AI for Social Good

- **10** Health
- **5** Environmental Sustainability
- **2** Hate speech
- **1** Assistive technology for people with disabilities

Unsupervised Learning

Machine Learning

Prof. Sandra Avila

Institute of Computing (IC/Unicamp)

MC886/MO444, October 6, 2022

Types of Machine Learning Systems

Types of Machine Learning Systems

Trained with human supervision (or not)

Supervised *vs.* Unsupervised *vs.* Reinforcement learning

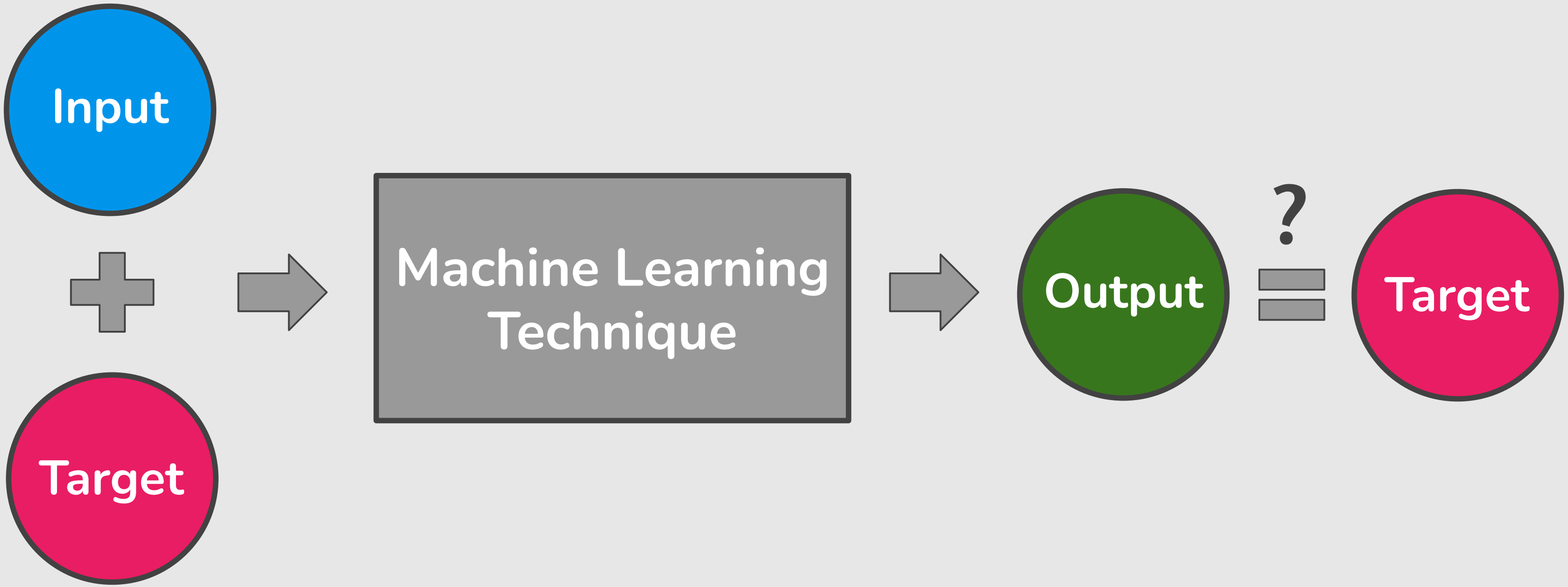
Can learn incrementally on the fly (or not)

Online *vs.* Batch Learning

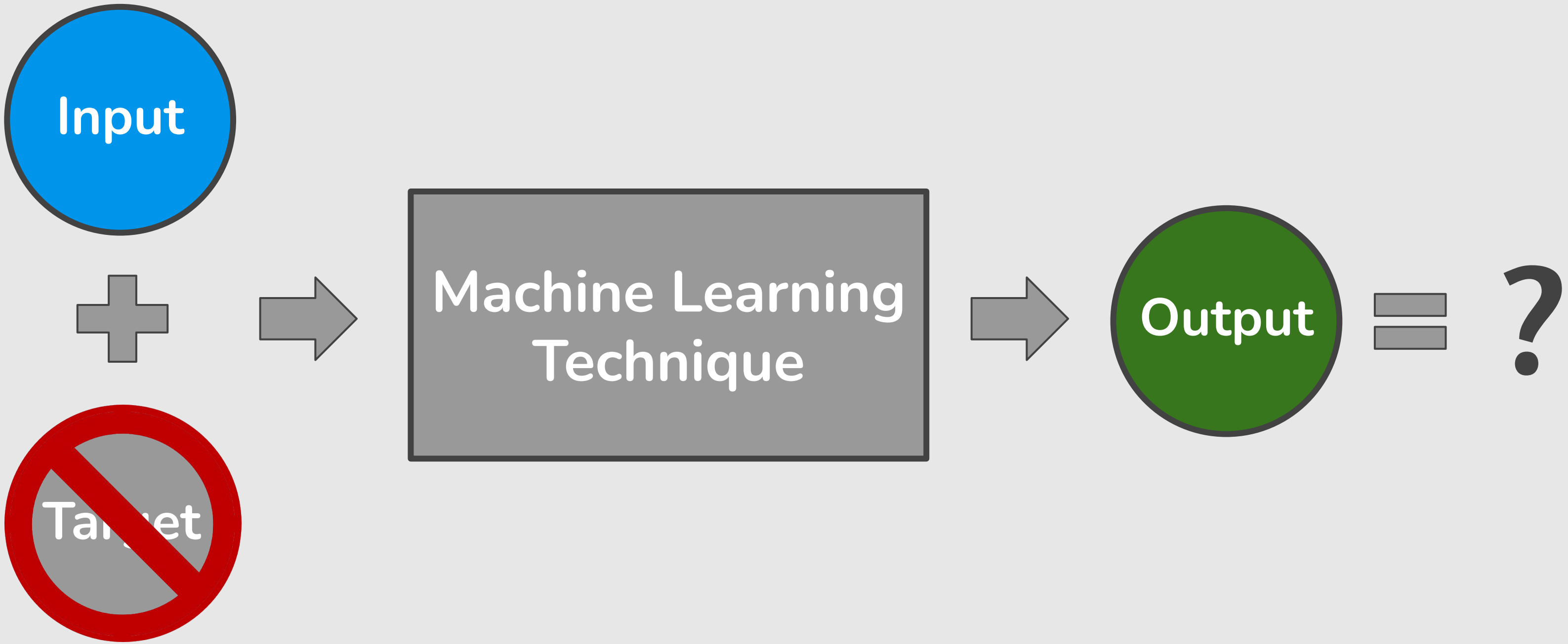
How they generalize

Instance based *vs.* Model based learning

Supervised Learning



Unsupervised Learning



Unsupervised Learning

The goal of unsupervised learning is **to find patterns** in the data, and build new and useful representations of it.

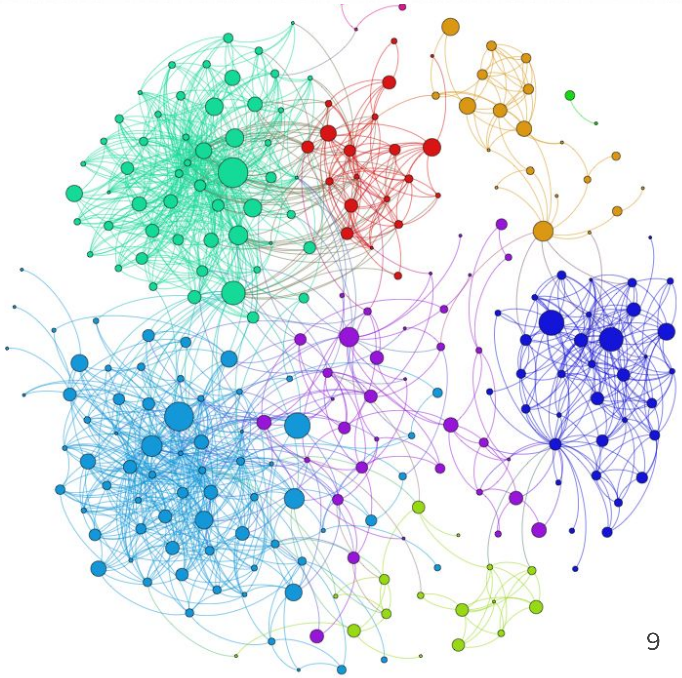
Unsupervised Learning

Clustering algorithm tries to detect similar groups.

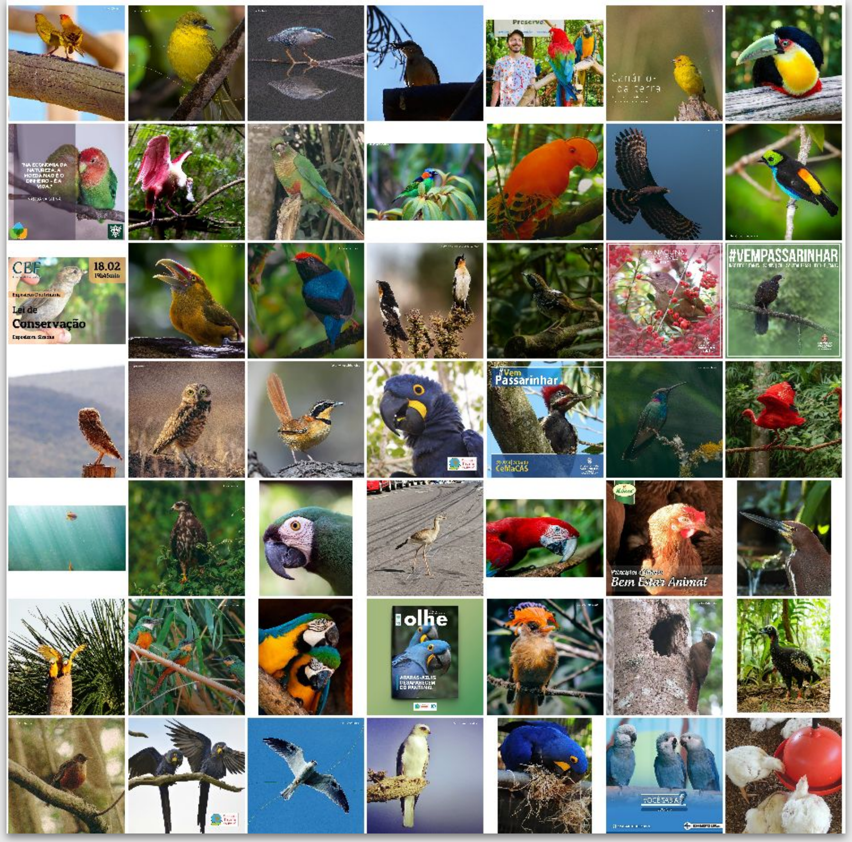
Dimensionality reduction tries to simplify the data without losing too much information.

Applications

- Social network analysis
- Market segmentation
- Information compression
- Information retrieval
- ...



