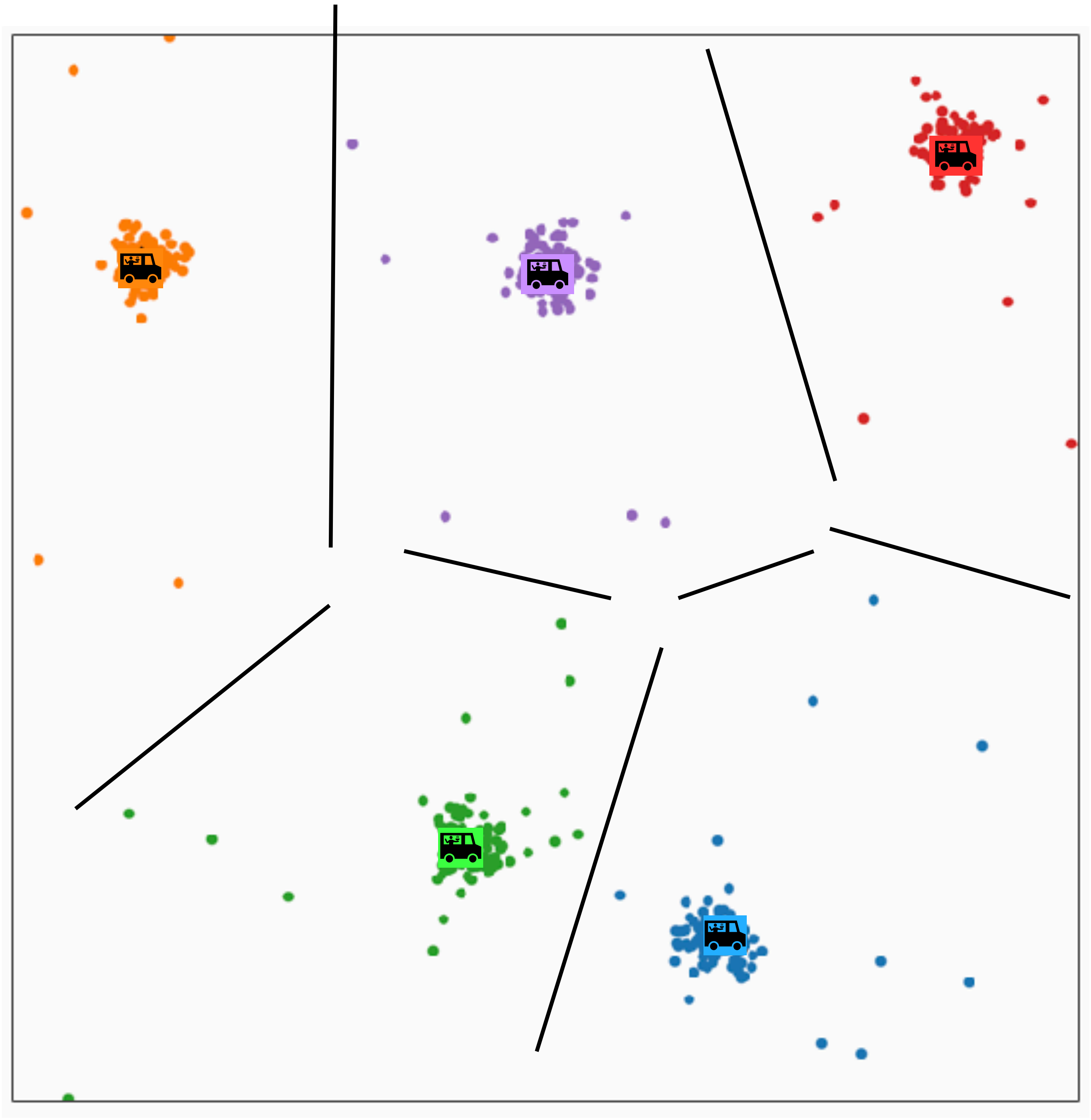

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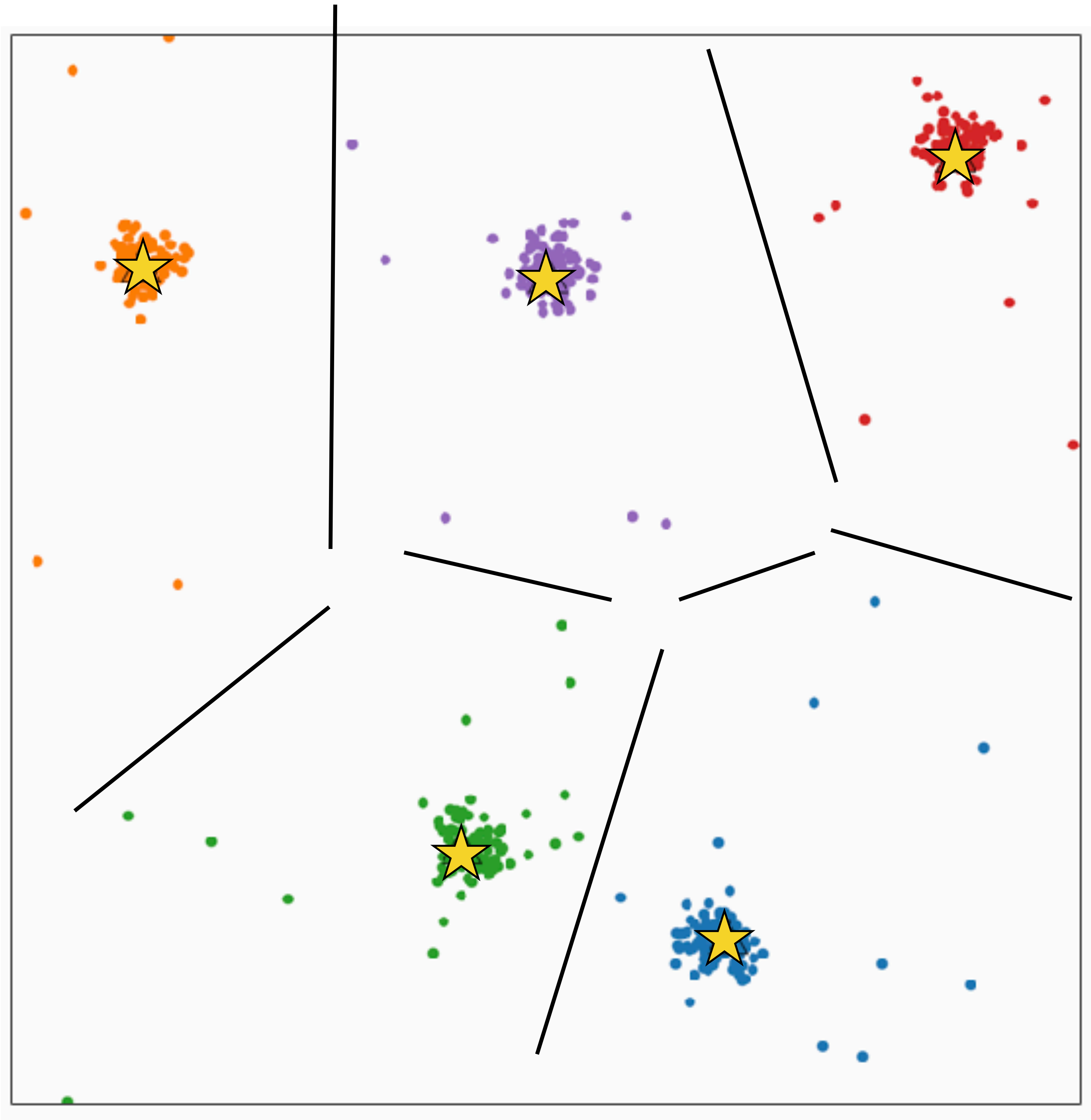

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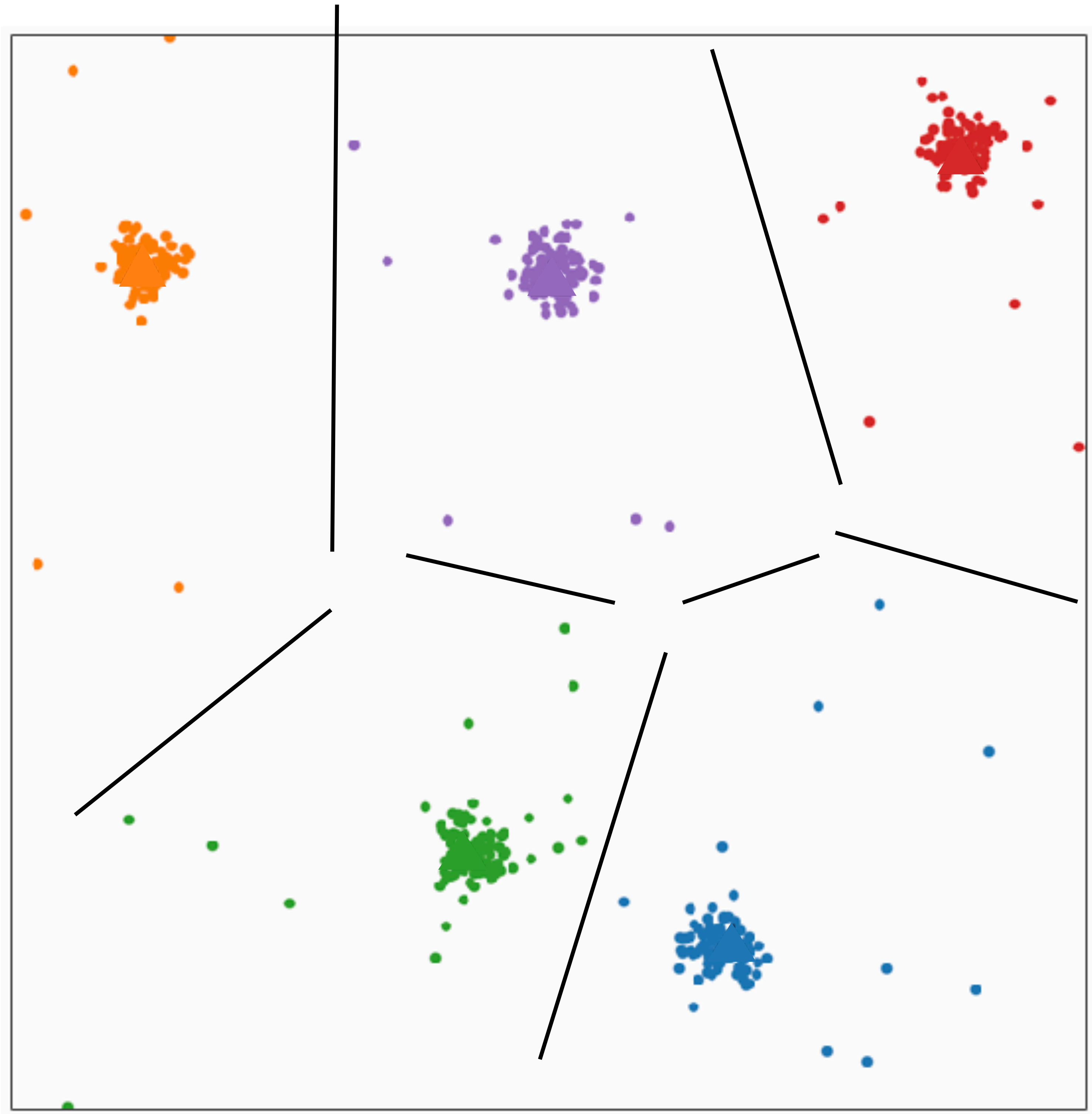

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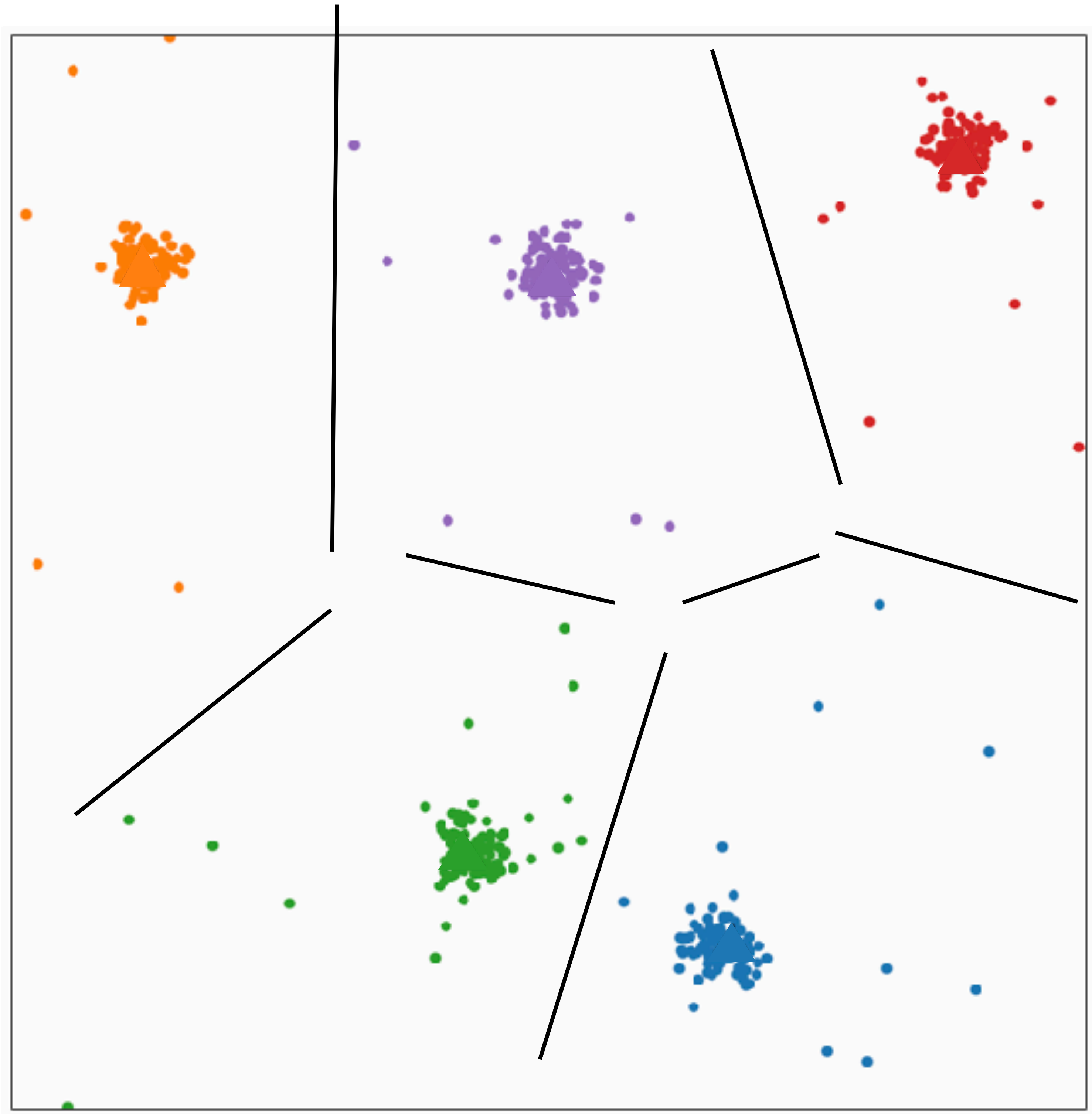

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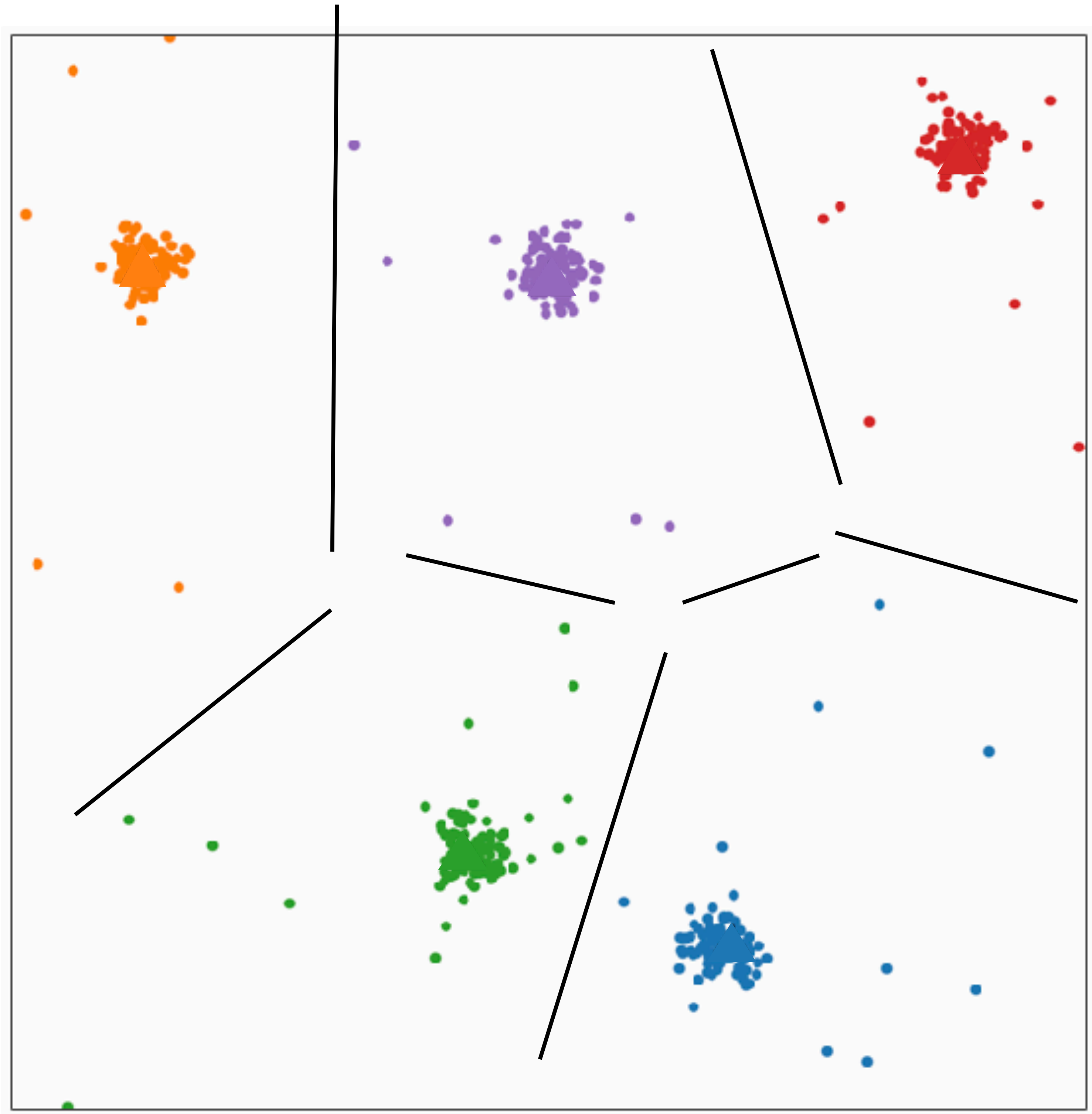

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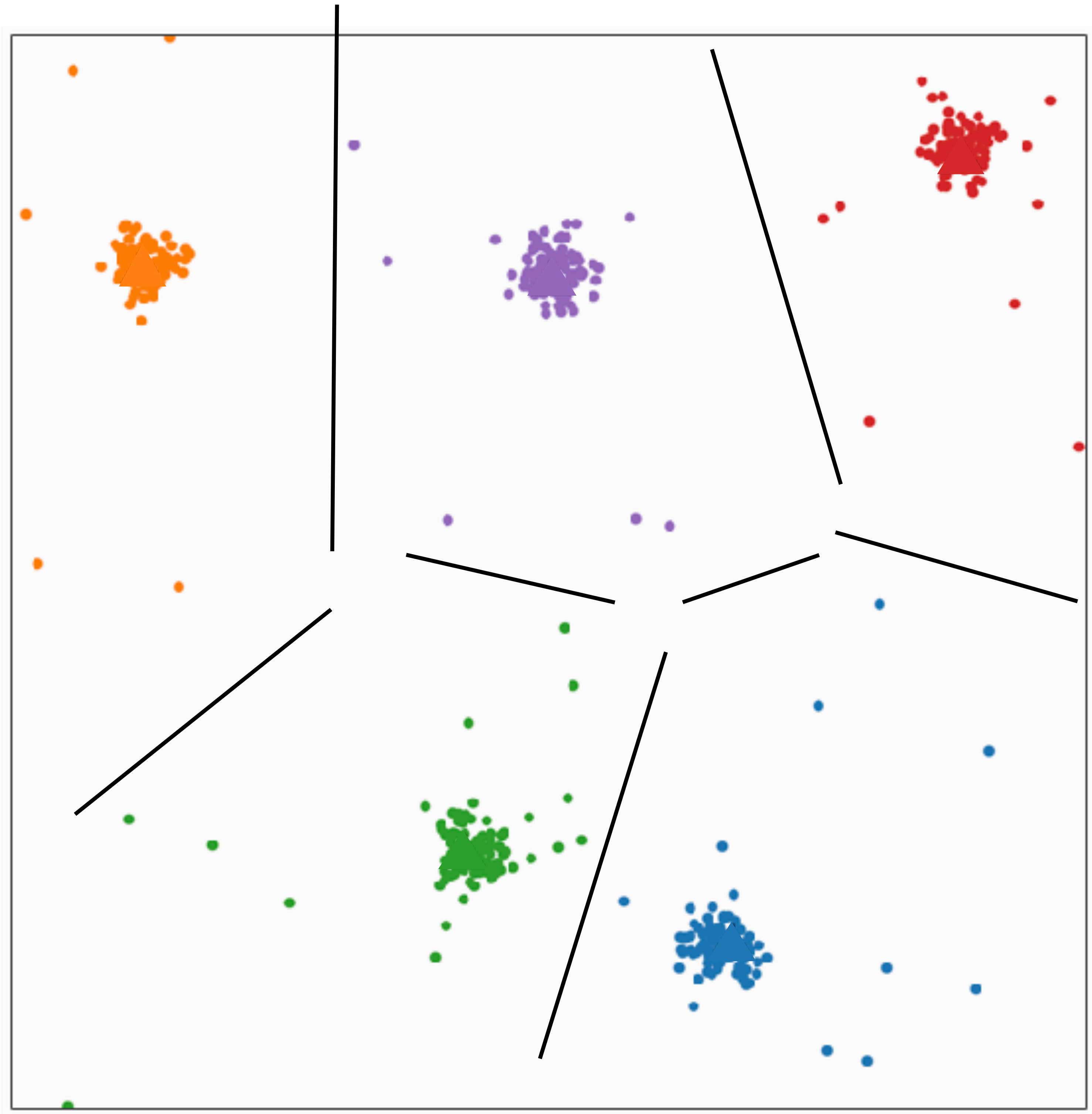

