

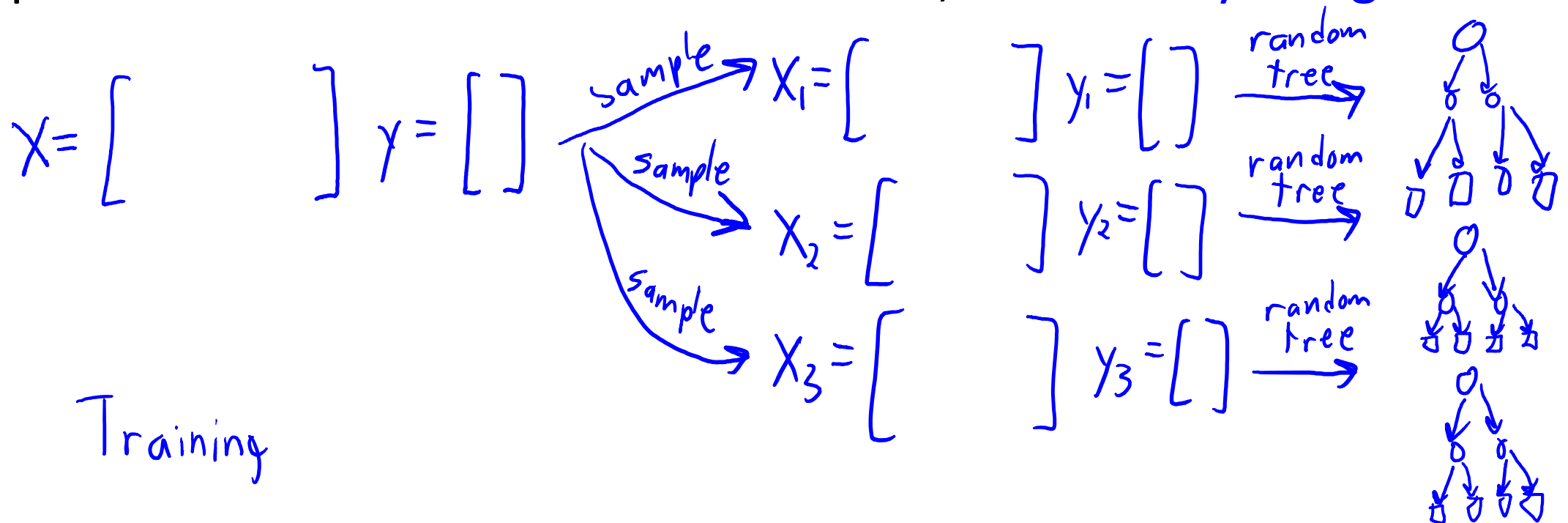
CPSC 340: Machine Learning and Data Mining

K-Means Clustering

Fall 2018

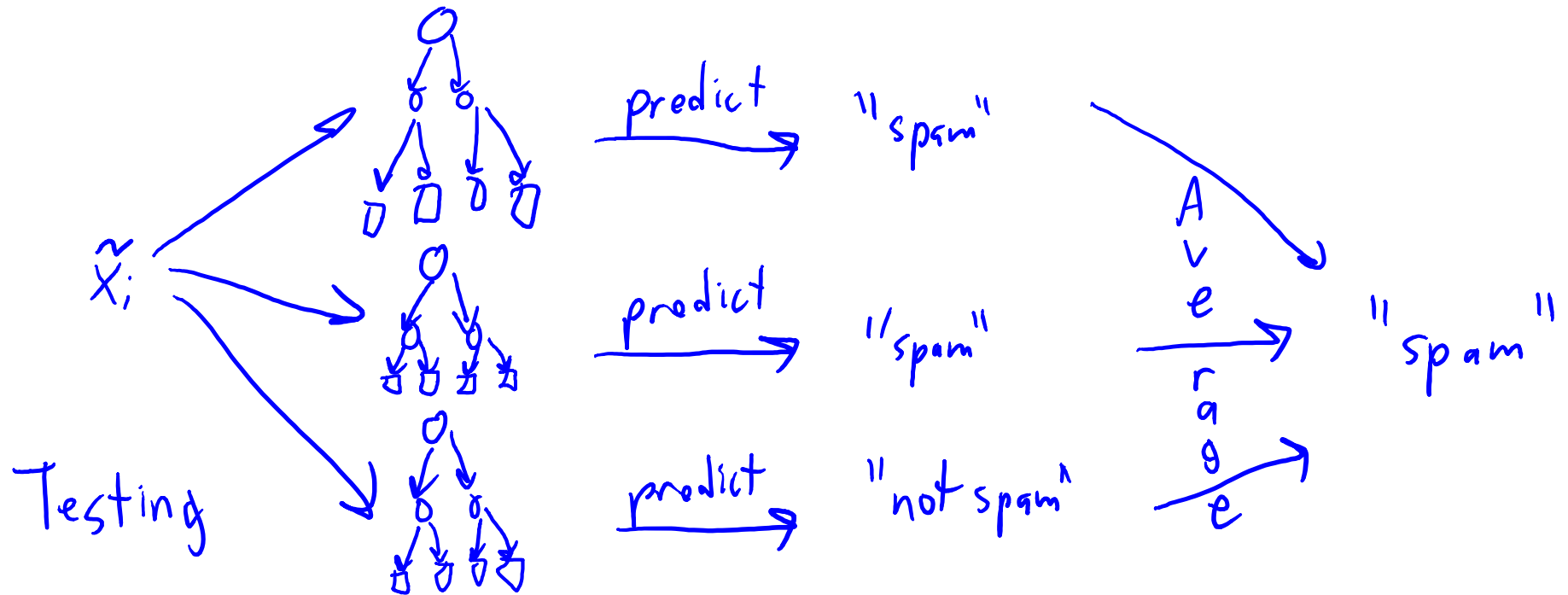
Last Time: Random Forests

- Random forests are one of the best 'out of the box' classifiers.
- Fit deep decision trees to random **bootstrap samples** of data, base splits on **random subsets** of the features, and **classify using mode**.



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End of Part 1: Key Concepts

- Fundamental ideas:
 - Training vs. test error (memorization vs. learning).
 - IID assumption (examples come independently from same distribution).
 - Golden rule of ML (test set should not influence training).
 - Fundamental trade-off (between training error vs. approximation error).
 - Validation sets and cross-validation (can approximate test error)
 - Optimization bias (we can overfit the training set and the validation set).
 - Decision theory (we should consider costs of predictions).
 - Parametric vs. non-parametric (whether model size depends on 'n').
 - No free lunch theorem (there is no “best” model).

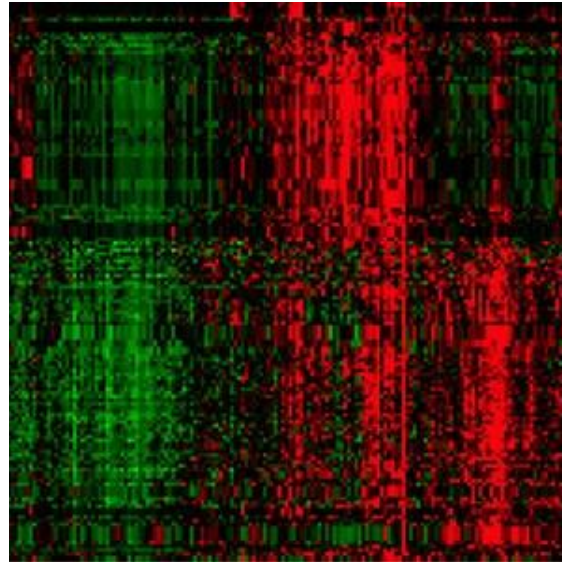
End of Part 1: Key Concepts

- We saw 3 ways of “learning”:
 - Searching for rules.
 - Decision trees (greedy recursive splitting using decision stumps).
 - Counting frequencies.
 - Naïve Bayes (probabilistic classifier based on conditional independence).
 - Measuring distances.
 - K-nearest neighbours (non-parametric classifier with universal consistency).
- We saw 2 generic ways of improving performance:
 - Encouraging invariances with data augmentation.
 - Ensemble methods (combine predictions of several models).
 - Random forests (averaging plus randomization to reduce overfitting).

Application: Classifying Cancer Types

- “I collected gene expression data for 1000 different types of cancer cells, can you tell me the different classes of cancer?”

$X =$



- We are not given the class labels y , but want **meaningful labels**.
- An example of **unsupervised learning**.

Unsupervised Learning

- Supervised learning:
 - We have features x_i and class labels y_i .
 - Write a program that produces y_i from x_i .
- Unsupervised learning:
 - We **only have x_i values**, but no explicit target labels.
 - You want to do “something” with them.
- Some unsupervised learning tasks:
 - Outlier detection: Is this a ‘normal’ x_i ?
 - Similarity search: Which examples look like this x_i ?
 - Association rules: Which x^j occur together?
 - Latent-factors: What ‘parts’ are the x_i made from?
 - Data visualization: What does the high-dimensional X look like?
 - Ranking: Which are the most important x_i ?
 - Clustering: What types of x_i are there?

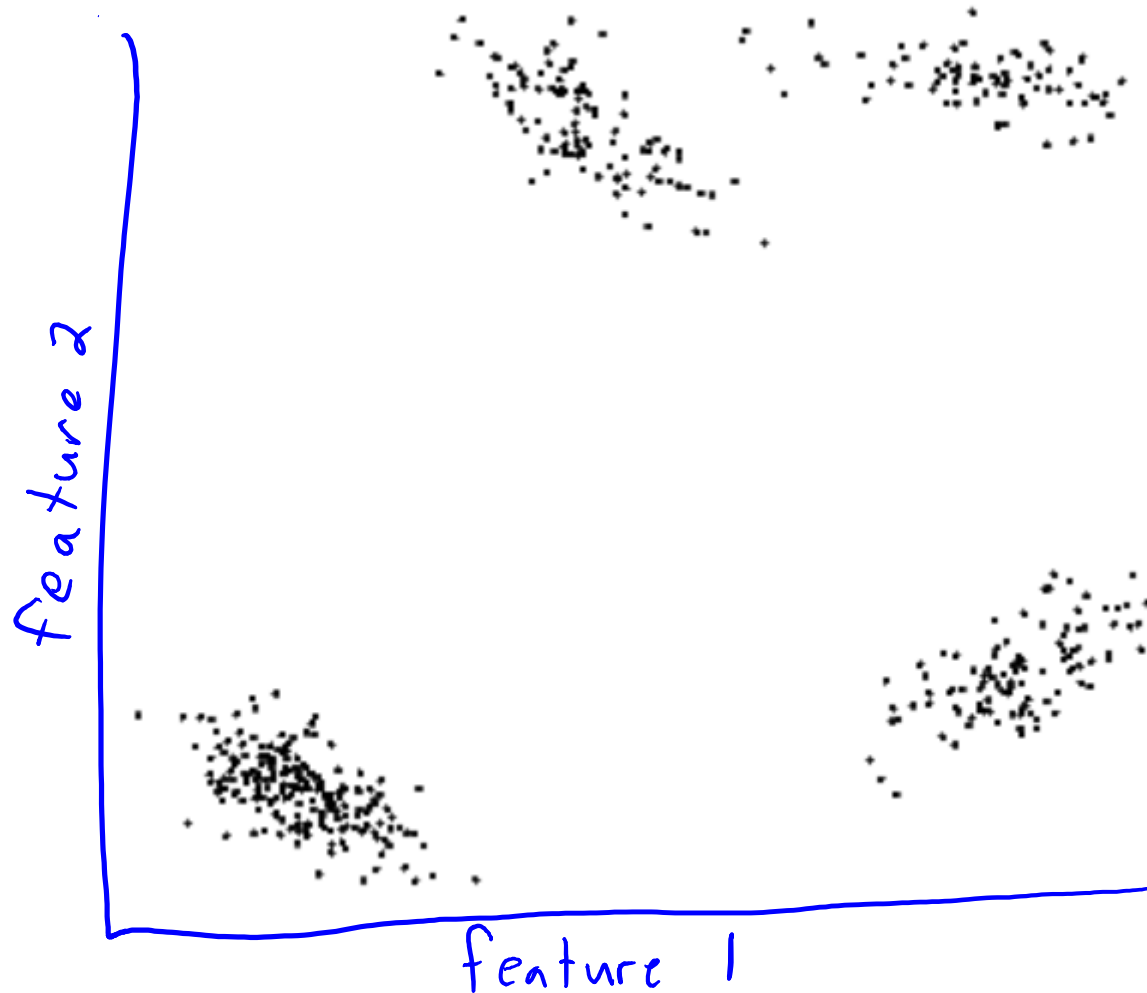
Clustering

- Clustering:
 - Input: set of examples described by features x_i .
 - Output: an assignment of examples to 'groups'.
- Unlike classification, we are not given the 'groups'.
 - Algorithm must discover groups.
- Example of groups we might discover in e-mail spam:
 - 'Lucky winner' group.
 - 'Weight loss' group.
 - 'Nigerian prince' group.
 - 'Russian bride' group.

Clustering Example

Input: data matrix 'X'.

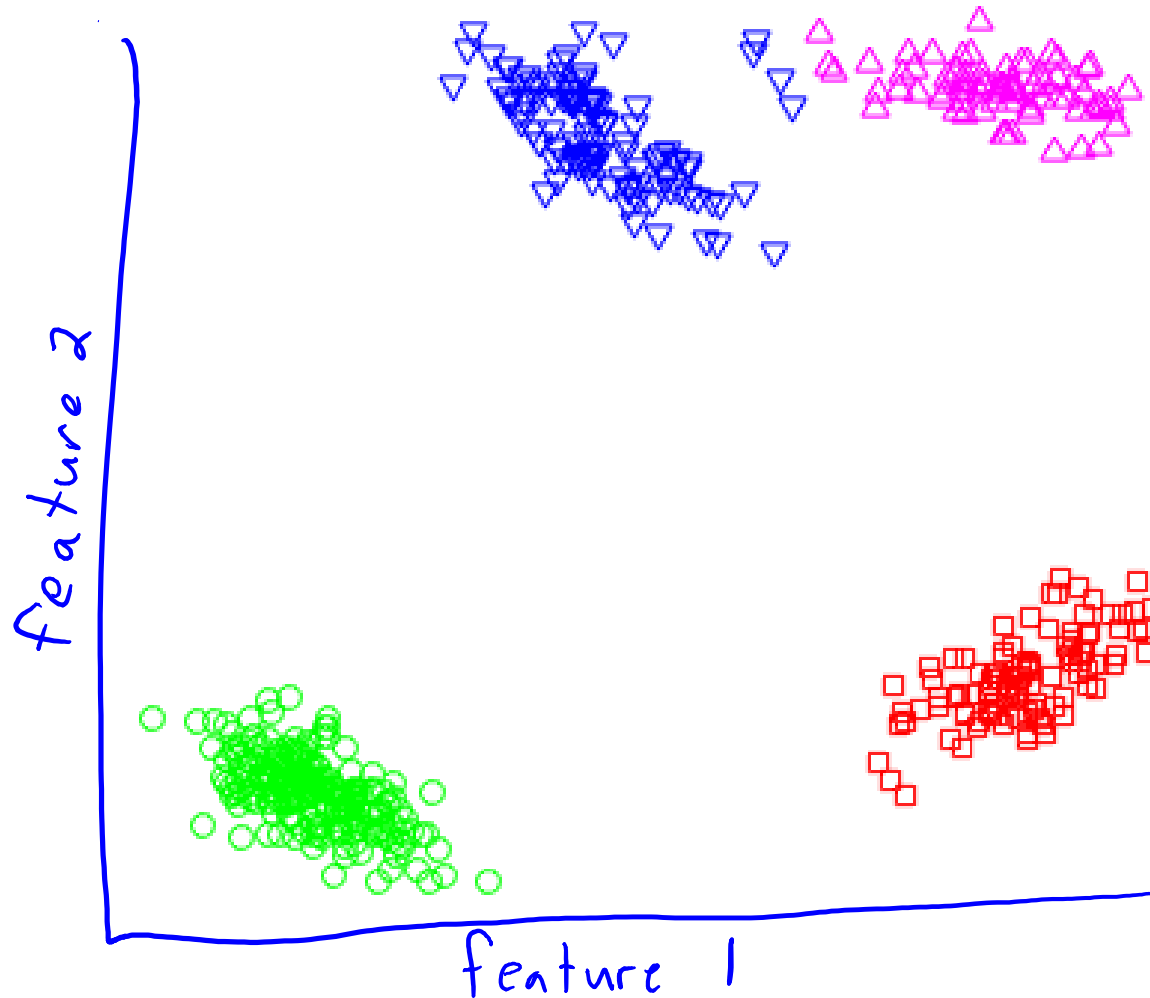
$$X = \begin{bmatrix} -9.0 & -7.3 \\ -10.9 & -9.0 \\ 13.7 & 19.3 \\ 13.8 & 20.4 \\ 12.8 & 20.6 \\ \vdots & \vdots \end{bmatrix}$$



Clustering Example

Input: data matrix 'X'.

$$X = \begin{bmatrix} -9.0 & -7.3 \\ -10.9 & -9.0 \\ 13.7 & 19.3 \\ 13.8 & 20.4 \\ 12.8 & 20.6 \\ \vdots & \vdots \end{bmatrix}$$