#PraCegoVer Dataset



Today's Agenda

- Clustering
  - k-Means Algorithm
  - Optimization Objective
  - Random Initialization
  - Choosing the Number of Clusters
  - Additional Issues

Clustering

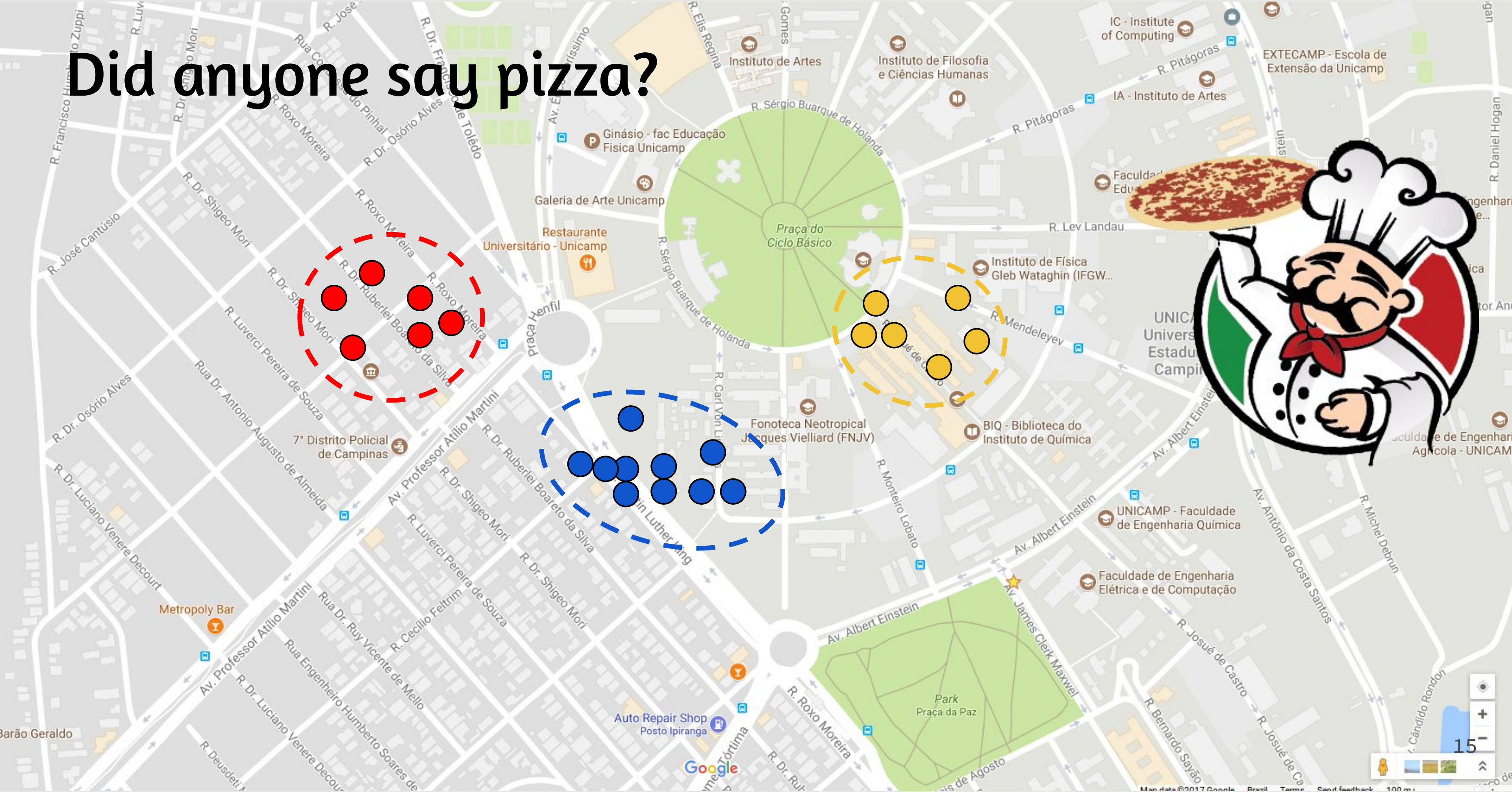
k-Means Algorithm

Did anyone say pizza?

https://www.youtube.com/watch?v=lpGxLWOIZy4

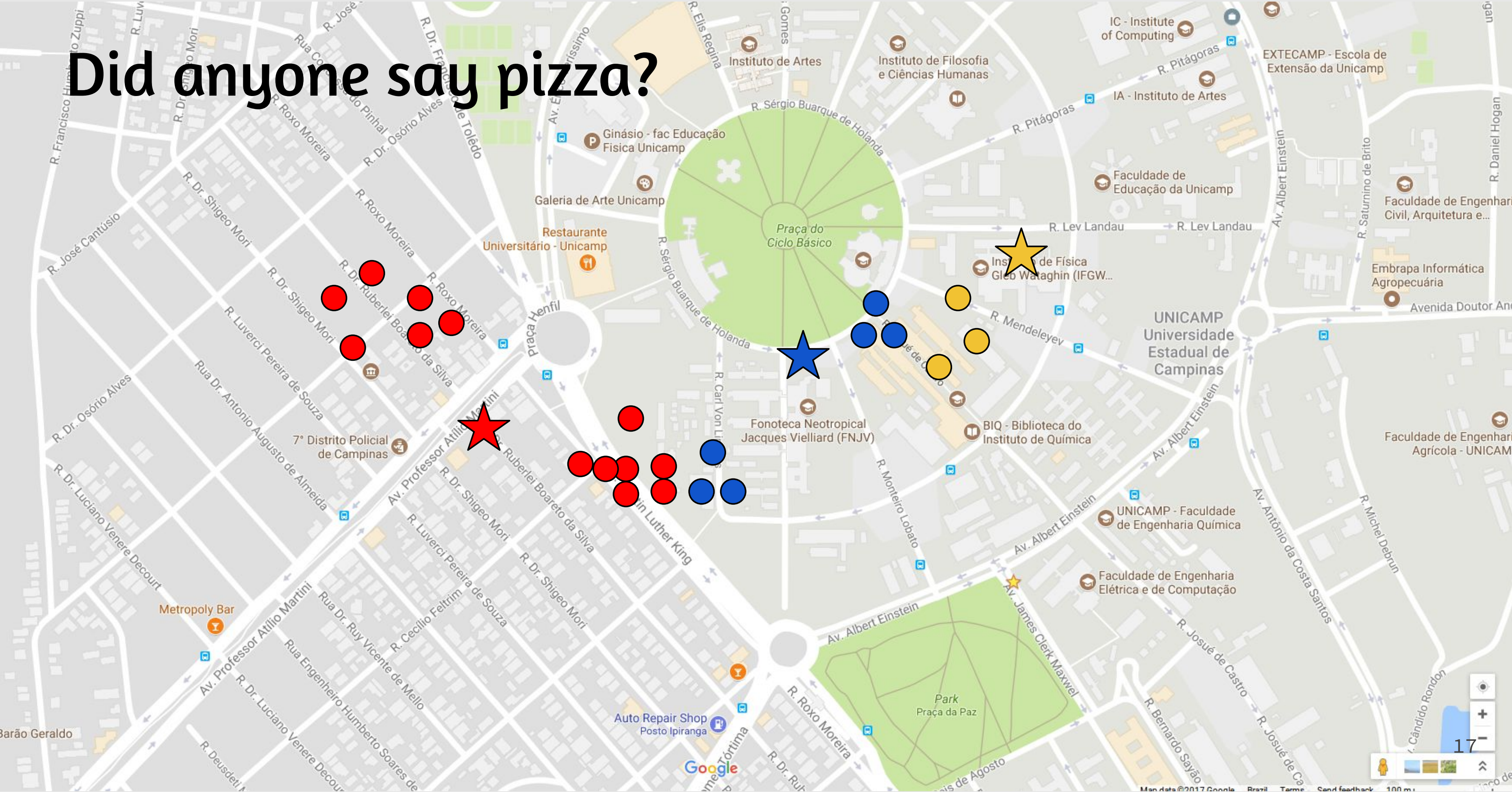
Did anyone say pizza?

Did anyone say pizza?



Did anyone say pizza?

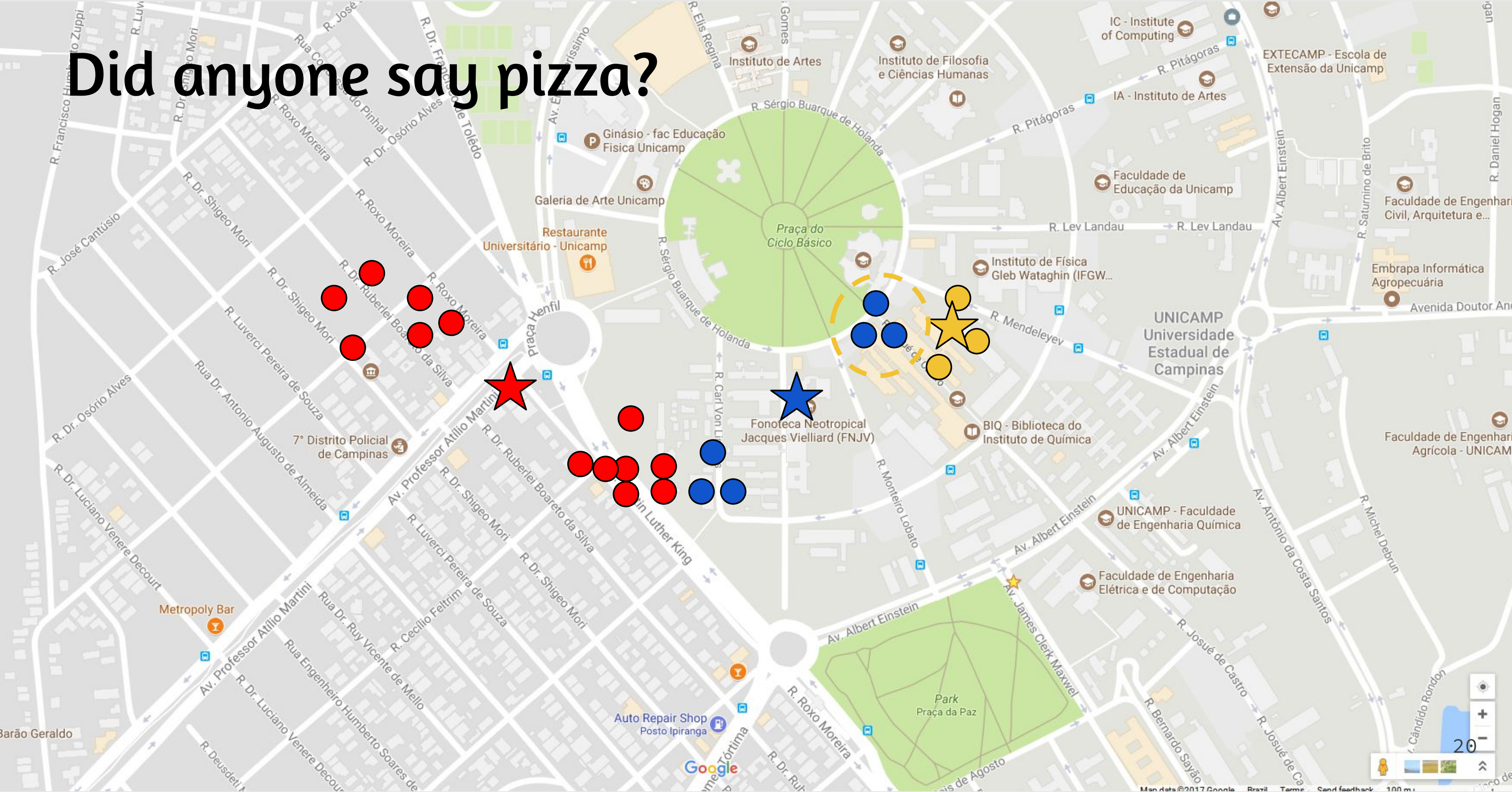
Did anyone say pizza?



