10-301/10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

K-Means
+
Ensemble Methods: Bagging

Matt Gormley
Lecture 25
Apr. 5, 2022

Reminders

- Homework 8: Reinforcement Learning
  - Out: Mon, Apr. 10
  - Due: Fri, Apr. 21 at 11:59pm
- Homework 9: Learning Paradigms
  - Out: Fri, Apr. 21
  - Due: Fri, Dec. 9 at 11:59pm
    (only two grace/late days permitted)

Crowdsourcing Exam Questions

Exercise

1. Select one of lecture-level learning objectives
   http://mlcourse.org/slides/10601-objectives.pdf
2. Write a question that assesses that objective
3. Adjust to avoid 'trivia style' question

Answer Here:

CLUSTERING

Clustering, Informal Goals

Goal: Automatically partition unlabeled data into groups of similar data points.

Question: When and why would we want to do this?

Useful for:

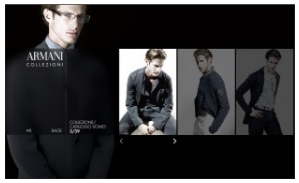
- Automatically organizing data.
- Understanding hidden structure in data.
- Preprocessing for further analysis.
    - Representing high-dimensional data in a low-dimensional space (e.g., for visualization purposes).

Slide courtesy of Nina Balcan

Applications (Clustering comes up everywhere…)

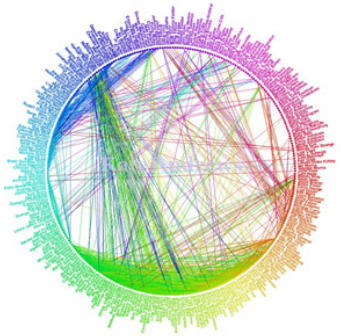
- Cluster news articles or web pages or search results by topic.



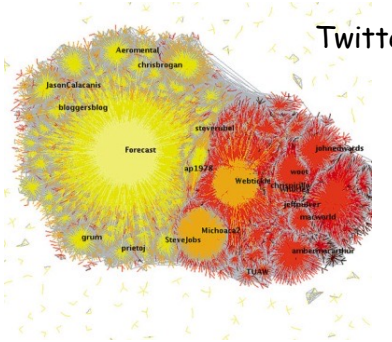


- Cluster protein sequences by function or genes according to expression profile.


- Cluster users of social networks by interest (community detection).



Facebook network

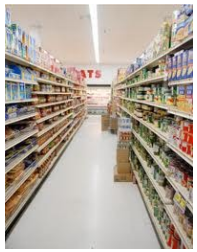


Twitter Network

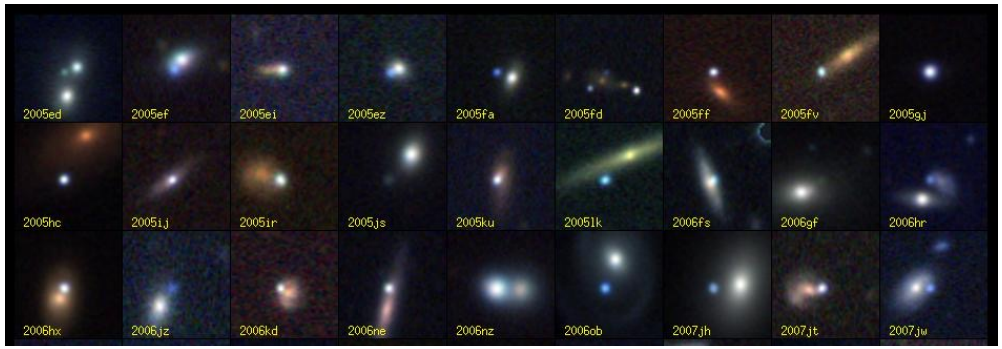
Slide courtesy of Nina Balcan

Applications (Clustering comes up everywhere…)

- Cluster customers according to purchase history.



- Cluster galaxies or nearby stars (e.g. Sloan Digital Sky Survey)

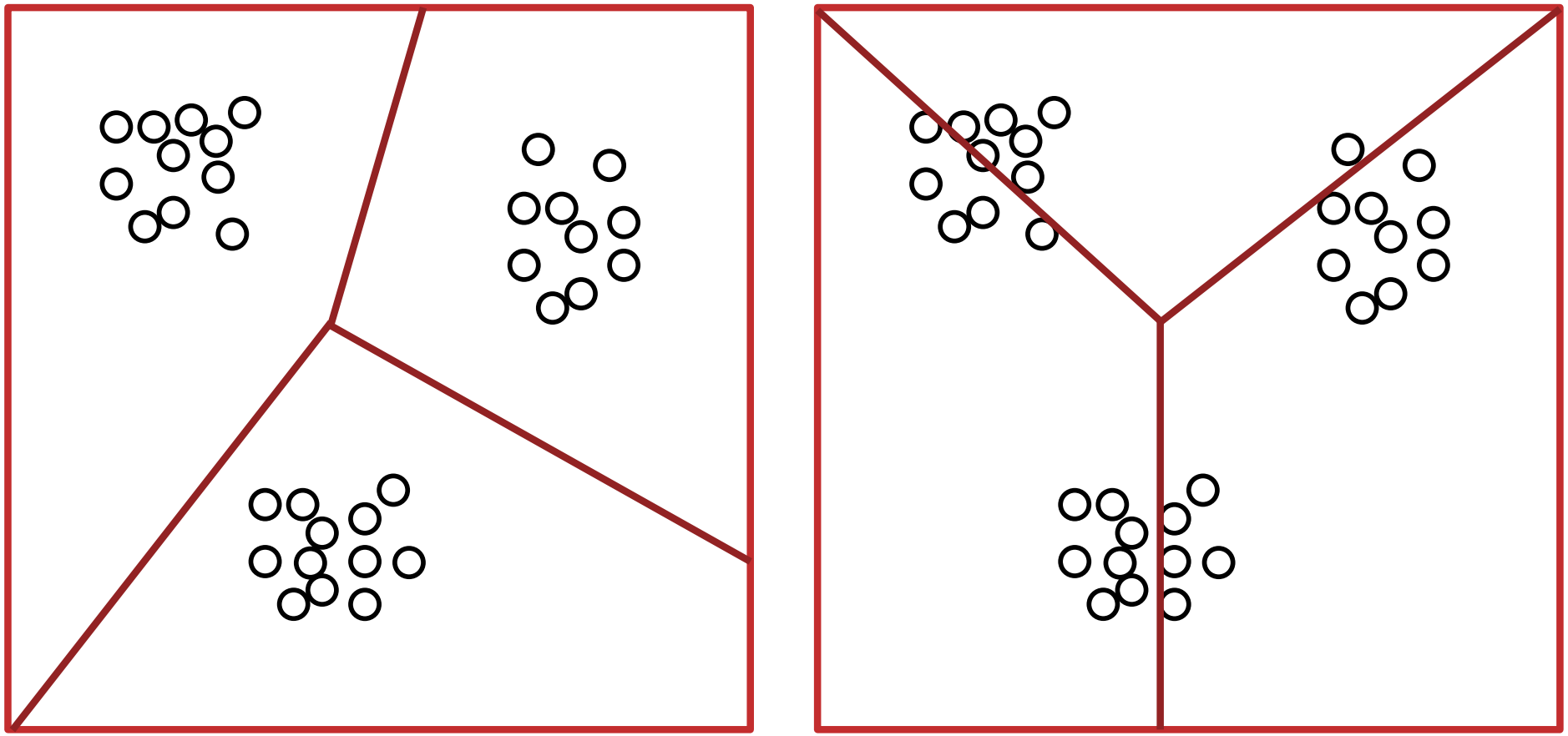


- And many many more applications….

Slide courtesy of Nina Balcan

Clustering

Question: Which of these partitions is "better"?



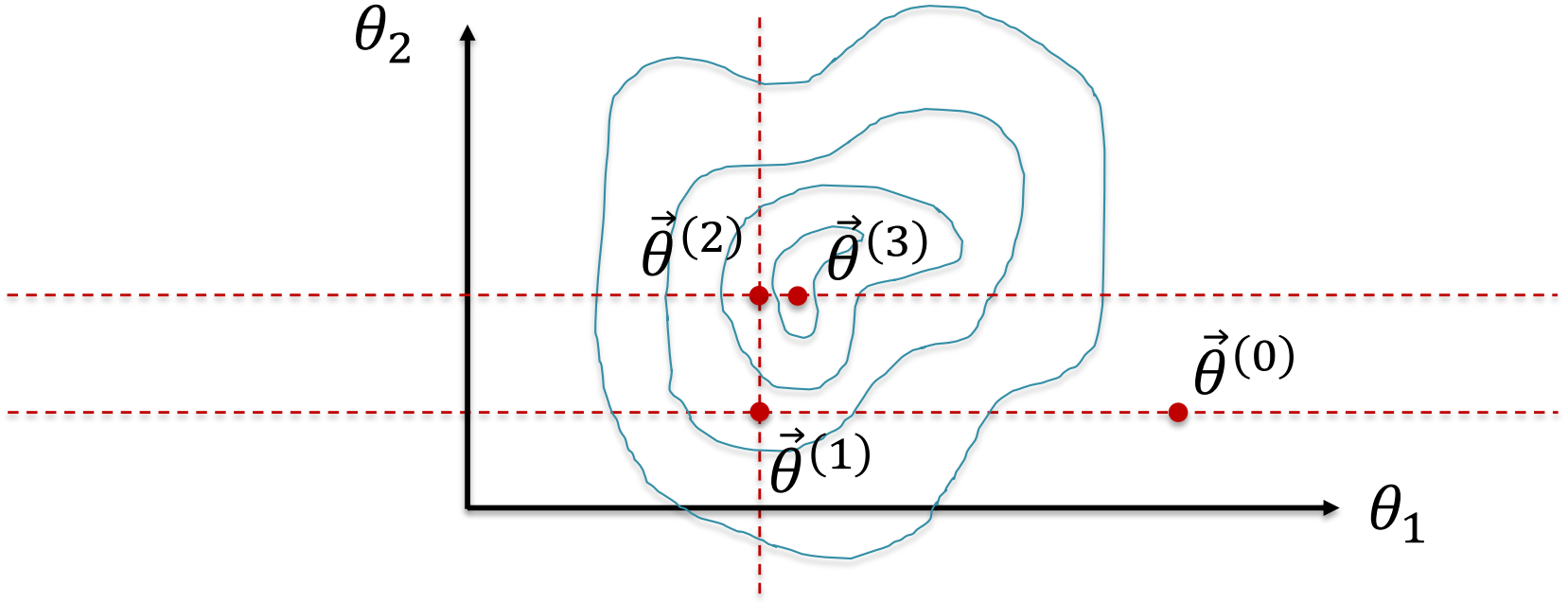
OPTIMIZATION BACKGROUND

Coordinate Descent

- Goal: minimize some objective

$$\vec{\theta}^* = \underset{\vec{\theta}}{\operatorname{argmin}} J(\vec{\theta})$$

- Idea: iteratively pick one variable and minimize the objective w.r.t. just that one variable, *keeping all the others fixed*.



