Lecture 11
Unsupervised learning

GEOL 4397: Data analytics and machine learning for geoscientists

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March. 26th, 2019

UNIVERSITY of HOUSTON
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EARTH AND ATMOSPHERIC SCIENCES

Week	Date	Topics	Comments
1	01/15 Tues	Overview of syllabus Lecture: Introduction to Machine learning: applications	
	01/17 Thur	Lecture: Review of linear algebra	
2	01/22 Tues	Lab: Linear algebra in Python	Not graded
	01/24 Thur	Lecture: Introduction to optimization	
3	01/29 Tues	Lab: Gradient descent + Linear regression	Report due on 02/05 at 5:30 pm
	01/31 Thur	Lecture: Introduction to machine learning: concepts	
4	02/05 Tues	Lecture: Logistic regression	
	02/07 Thur	Lab: Logistic regression	Report due on 02/14 at 5:30 pm
5	02/12 Tues	Lecture: Support vector machine	
	02/14 Thur	Lab: Support vector machine	Report due on 02/21 at 5:30 pm
6	02/19 Tues	Lecture: Decision trees	
	02/21 Thur	Lab: Decision trees	Report due on 02/28 at 5:30 pm
7	02/26 Tues	Lecture: Random Forest	
	02/28 Thur	Lab: Random forest	Report due on 03/07 at 5:30 pm
8	03/05 Tues	Lecture: Ensemble learning	
	03/07 Thur	Lab: Ensemble learning	Reprot due on 03/19 at 5:30 pm
9	03/12 Tues	No class due to spring break	
	03/14 Thur	No class due to spring break	
10	03/19 Tues	Review & Recap	
	03/21 Thur	Exam	
11	03/26 Tues	Lecture: Clustering	
	03/28 Thur	Lab: Clustering	Report due on 04/04 at 5:30 pm
12	04/02 Tues	Lecture: Introduction to TensorFlow	
	04/04 Thur	Lab: TensorFlow	Not graded
13	04/09 Tues	Lecture: Introduction to neural networks 1	
	04/11 Thur	Lecture: Introduction to neural networks 2	
14	04/16 Tues	Lab: Deep learning	Report due on 04/23 at 5:30pm
	04/18 Thur	Lecture: Convolutional neural networks 1	
15	04/23 Tues	Guest lecture: Convolutional neural networks 2	
	04/25 Thur	Lab: CNN (optional)	Report due on 05/02 at 5:30 pm
16	04/30 Tues	final presentation??	
	05/02 Thur	final presentation??	
Note	28 class meetings		04/29 last day of class

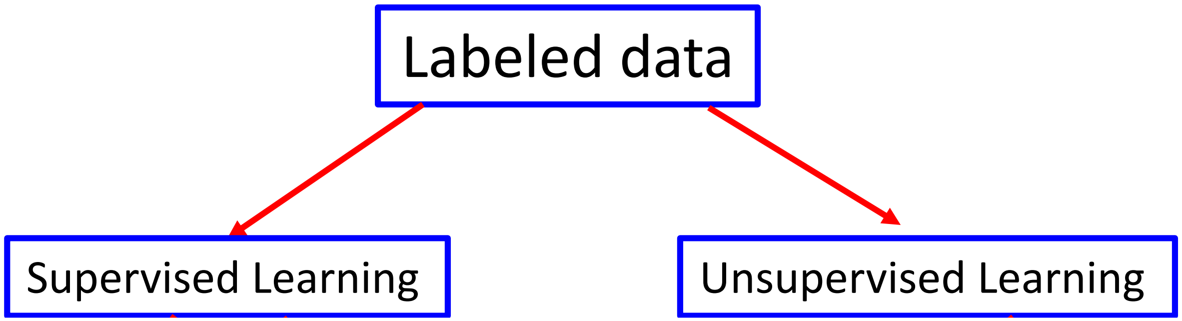
Outline

- Dimensionality reduction
- K-means Clustering
- Implementation in Scikit-Learn

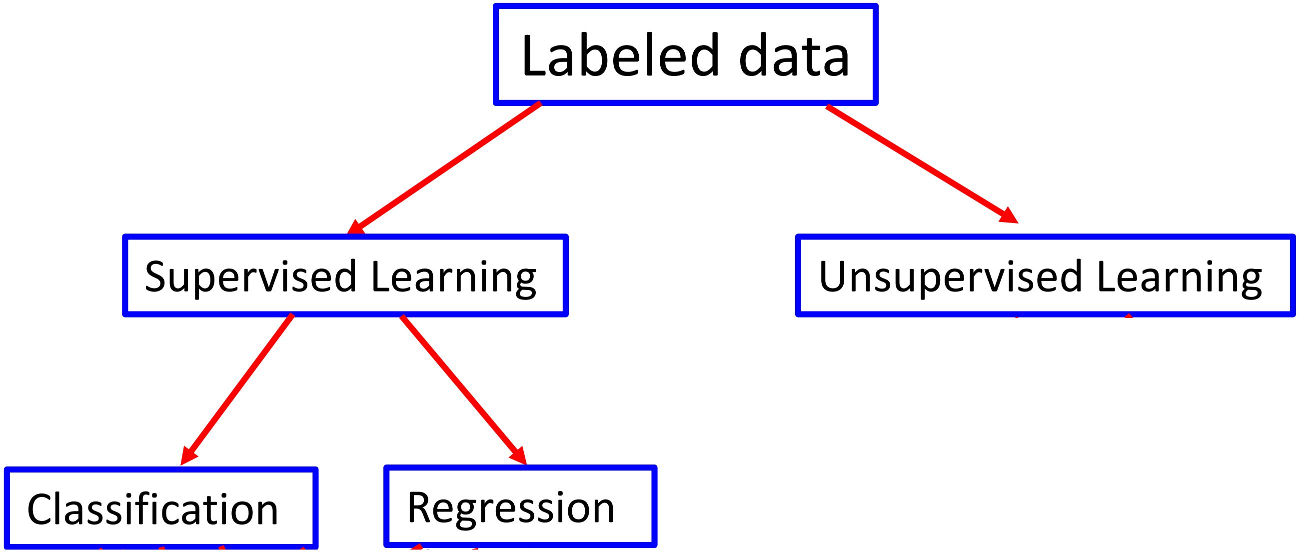
Acknowledgments

- Youtube video by Joshua Starmer: https://goo.gl/RDMb4P
- Youtube video by Luis Serrano: https://goo.gl/wuSYXK

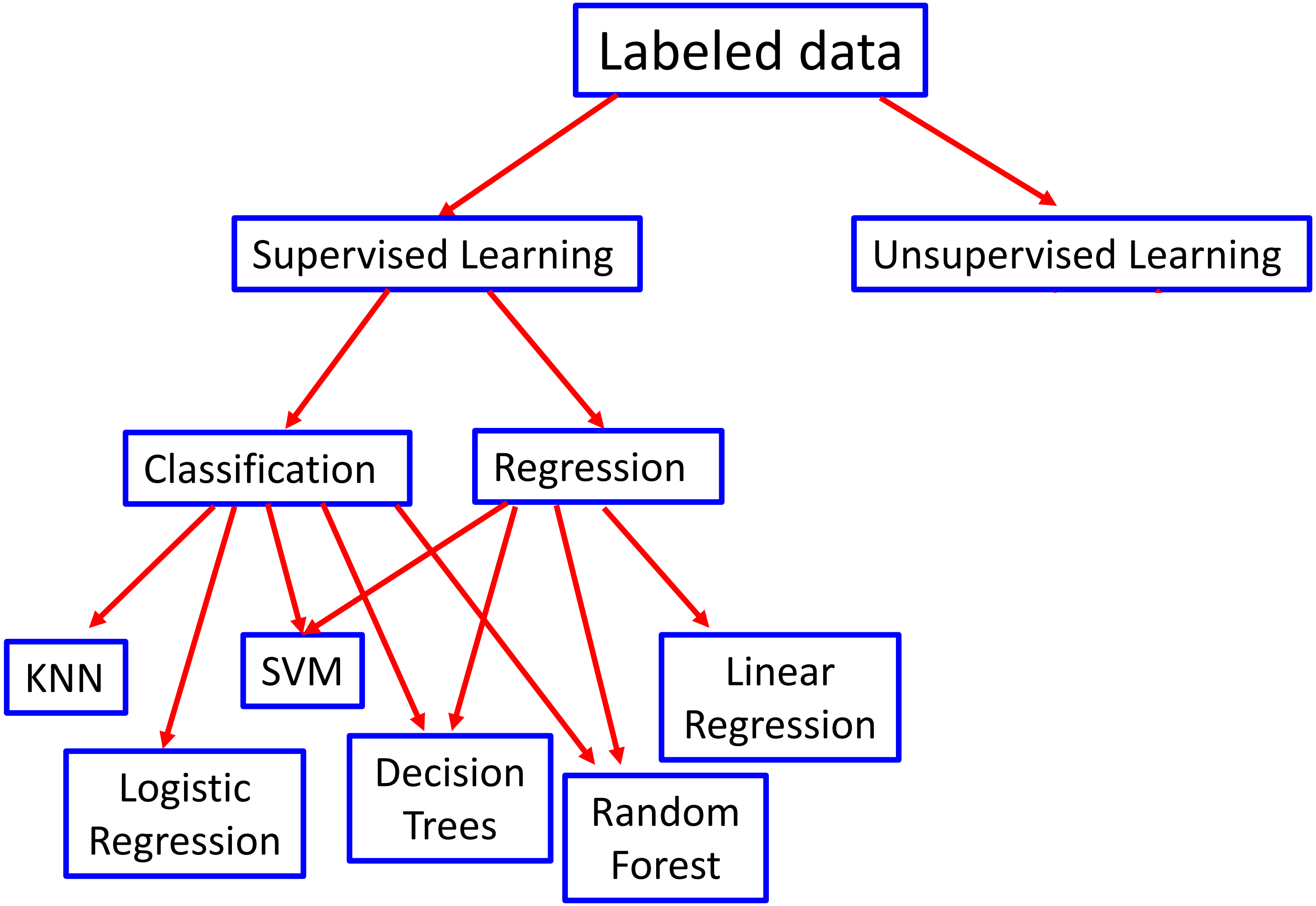
Machine learning algorithms



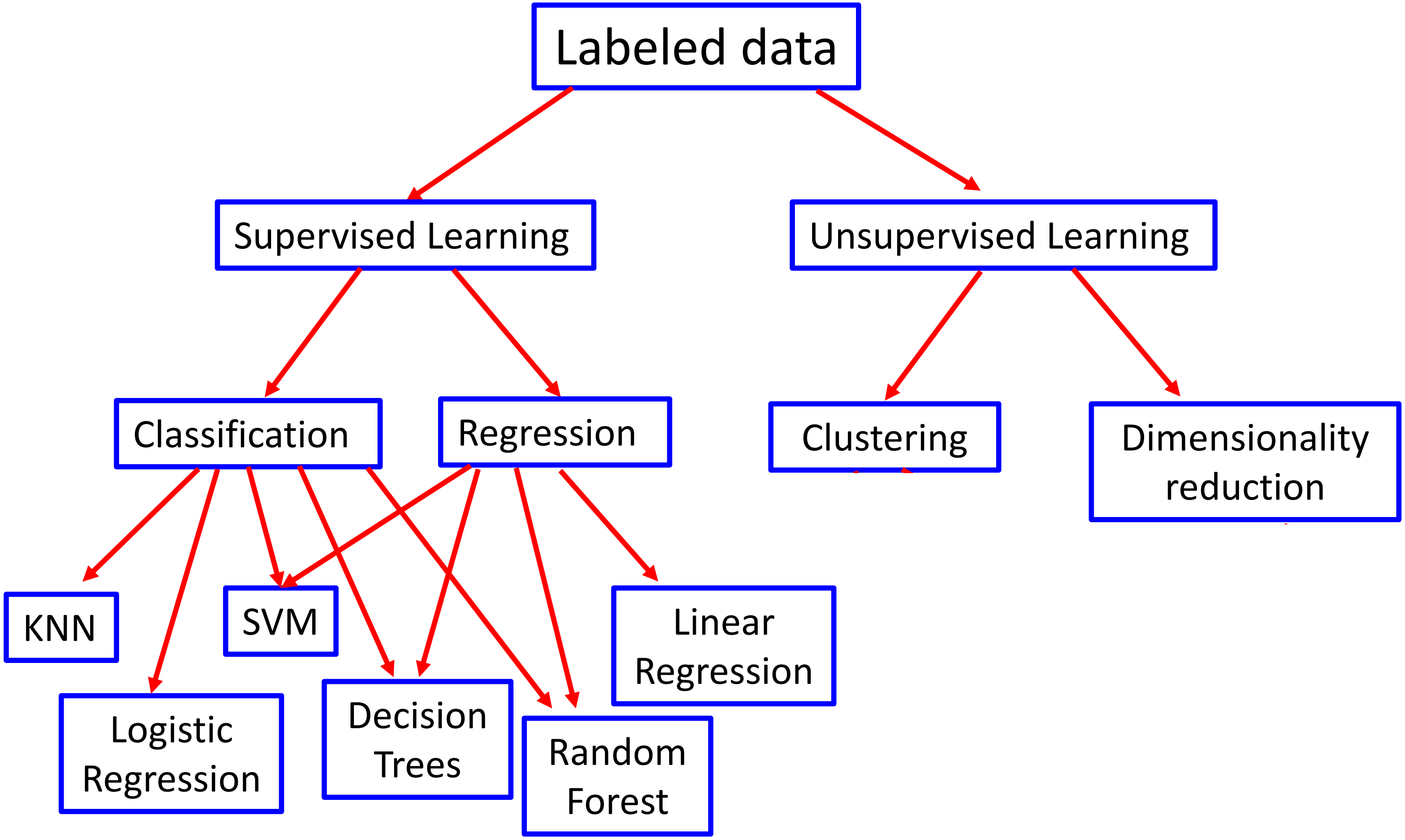
Machine learning algorithms



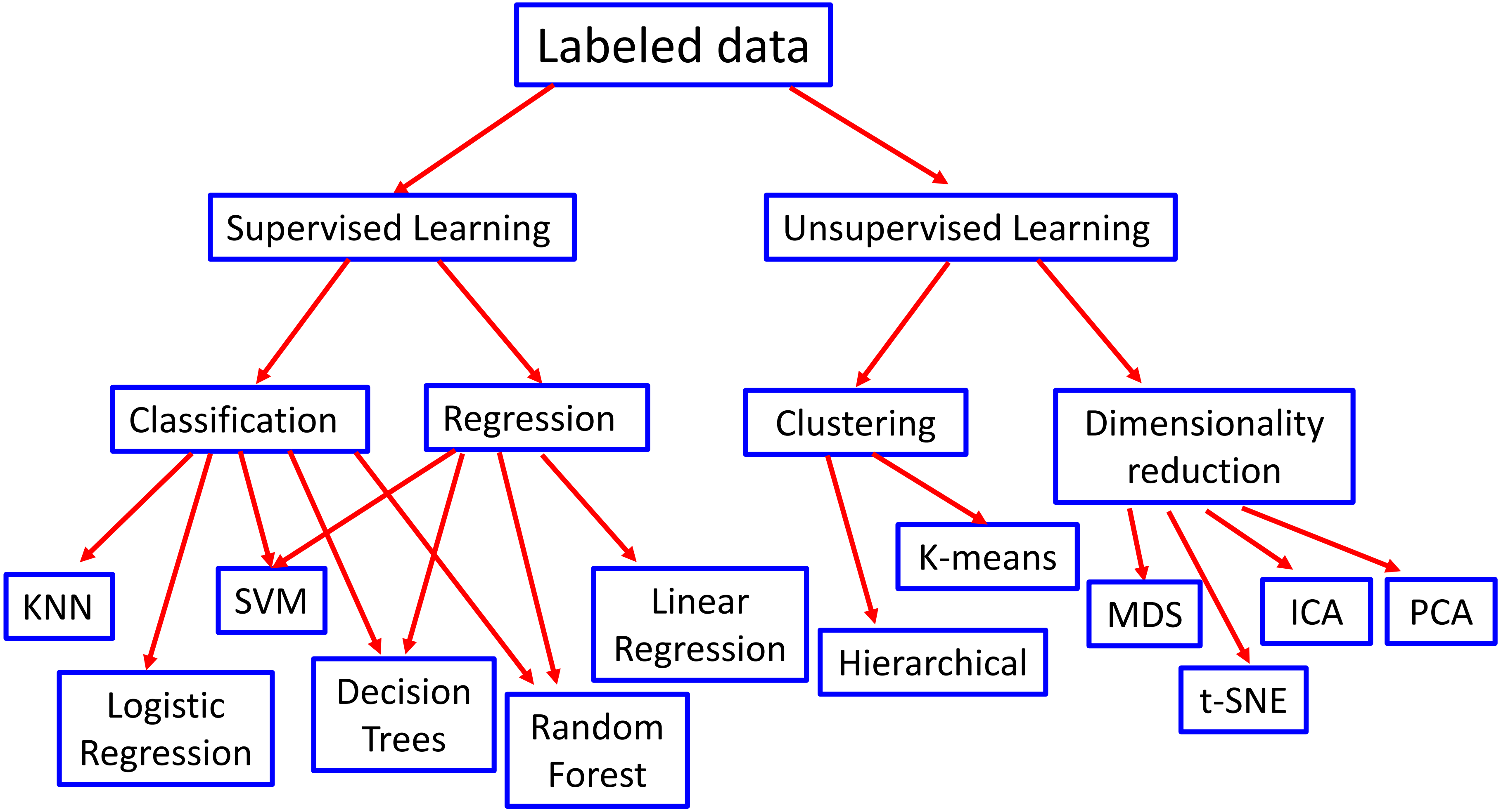
Machine learning algorithms



Machine learning algorithms



Machine learning algorithms



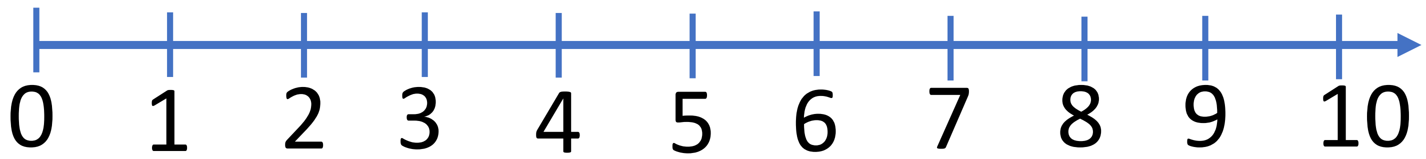
Dimensionality reduction

- Reduces high-dimensional data into 2D (or 3D) space for better visualization and analysis

Introduction to dimensions

- Fundamental yet important concepts

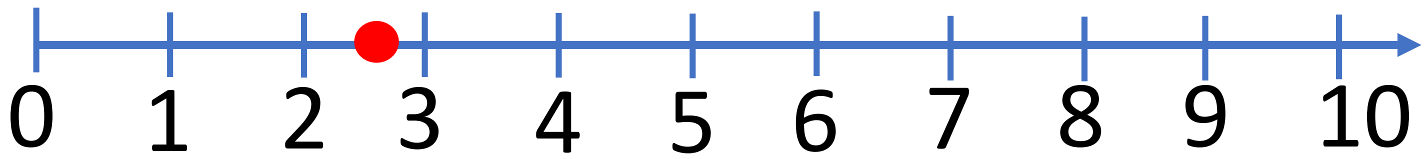
1-Dimension (1D)



1-Dimension (1D) = a number line

1-Dimension (1D)

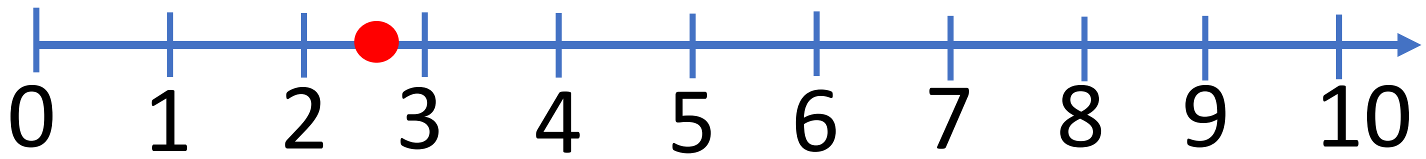
1-Dimension (1D) = a number line



Suppose I measure the average density of some crustal rocks:
2.67 g/cc

1-Dimension (1D)

