CS150A Database

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Today:

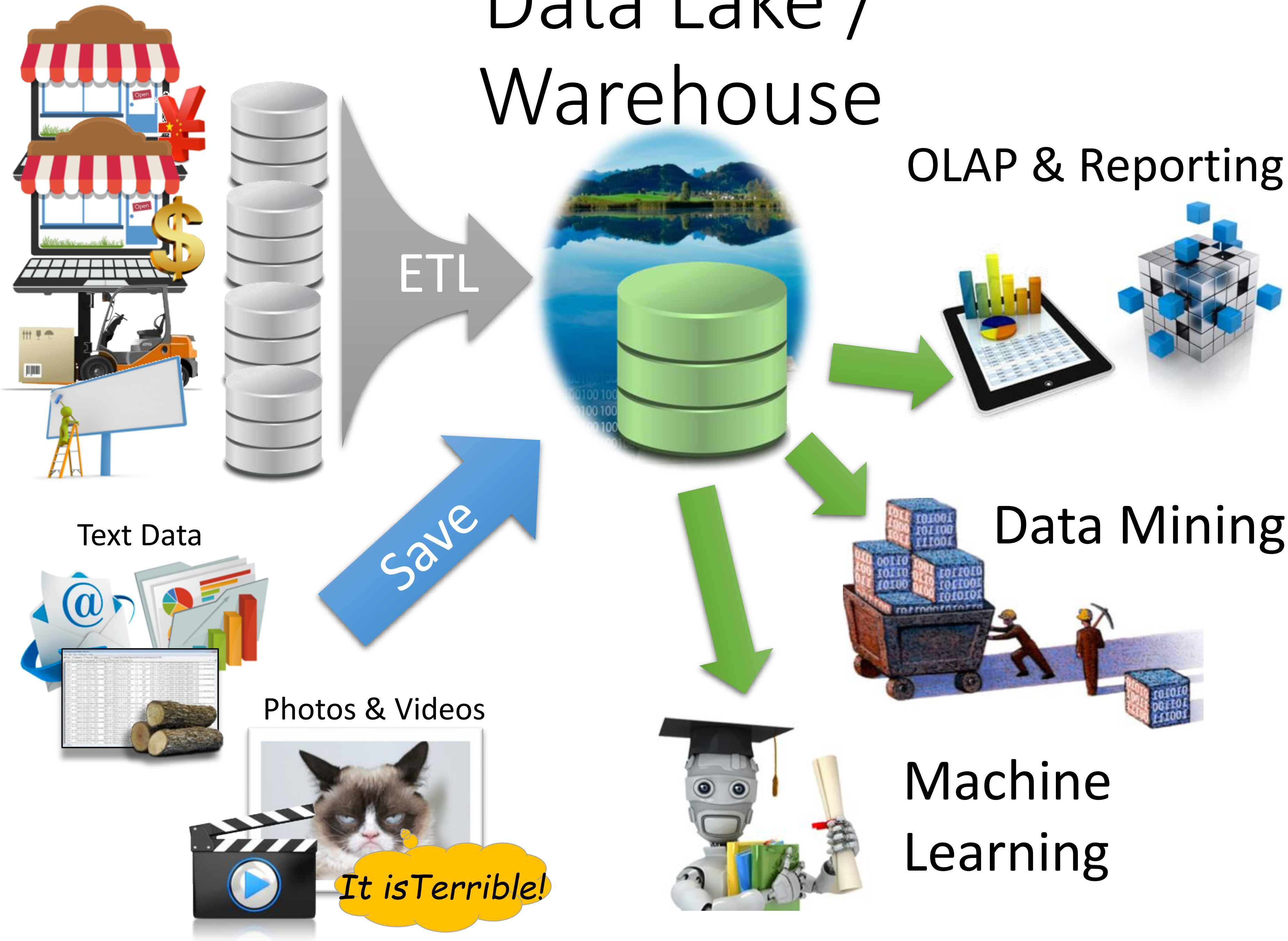
- Analytics and ML in Data Systems:
  - Part 2
  - Clustering

Readings:

- Database Management Systems (DBMS), Chapter 26

Acknowledgement: Joseph E. Gonzalez@UCBerkeley's scourse notes

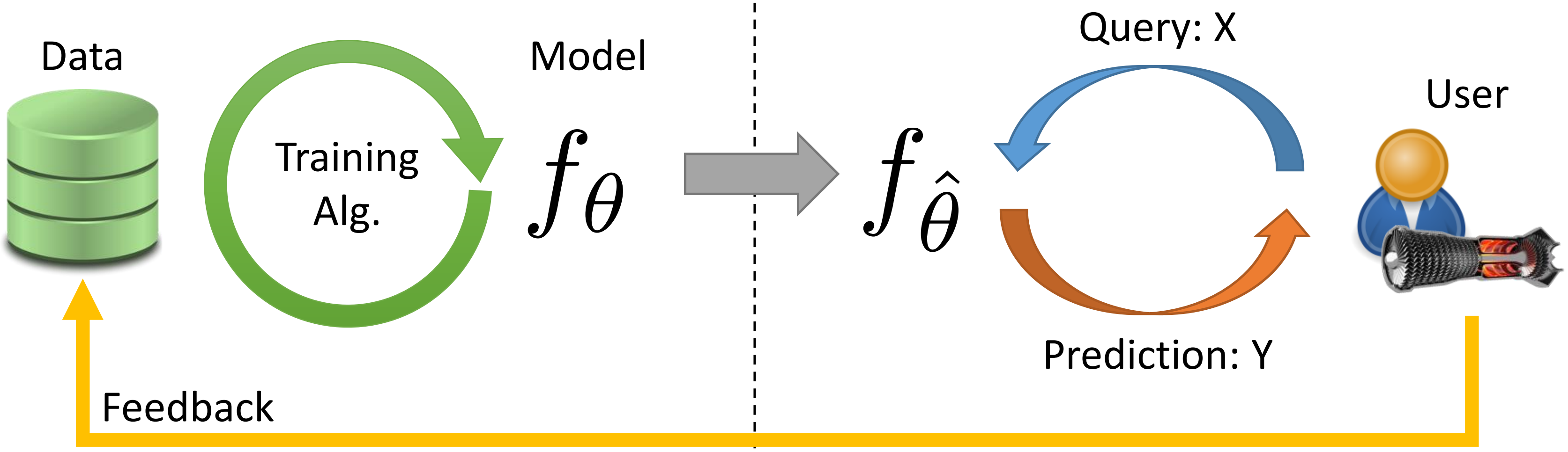
Data Lake / Warehouse



Machine Learning Lifecycle

Learning

Inference



- Typically a time consuming iterative batch process
  - Feature engineering
  - Validation

➢ Focus is on making fast robust predictions
  - Monitoring and tracking feedback
  - Materialization + fast model inference

Taxonomy
of Machine Learning

Labeled Data

Indirect (reward)

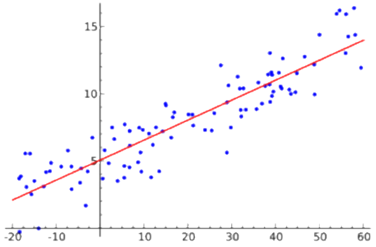
Unlabeled Data

Supervised Learning

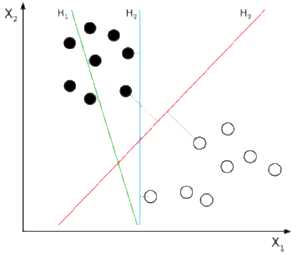
Reinforcement & Bandit Learning

Unsupervised Learning

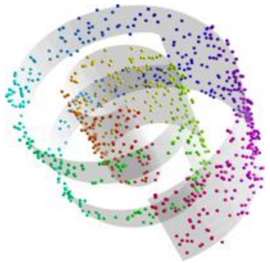
Regression



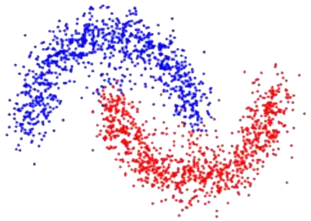
Classification



Dimensionality Reduction



Clustering



Clustering Images

- Given a collection of images cluster them into *meaningful groups*.

Clustering Images

- Given a collection of images cluster them into meaningful groups.

“Forest”

“Mountains”

“Beaches”

Clustering Images

- Given a collection of images cluster them into meaningful groups.

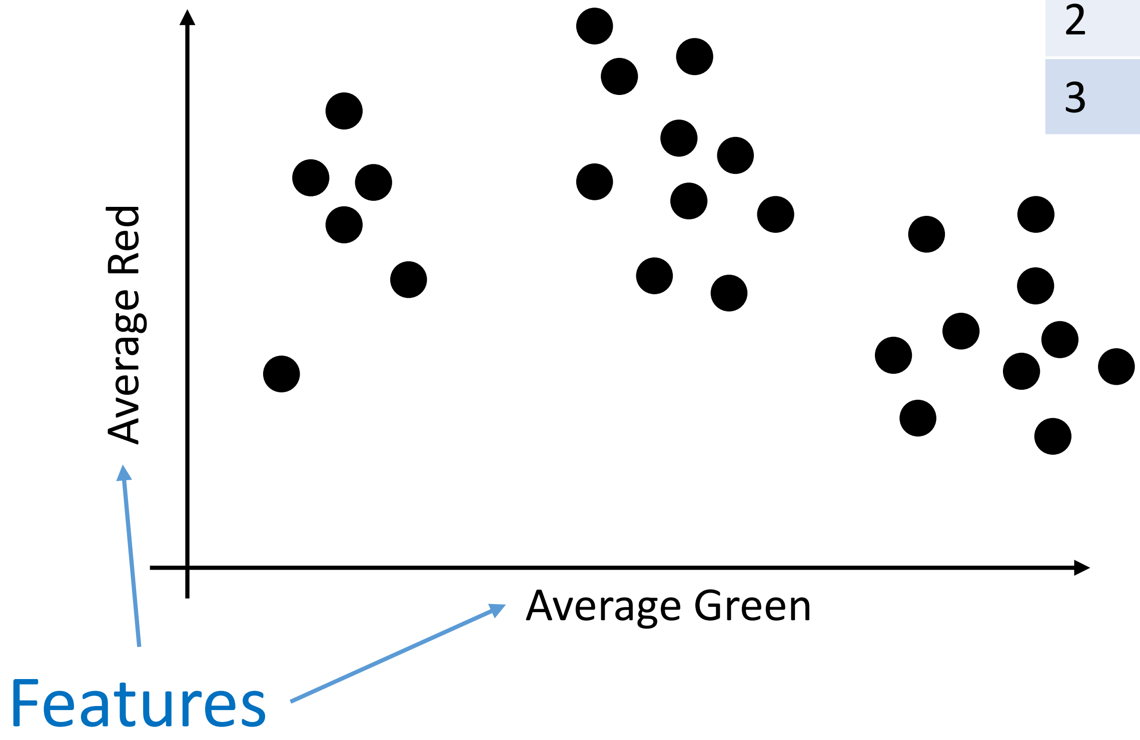
- **Unsupervised:** The labels of the groups are not given in the training data
- **Exploratory:** overlaps with data mining

Clustering Images

- Given a collection of images cluster them into meaningful groups.

Image Id	Average Red	Average Green
1	123	200
2	212	103
3	55	35

Simplified Illustration



- How many clusters?
- Where are the clusters?

Clustering Images

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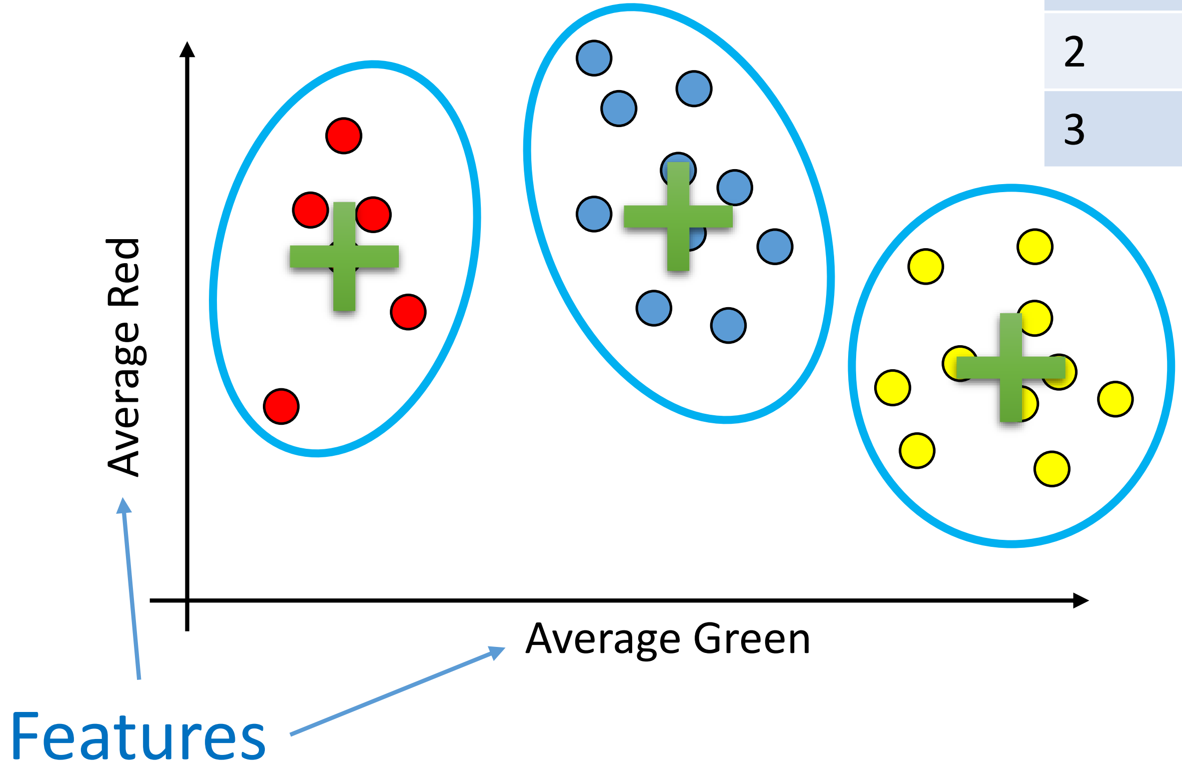
Simplified Illustration



- Where are the clusters?
- How many clusters?

Clustering Images

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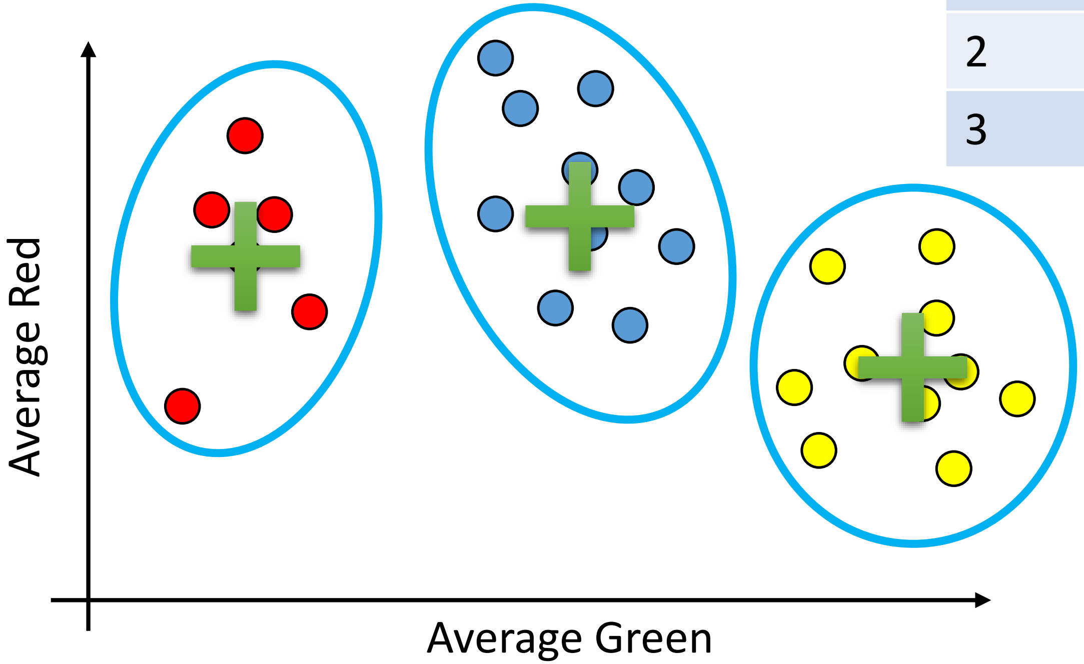

What makes a **good** clustering?