Block Coordinate Descent

- Goal: minimize some objective (with 2 blocks)

$$\vec{\alpha}^*, \vec{\beta}^* = \underset{\vec{\alpha},\vec{\beta}}{\operatorname{argmin}} J(\vec{\alpha}, \vec{\beta})$$

- Idea: iteratively pick one *block* of variables ($\vec{\alpha}$ or $\vec{\beta}$) and minimize the objective w.r.t. that block, keeping the other(s) fixed.

while not converged:

$$\vec{\alpha} = \underset{\vec{\alpha}}{\operatorname{argmin}} J(\vec{\alpha}, \vec{\beta})$$

$$\vec{\beta} = \underset{\vec{\beta}}{\operatorname{argmin}} J(\vec{\alpha}, \vec{\beta})$$

K-MEANS

K-Means Algorithm (Derivation)

Recipe for K-Means Derivation:

1) Define a Model.
2) Choose an objective function.
3) Optimize it!

K-Means Algorithm (Derivation)

- Input: unlabeled data $\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^{N},\ \mathbf{x}^{(i)} \in \mathbb{R}^M$
- Goal: Find an assignment of points to clusters
- Model Paramters:
  - cluster centers: $\mathbf{C} = [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_K],\ \mathbf{c}_j \in \mathbb{R}^M$
  - cluster assignments: $\mathbf{z} = [z^{(1)}, z^{(2)}, \ldots, z^{(N)}],\ z^{(i)} \in \{1, \ldots, K\}$
- Decision Rule: assign each point $\mathbf{x}^{(i)}$ to its nearest cluster center $\mathbf{c}_j$

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$$\hat{\mathbf{C}} = \underset{\mathbf{C}}{\operatorname{argmin}} \sum_{i=1}^{N} \min_{j} ||\mathbf{x}^{(i)} - \mathbf{c}_j||_2^2$$

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$$= \boxed{\underset{\mathbf{C},\mathbf{z}}{\operatorname{argmin}}\ J(\mathbf{C}, \mathbf{z})}$$

Now apply
Block Coordinate Descent!

K-Means Algorithm

1) **Given** unlabeled feature vectors
   $D = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\}$
2) **Initialize** cluster centers $c = \{\mathbf{c}_1, \ldots, \mathbf{c}_K\}$
3) **Repeat** until convergence:
   a) $\mathbf{z} \leftarrow \text{argmin}_{\mathbf{z}}\ J(\mathbf{C}, \mathbf{z})$
      (pick each *cluster assignment* to minimize distance)
   b) $\mathbf{C} \leftarrow \text{argmin}_{\mathbf{C}}\ J(\mathbf{C}, \mathbf{z})$
      (pick each *cluster center* to minimize distance)

This is an application of
Block Coordinate Descent!
The only remaining step is to figure out
what the argmins boil down to…

K-Means Algorithm

1) **Given** unlabeled feature vectors
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2) **Initialize** cluster centers $c = \{\mathbf{c}_1, \ldots, \mathbf{c}_K\}$
3) **Repeat** until convergence:

a) for i in {1,…, N}

$$z^{(i)} \leftarrow \textbf{argmin}_j \left(\| \mathbf{x}^{(i)} - \mathbf{c}_j \|_2\right)^2$$

b) for j in {1,…,K}

$$\mathbf{c}_j \leftarrow \textbf{argmin}_{\mathbf{c}_j} \sum_{i:z^{(i)}=j} \left(\| \mathbf{x}^{(i)} - \mathbf{c}_j \|_2\right)^2$$

The minimization over cluster assignments decomposes, so that we can find each $z^{(i)}$ independently of the others

Likewise, the minimization over cluster centers decomposes, so we can find each $\mathbf{c}_j$ independently

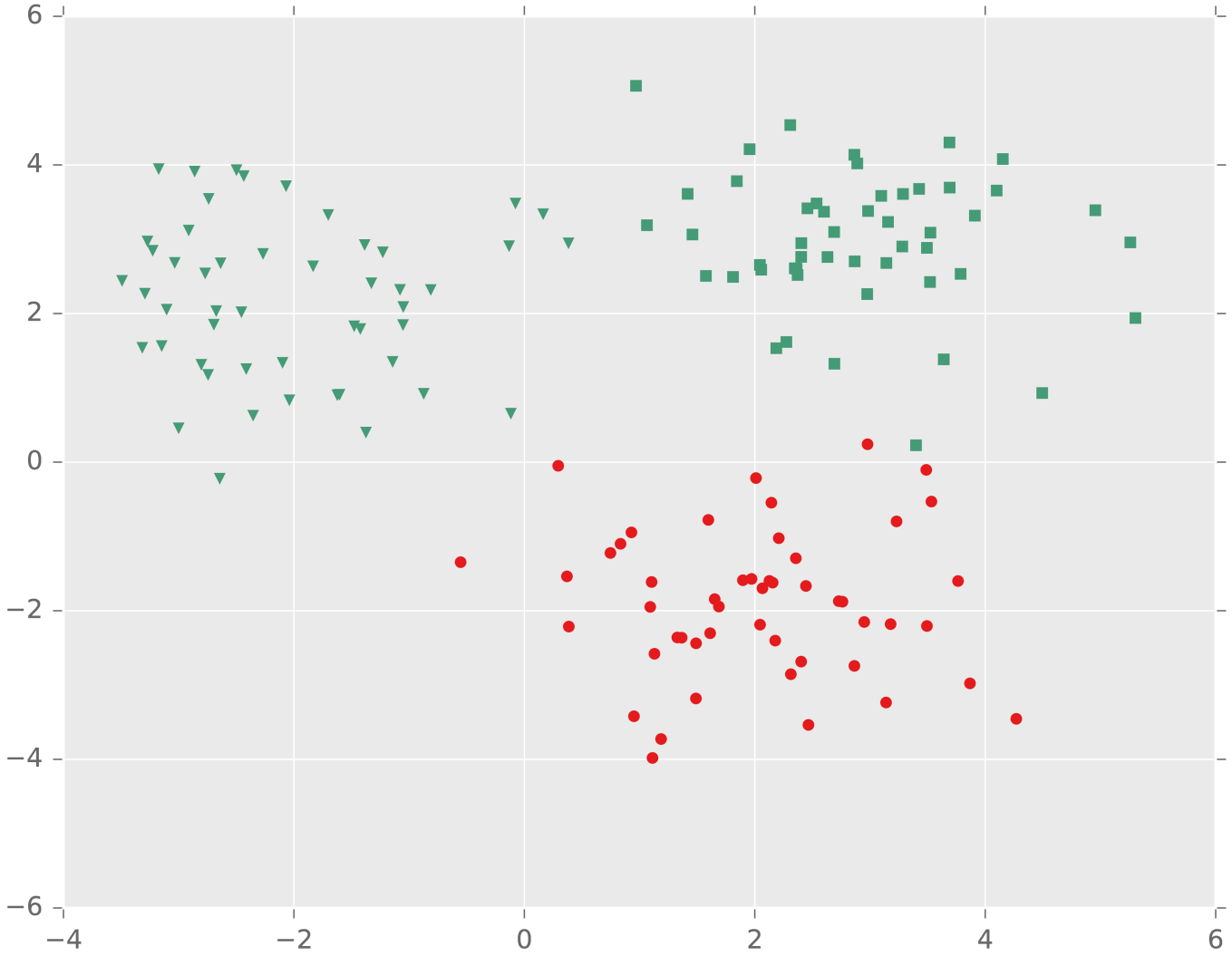
K-Means Algorithm

1) **Given** unlabeled feature vectors
   $D = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\}$
2) **Initialize** cluster centers $c = \{\mathbf{c}_1, \ldots, \mathbf{c}_K\}$
3) **Repeat** until convergence:
   a) for i in {1,…, N}
      $z^{(i)} \leftarrow$ **index** j of cluster center **nearest** to $\mathbf{x}^{(i)}$
   b) for j in {1,…,K}
      $\mathbf{c}_j \leftarrow$ **mean** of **all** points assigned to cluster j

K=3 cluster centers

K-MEANS EXAMPLE

Example: K-Means



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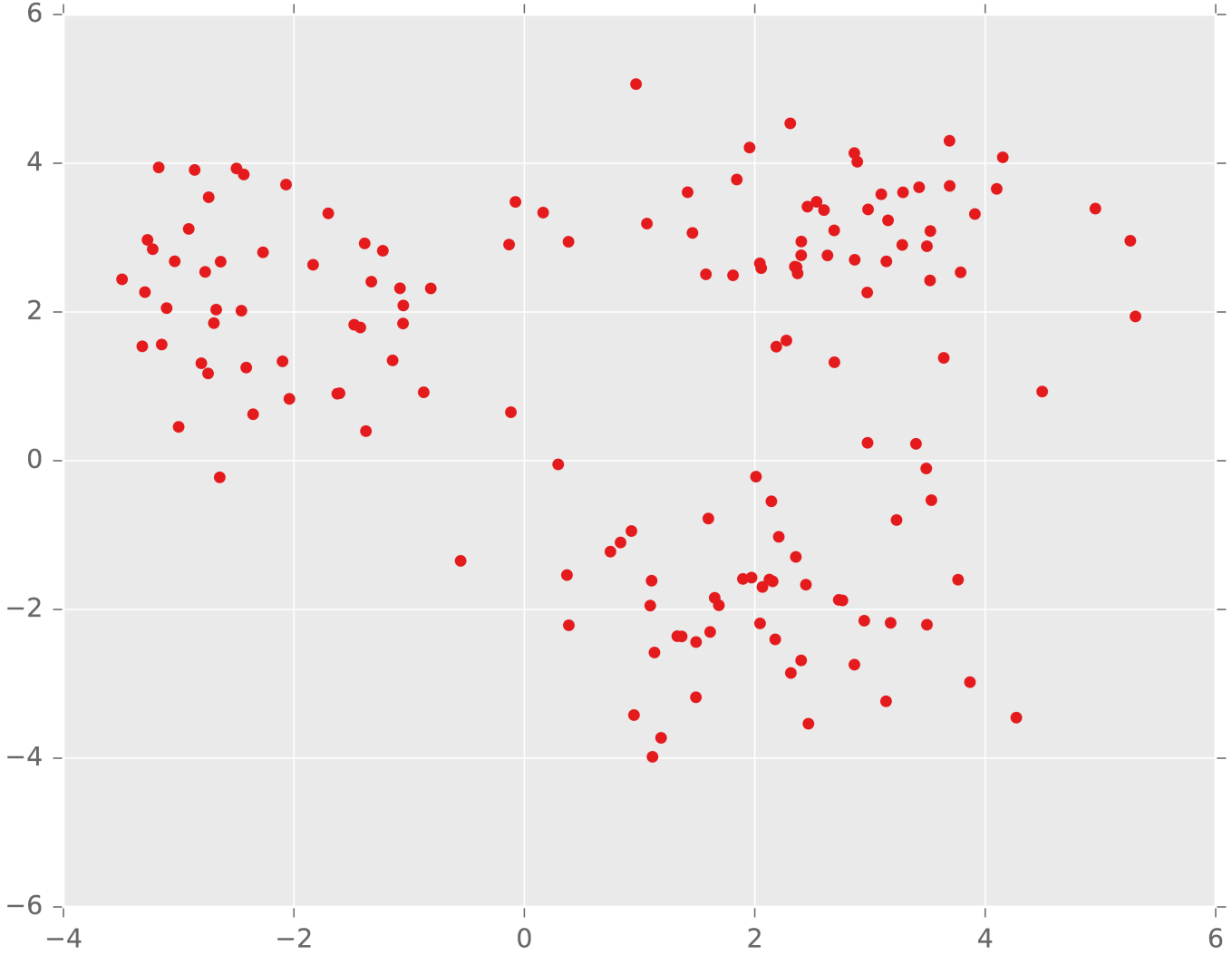