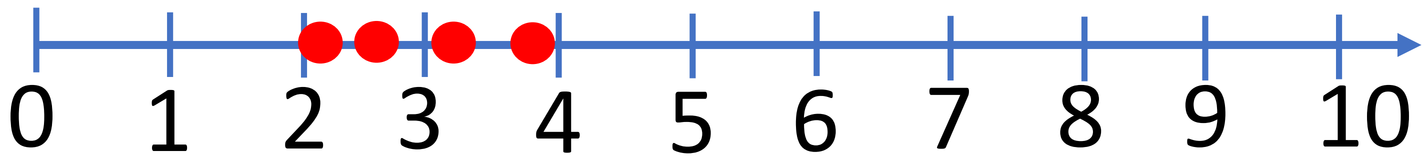
1-Dimension (1D) = a number line



Suppose I measured densities on several different rocks:
2.14 g/cc, 2.67 g/cc, 3.25 g/cc, 3.86 g/cc

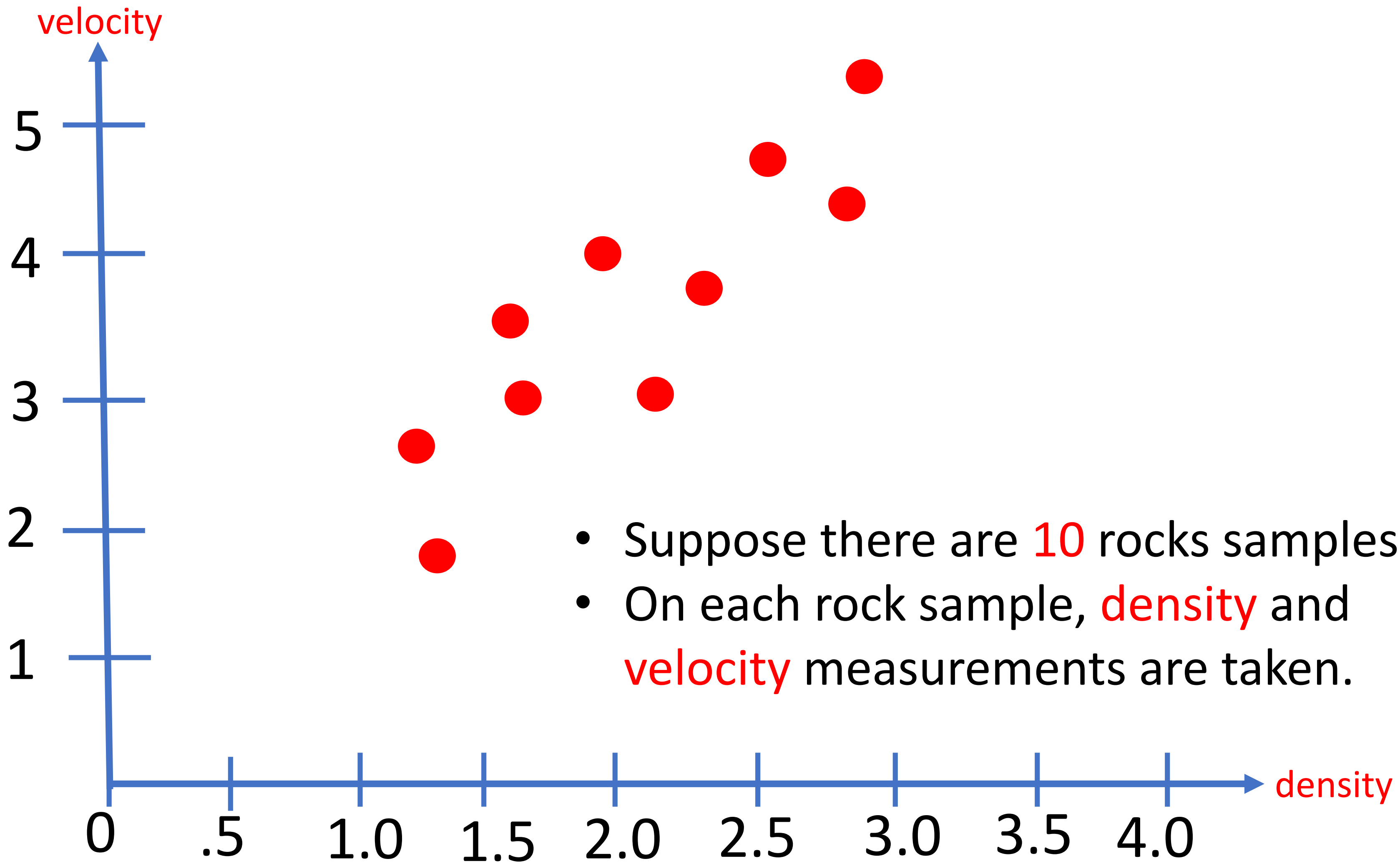
1-Dimension (1D)

1-Dimension (1D) = a number line



Suppose I measured densities on several different rocks:
2.14 g/cc, 2.67 g/cc, 3.25 g/cc, 3.86 g/cc

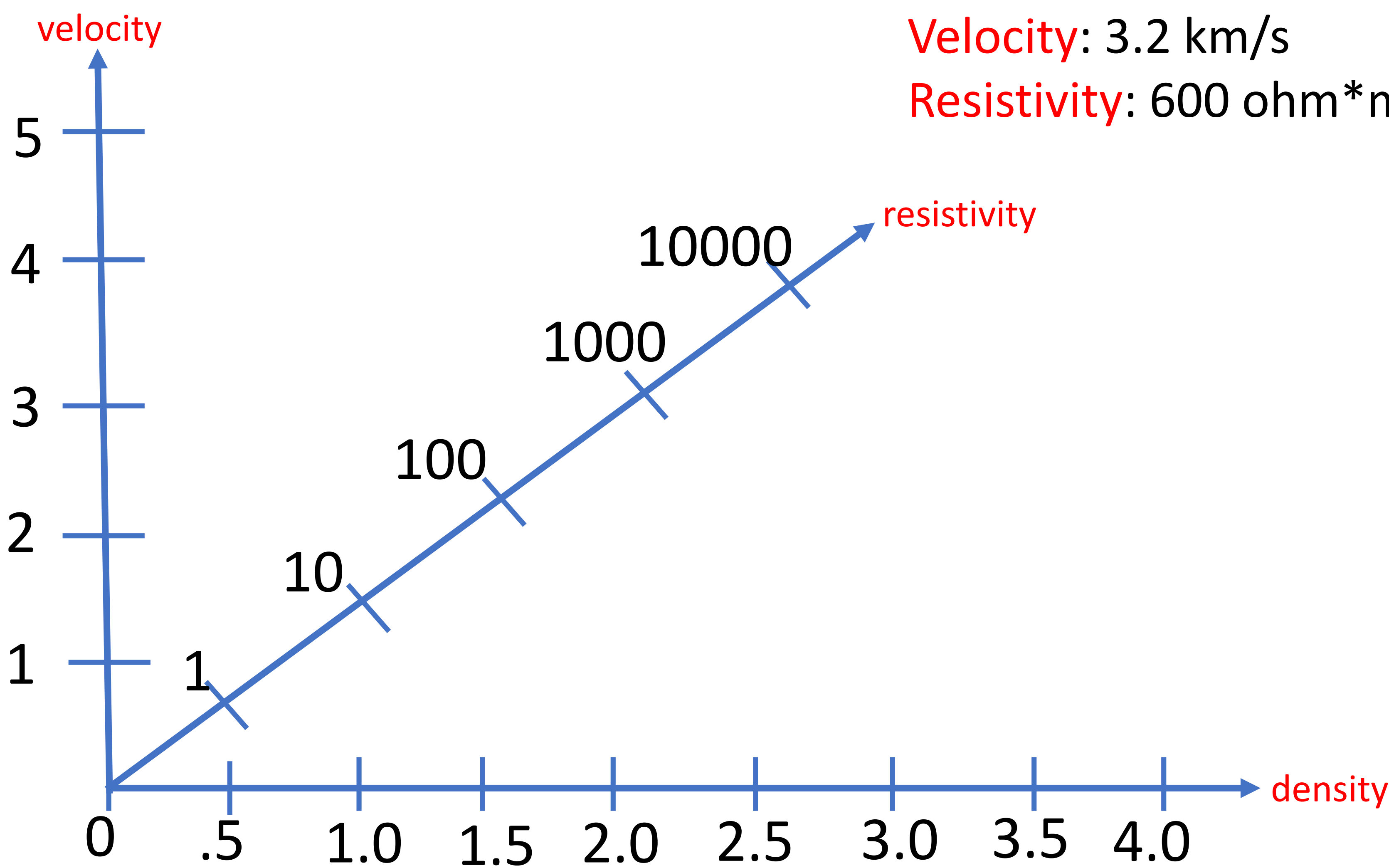
2-Dimension (2D)



- Suppose there are 10 rocks samples.
- On each rock sample, density and velocity measurements are taken.

3-Dimension (3D)

Density: 2.65 g/cc
Velocity: 3.2 km/s
Resistivity: 600 ohm*m



Dimensions so far …

- 1 measurement = 1D graph
- 2 measurements = 2D graph
- 3 measurements = 3D graph

Dimensions so far …

- 1 measurement = 1D graph
- 2 measurements = 2D graph
- 3 measurements = 3D graph
- 4 measurements = 4D graph (you cannot draw it)

Dimensions so far …

- 1 measurement = 1D graph
- 2 measurements = 2D graph
- 3 measurements = 3D graph
- 4 measurements = 4D graph (you cannot draw it)
- 200 measurements = 200D graph

Dimensions so far …

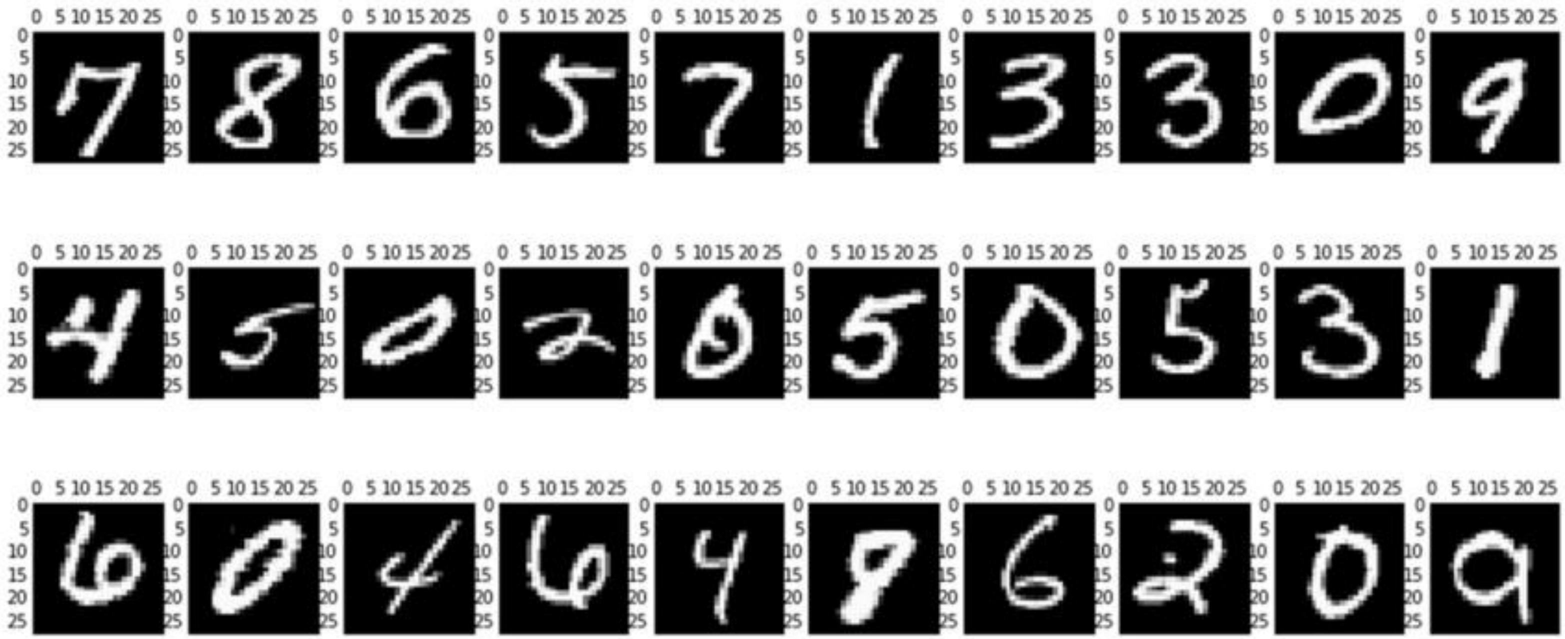
- 1 measurement = 1D graph
- 2 measurements = 2D graph
- 3 measurements = 3D graph
- 4 measurements = 4D graph (you cannot draw it)
- 200 measurements = 200D graph

Each more physical property measurement we make on one rock sample adds one more dimension.

In-class quiz

- Geochemical facies analysis
- Data consists of XRF measurements of cuttings from the lateral section of an unconventional well
- Measurements made at approximately 10 m intervals
- For each cutting sample, there were 22 measurements.
- A total of 269 cutting samples
- Question: If we plot up the measurements, what is the dimension of the space? How many points are there in this high dimensional space?

In-class quiz 2



Some examples of MNIST handwritten digits
Each image is a 28 X 28 pixel images
A total of 70,000 images
Question: Suppose we want to plot up all 70,000 images in a high dimensional space, what should the dimension of this space be?

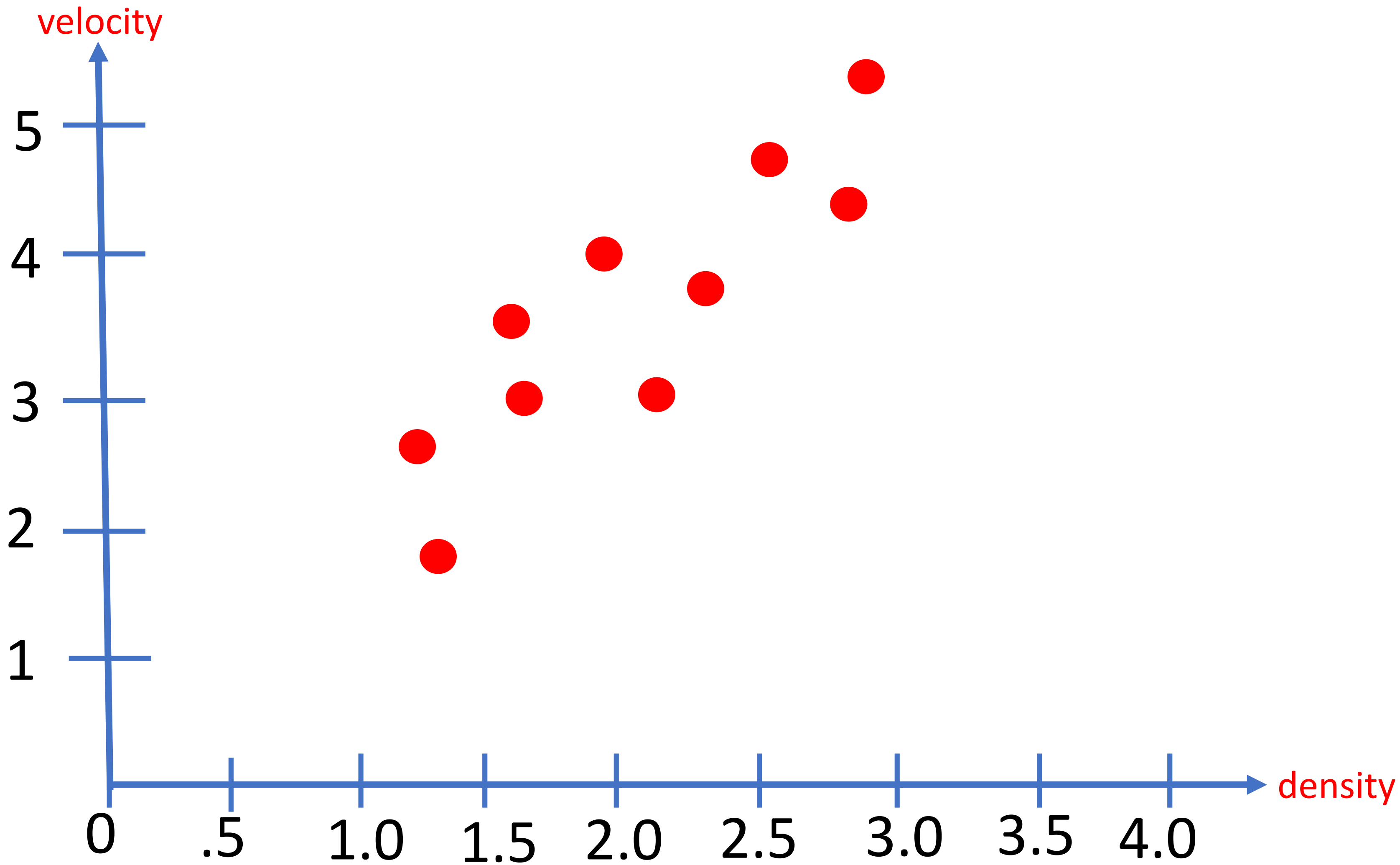
Questions

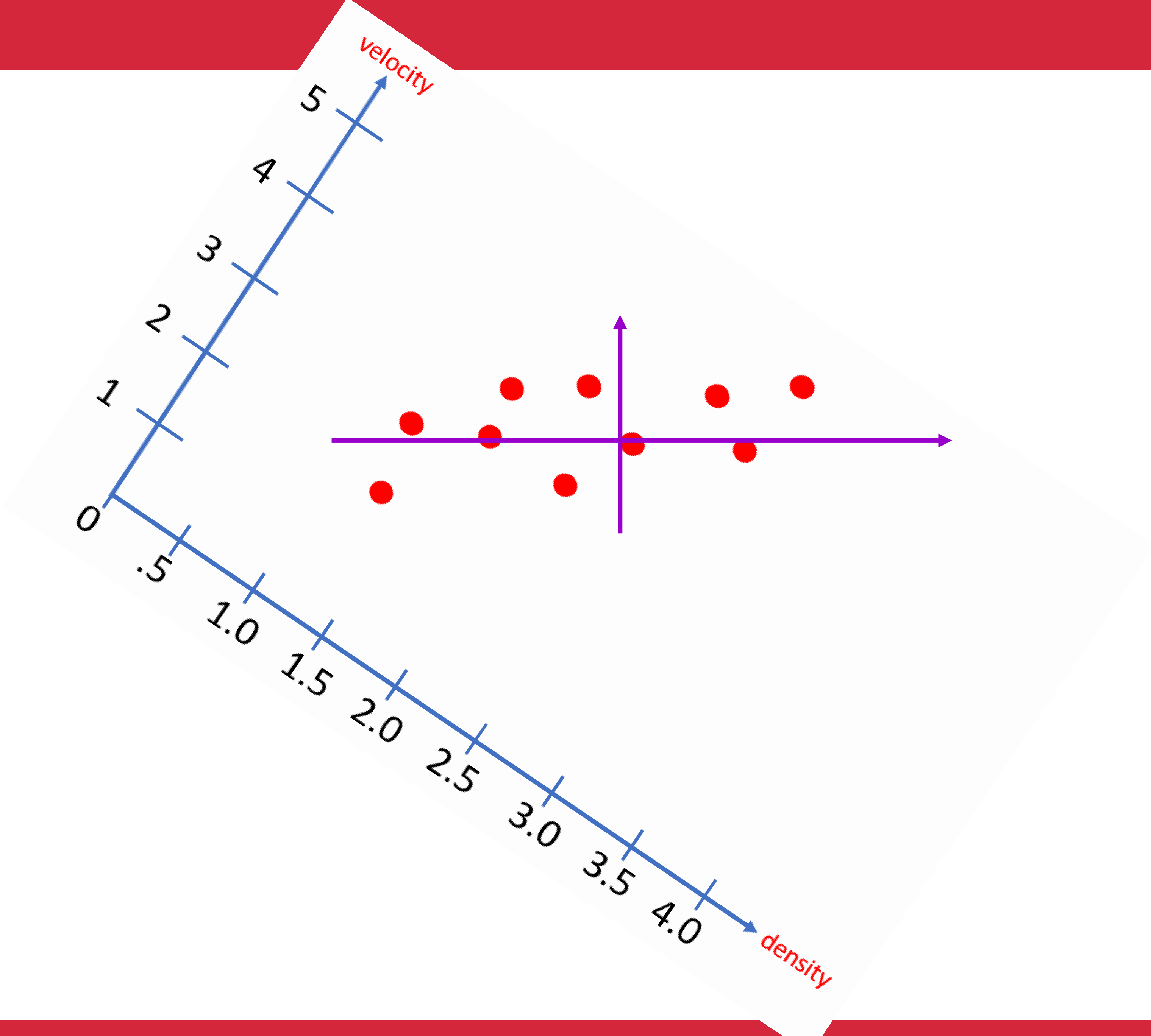
- How to visualize high-dimensional data?
- Are all those dimensional equally important? Or some more important than others?