- All points are **near** the cluster center
- **Spread** between clusters > spread within clusters

Clustering Images

- Given a collection of images cluster them into meaningful groups.

Image Id	Average Red	Average Green
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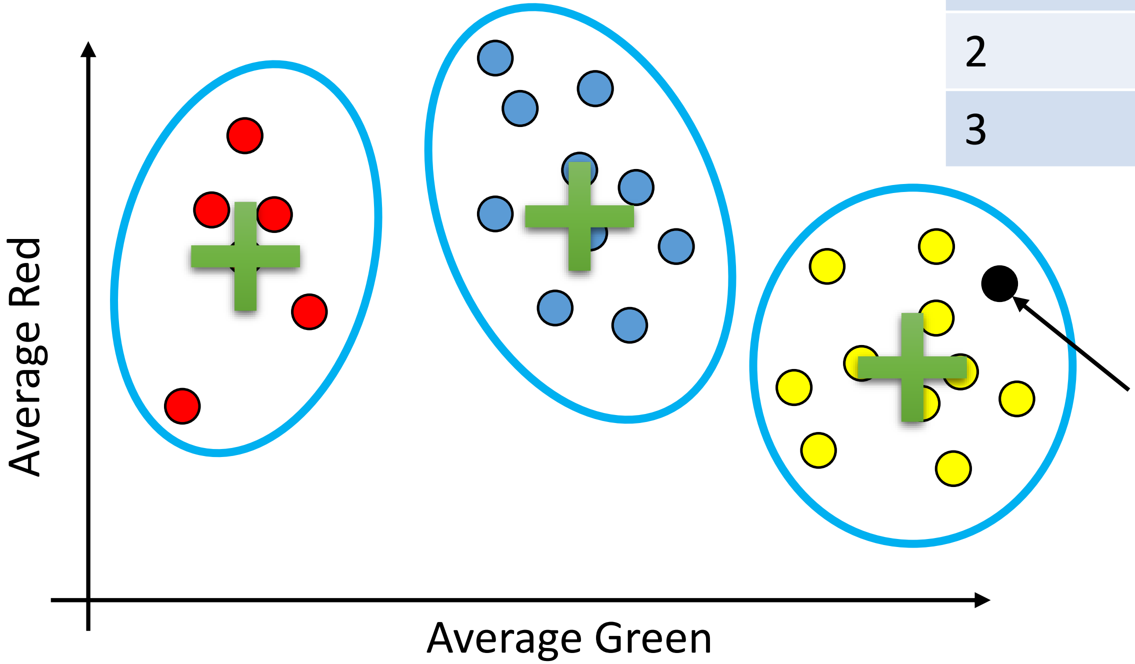

What happens when a new point arrives?

Clustering Images

- Given a collection of images cluster them into meaningful groups.

Image Id	Average Red	Average Green
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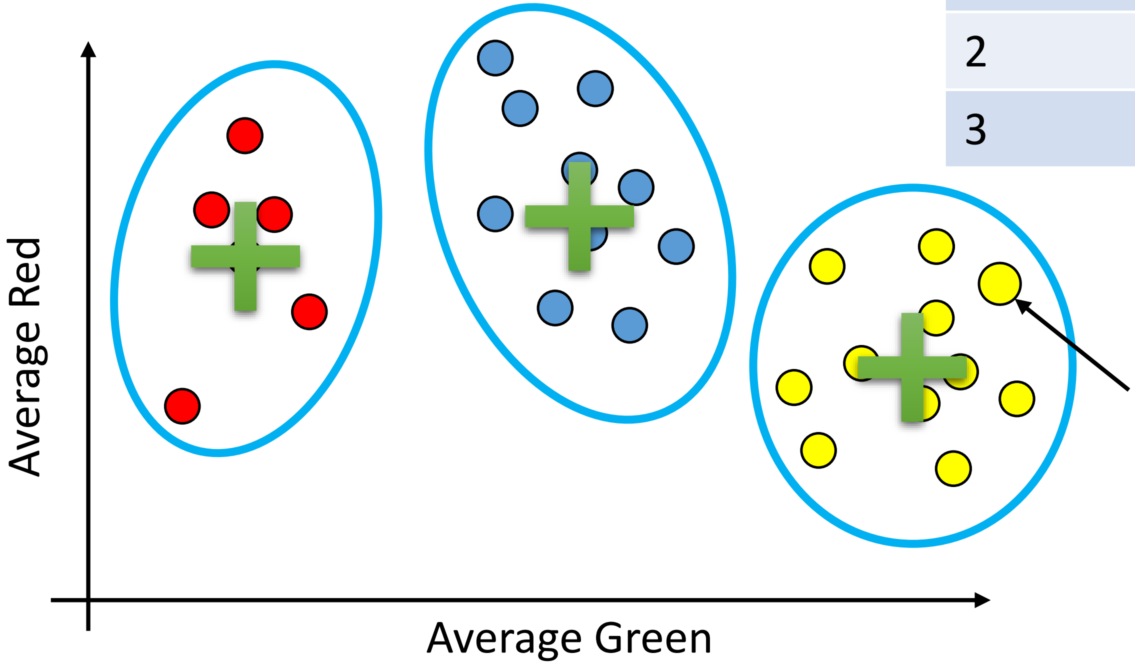

What happens when a new point arrives?

Predict "label" based on existing clusters (Yellow)

Clustering Images

- Given a collection of images cluster them into meaningful groups.

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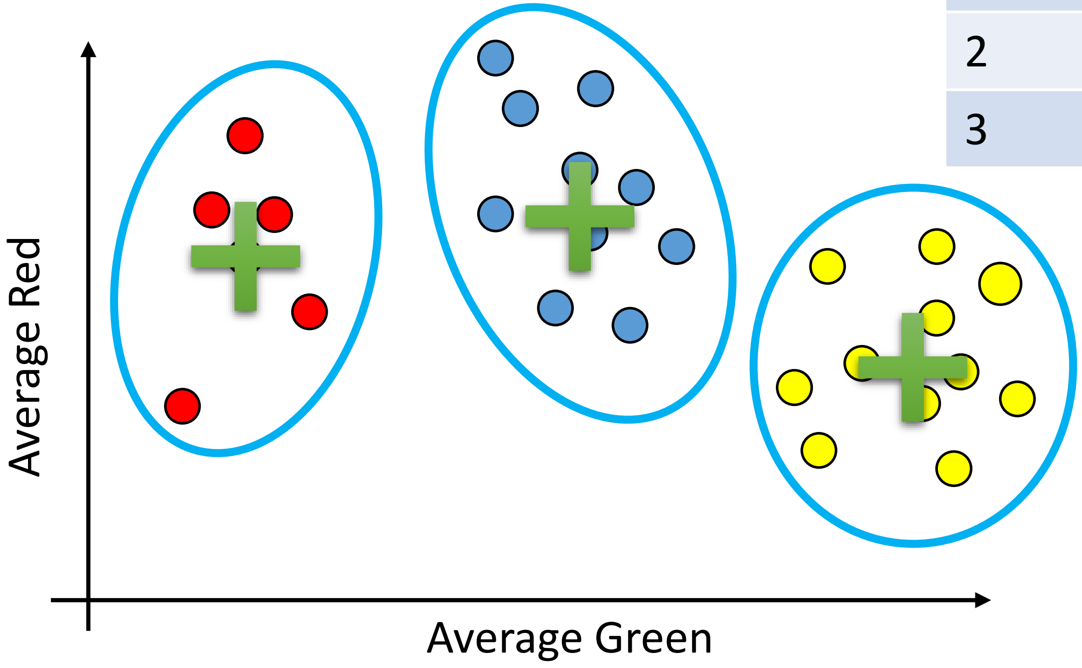


How do we automatically cluster data?

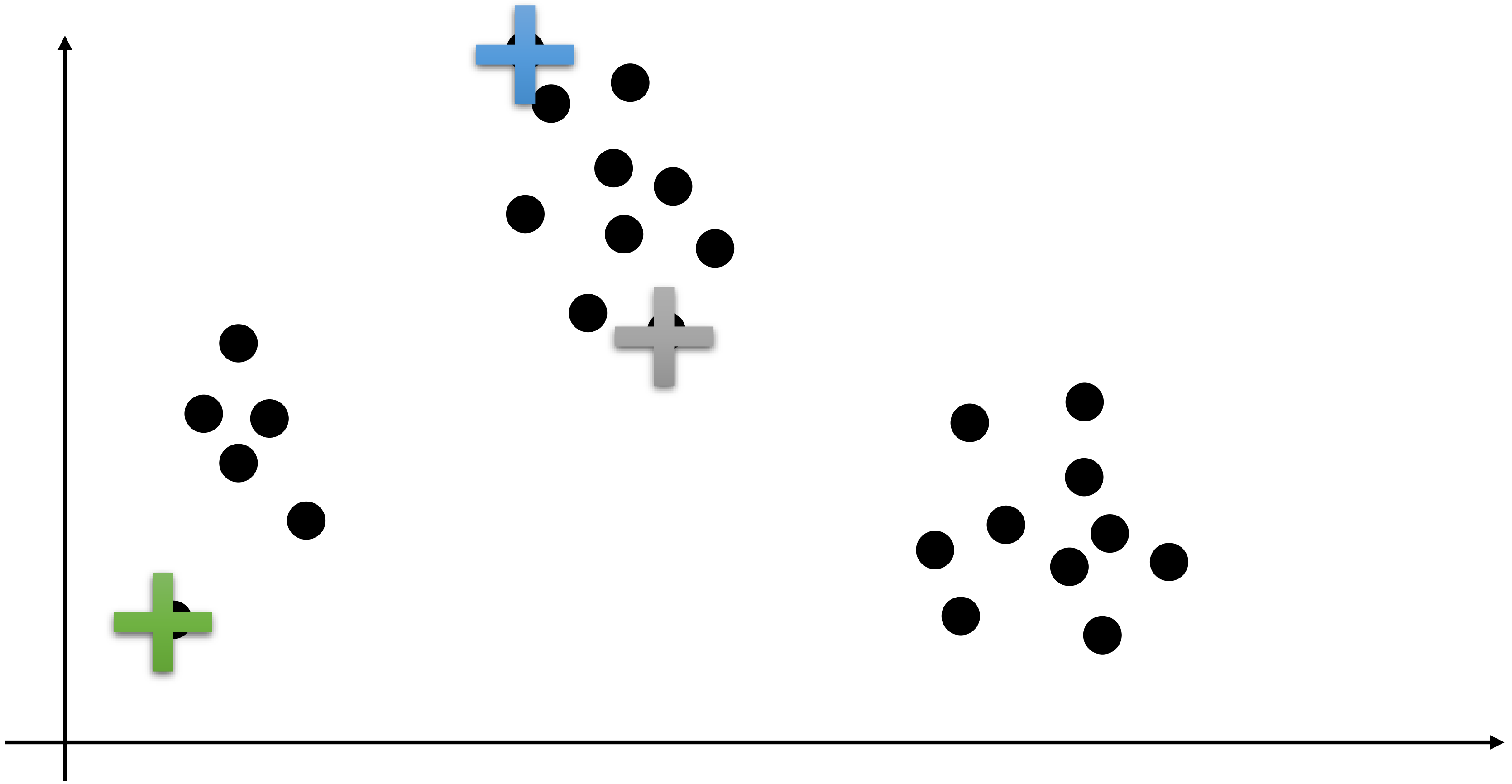
How do we Compute a Clustering?

Many different clustering models and algorithms:

- <u>Feature Based Clustering:</u> *Points in R^d*
  - **K-Means:** EM on Symmetric Gaussians ← We will learn this one
  - **Mixture Models:** Generalized k-means
  - …
- <u>Spectral Methods:</u> *Similarity Function Between Items*
  - **Similarity based clustering:** *A and B are co-purchased*
  - **Graph clustering:** *Cities based on road network*
  - …
- <u>Hierarchical Clustering:</u> *clustering nested items*
  - **Latent Dirichlet Allocation:** *Documents based on words*
    - *Developed at Berkeley and widely used!*
  - …

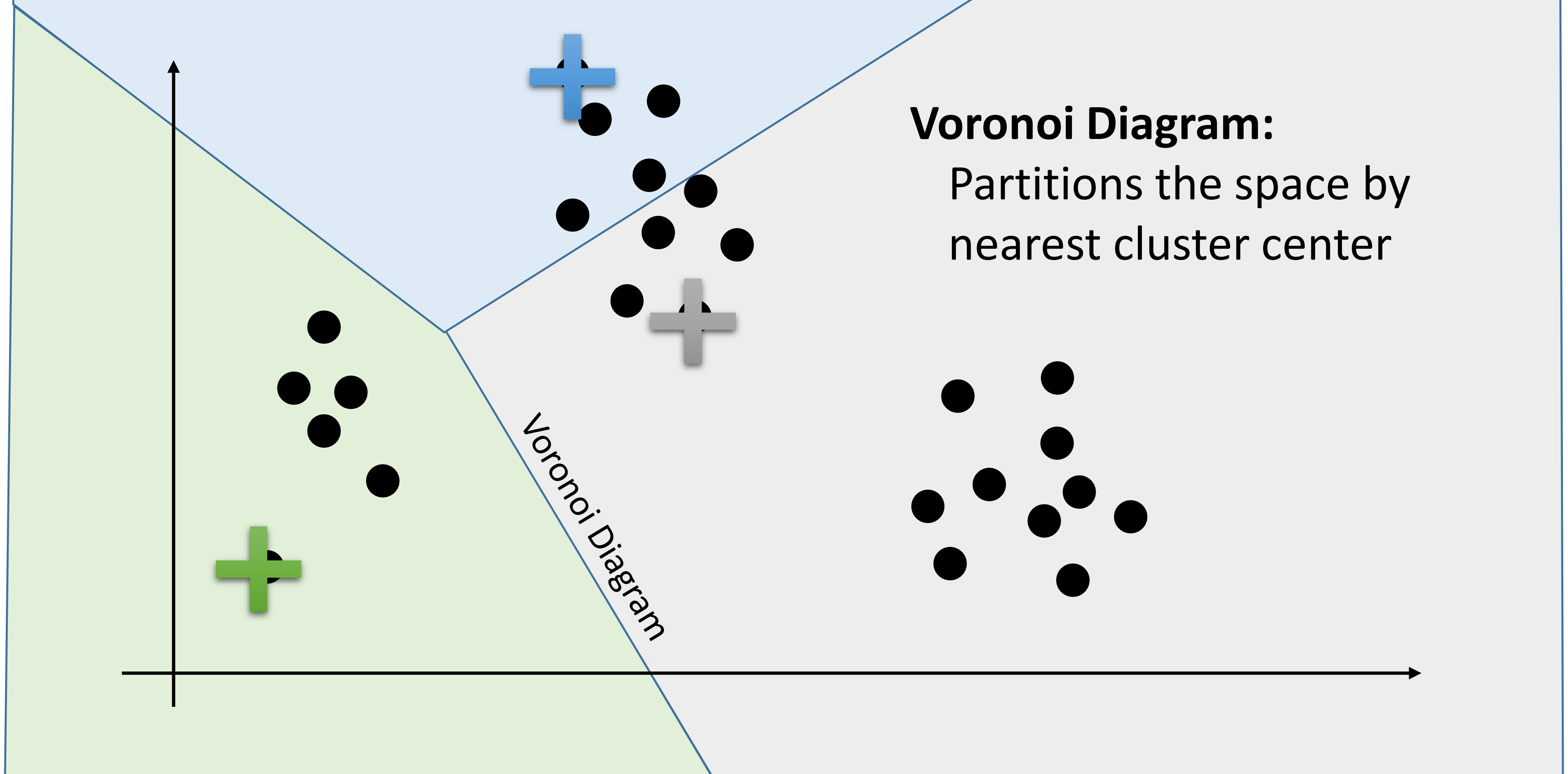
K-Means Clustering: *Intuition*

- Input K: The number of clusters to find
- Pick an initial set of points as cluster centers