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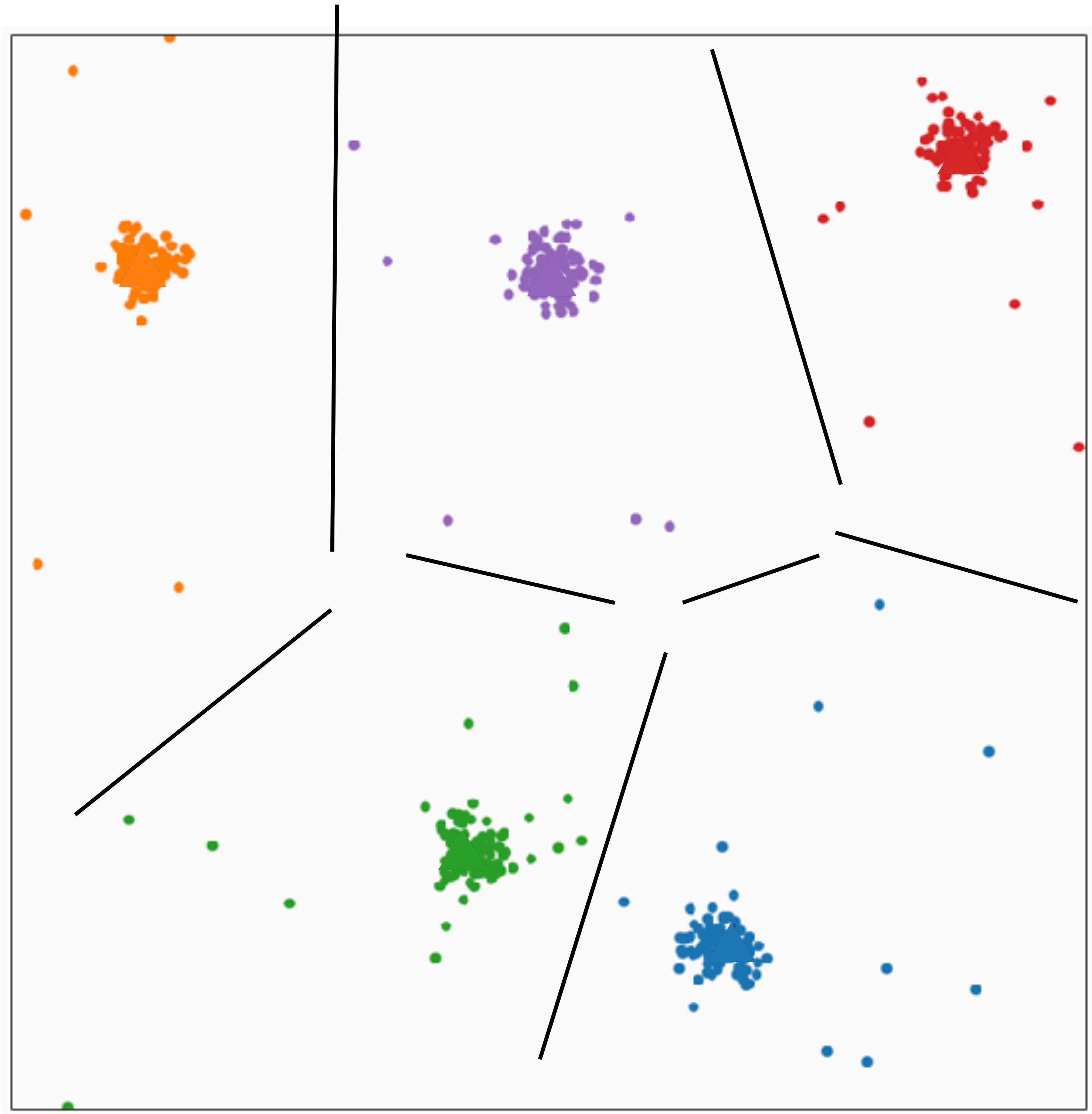

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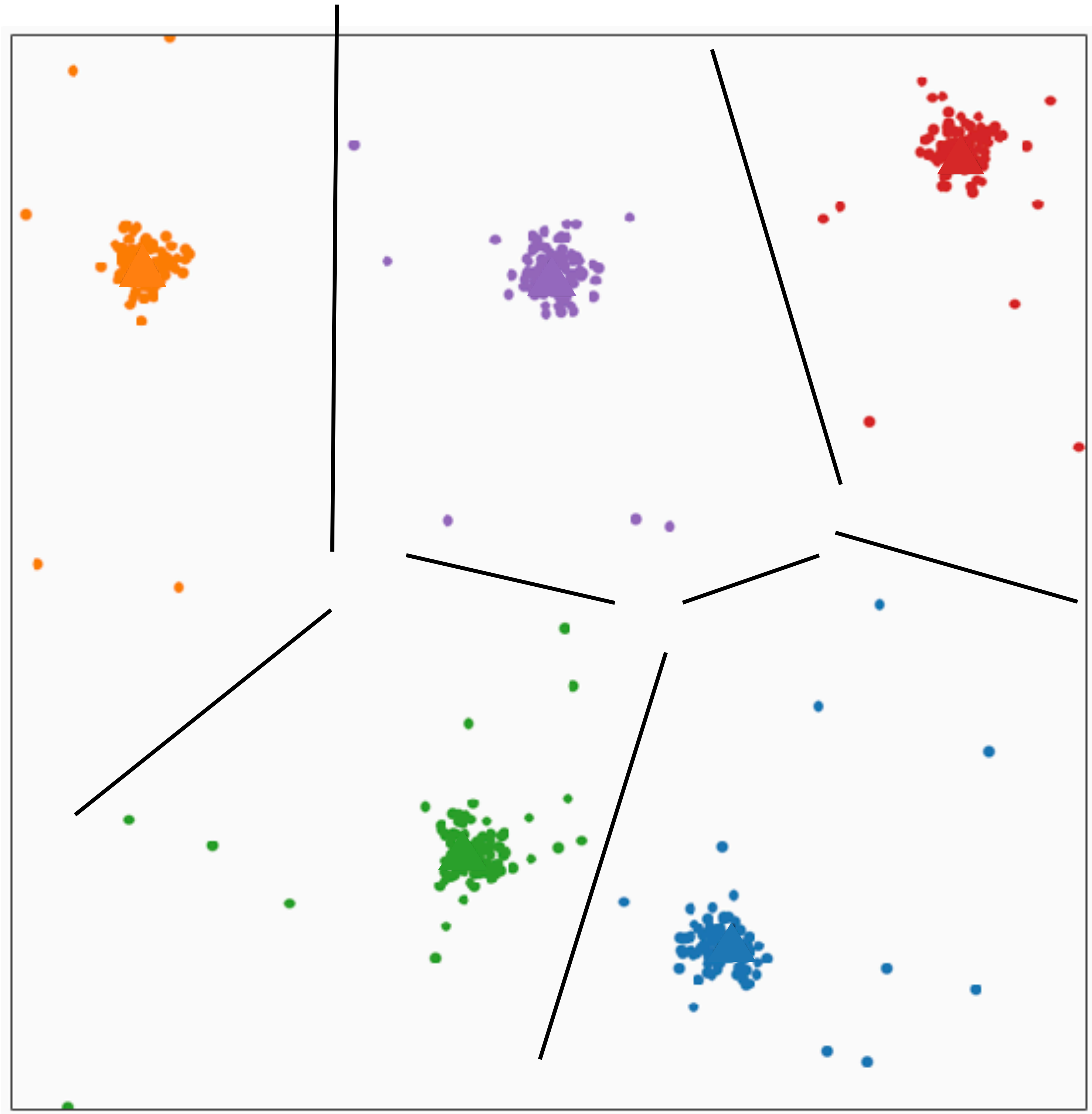

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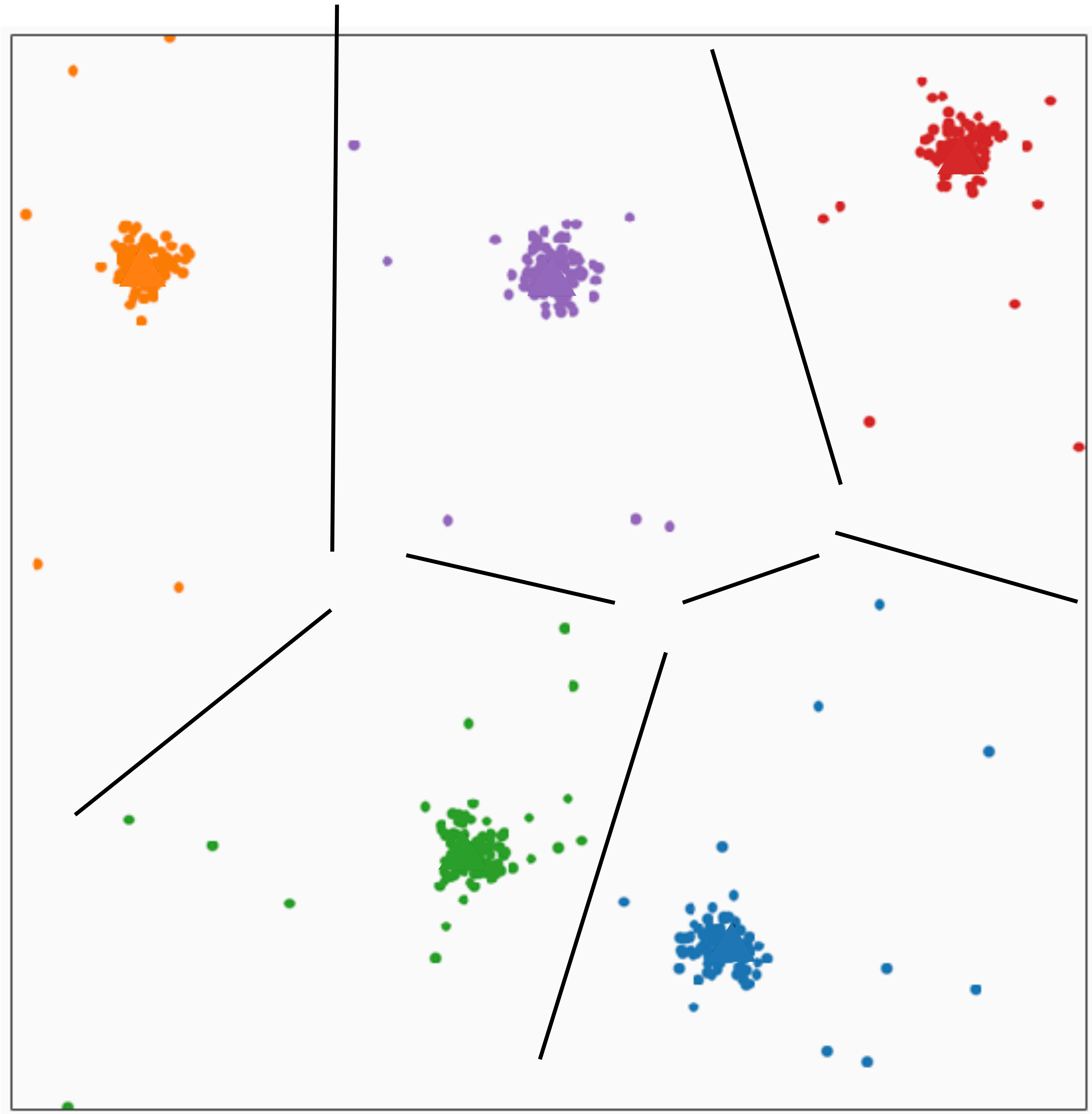

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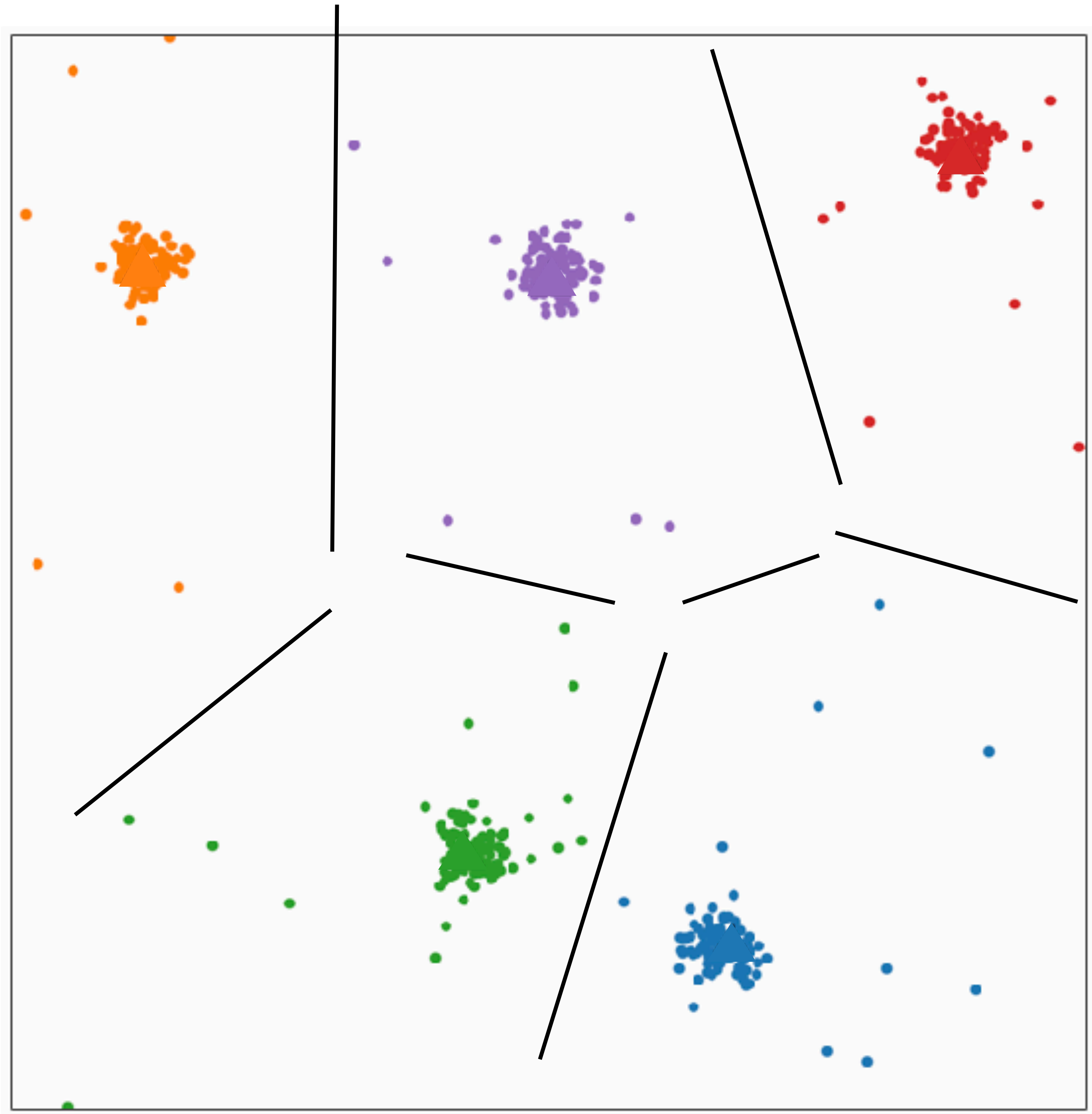

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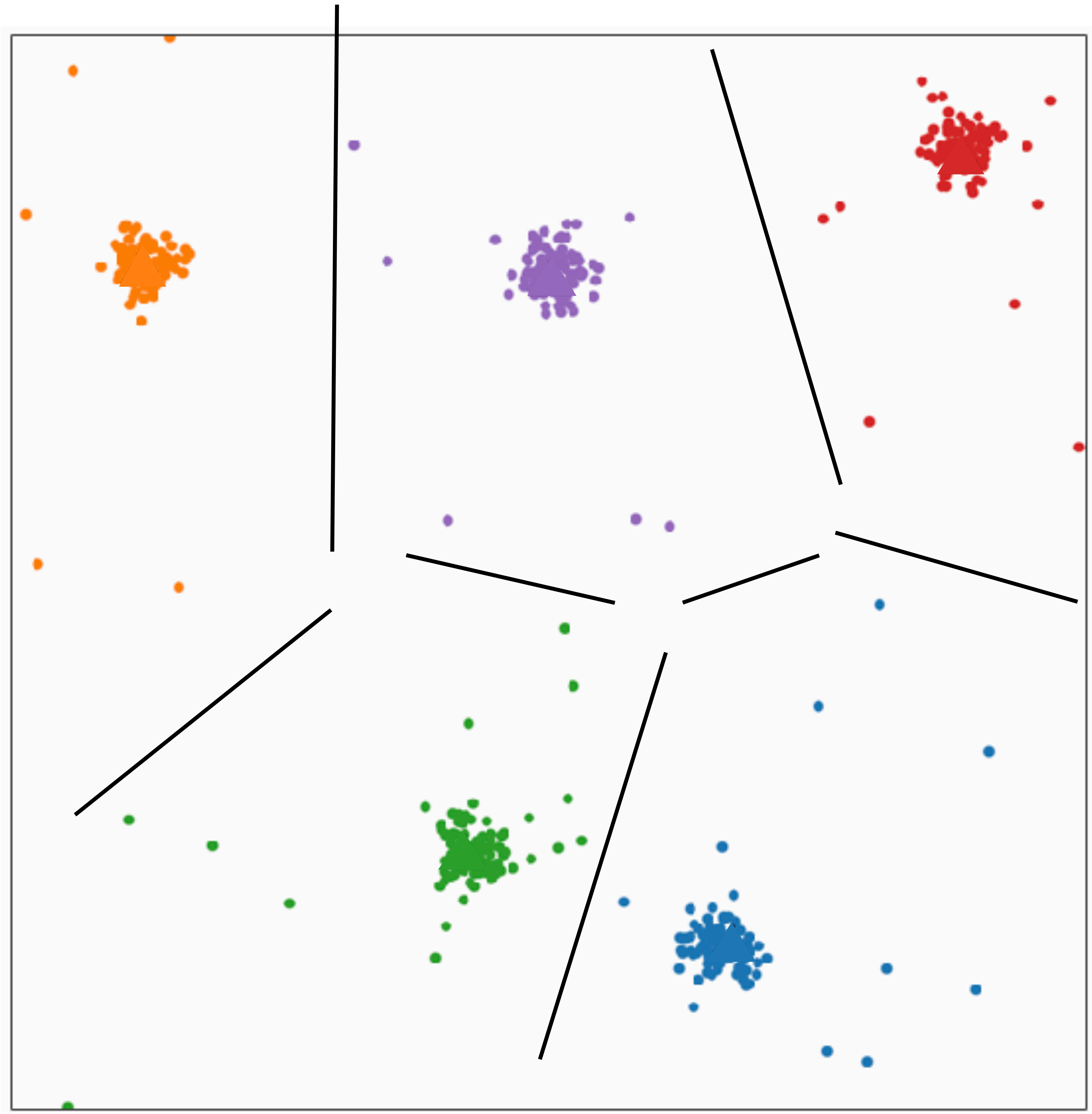

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Clustering & related

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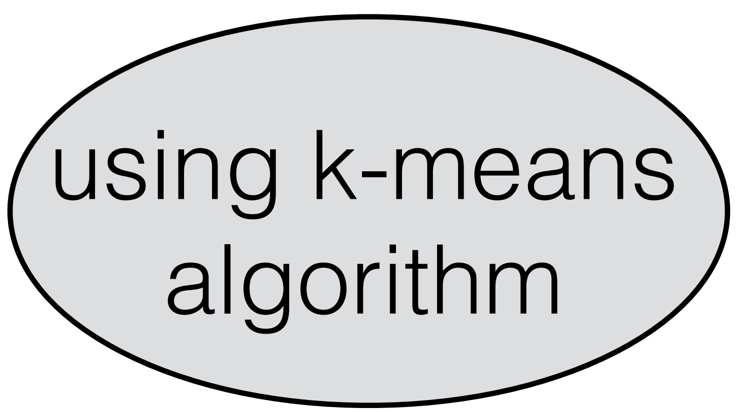

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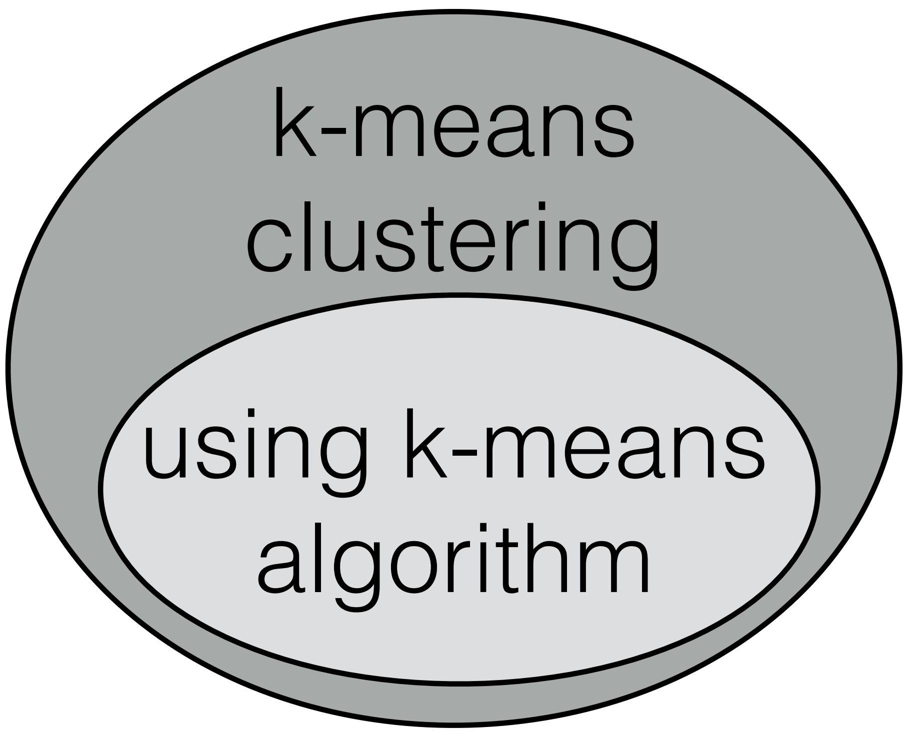

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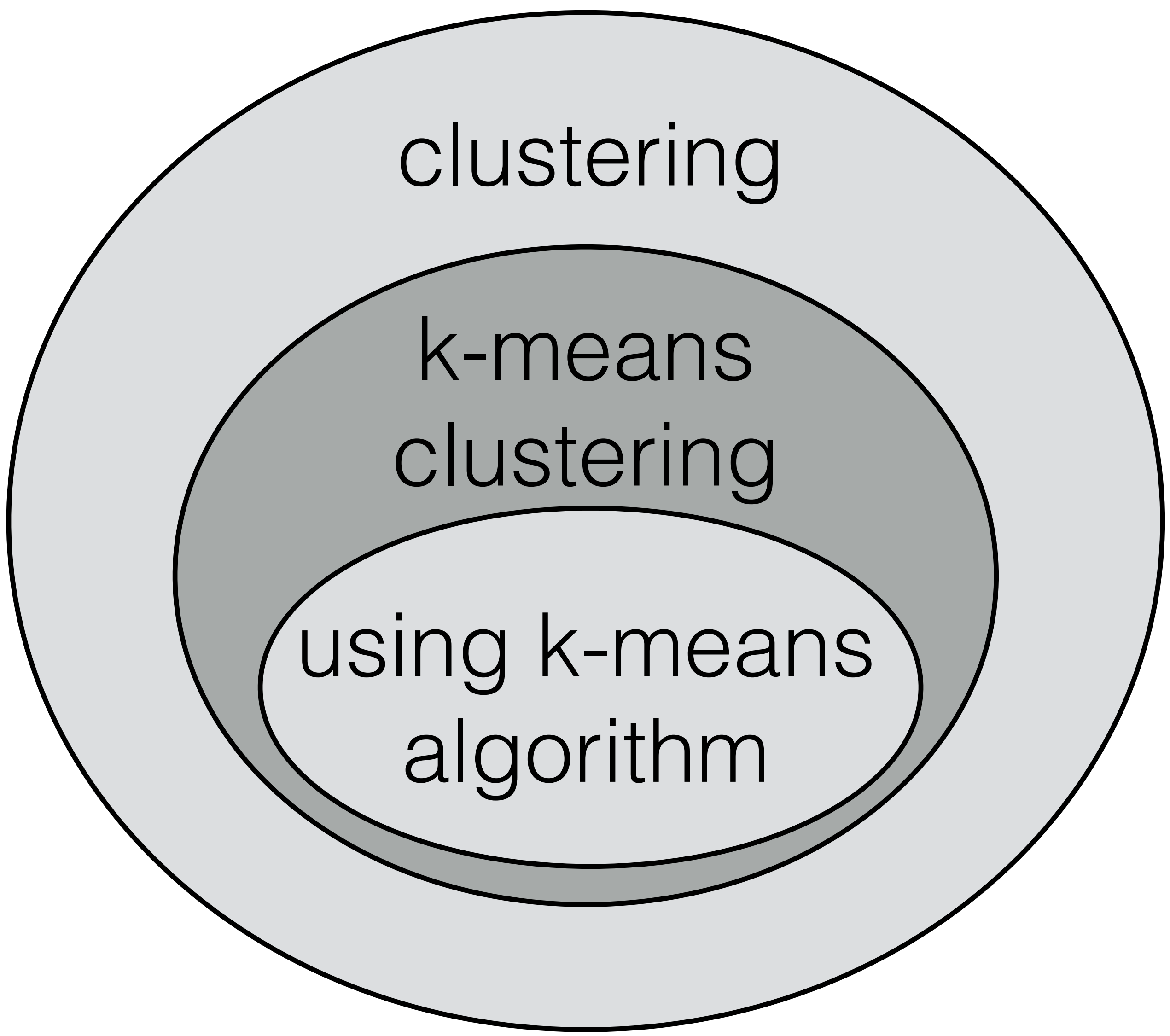