PCA

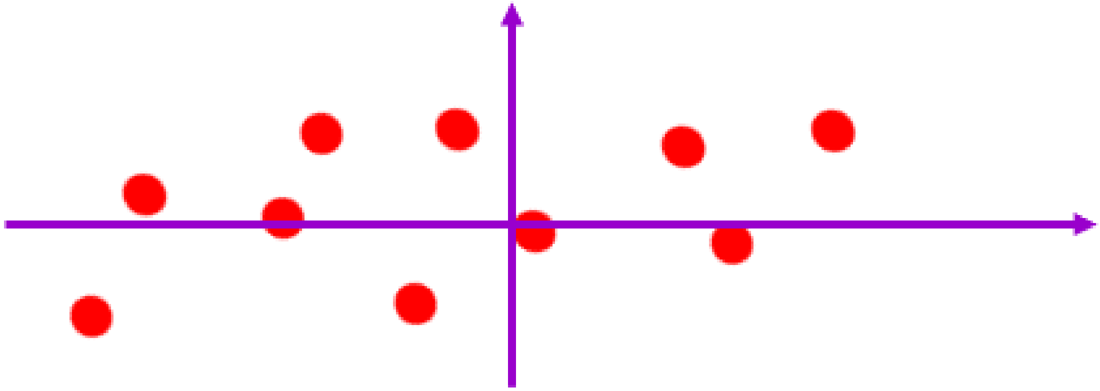
- Reduces a high-dimensional dataset (e.g., 22-D dimensional) to 2 or 3 dimensions for better visualization

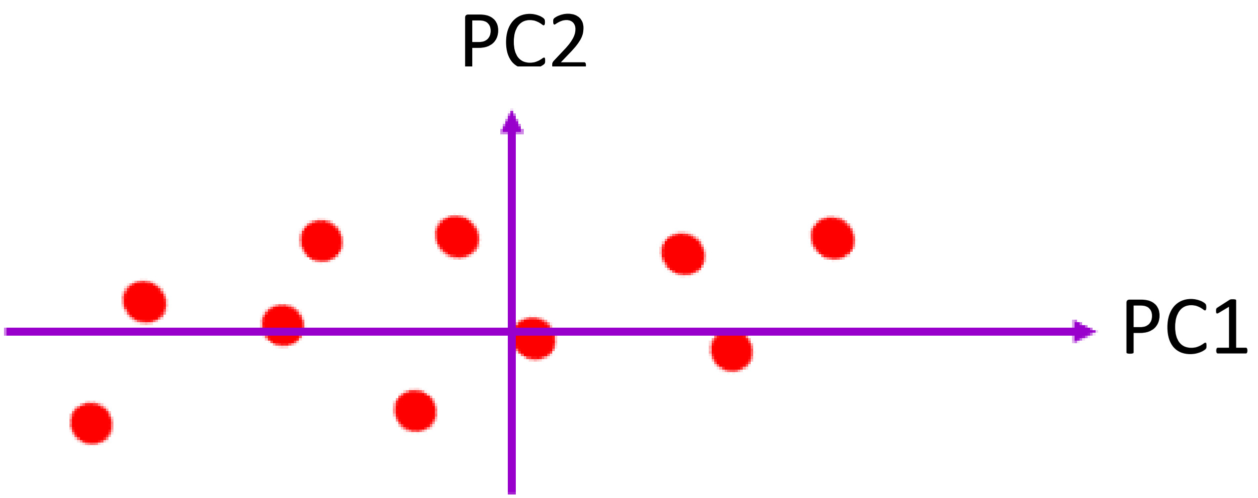
2-Dimension (2D)





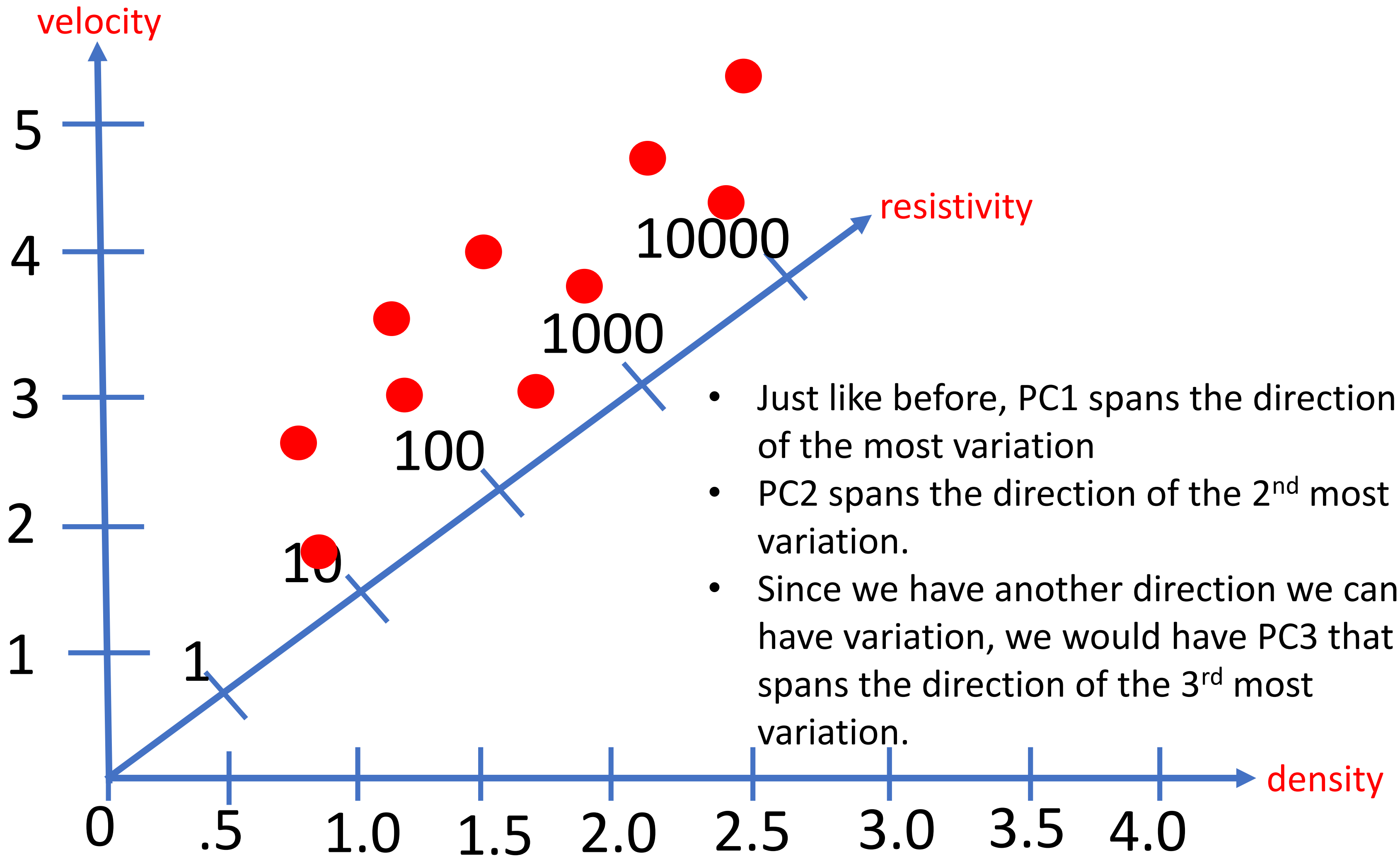
velocity
5
4
3
2
1
0
.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
density





- PC1 (the first component) is the axis that spans the most variation
- PC2 (the second component) is the axis that spans the second most variation

What if we 3-Dimension (3D) data?



- Just like before, PC1 spans the direction of the most variation
- PC2 spans the direction of the 2nd most variation.
- Since we have another direction we can have variation, we would have PC3 that spans the direction of the 3rd most variation.

What if we had 4-D data?

- PC1 would span the direction of the most variation.
- PC2 would span the direction of the 2^{nd} most variation.
- PC3 would span the direction of the 3^{rd} most variation.
- PC4 would span the direction of the 4^{th} most variation.

What if we had 4-D data?

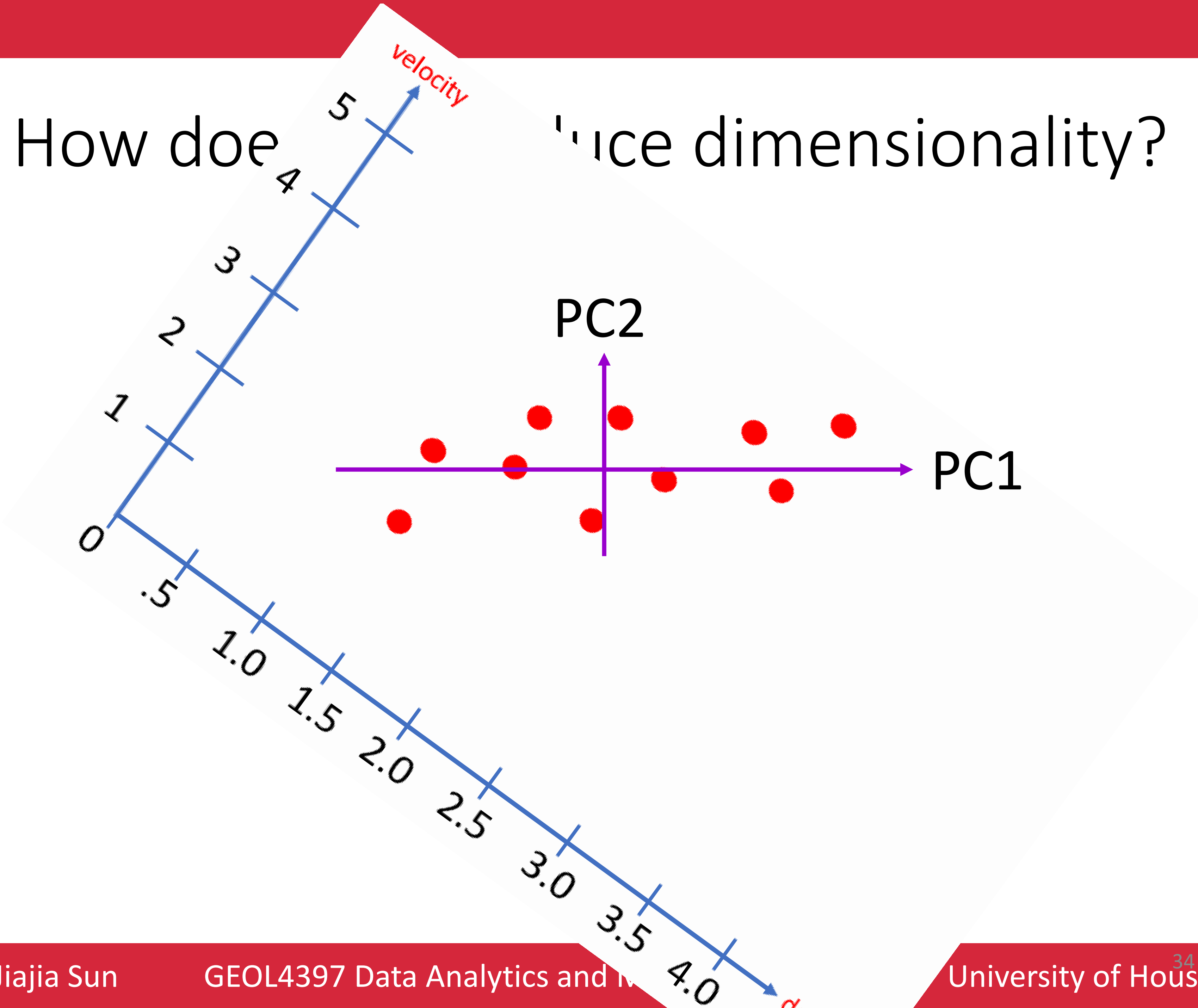
- PC1 would span the direction of the most variation.
- PC2 would span the direction of the 2^{nd} most variation.
- PC3 would span the direction of the 3^{rd} most variation.
- PC4 would span the direction of the 4^{th} most variation.

In general,

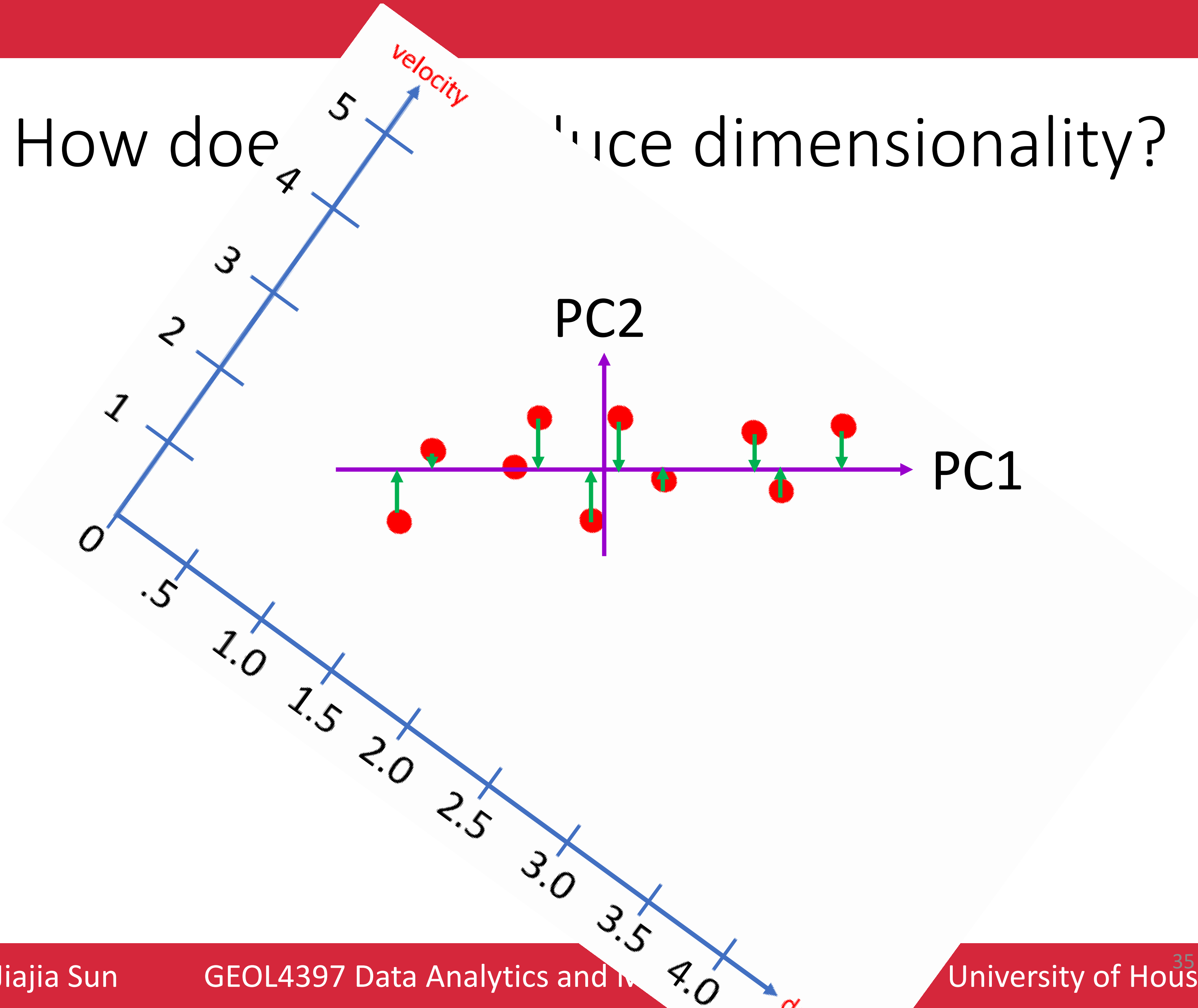
- There is a PC for each physical property measurement.
- If we had 22 measurements on each cutting sample, we would have 22 PCs.
- PC22 would span the direction of the 22^{nd} most variation.

How does PCA reduce dimensionality?

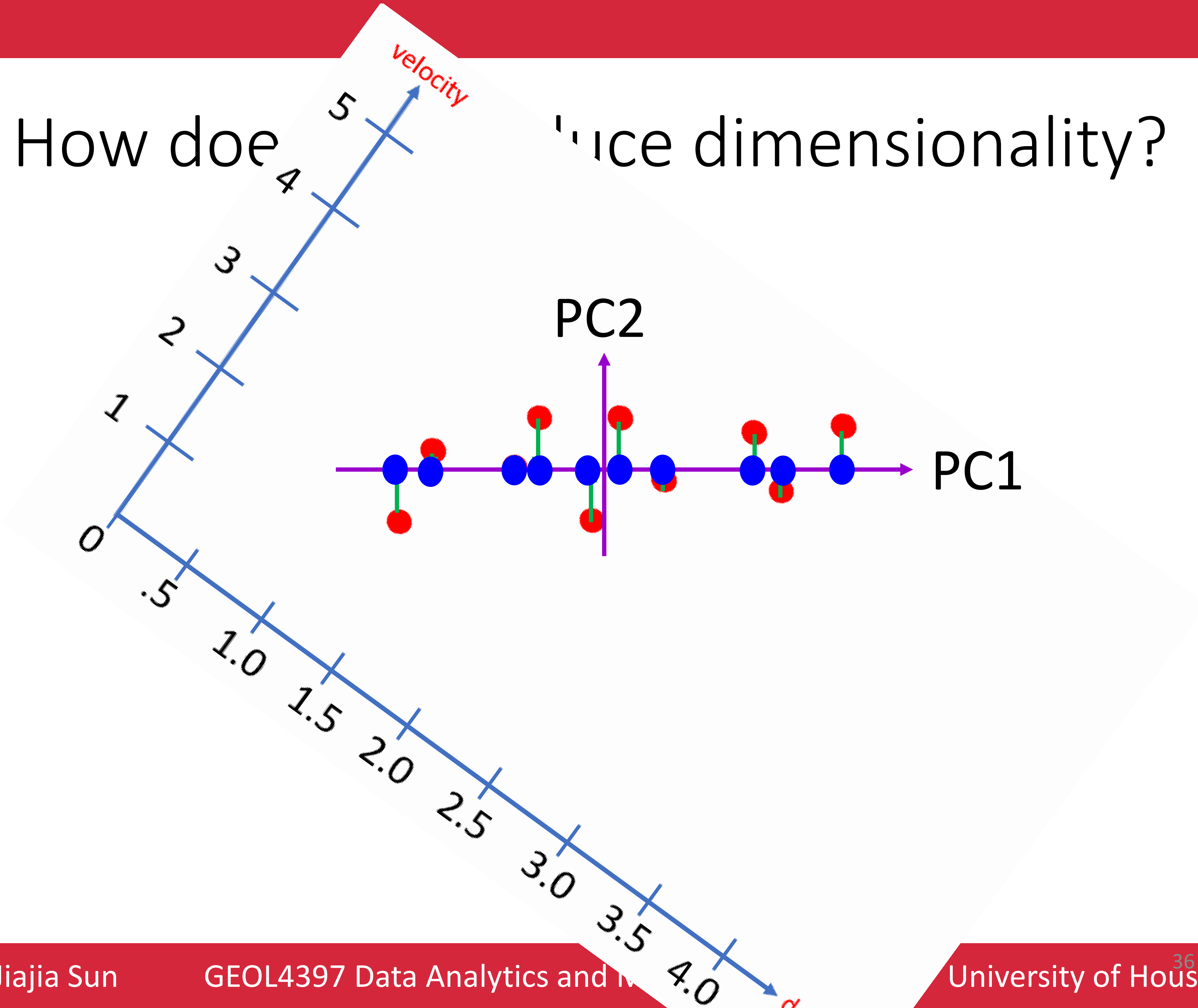
How doe… …uce dimensionality?