K-Means Clustering: *Intuition*

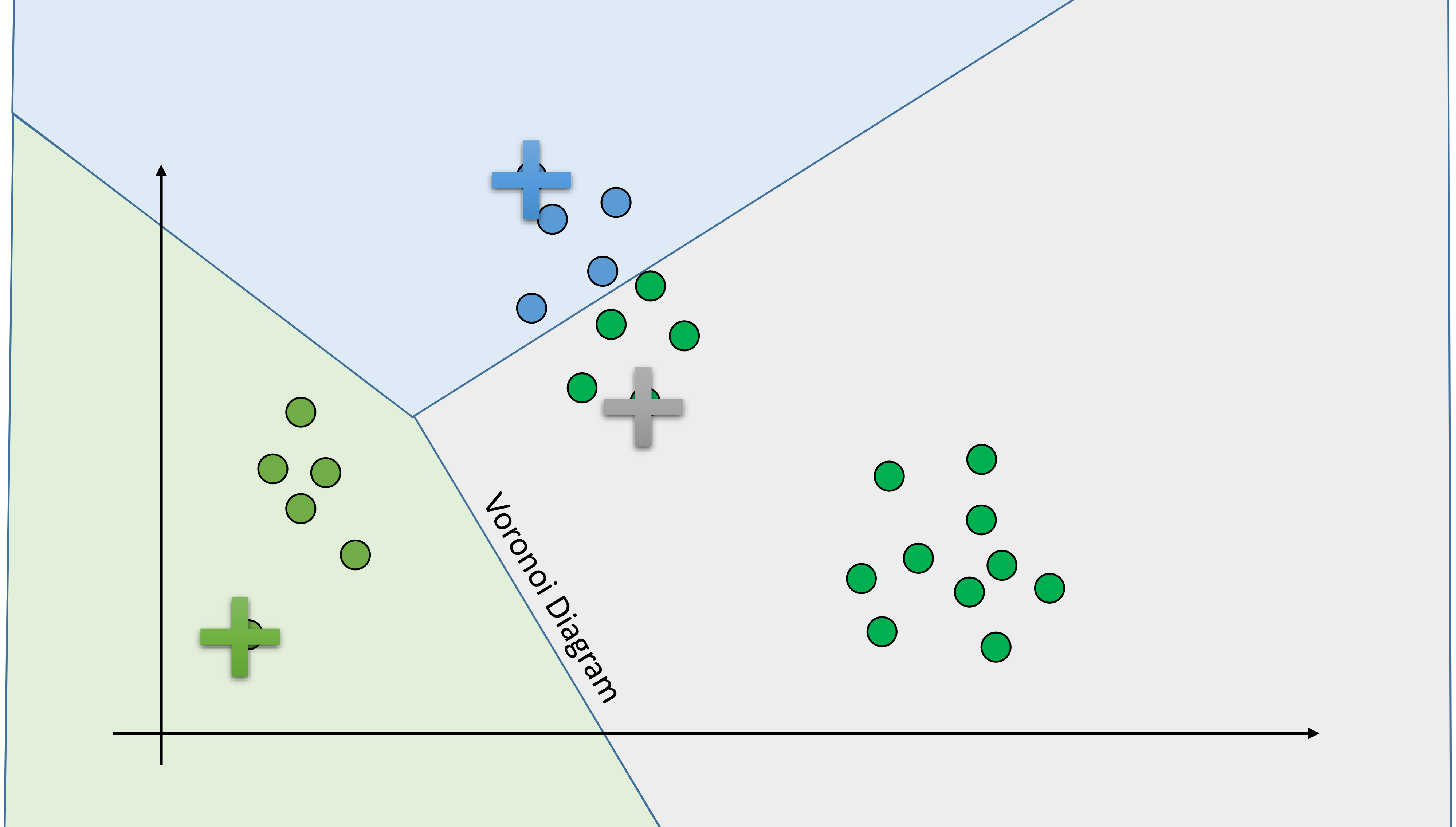
- For each data point find the cluster nearest center



Voronoi Diagram:
Partitions the space by nearest cluster center

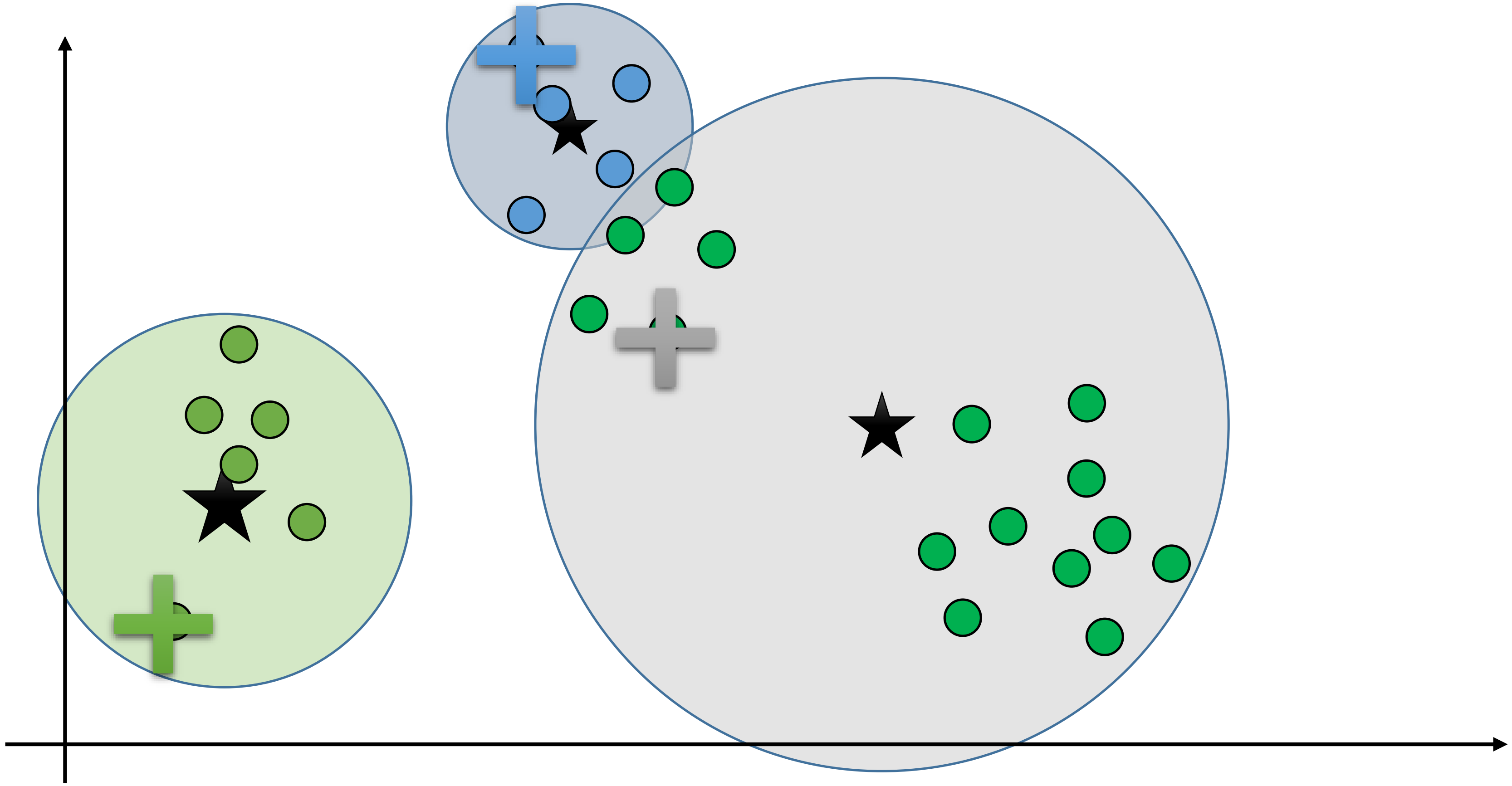
K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



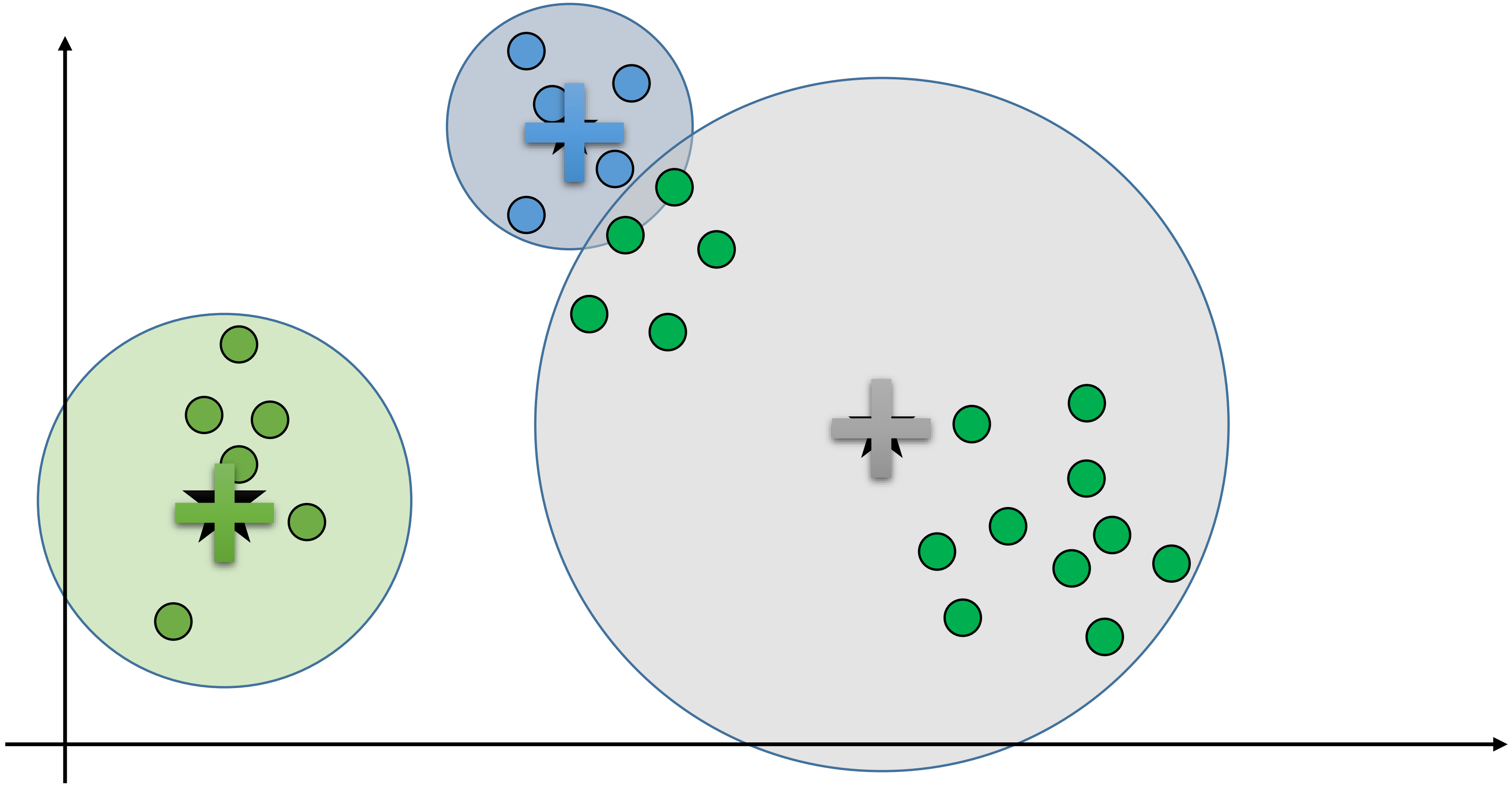
K-Means Clustering: *Intuition*

- Compute mean of points in each "cluster"



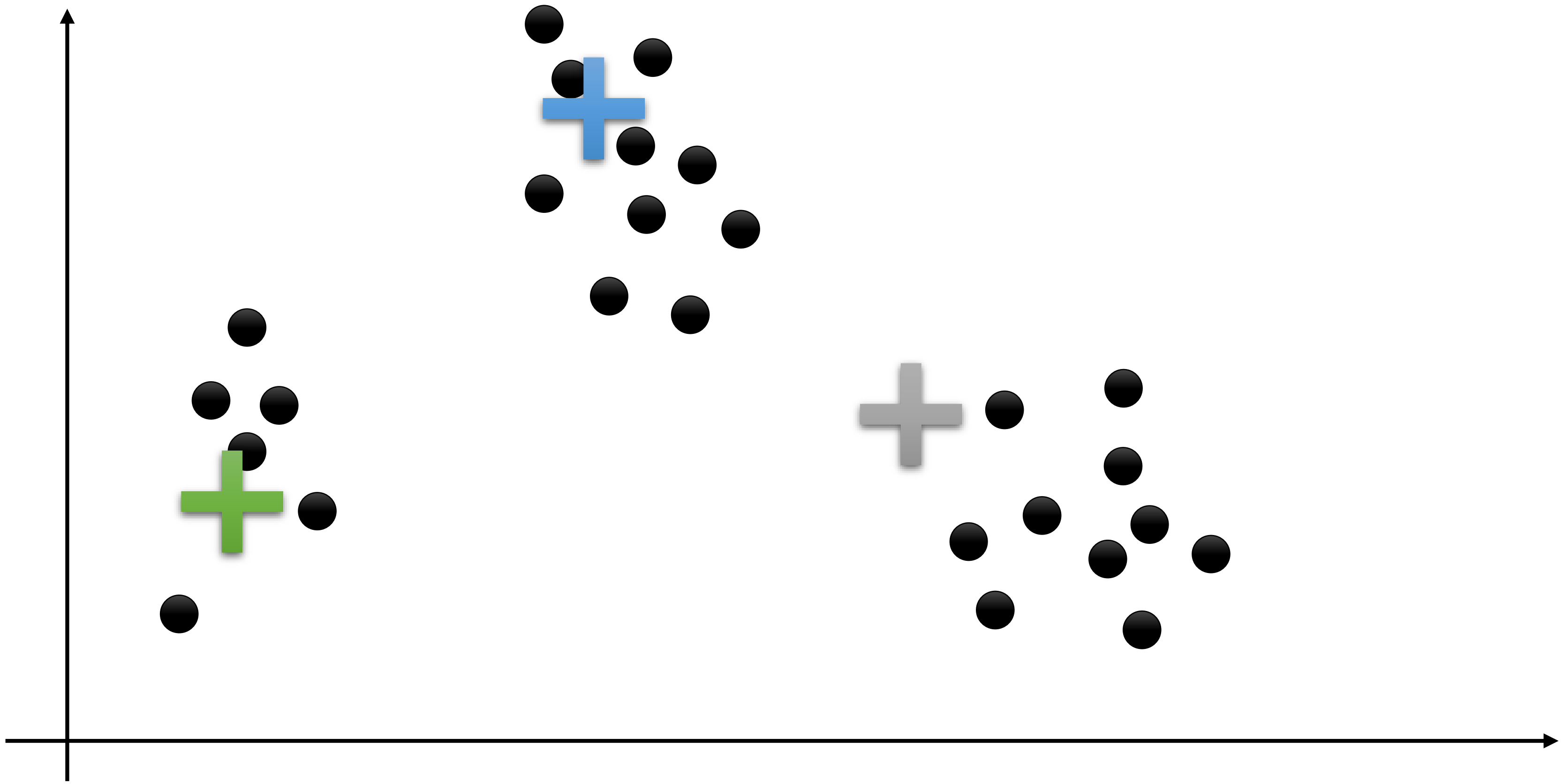
K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster



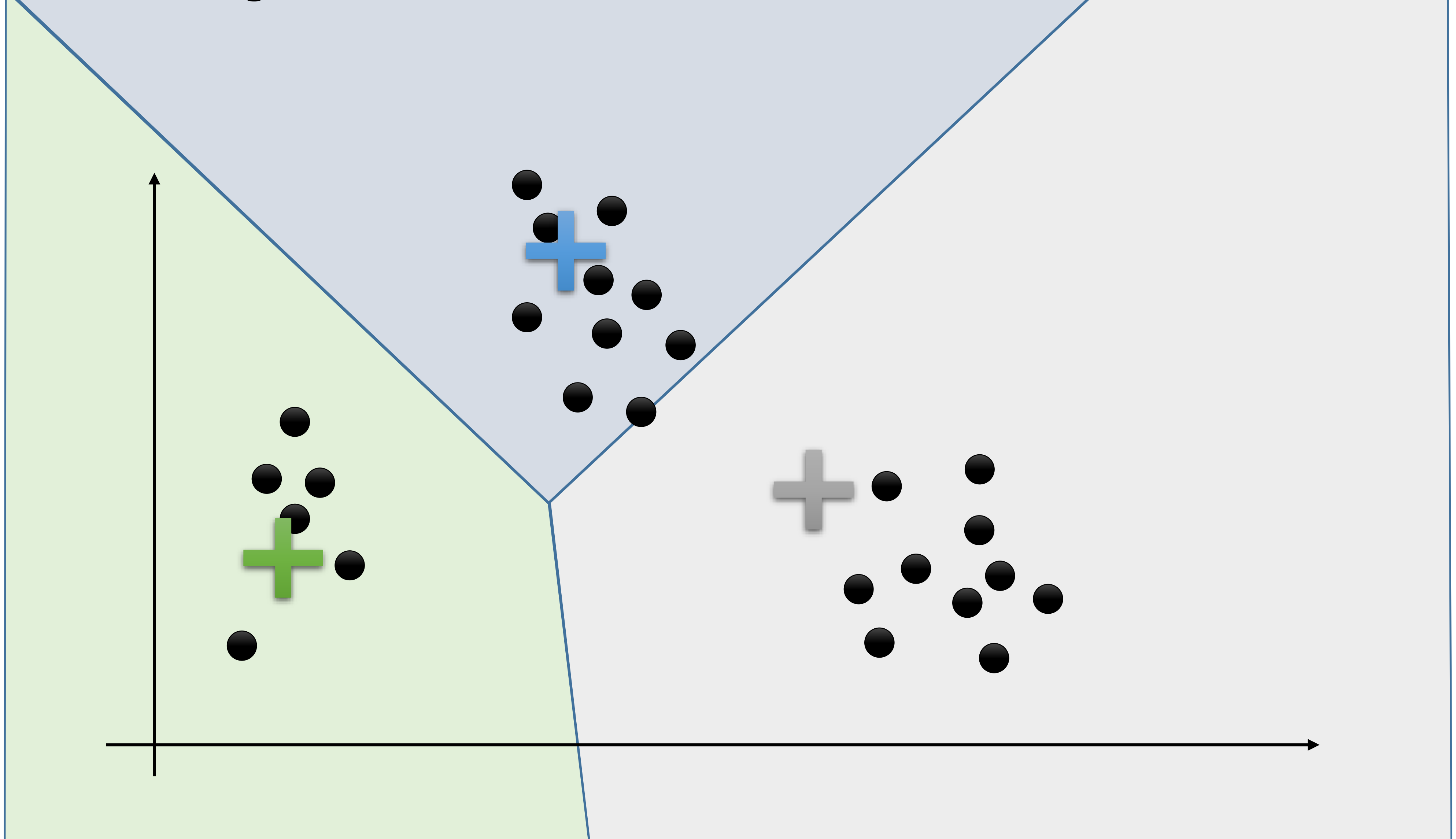
K-Means Clustering: *Intuition*

- Improved?
- Repeat



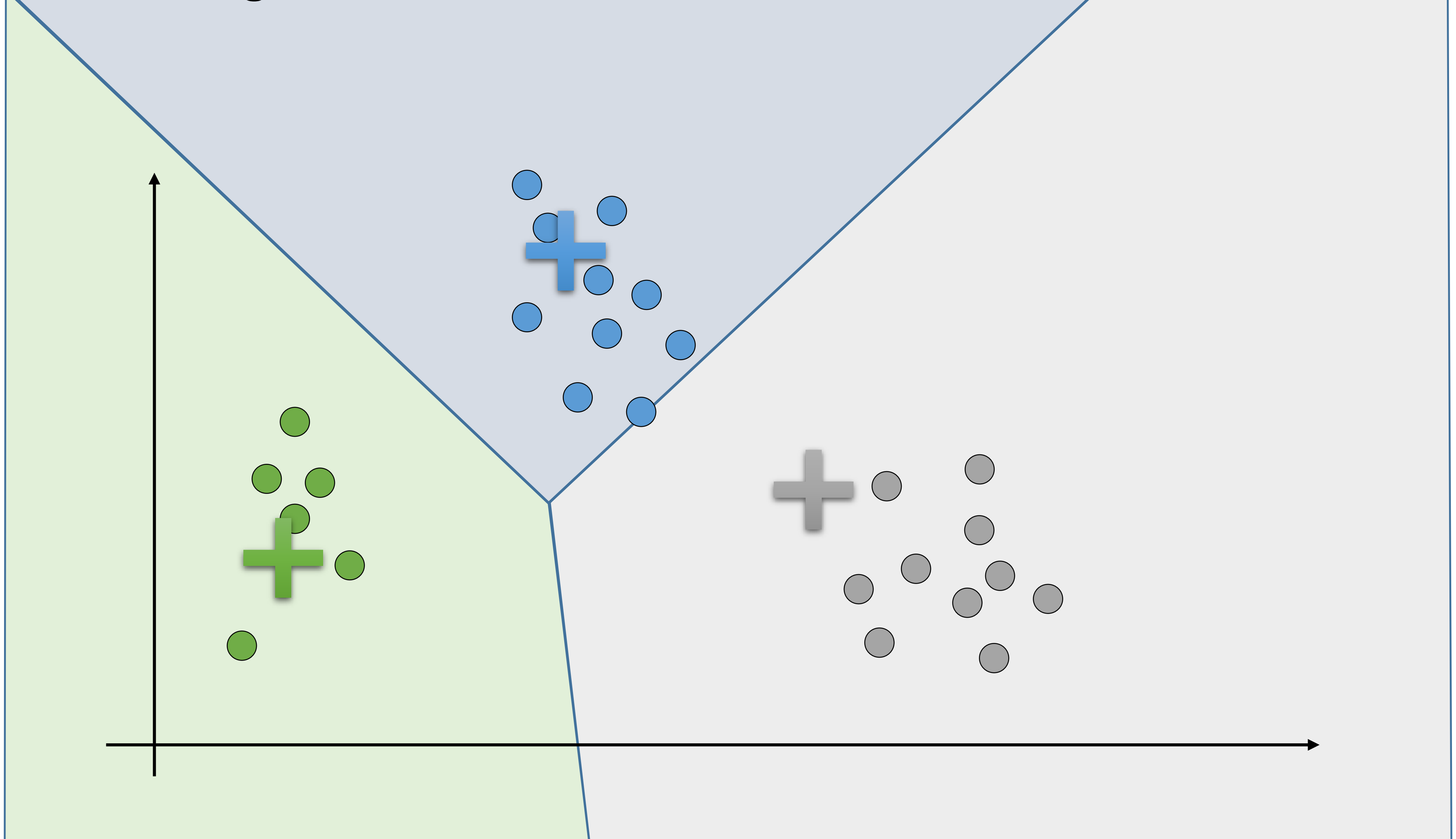
K-Means Clustering: *Intuition*

- Assign Points



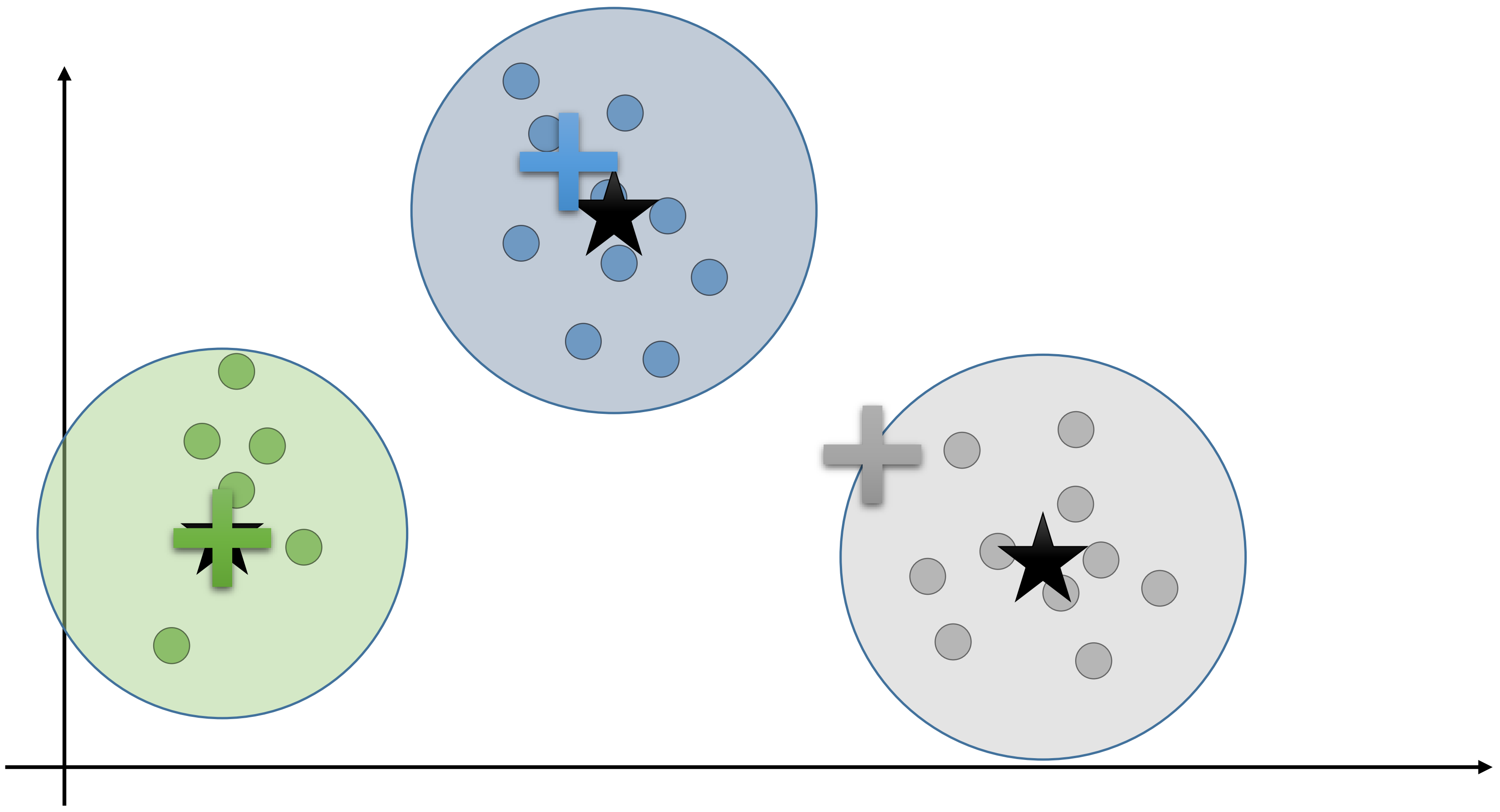
K-Means Clustering: *Intuition*

- Assign Points



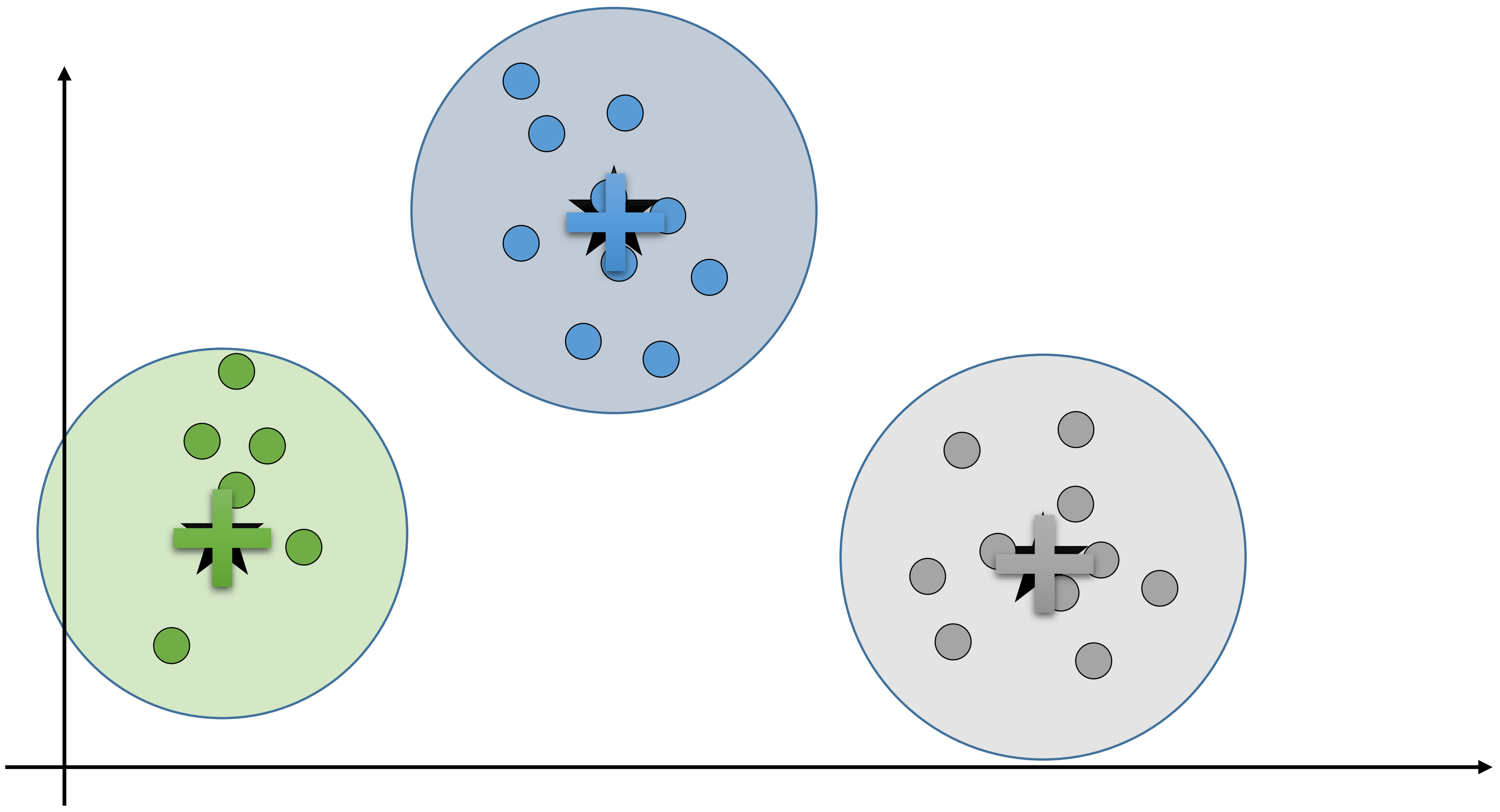
K-Means Clustering: *Intuition*

- Compute cluster means



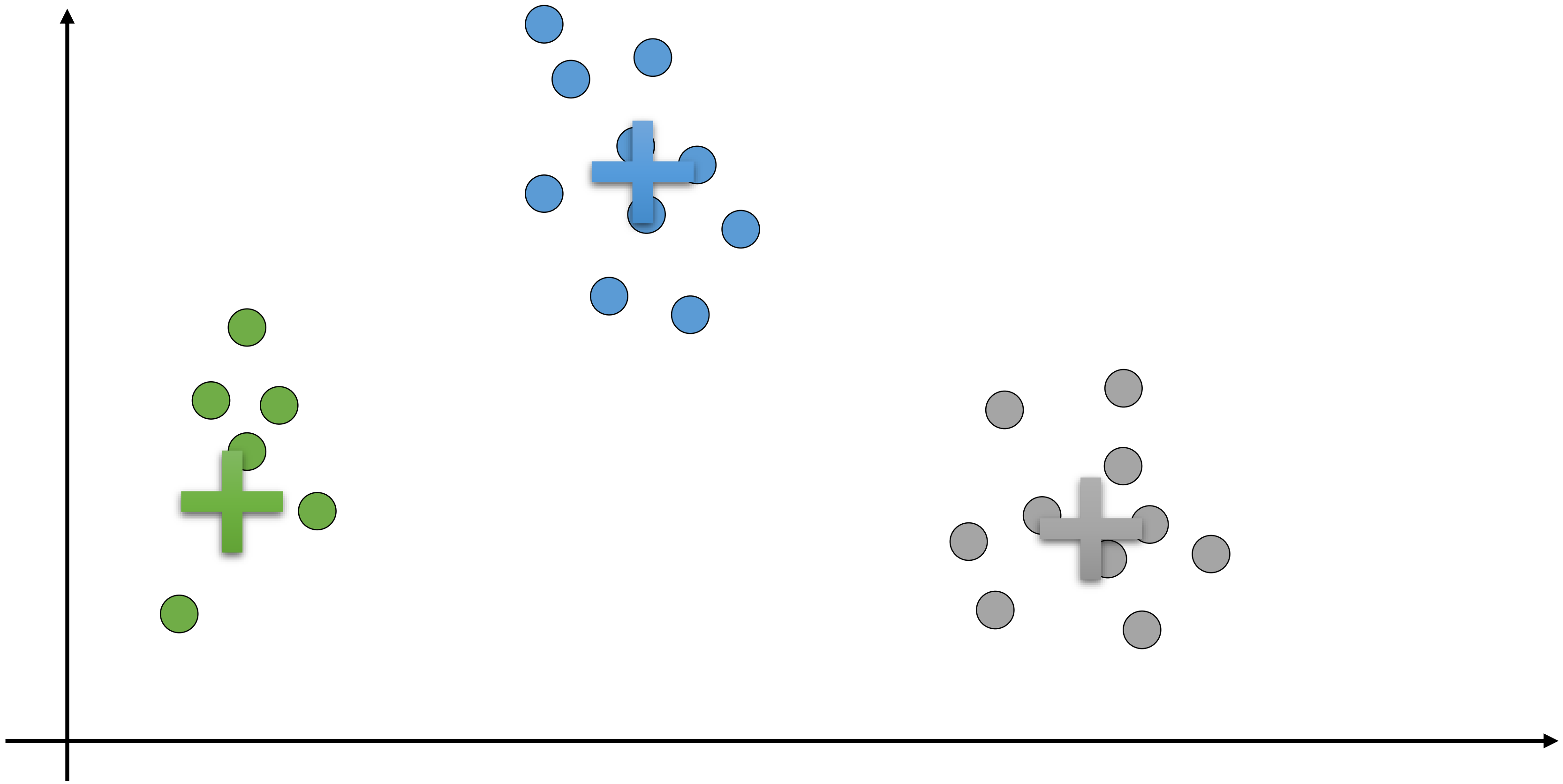
K-Means Clustering: *Intuition*

- Update cluster centers



K-Means Clustering: *Intuition*

- Repeat?
  - Yes to check that nothing changes → Converged!



K-Means Algorithm: **Details**

```
centers ← pick k initial Centers

while (centers are changing) {
   // Compute the assignments (E-Step)
   asg ← [(x, nearest(centers, x)) for x in data]
```

What do we mean by "nearest":

A: Euclidean Distance

$$\arg\min_{c \in \text{centers}} ||c - x||_2^2 = \sum_{i=1}^{d} (c_i - x_i)^2$$

K-Means Algorithm: **Details**

```
centers ← pick k initial Centers

while (centers are changing) {
   // Compute the assignments (E-Step)
   asg ← [(x, nearest(centers, x)) for x in data]

   // Compute the new centers (M-Step)
   for i in range(k):
      centers[i] =
         mean([x for (x, c) in asg if c == i])
}
```

Compute the
"Expected" Assignment

Find centers that maximize the
data "likelihood"

K-Means Algorithm: **Details**

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```