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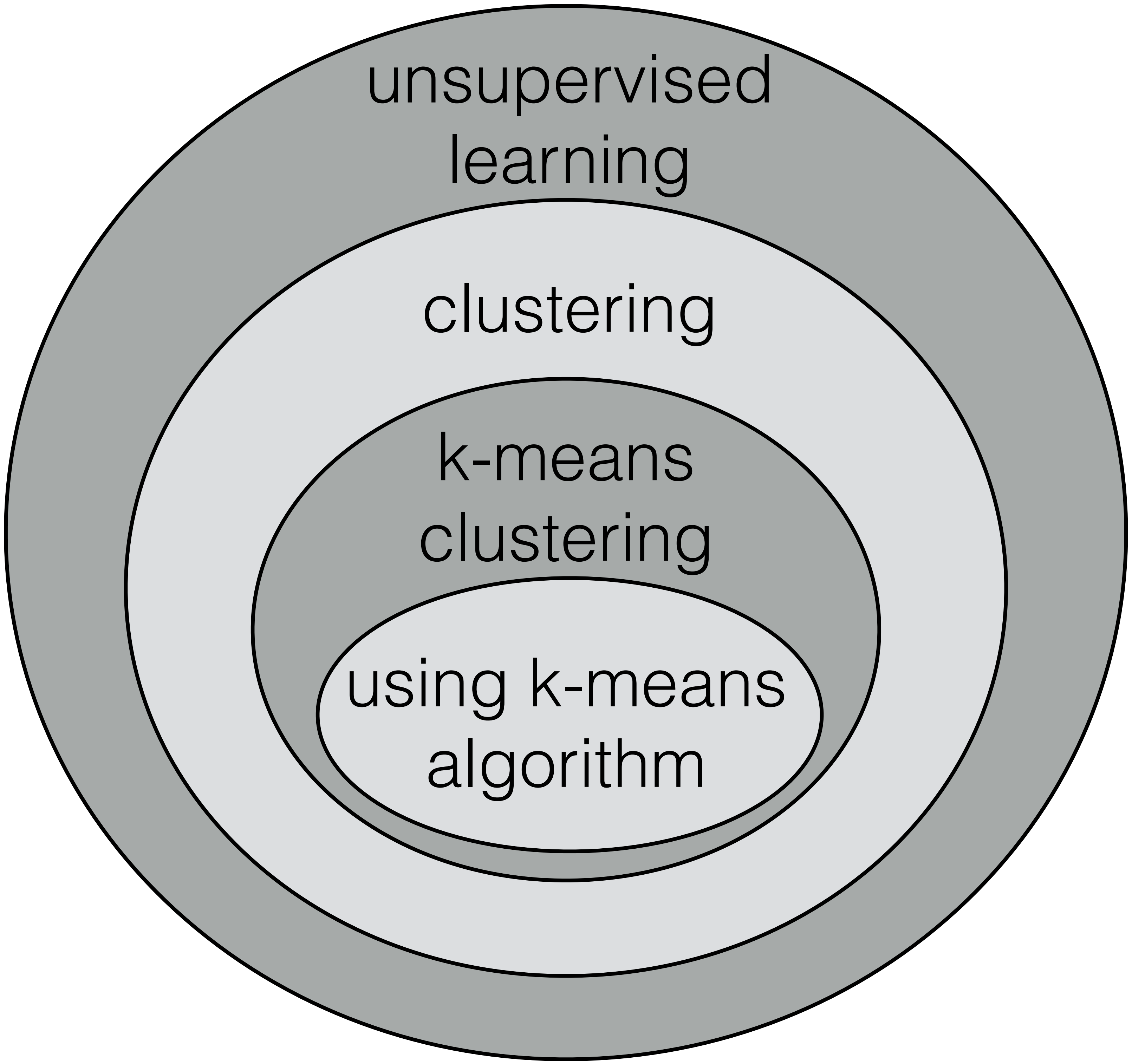

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k-means algorithm: initialization

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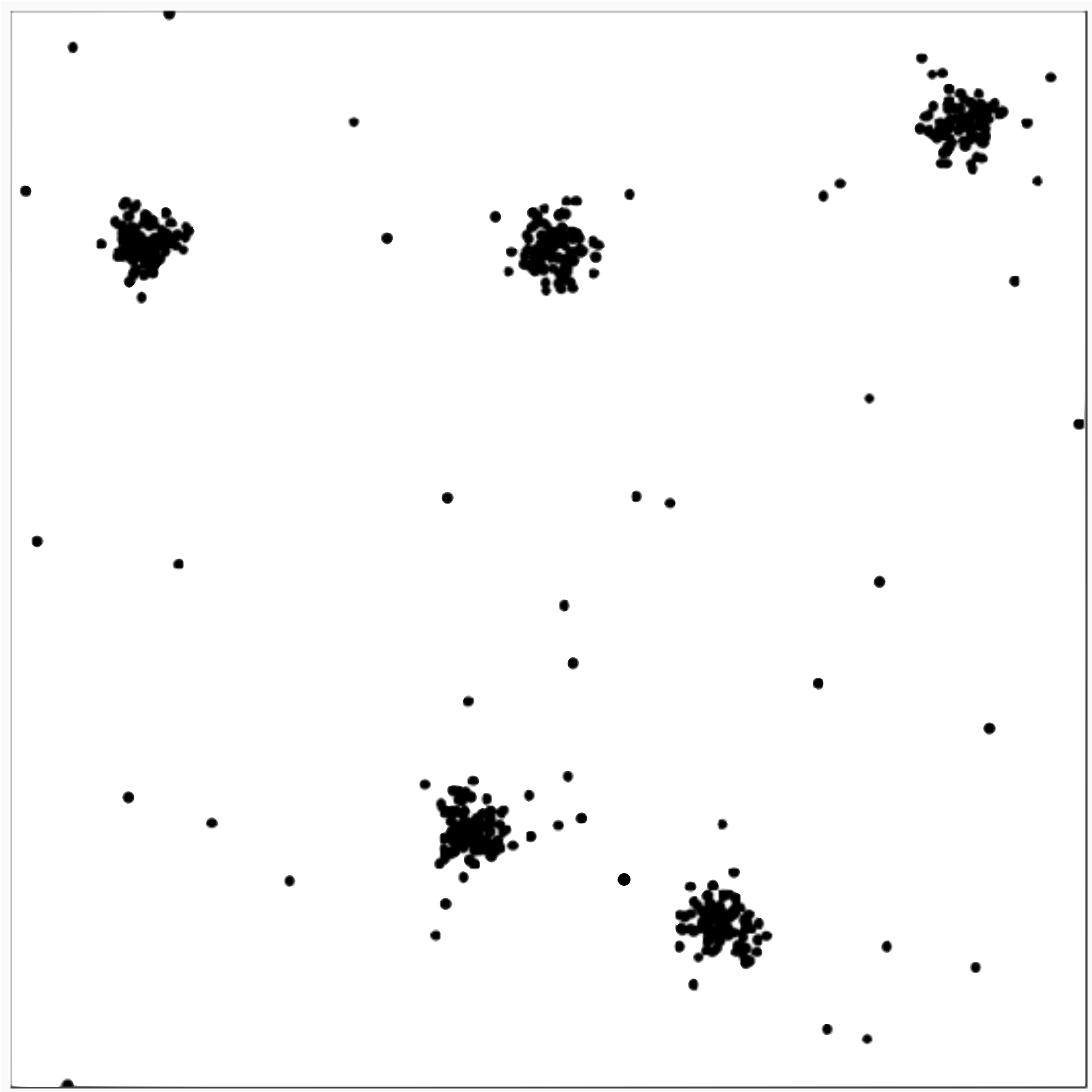
- **Theorem**. If run for enough outer iterations, the k-means algorithm will converge to a local minimum of the k-means objective

k-means algorithm: initialization



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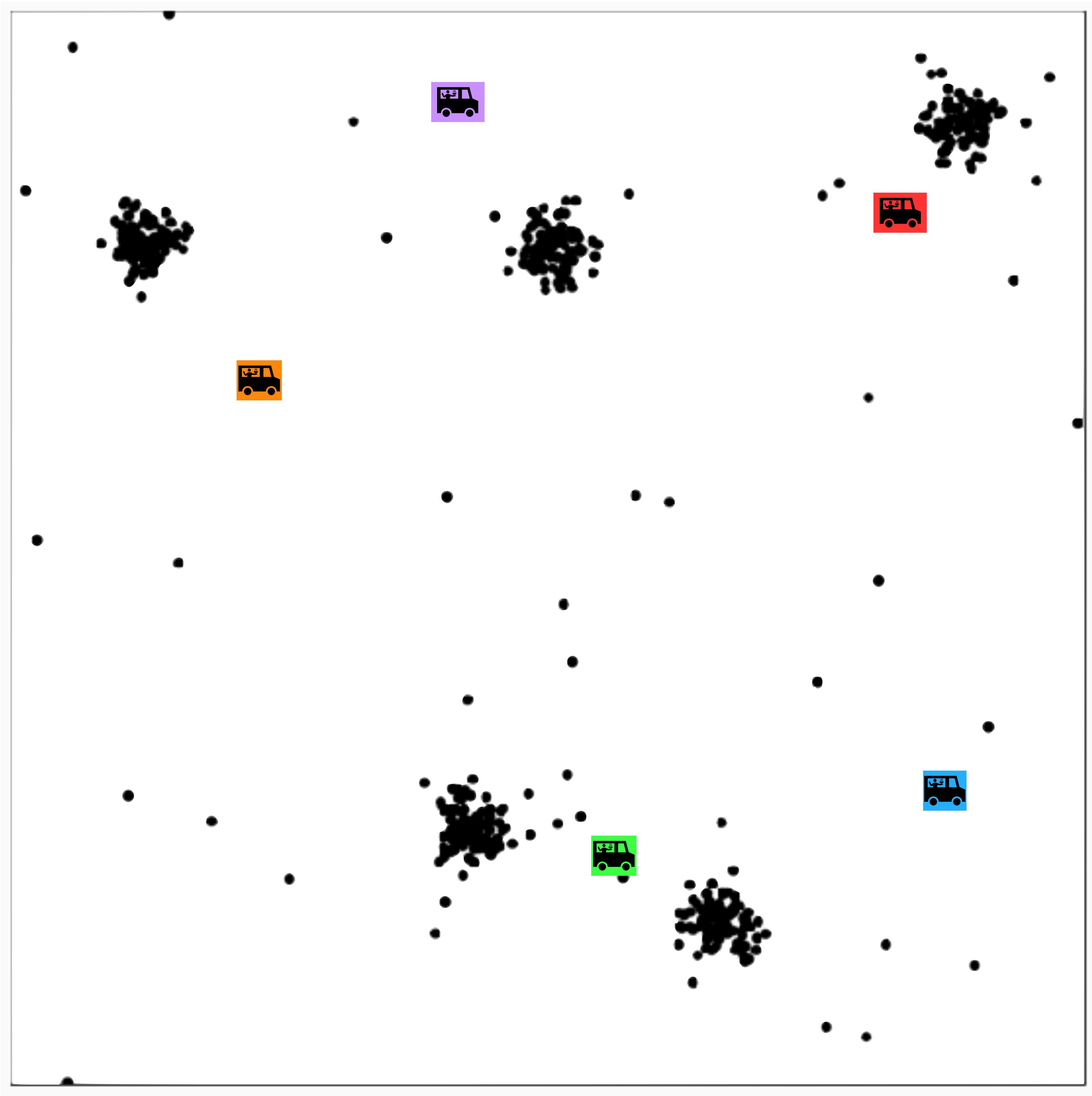

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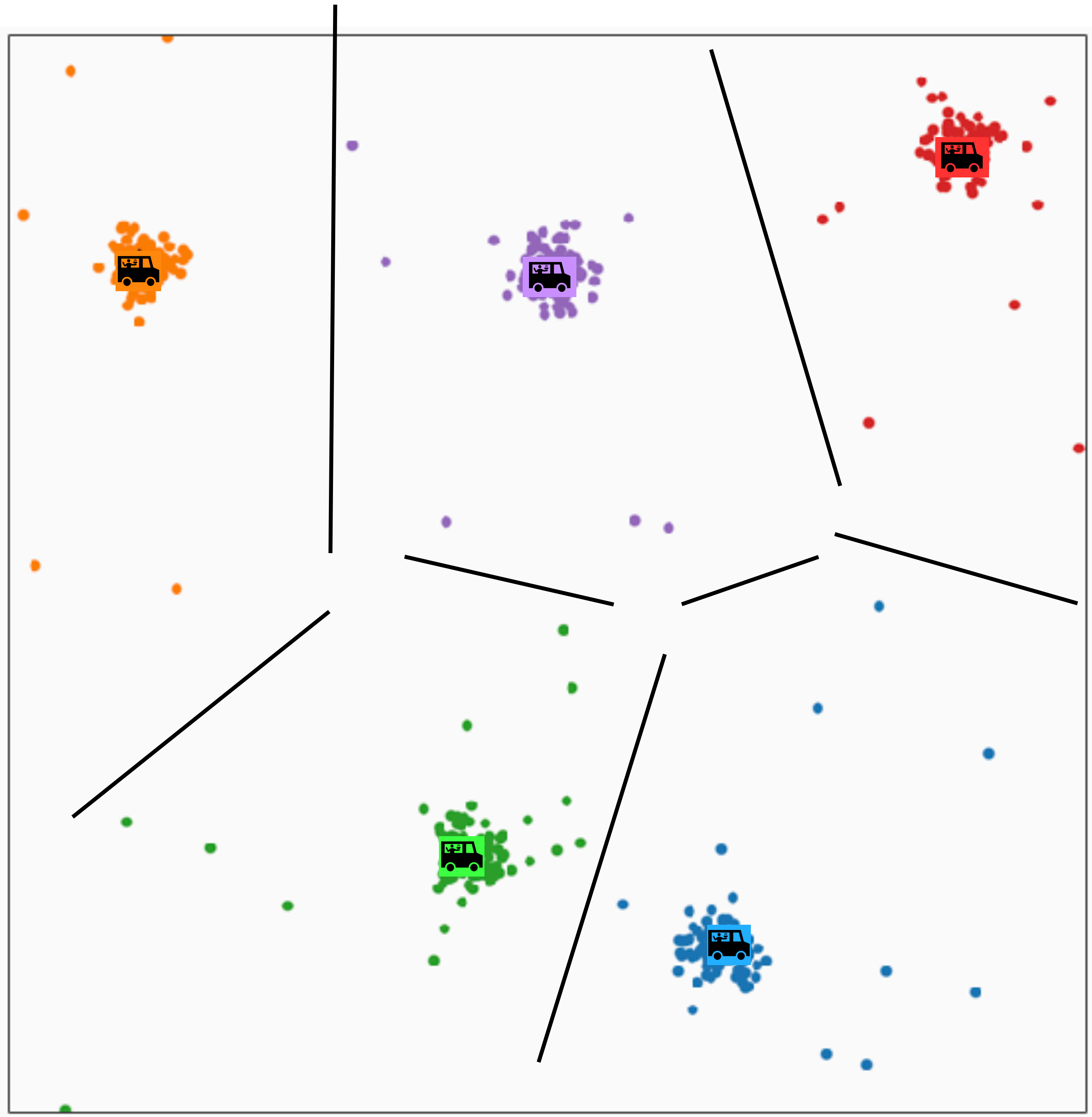

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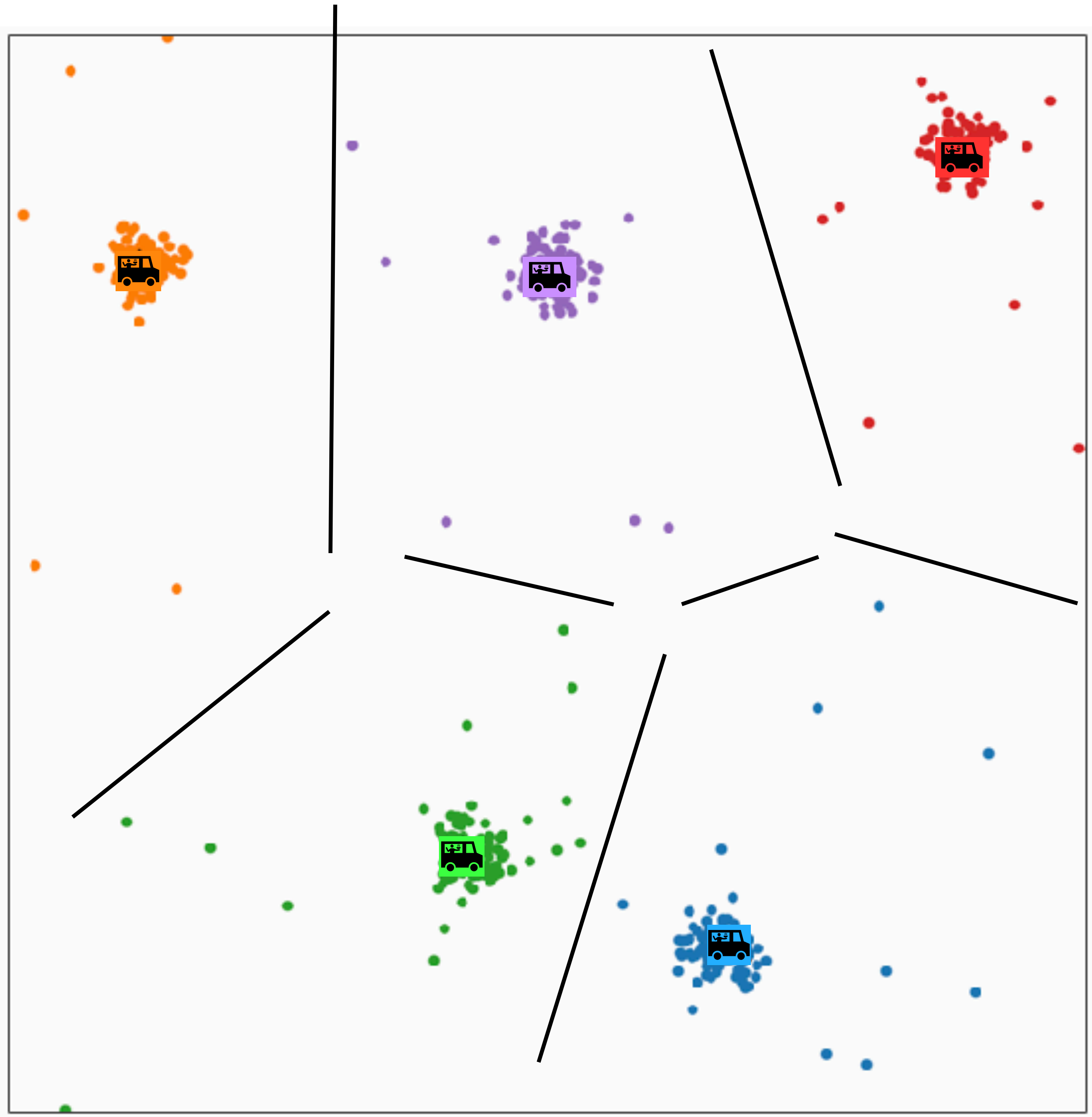

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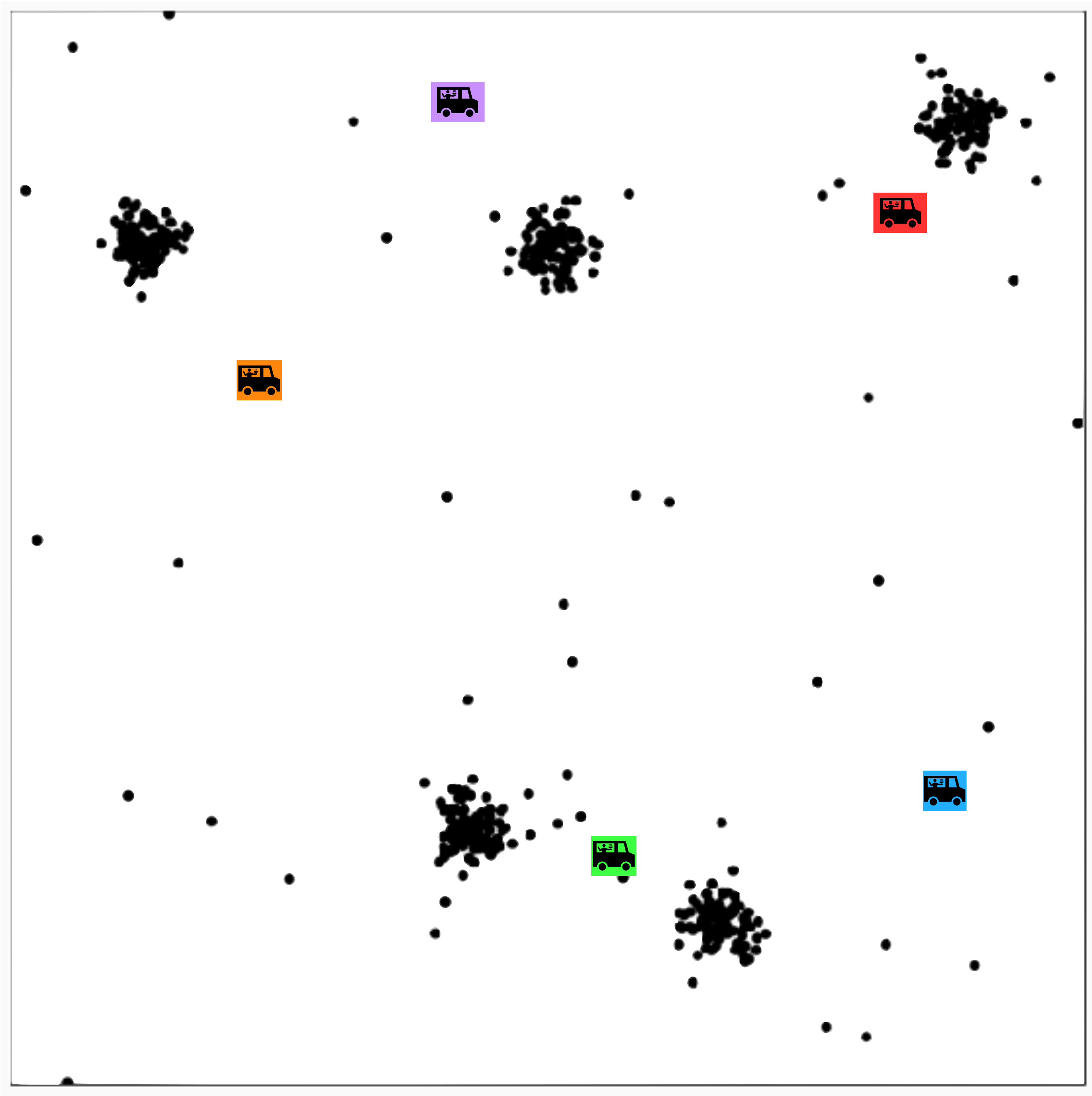

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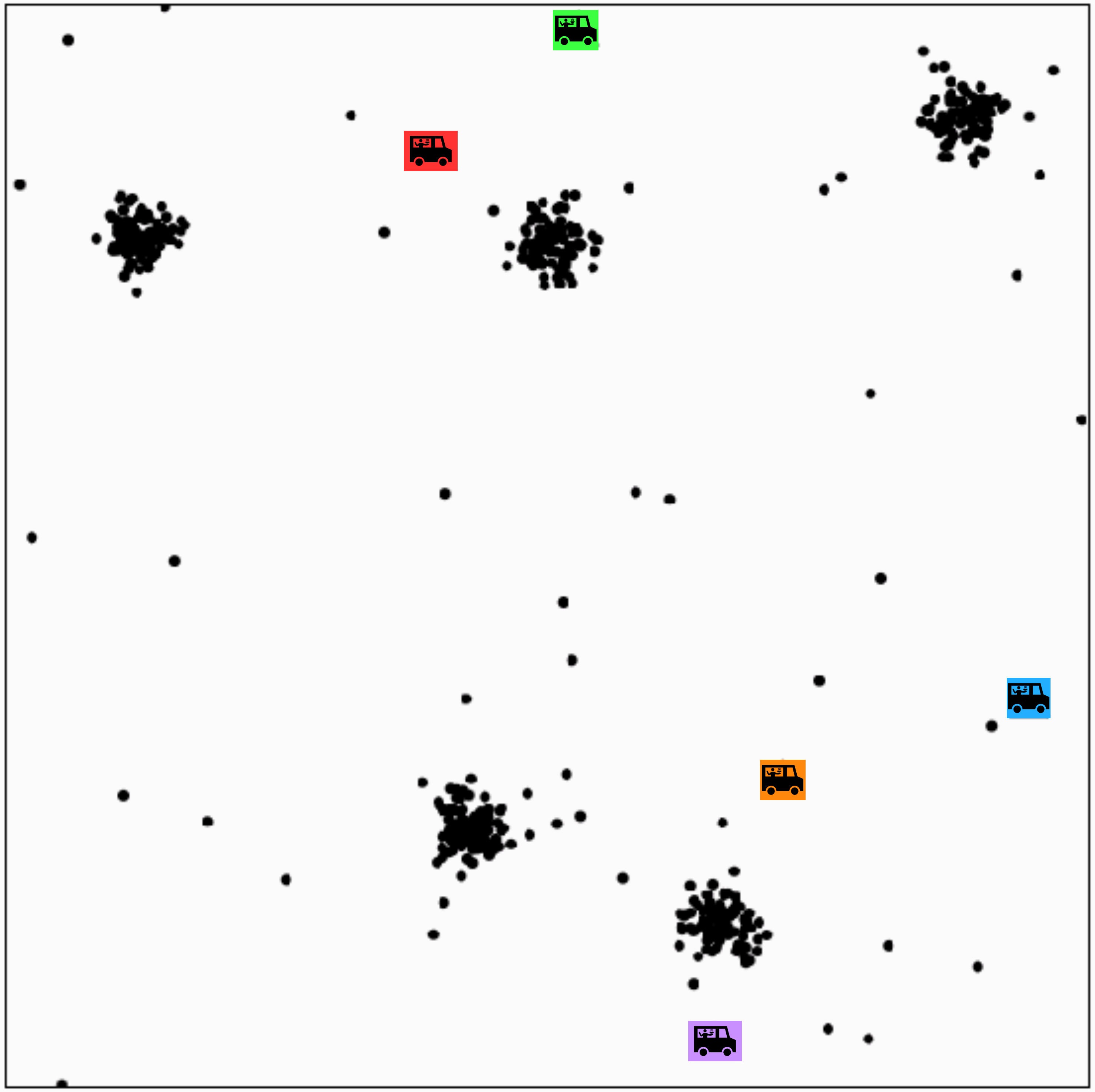