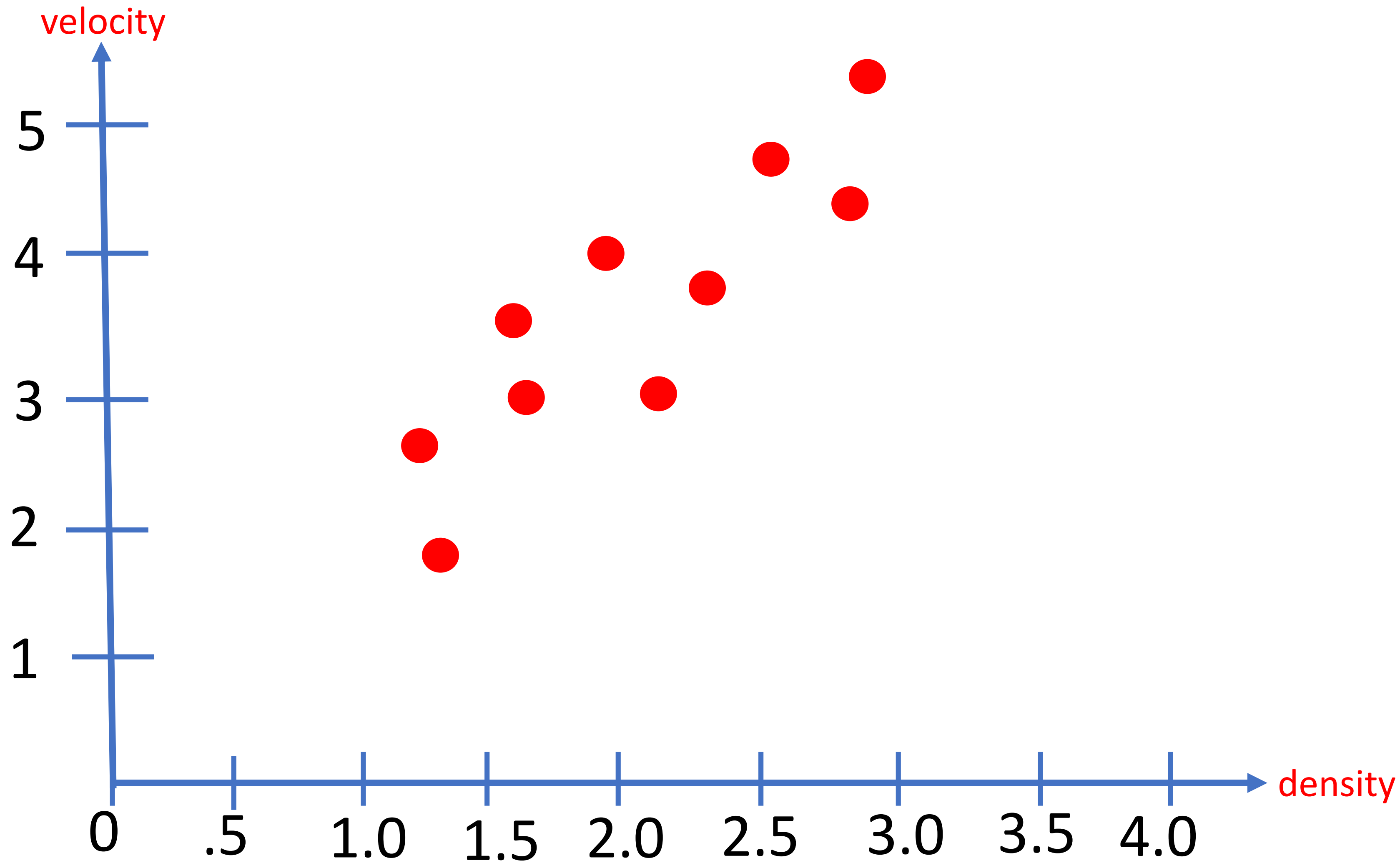
How doe … uce dimensionality?



How doe ... 'uce dimensionality?



Dimensionality reduction



MNIST dataset: PCA

- Original data in 784 dimensional space

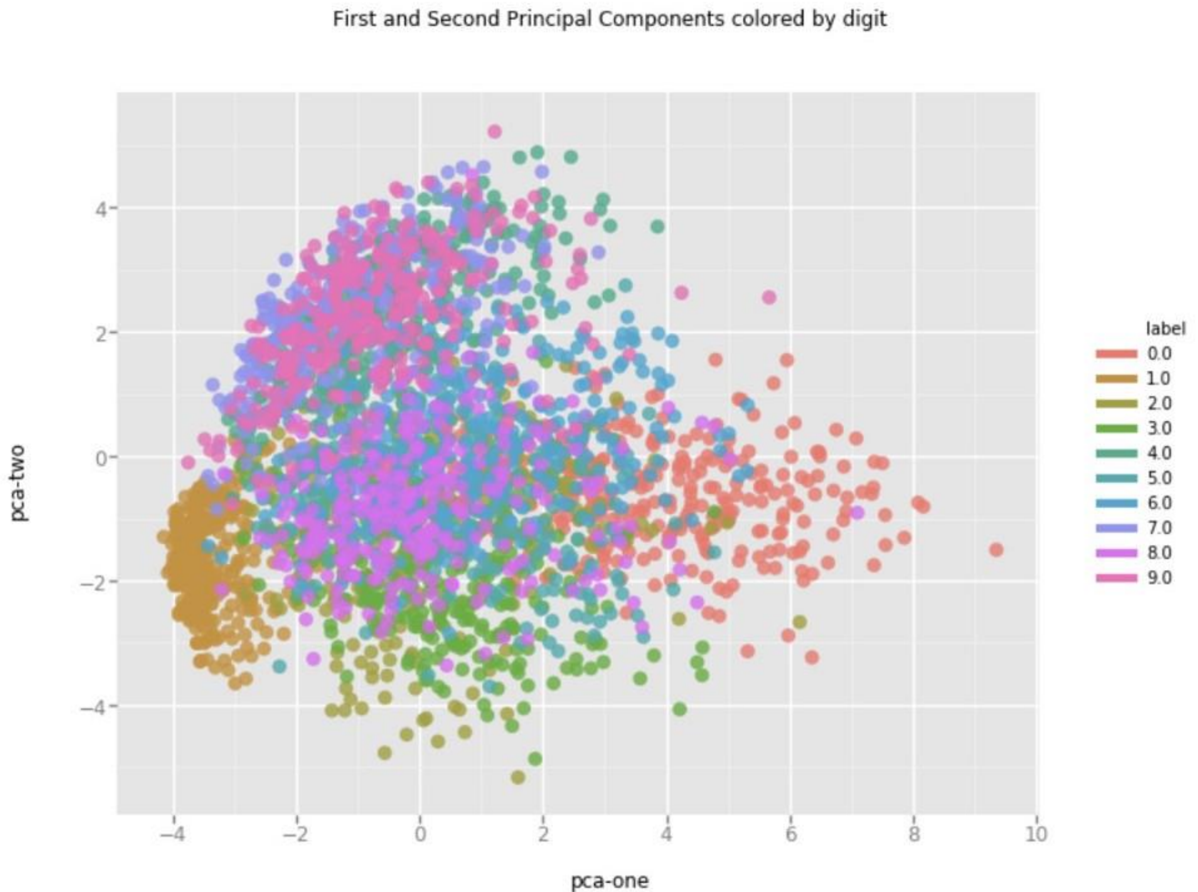


Image source: https://goo.gl/Dj97T7

MNIST dataset: t-SNE

- Original data in 784 dimensional space

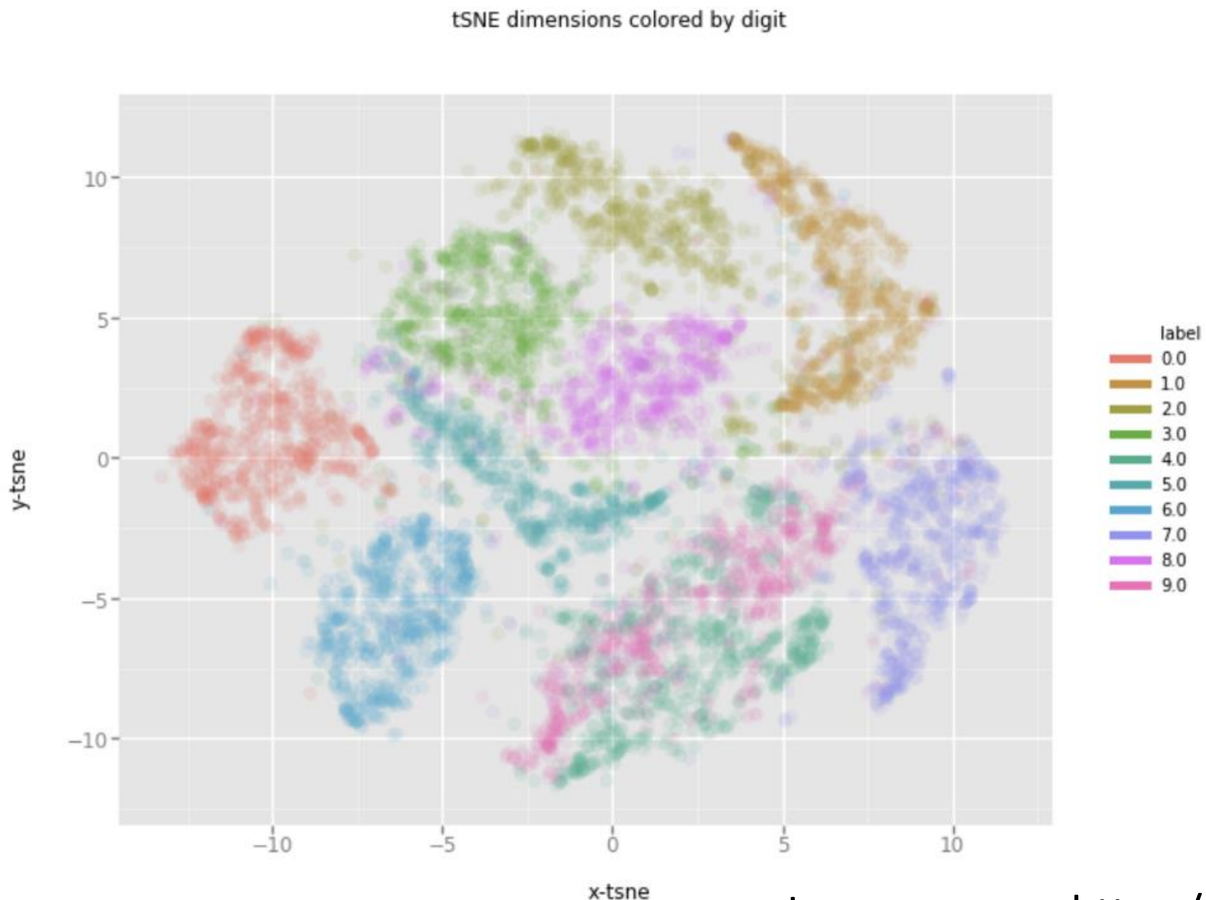
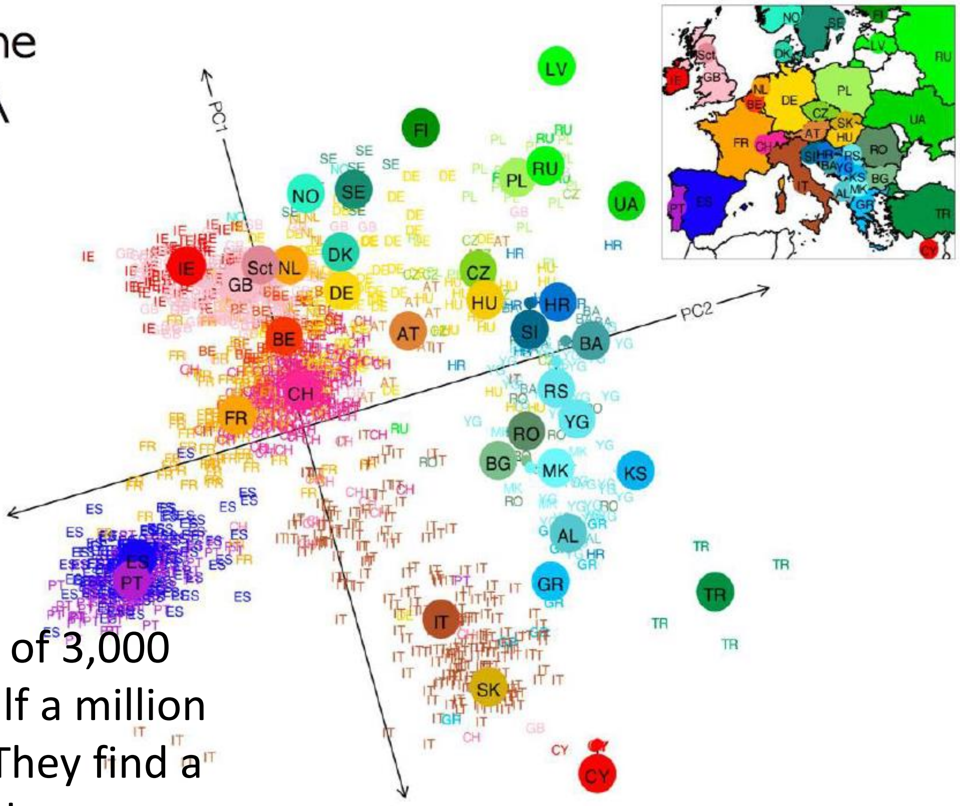


Image source: https://goo.gl/Dj97T7

Example: PCA for high-dimensional data

500,000 DNA sites in human genome projected to 2 dimensions with PCA

Principal components correspond to geography → ancestry



Novembre et al. (2008), Nature

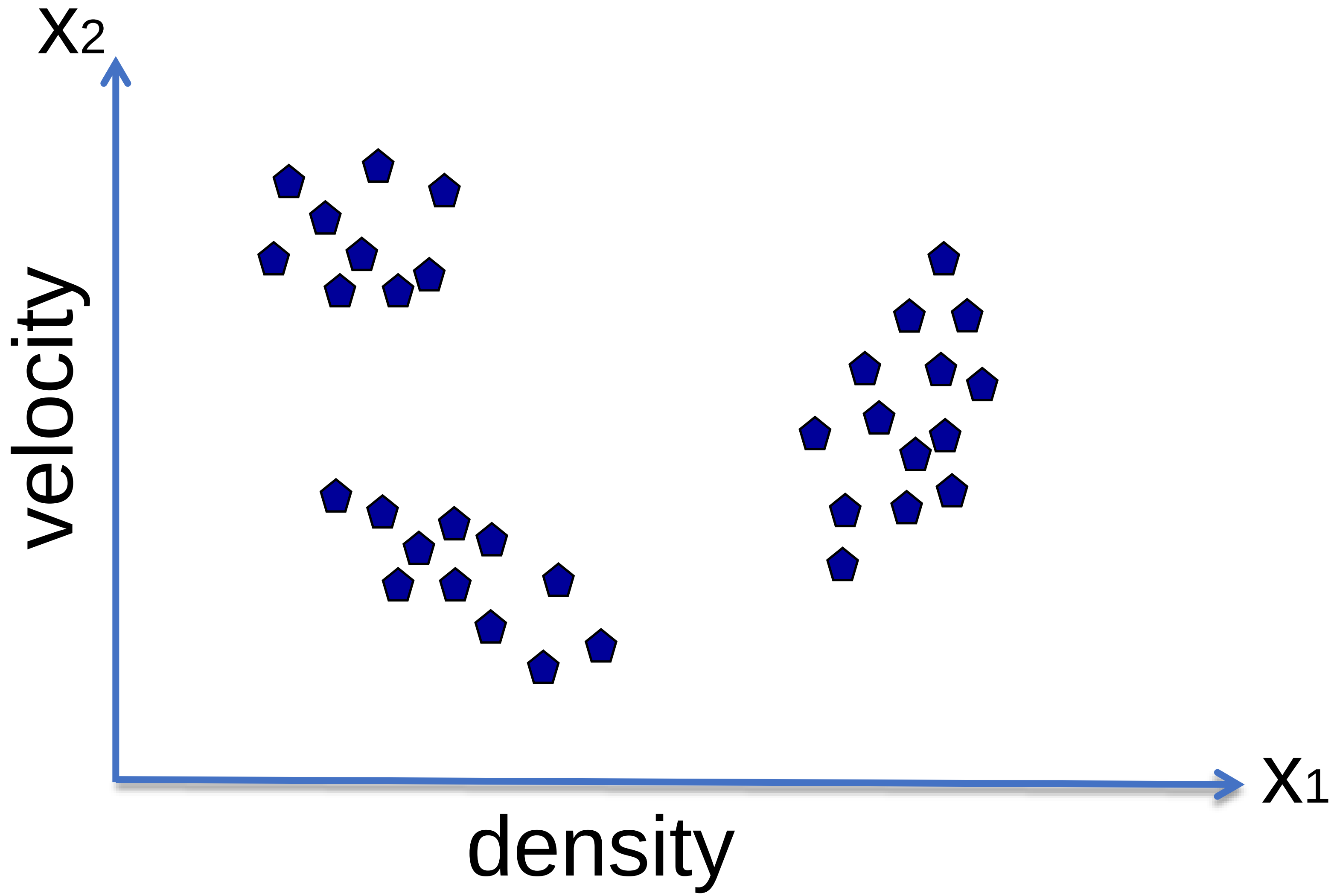
Characterize genetic variations in a sample of 3,000 European individuals genotyped at over half a million variable DNA sites in the human genome. They find a close correspondence between genetic and geographic distances. → genetic ancestry testing an individual's DNA can be used to infer their geographic origin with surprising accuracy—often to within a few hundred kilometers.