Guaranteed to converge!

… to what?

To a local optimum. ☹

Depends on Initial Centers

K-Means Algorithm: **Details**

```
centers ← pick k initial Centers
```

How do we pick initial centers?

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while (centers are changing) {
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```

Guaranteed to converge!

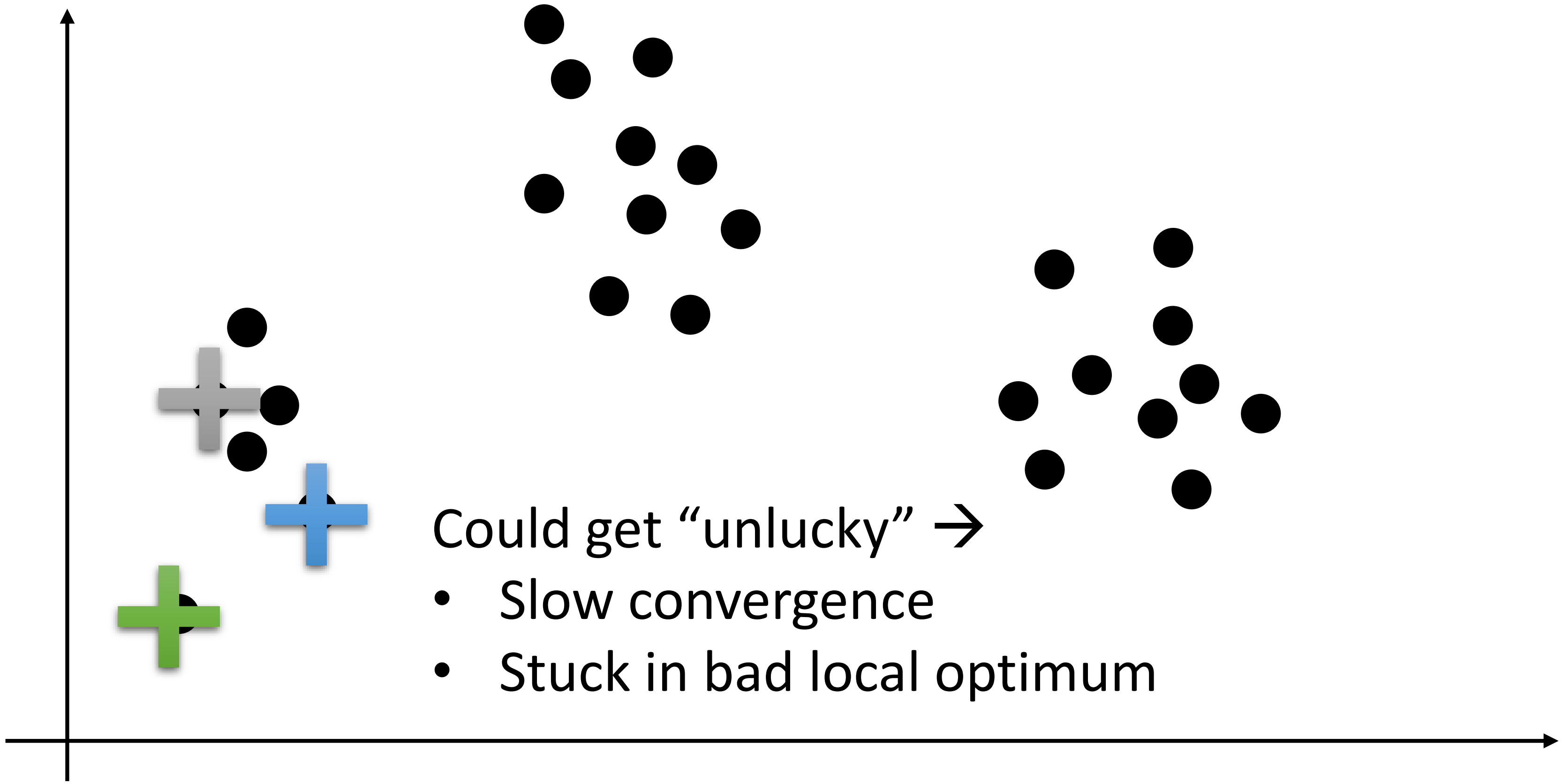
... to what?

To a local optimum. ☹

Depends on Initial Centers

Picking the Initial Centers

- **Simple Strategy:** select *k* points at random
  - What could go wrong?

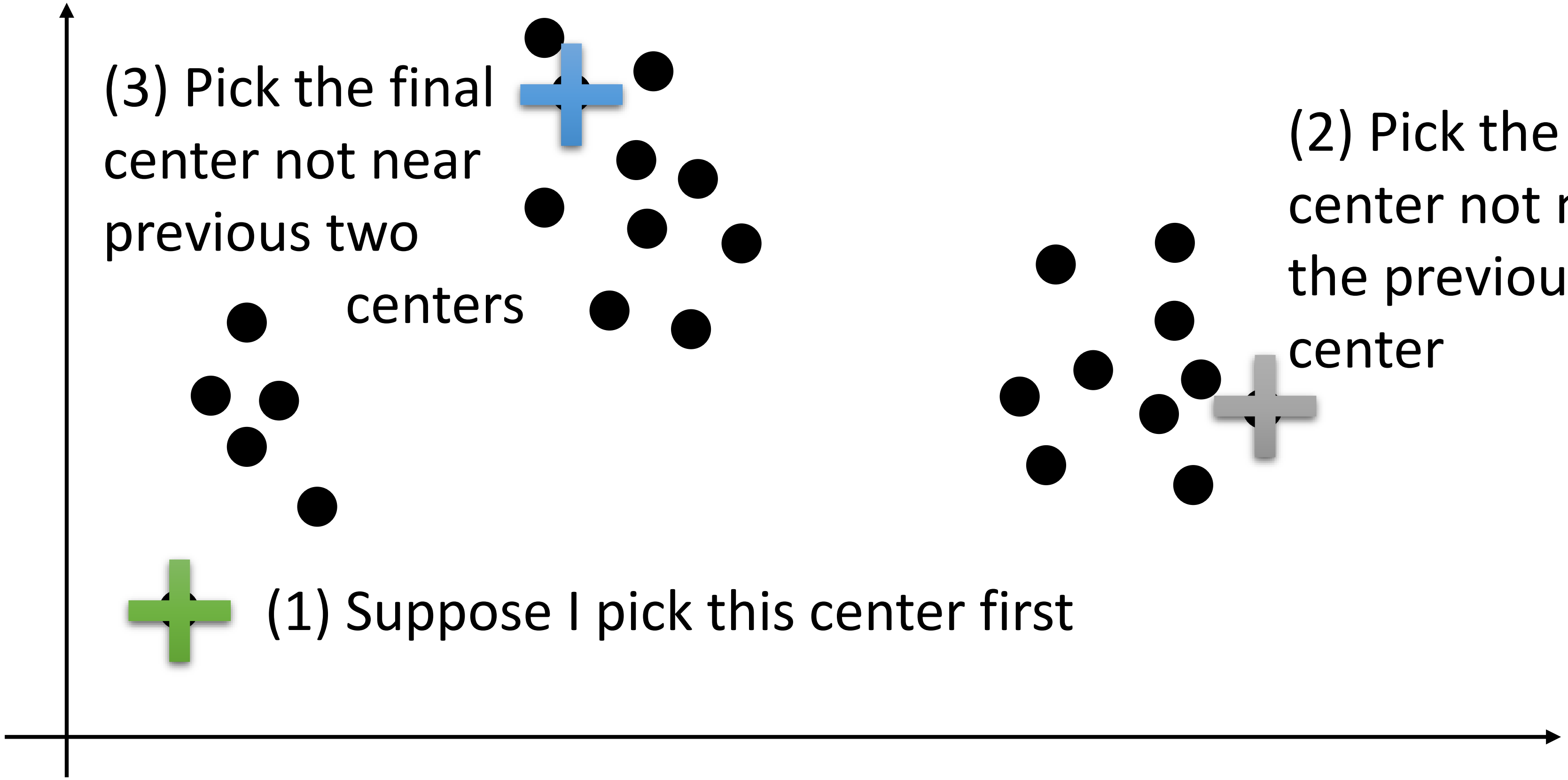


Could get "unlucky" →

- Slow convergence
- Stuck in bad local optimum

Picking the Initial Centers

- **Better Strategy:** kmeans++
  - Randomized approx. algorithm
  - Intuition select points that are not near existing centers

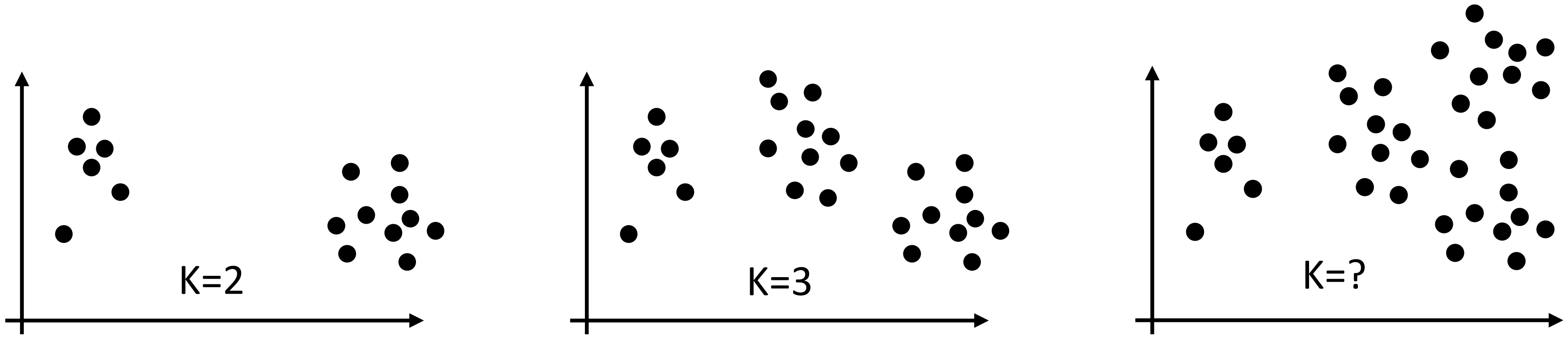


K-Means++ Algorithm

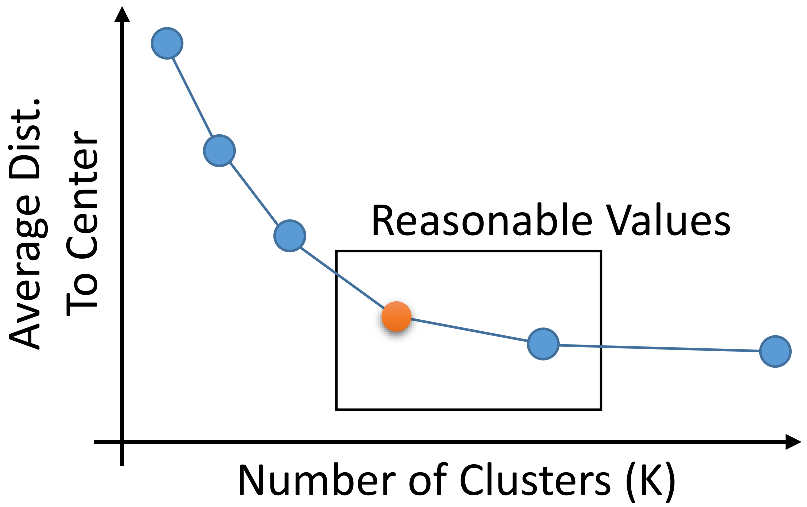
```
centers ← set(randomly select a single point)

while len(centers) < k:
  # Compute the distance of each point
  # to its nearest center dSq = d^2
  dSq ← [(x, dist_to_nearest(centers, x)^2) for x in data]
  # Sample a new point with probability
  # proportional to dSq
  c ← sample_one(data, prob = dSq / sum(dSq))
  # Update the clusters
  centers.add(c)
```


http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf

How do we choose K?