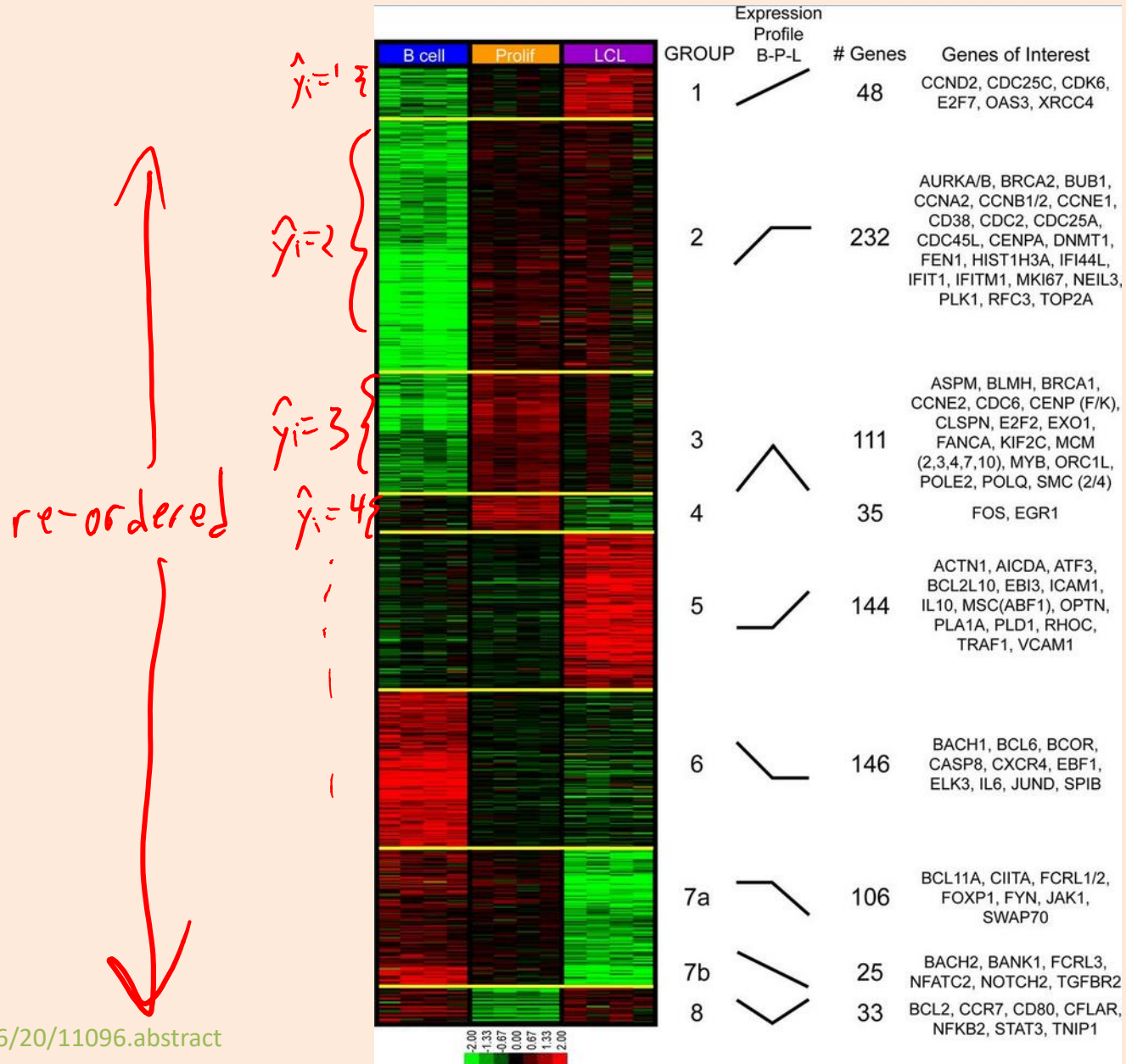
Output: clusters \hat{y} .

$$\hat{y} = \begin{bmatrix} 2 \\ 2 \\ 3 \\ 3 \\ 1 \\ \vdots \end{bmatrix}$$

Data Clustering

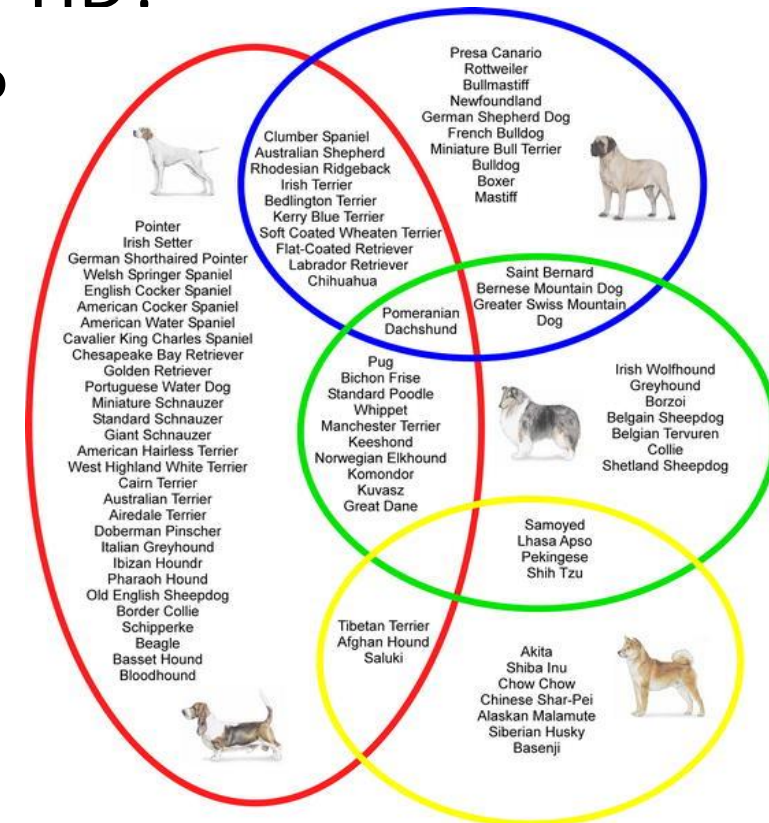
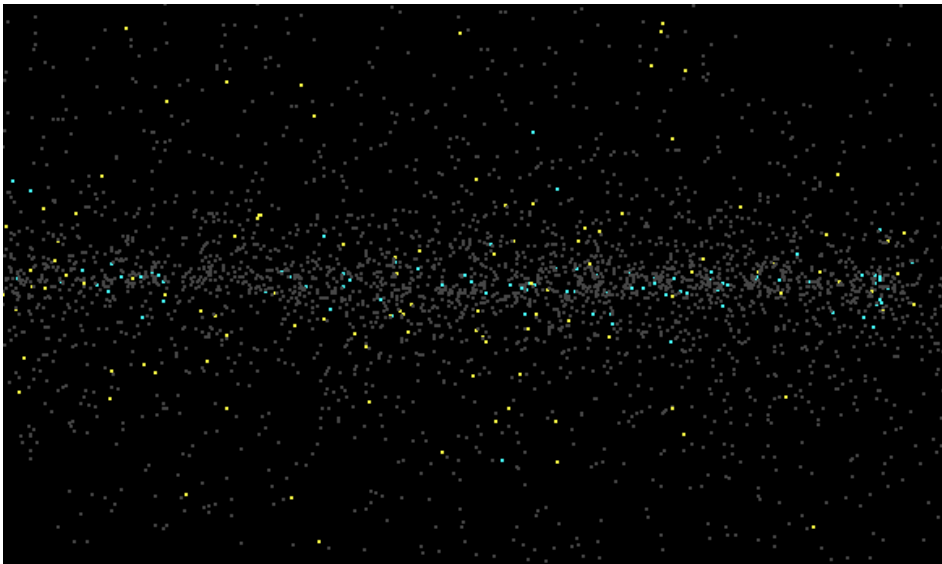
- General goal of clustering algorithms:
 - Examples in the same group should be ‘similar’.
 - Examples in different groups should be ‘different’.
- But the ‘best’ clustering is hard to define:
 - We don’t have a test error.
 - Generally, there is no ‘best’ method in unsupervised learning.
 - So there are lots of methods: we’ll focus on important/representative ones.
- Why cluster?
 - You could want to know what the groups are.
 - You could want a ‘prototype’ example for each group.
 - You could want to find the group for a new example x_i .
 - You could want to find examples related to a new example x_i .

Clustering of Epstein-Barr Virus



Other Clustering Applications

- NASA: what types of stars are there?
- Biology: are there sub-species?
- Documents: what kinds of documents are on my HD?
- Commercial: what kinds of customers do I have?



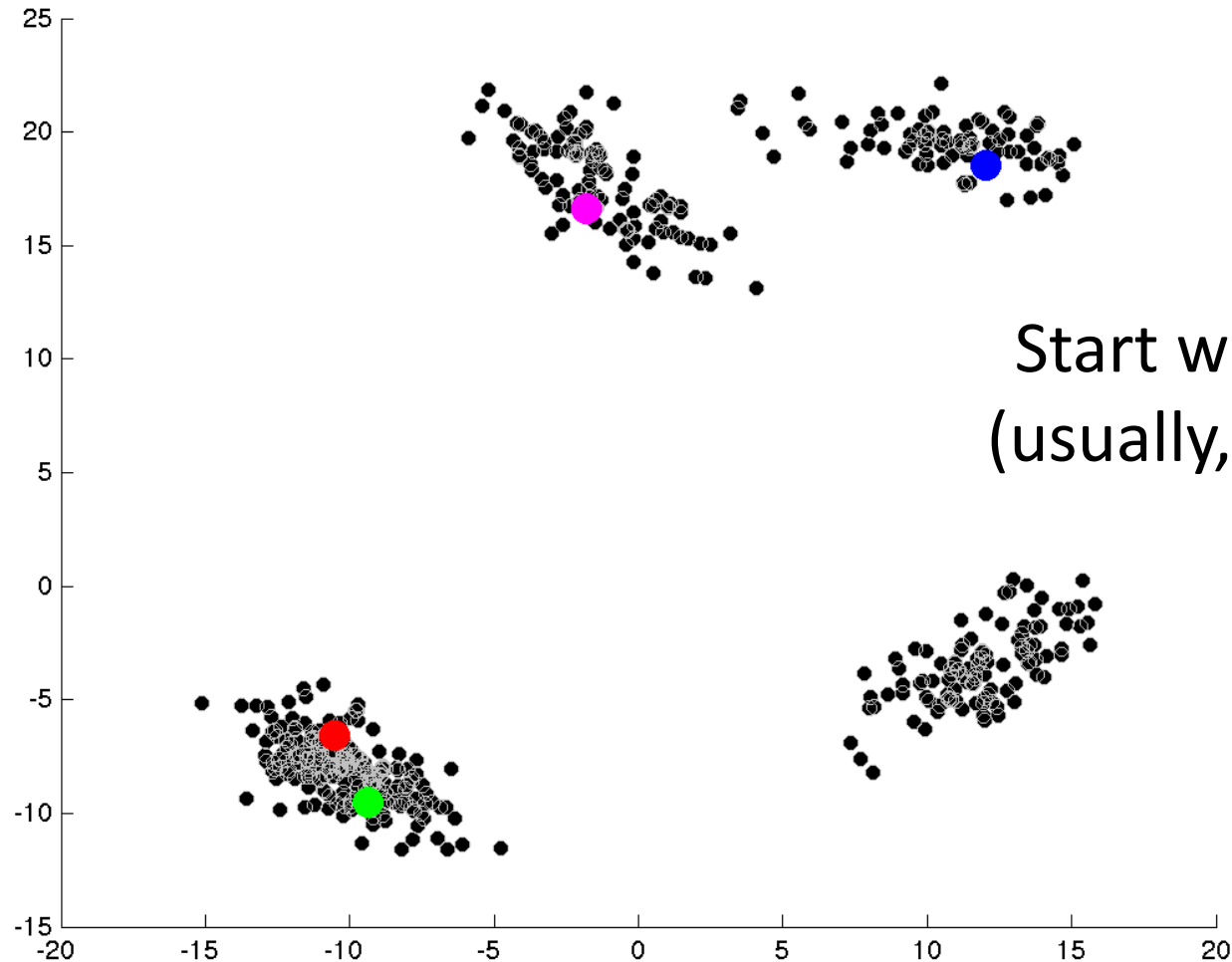
K-Means

- Most popular clustering method is **k-means**.
- Input:
 - The **number of clusters 'k'** (hyper-parameter).
 - Initial guess of the center (the “mean”) of each cluster.
- Algorithm:
 - **Assign each x_i** to its closest mean.
 - **Update the means** based on the assignment.
 - Repeat until convergence.

K-Means Example

Input: data matrix 'X'.

$$X = \begin{bmatrix} -9.0 & -7.3 \\ -10.9 & -9.0 \\ 13.7 & 19.3 \\ 13.8 & 20.4 \\ 12.8 & 20.6 \\ \vdots & \vdots \end{bmatrix}$$

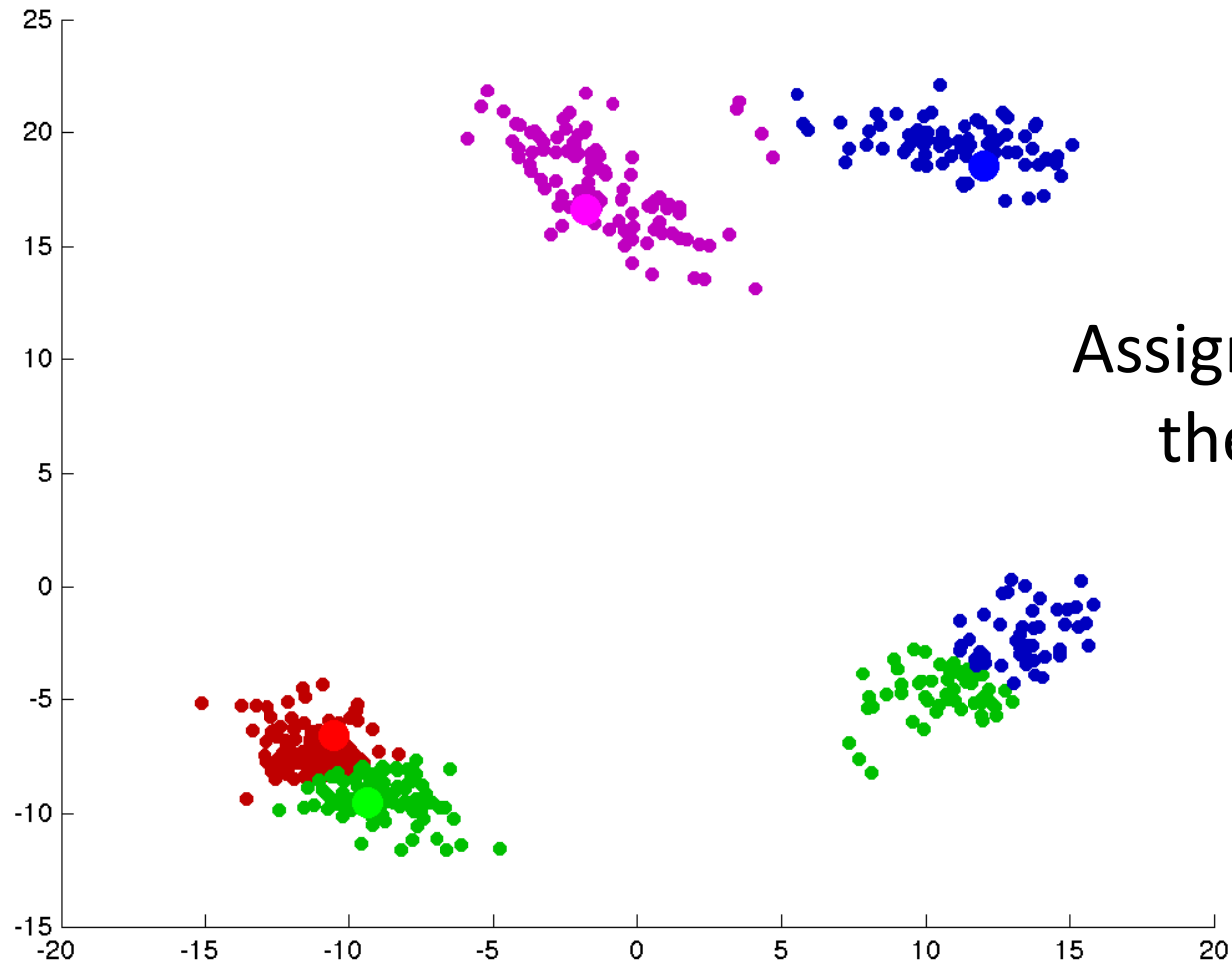


Start with 'k' initial 'means'
(usually, random data points)

K-Means Example

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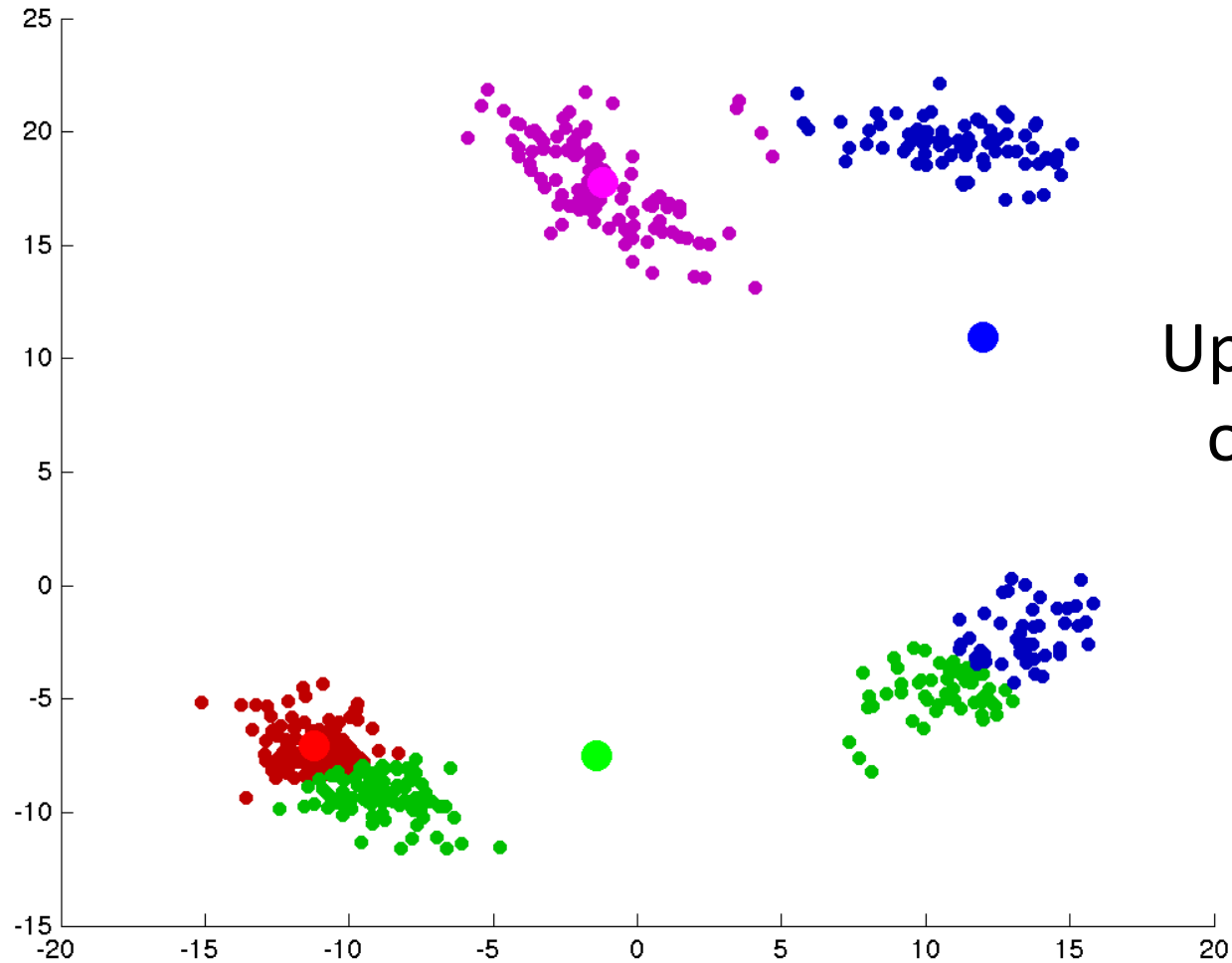


Assign each example to the closest mean.