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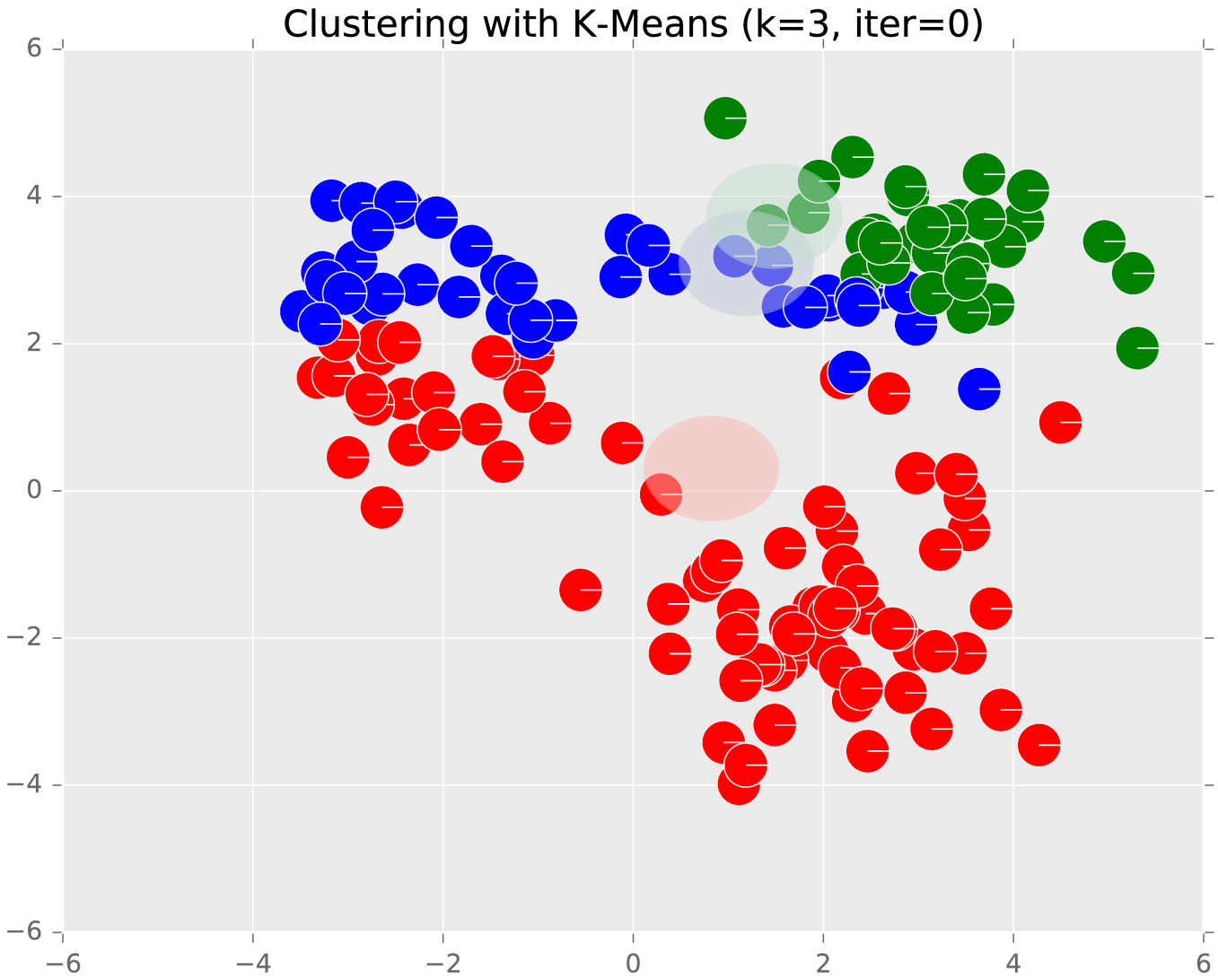

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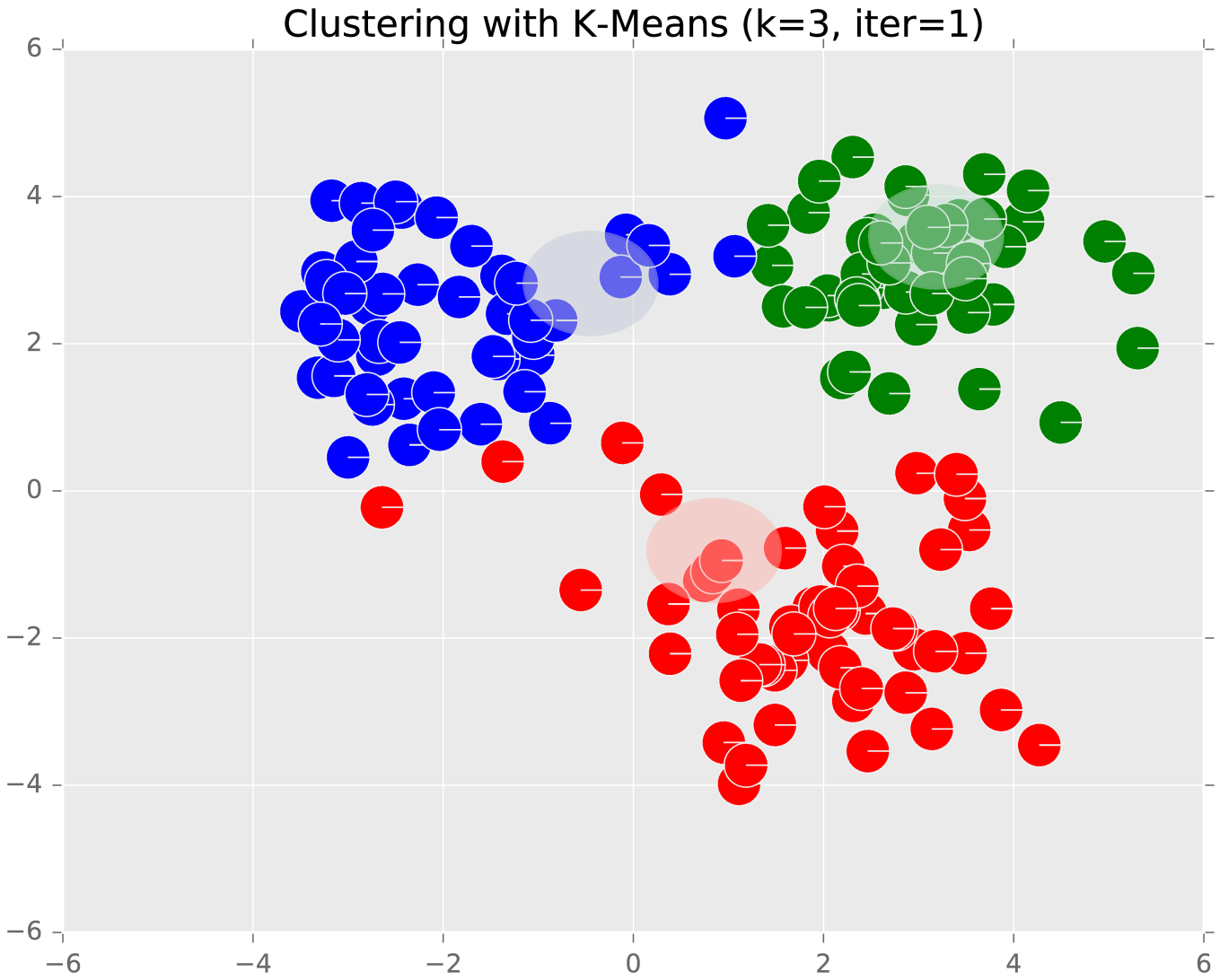

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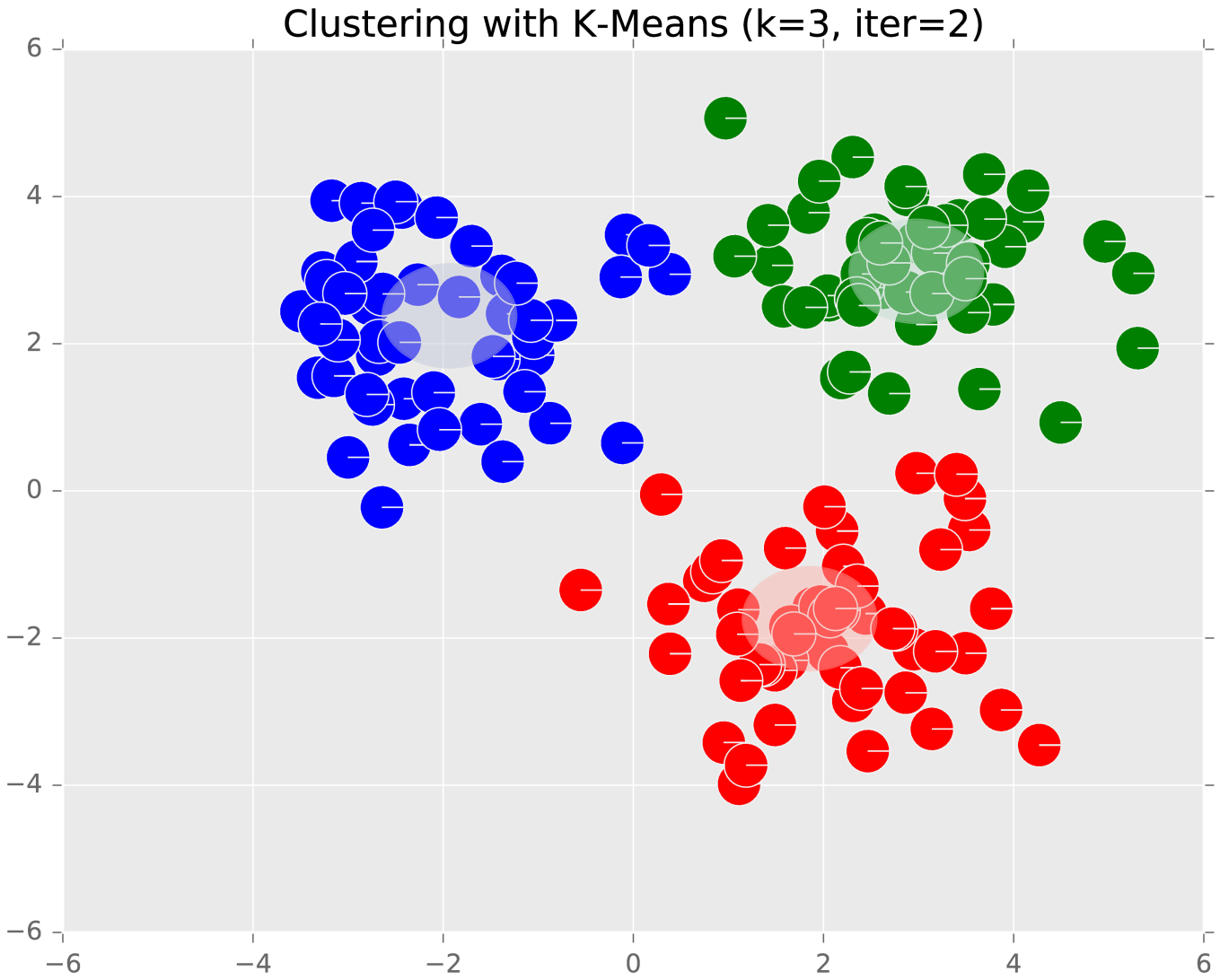