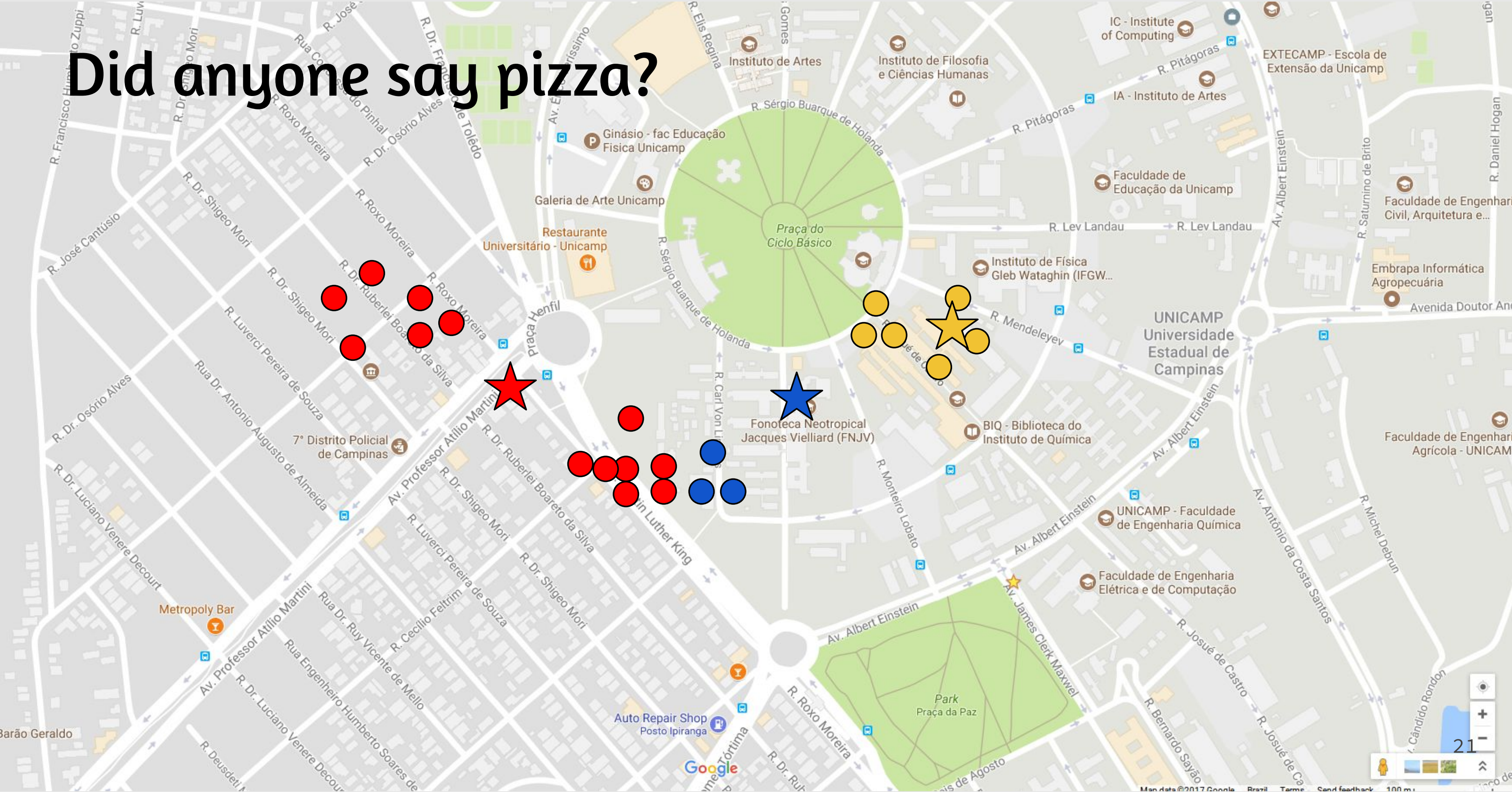
Did anyone say pizza?

Did anyone say pizza?

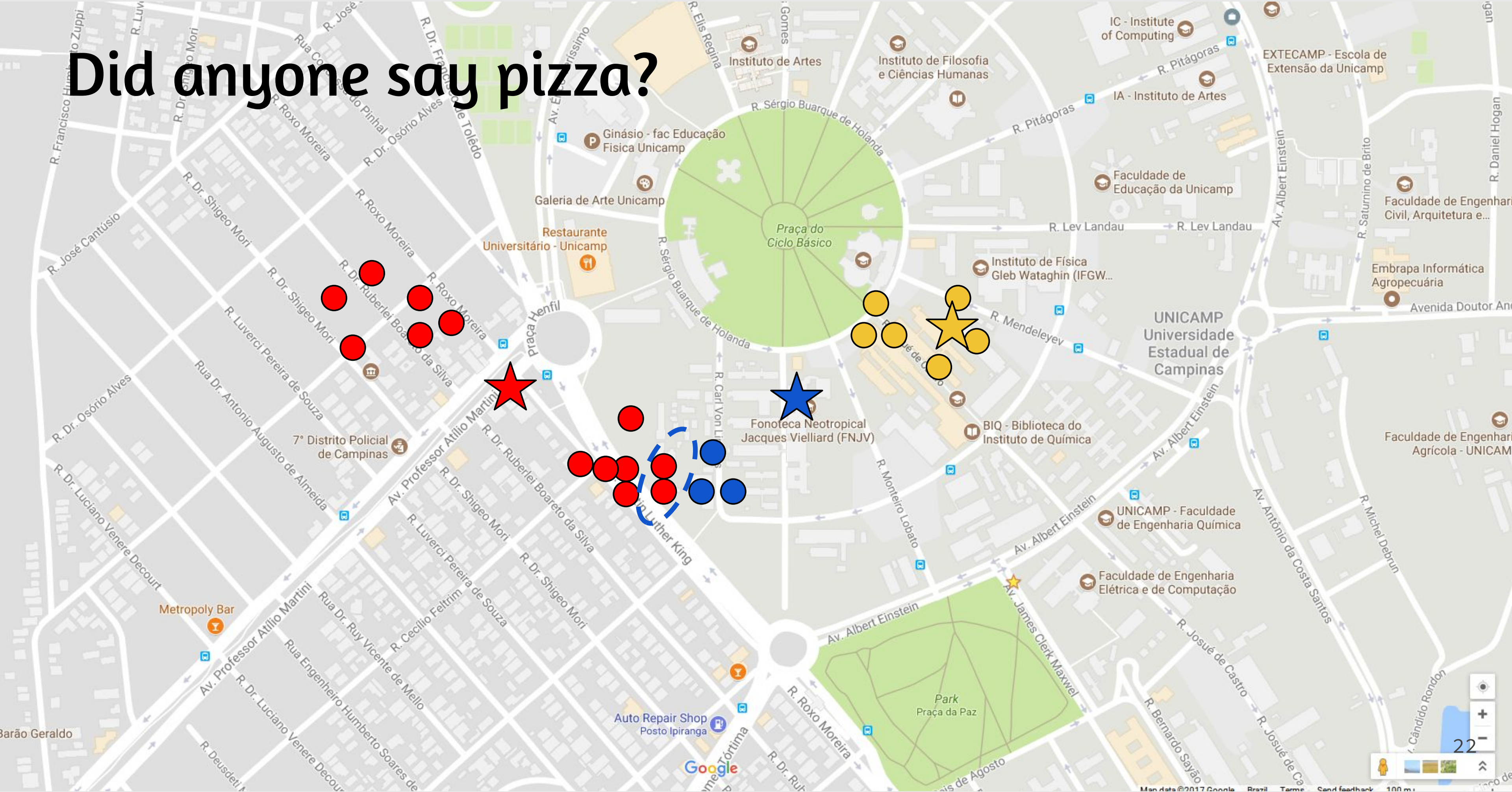
Did anyone say pizza?



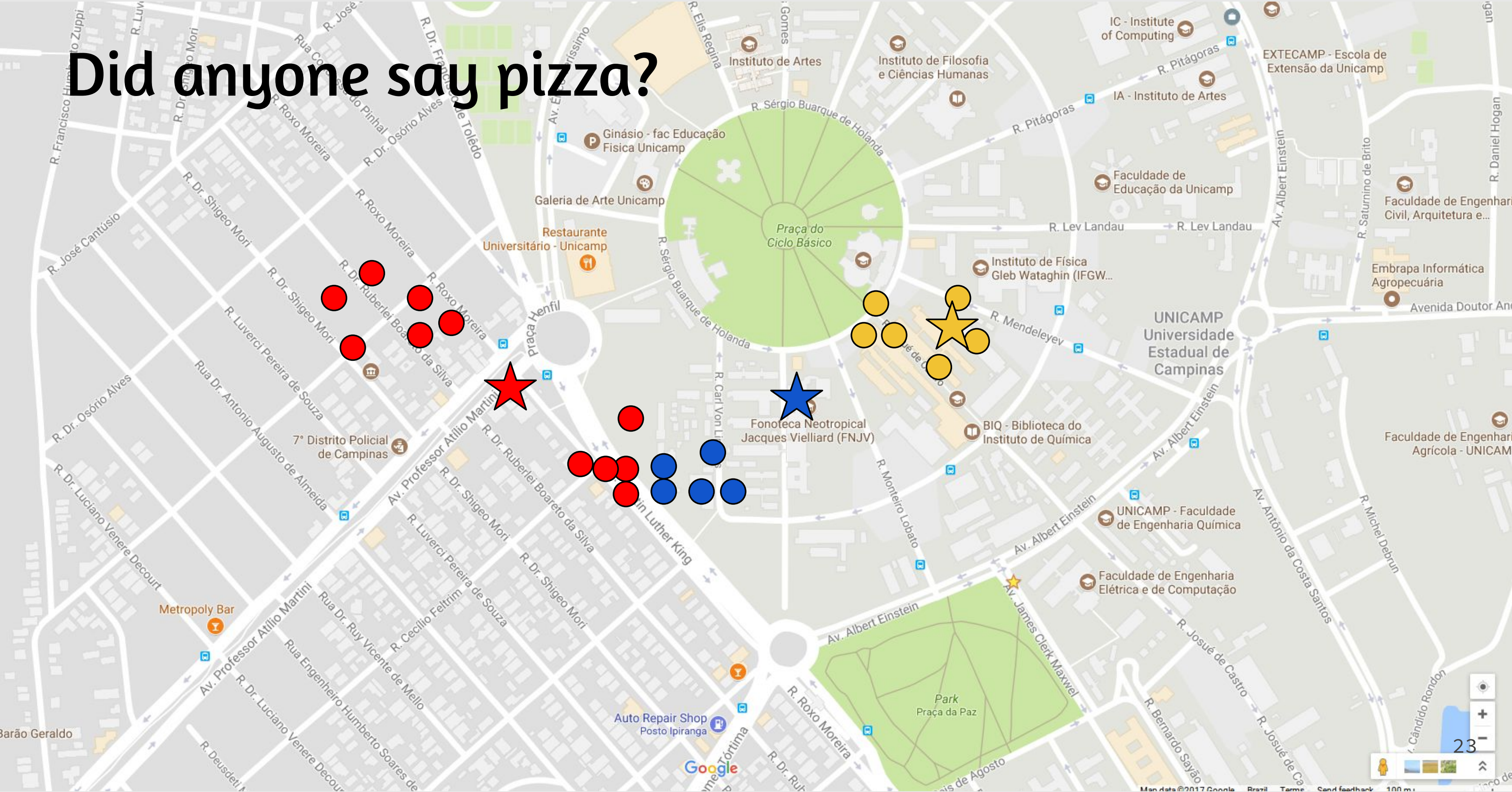
Did anyone say pizza?