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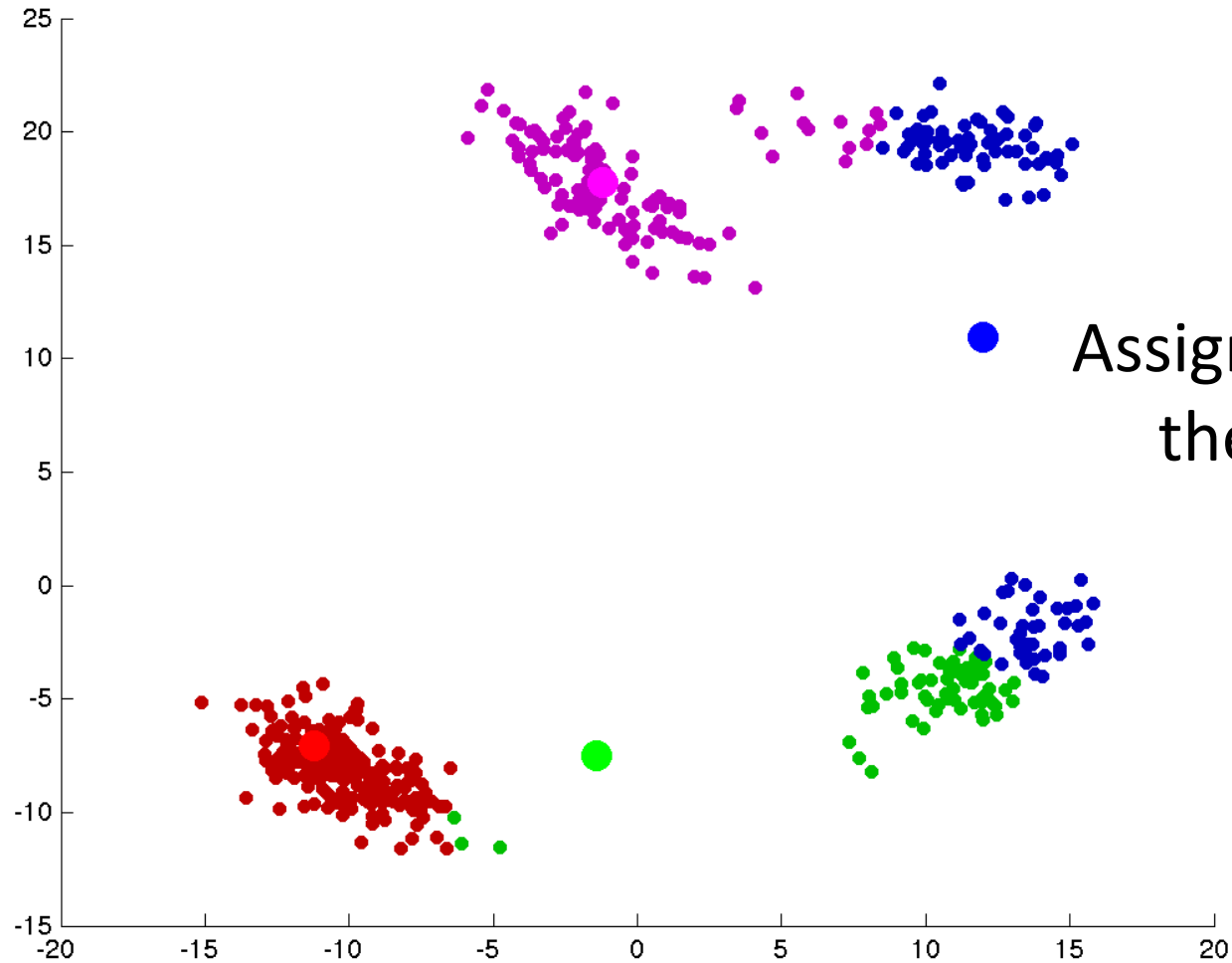


Update the mean
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K-Means Example

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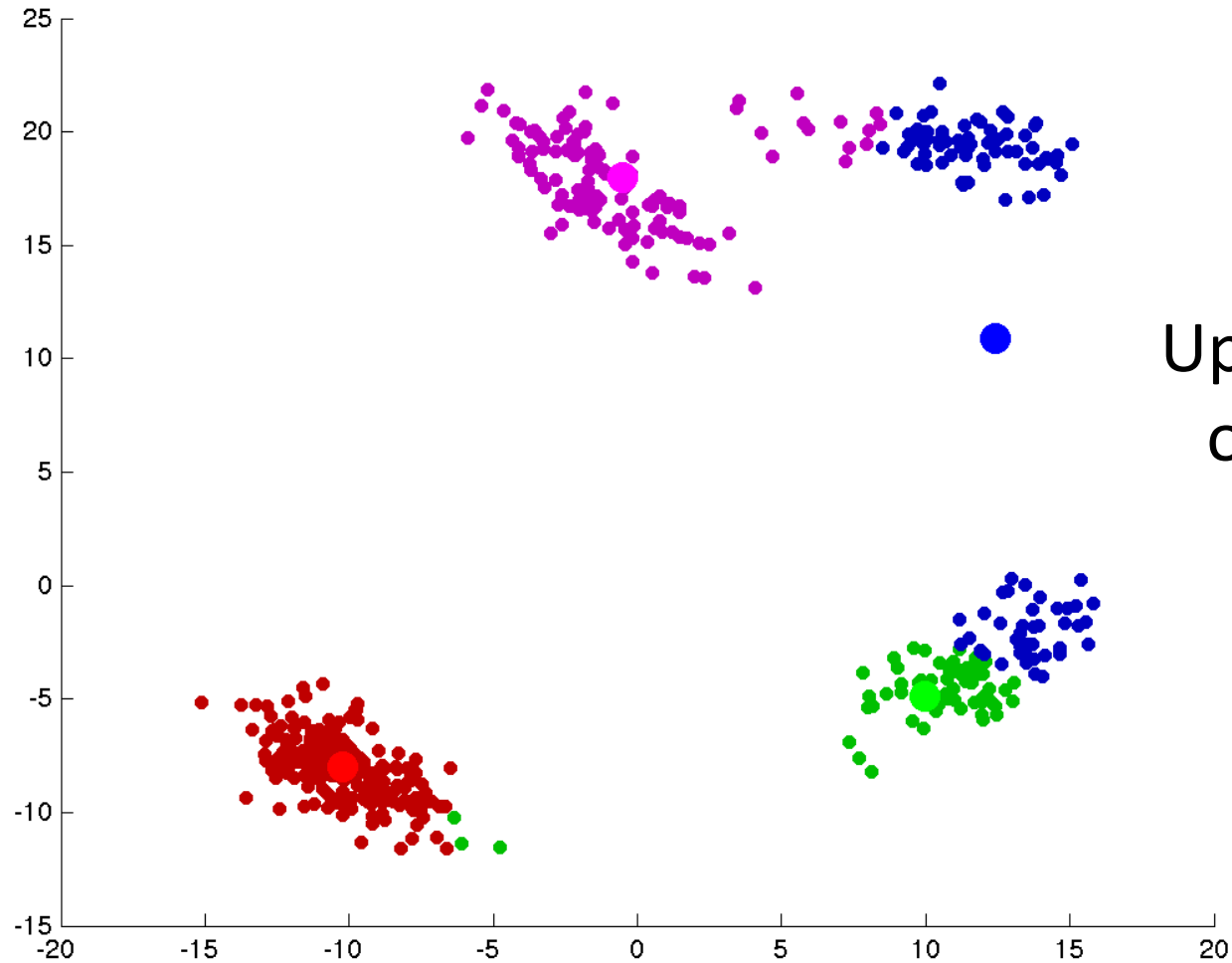
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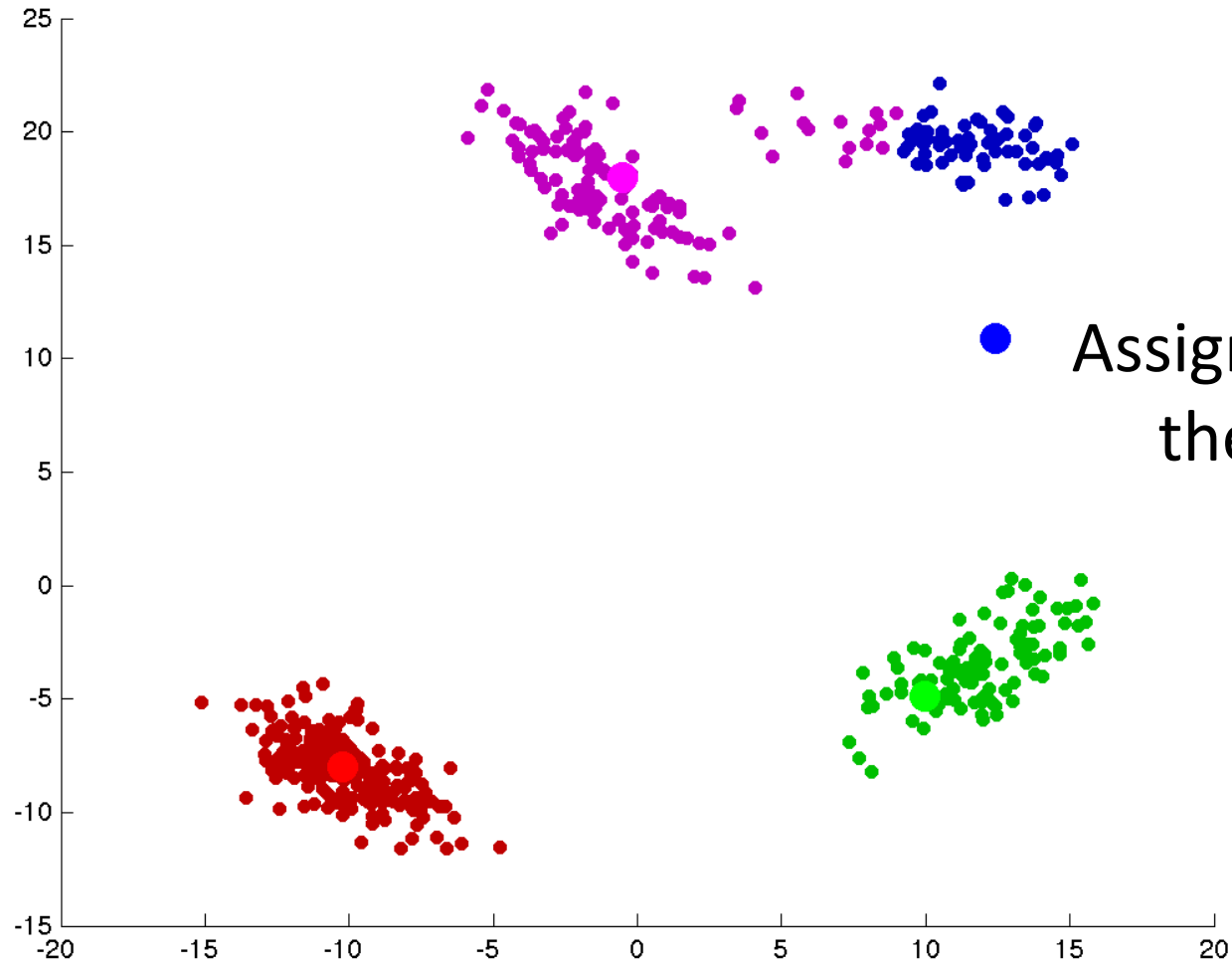


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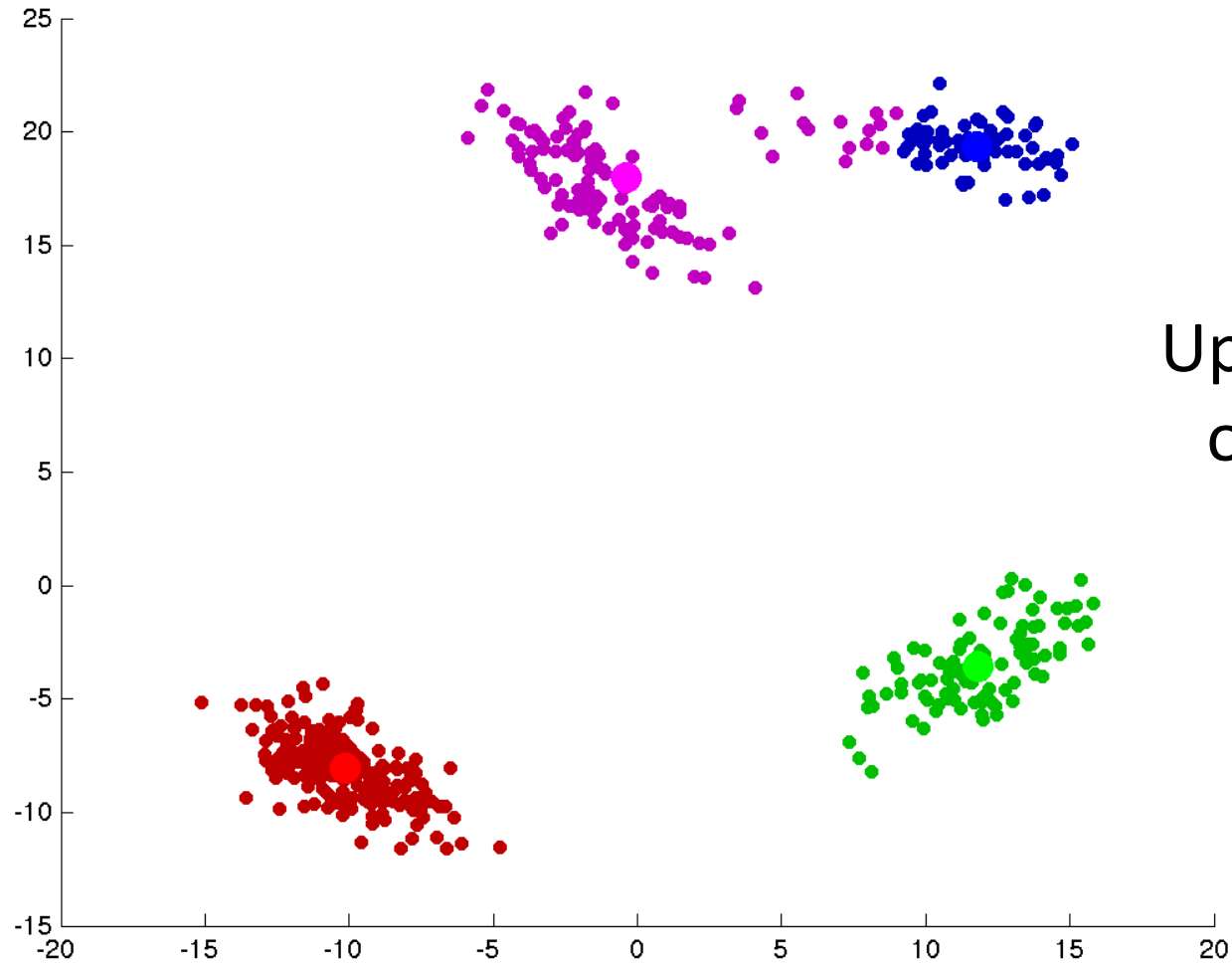
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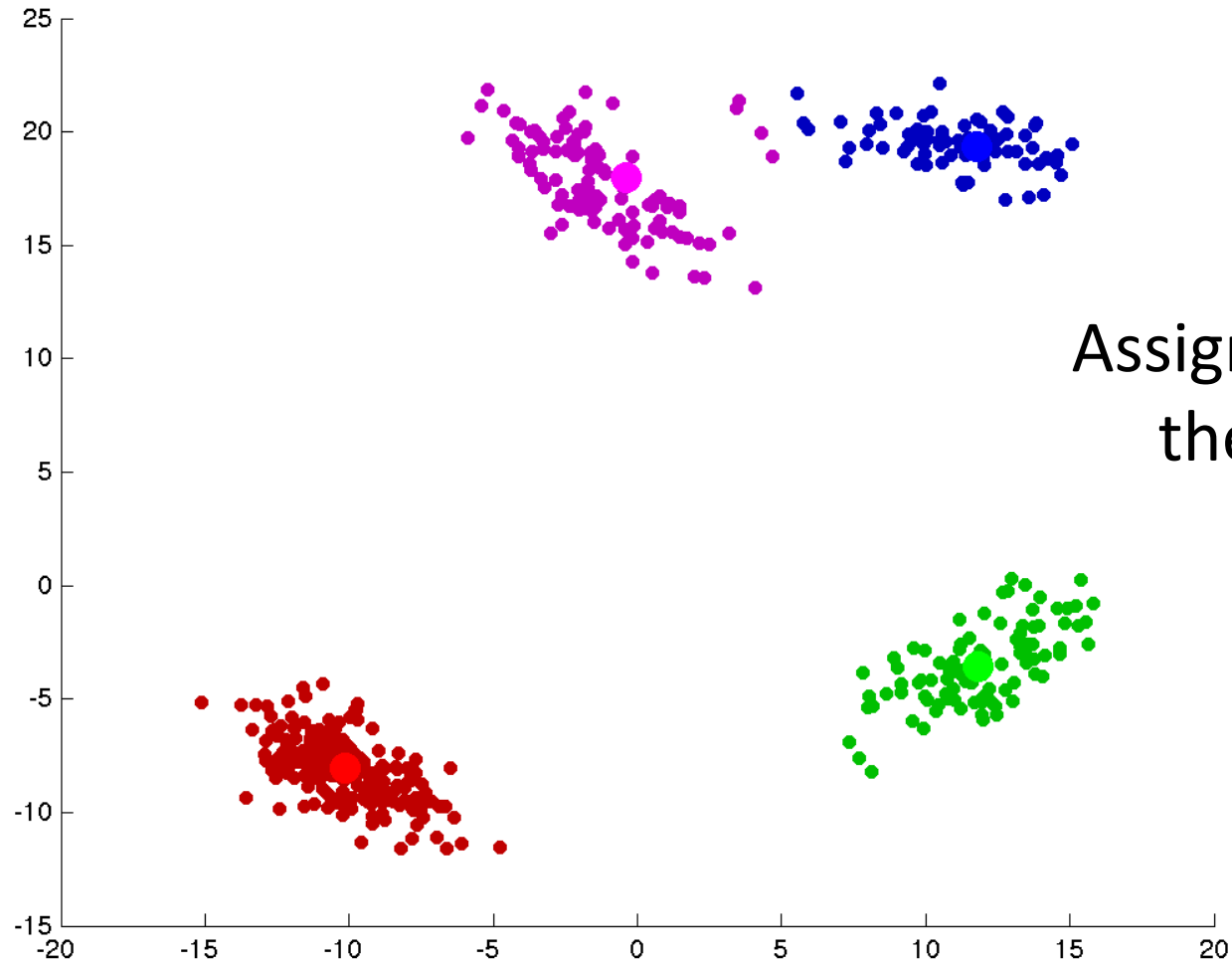