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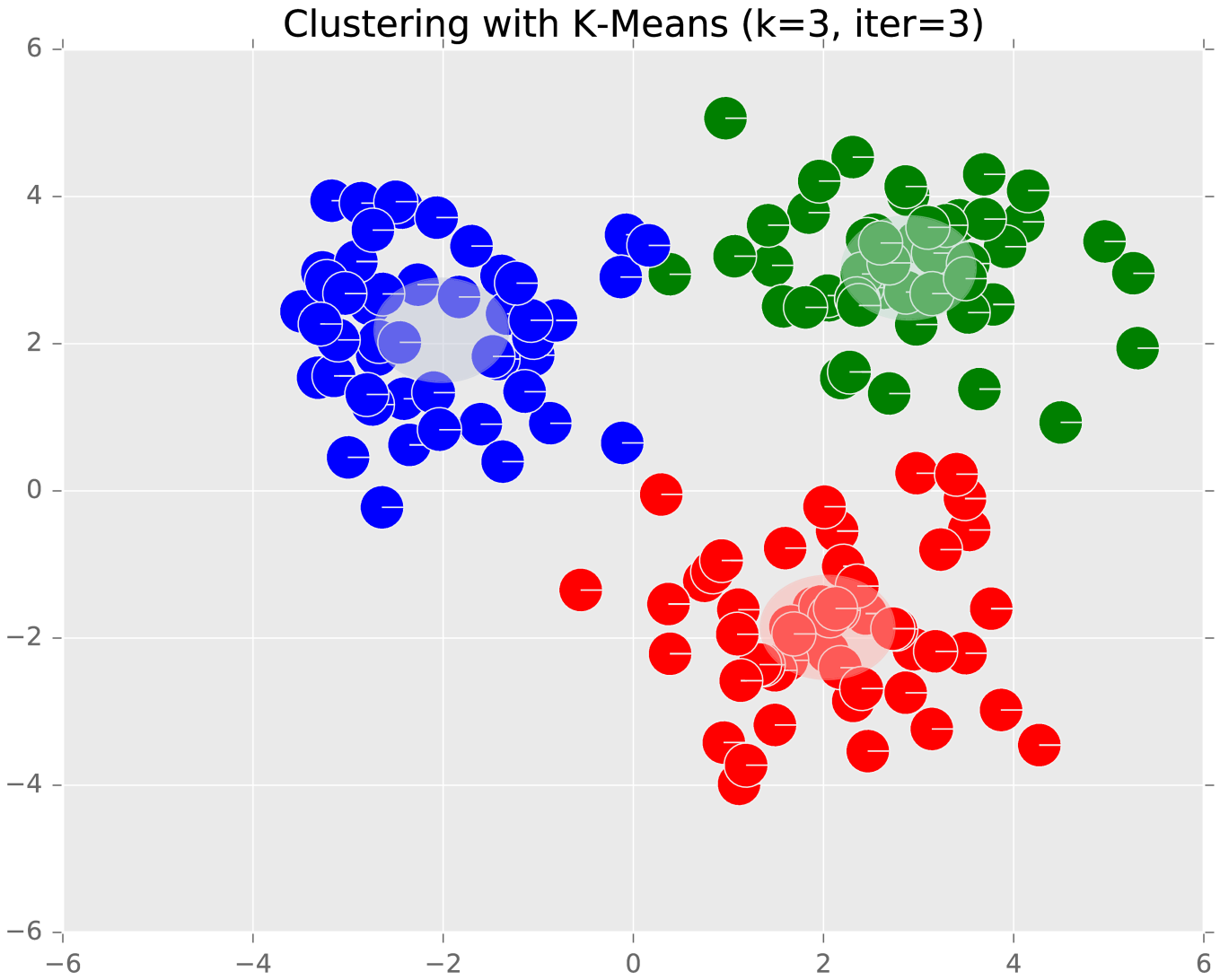

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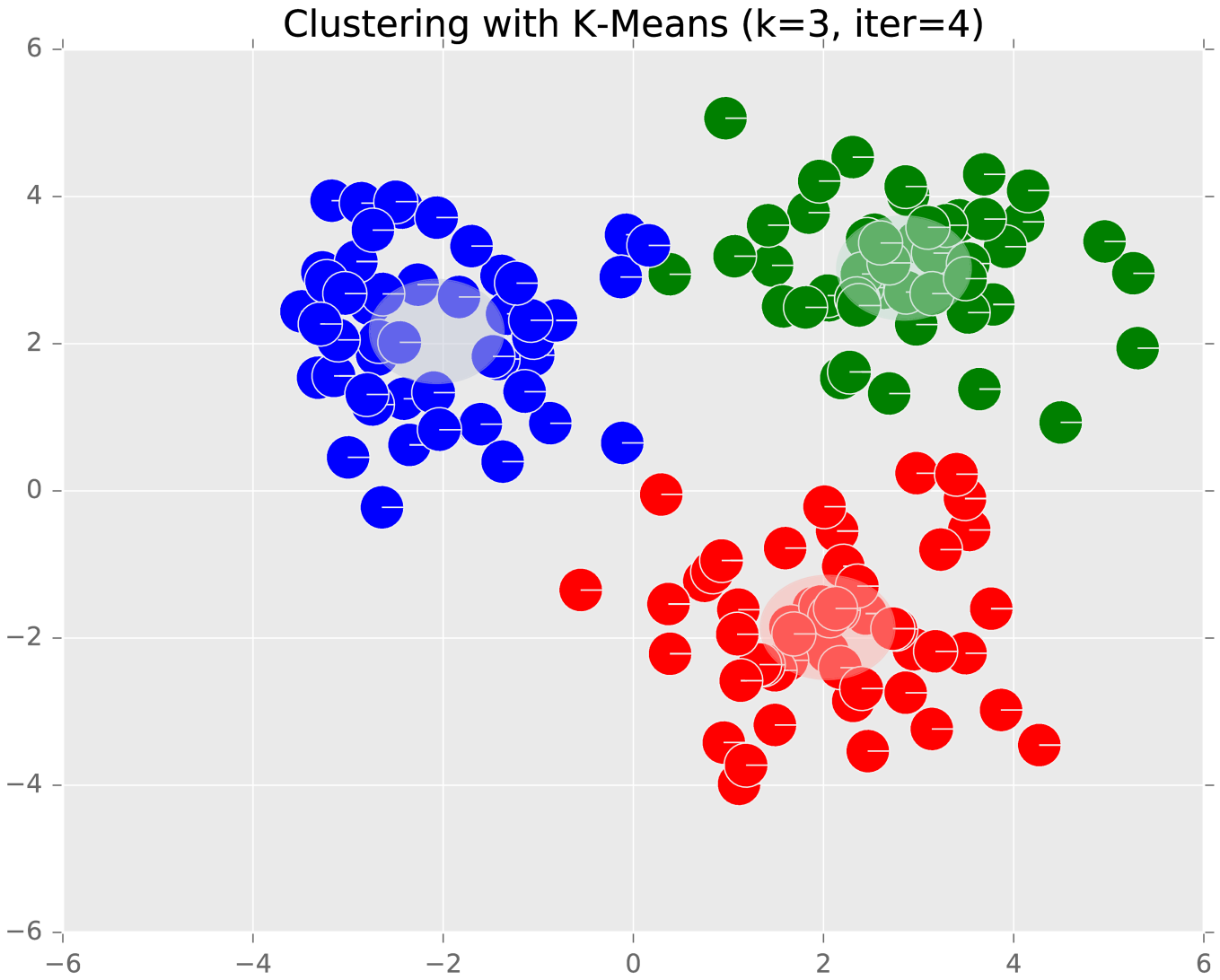
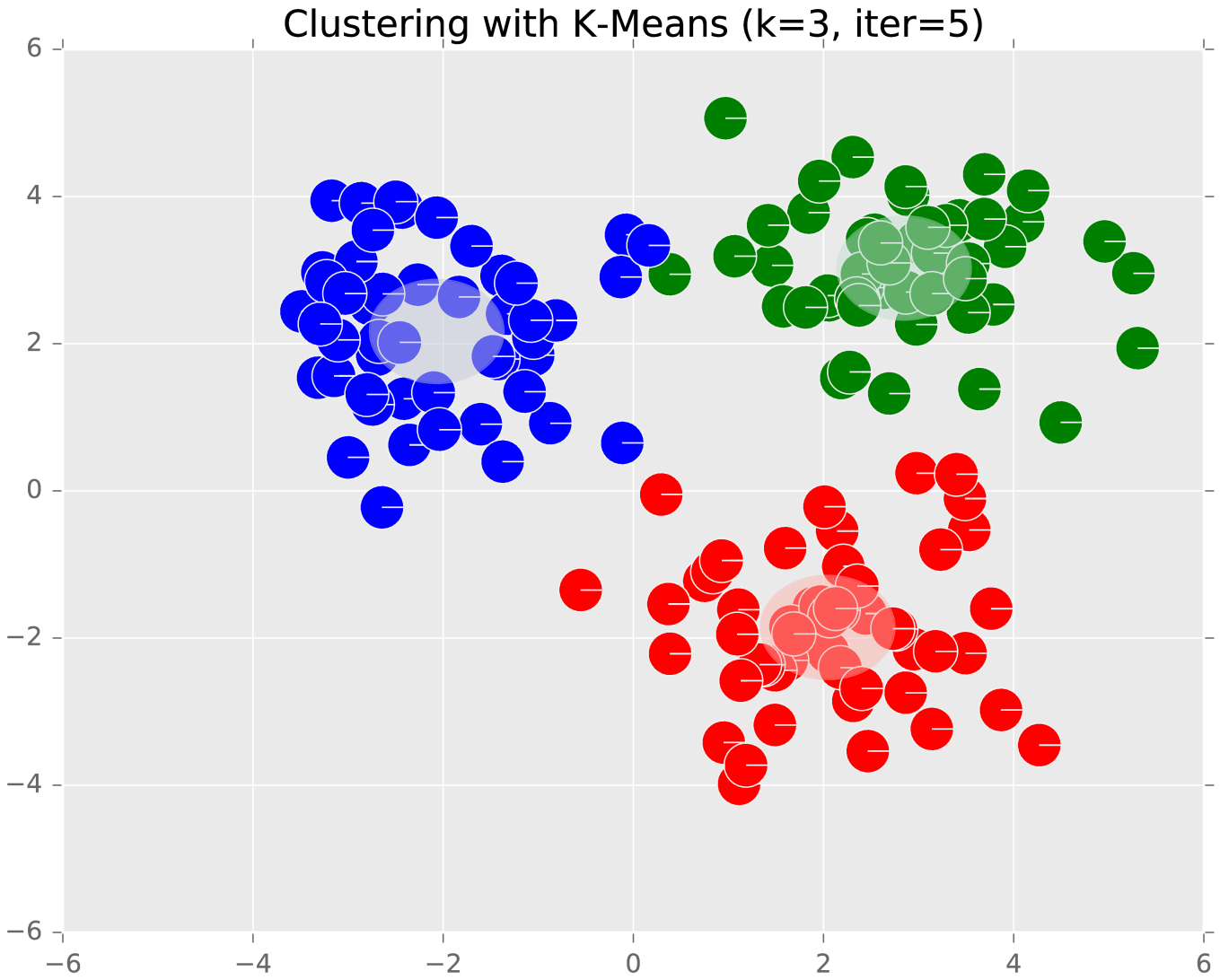