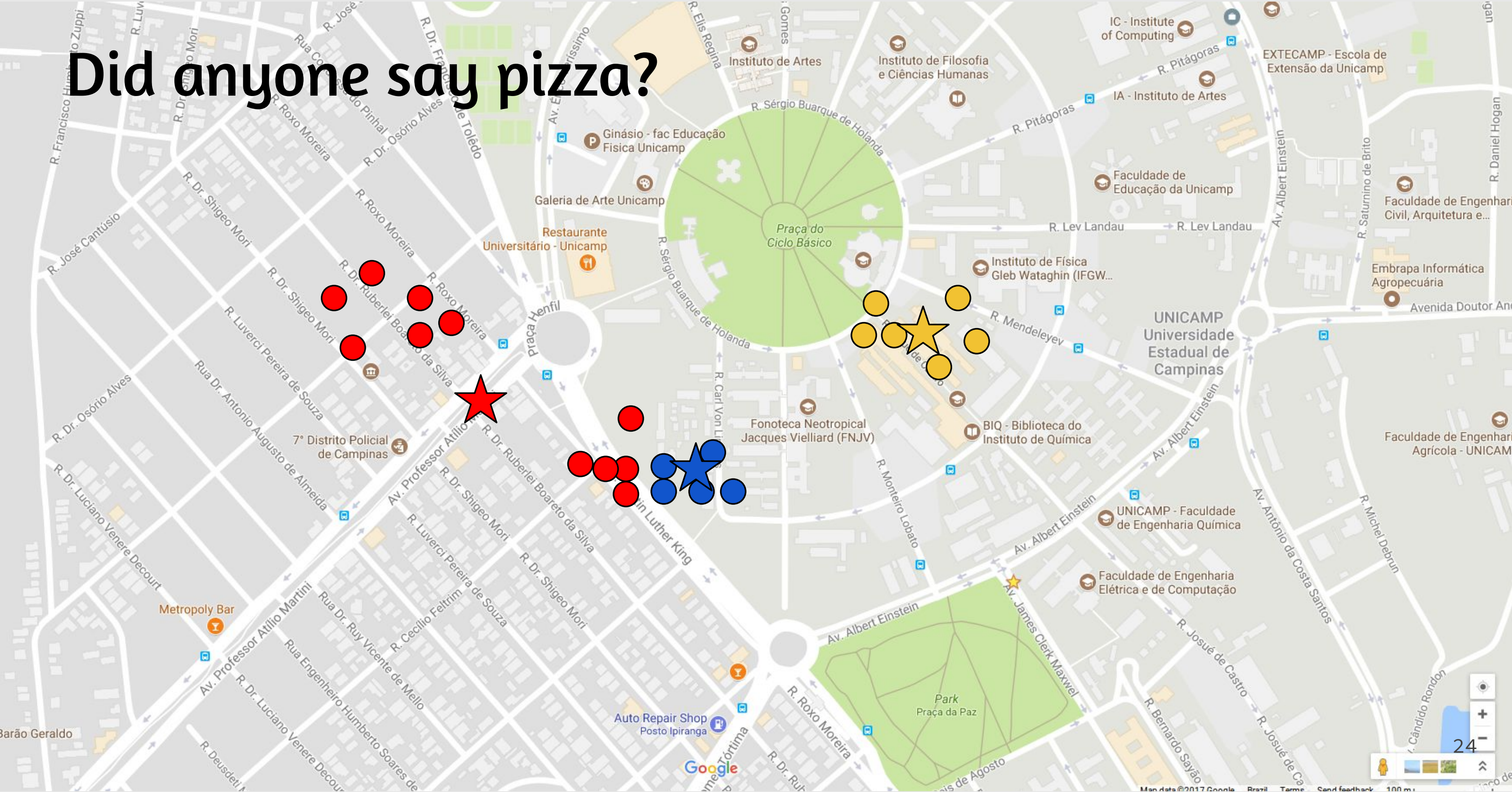
Did anyone say pizza?



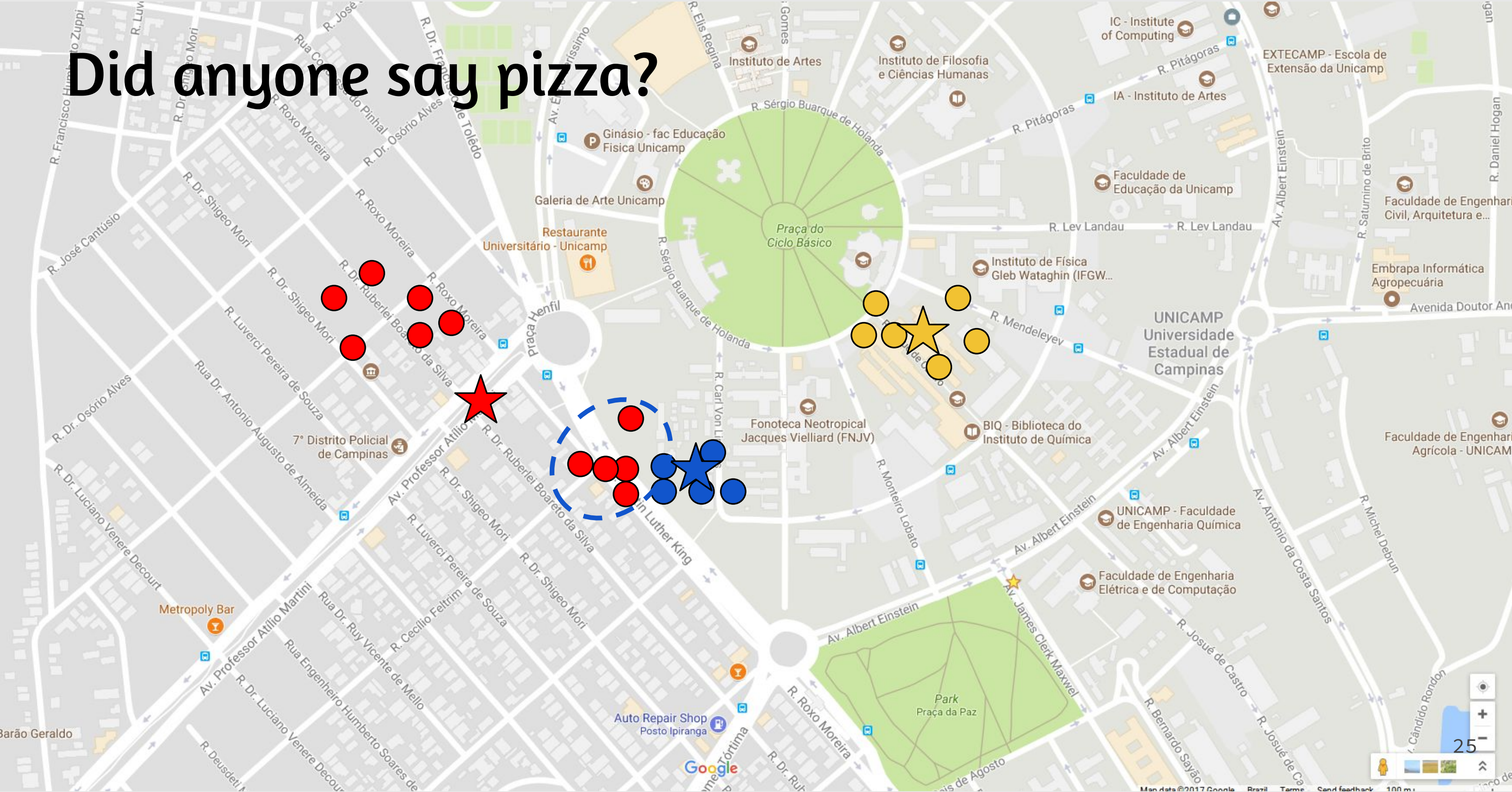
Did anyone say pizza?



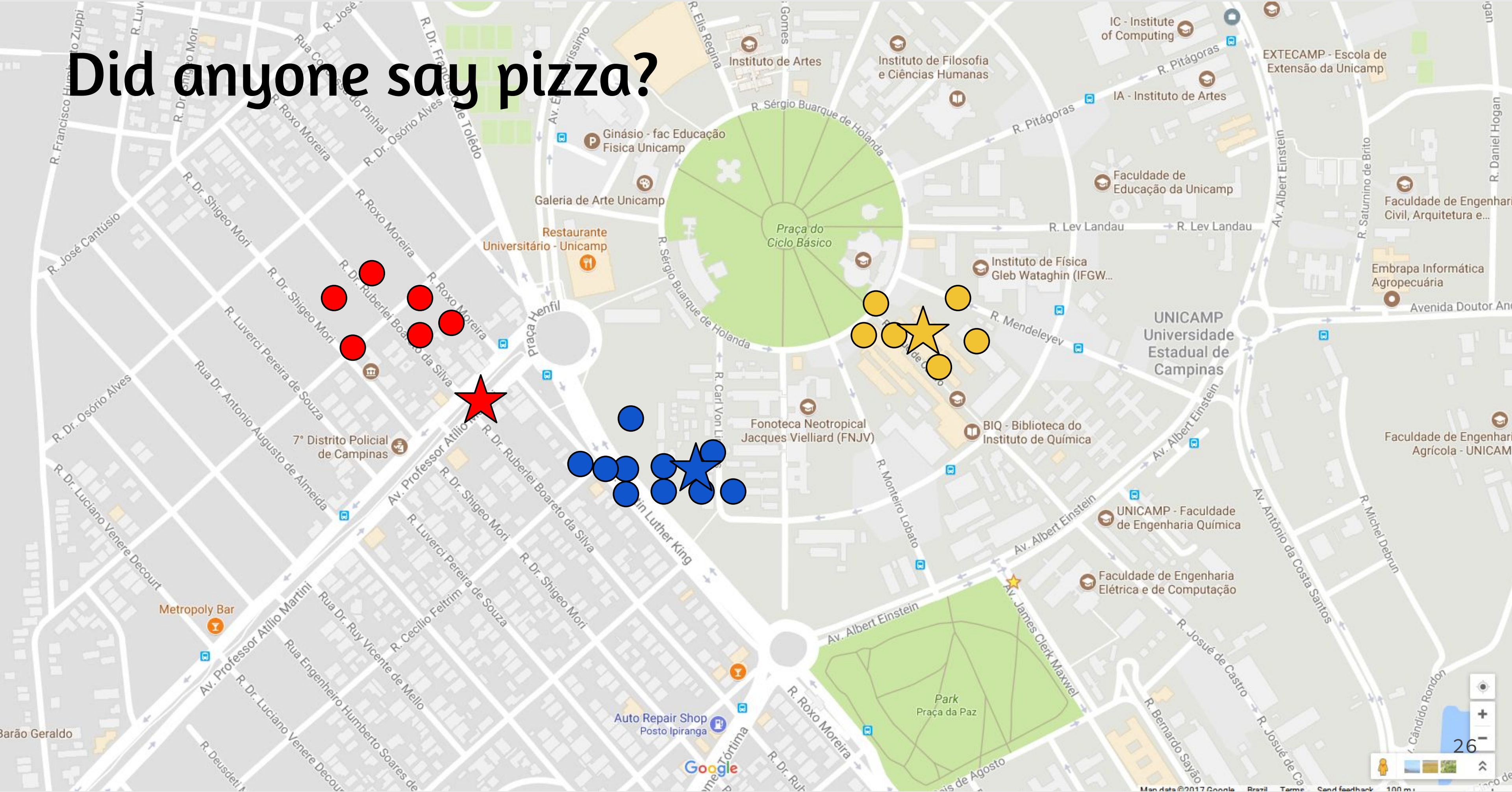
Did anyone say pizza?