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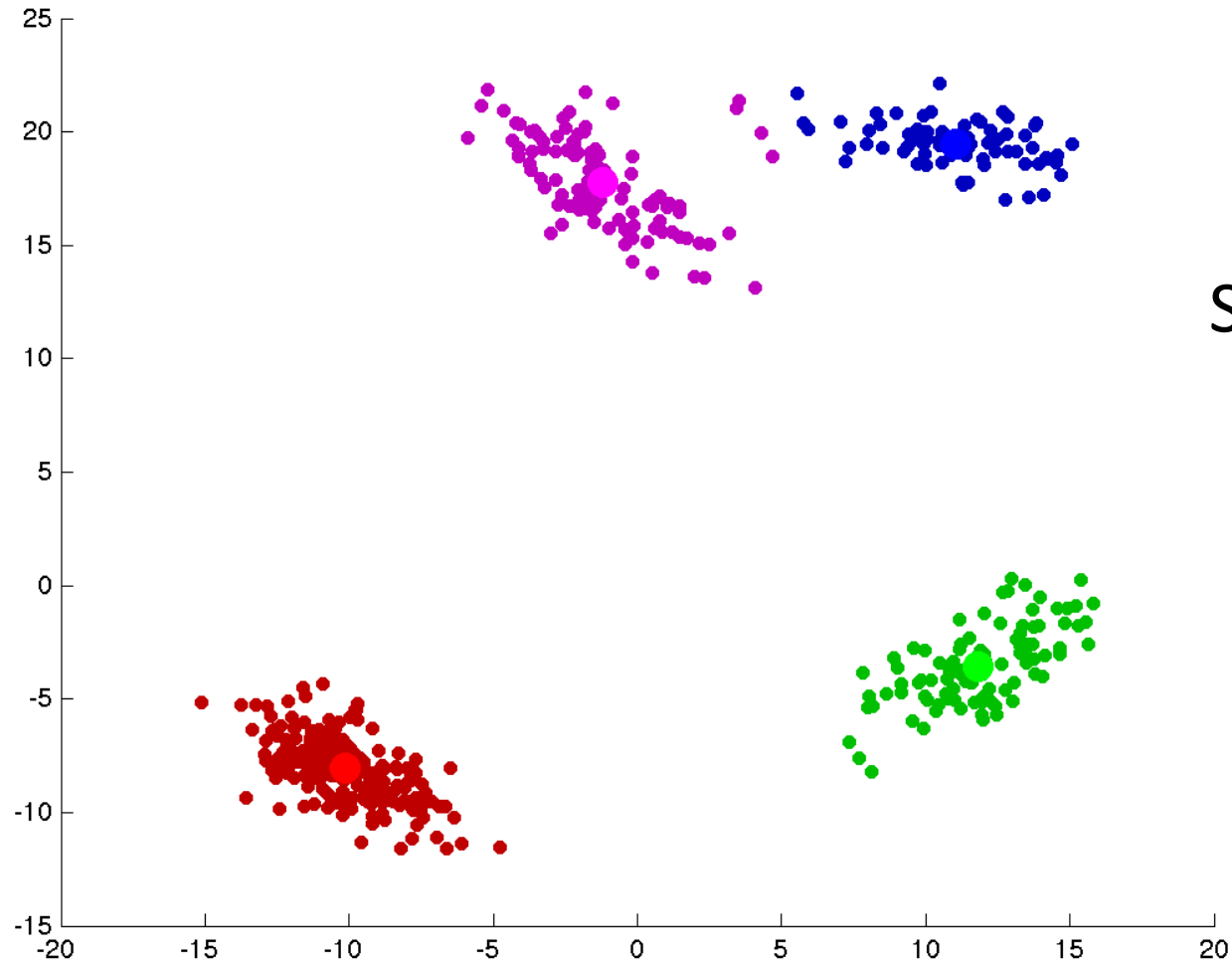


Assign each example to the closest mean.

K-Means Example

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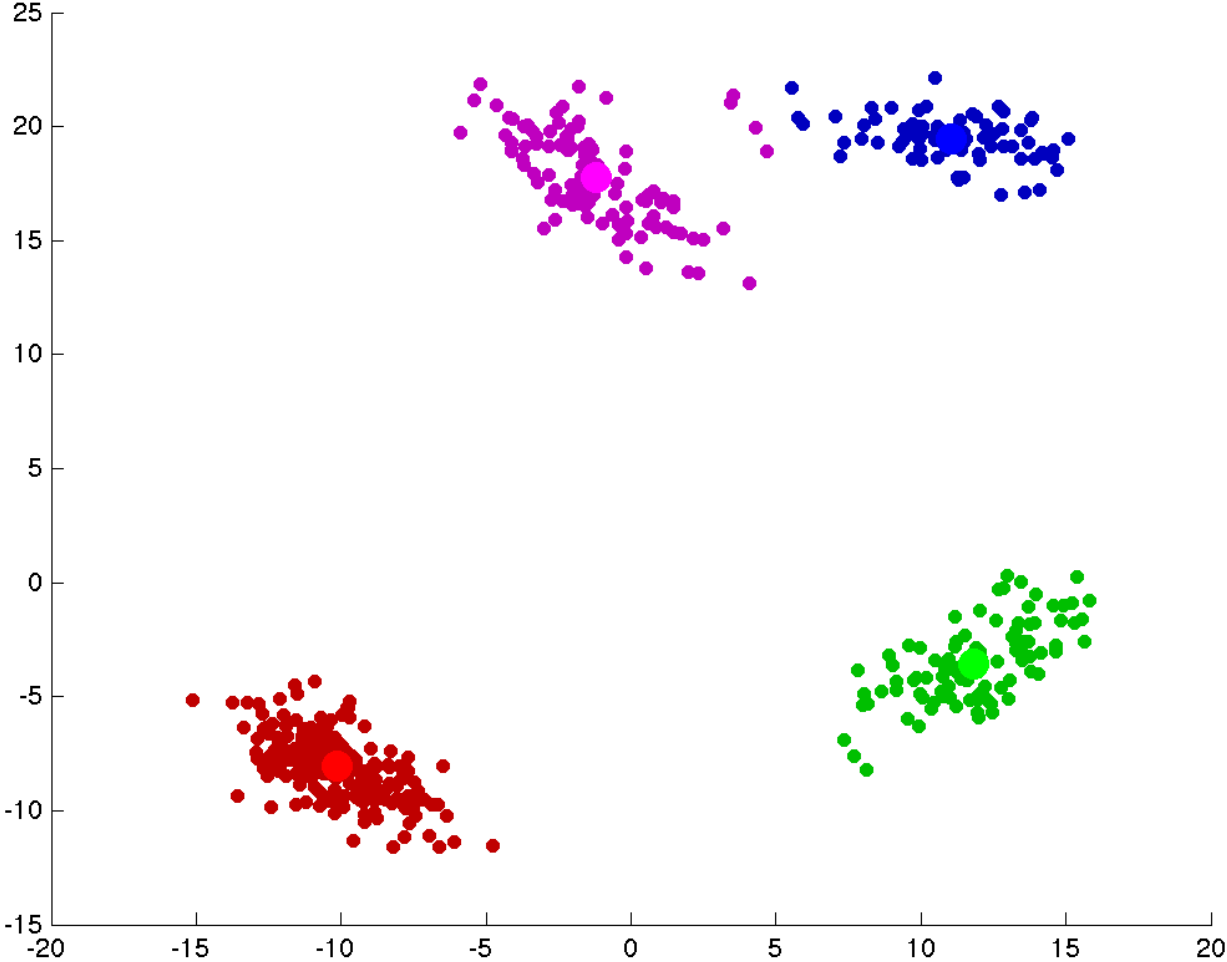


Stop if no examples change groups.

K-Means Example

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Output:

- Clusters ' \hat{y} '.
- Means ' W '.

$$\hat{y} = \begin{bmatrix} 2 \\ 2 \\ 3 \\ 3 \\ 1 \\ \vdots \end{bmatrix}$$

$$W = \begin{bmatrix} -1.2 & 17.8 \\ -10.2 & -8.0 \\ 11.0 & 19.5 \\ 11.8 & -3.6 \end{bmatrix}$$

Handwritten green annotations: a bracket on the right side of the matrix labeled 'k', and a bracket below the matrix labeled 'd'.

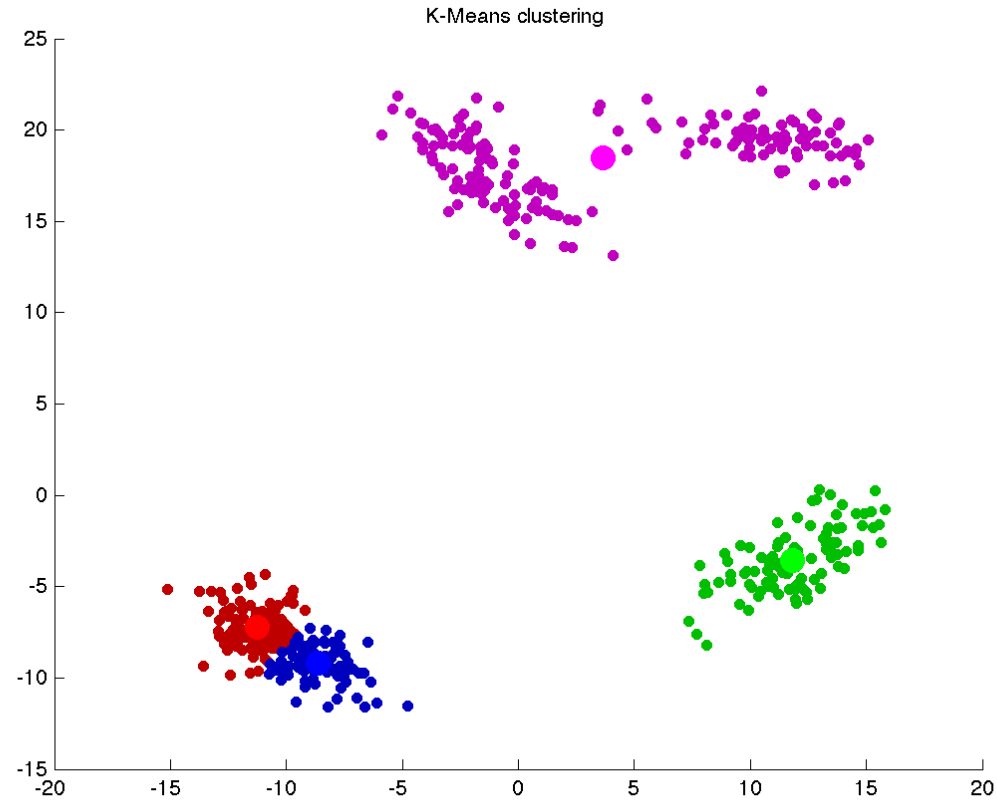
Interactive demo:

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

K-Means Issues

- **Guaranteed to converge** when using Euclidean distance.
- Given a new test example:
 - **Assign it to the nearest mean** to cluster it.
- Assumes you **know number of clusters 'k'**.
 - Lots of heuristics to pick 'k', none satisfying:
 - https://en.wikipedia.org/wiki/Determining_the_number_of_clusters_in_a_data_set
- Each example is assigned to **one (and only one) cluster**:
 - No possibility for overlapping clusters or leaving examples unassigned.
- It may converge to **sub-optimal solution...**

K-Means Clustering with Different Initialization



- Classic approach to dealing with sensitivity to initialization: [random restarts](#).
 - Try several different random starting points, choose the “best”.
- See bonus slides for a more clever approach called k-means++.

KNN vs. K-Means

- Don't confuse KNN classification and k-means clustering:

Property	KNN Classification	K-Means Clustering
Task	Supervised learning (given y_i)	Unsupervised learning (no given y_i).
Meaning of 'k'	Number of neighbours to consider (not number of classes).	Number of clusters (always consider single nearest mean).
Initialization	No training phase.	Training that is sensitive to initialization.
Model complexity	Model is complicated for small 'k', simple for large 'k'.	Model is simple for small 'k', complicated for large 'k'.
Parametric?	Non-parametric: - Stores data 'X'	Parametric (for 'k' not depending on 'n') - Stores means 'W'

What is K-Means Doing?

- We can interpret K-means steps as minimizing an objective:
 - Total sum of squared distances from example x_i to their centers $w_{\hat{y}_i}$:

$$f(w_1, w_2, \dots, w_k, \hat{y}_1, \hat{y}_2, \dots, \hat{y}_n) = \sum_{i=1}^n \|w_{\hat{y}_i} - x_i\|^2$$

- The k-means steps:
 - Minimize 'f' in terms of the \hat{y}_i (update cluster assignments).
 - Minimize 'f' in terms of the w_c (update means).

- Termination of the algorithm follows because:
 - Each step does not increase the objective.
 - There are a finite number of assignments to k clusters.

Cluster of example 'i',
 $\hat{y}_i \in \{1, 2, \dots, k\}$

$$W = \begin{bmatrix} \text{---} w_1 \text{---} \\ \text{---} w_2 \text{---} \\ \vdots \\ \text{---} w_k \text{---} \end{bmatrix} \left. \vphantom{\begin{bmatrix} \text{---} w_1 \text{---} \\ \text{---} w_2 \text{---} \\ \vdots \\ \text{---} w_k \text{---} \end{bmatrix}} \right\}^k$$

d

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- The k-means steps:
 - Minimize 'f' in terms of the \hat{y}_i (update cluster assignments).
 - Minimize 'f' in terms of the w_c (update means).

- Use 'f' to choose between initializations (fixed 'k').
- Need to change w_c update under other distances:
 - L1-norm: set w_c to median ("k-medians", see bonus).

Cluster of example 'i',
 $\hat{y}_i \in \{1, 2, \dots, k\}$

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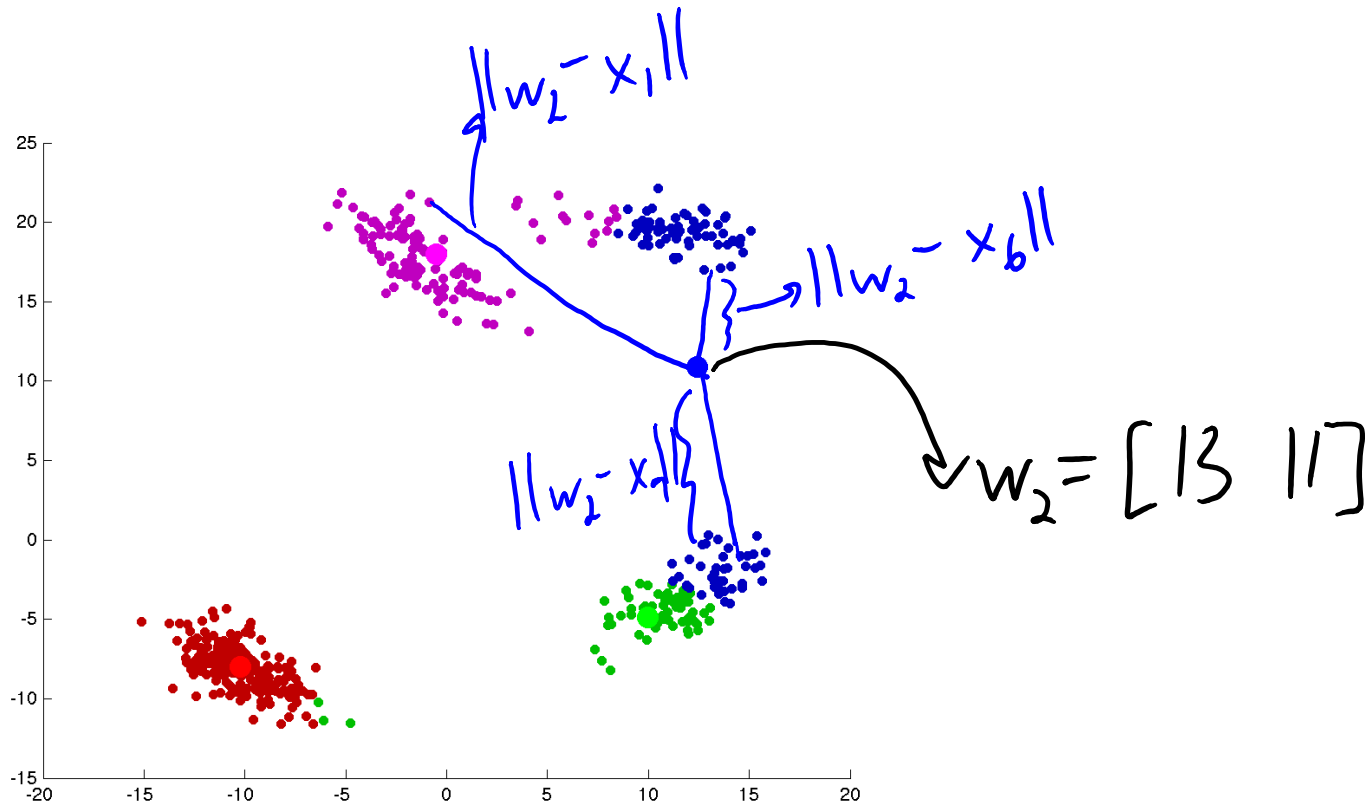
d

Cost of K-means

- Bottleneck is calculating distance from each x_i to each mean w_c :

$$\|w_c - x_i\|^2 = \sum_{j=1}^d (w_{cj} - x_{ij})^2$$

d-dimensional vector



Cost of K-means

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$$\|w_c - x_i\|^2 = \sum_{j=1}^d (w_{cj} - x_{ij})^2$$

d-dimensional vector

- Each time we do this costs $O(d)$.
- We need to compute distance from 'n' examples to 'k' clusters.
- Total cost of assigning examples to clusters is $O(ndk)$.
 - Fast if k is not too large.
- Updating means is cheaper: $O(nd)$.

– For each cluster 'c', compute $w_c = \frac{1}{n_c} \sum_{i \in C} x_i$

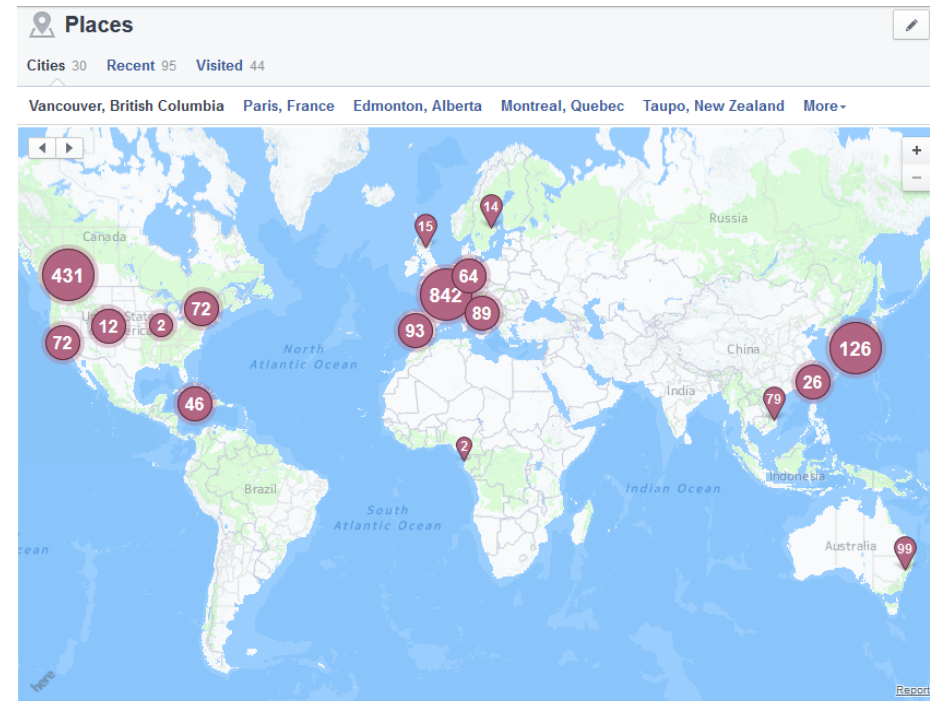
Object in cluster.