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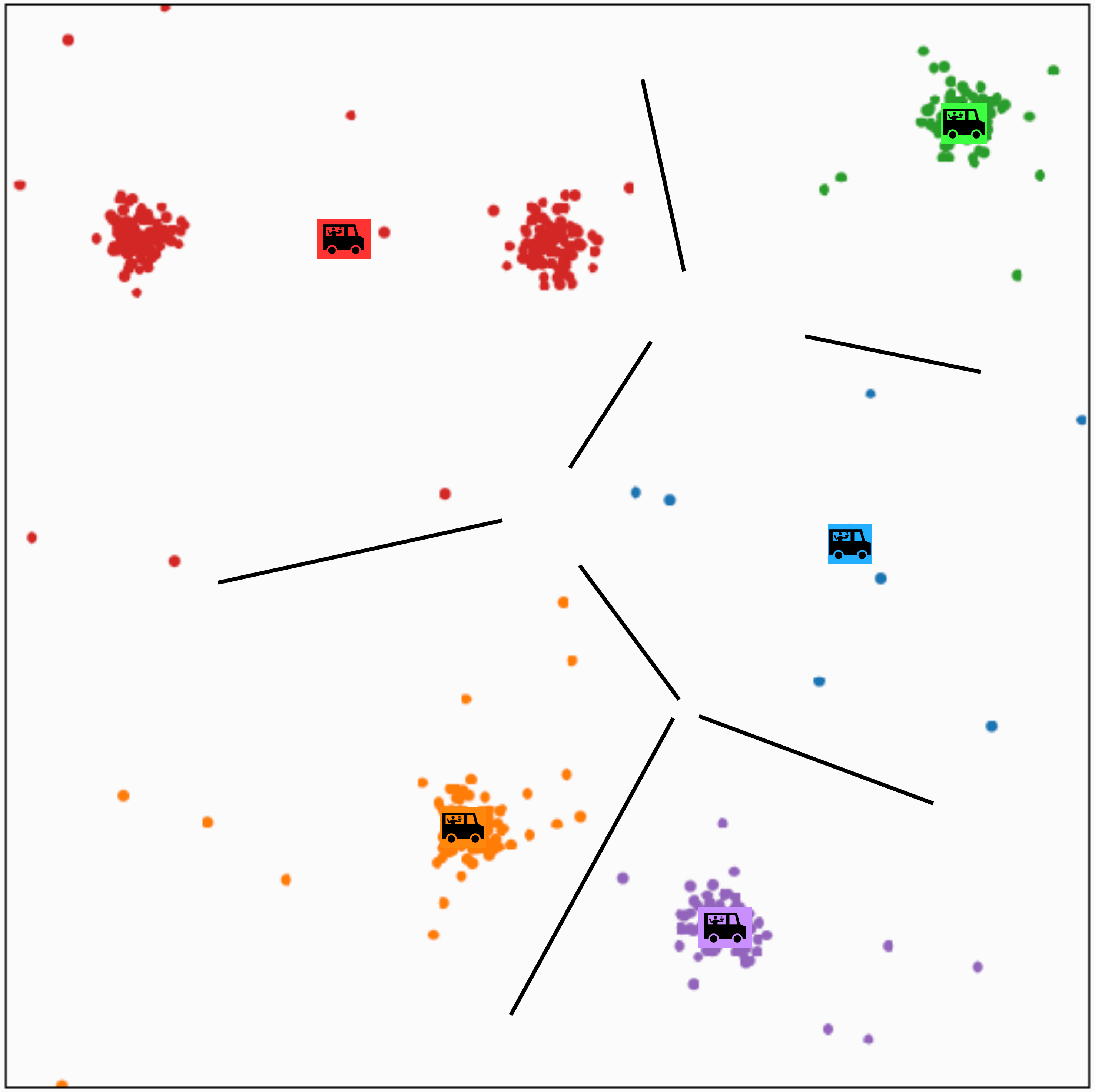

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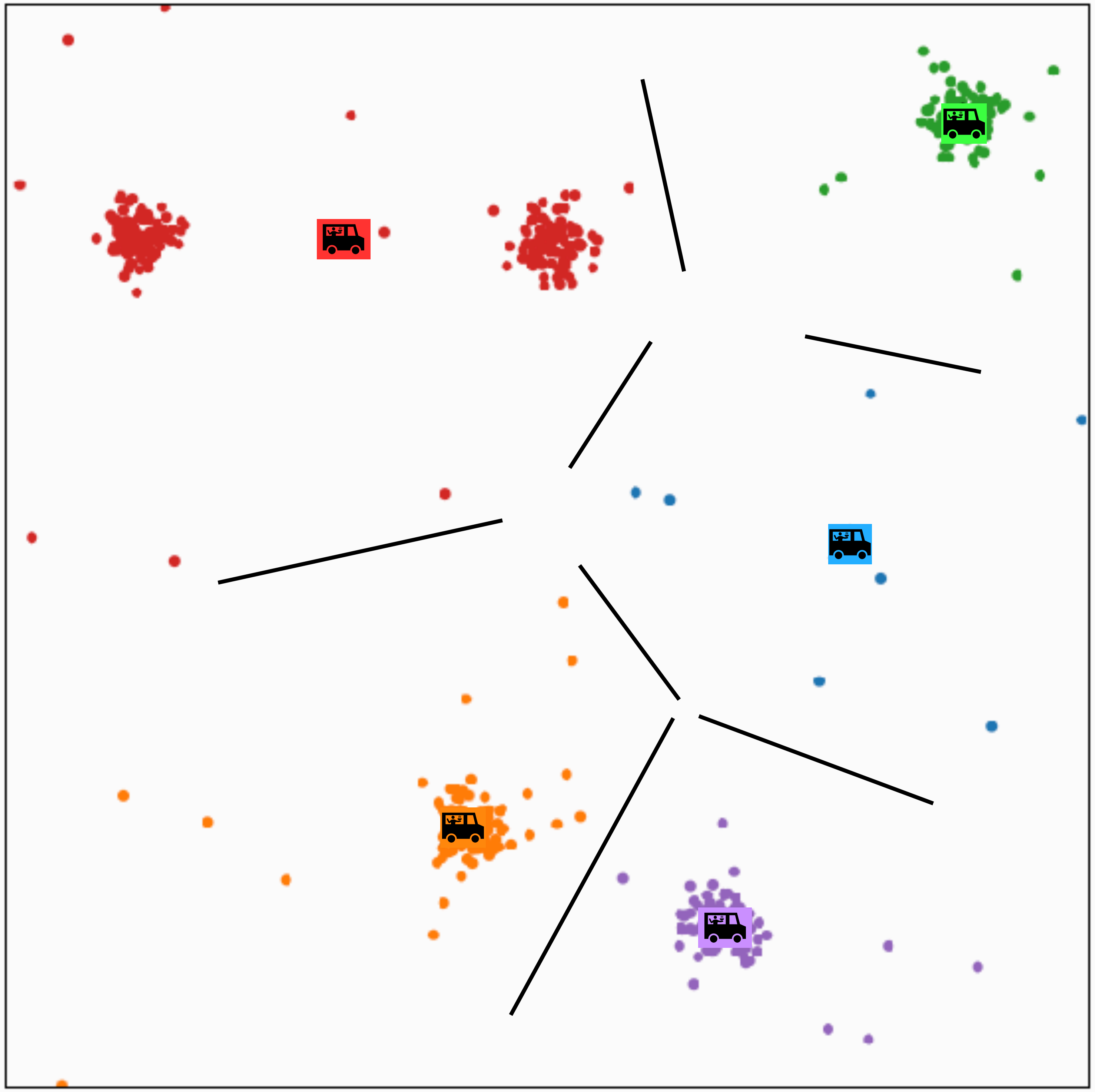

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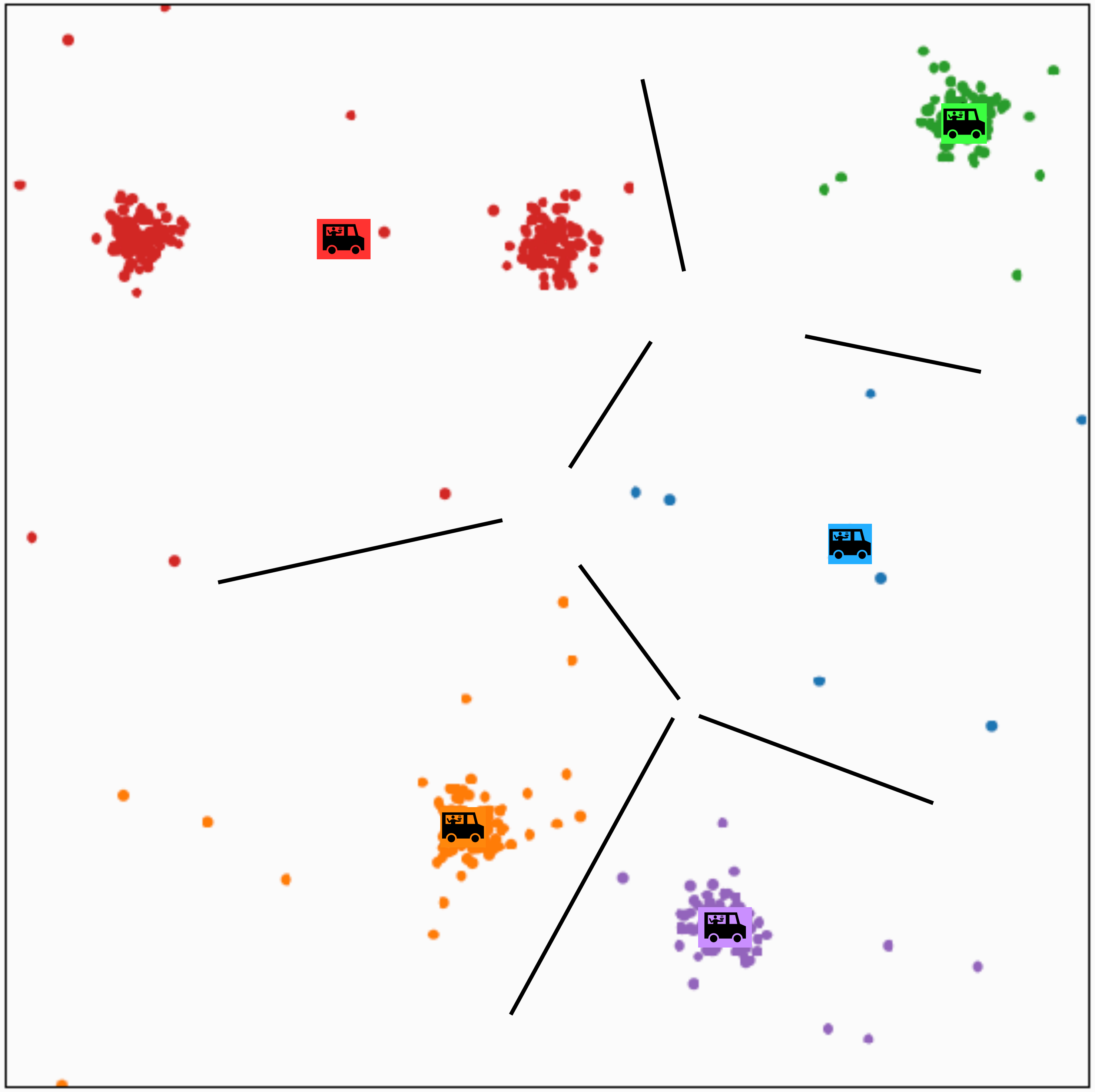

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Why or why not?

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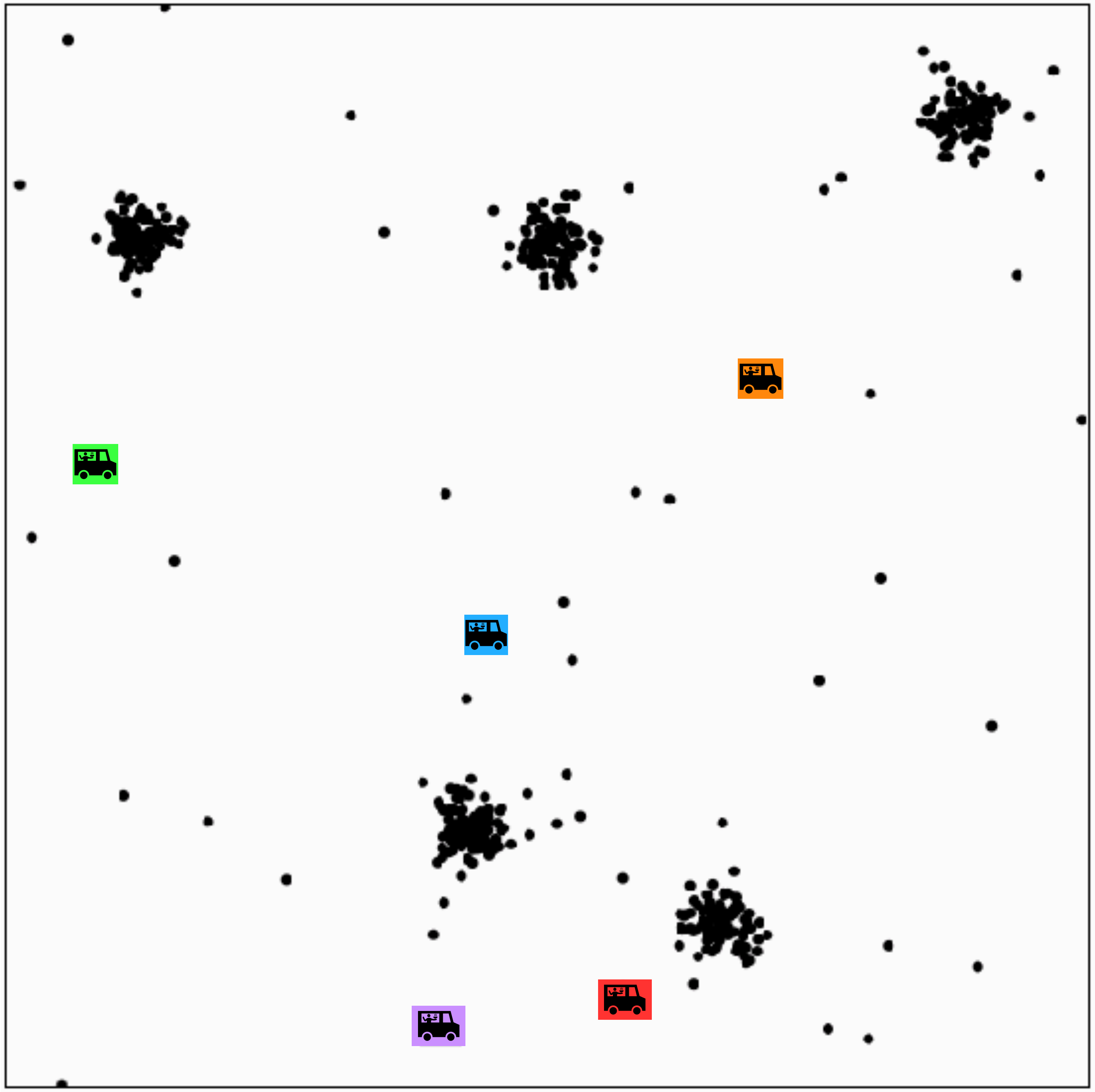

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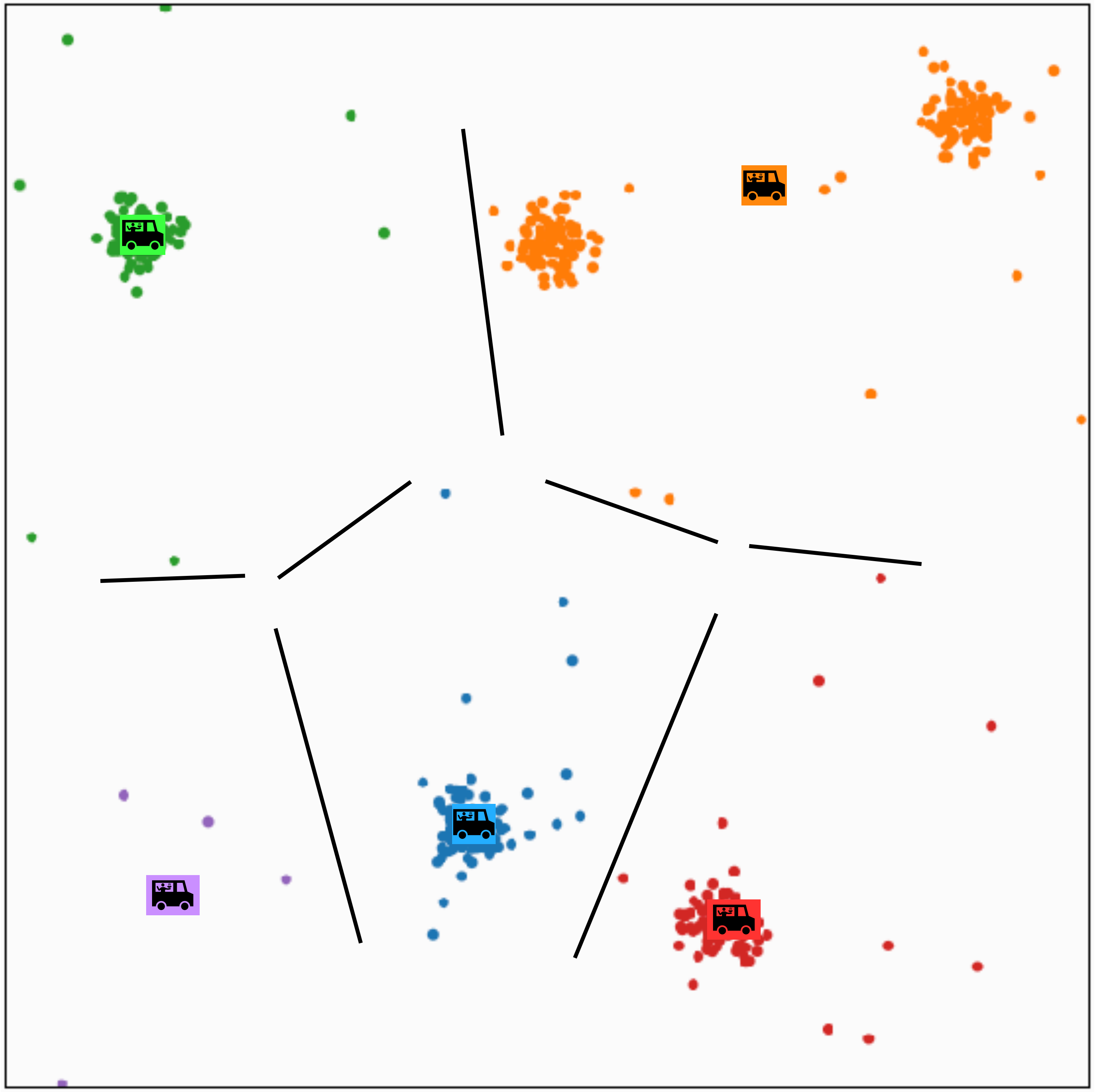

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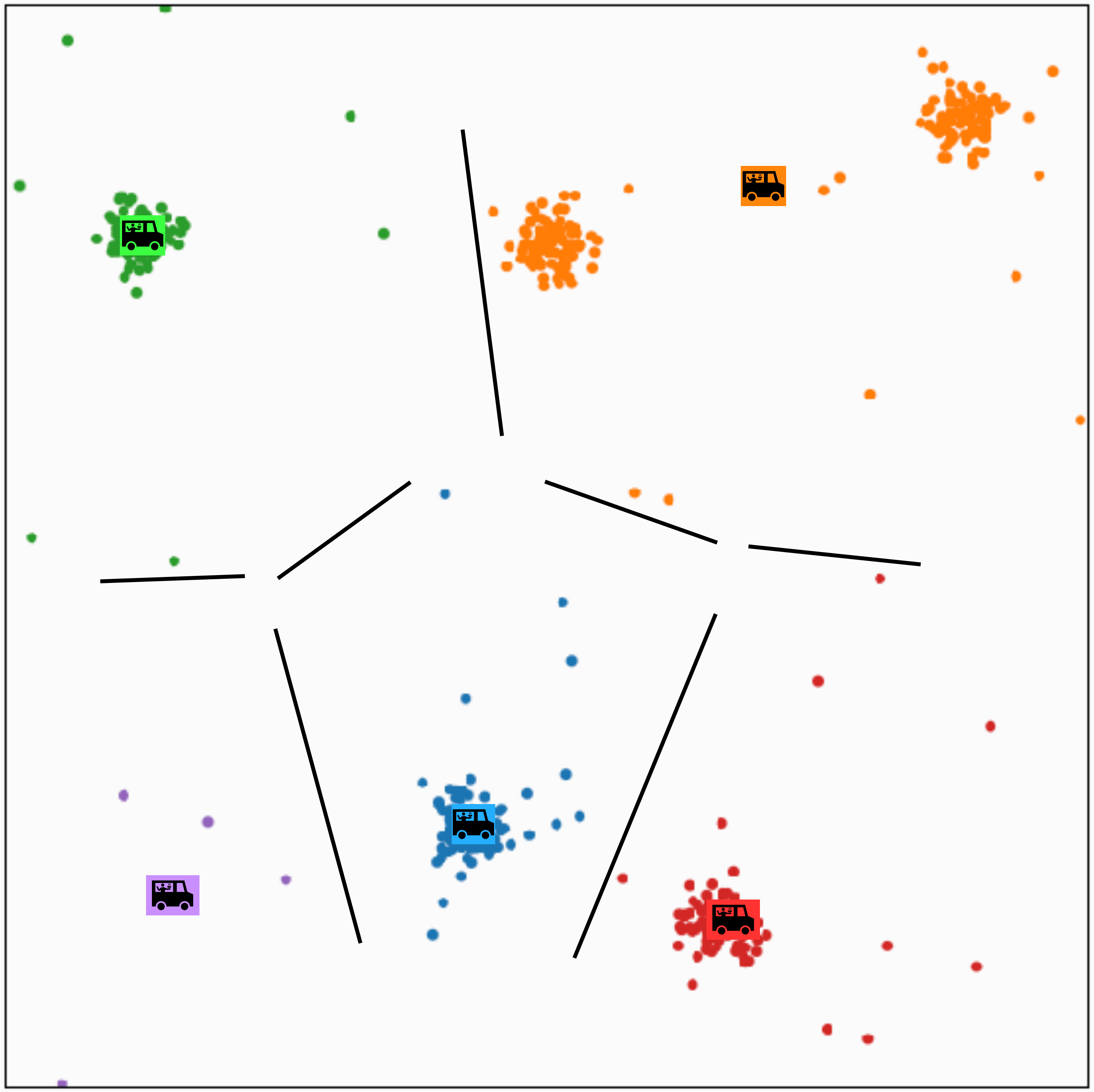