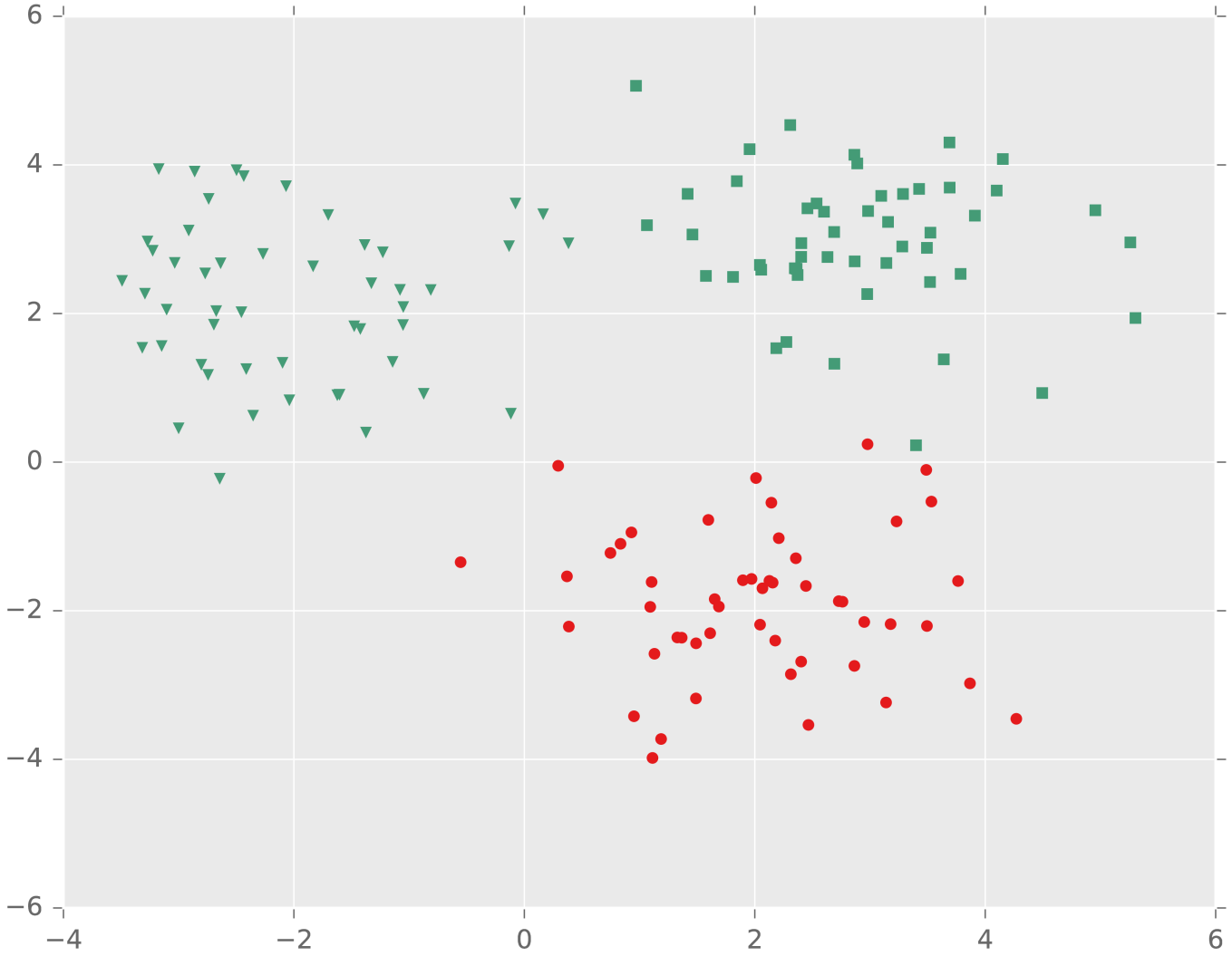
Example: K-Means



K=2 cluster centers

K-MEANS EXAMPLE

Example: K-Means



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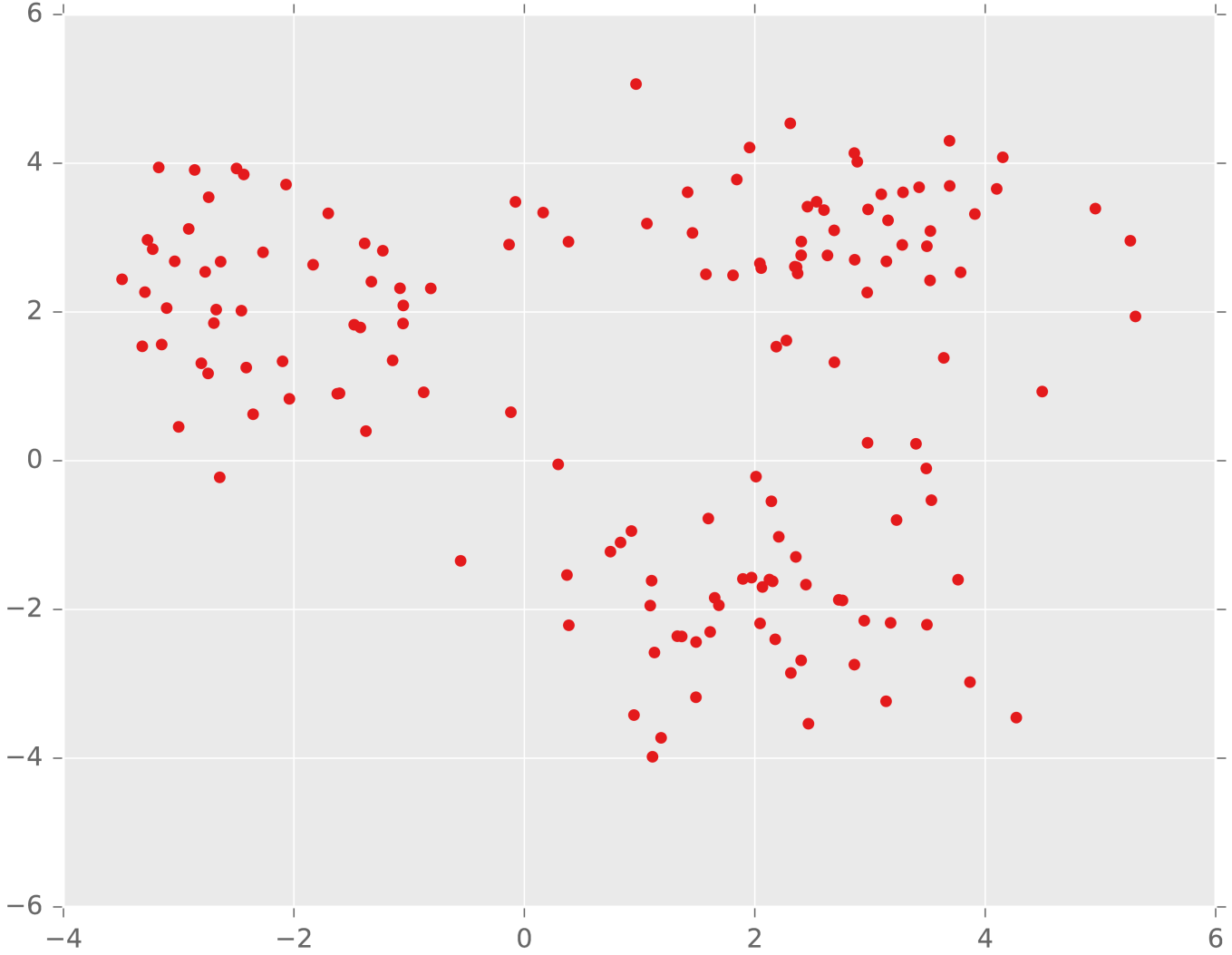