Loop over objects in cluster.

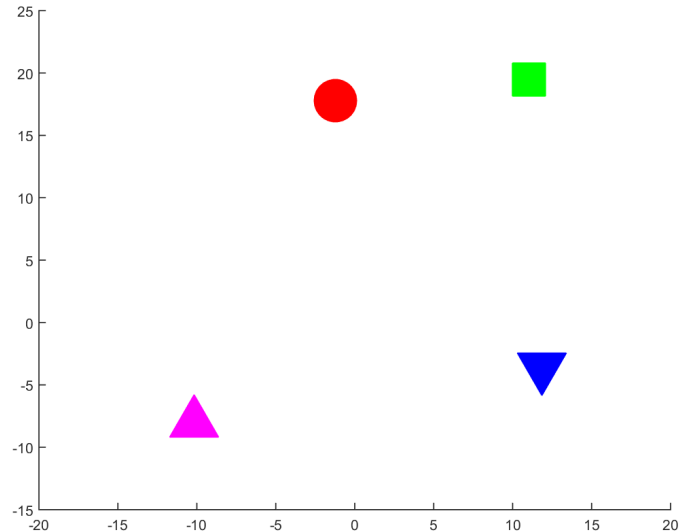
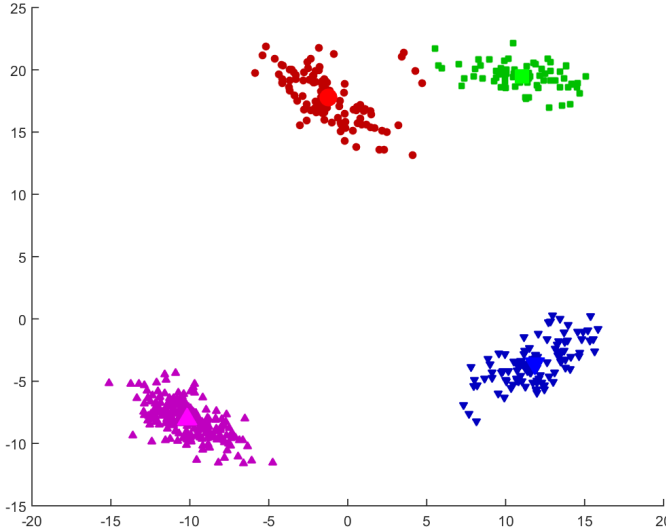
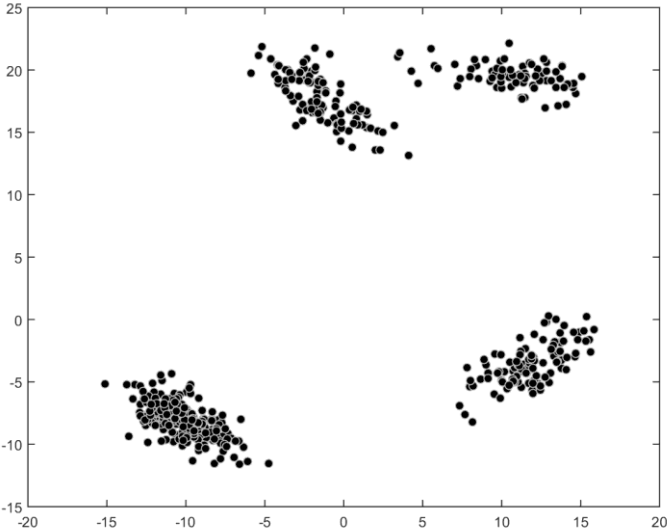
Number of objects in cluster 'c'

Vector Quantization

- K-means originally comes from signal processing.
- Designed for **vector quantization**:
 - Replace examples with the mean of their cluster (“prototype”).
- Example:
 - Facebook places: 1 location summarizes many.
 - What sizes of clothing should I make?



Vector Quantization



$n \times d$

$$X = \begin{bmatrix} -9.0 & -7.3 \\ -10.9 & -9.0 \\ 13.7 & 19.3 \\ 13.8 & 20.4 \\ 12.8 & 20.6 \\ \vdots & \vdots \end{bmatrix}$$

Run k-means

$k \times d$

$$W = \begin{bmatrix} -1.2 & 17.8 \\ -10.2 & -8.0 \\ 11.0 & 19.5 \\ 11.8 & -3.6 \end{bmatrix}$$

$n \times 1$

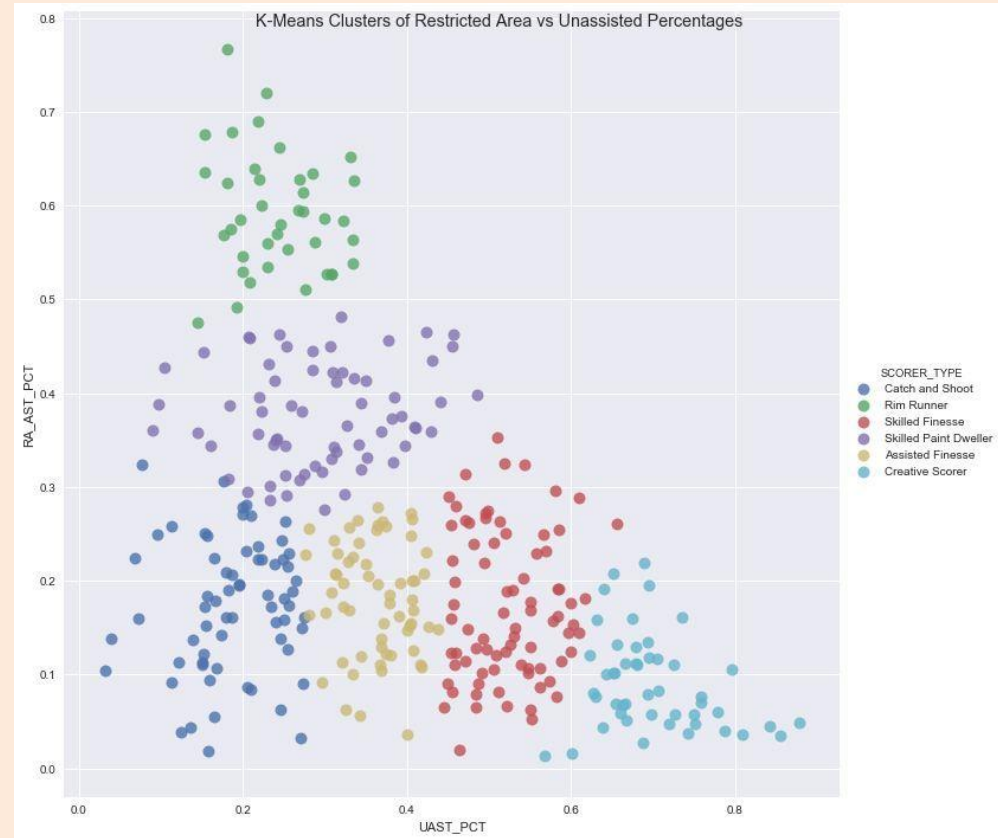
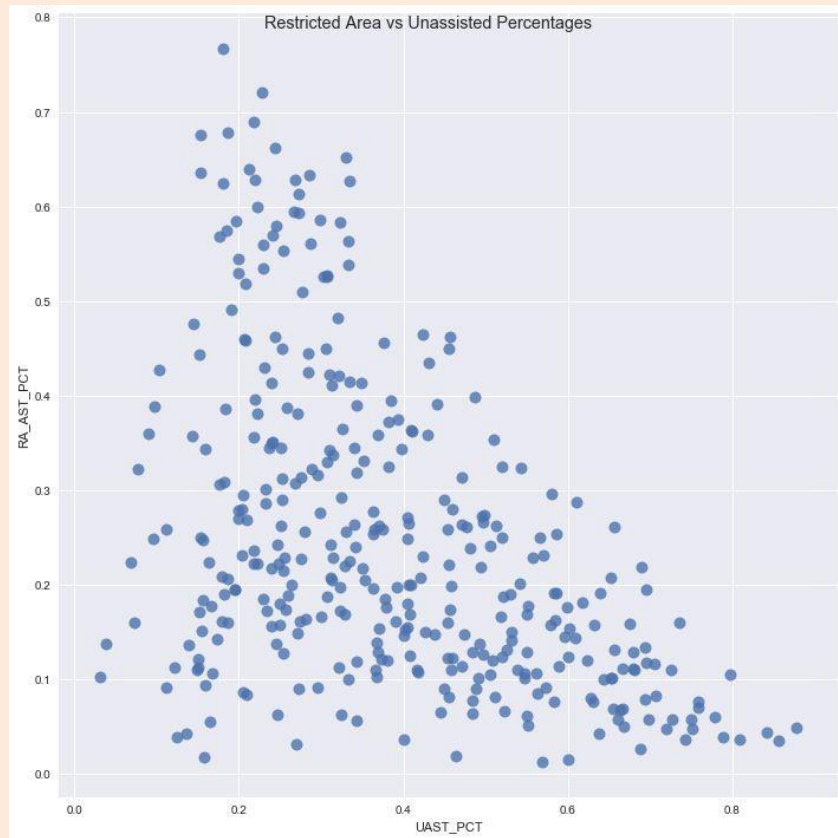
$$\hat{y} = \begin{bmatrix} 2 \\ 2 \\ 3 \\ 3 \\ 1 \\ \vdots \end{bmatrix}$$

Approximate objects with means.

$$\hat{X} = \begin{bmatrix} -10.2 & -8.0 \\ -10.2 & -8.0 \\ 11.0 & 19.5 \\ 11.0 & 19.5 \\ -1.2 & 17.8 \\ \vdots & \vdots \end{bmatrix}$$

Vector Quantization for Basketball Players

- Clustering NBA basketball players based on shot type/percentage:



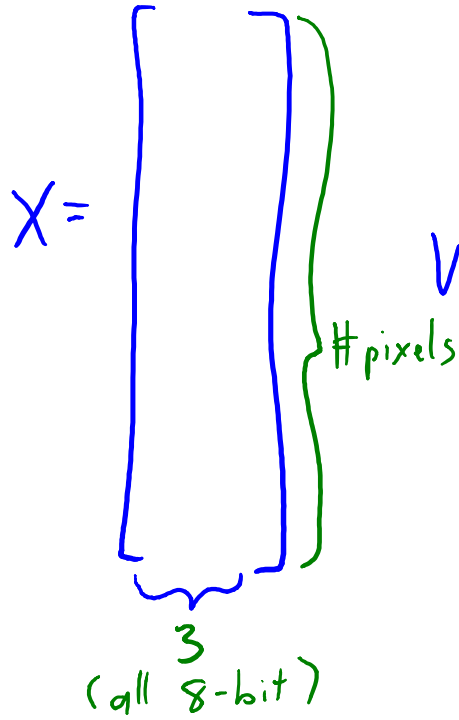
- The “prototypes” represent offensive styles (like “catch and shoot”).

Vector Quantization: Image Colors

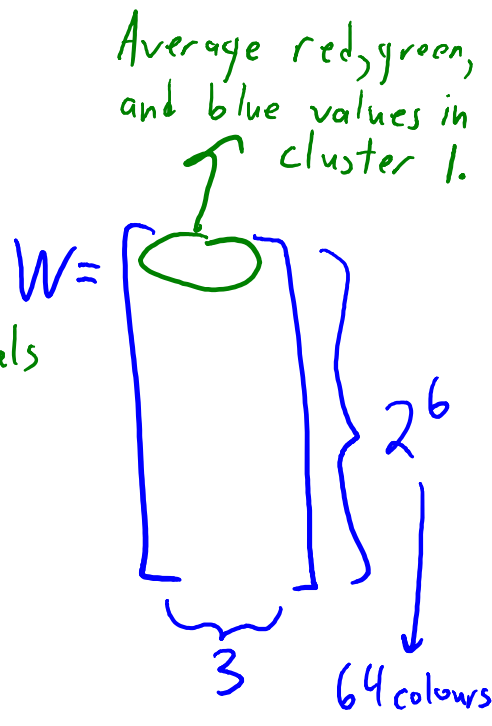
- Usual RGB representation of a pixel's color: three 8-bit numbers.
 - For example, [241 13 50] = ■.
 - Can apply k-means to find set of prototype colours.



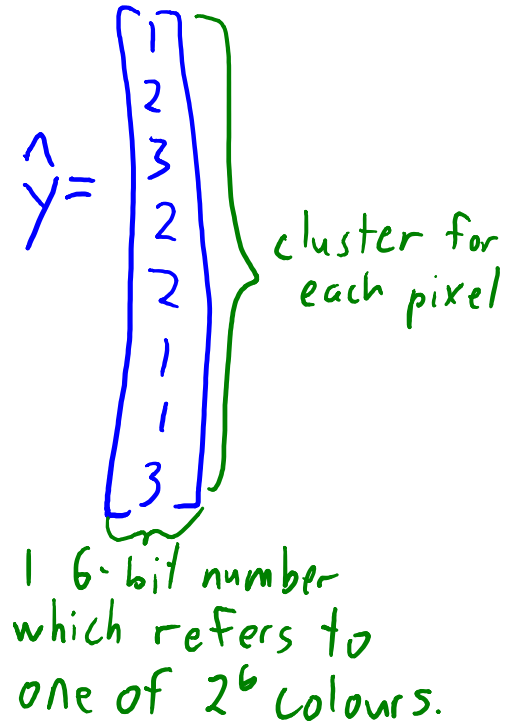
Original:
(24-bits/pixel)



Run k-means with
 2^6 clusters:



K-means predictions:
(6-bits/pixel)

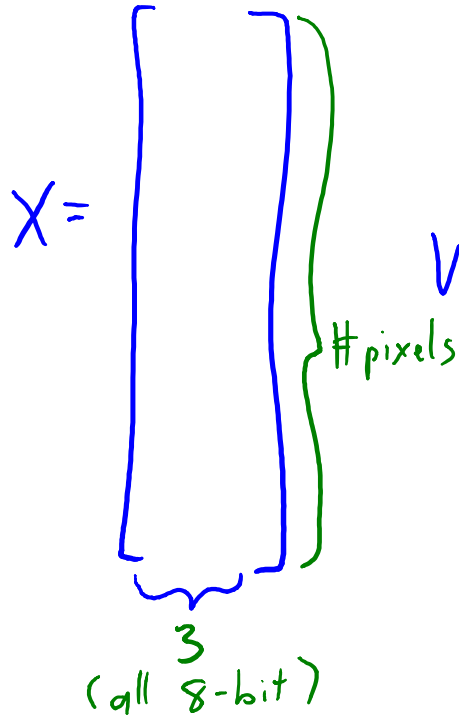


Vector Quantization: Image Colors

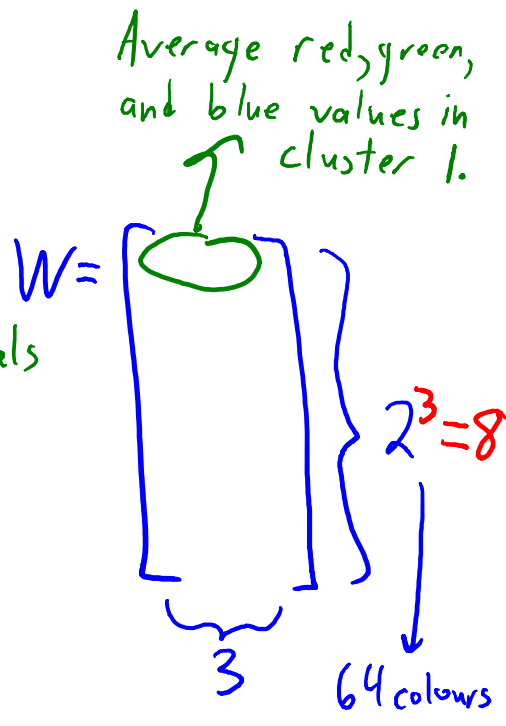
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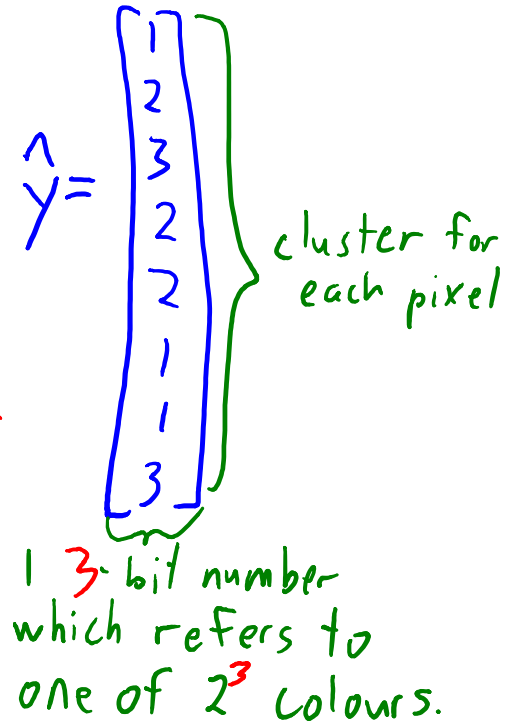
Original:
(24-bits/pixel)



Run k-means with
 2^6 clusters:



K-means predictions:
(3-bits/pixel)