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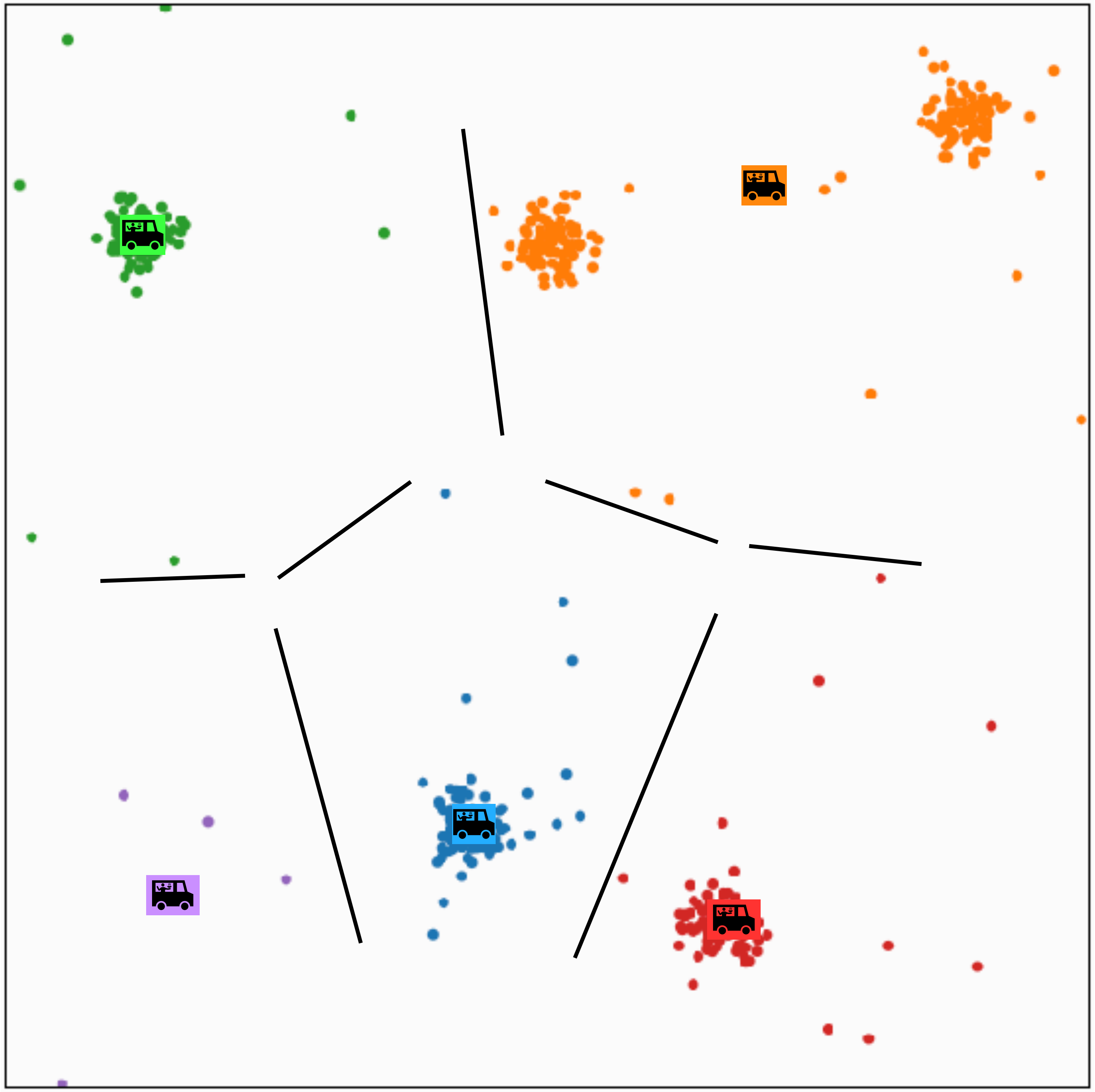

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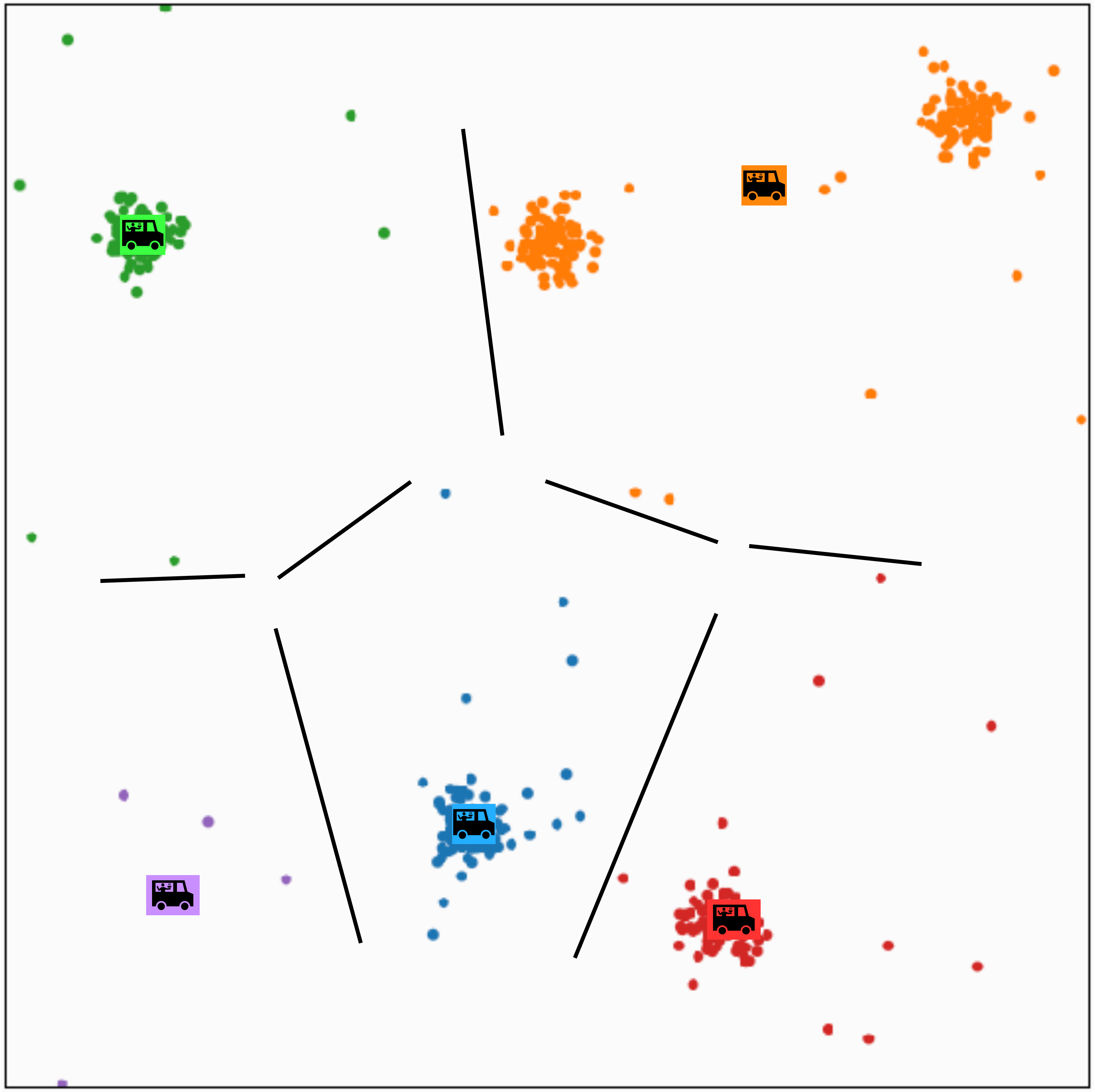

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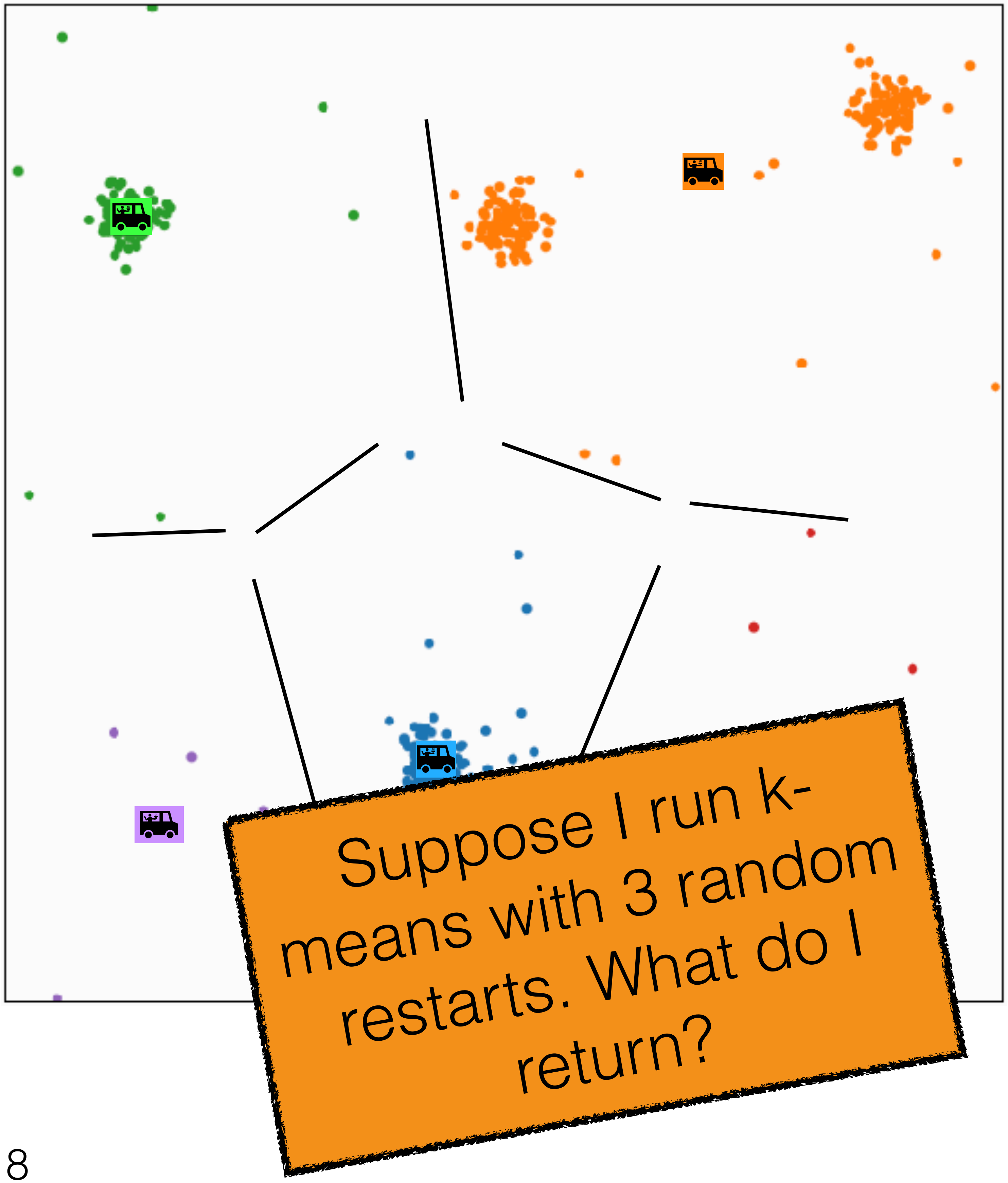

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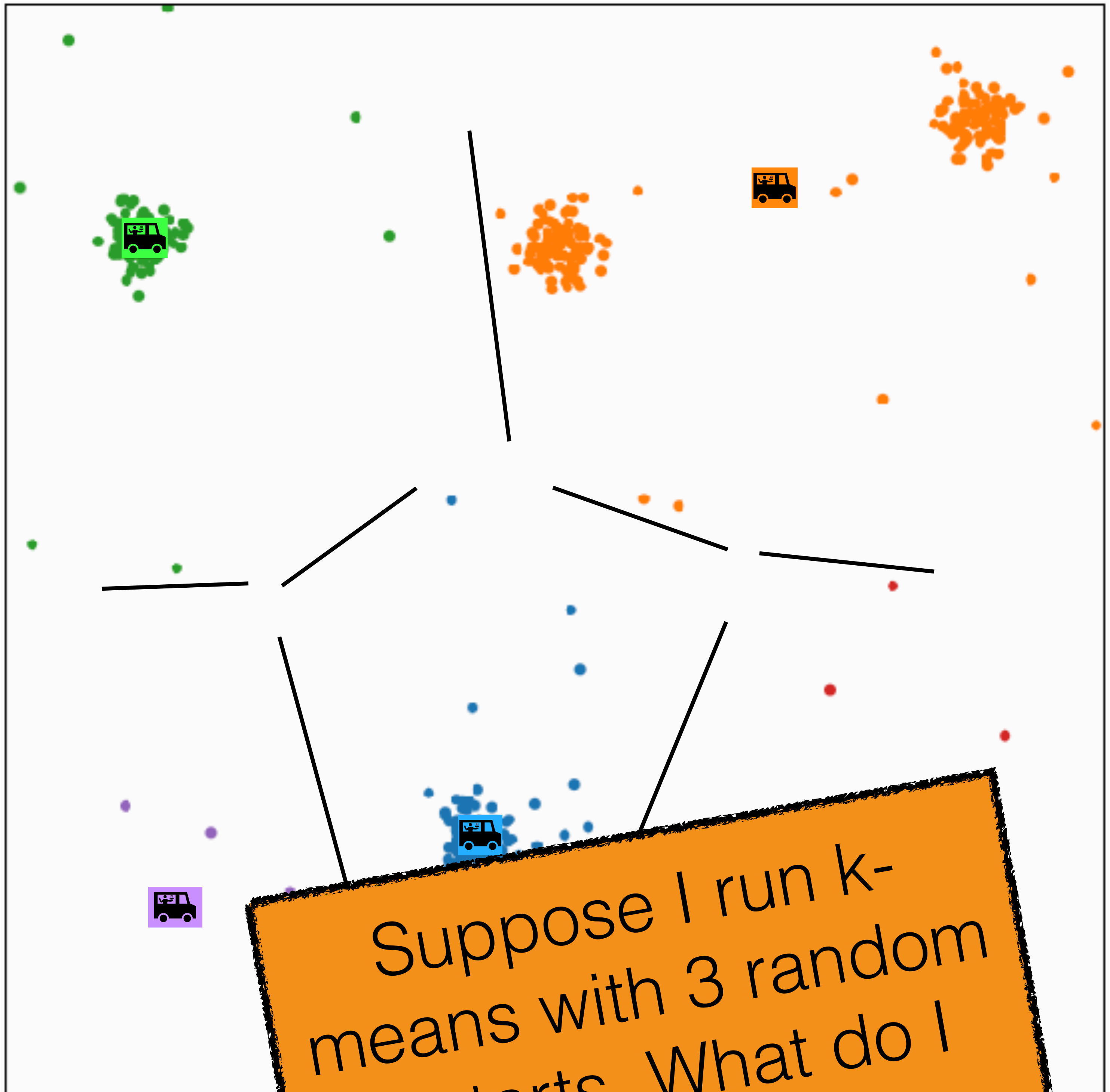

Suppose I run k-means with 3 random restarts. What do I return?

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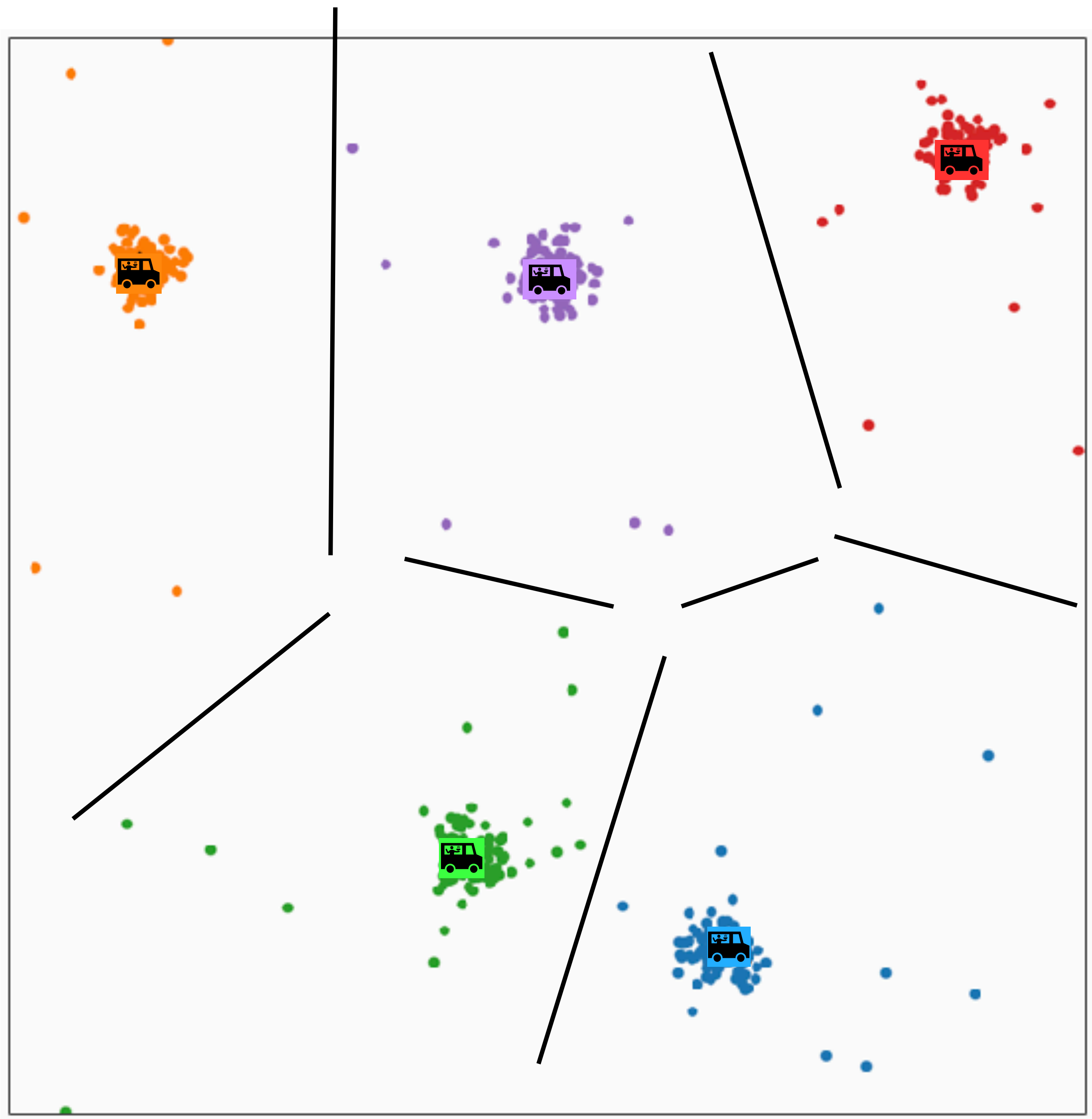
k-means algorithm: effect of *k*

[https://stanford.edu/class/engr108/visualizations/kmeans/kmeans.html]

k-means algorithm: effect of *k*



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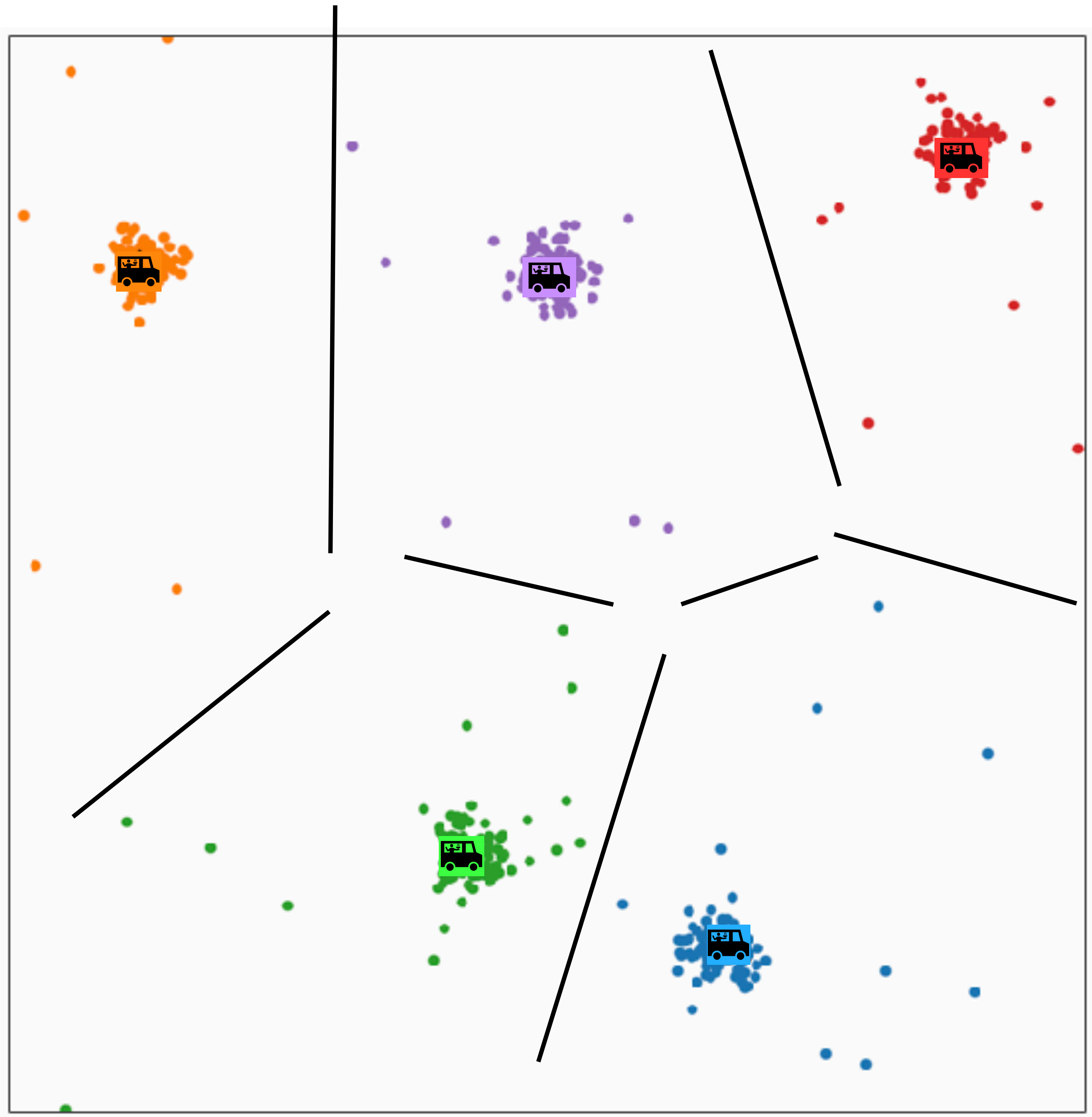
k-means algorithm: effect of *k*

- Different *k* will give us different results



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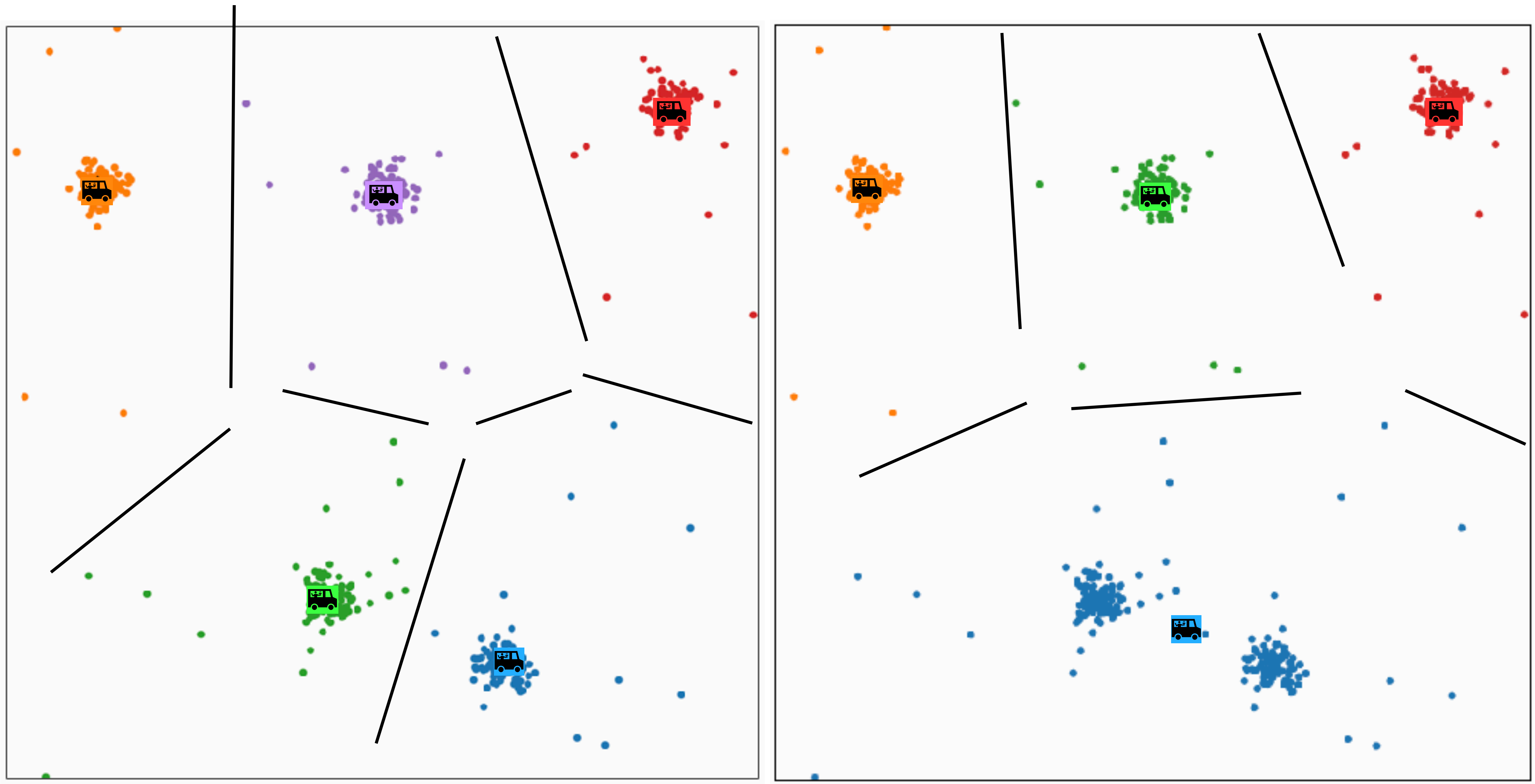