- Basic Elbow Method (Easy and what you do in HW)
  - Try range of K-values and plot average distance to centers
- Cross-Validation (Better)
  - Repeatedly split the data into training and validation datasets
  - Cluster the training dataset
  - Measure Avg. Dist. To Centers on validation data



K-Means +

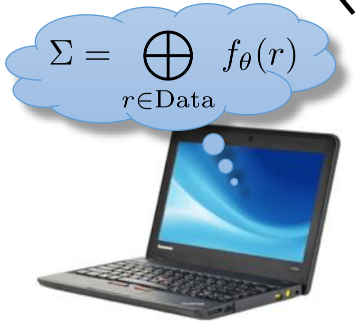
How do we run k-means on the data warehouse / data lake?

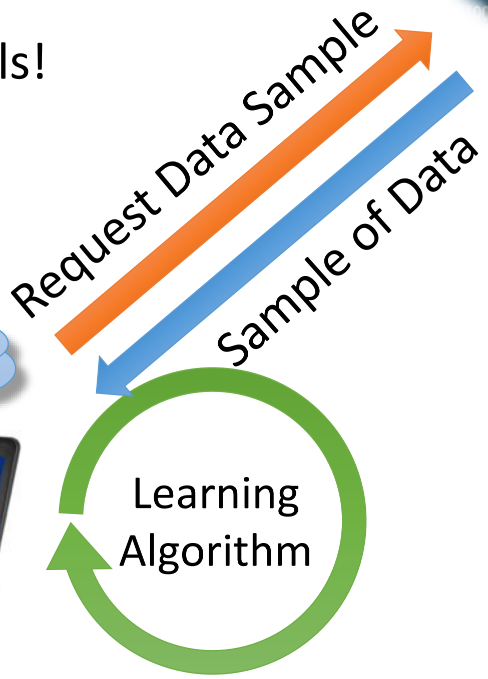
Interacting With the Data

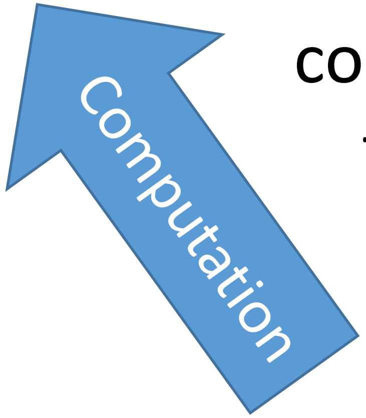
Good for smaller datasets

- Faster more natural interaction
- Lots of tools!

Compute Locally





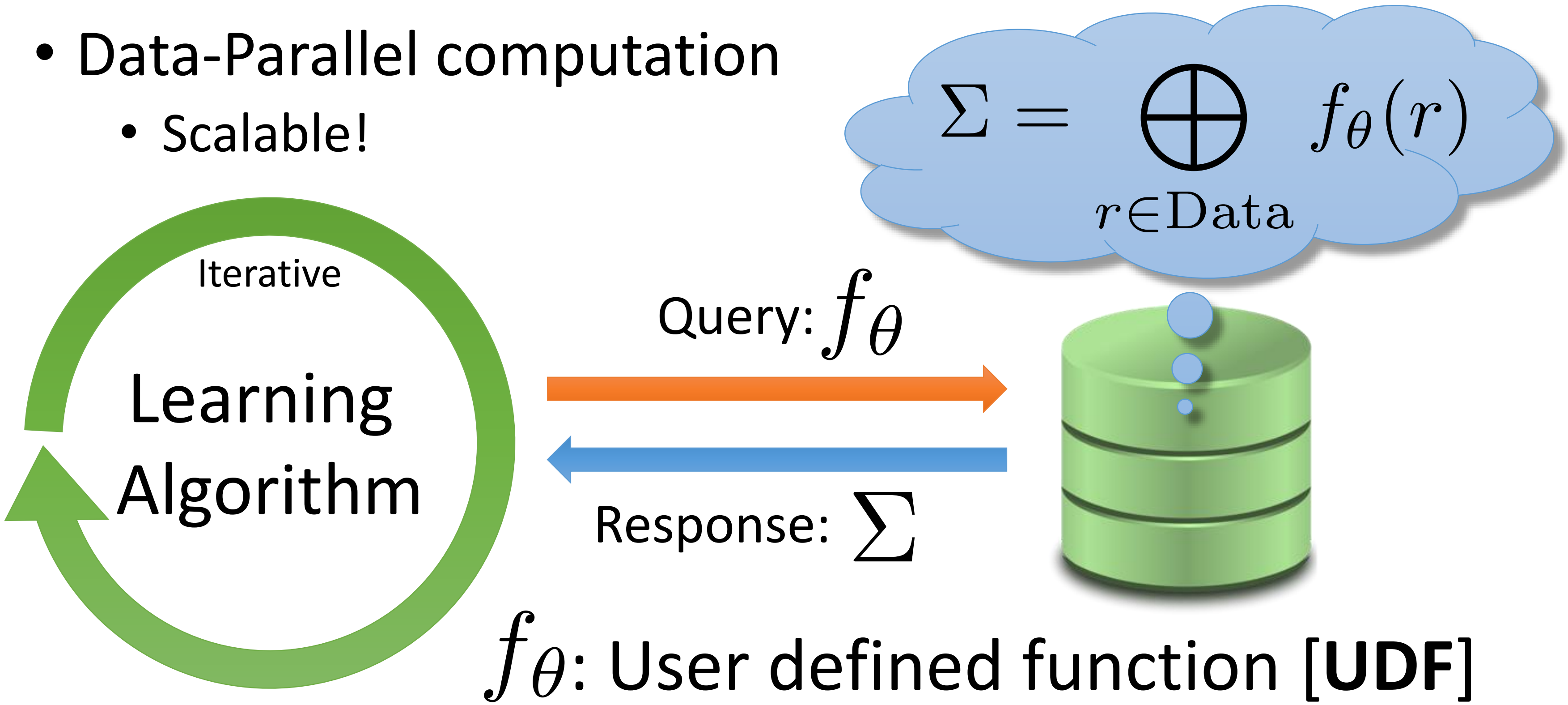


Can we send the computation to the data?

Yes!

Statistical Query Pattern
Common Machine Learning Pattern

- Computing aggregates of user defined functions
- Data-Parallel computation
  - Scalable!



f_θ: User defined function [**UDF**]

$\bigoplus$: User defined aggregate [**UDA**]

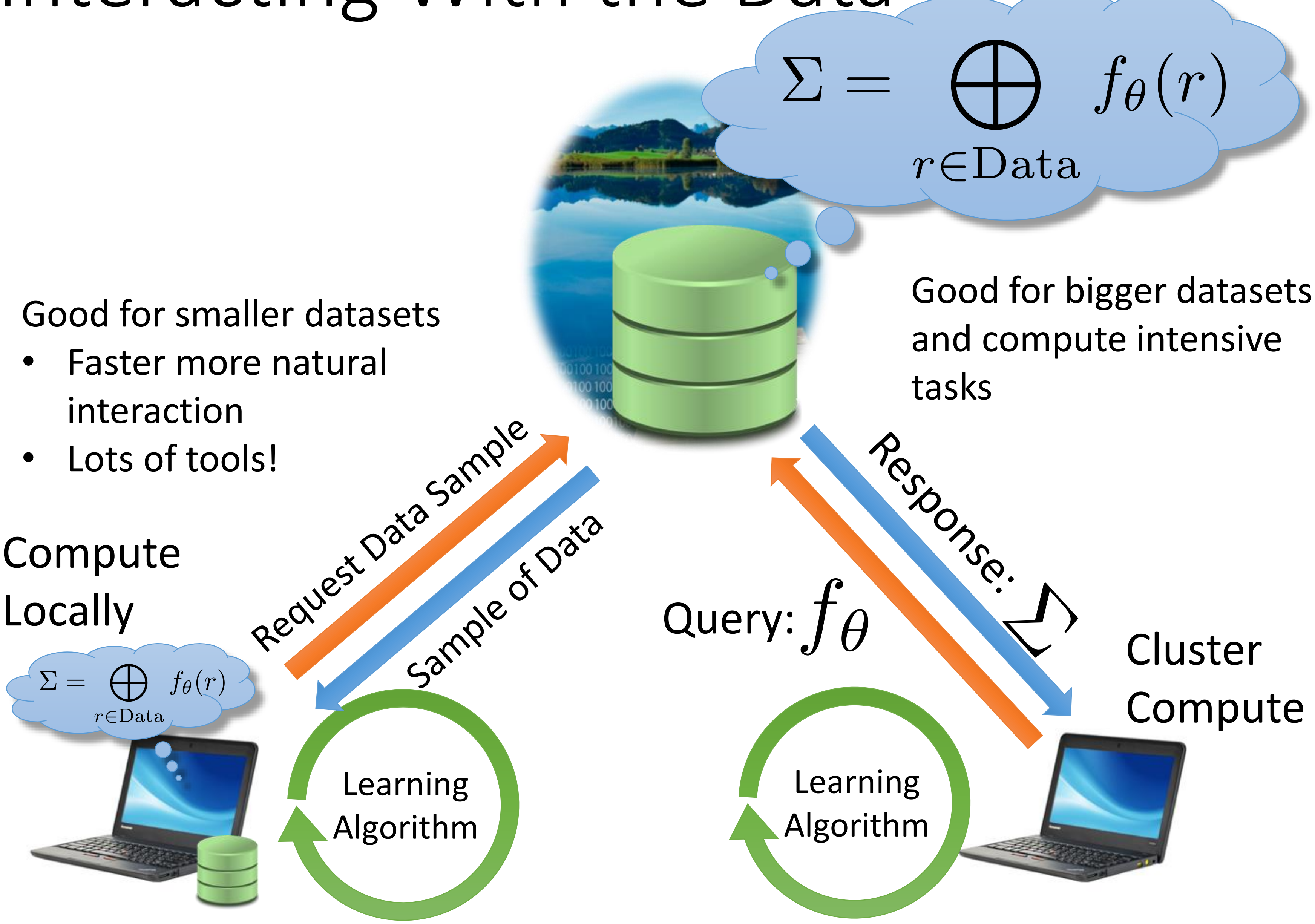
D. Caragea et al., *A Framework for Learning from Distributed Data Using Sufficient Statistics and Its Application to Learning Decision Trees*. Int. J. Hybrid Intell. Syst. 2004

Interacting With the Data

Good for smaller datasets

- Faster more natural interaction
- Lots of tools!

Good for bigger datasets and compute intensive tasks



Can we express K-Means in the **Statistical Query Pattern?**

```
centers ← pick k initial Centers
while (centers are changing):
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    for i in range(k): // Compute the new centers (M-Step)
        centers[i] = mean([x for (x, c) in asg if c == i])
```

Query returns all the data ...

Merge with M-Step → **Statistical Query Pattern**

```
centers ← pick k initial Centers
while (centers are changing):
    for i in range(k):
        new_centers[i] =
            mean([x for x in data if nearest(centers, x) == i])
    centers = new_centers
```

Can we express K-Means in the **Statistical Query Pattern?**

```
centers ← pick k initial Centers
while (centers are changing):
    for i in range(k):
        new_centers[i] =
            mean([x for x in data if nearest(centers, x) == i])
    centers = new_centers
```

Group by query:

```
SELECT nearest_UDF(centers, x) AS cid, mean_UDA(x)
FROM data GROUPBY cid
```

K-Means in Map-Reduce

- **MapFunction**(*old_centers, x*)
  - Compute the index of the nearest old center
  - Return (**key** = *nearest_centers*, **value** = (*x*, 1))
- **ReduceFunction** combines values and counts
  - For each cluster center (Group By)
- Data system returns aggregate statistics:

$$s_i = \sum_{x \in \text{Cluster } i} x_i \qquad \text{and} \qquad n_i = \sum_{x \in \text{Cluster } i} 1$$

- ML algorithm computes new centers: $\mu_i = s_i / n_i$

Can we express K-Means++ in the **Statistical Query Pattern**?

- *Yes*, however there is a better version: **K-Means||**
  - More complex but much faster
- Or you can parallelize **K-Means++** directly
  - Requires more passes
- Challenging Step?
  - Parallel weighted sampling:

```
sample_one(data, prob = dSq / sum(dSq))
```

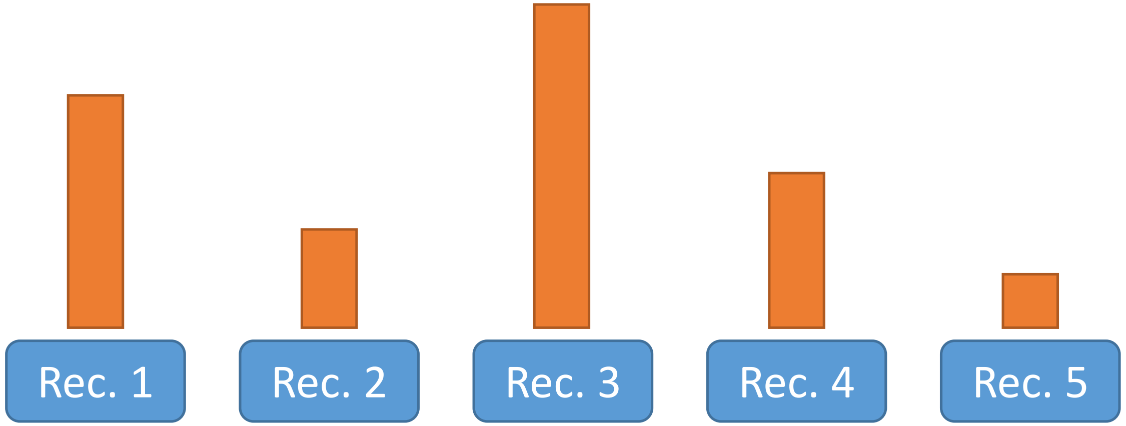
  - How do you select one point uniformly at random?

Res-A: weighted reservoir sampling

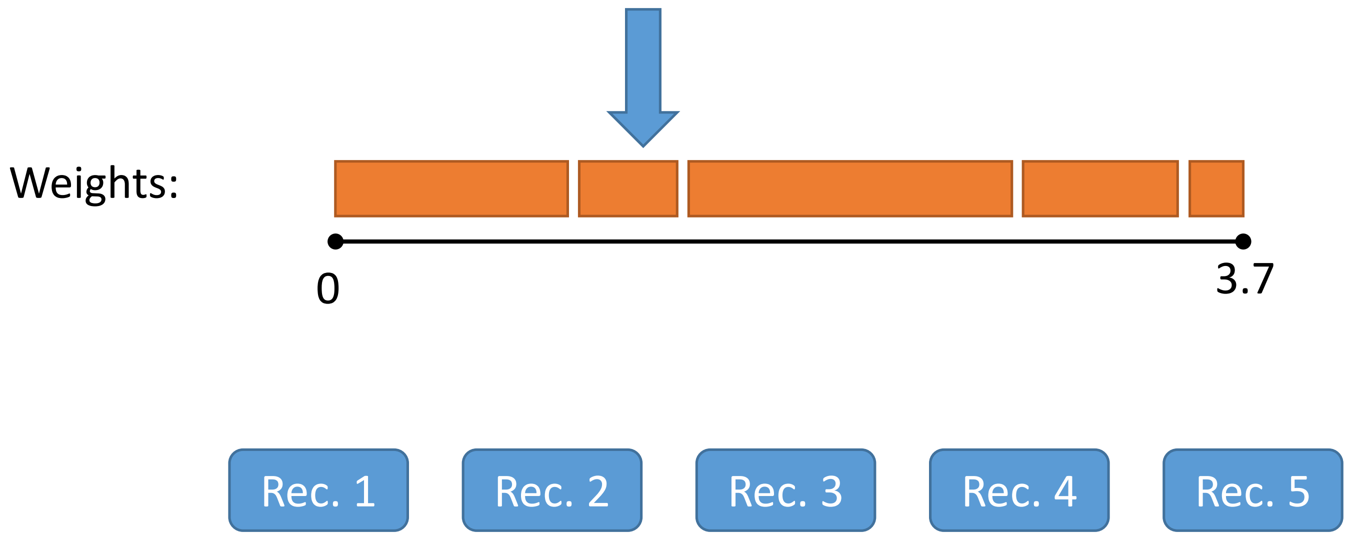
- **Goal:** *Sample* ***k*** *records from a stream where record* ***i*** *is included in the sample with probability* ***proportional*** *to* w_i

How would we normally sample k records?