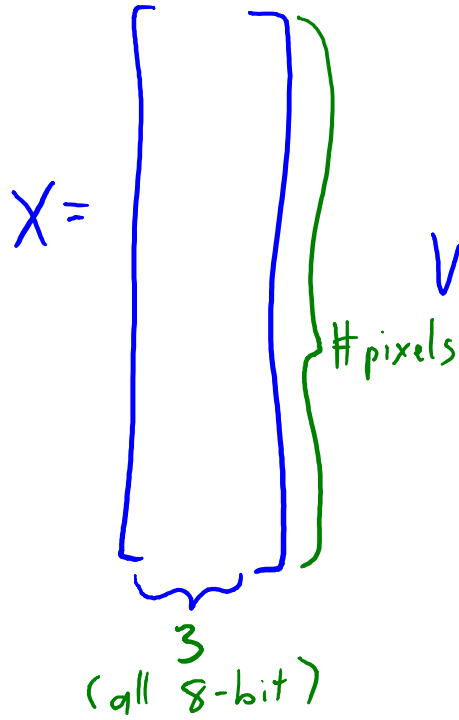


Vector Quantization: Image Colors

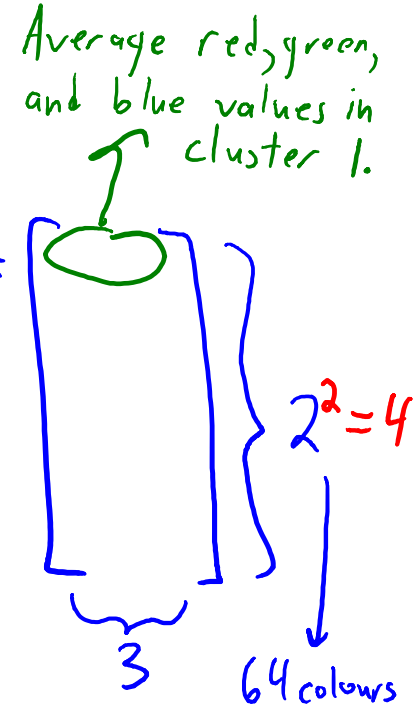
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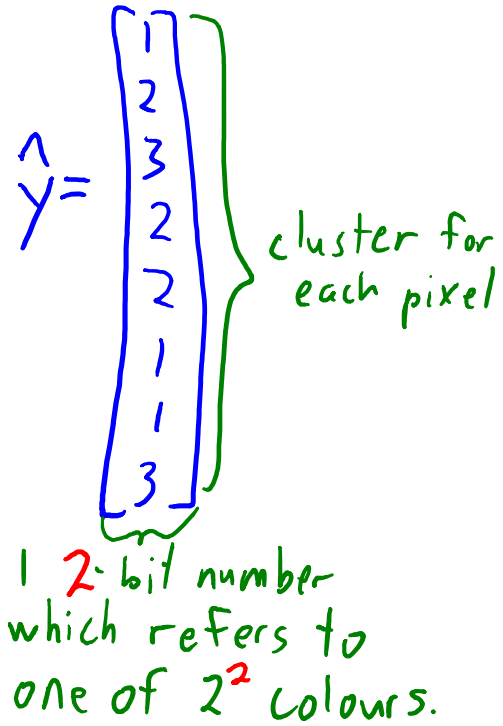
Original:
(24-bits/pixel)



Run k-means with
 2^6 clusters:



K-means predictions:
(2-bits/pixel)

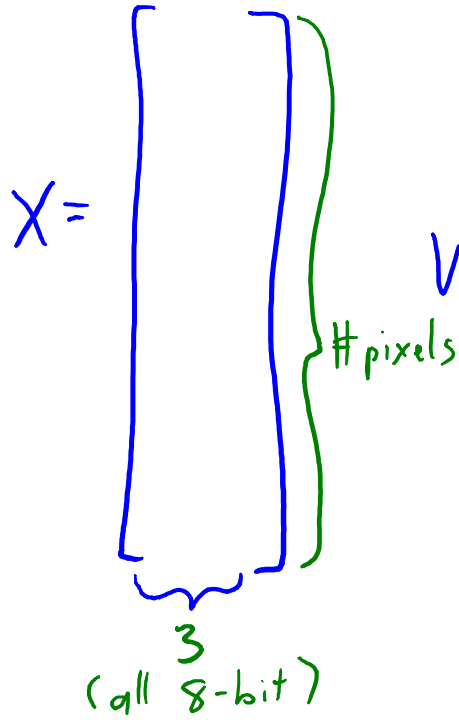


Vector Quantization: Image Colors

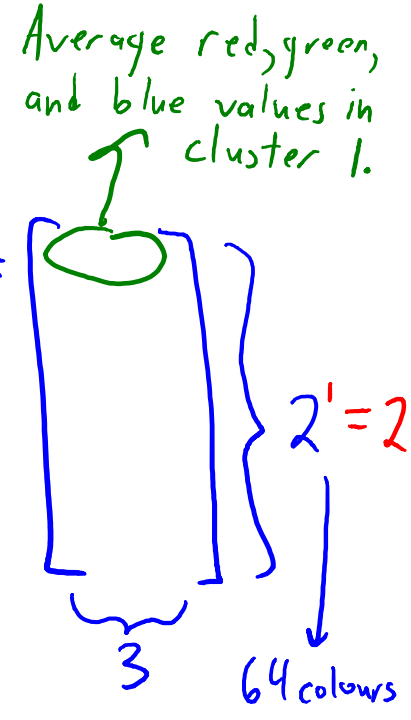
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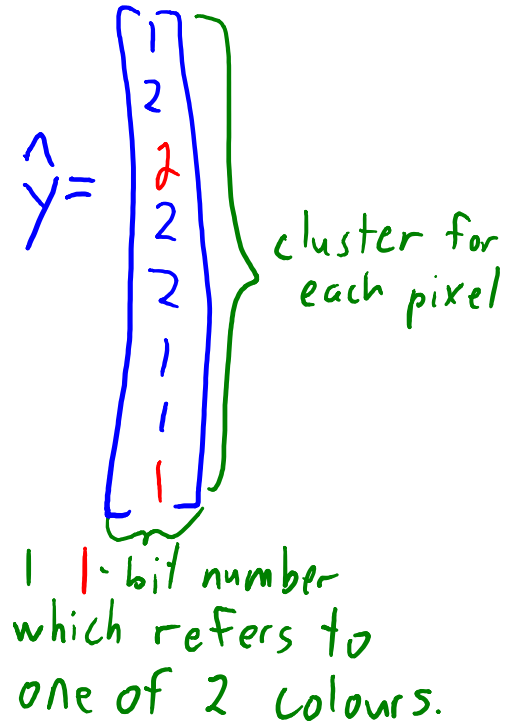
Original:
(24-bits/pixel)



Run k-means with
 2^6 clusters:



K-means predictions:
(1-bit/pixel)



Summary

- **Unsupervised learning**: fitting data without explicit labels.
- **Clustering**: finding 'groups' of related examples.
- **K-means**: simple iterative clustering strategy.
 - Fast but sensitive to initialization.
- **Vector quantization**:
 - Compressing examples by replacing them with the mean of their cluster.
- **Next time**:
 - John Snow and non-parametric clustering.

What is K-Means Doing?

- How are are k-means step decreasing this objective?

$$f(w_1, w_2, \dots, w_k, \hat{y}_1, \hat{y}_2, \dots, \hat{y}_n) = \sum_{i=1}^n \|w_{\hat{y}_i} - x_i\|^2$$

- If we just write as function of a particular \hat{y}_i , we get:

$$f(\hat{y}_i) = \|w_{\hat{y}_i} - x_i\|^2 + (\text{constant})$$

- The “constant” includes all other terms, and doesn’t affect location of min.
- We can minimize in terms of \hat{y}_i by setting it to the ‘c’ with w_c closest to x_i .

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- How are are k-means step decreasing this objective?

$$f(w_1, w_2, \dots, w_k, \hat{y}_1, \hat{y}_2, \dots, \hat{y}_n) = \sum_{i=1}^n \|w_{\hat{y}_i} - x_i\|^2$$

- If we just write as function of a particular w_{c_j} we get:

$$f(w_{c_j}) = \sum_{i \in C_j} \sum_{j=1}^d (w_{c_j} - x_{ij})^2 + (\text{constant})$$

$\underbrace{\hspace{10em}}_{\text{set of examples with } \hat{y}_i = c}$

- Derivative is given by: $f'(w_{c_j}) = 2 \sum_{i \in C_j} (w_{c_j} - x_{ij})$

- Setting equal to 0 and solving for w_{c_j} gives: $\sum_{i \in C_j} w_{c_j} = \sum_{i \in C_j} x_{ij}$ or $w_{c_j} * n_{c_j} = \sum_{i \in C_j} x_{ij}$
or $w_{c_j} = \frac{1}{n_{c_j}} \sum_{i \in C_j} x_{ij}$

K-Medians Clustering

- With **other distances k-means may not converge.**
 - But we can **make it converge by changing the updates** so that they are minimizing an objective function.
- E.g., we can use the L1-norm objective: $\sum_{i=1}^n \|w_{y_i} - x_i\|_1$
- Minimizing the L1-norm objective gives the ‘k-medians’ algorithm:
 - Assign points to clusters by finding “mean” with smallest L1-norm distance.
 - Update ‘means’ as median value (dimension-wise) of each cluster.
 - This minimizes the L1-norm distance to all the points in the cluster.
- This approach is more robust to outliers.


↑ k-means will put a cluster here.



What is the “L1-norm and median” connection?

- Point that minimizes the sum of squared L2-norms to all points:

$$f(w) = \sum_{i=1}^n \|w - x_i\|^2$$

- Is given by the **mean** (just take derivative and set to 0):

$$w = \frac{1}{n} \sum_{i=1}^n x_i$$

- Point that minimizes the sum of L1-norms to all all points:

$$f(w) = \sum_{i=1}^n \|w - x_i\|_1$$

- Is given by the **median** (derivative of absolute value is +1 if positive and -1 if negative, so any point with half of points larger and half of points smaller is a solution).

K-Medoids Clustering

- A disadvantage of k-means in some applications:
 - The **means might not be valid data** points.
 - May be important for vector quantization.
- E.g., consider bag of words features like $[0,0,1,1,0]$.
 - We have words 3 and 4 in the document.
- A mean from k-means might look like $[0.1\ 0.3\ 0.8\ 0.2\ 0.3]$.
 - What does it mean to have 0.3 of word 2 in a document?
- Alternative to k-means is **k-medoids**:
 - Same algorithm as k-means, except the means must be data points.
 - Update the means by finding example in cluster minimizing squared L2-norm distance to all points in the cluster.

K-Means Initialization

- K-means is fast but **sensitive to initialization**.
- Classic approach to initialization: **random restarts**.
 - Run to convergence using different random initializations.
 - Choose the one that minimizes average squared distance of data to means.
- Newer approach: **k-means++**
 - Random initialization that **prefers means that are far apart**.
 - Yields **provable bounds** on expected approximation ratio.

K-Means++

- Steps of **k-means++**:

1. Select initial mean w_1 as a **random x_i** .

2. **Compute distance d_{ic}** of each example x_i to each mean w_c .

$$d_{ic} = \sqrt{\sum_{j=1}^d (x_{ij} - w_{cj})^2} = \|x_i - w_c\|_2$$

3. For each example 'i' **set d_i to the distance to the closest mean.**

$$d_i = \min_c \{d_{ic}\}$$

4. Choose next mean by **sampling an example 'i' proportional to $(d_i)^2$.**

$$p_i \propto d_i^2 \Rightarrow p_i = \frac{d_i^2}{\sum_{j=1}^n d_j^2}$$

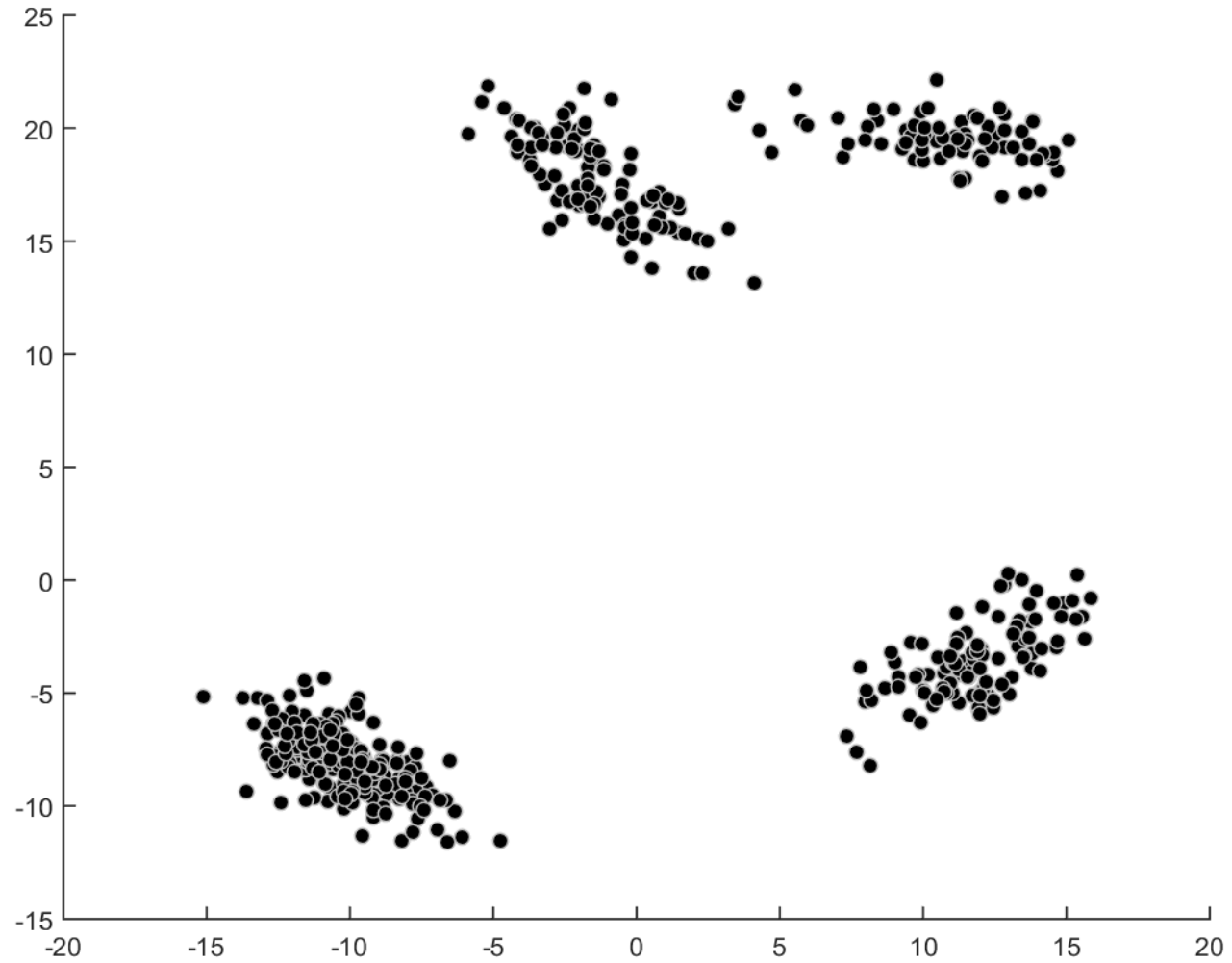
5. Keep returning to step 2 until we have k-means.

- Expected approximation ratio is $O(\log(k))$.

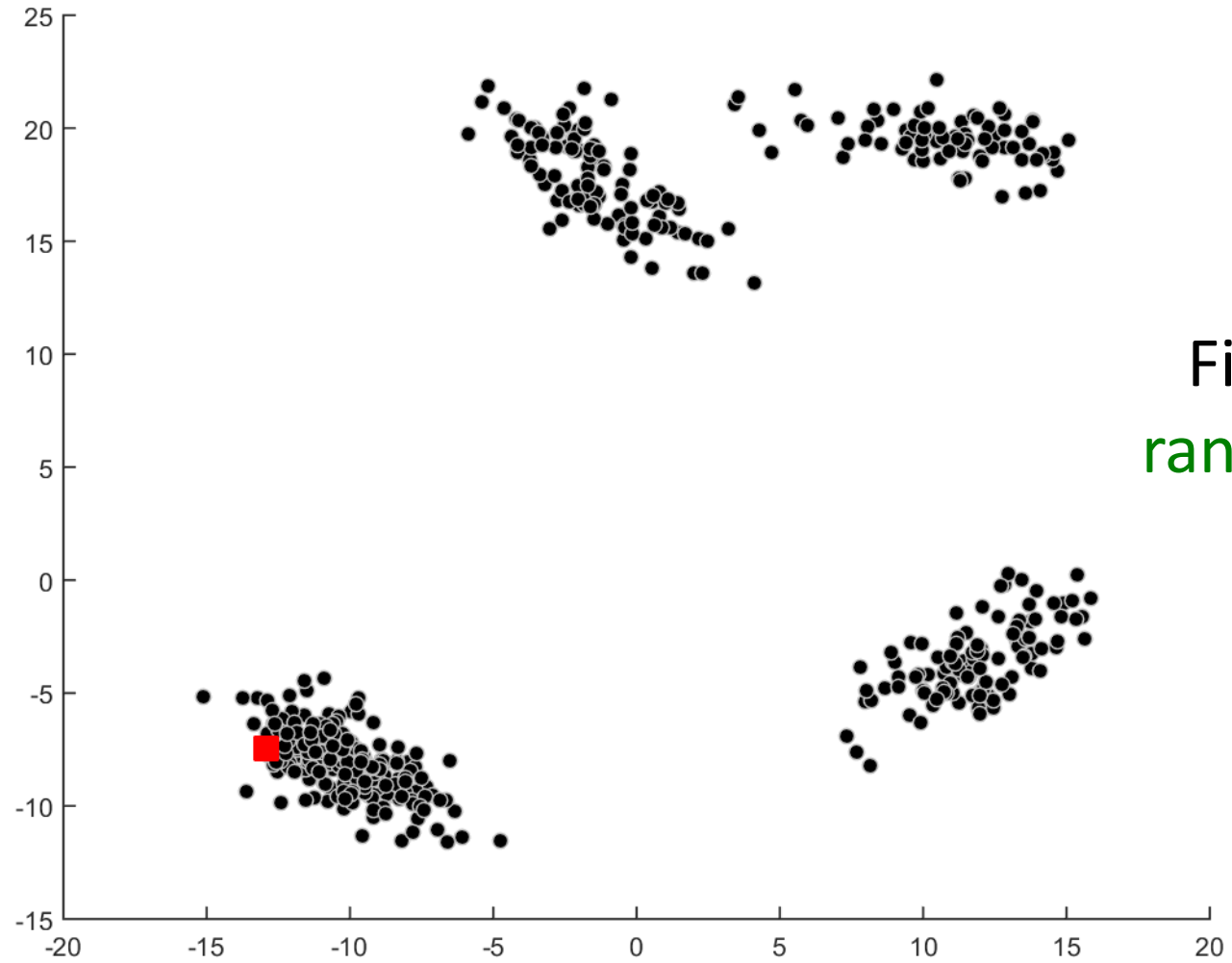
Can be
done in
 $O(n)$.