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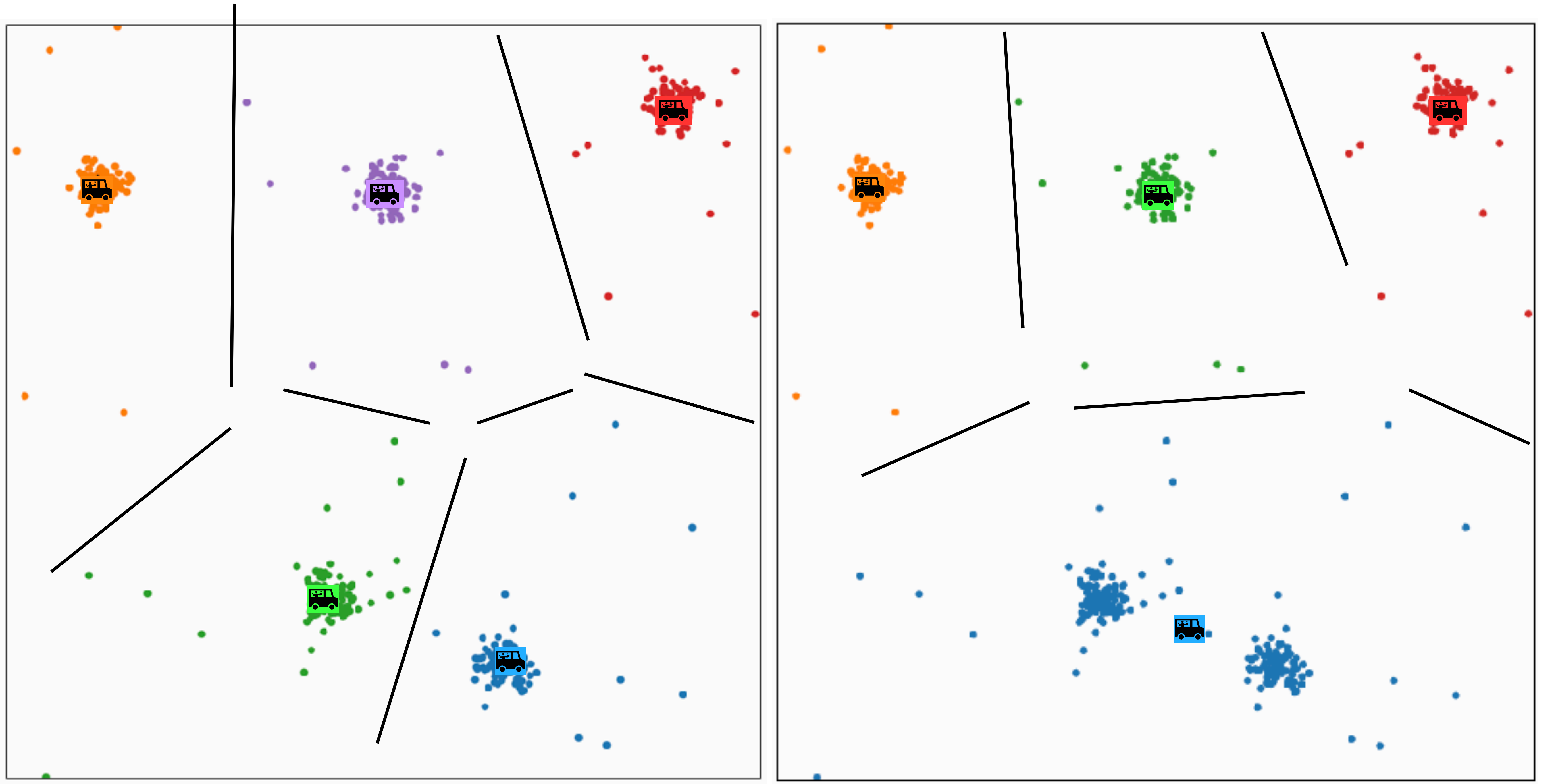
k-means algorithm: effect of *k*

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



[https://stanford.edu/class/engr108/visualizations/kmeans/kmeans.html]

k-means algorithm: effect of *k*

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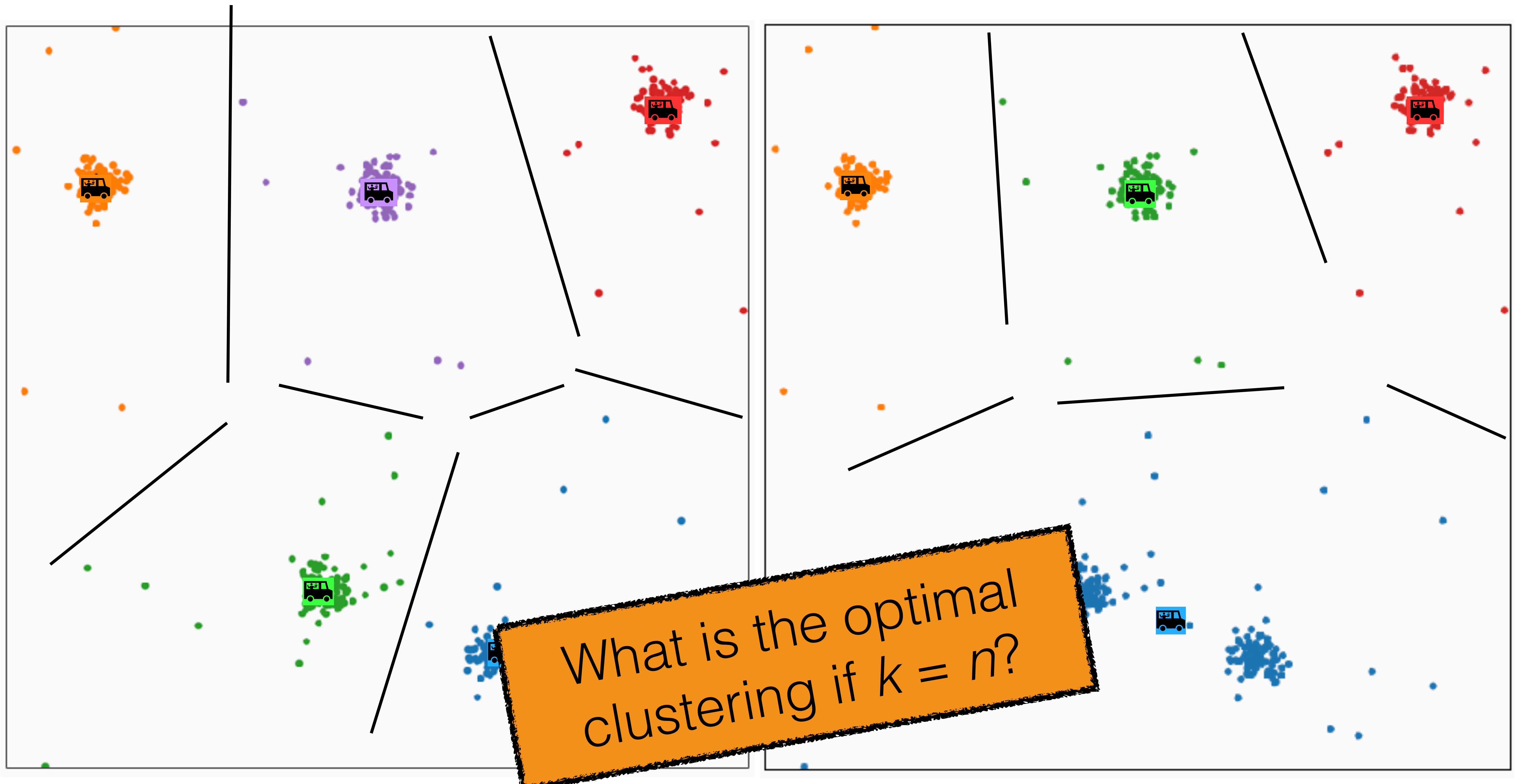

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k-means algorithm: choosing *k*

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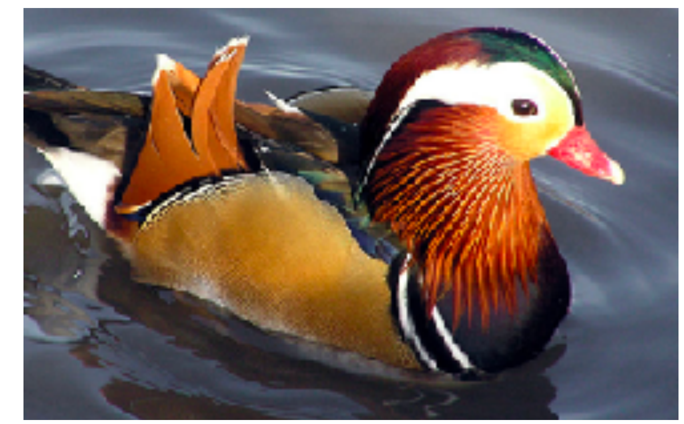

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   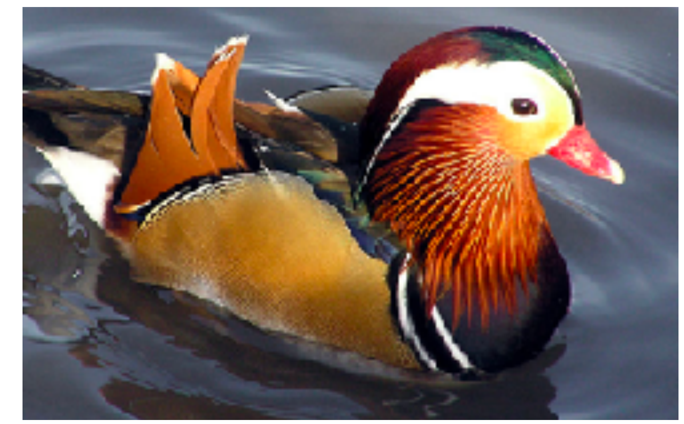

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Why not?

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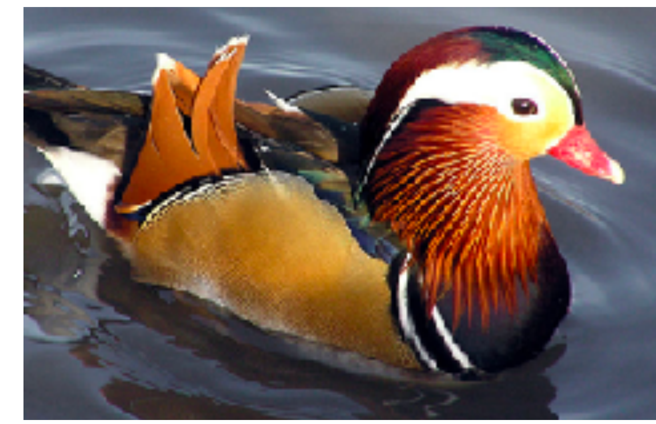

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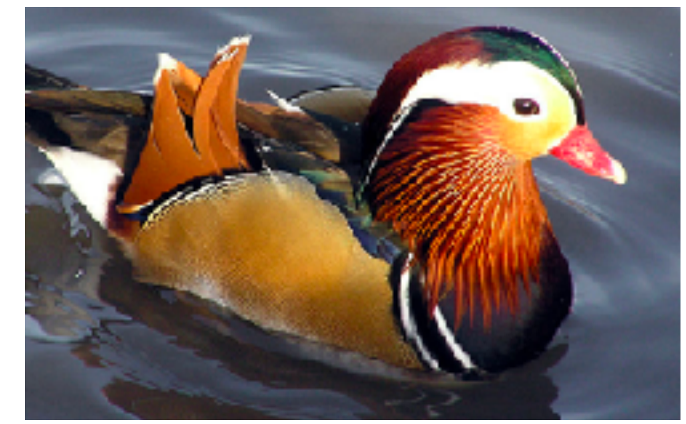

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- How to choose *k* depends on what you'd like to do
  - E.g. cost-benefit trade-off
  - Often no single "right answer"

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Cluster shape

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

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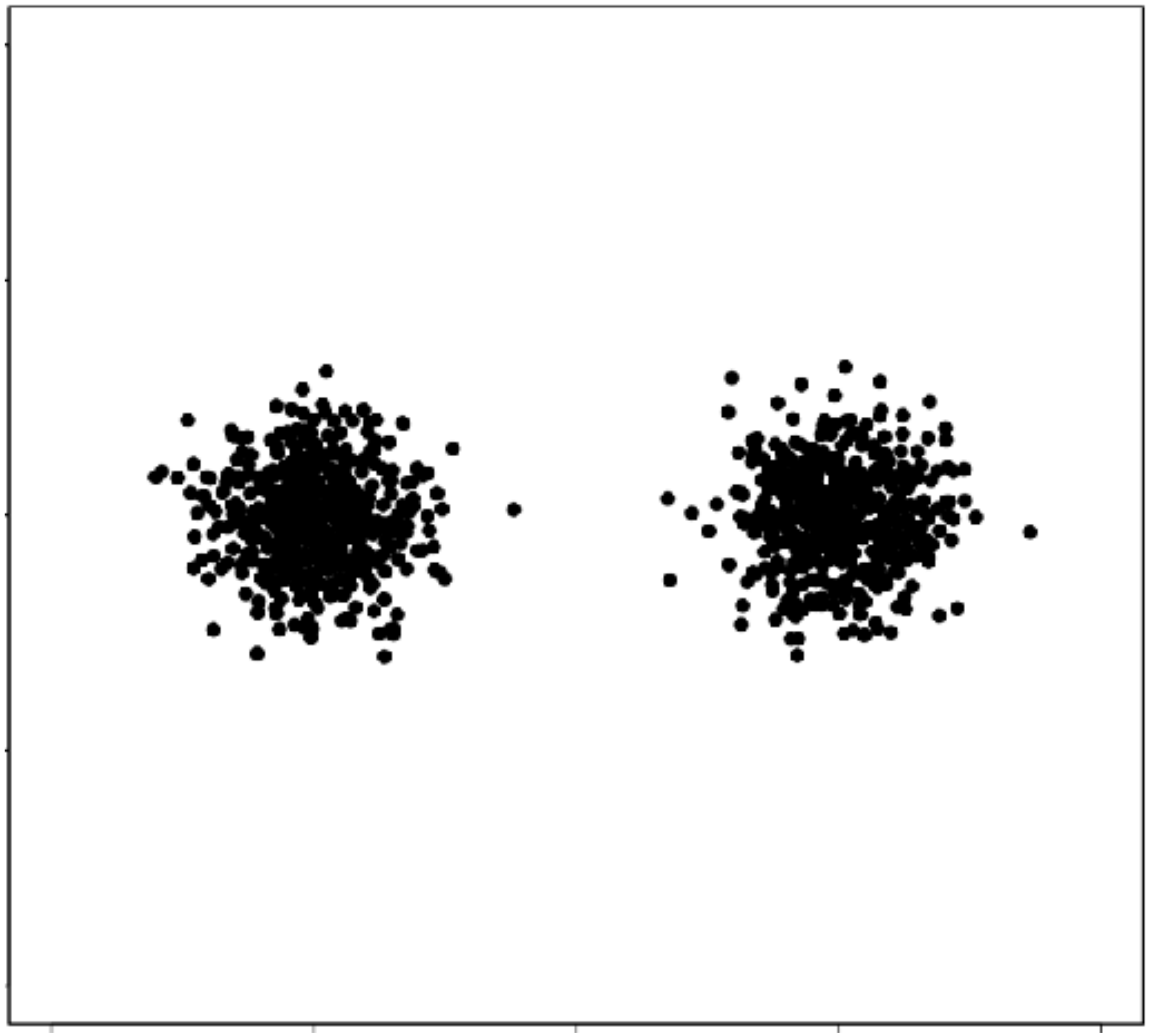

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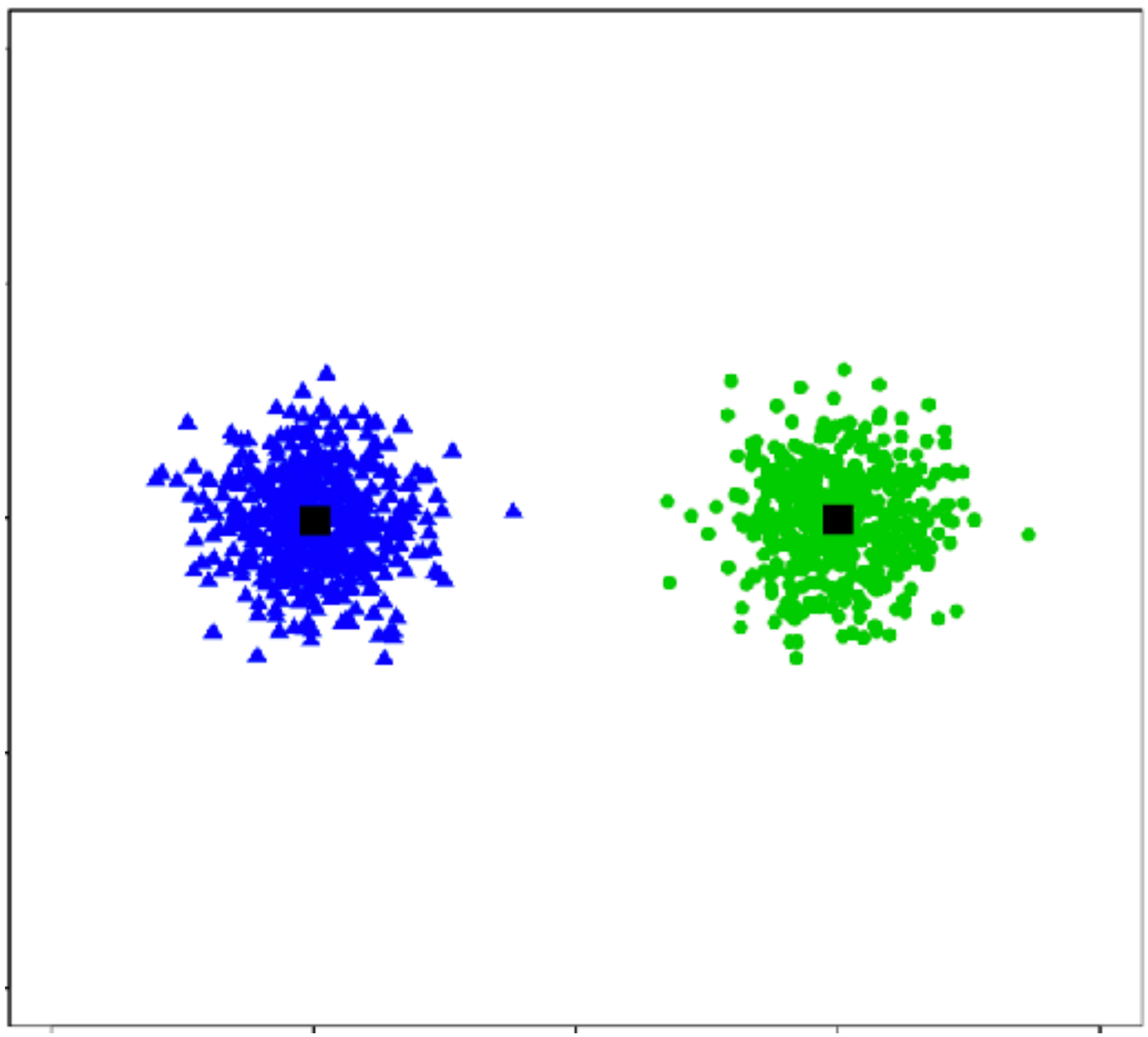

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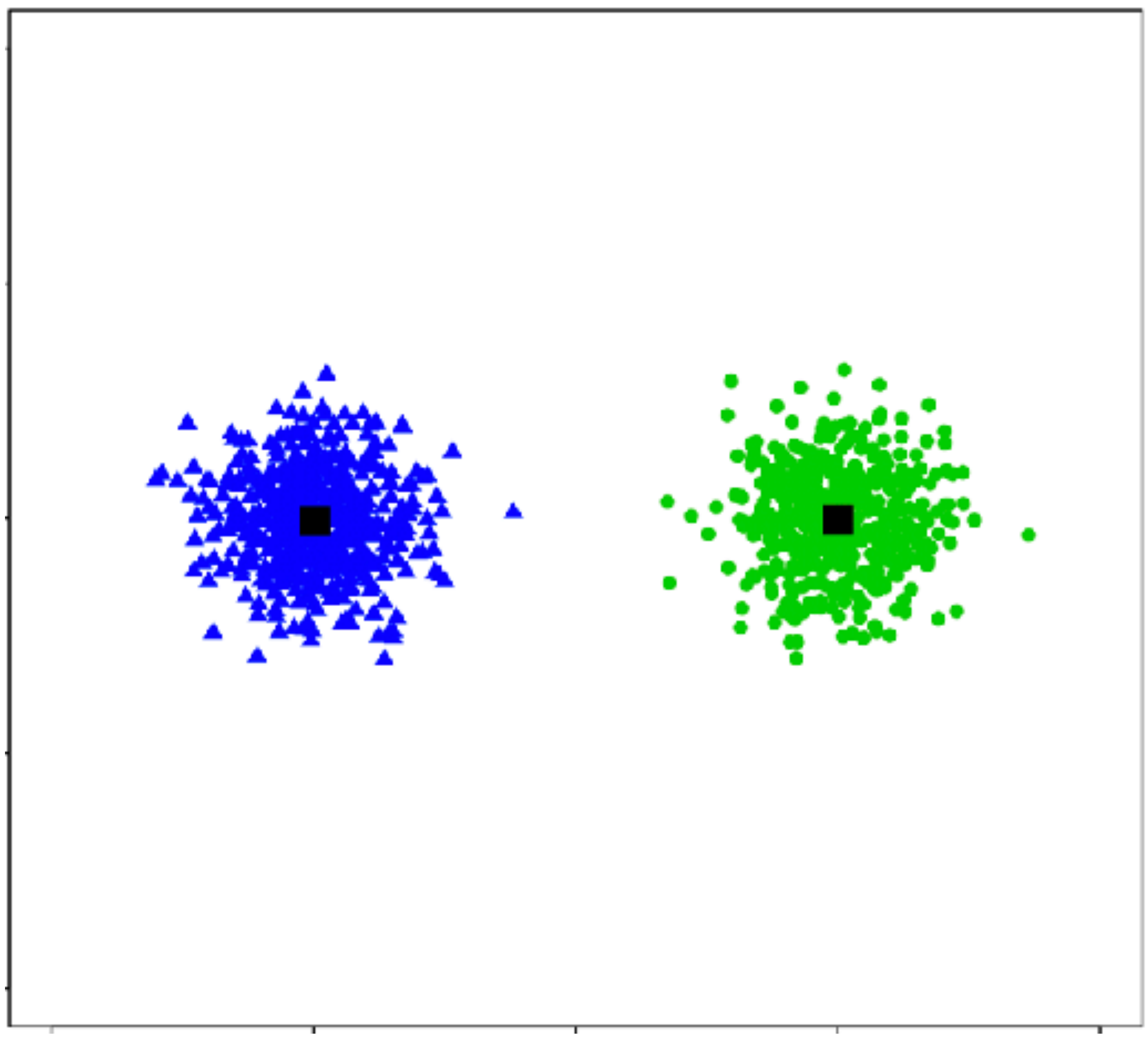