Thanks to Karianne Bergen

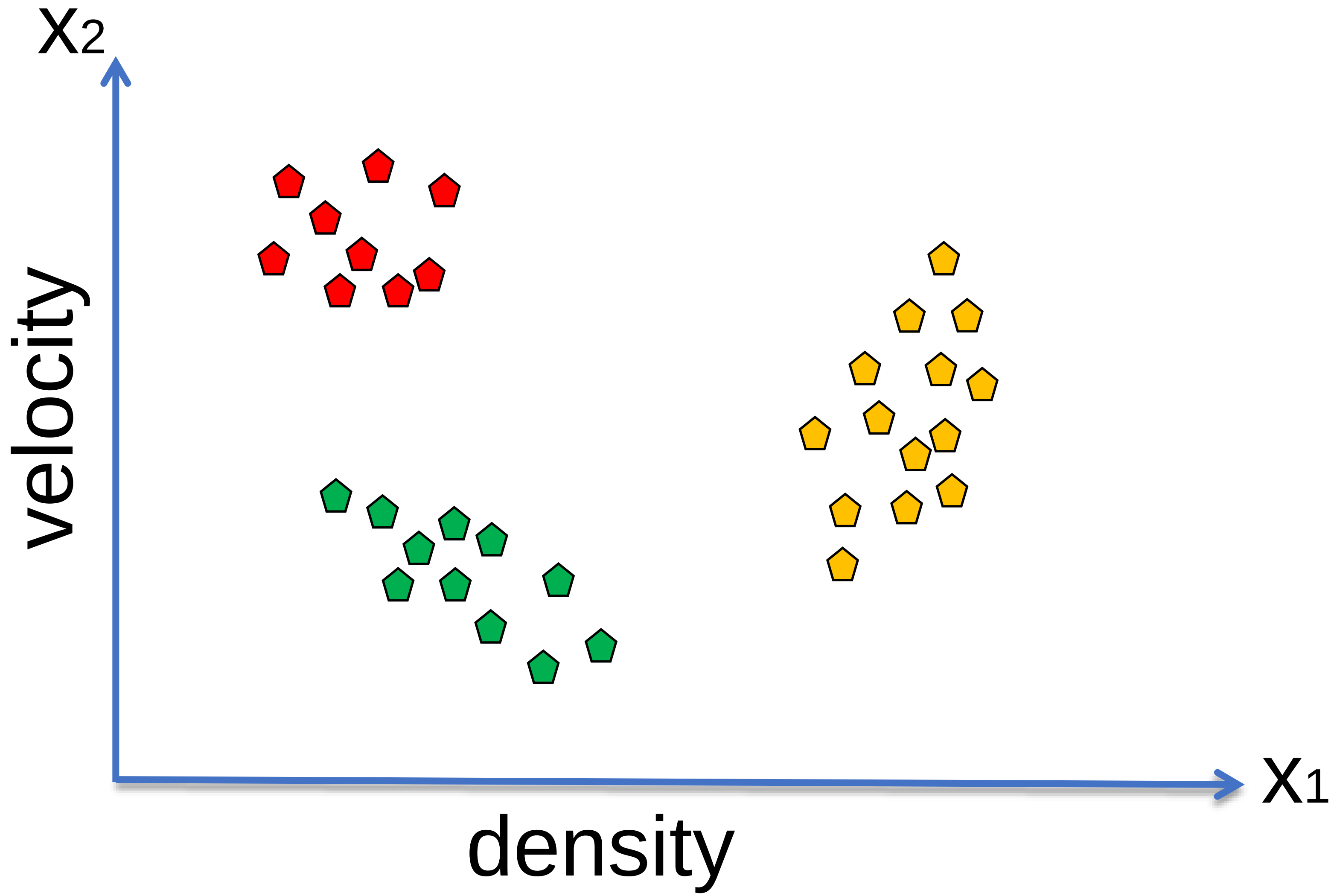
Outline

- Dimensionality reduction
- K-means Clustering
- Implementation in Scikit-Learn

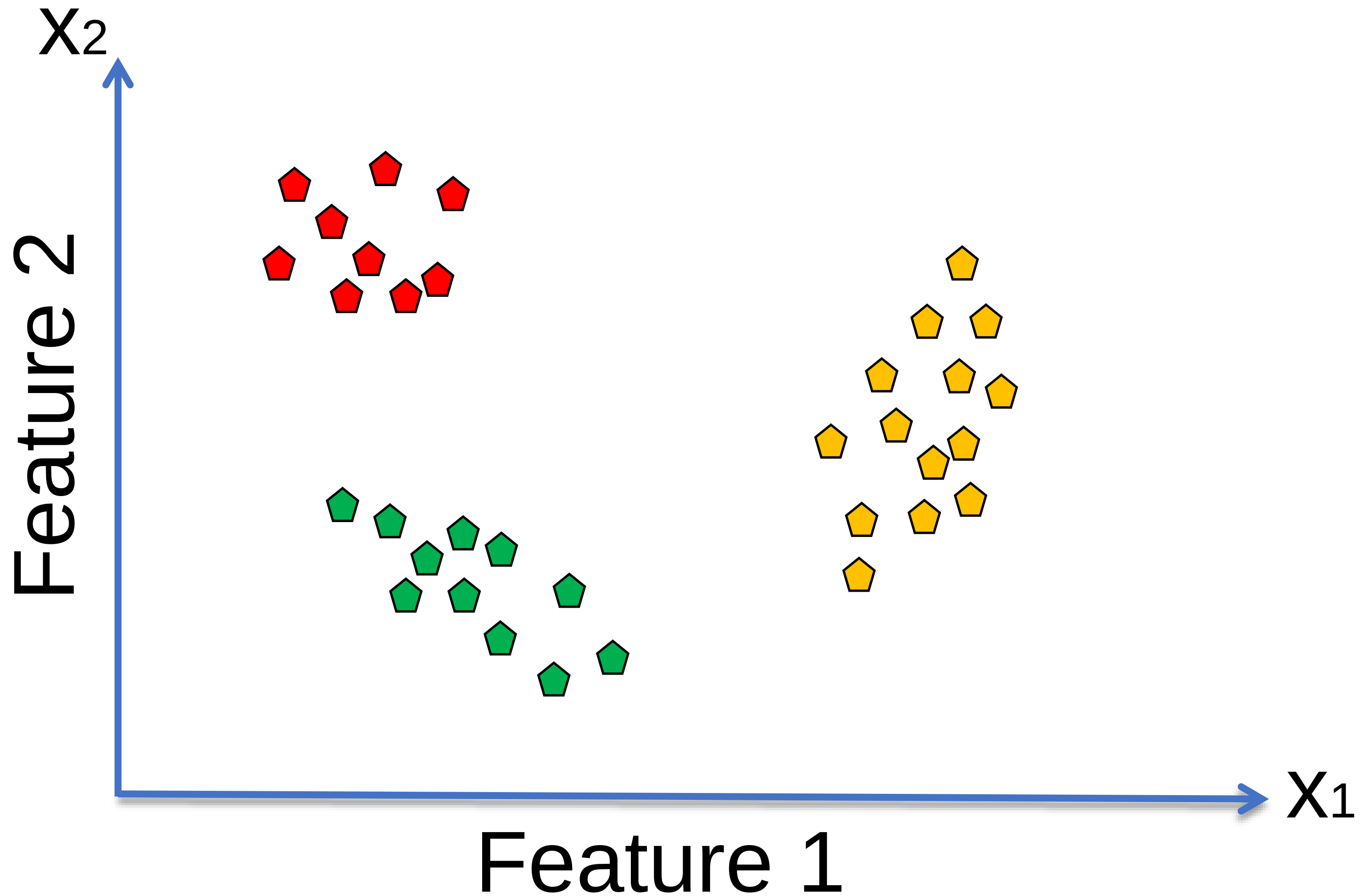
Clustering



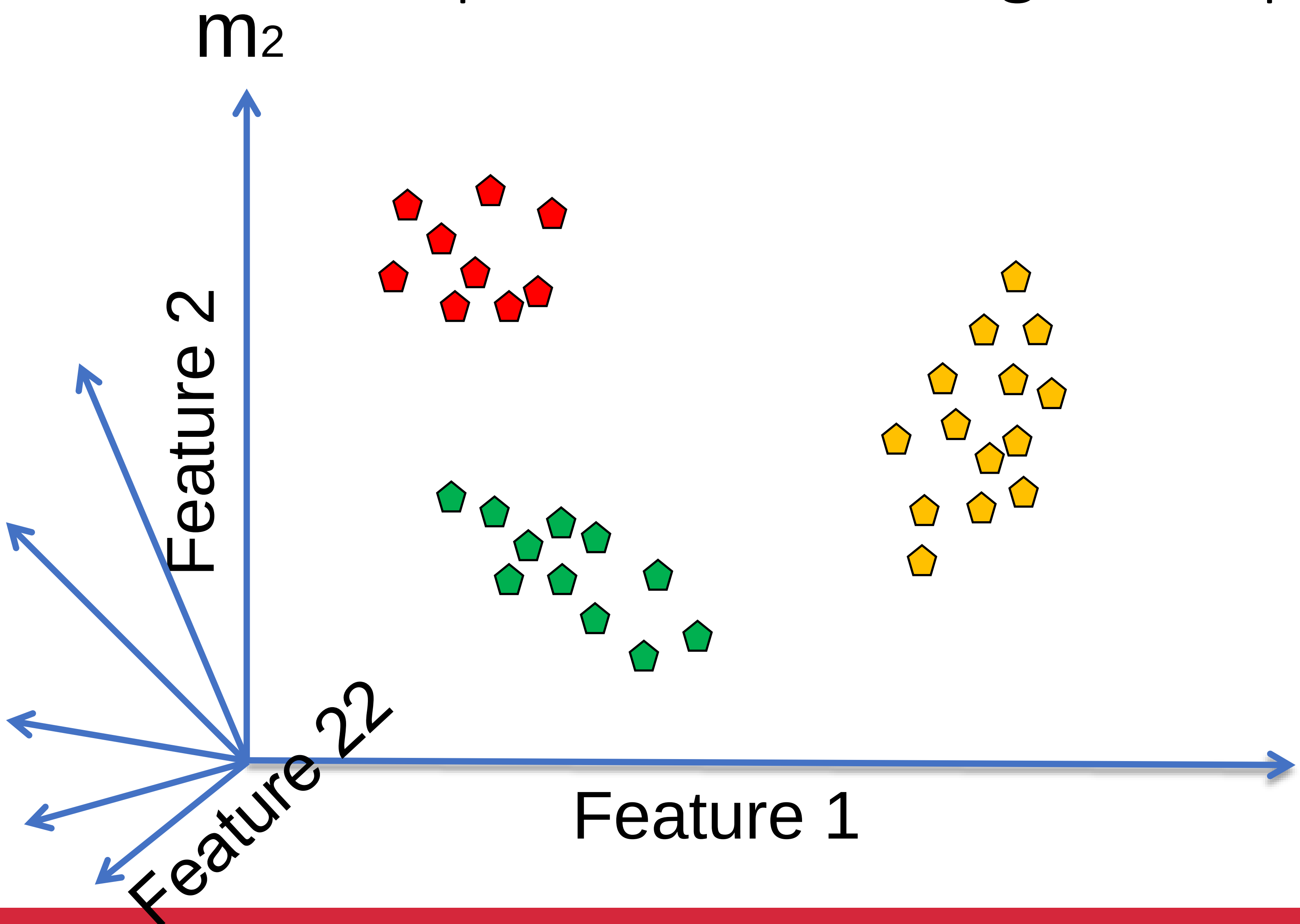
Clustering



Clustering



Unsupervised learning: example



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Headlines

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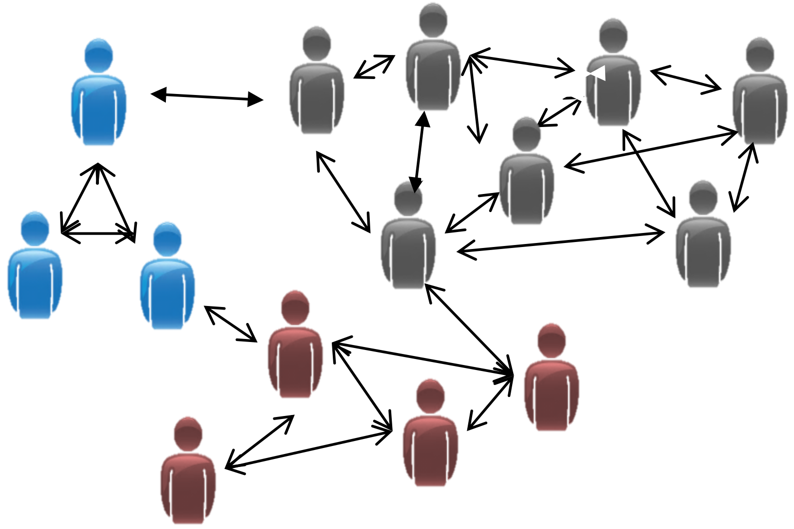
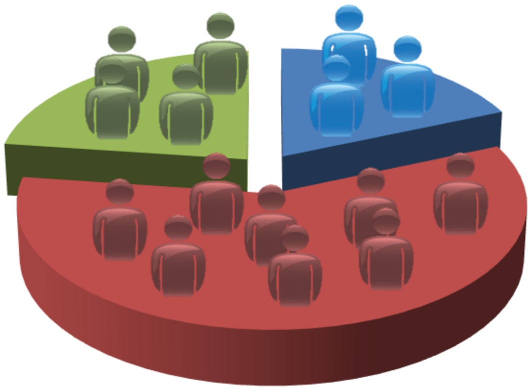
Unsupervised learning: applications