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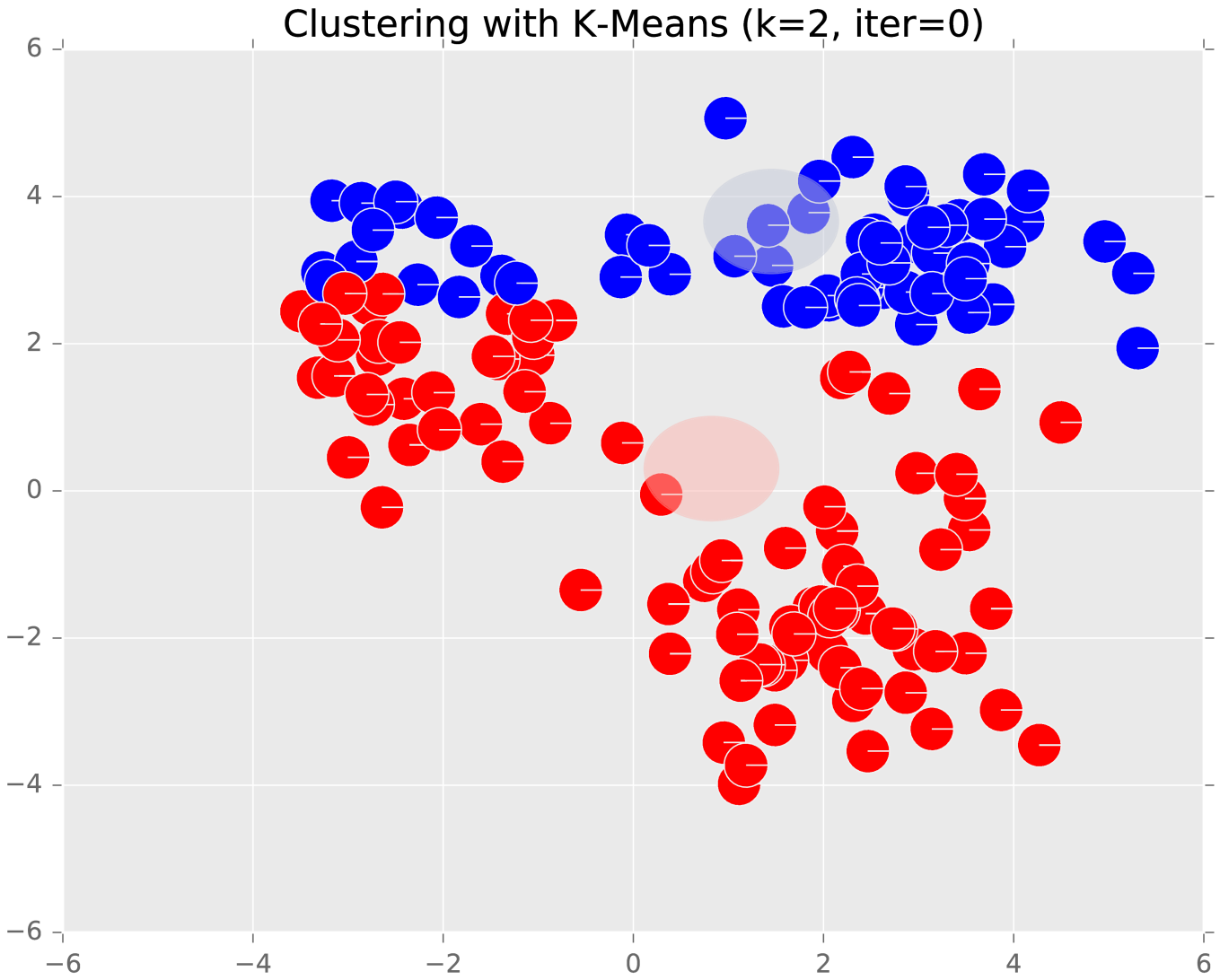

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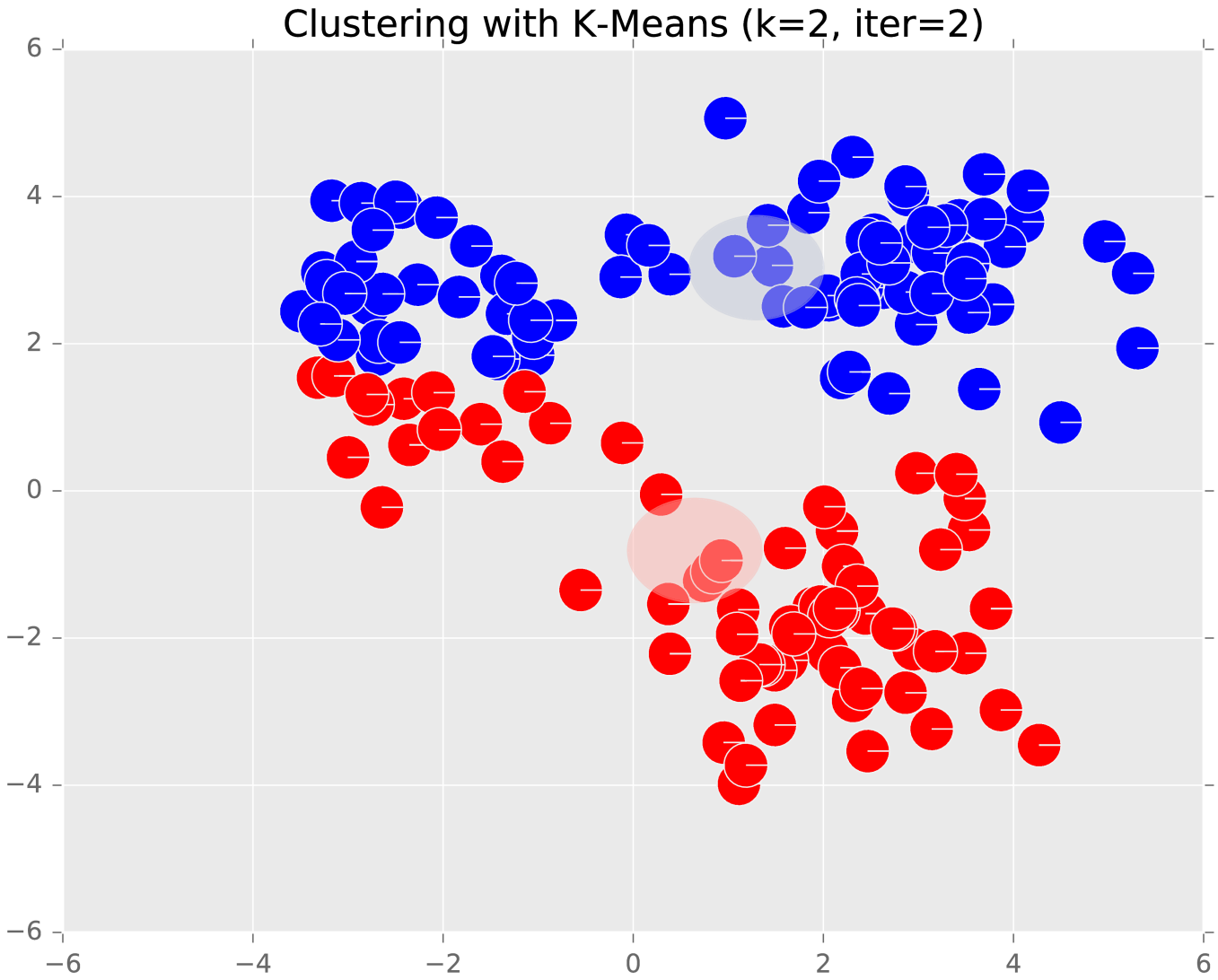

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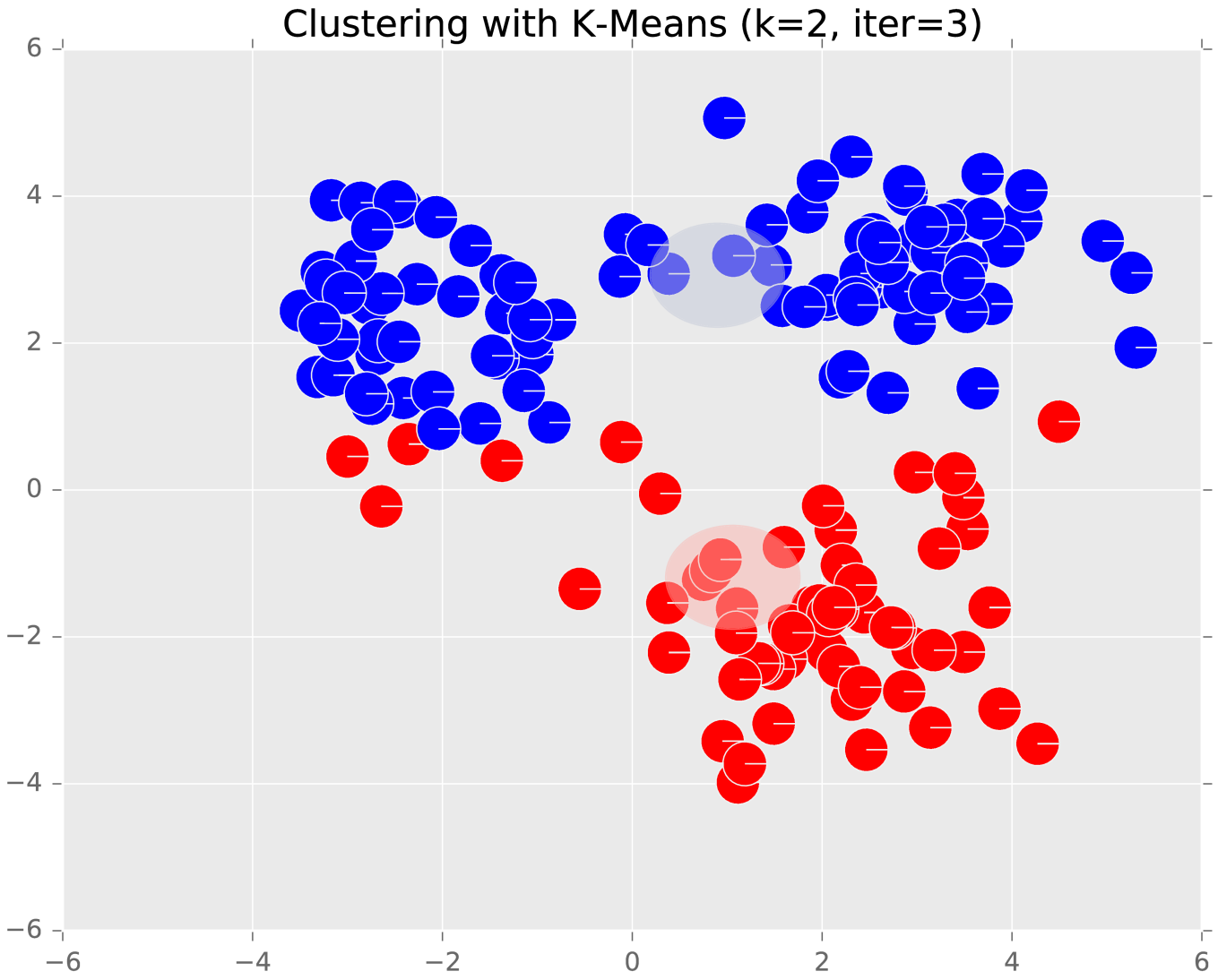