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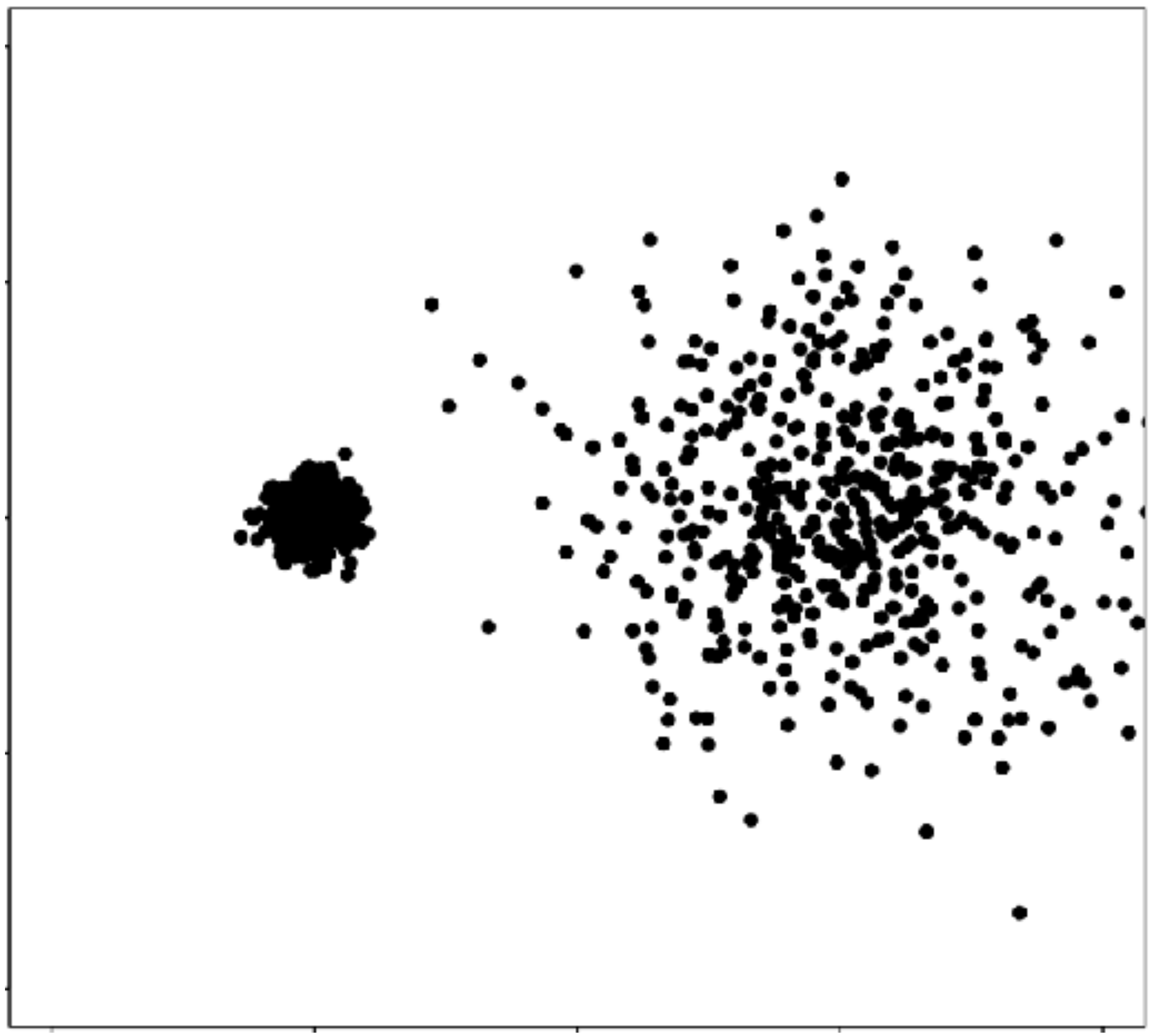

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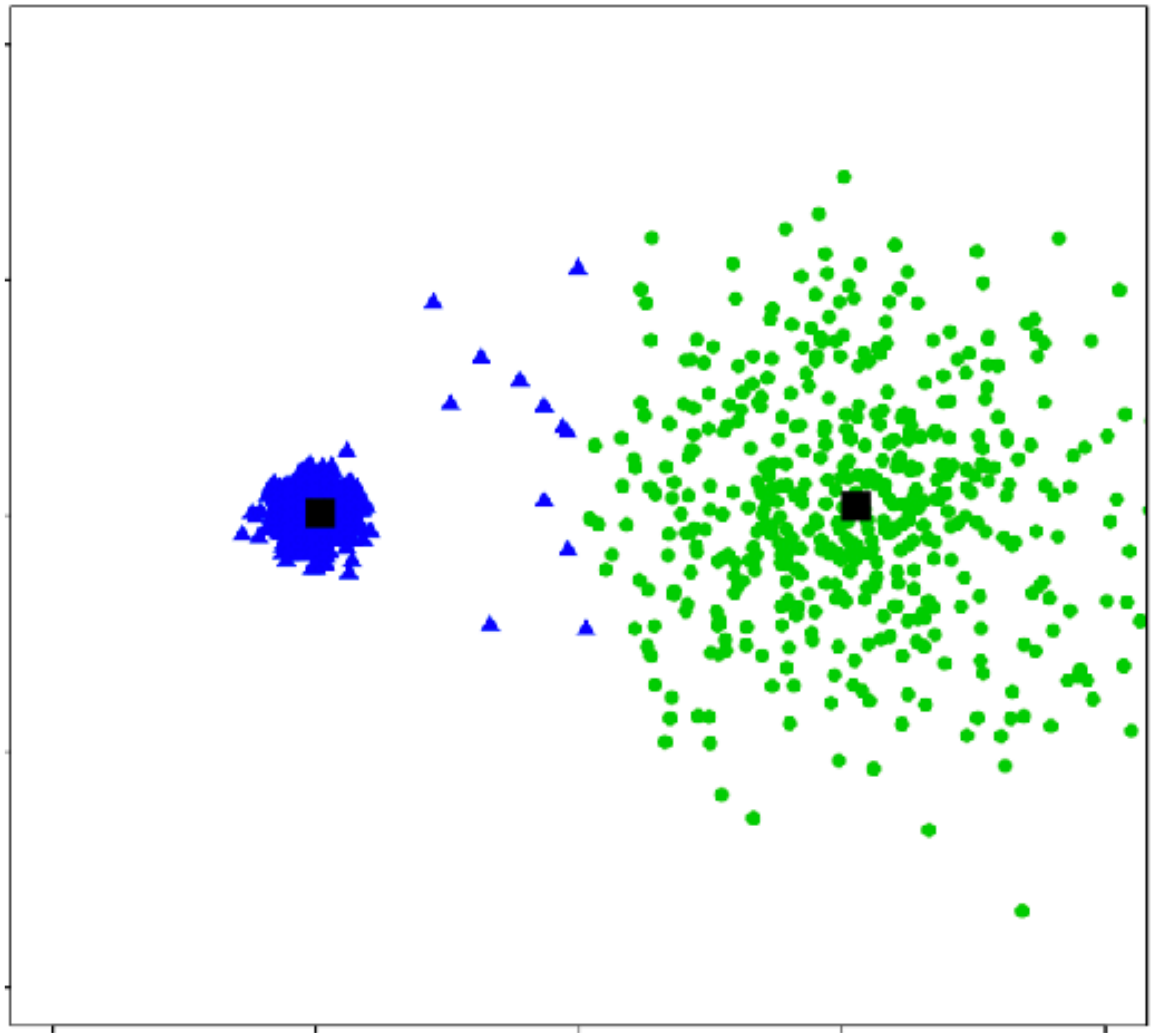

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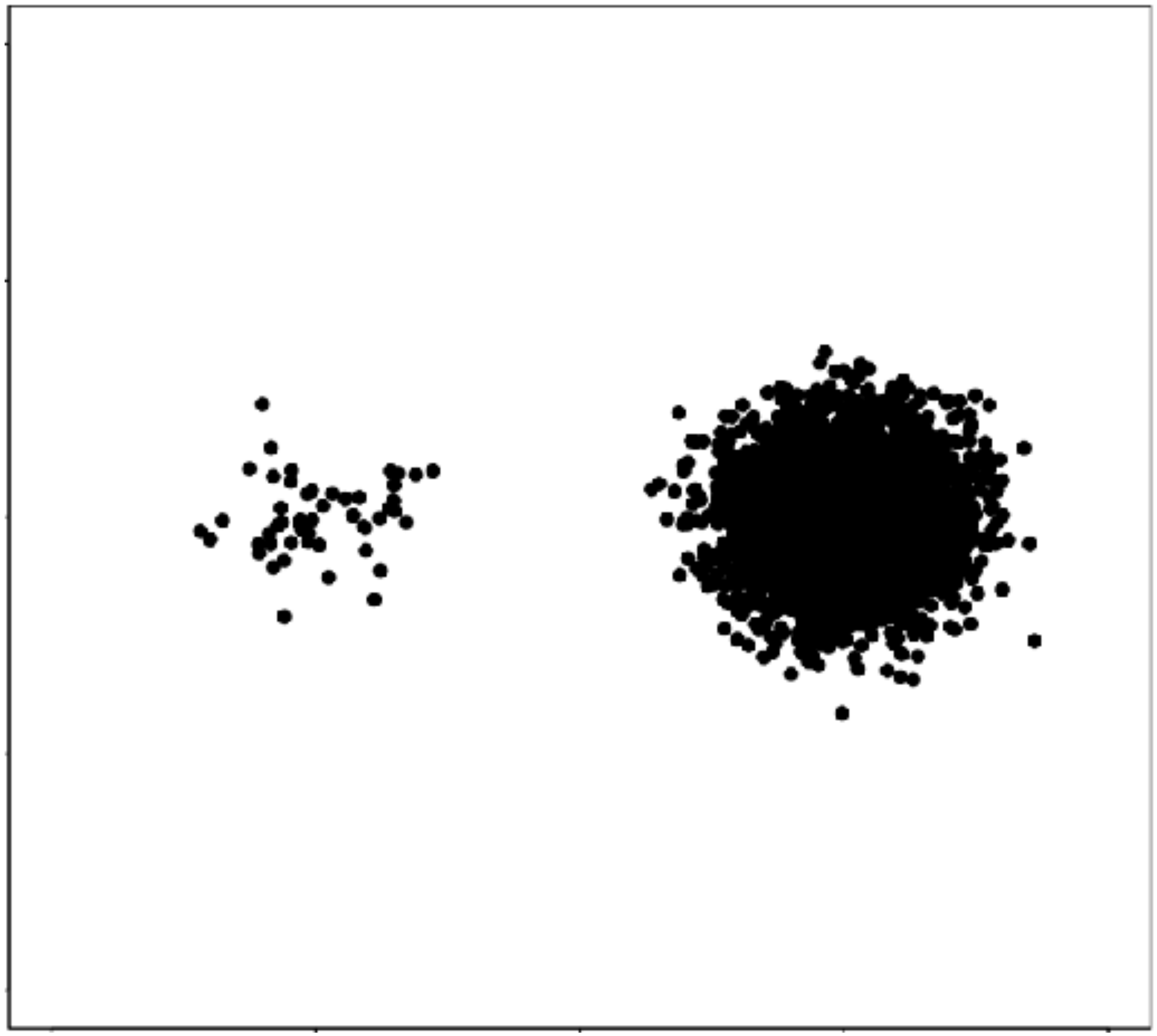

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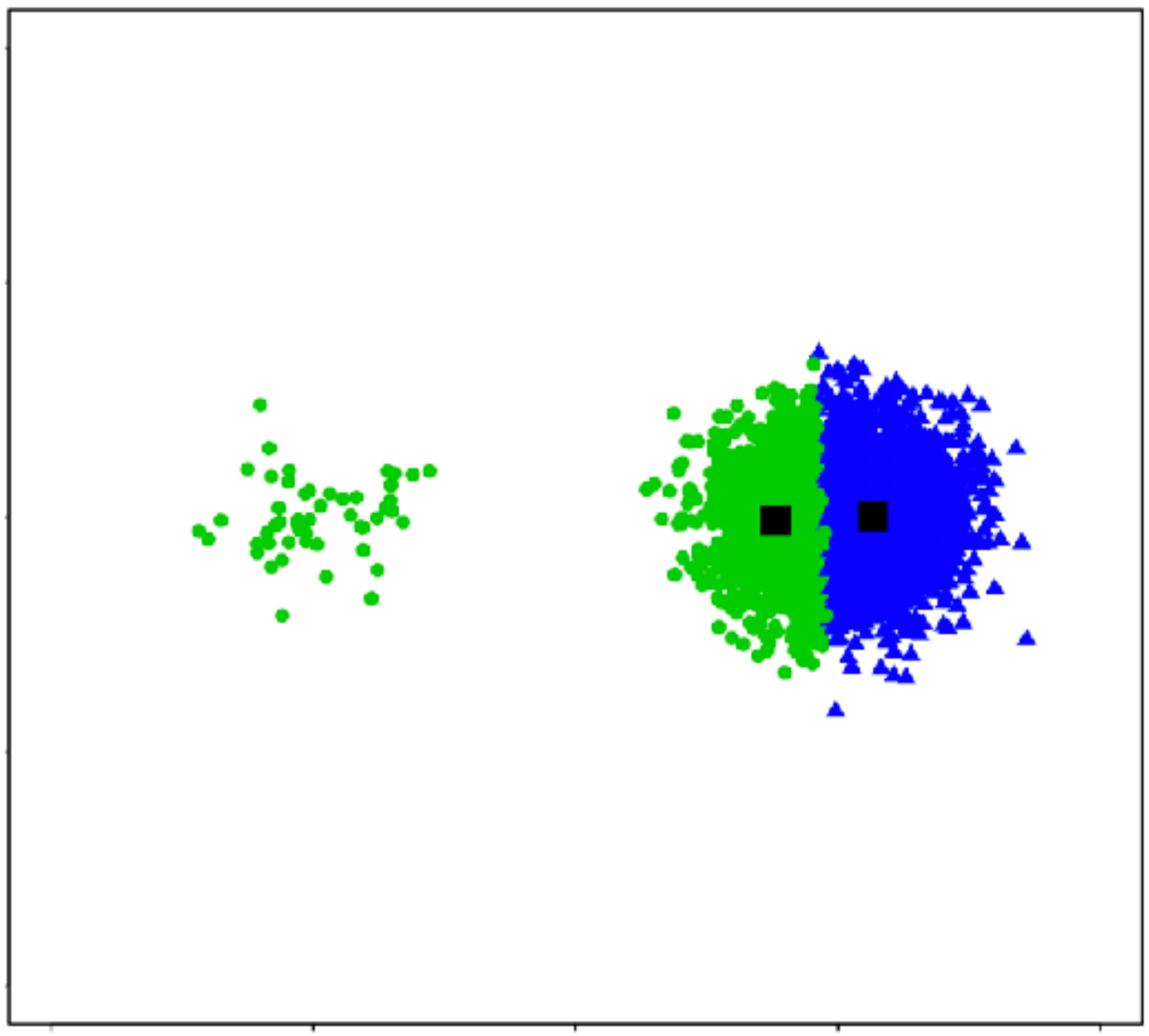

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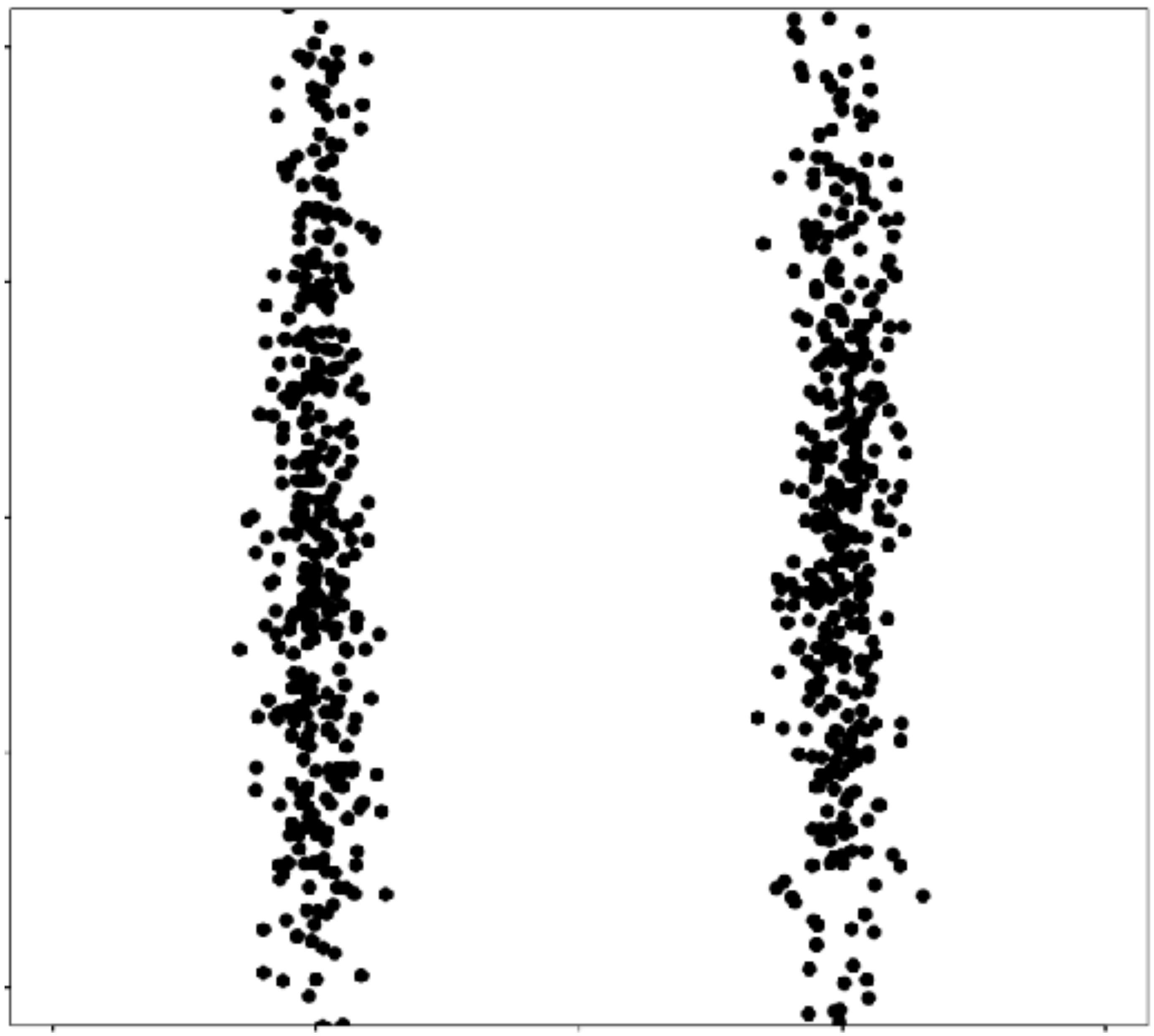

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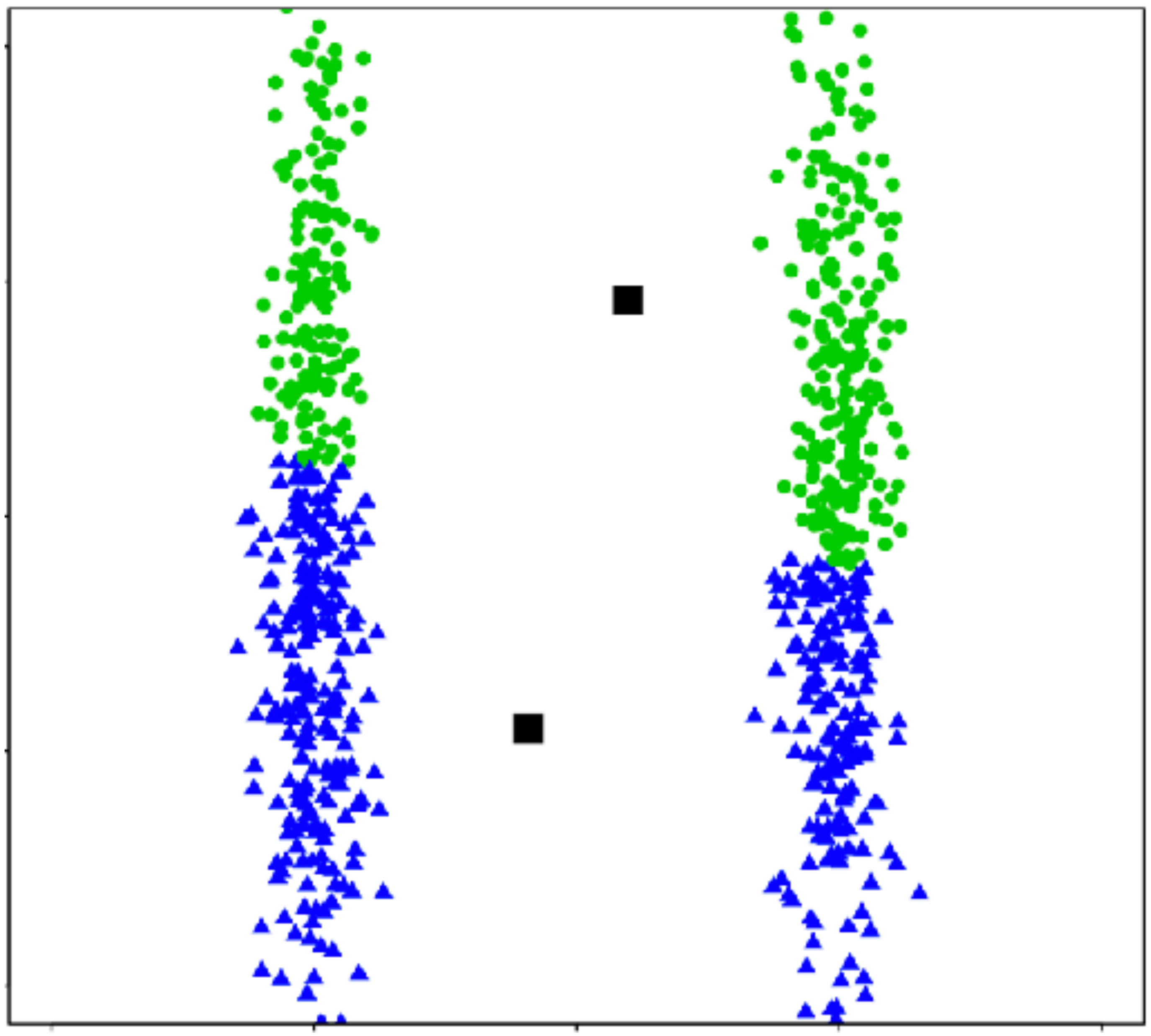