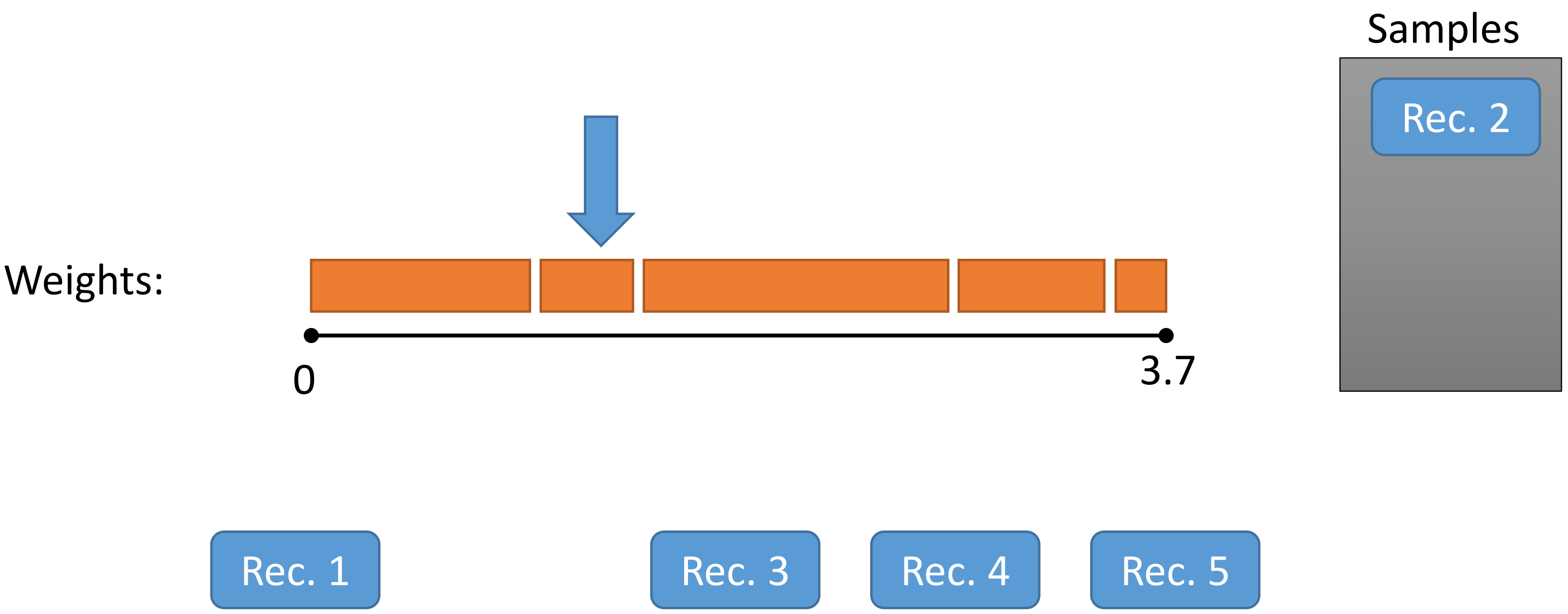
Weights:



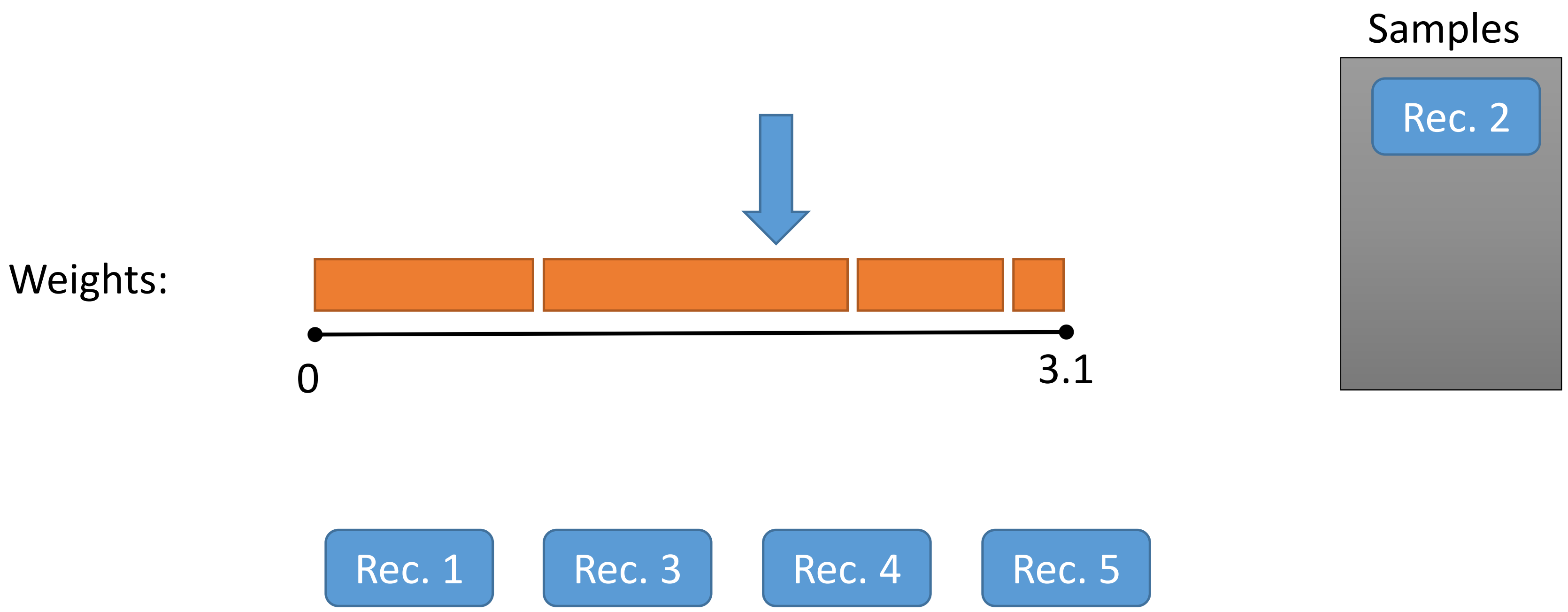
Draw a random number uniformly between **0** and **3.7**



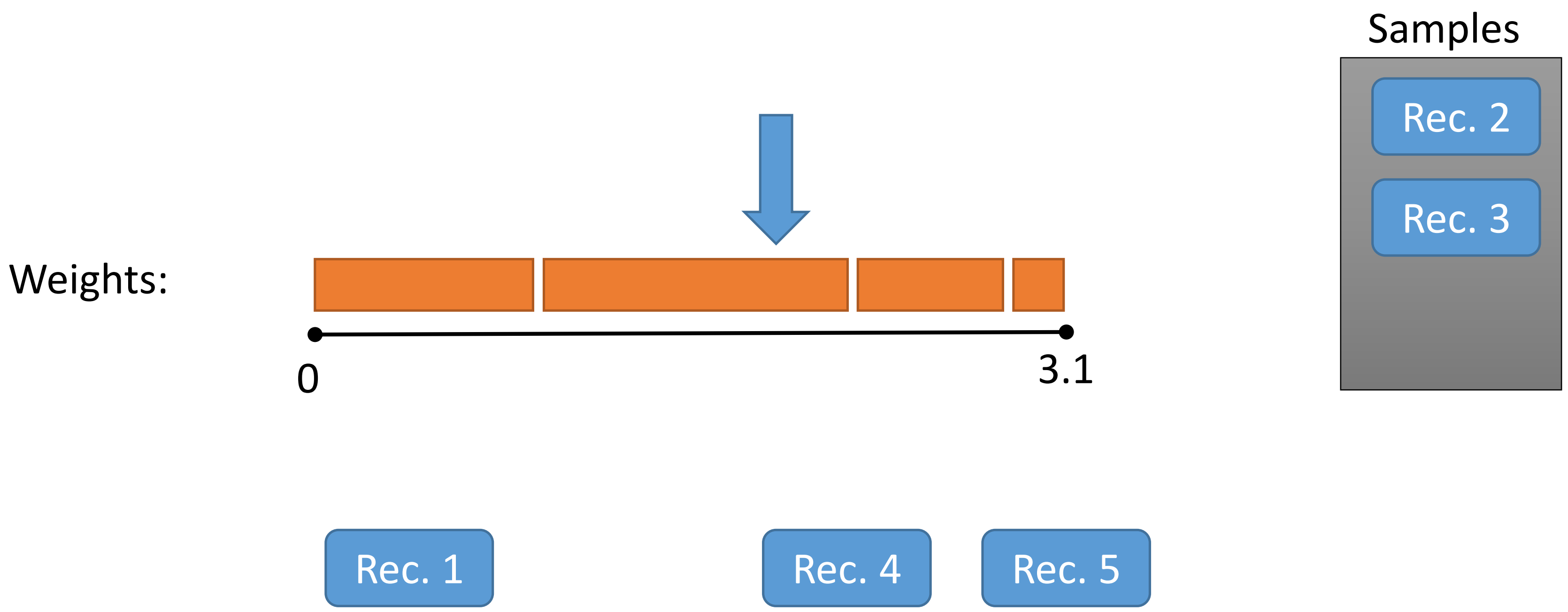
Sample the corresponding record and remove the weight.



Draw a random number uniformly between **0** and **3.1**



We want to do this in **one pass** *without* ever knowing the **sum** of the weights!



Res-A: weighted reservoir sampling

- **Goal:** *Sample **k** records from a stream where record **i** is included in the sample with probability proportional to w_i*
- **Algorithm:**
  - For each record ***i*** draw a uniform random number:

$$u_i \sim \mathbf{Unif}(0, 1)$$

  - Select the top-k records ordered by: u_i^{1/w_i}

- **Common ML Pattern?**
  - **Query Function:** *`[pow(rand(), 1 / record.w), record]`*
  - **Agg. Function:** *top-k heap*

Pavlos S. Efraimidis and Paul G. Spirakis. 2006. Weighted random sampling with a reservoir. *Inf. Process. Lett.* 97, 5 (March 2006), 181-185

Illustrating Res-A Algorithm

Weights:		Uniform Random Number	u_i^{1/w_i}
1.0	Rec. 1	0.31	0.31
2.0	Rec. 2	0.20	0.45
1.4	Rec. 3	0.45	0.56
2.5	Rec. 4	0.14	0.46
0.7	Rec. 5	0.55	0.43
3.0	Rec. 6	0.69	0.88

Top 2

Basic Analysis Behind **Res-A**

- Define the random variable: $X_i = u_i^{1/w_i}$
- Then:

$$\mathbf{P}\left(X_i < \alpha\right) = \mathbf{P}\left(u_i^{1/w_i} < \alpha\right) = \mathbf{P}\left(u_i < \alpha^{w_i}\right) = \alpha^{w_i}$$

$$\mathbf{p}\left(X_i = \alpha\right) = w_i \alpha^{w_i - 1}$$

Derivative of CDF → PDF

- Suppose we want to pick just one element (k=1)
  - Probability of selecting X_i is:

$$\int_0^1 \mathbf{p}\left(X_i = \alpha\right) \prod_{j \neq i} \mathbf{P}\left(X_j < \alpha\right) d\alpha = \int_0^1 \left(w_i \alpha^{w_i - 1}\right) \prod_{j \neq i} \alpha^{w_j} d\alpha$$

$$= \frac{w_i}{\sum_j w_j}$$

We won't test you on this derivation

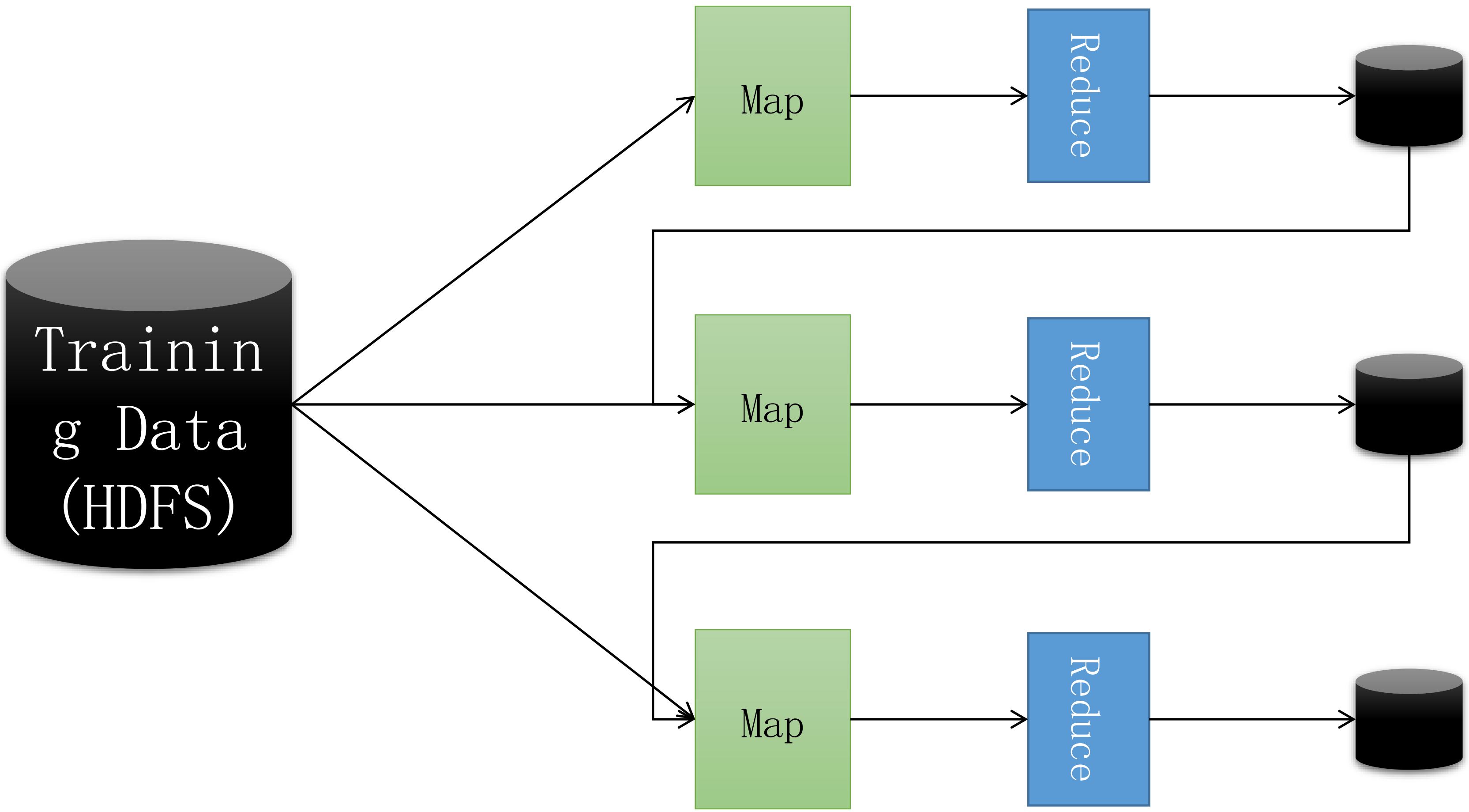
People who like Res-A also like…

- Algorithm R
  - Another reservoir filtering algorithm (recitation?)
- Bloom Filters
  - Efficient set membership with limited memory
- Count-Min
  - Efficient key-counting with limited memory
- Heavy Hitters Sketch
  - Top-k Elements with limited memory