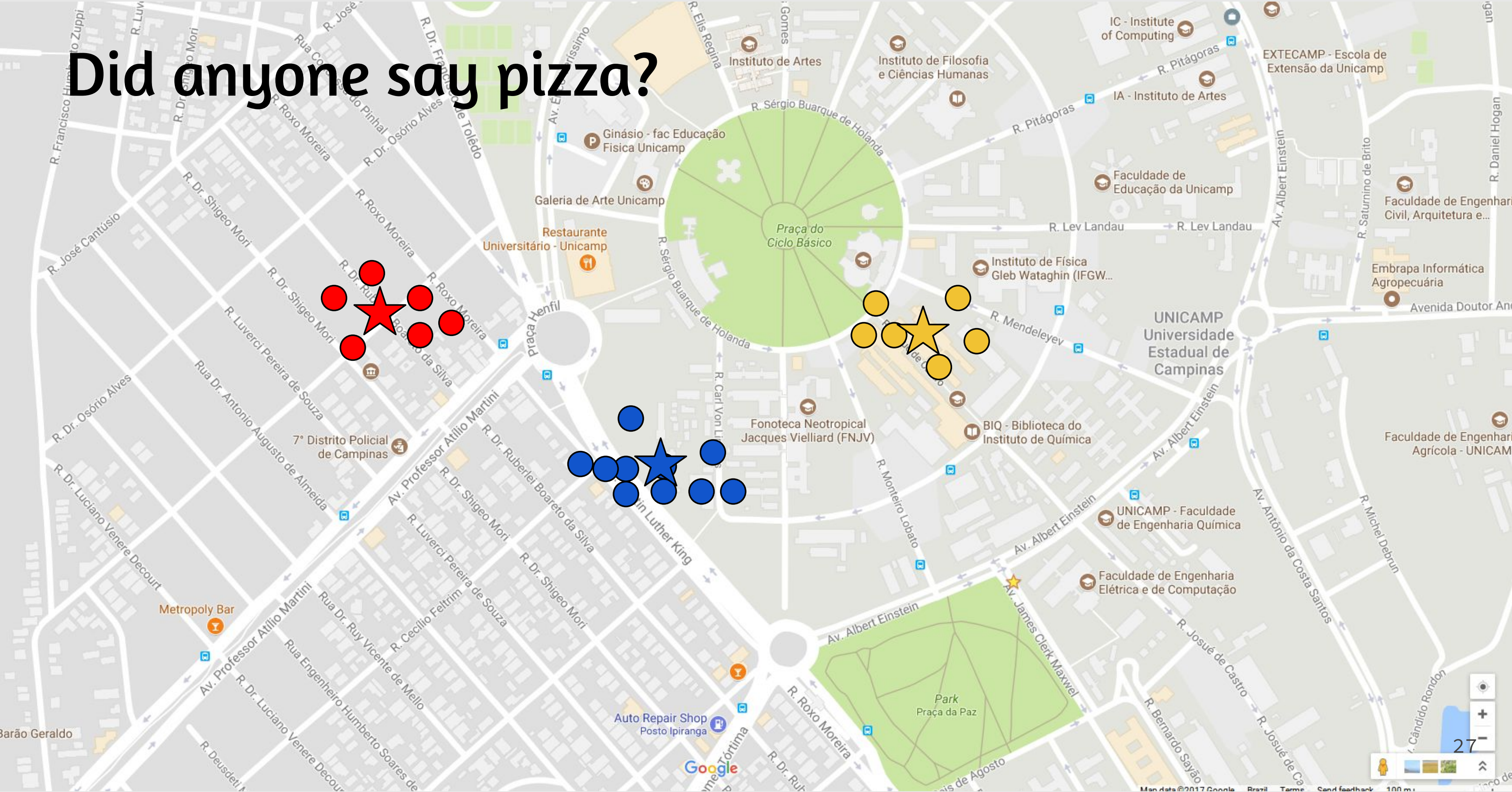
Did anyone say pizza?



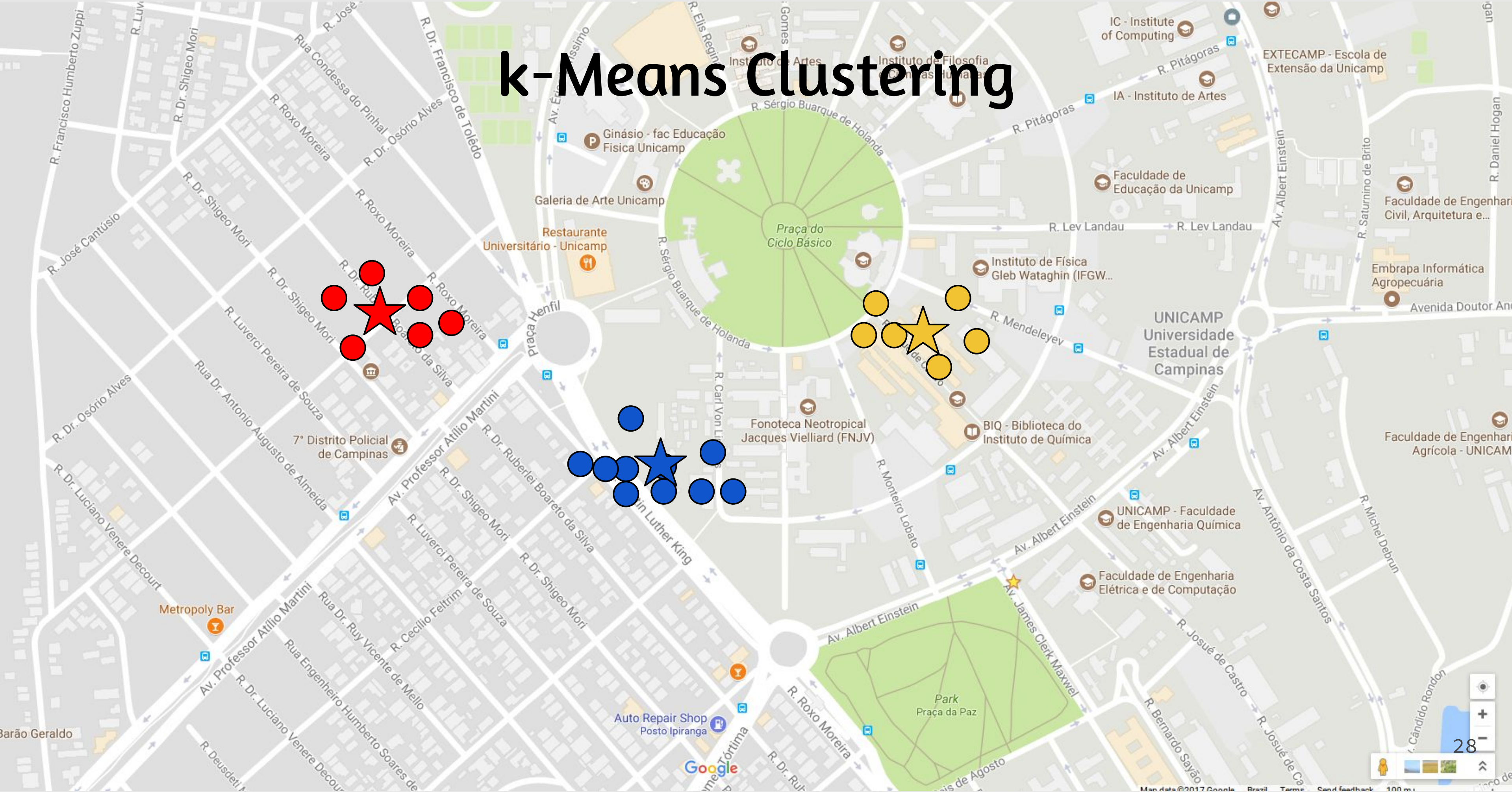
Did anyone say pizza?



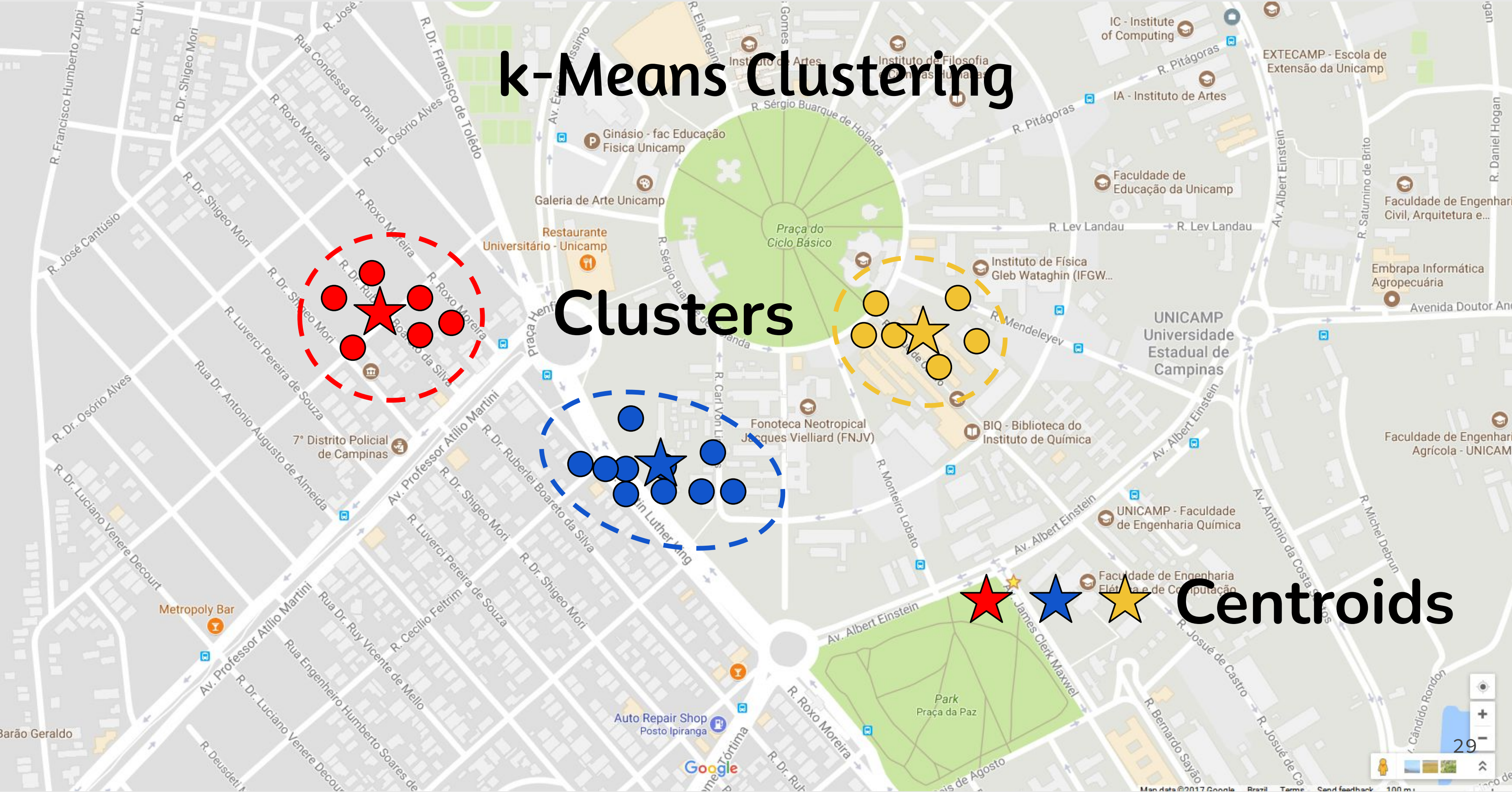
Did anyone say pizza?



k-Means Clustering



k-Means Clustering



k-Means: Image Segmentation

Credit: Christopher Bishop

k-Means: Image Segmentation

Credit: Christopher Bishop

k-Means Algorithm

1. **Define the *k* centroids.**
2. **Find the closest centroid & update cluster assignments.**
3. **Move the centroids to the center of their clusters.**
4. **Repeat steps 2 and 3** until the centroid stop moving a lot at each iteration.

k-Means Algorithm

1. **Define the *k* centroids**.
   Initialize these at random.

k-Means Algorithm

1. **Define the *k* centroids.**
2. **Find the closest centroid & update cluster assignments.**
   Assign each data point to one of the *k* clusters.
   Each data point is assigned to the nearest centroid's cluster (Euclidean distance).

k-Means Algorithm

1. **Define the *k* centroids.**
2. **Find the closest centroid & update cluster assignments.**
3. **Move the centroids to the center of their clusters.**
   The new position of each centroid is calculated as the average position of all the points in its cluster.

k-Means Algorithm

1. **Define the *k* centroids.**
2. **Find the closest centroid & update cluster assignments.**
3. **Move the centroids to the center of their clusters.**
4. **Repeat steps 2 and 3** until the centroid stop moving a lot at each iteration (i.e., until the algorithm converges).

k-Means Algorithm

Input:

- K (number of clusters)
- Training set $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \ \mu_2, \ \ldots, \ \mu_K \in \mathbb{R}^n$

repeat {

}

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

}

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

$$\min_k ||x^{(i)} - \mu_k||$$

repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

}

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

Cluster assignment step

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

}

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

for k = 1 to K

μ_k := mean of points assigned to cluster k

}

k-Means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

for $i = 1$ to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

for $k = 1$ to K

μ_k := mean of points assigned to cluster k

} **Move centroid step**

k-Means Algorithm

Q: What if a cluster doesn't have any element?