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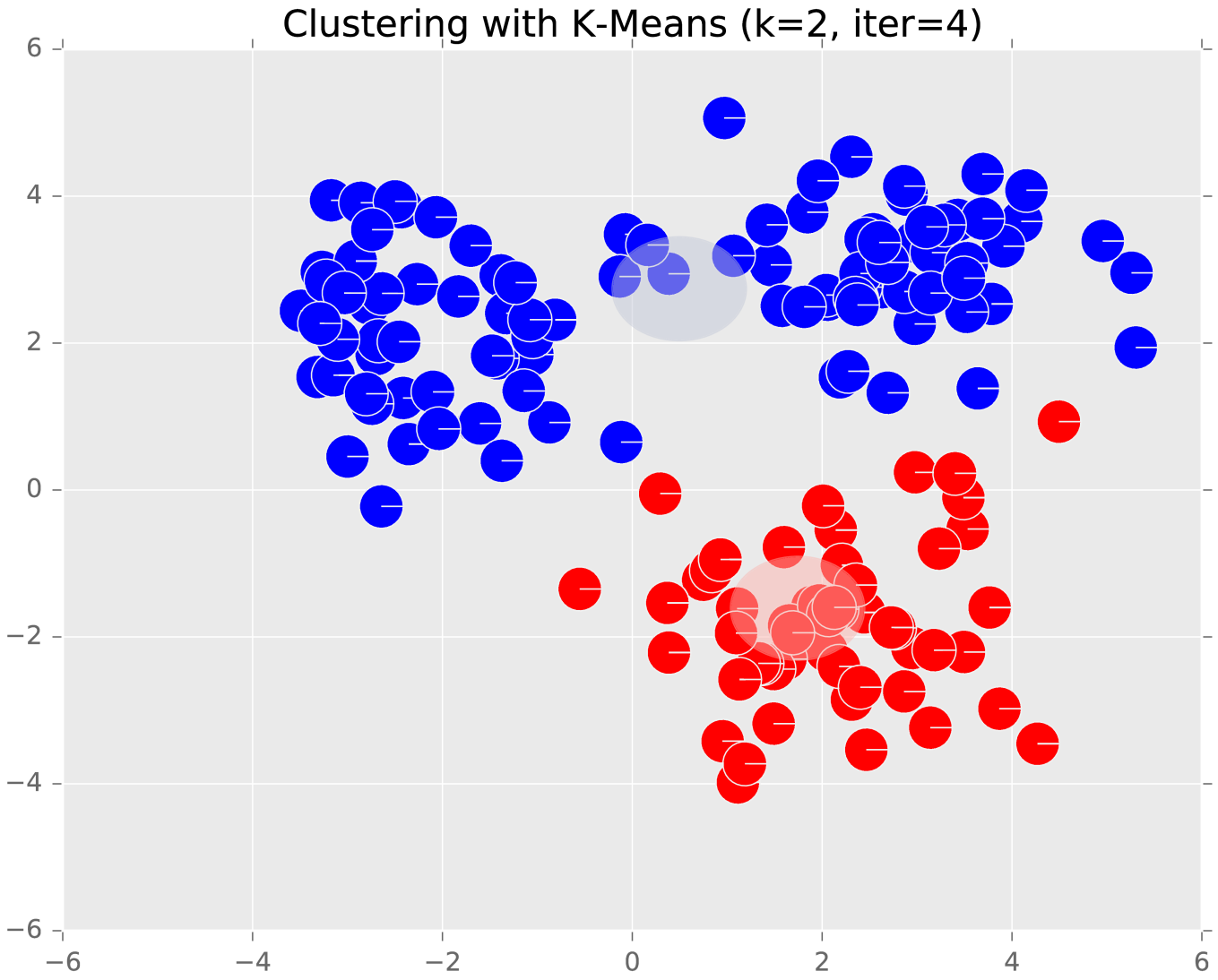

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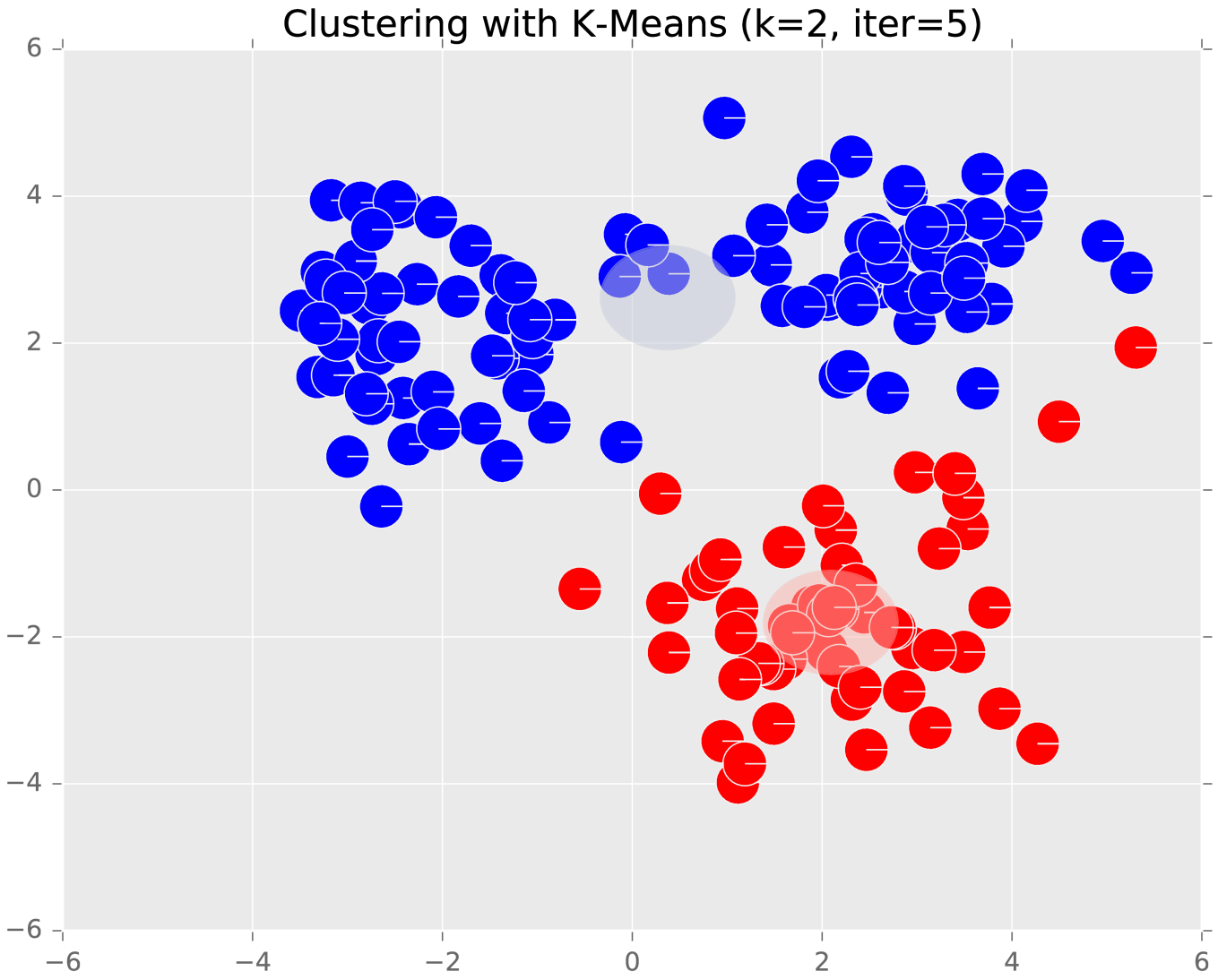

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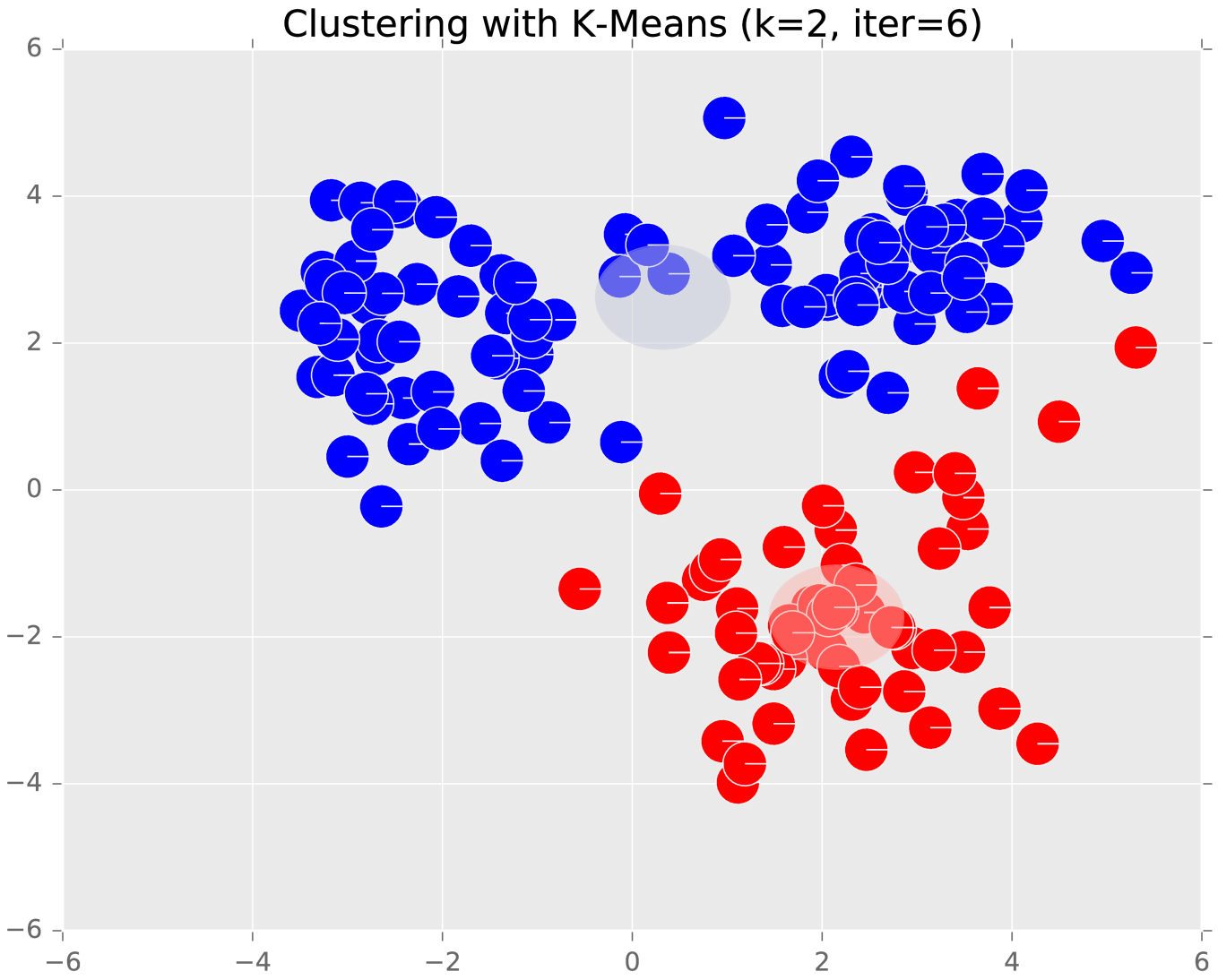