"probability that we
choose x_i as next mean"

K-Means++

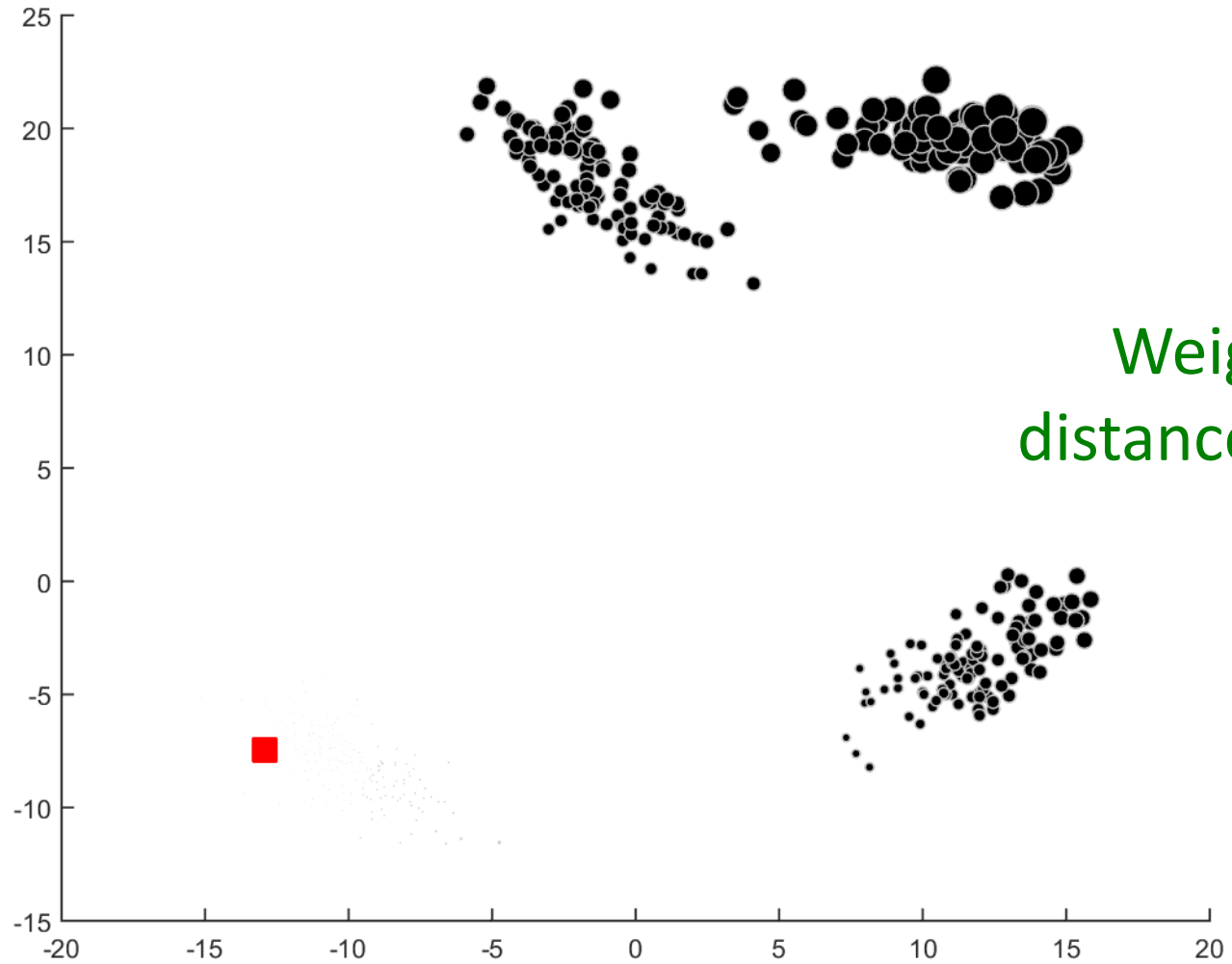


K-Means++



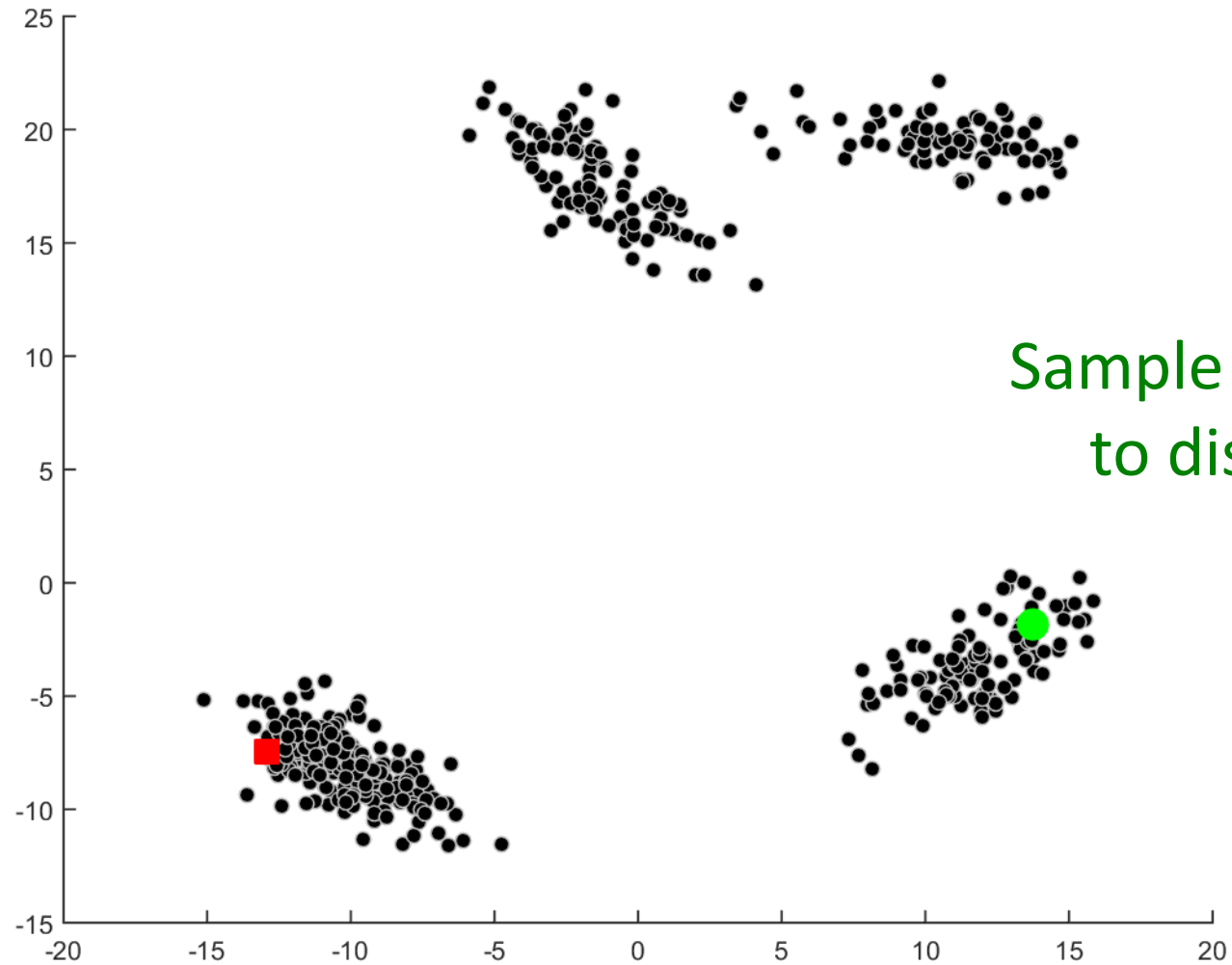
First mean is a
random example.

K-Means++



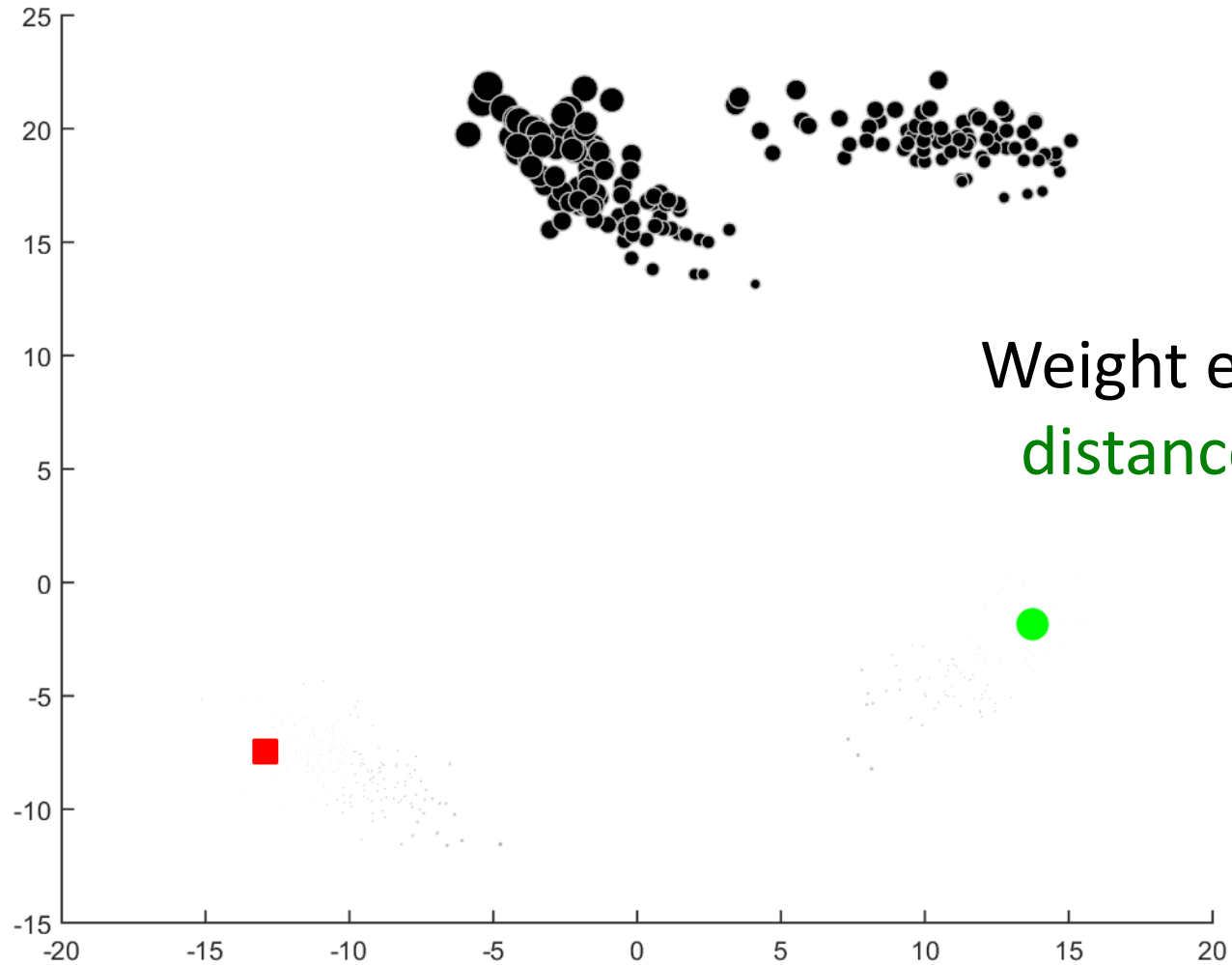
Weight examples by
distance to mean squared.

K-Means++



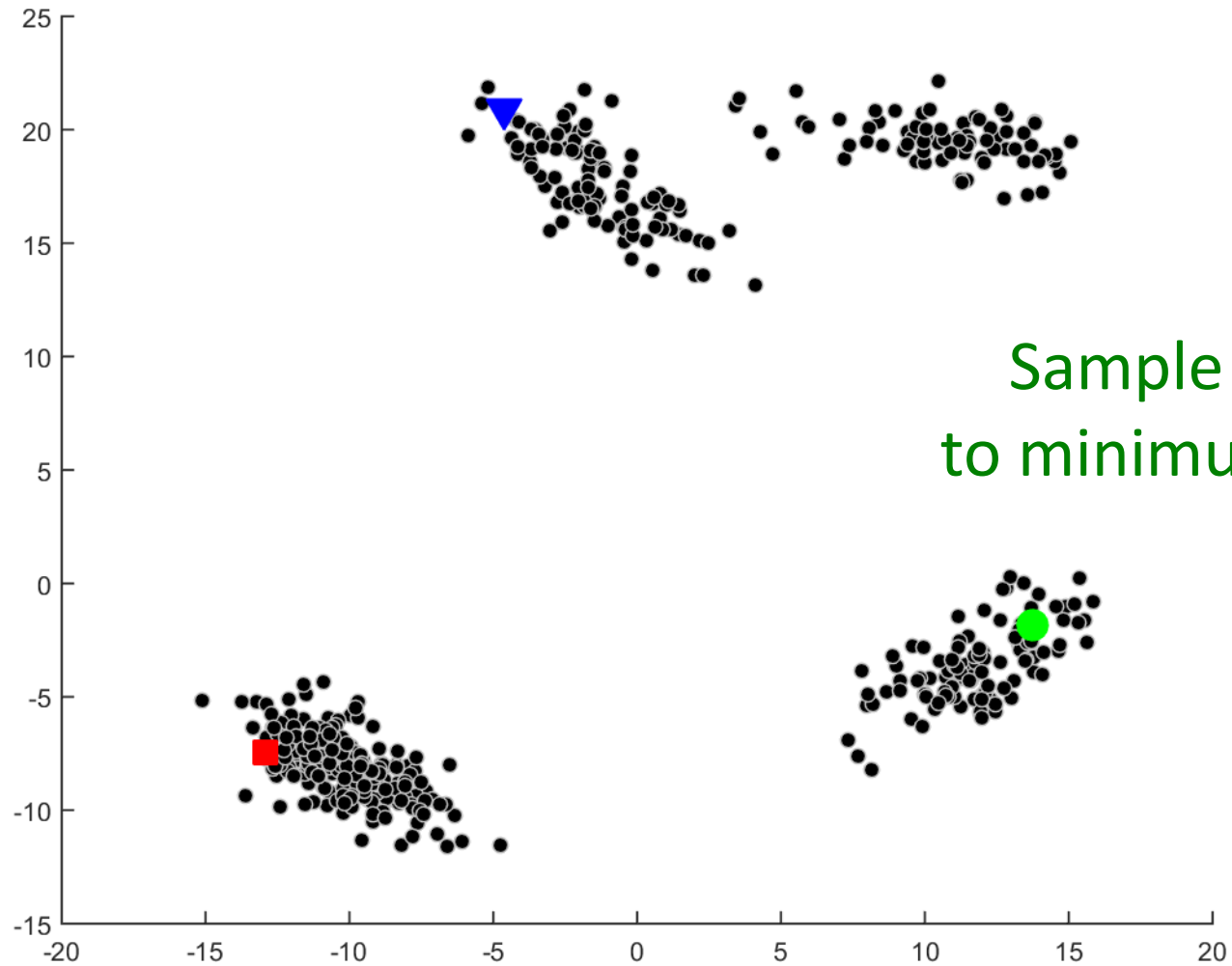
Sample mean proportional
to distances squared.

K-Means++



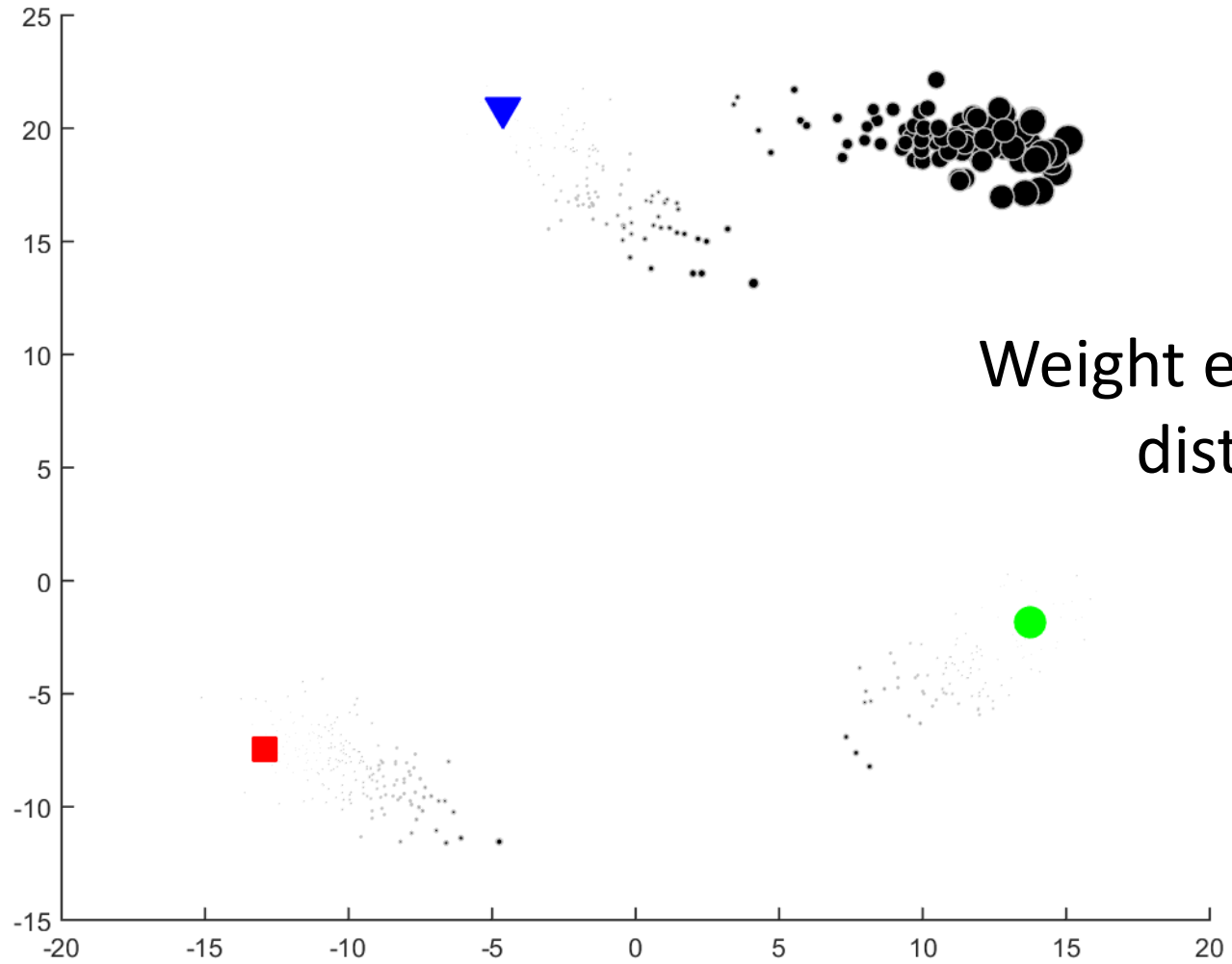
Weight examples by squared
distance to nearest mean.