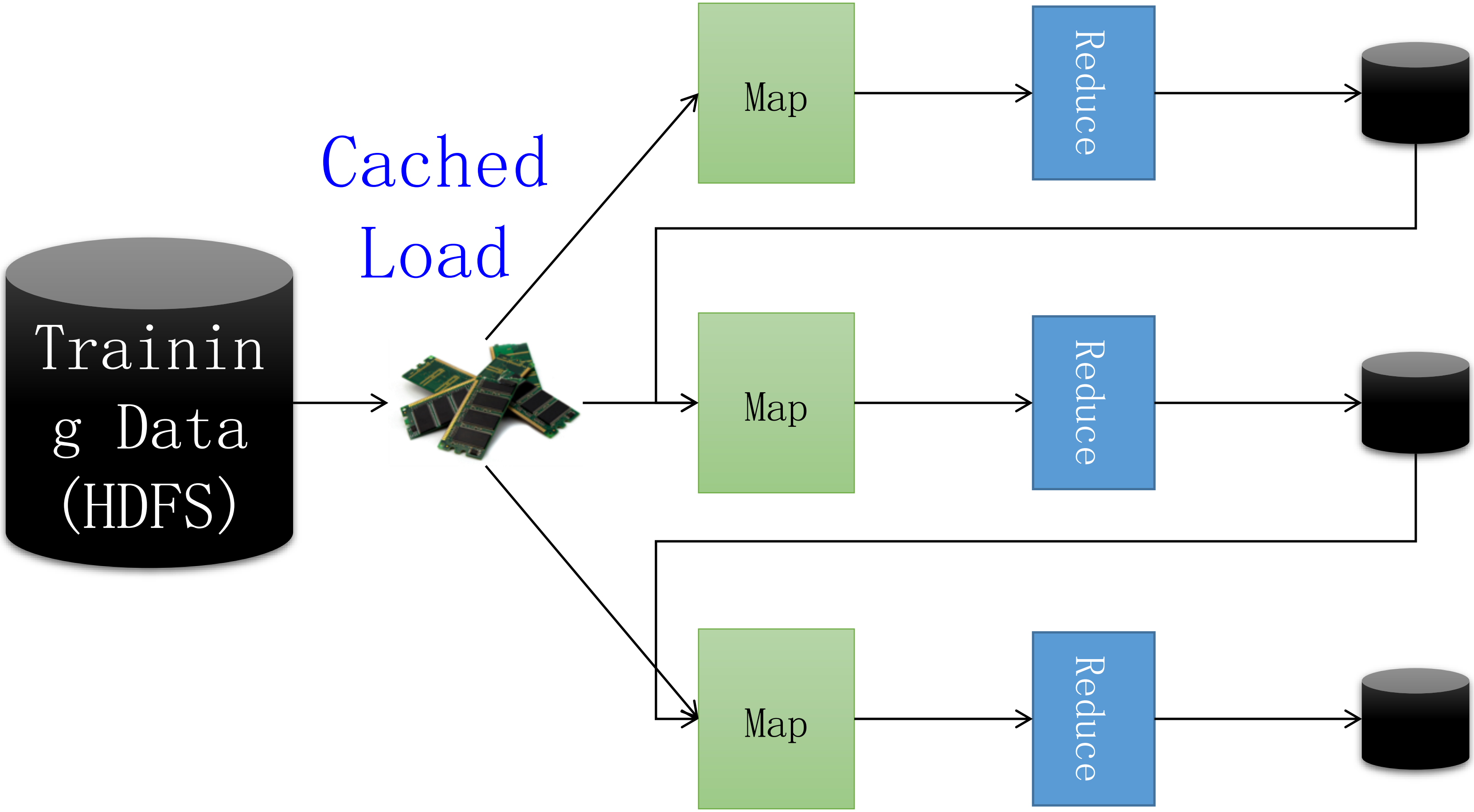
Implementation Details: Statistical Query Pattern

- **Iterative** ML ➔ Data caching is important
  - Motivation behind Spark project

Map Reduce Dataflow View

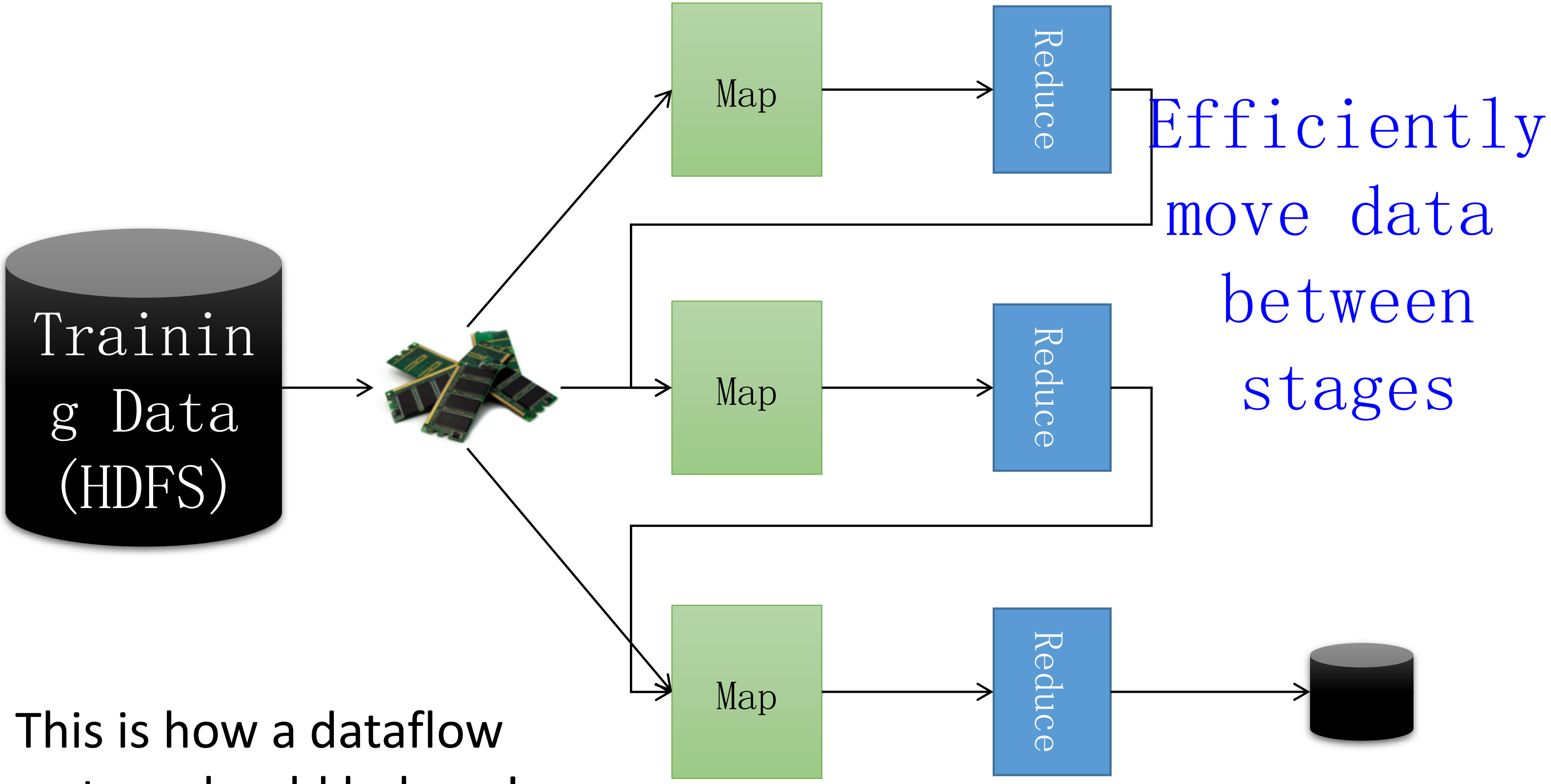


Spark Opt. Dataflow



10–100× faster than network and disk

Spark Opt. Dataflow View

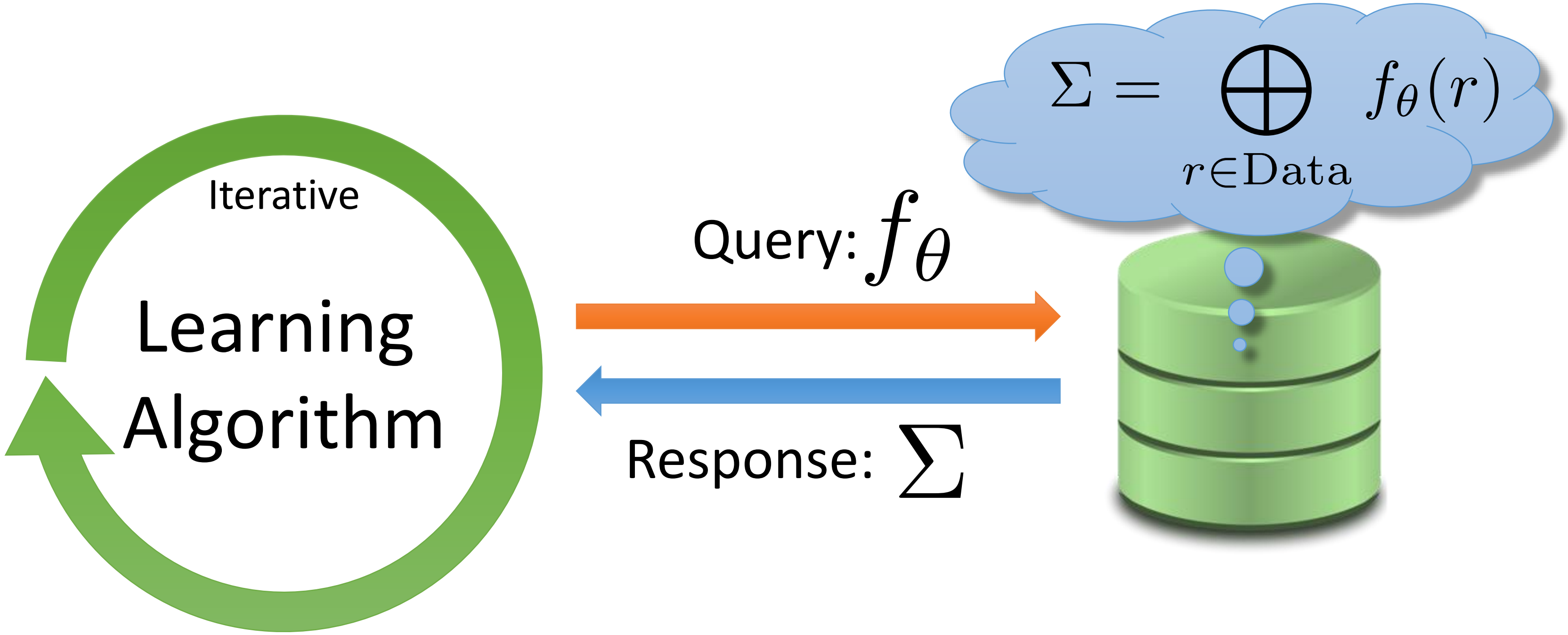


This is how a dataflow system should behave!

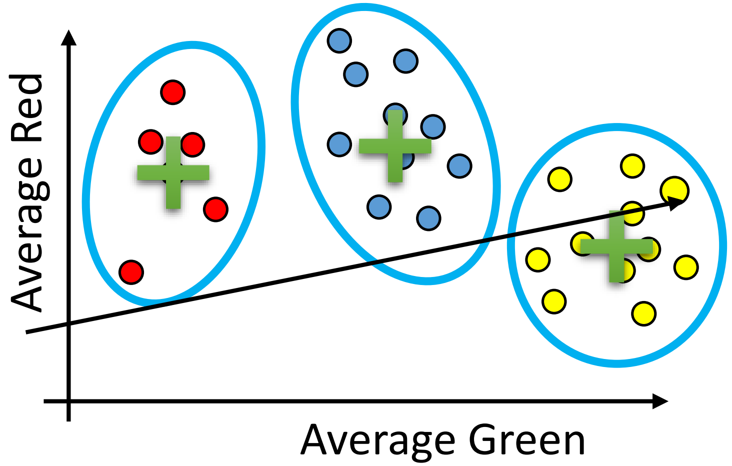
- What happened to map-reduce?

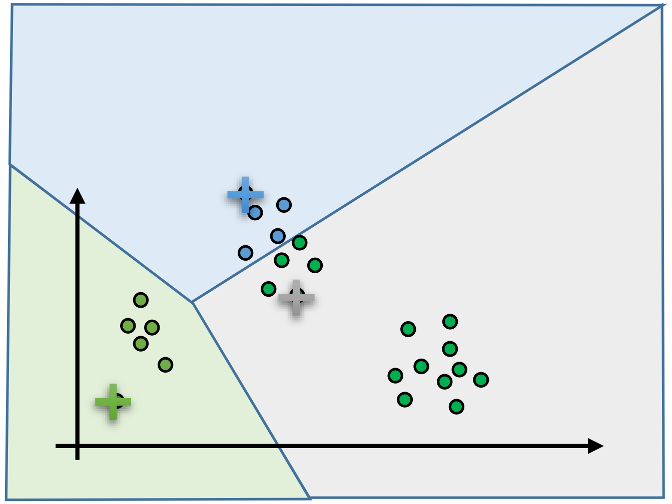
Implementation Details: Common Machine Learning Pattern

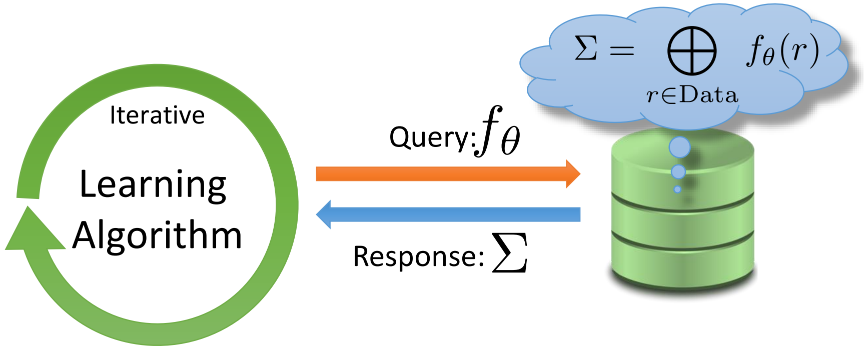
- Iterative ML ➔ Data caching is important
  - Motivation behind Spark project
- Need to watch out for large $\boldsymbol{\theta}$ and $\boldsymbol{\Sigma}$



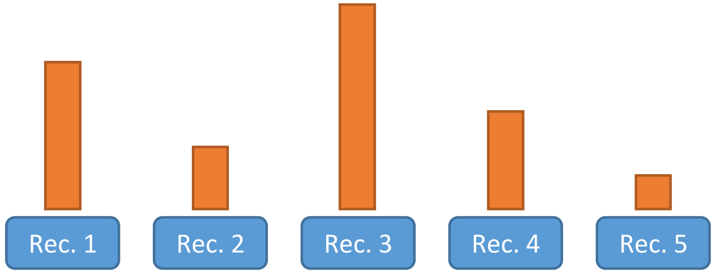
Summary of Clustering








```
SELECT nearest_UDF(centers, x) AS cid, mean_UDA(x)
FROM data GROUPBY cid
```



Taxonomy
of Machine Learning

Labeled Data

Indirect (reward)

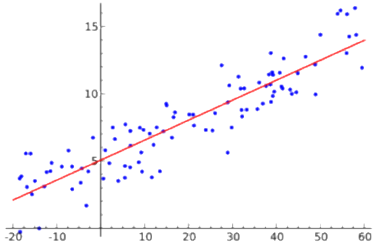
Unlabeled Data

Supervised Learning

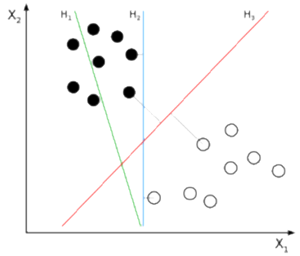
Reinforcement & Bandit Learning

Unsupervised Learning

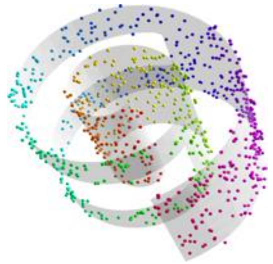
Regression



Classification



Dimensionality Reduction



Clustering