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

for k = 1 to K

μ_k := mean of points assigned to cluster k

}

k-Means Algorithm

Q: What happens when we don't have very well separated clusters?

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

for k = 1 to K

μ_k := mean of points assigned to cluster k

}

Clustering

Optimization Objective

k-Means Optimization Objective

$c^{(i)}$ = index of cluster (from 1 to K) to which example $x^{(i)}$ is currently assigned

μ_k = cluster centroid k

$\mu_{c^{(i)}}$ = cluster centroid of cluster to which example $x^{(i)}$ has been assigned

Optimization objective:

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} \|x^{(i)} - \mu_{c^{(i)}}\|$$

$$\min_{\substack{c^{(1)}, \ldots, c^{(m)} \\ \mu_1, \ldots, \mu_K}} J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

k-Means Optimization Objective

Randomly initialize K cluster centroids $\mu_1,\ \mu_2,\ \ldots,\ \mu_K \in \mathbb{R}^n$

repeat {

for $i = 1$ to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid **closest** to $x^{(i)}$

for $k = 1$ to K

μ_k := mean of points assigned to cluster k

}

Clustering

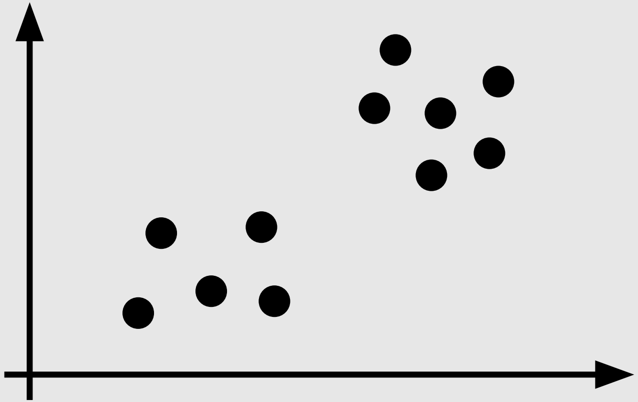
Random Initialization

Random Initialization

Should have $K < m$.

Randomly pick K training examples.

Set $\mu_1, \ldots, \mu_K$ equal to these K examples.



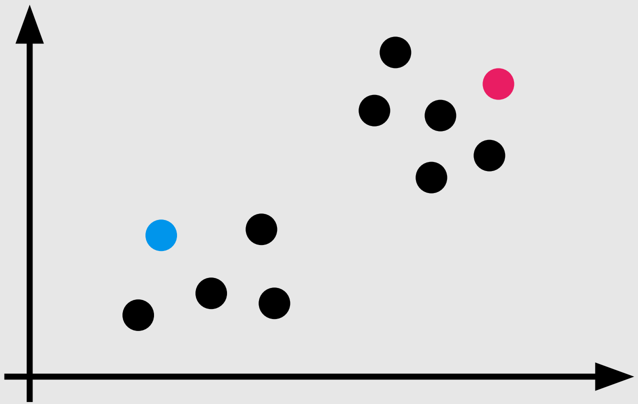
Random Initialization

Should have $K < m$.

Randomly pick K training examples.

Set $\mu_1, \ldots, \mu_K$ equal to these K examples.

$K = 2$



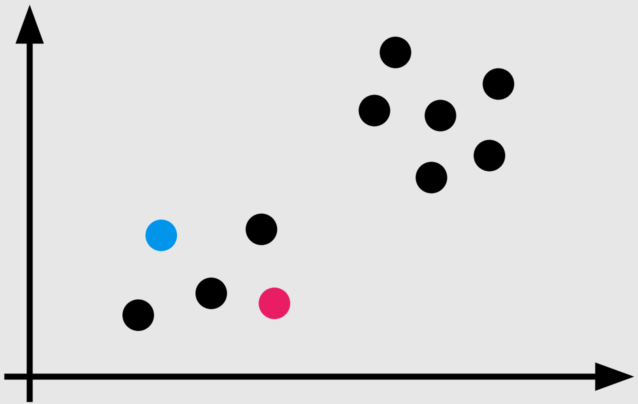
Random Initialization

Should have $K < m$.

Randomly pick K training examples.

Set $\mu_1, \ldots, \mu_K$ equal to these K examples.

$K = 2$



https://www.naftaliharris.com/blog/visualizing-k-means-clustering

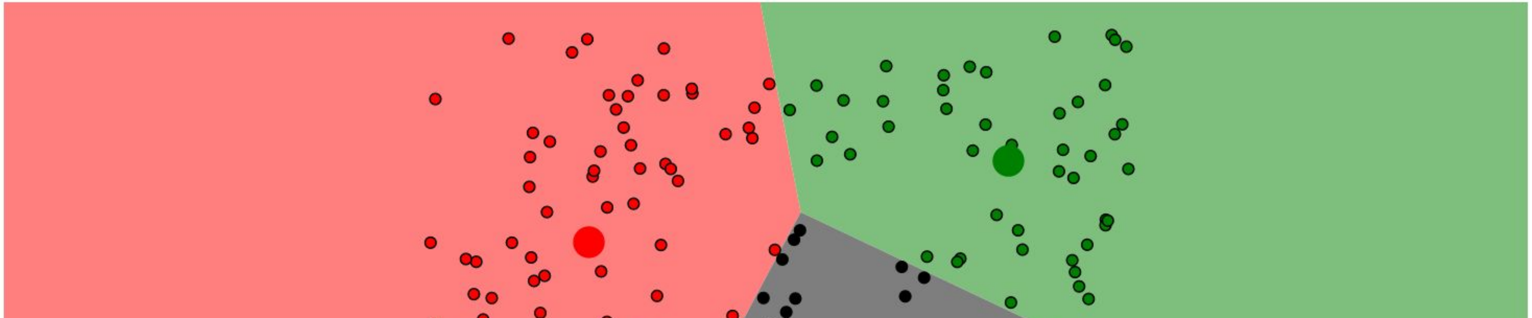
naftali harris

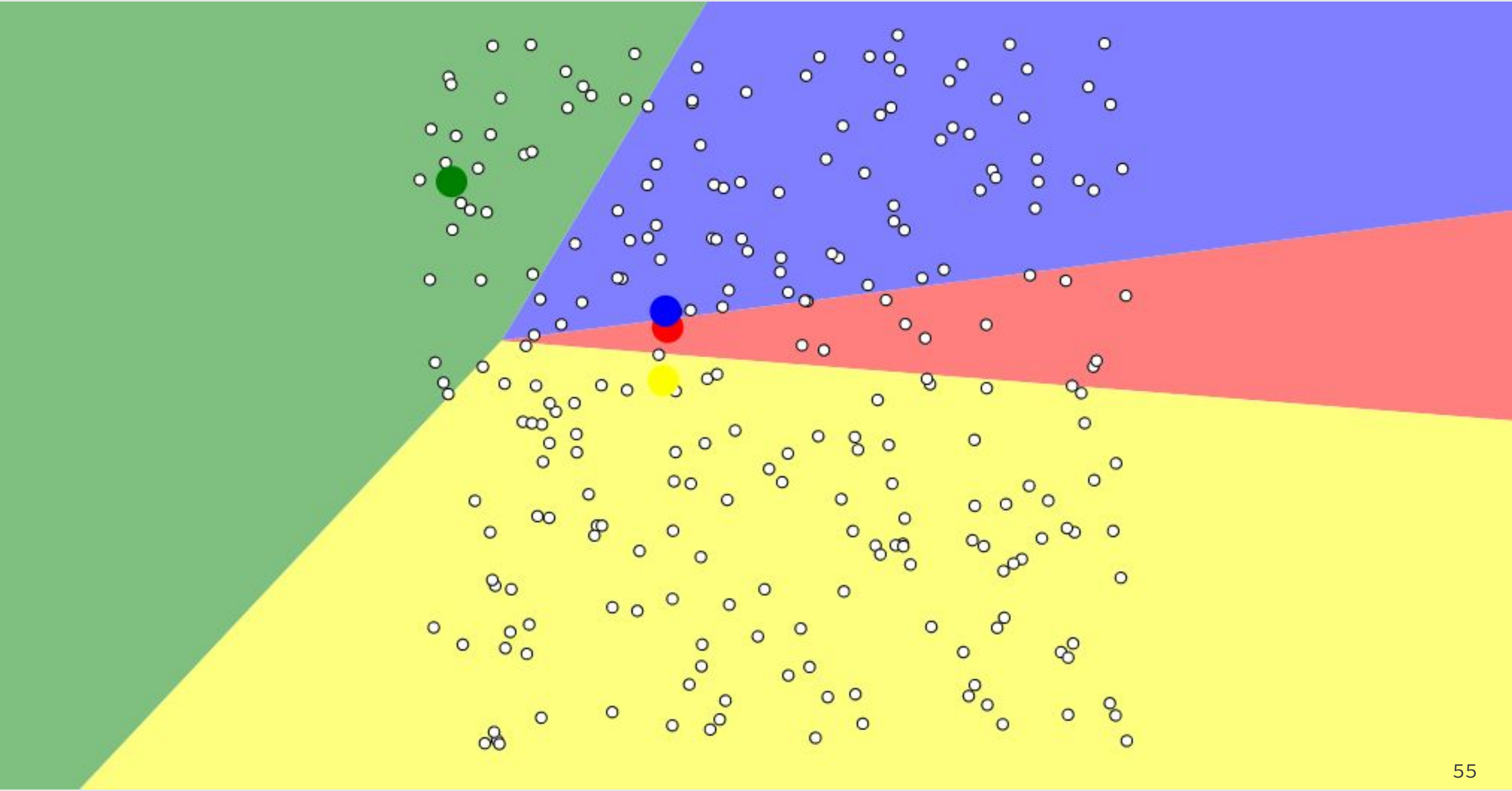
Blog | About | Contact | I'm Feeling Lucky

Visualizing K-Means Clustering

January 19, 2014

Suppose you plotted the screen width and height of all the devices accessing this website. You'd probably find that the points form three clumps: one clump with small dimensions, (smartphones), one with moderate dimensions, (tablets), and one with large dimensions, (laptops and desktops). Getting an algorithm to recognize these clumps of points without help is called *clustering*. To gain insight into how common clustering techniques work (and don't work), I've been making some visualizations that illustrate three fundamentally different approaches. This post, the first in this series of three, covers the k-means algorithm. To begin, click an initialization strategy below:





Random Initialization

for i = 1 to 100 {

Randomly initialize k-Means.

Run k-Means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.