K-Means++



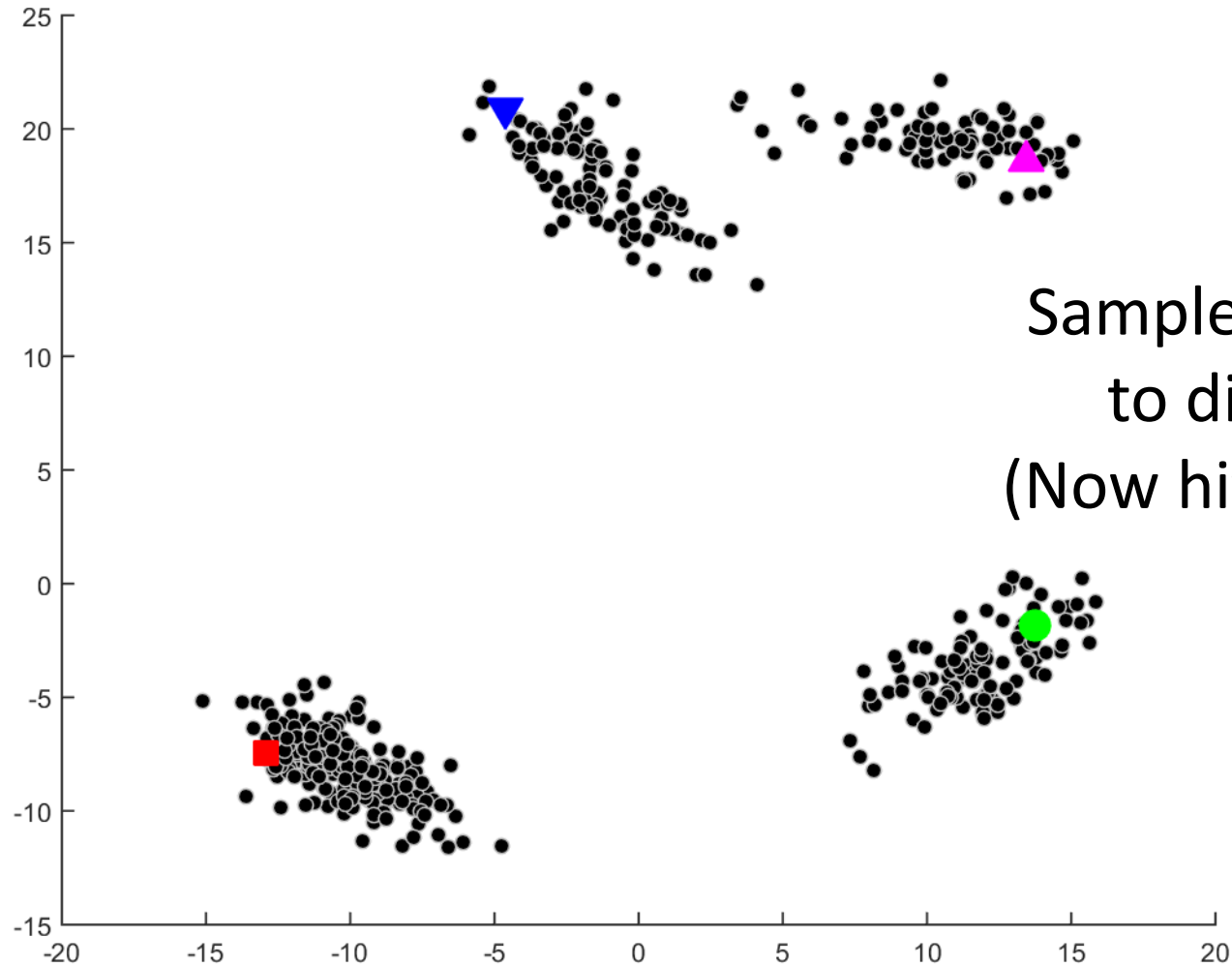
Sample mean proportional
to minimum distances squared

K-Means++



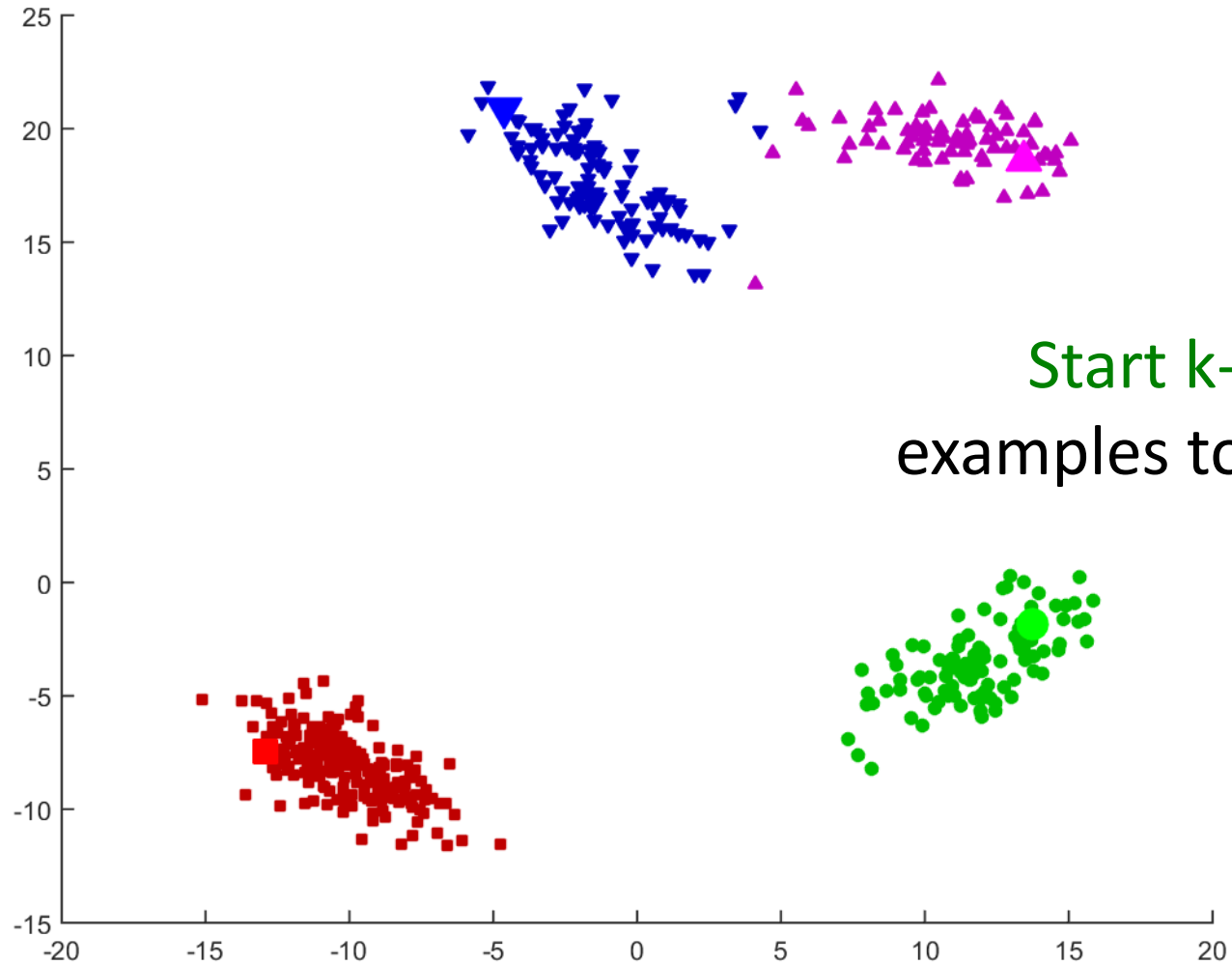
Weight examples by squared distance to mean.

K-Means++



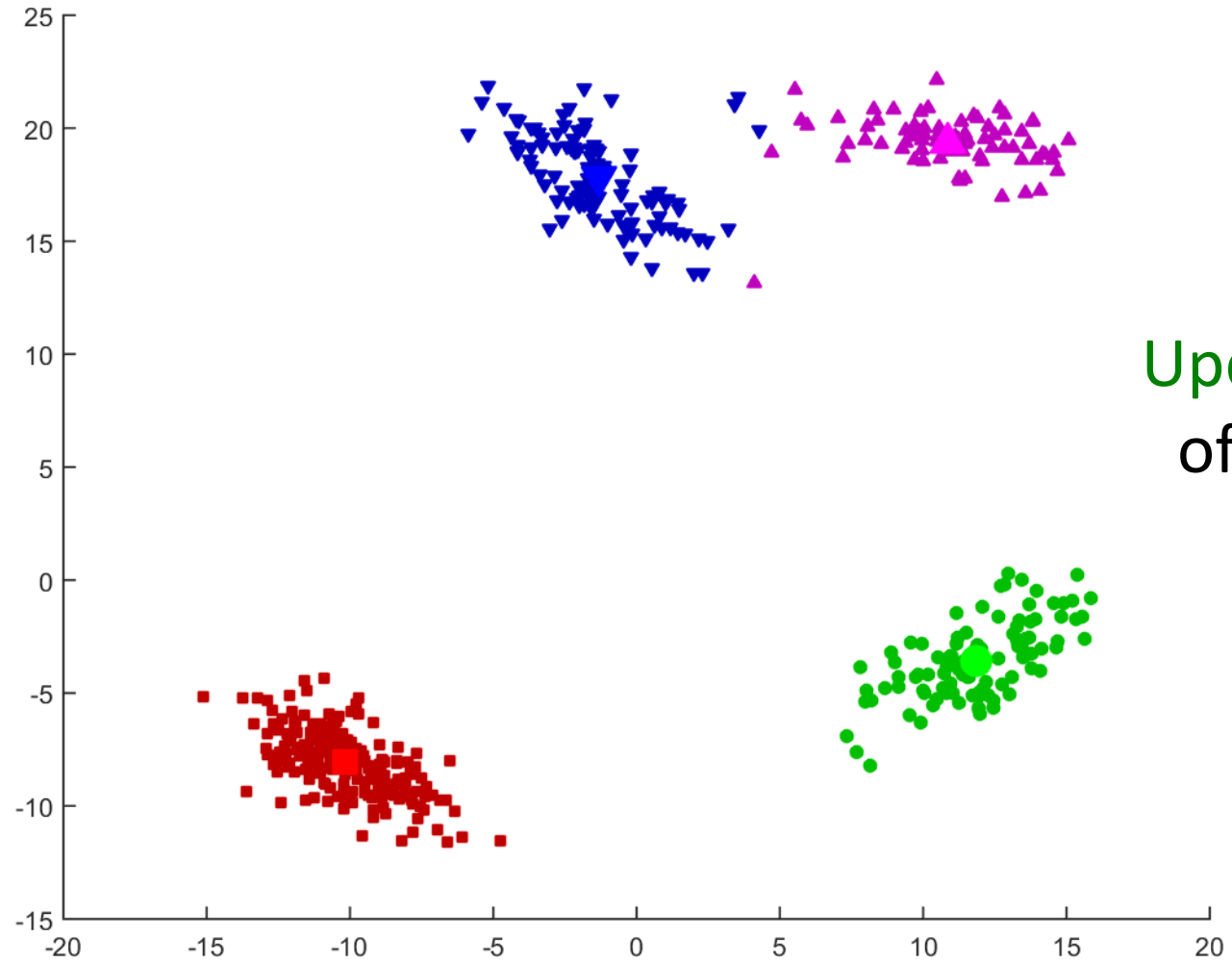
Sample mean proportional
to distances squared.
(Now hit chosen target $k=4$.)

K-Means++



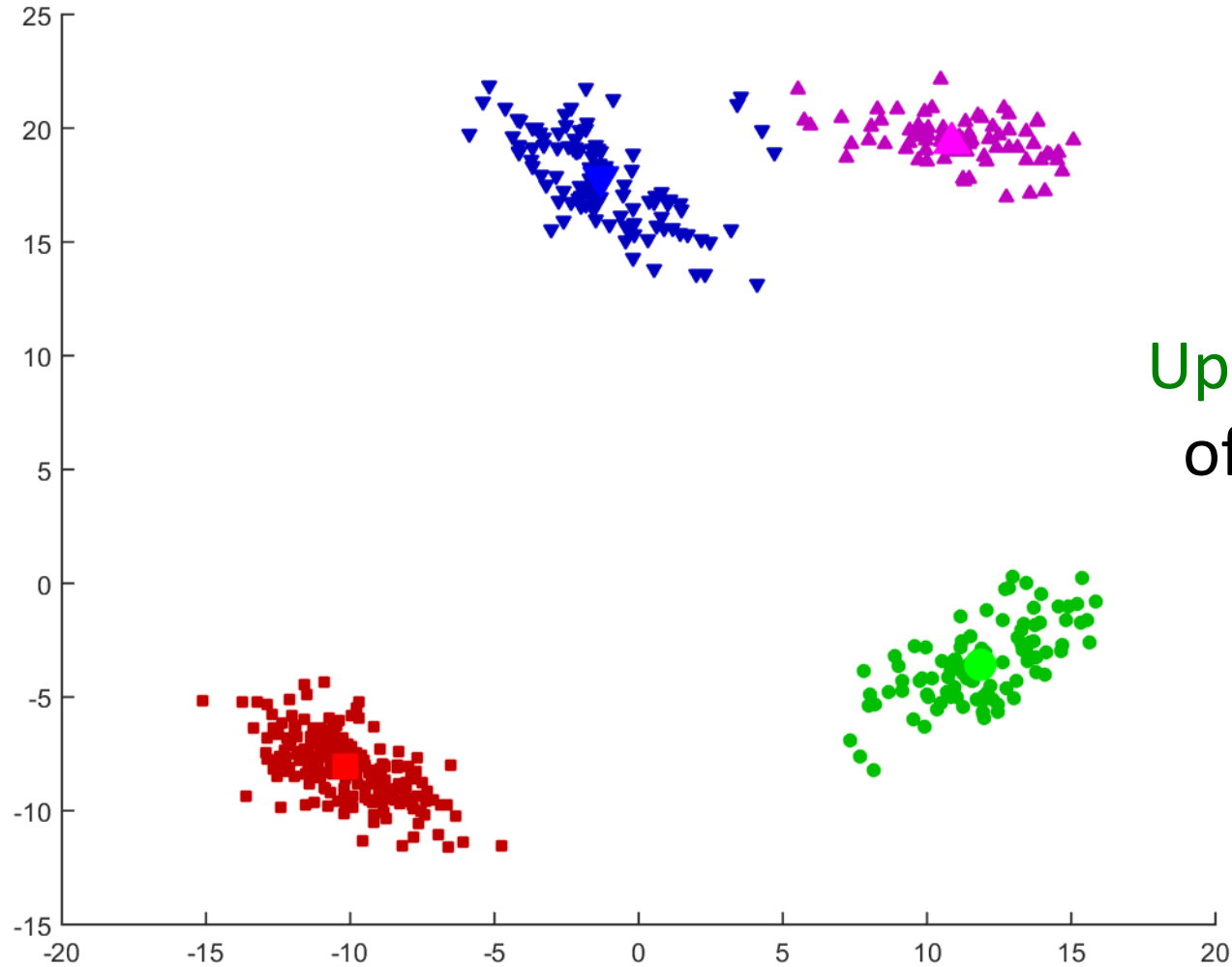
Start k-means: assign examples to the closest mean.

K-Means++



Update the mean
of each cluster.

K-Means++



Update the mean
of each cluster.

In this case: just 2 iterations!

Discussion of K-Means++

- Recall the objective function k-means tries to minimize:

$$f(W, c) = \sum_{i=1}^n \|x_i - w_{c(i)}\|_2^2$$

↑ ↑
all means all assignments

- The initialization of 'W' and 'c' given by k-means++ satisfies:

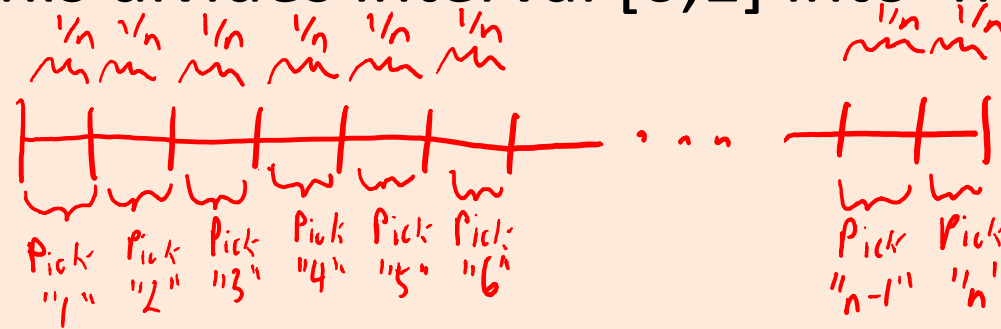
$$\underbrace{E [f(W, c)]}_{\substack{\text{Expectation over} \\ \text{random samples}}} = O(\log(k))$$

↑ ↑ ↑
"Best" mean and clustering according to objective.

- Get good clustering with high probability by re-running.
- However, there is no guarantee that c^* is a good clustering.

Uniform Sampling

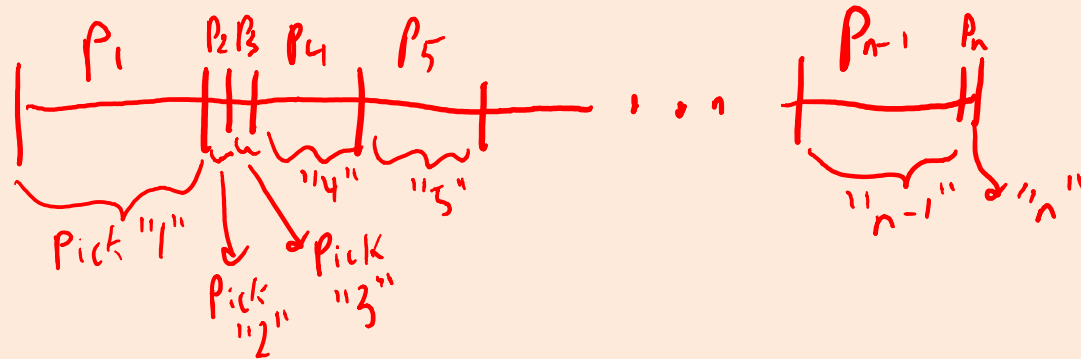
- Standard approach to generating a random number from $\{1,2,\dots,n\}$:
 1. Generate a uniform random number 'u' in the interval $[0,1]$.
 2. Return the largest index 'i' such that $u \leq i/n$.
- Conceptually, this divides interval $[0,1]$ into 'n' equal-size pieces:



- This assumes $p_i = 1/n$ for all 'i'.
↑ probability of picking number 'i'.

Non-Uniform Sampling

- Standard approach to generating a random number for general p_i .
 1. Generate a uniform random number 'u' in the interval [0,1].
 2. Return the largest index 'i' such that $u \leq \sum_{j=1}^i p_j$
- Conceptually, this divides interval [0,1] into non-equal-size pieces:



- Can sample from a generic discrete probability distribution in $O(n)$.
- If you need to generate 'm' samples:
 - Cost is $O(n + m \log(n))$ with binary search and storing cumulative sums.

How many iterations does k-means take?

- Each update of the ' \hat{y}_i ' or ' w_c ' does not increase the objective 'f'.
- And there are k^n possible assignments of the \hat{y}_i to 'k' clusters.
- So within k^n iterations you cannot improve the objective by changing \hat{y}_i , and the algorithm stops.

- Tighter-but-more-complicated “smoothed” analysis:
 - <https://arxiv.org/pdf/0904.1113.pdf>