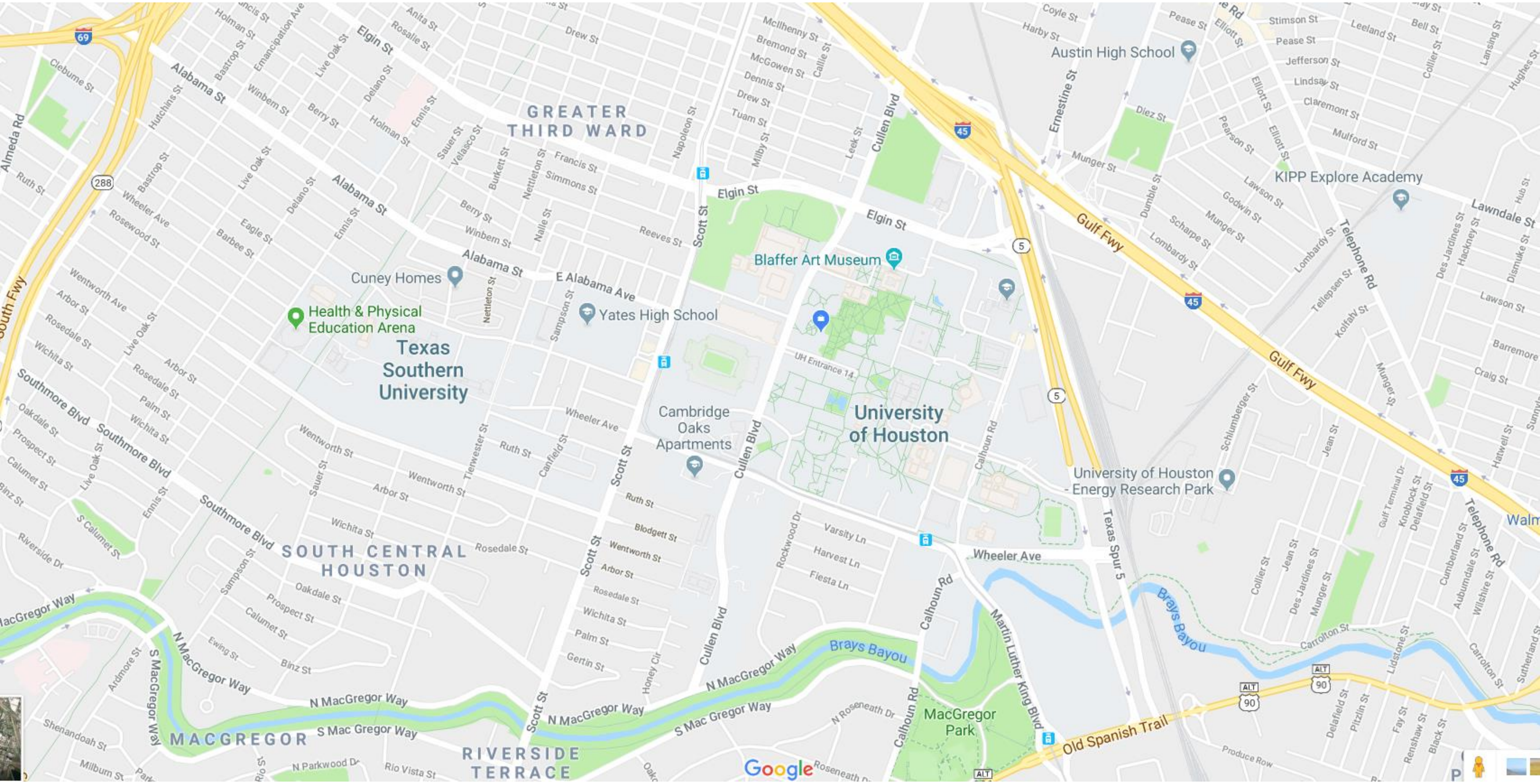


Social network analysis

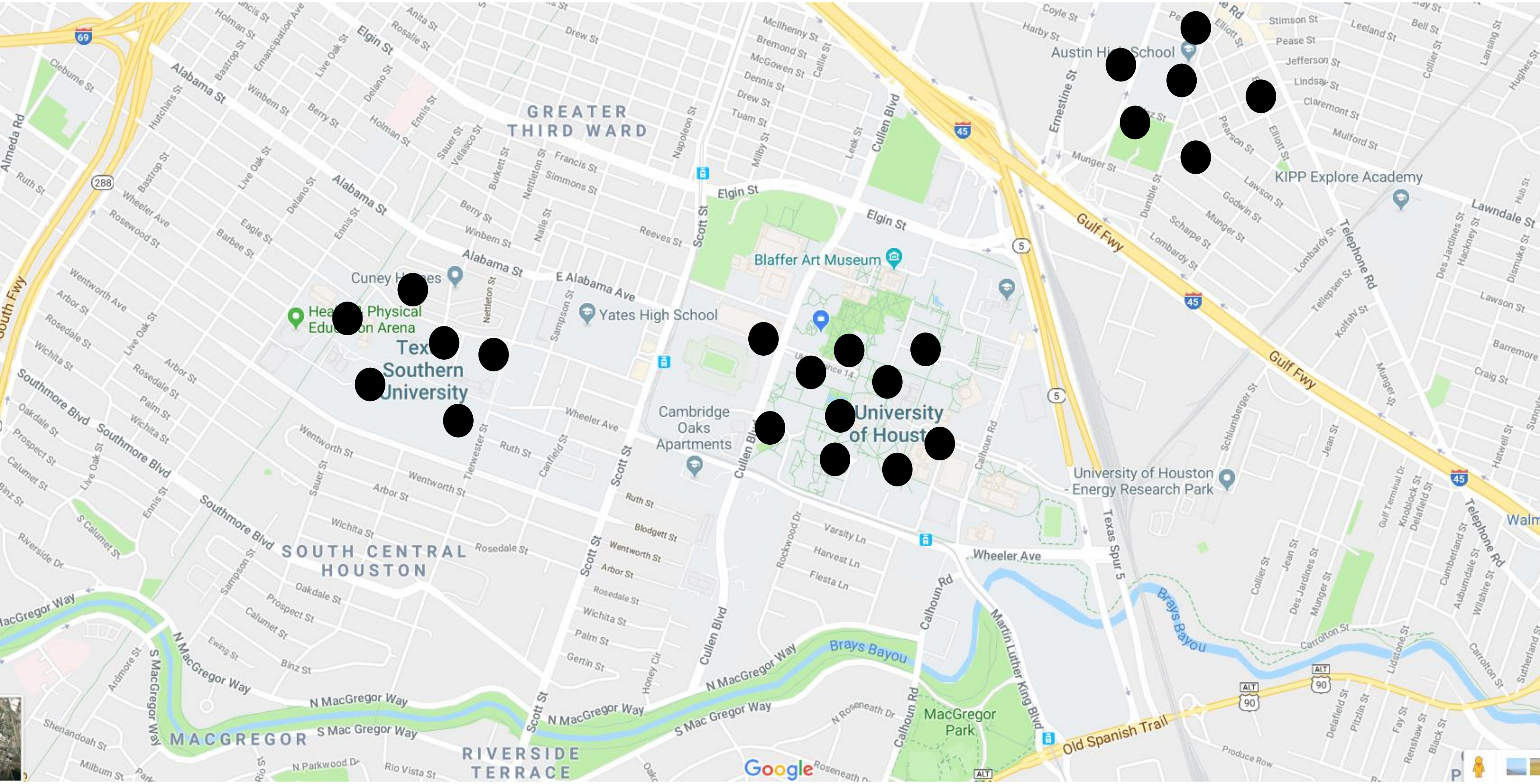


Market segmentation

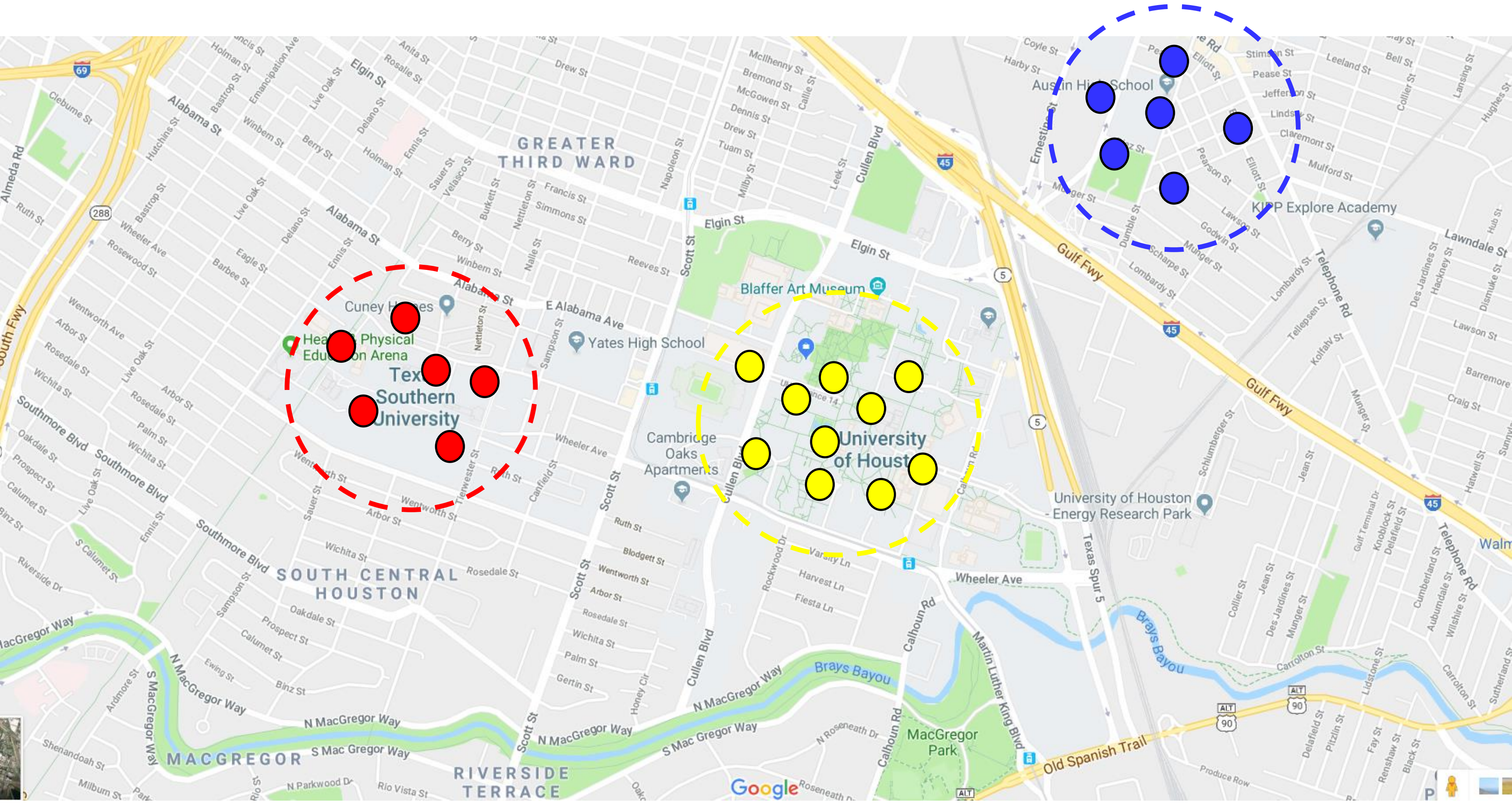
Investing in pizza stores in Houston



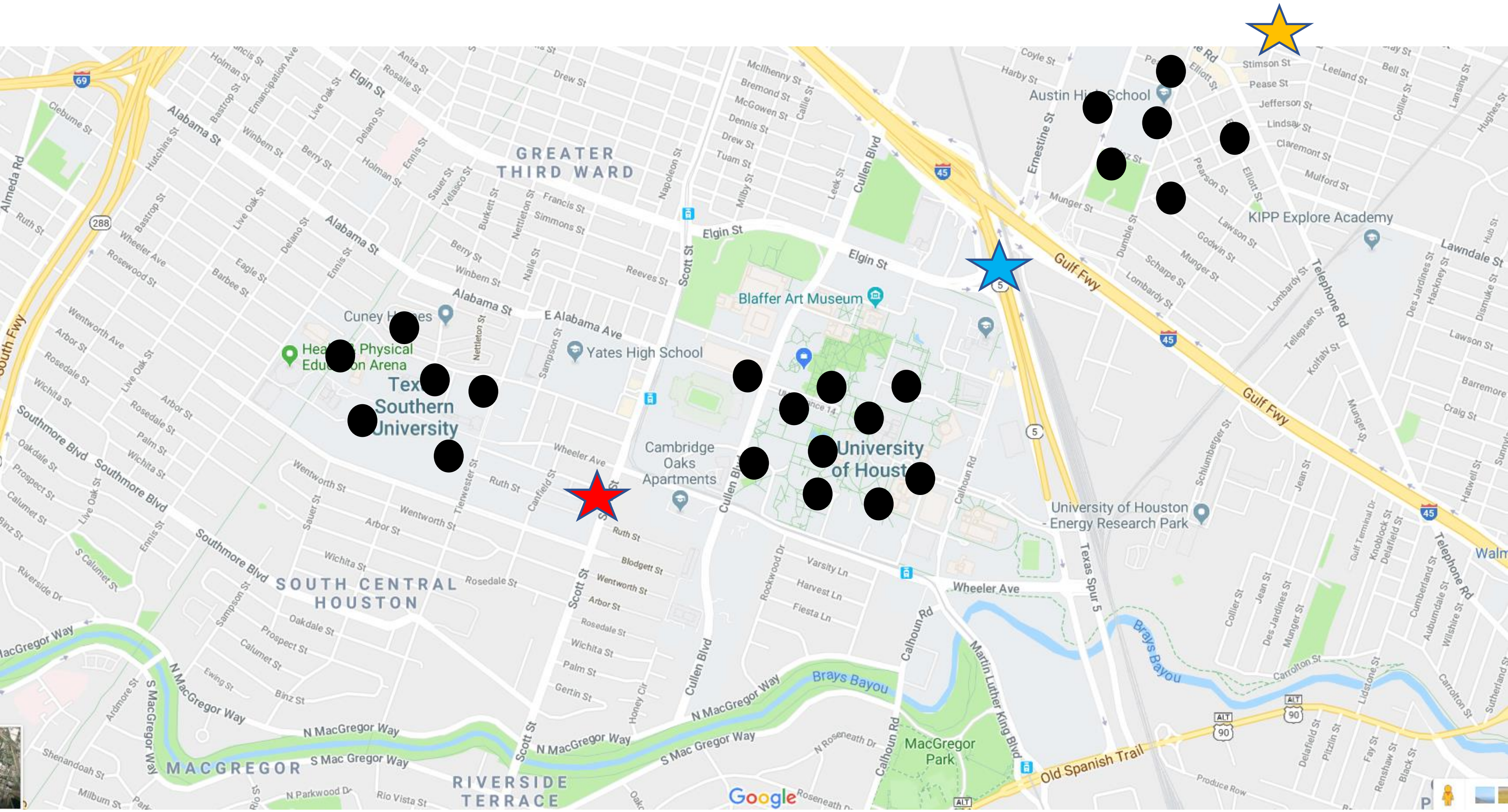
Customer data



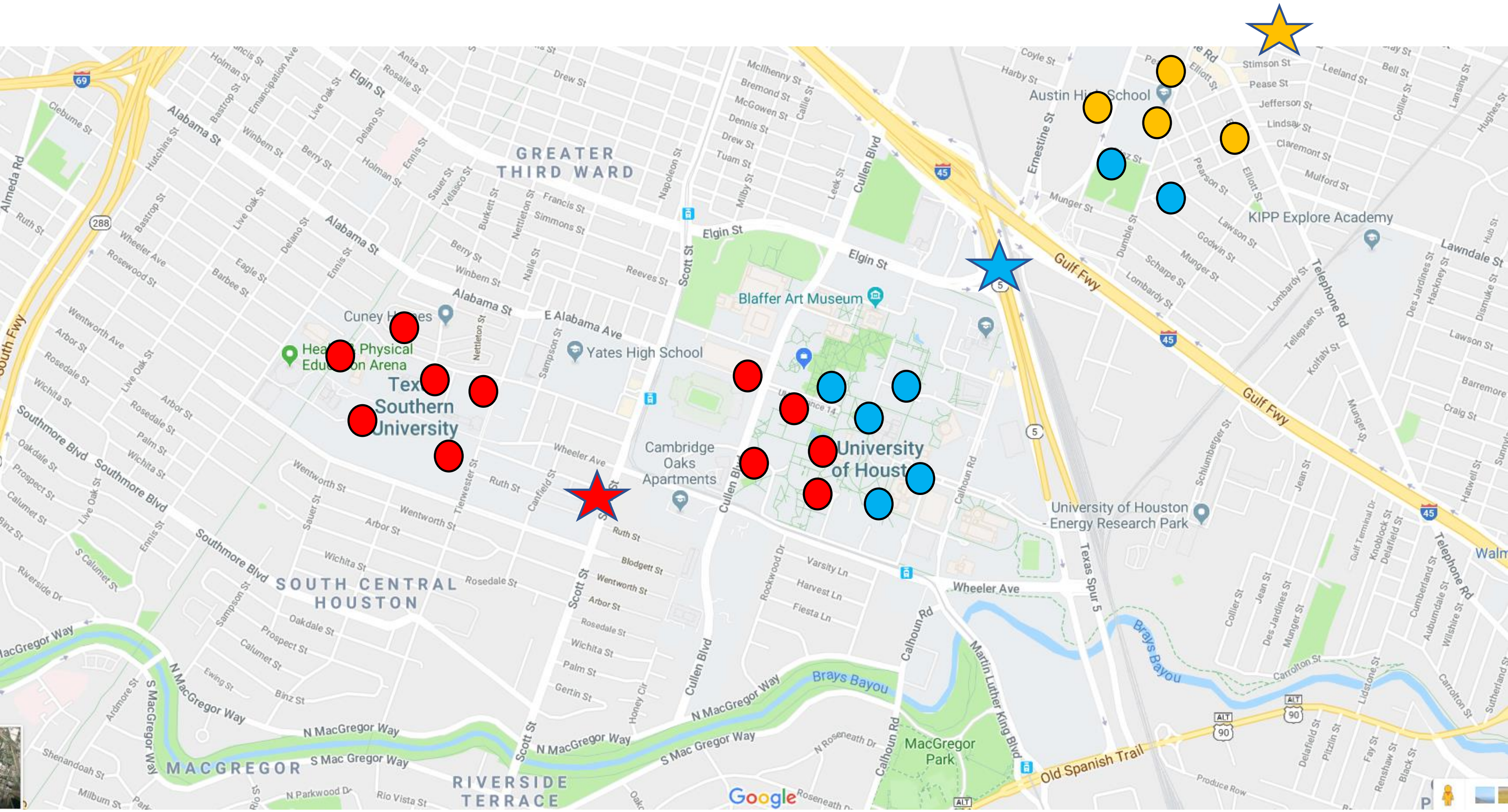
Human wisdom



Start with random locations



Distribution of customers



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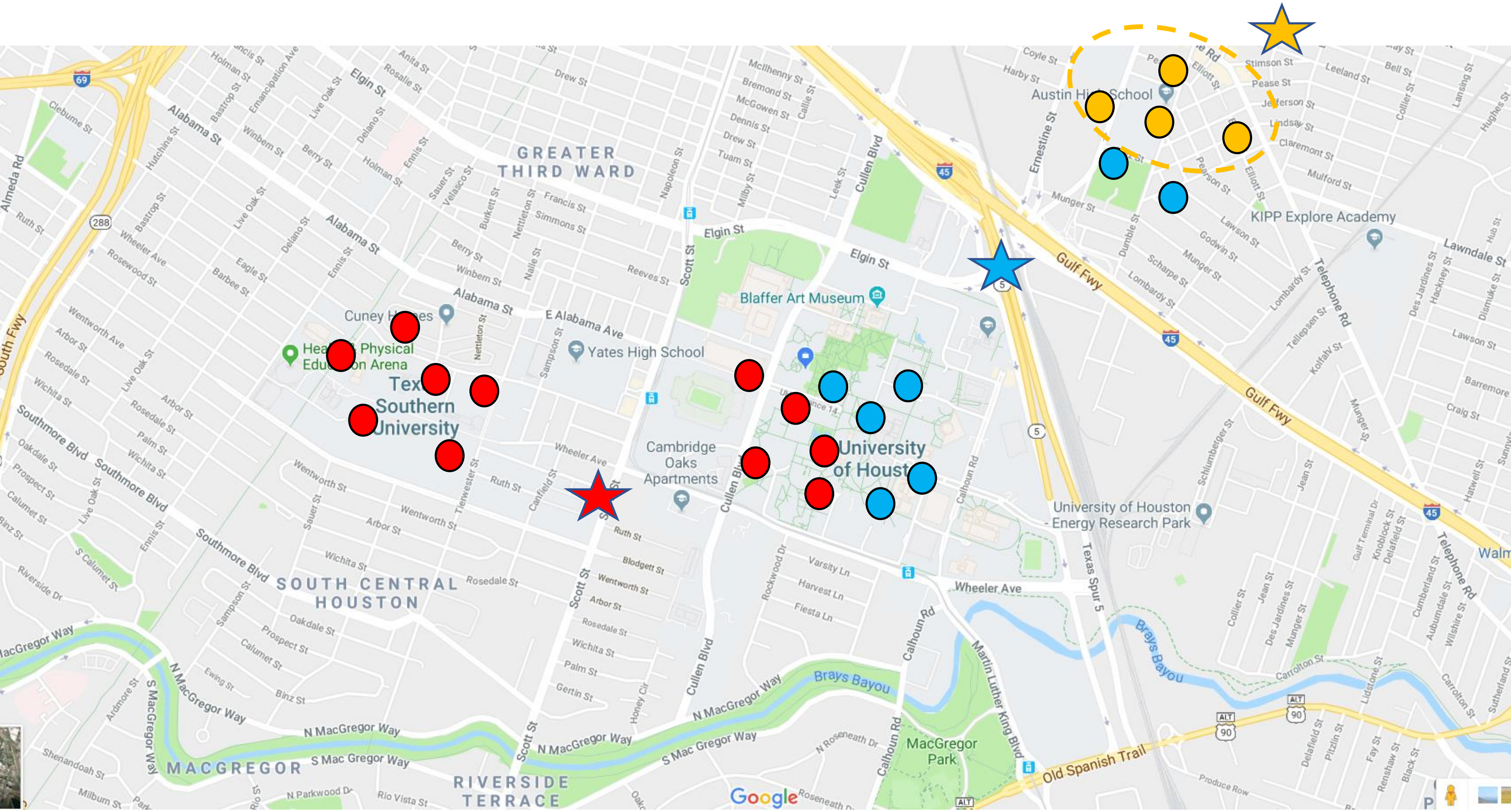
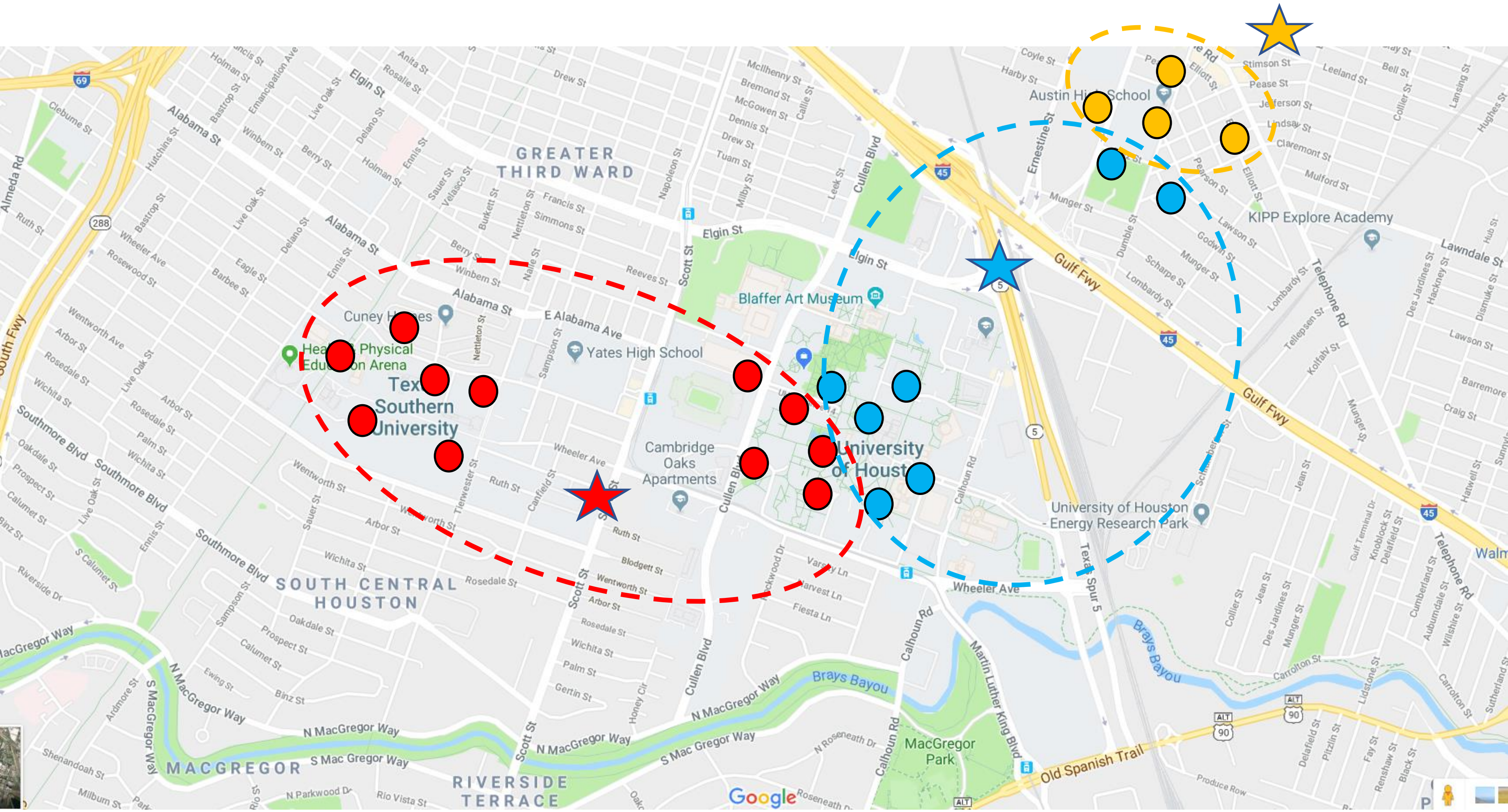
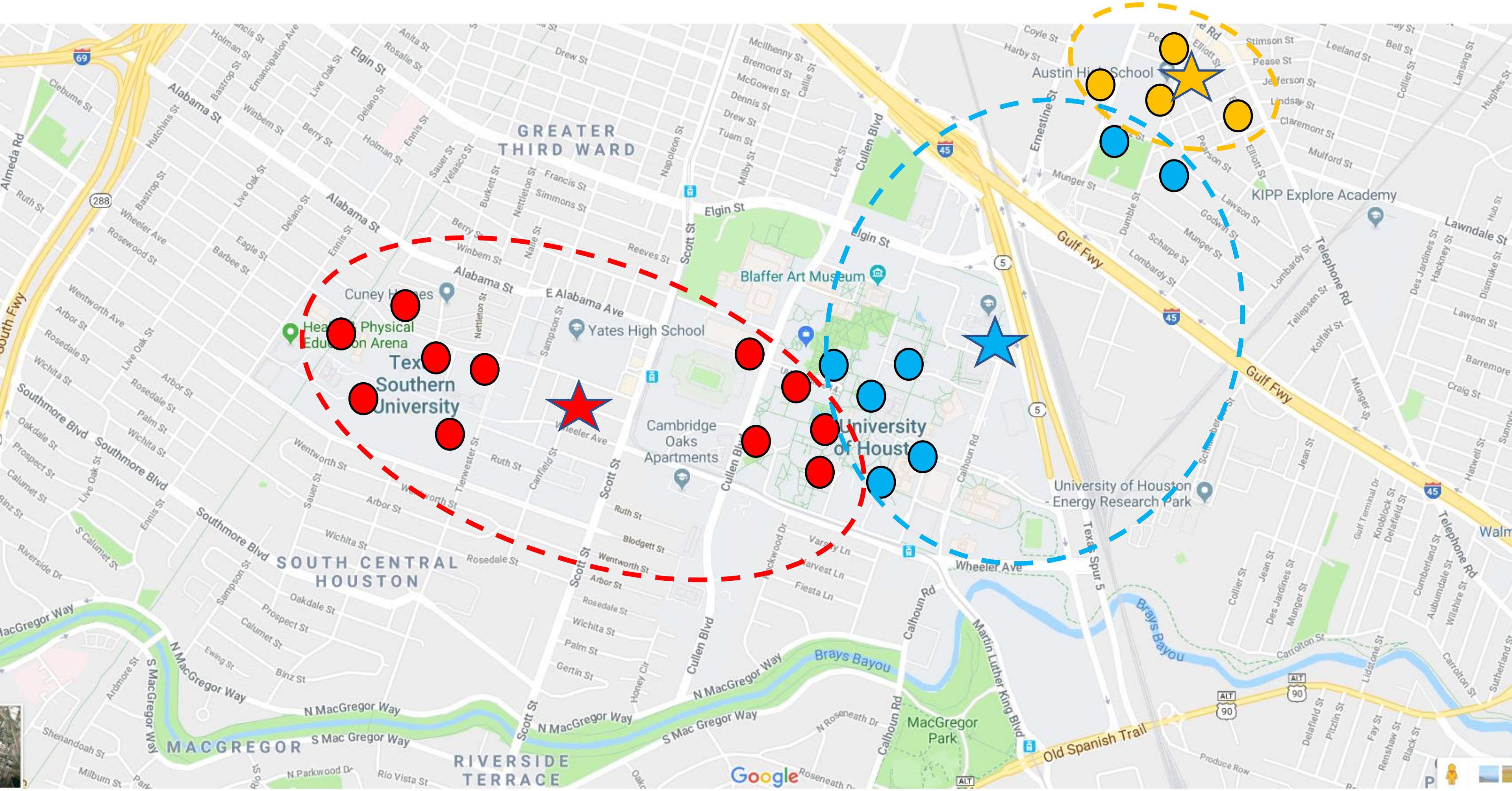