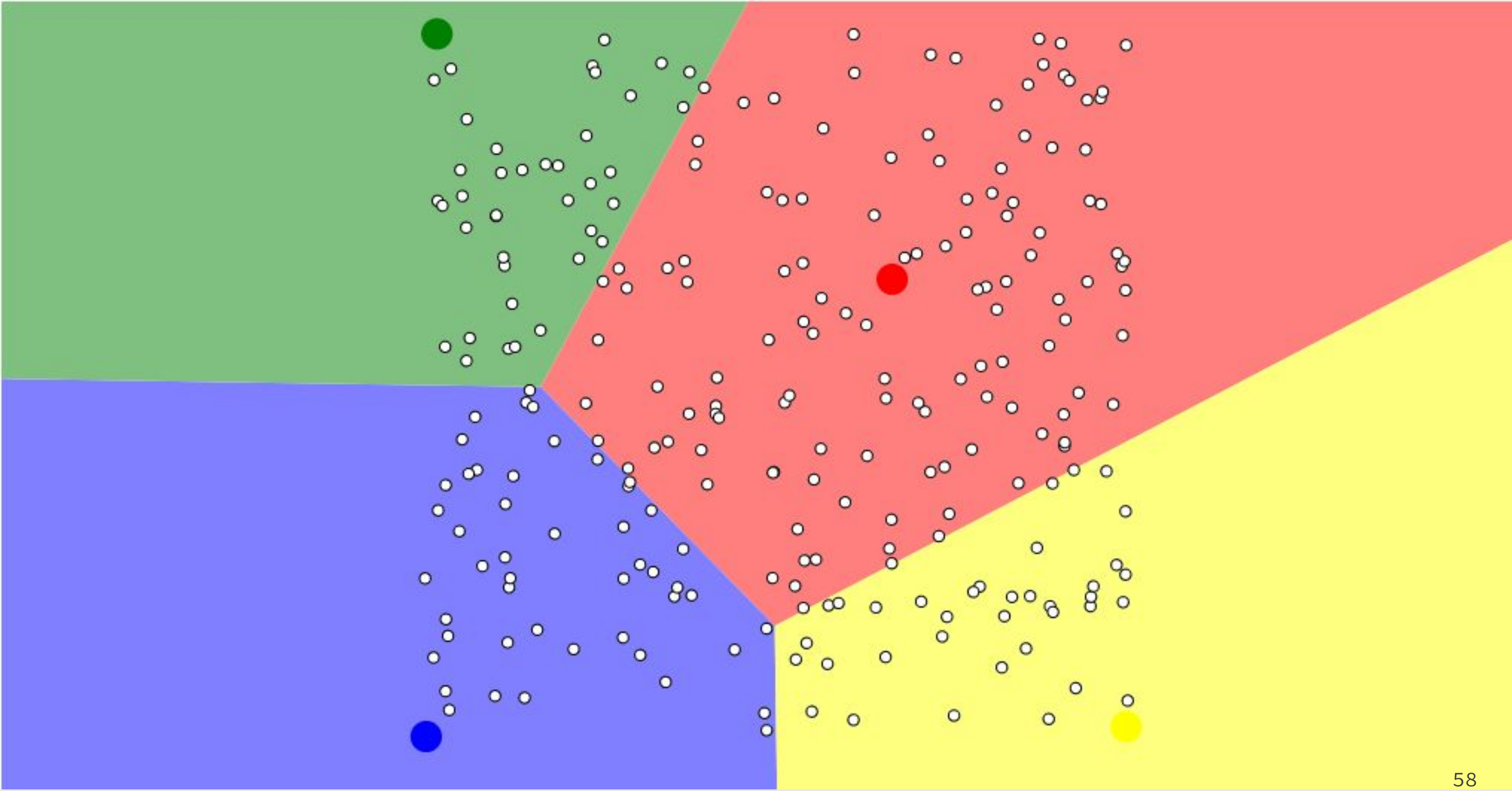
Compute cost function J.

}

Pick clustering that gave lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$.

Can we do better?

- One idea for initializing k-Means is to use a farthest-first traversal on the data set, **to pick K points that are far away from each other**.



Can we do better?

- One idea for initializing k-Means is to use a farthest-first traversal on the data set, to pick K points that are far away from each other.

- However, this is **too sensitive to outliers**.

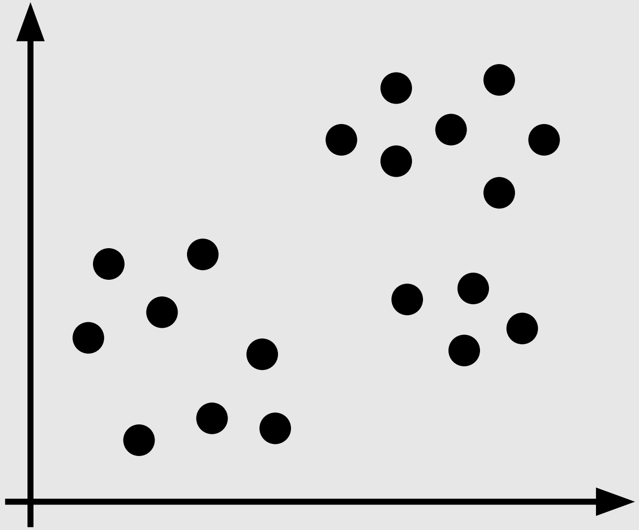
k-Means++ (Arthur & Vassilvitski, 2007)

- It works similarly to the “farthest” heuristic.
- Choose each point at random, with probability proportional to its squared distance from the centers chosen already.

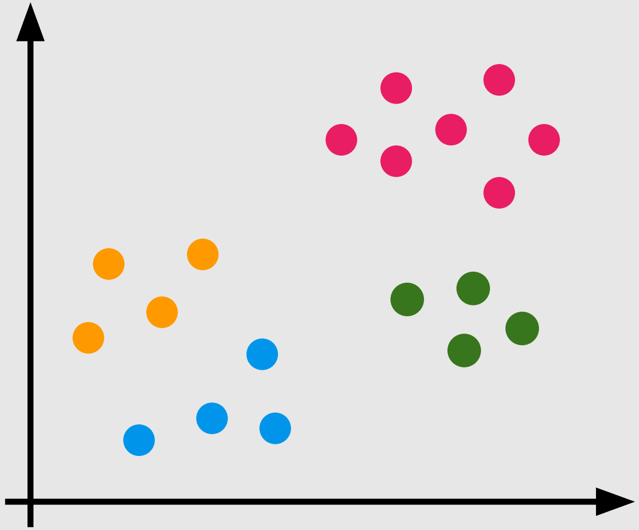
scikit-learn (default)

Clustering
Choosing the number of clusters

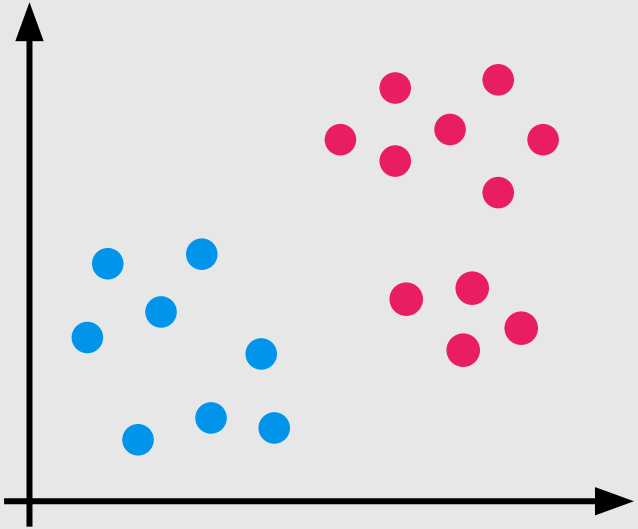
What is the right value of K?



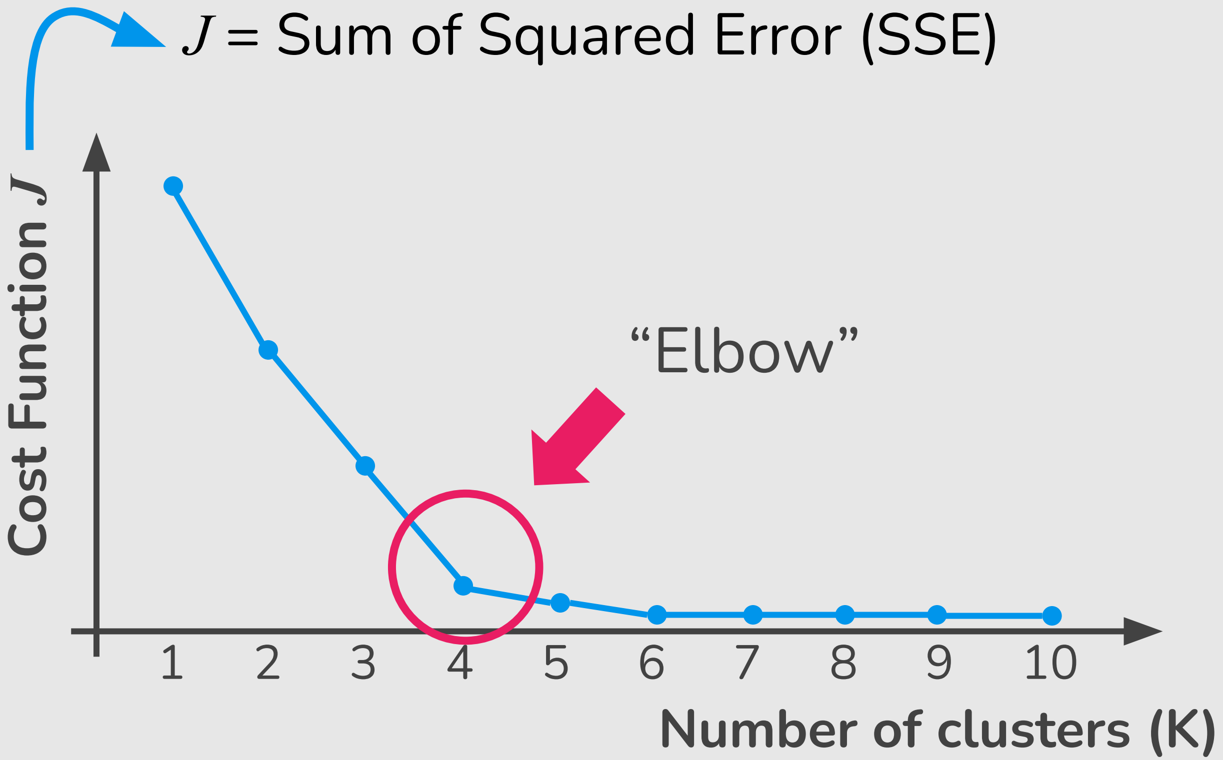
What is the right value of K?



What is the right value of K?