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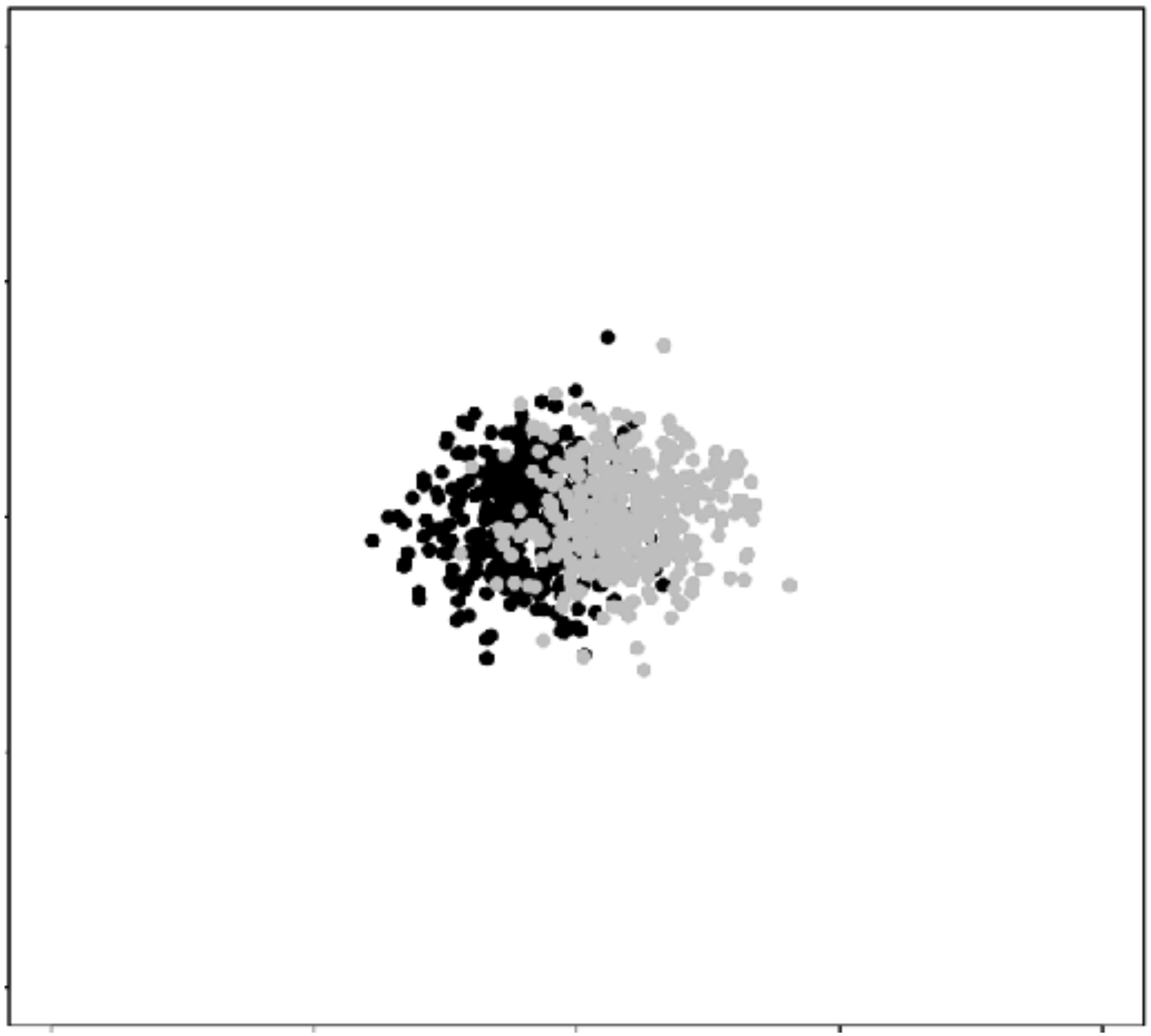

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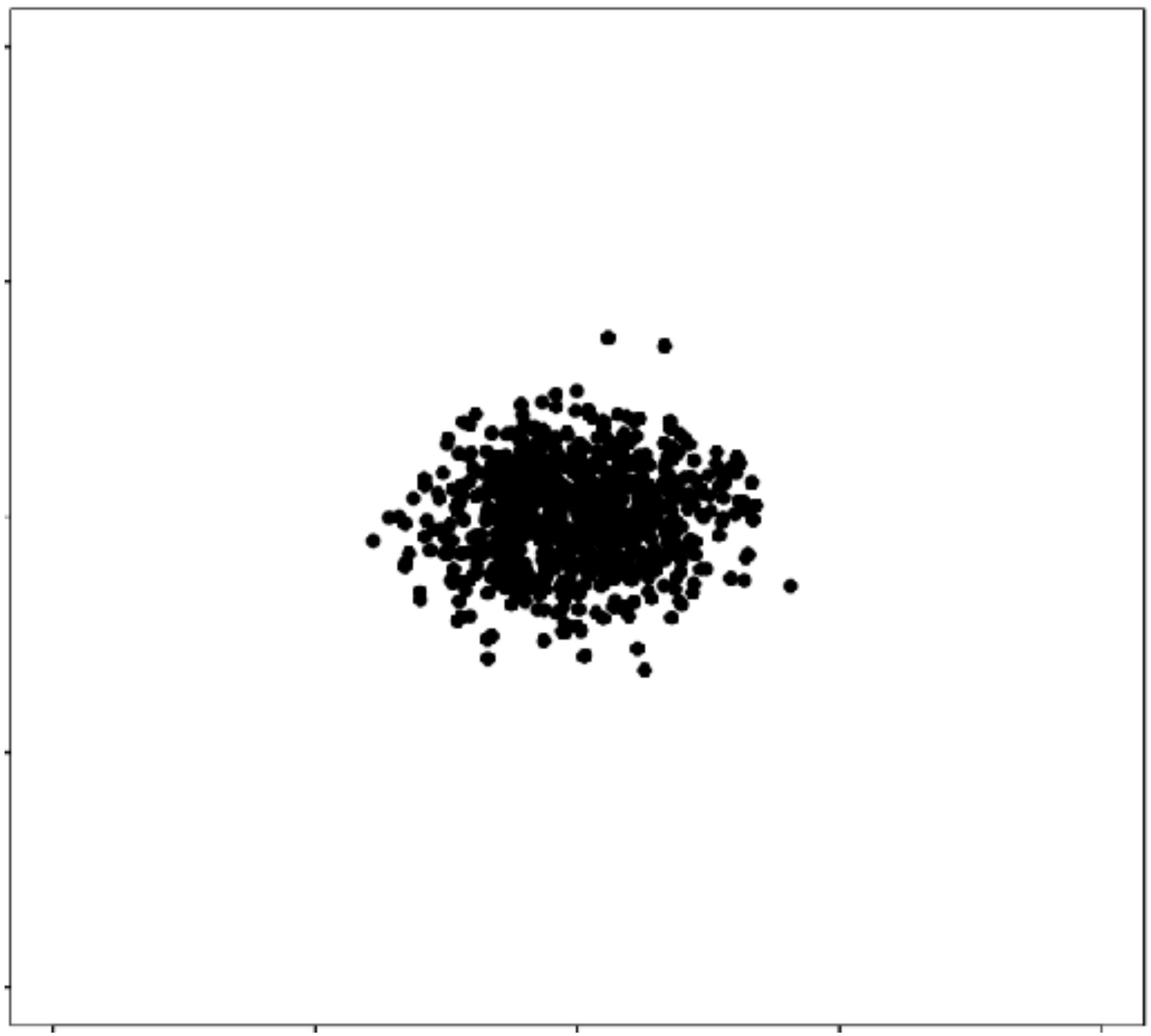

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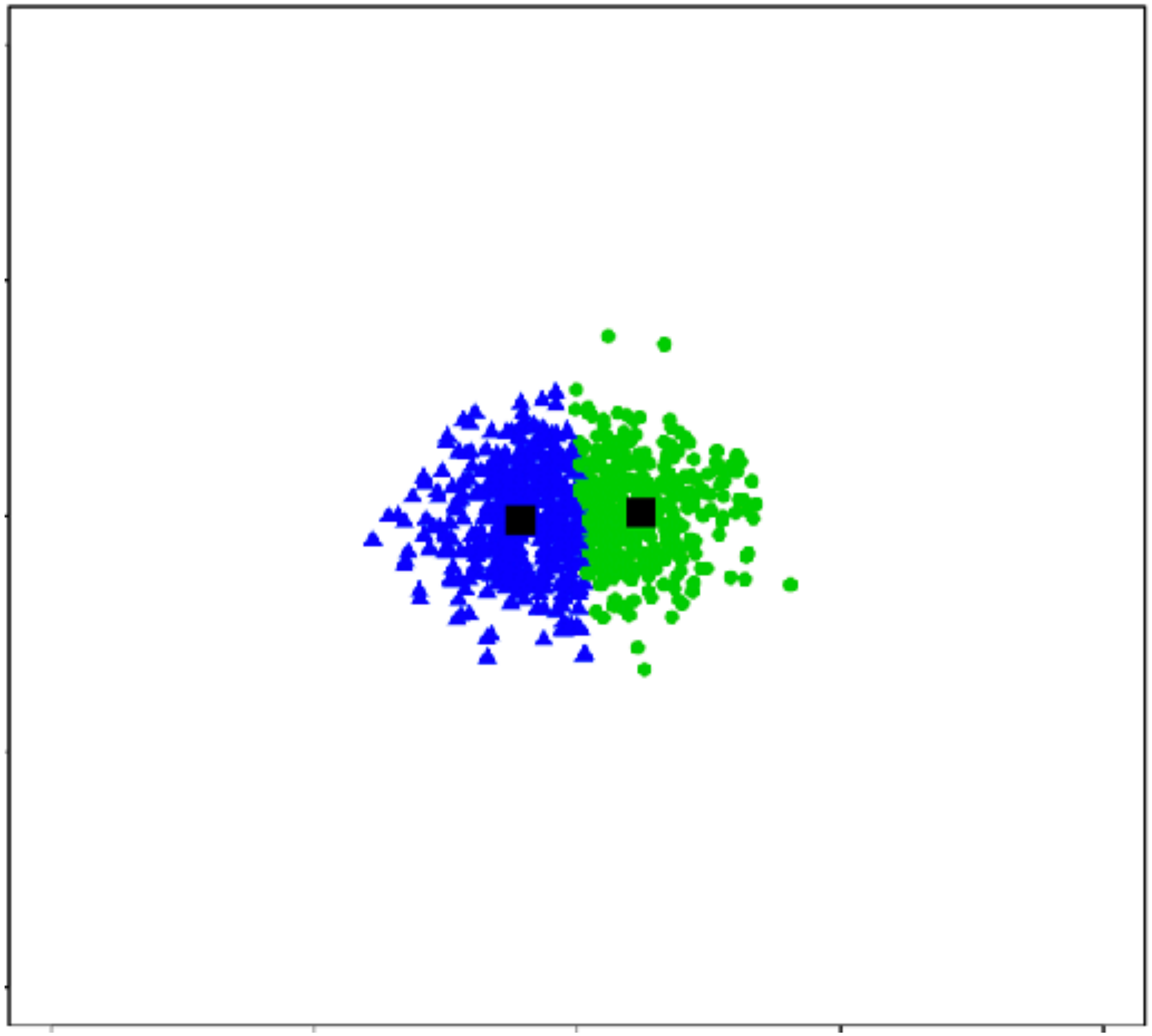

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Machine learning (ML): why & what

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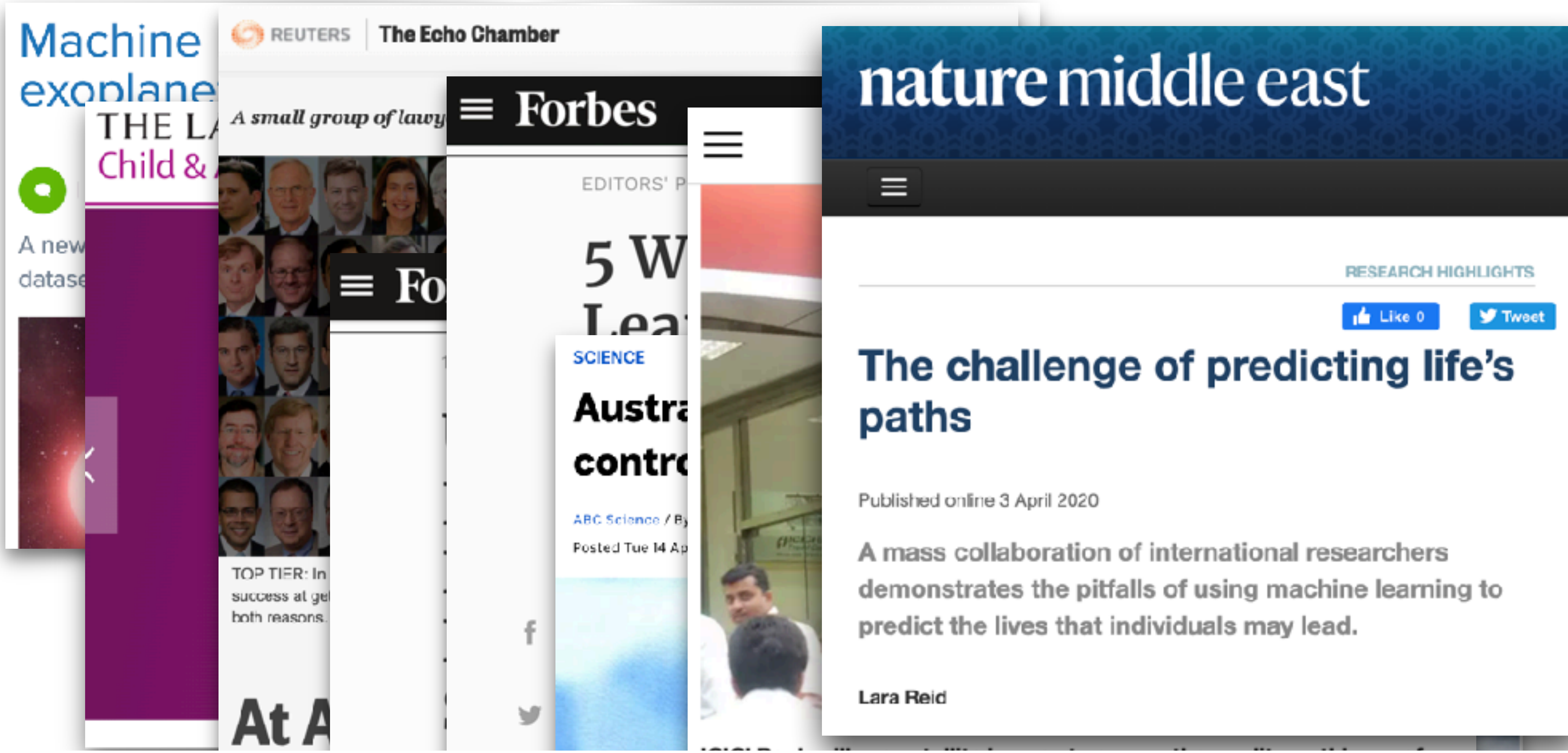

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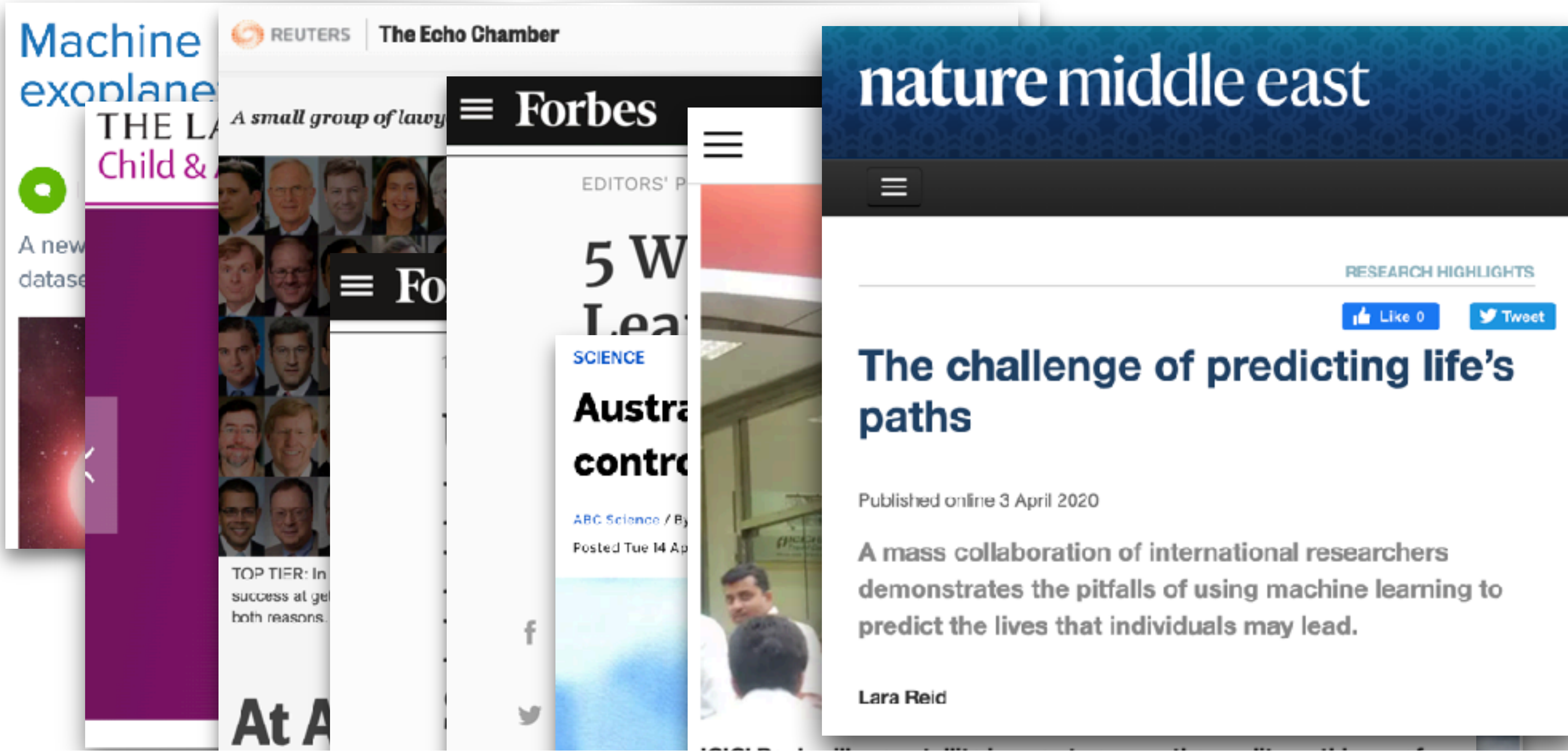

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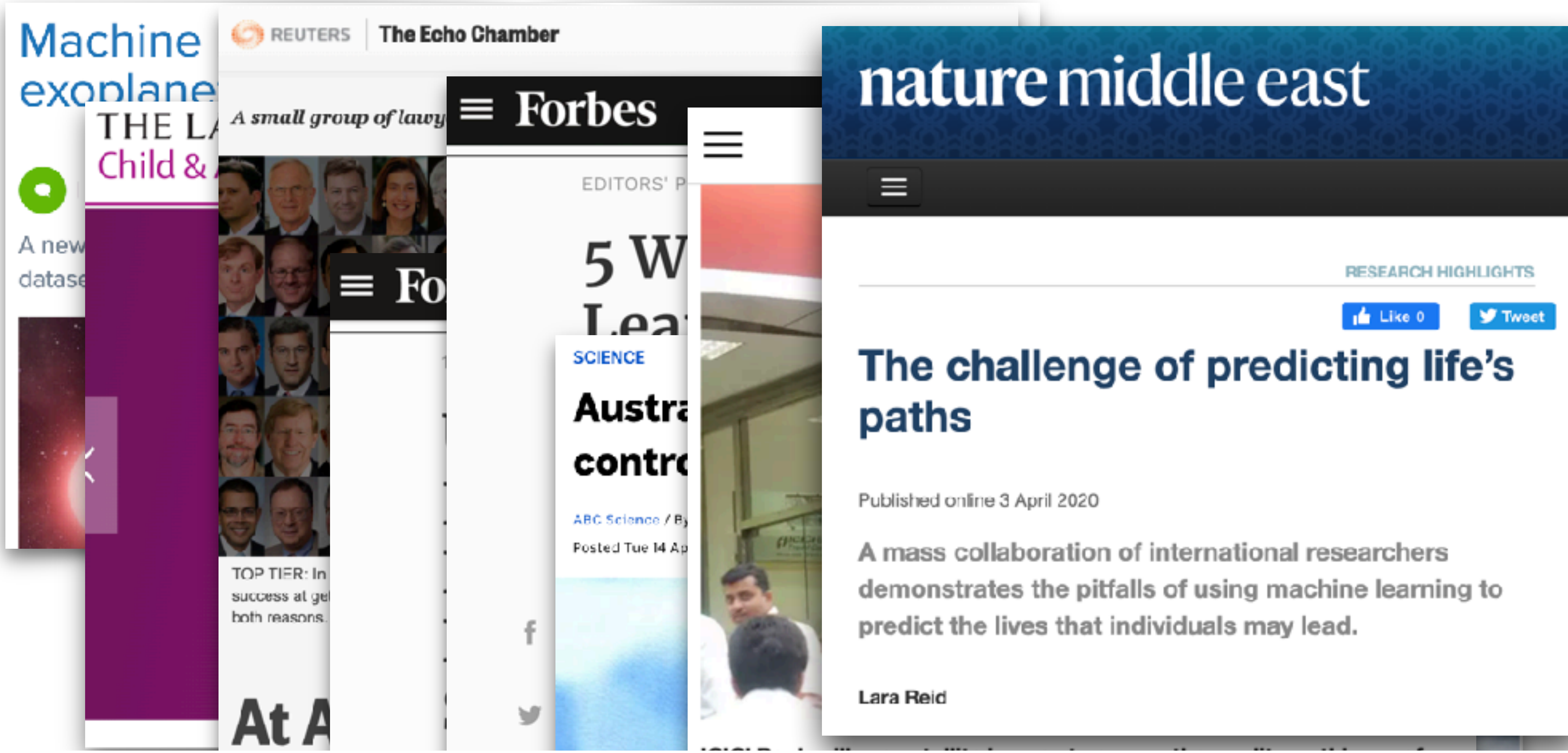

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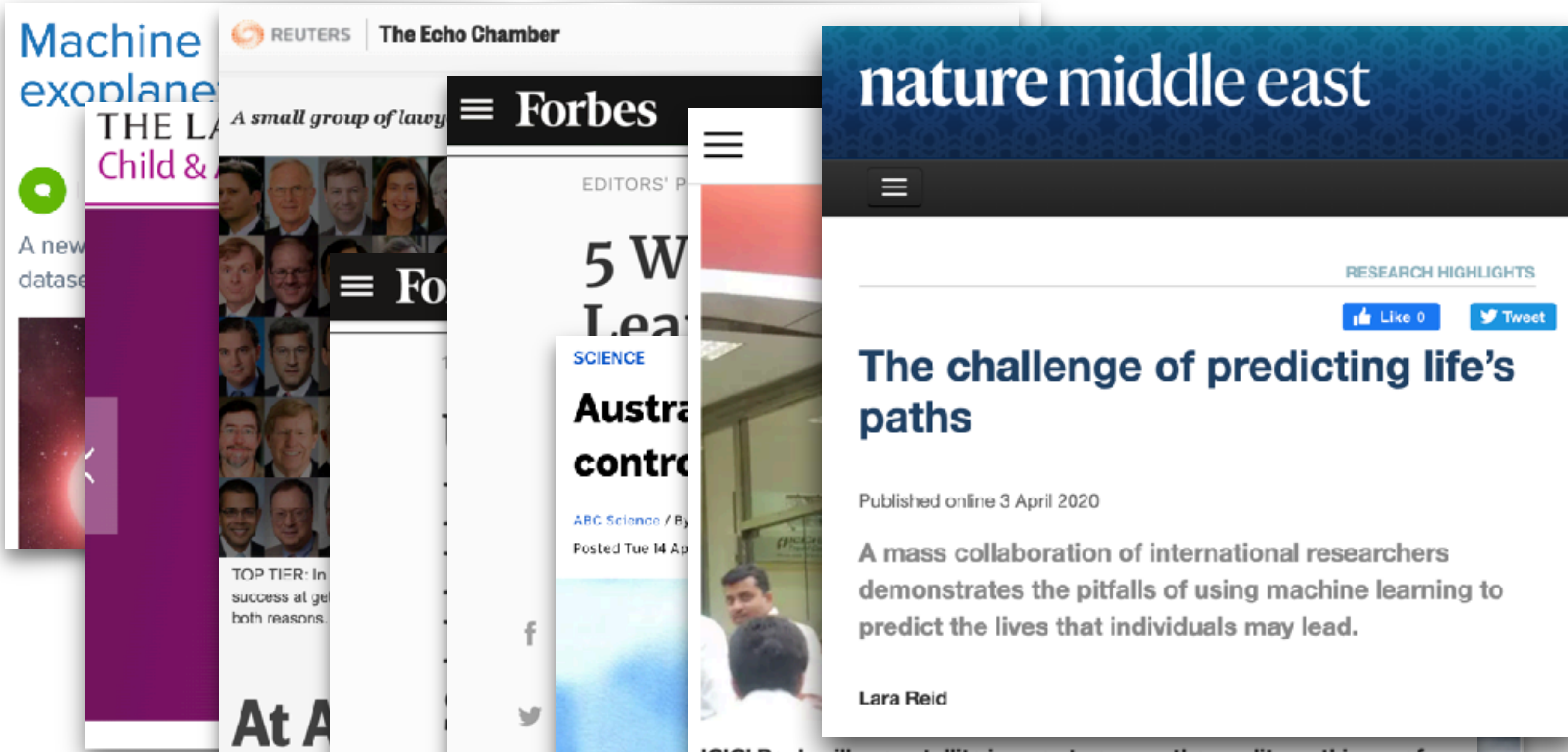

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- **Notes:** ML is not magic. ML is built on math.