Distribution of customers



Update store locations



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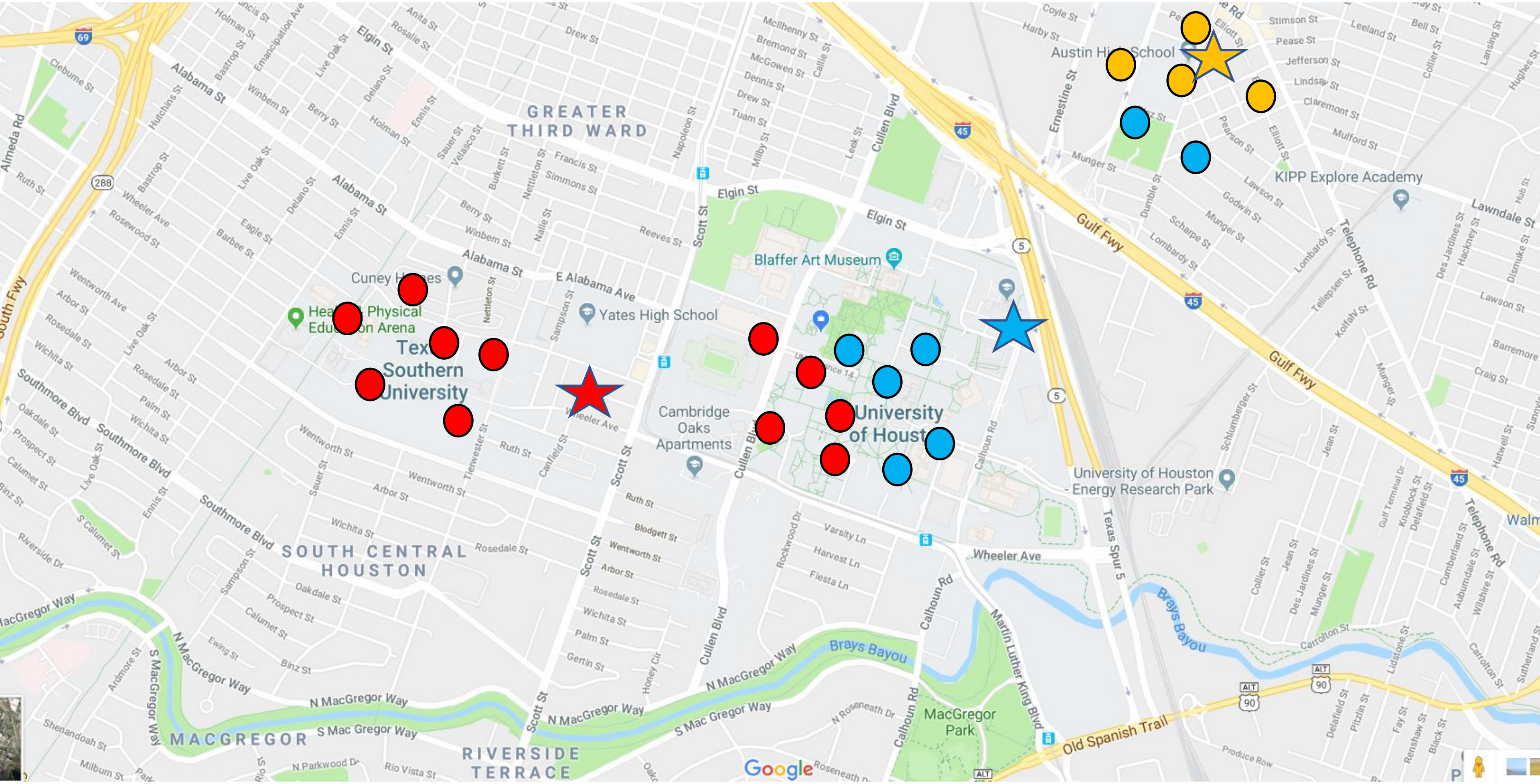
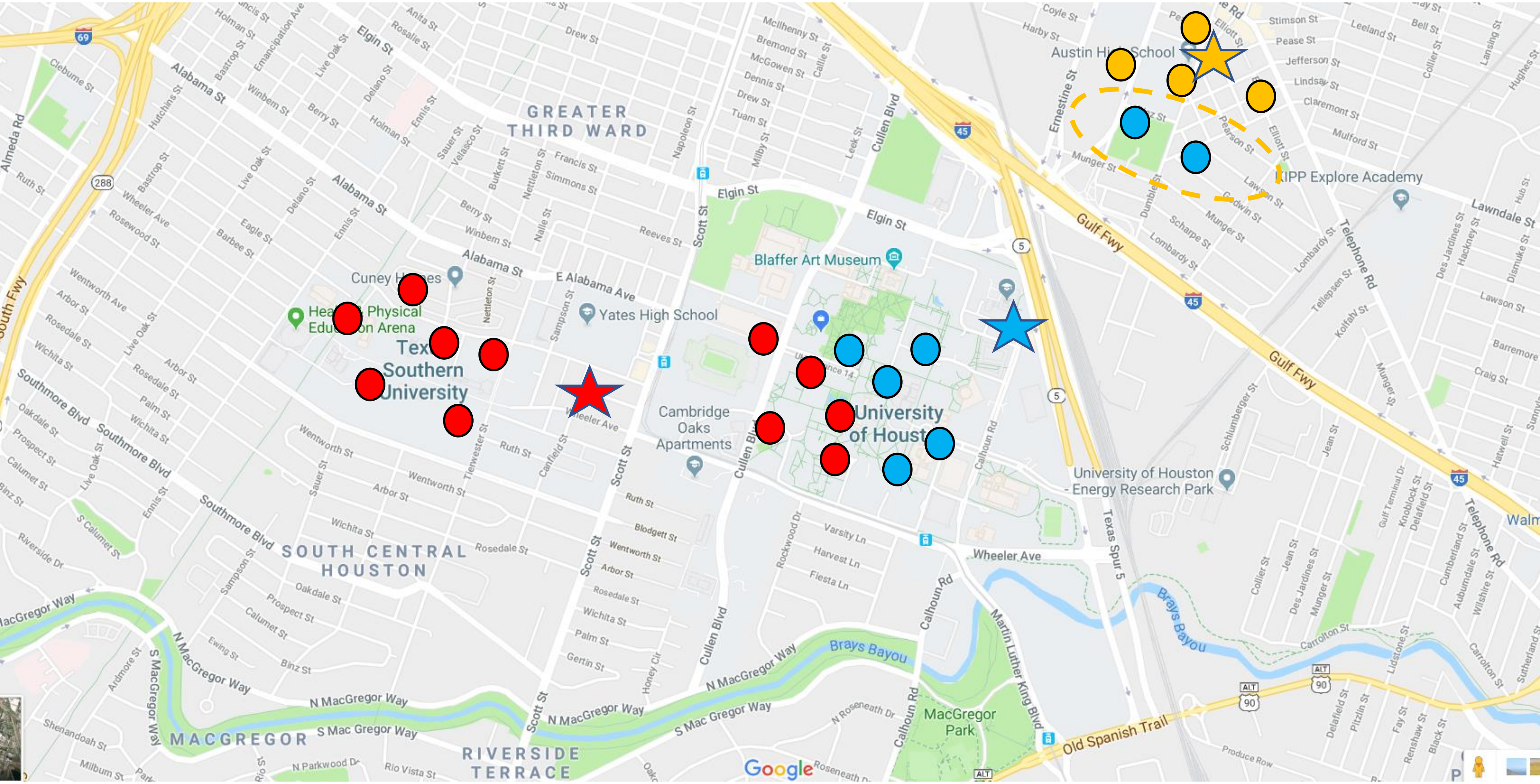
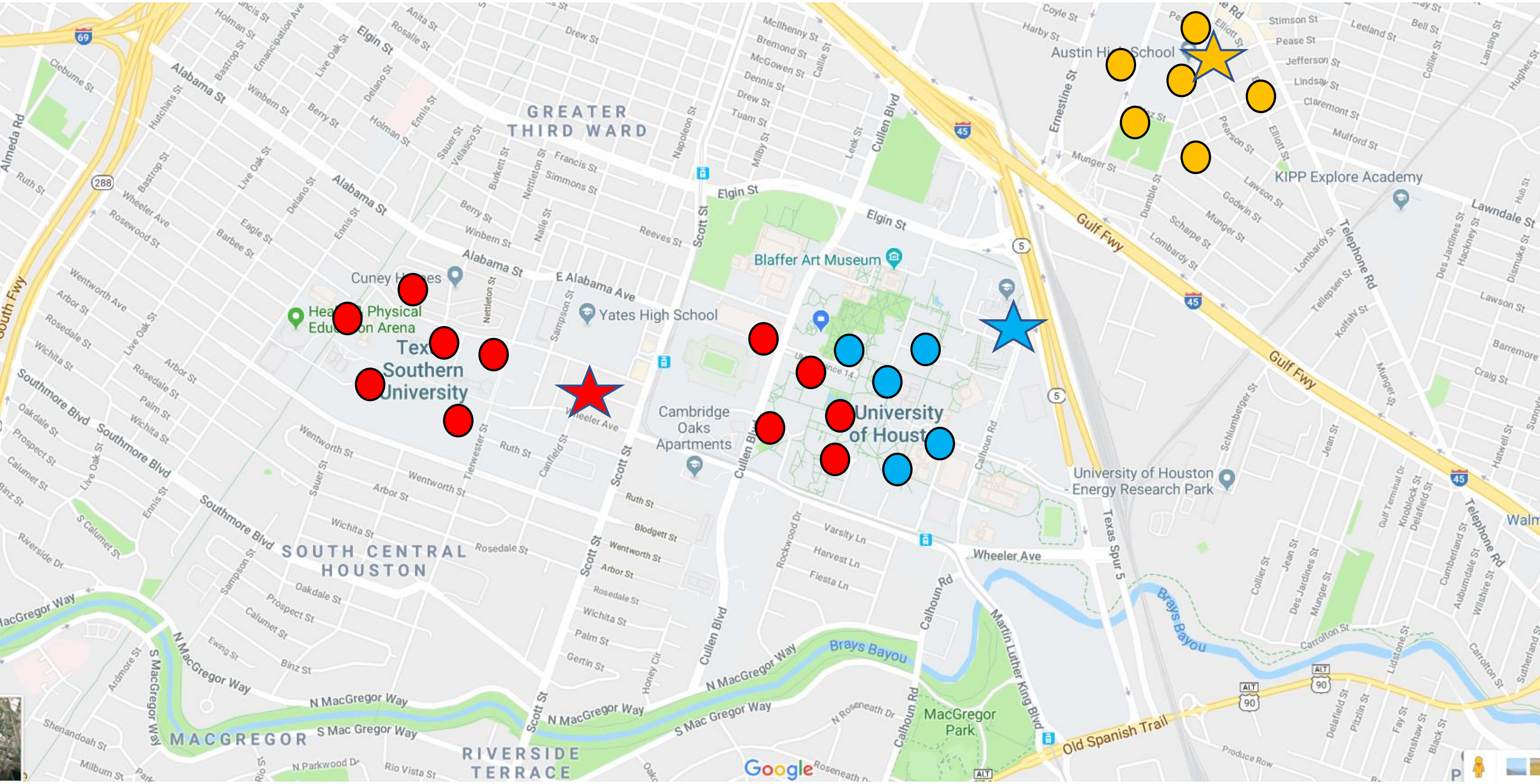