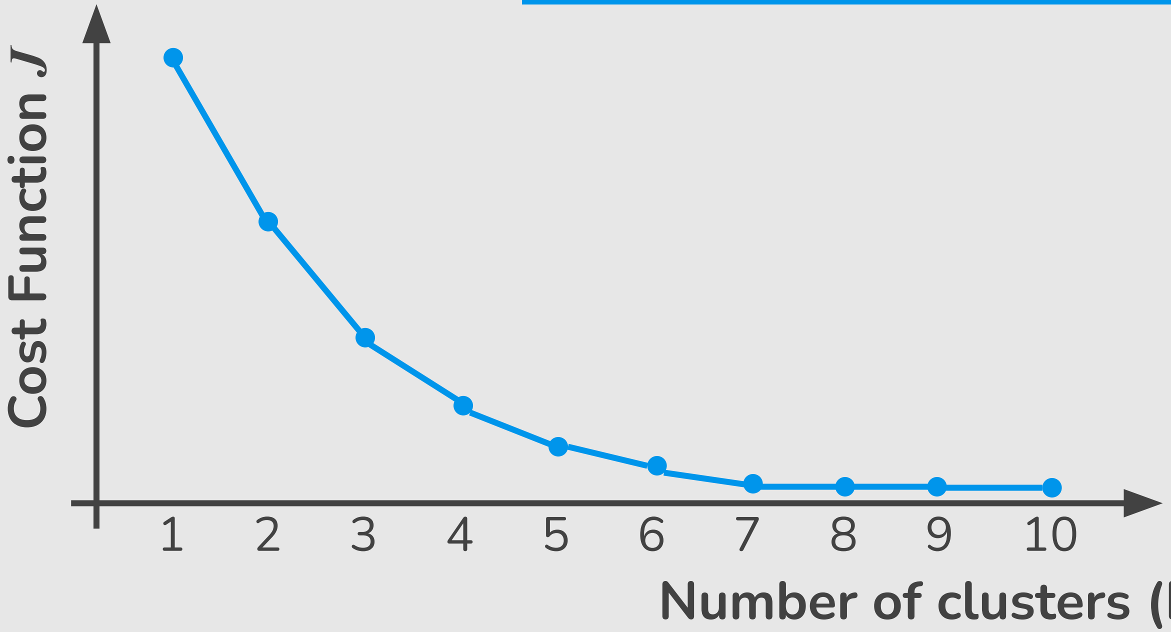


Elbow Method

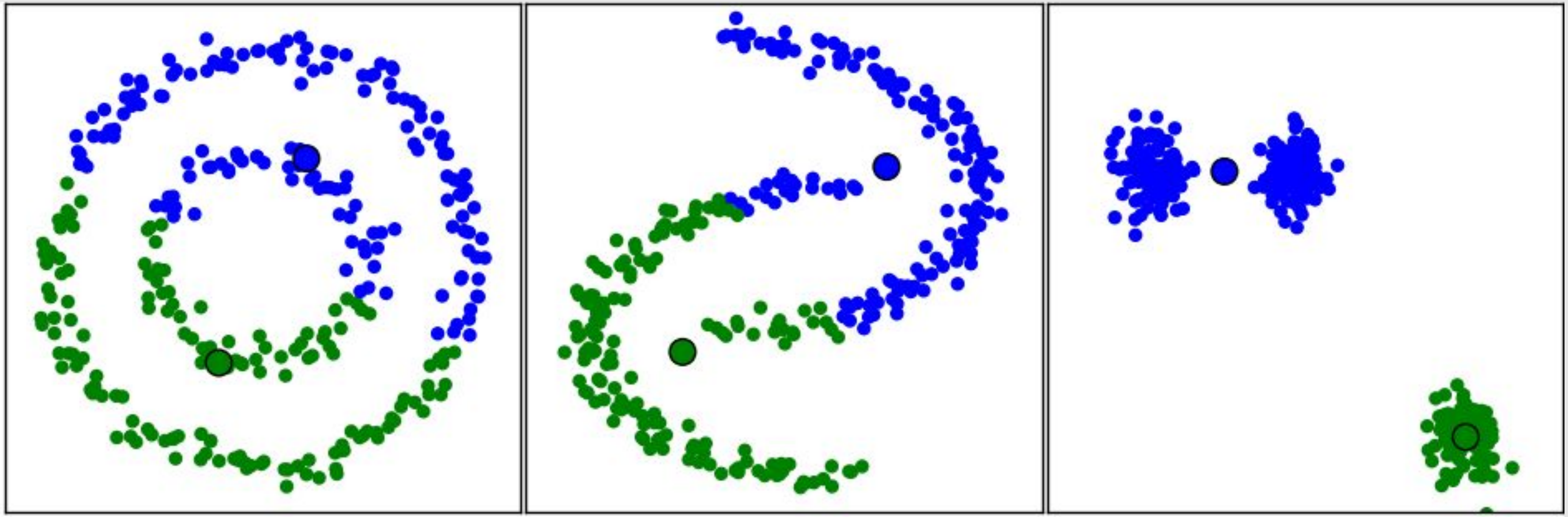


~~Elbow~~ Method

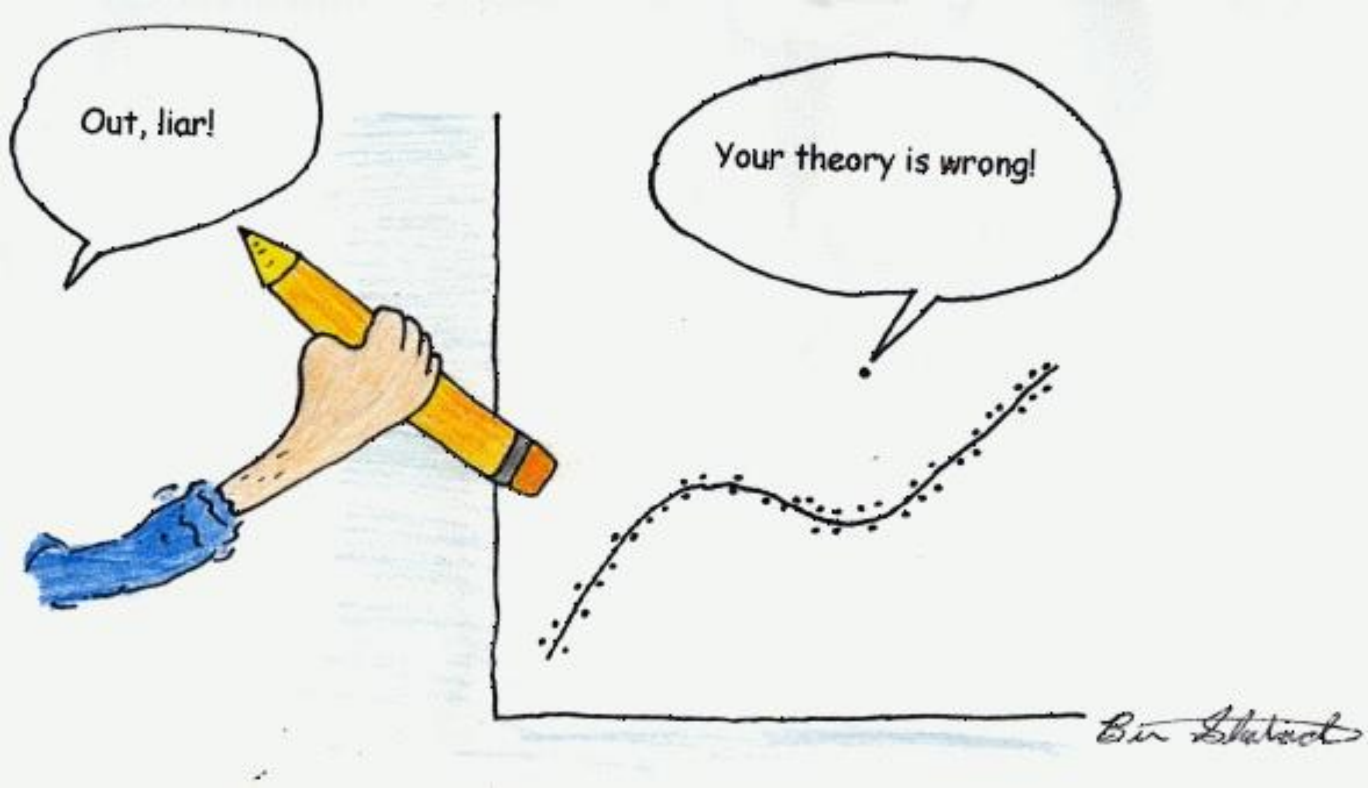
Q: You find that cost function J is much higher for k = 5 than for k =3. What can you conclude?



k-Means: Additional Issues



Outliers

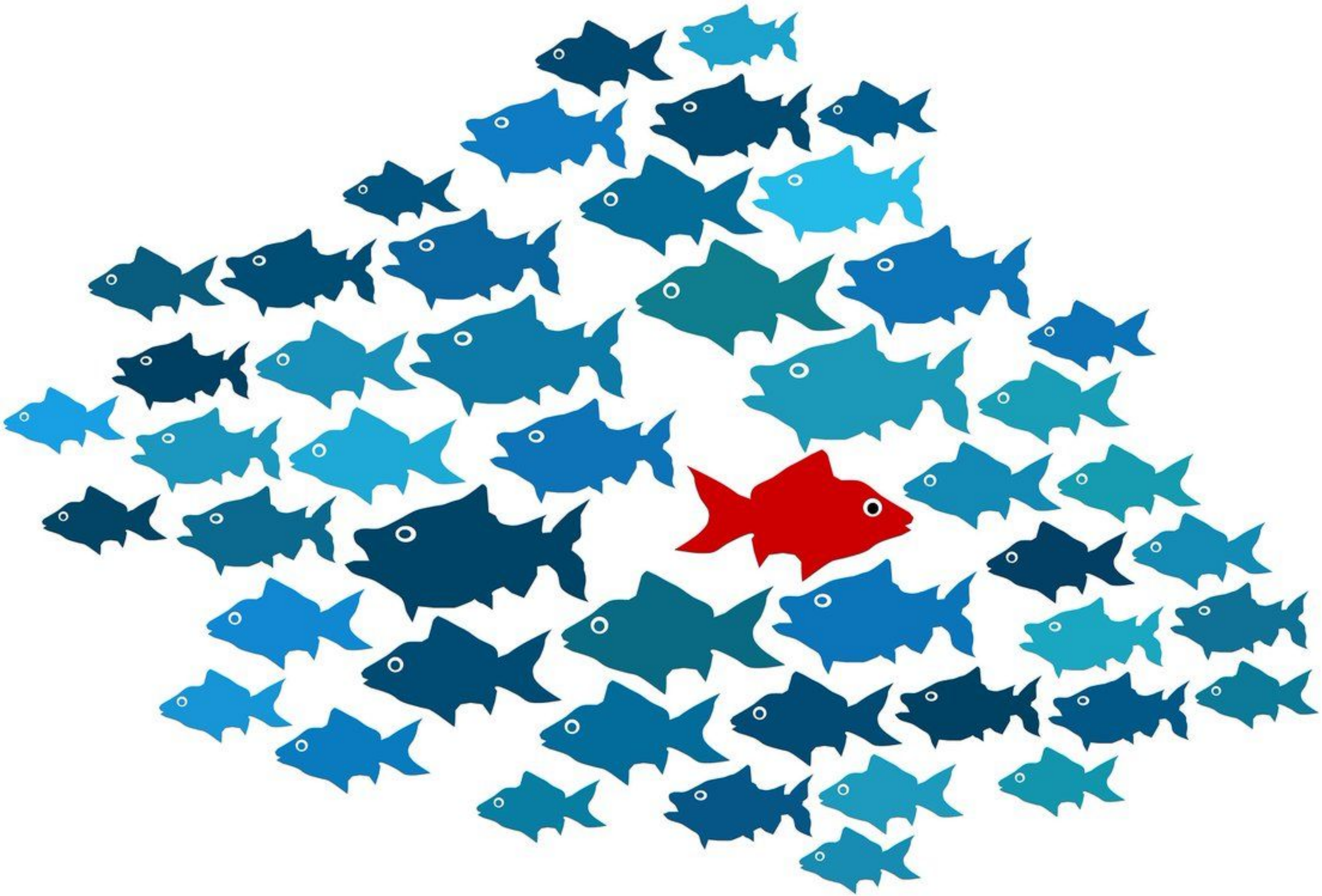


Outliers

- It is often useful to discover outliers and eliminate them before clustering.

Outliers

- It is often useful to discover outliers and eliminate them before clustering.
- Techniques for identifying outlier: *"Anomaly Detection" [chap. 9], Introduction to Data Mining, 2018.*



Outliers

- It is often useful to discover outliers and eliminate them before clustering.
- Techniques for identifying outlier: "*Anomaly Detection*" *[chap. 9], Introduction to Data Mining, 2018.*
- Also, we often want to eliminate small clusters because they frequently represent groups of outliers.

Reducing the SSE with Postprocessing

- **Split a cluster**: the cluster with the largest SSE is usually chosen.

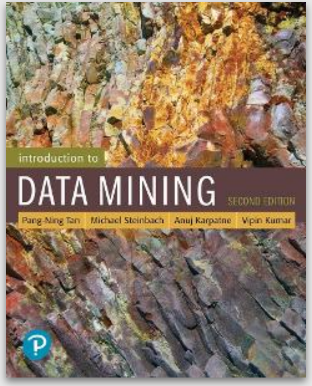
Reducing the SSE with Postprocessing

- **Split a cluster**: the cluster with the largest SSE is usually chosen.
- **Introduce a new cluster centroid**: often the point that is farthest from any cluster center is chosen.

Reducing the SSE with Postprocessing

- **Split a cluster**: the cluster with the largest SSE is usually chosen.
- **Introduce a new cluster centroid**: often the point that is farthest from any cluster center is chosen.
- **Merge two clusters**: The clusters with the closest centroids are typically chosen.

References



Machine Learning Books

- Pattern Recognition and Machine Learning, Chap. 9 “Mixture Models and EM”
- Pattern Classification, Chap. 10 “Unsupervised Learning and Clustering”
- Introduction to Data Mining, Chap. 7 “Cluster Analysis: Basic Concepts and Algorithms” https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 8