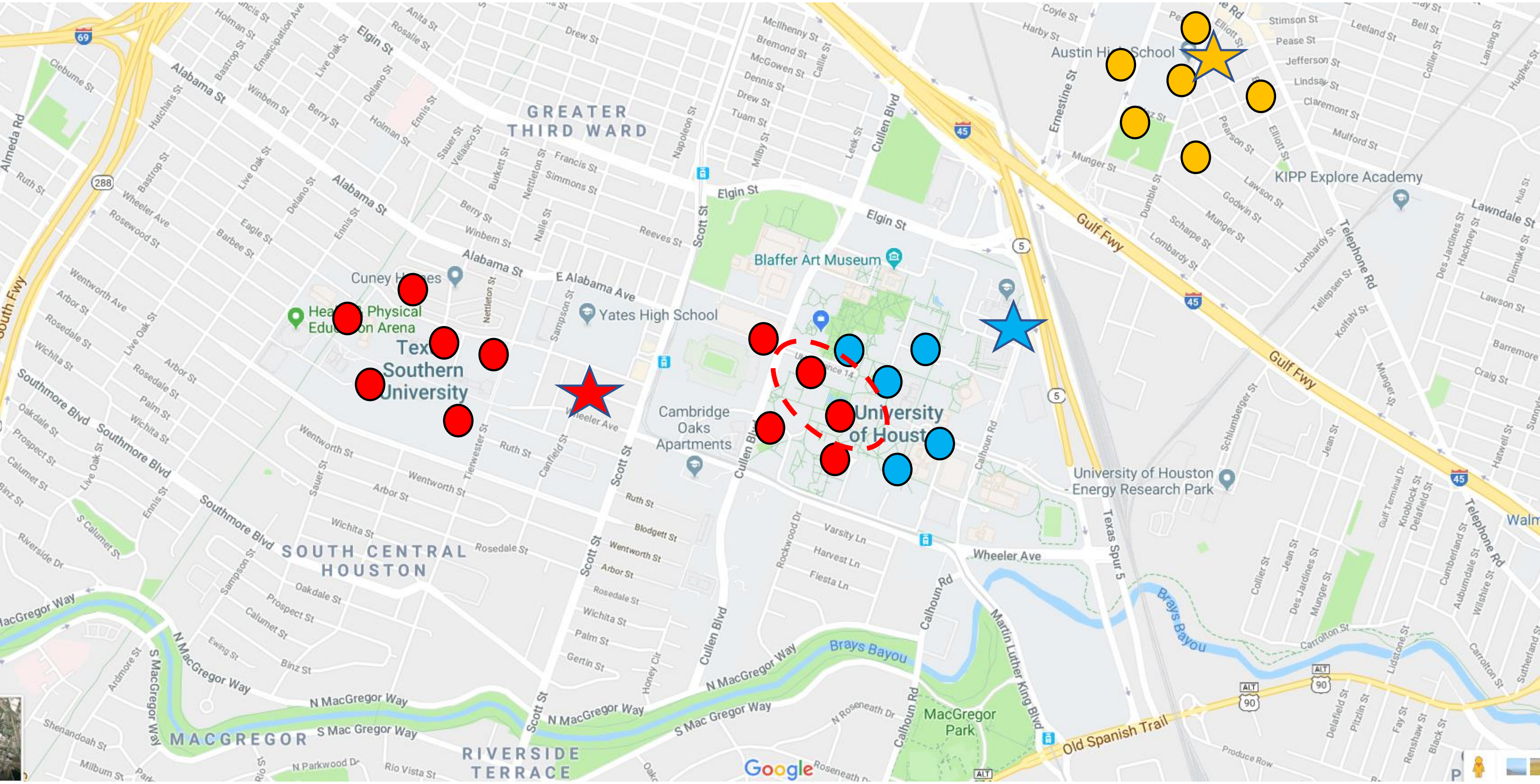
Customer distribution update



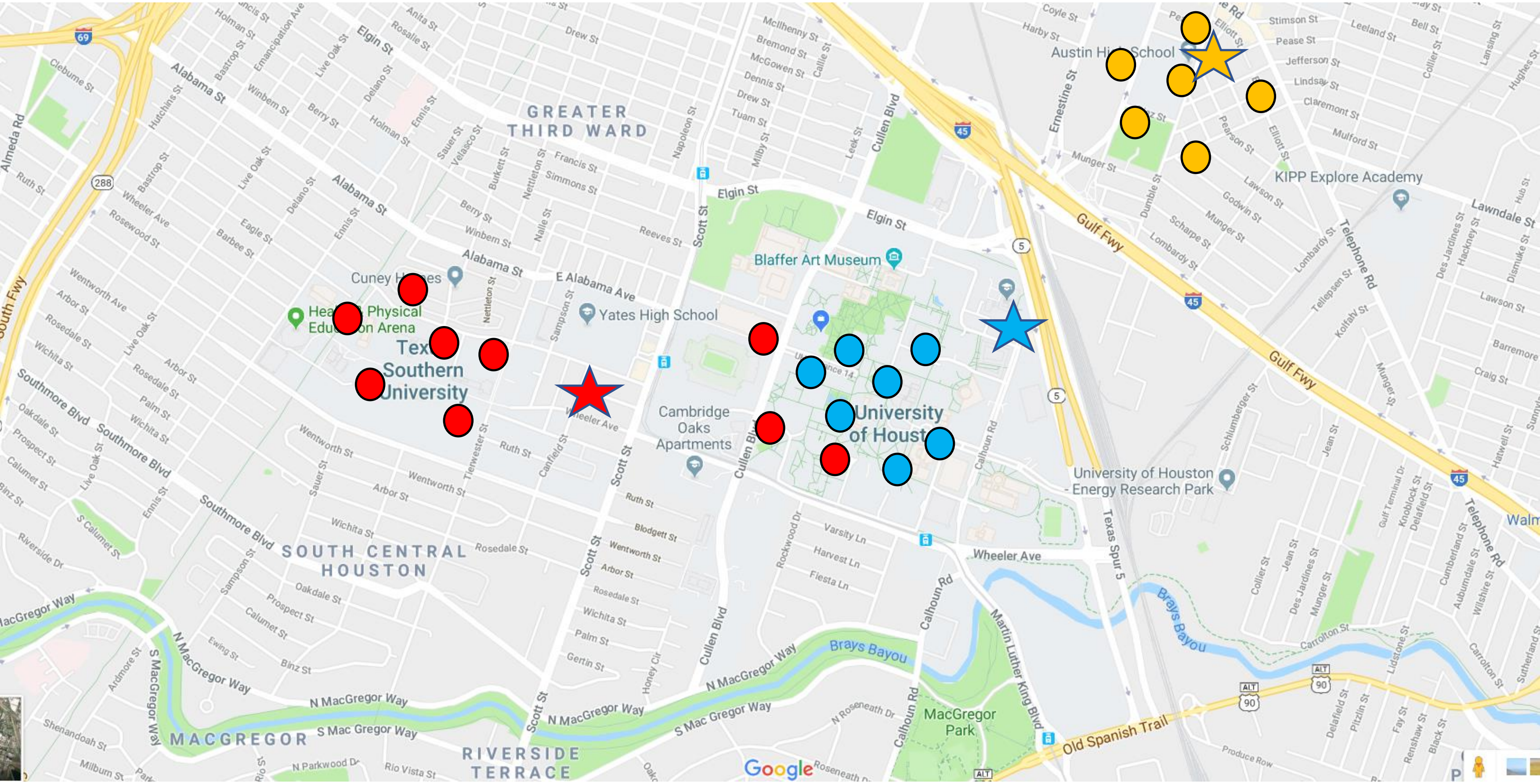
Customer distribution update



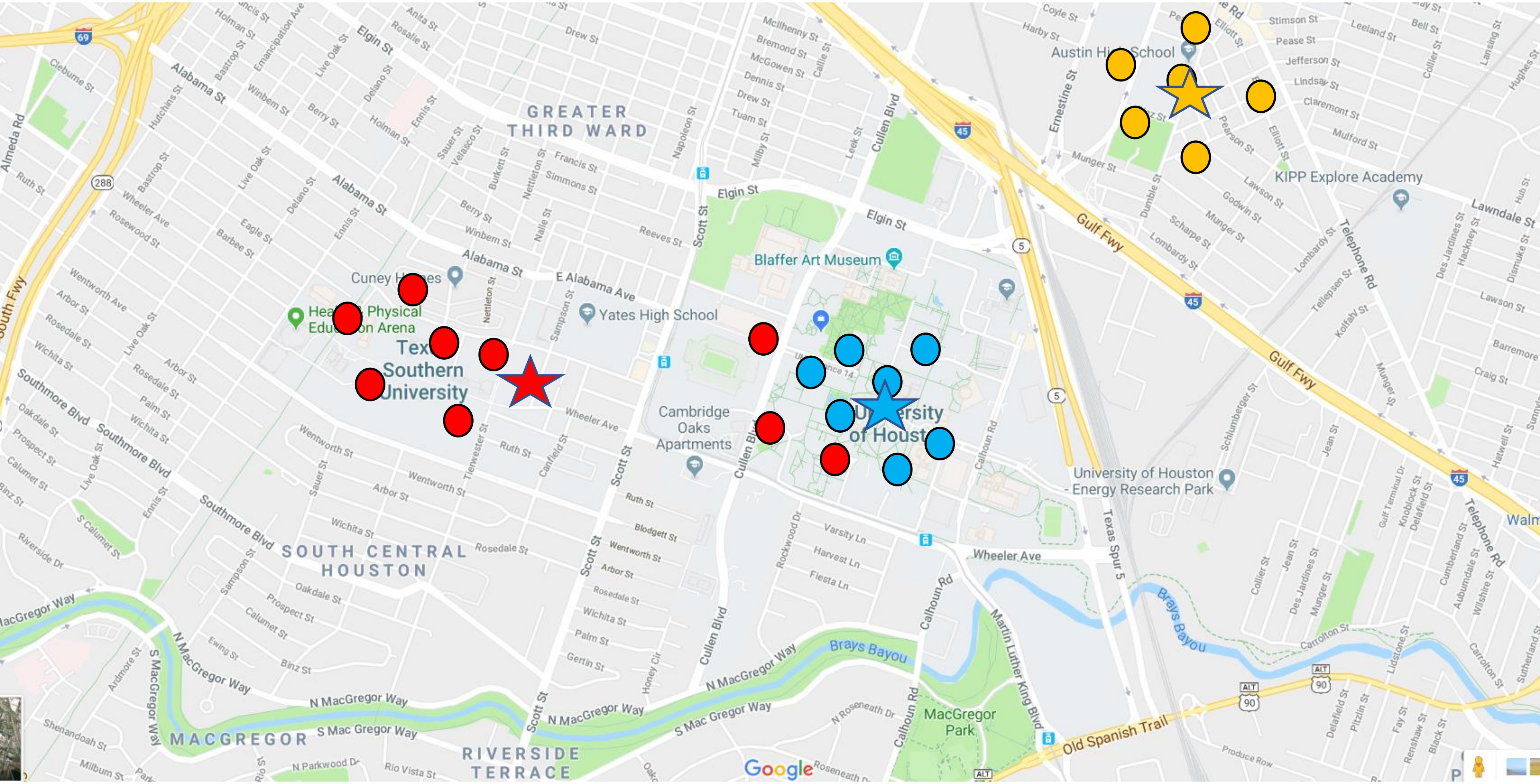
Customer distribution update



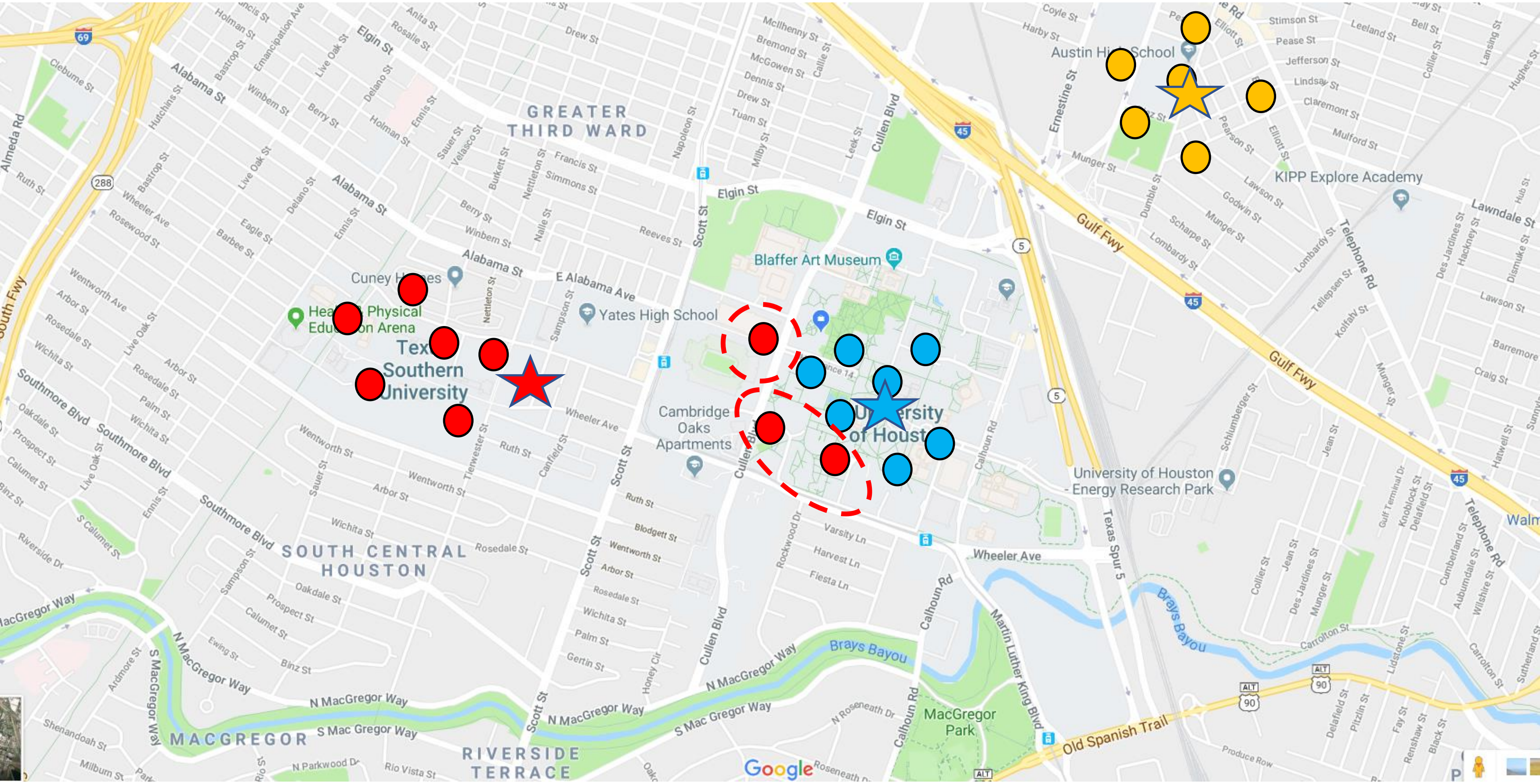
Customer distribution update



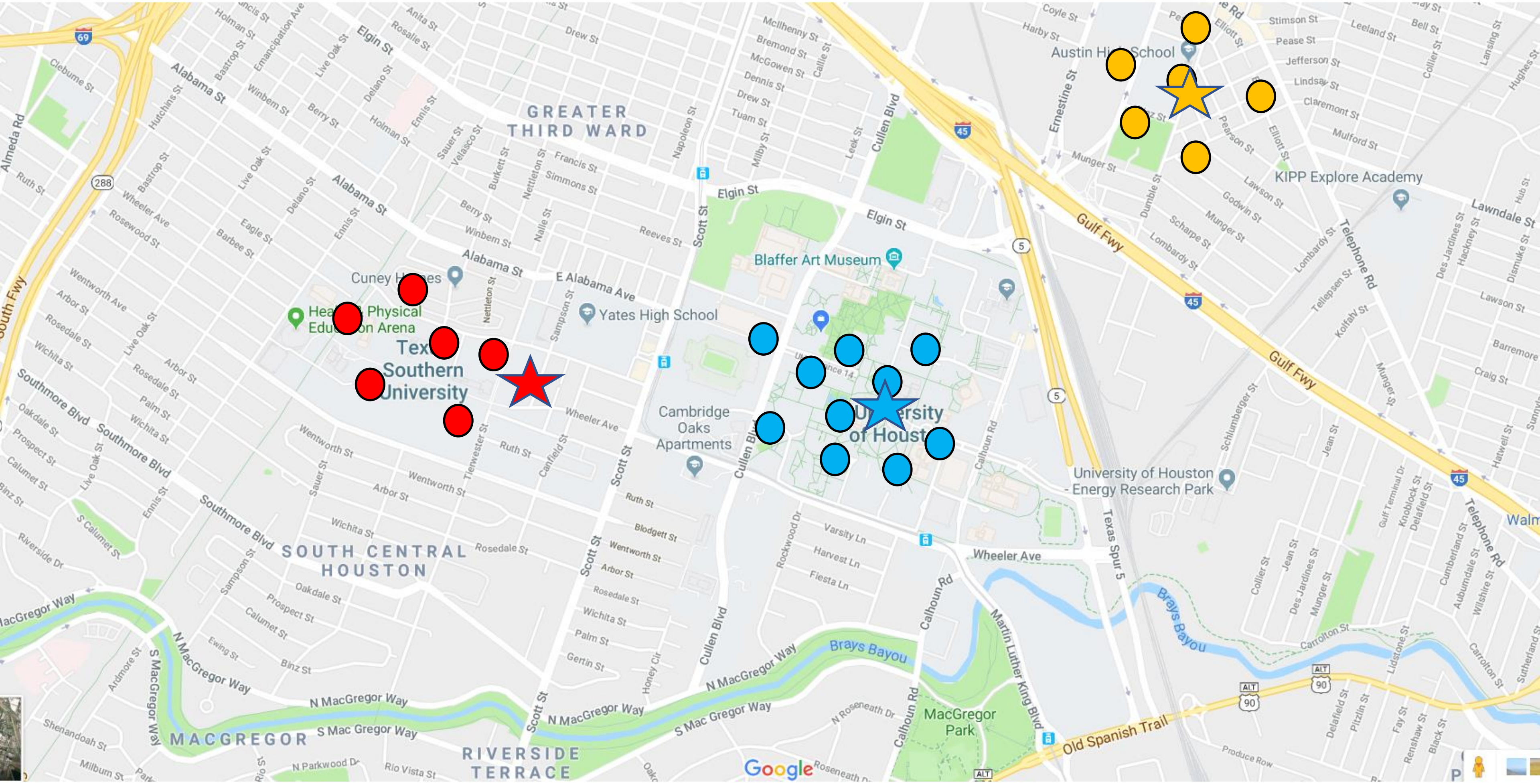
Update store locations



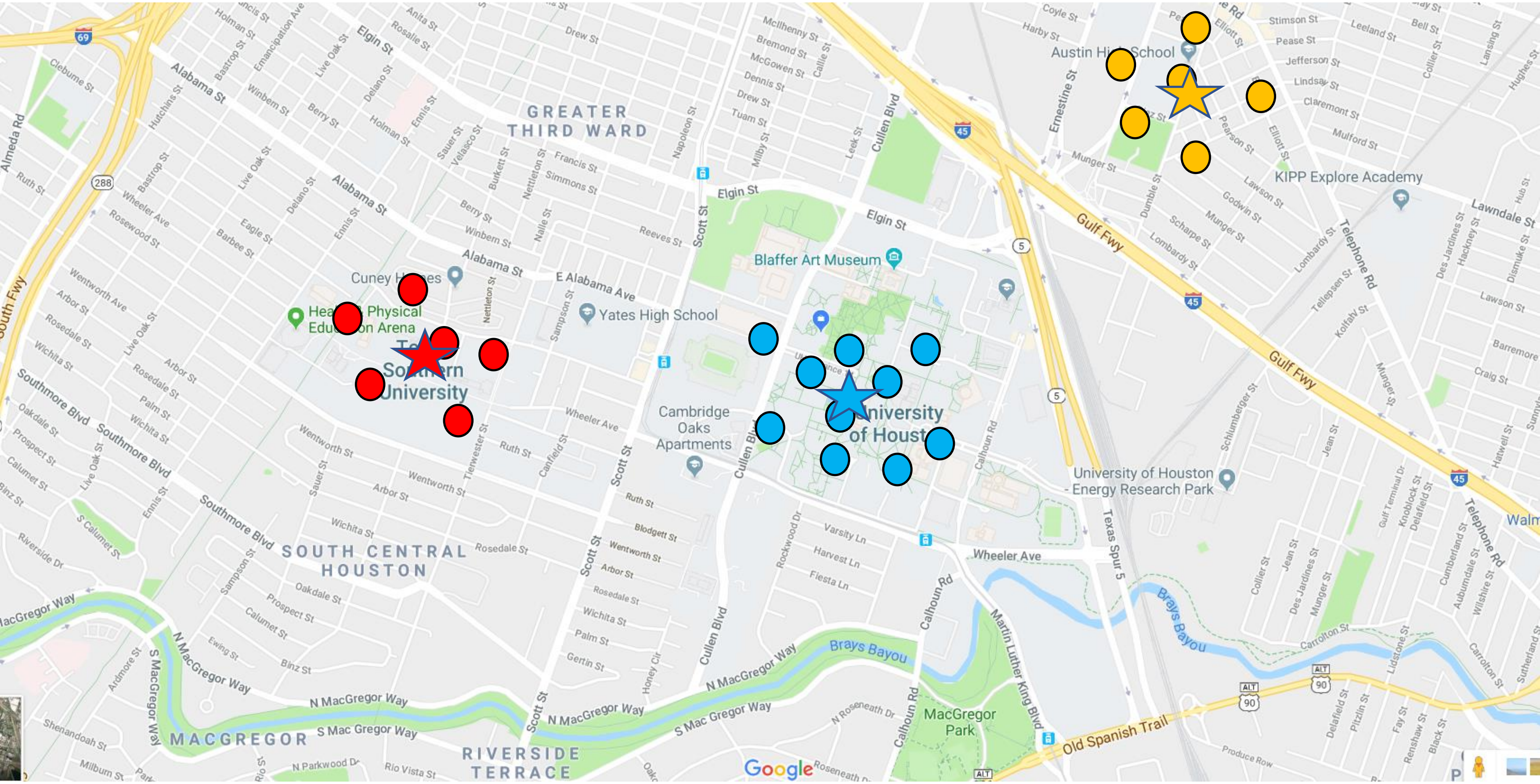
Update customer distributions



K-means clustering



Update store locations



K-means clustering: terminology

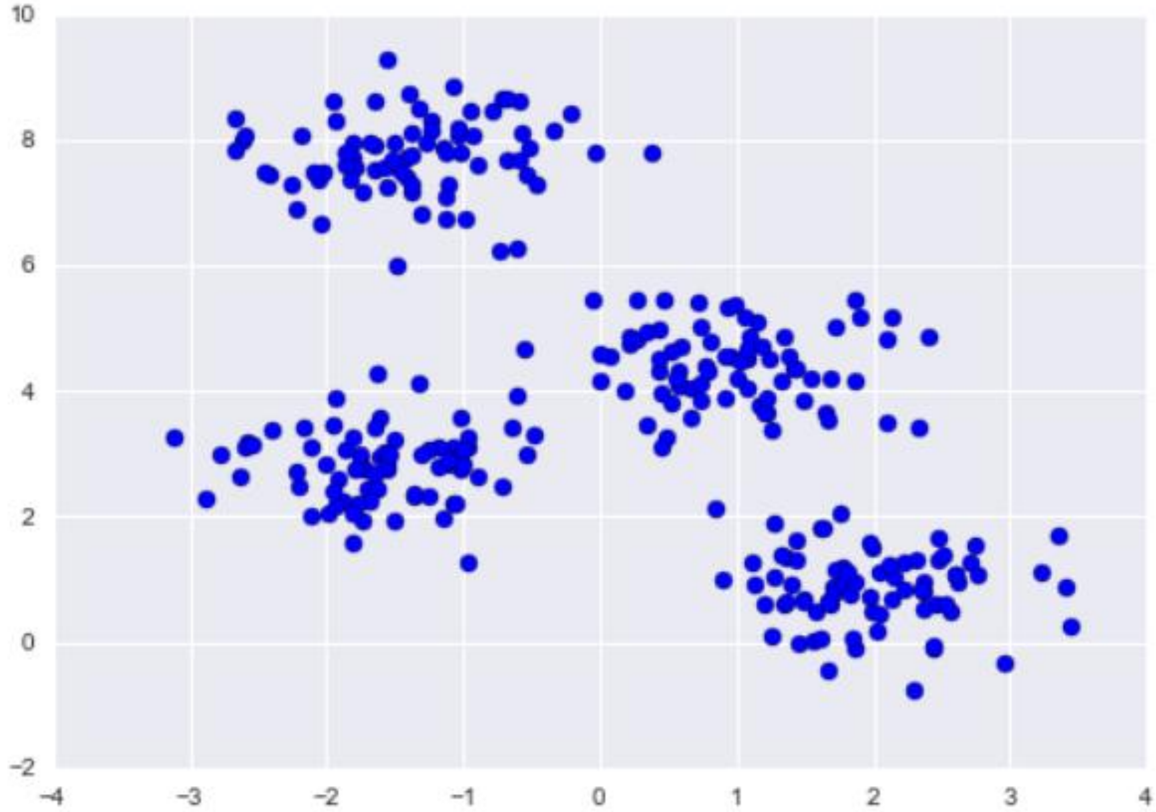
- The pizza store locations are called cluster centers or centroids.
- Each group of customers is called a cluster
- Each location or building is called an observation (or an object/instance).

K-means clustering: how it works

- Start with random initial cluster centers
- While (not converge)
  - Calculate distance between each cluster center and each instance.
  - Assign each instance to the nearest cluster center
  - Update cluster centers by calculating the mean of all the instances assigned to the same cluster
- end

Implementation in Scikit-learn

```
from sklearn.datasets.samples_generator import make_blobs
X, y_true = make_blobs(n_samples=300, centers=4,
                       cluster_std=0.60, random_state=0)
plt.scatter(X[:, 0], X[:, 1], s=50);
```



Implementation in Scikit-learn

```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=4)
kmeans.fit(X)
y_kmeans = kmeans.predict(X)
```

Implementation in Scikit-learn

```
plt.scatter(X[:, 0], X[:, 1], c=y_kmeans, s=50, cmap='viridis')

centers = kmeans.cluster_centers_
plt.scatter(centers[:, 0], centers[:, 1], c='black', s=200, alpha=0.5);
```