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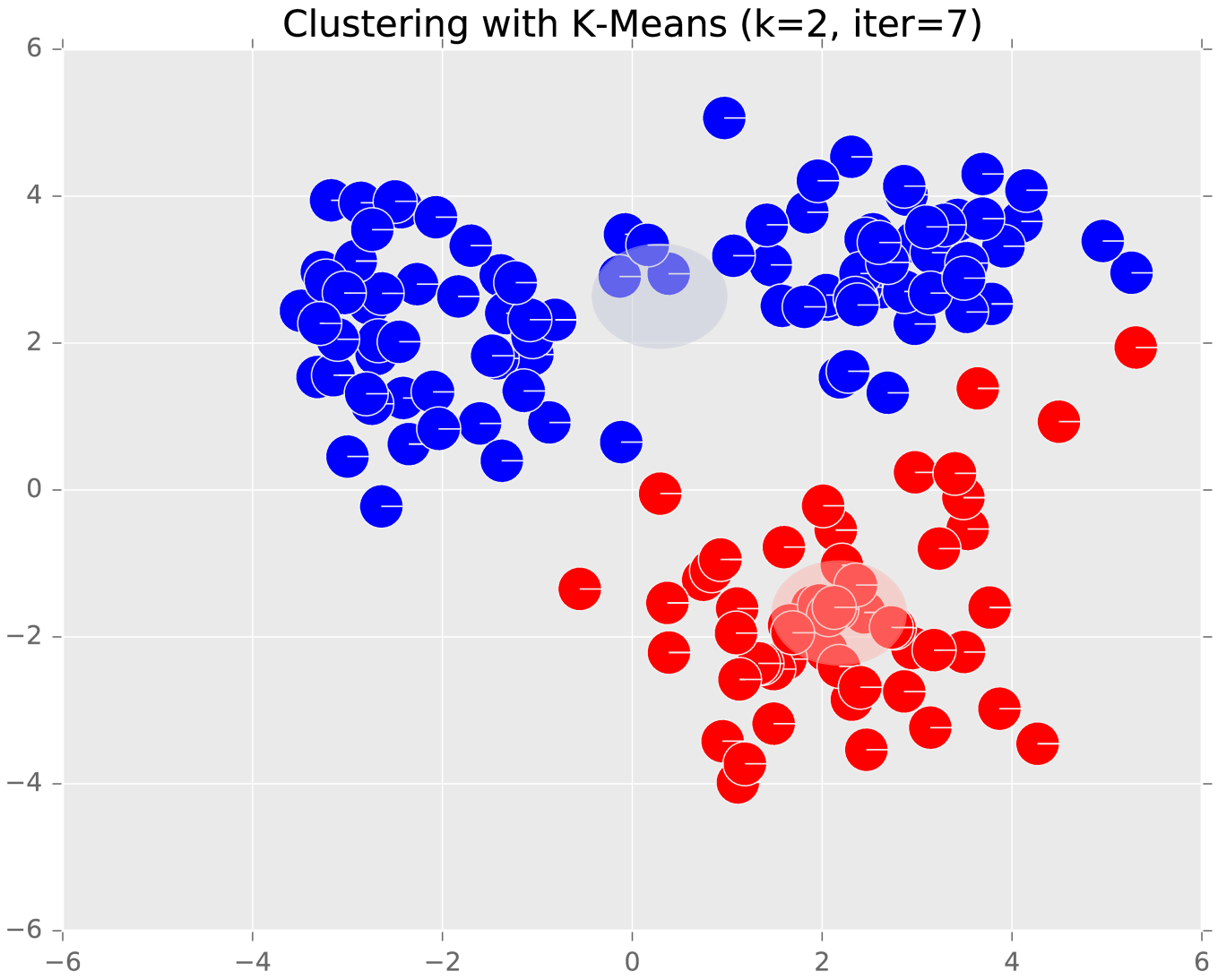


INITIALIZING K-MEANS

Initialization of K-Means

K-Means Algorithm

1) **Given** unlabeled feature vectors
   $D = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\}$
2) **Initialize** cluster centers $c = \{\mathbf{c}_1, \ldots, \mathbf{c}_K\}$
3) **Repeat**
   a) for i in
   b) for j in

Remaining Question:
How should we initialize the cluster centers?

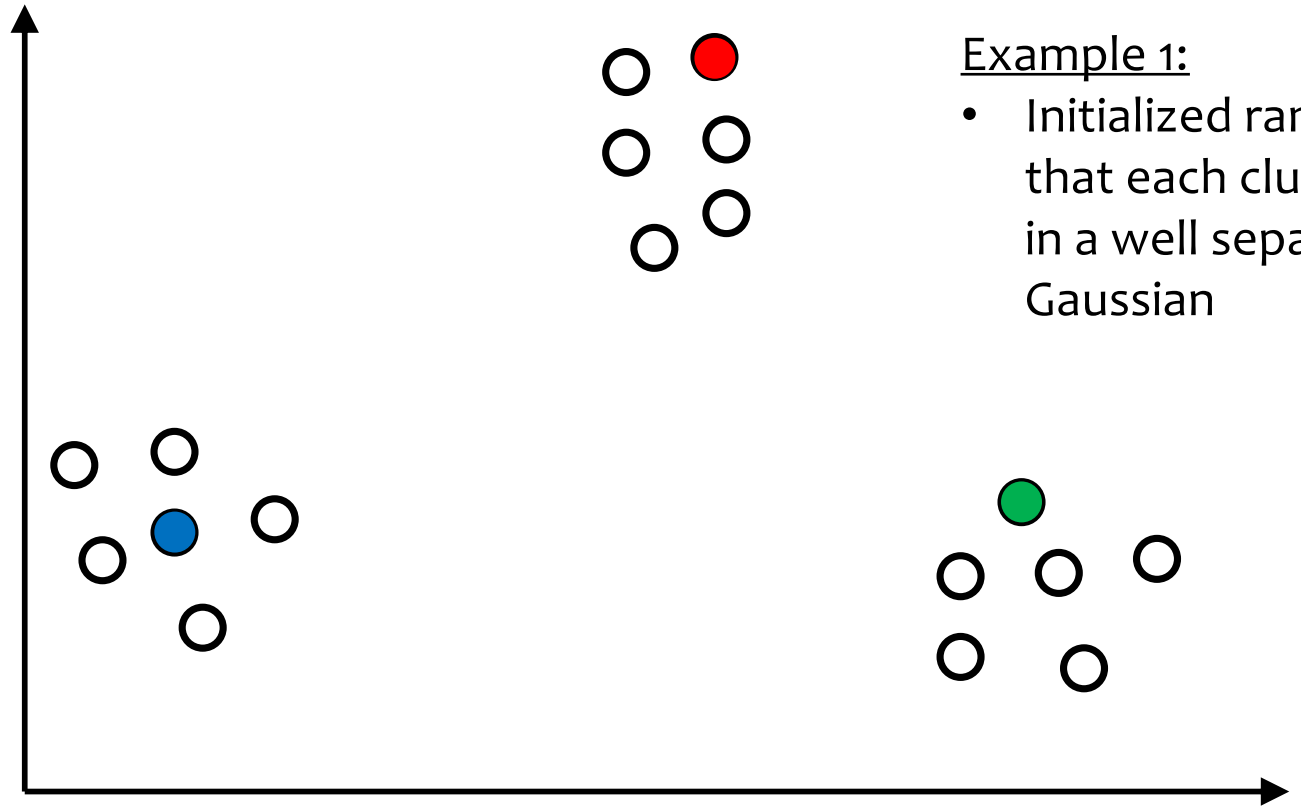
Three Solutions:

1. Random centers (picked from the data points)
2. Furthest point heuristic
3. K-Means++

Initialization for K-Means

Algorithm #1: Random Initialization
Select each cluster center uniformly at random from the data points in the training data

Observations:
Even when data comes from well-separated Gaussians…
- … sometimes works great!
- … sometimes get stuck in poor local optima.



Example 1:
- Initialized randomly such that each cluster center is in a well separated Gaussian

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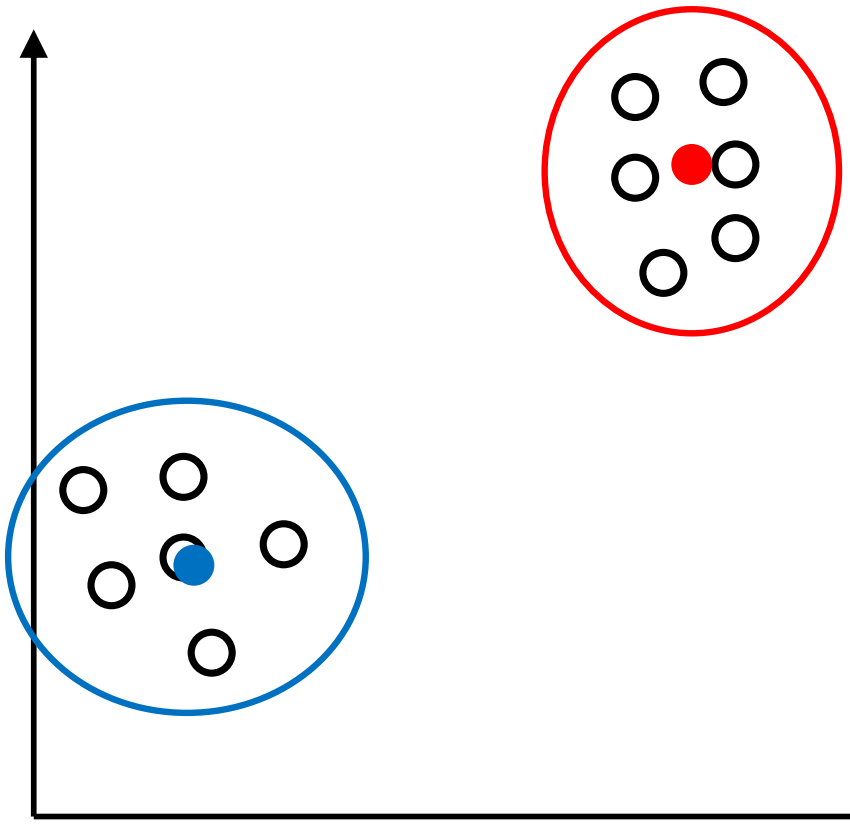

Example 1:
- Initialized randomly such that each cluster center is in a well separated Gaussian
- Good overall performance

Initialization for K-Means

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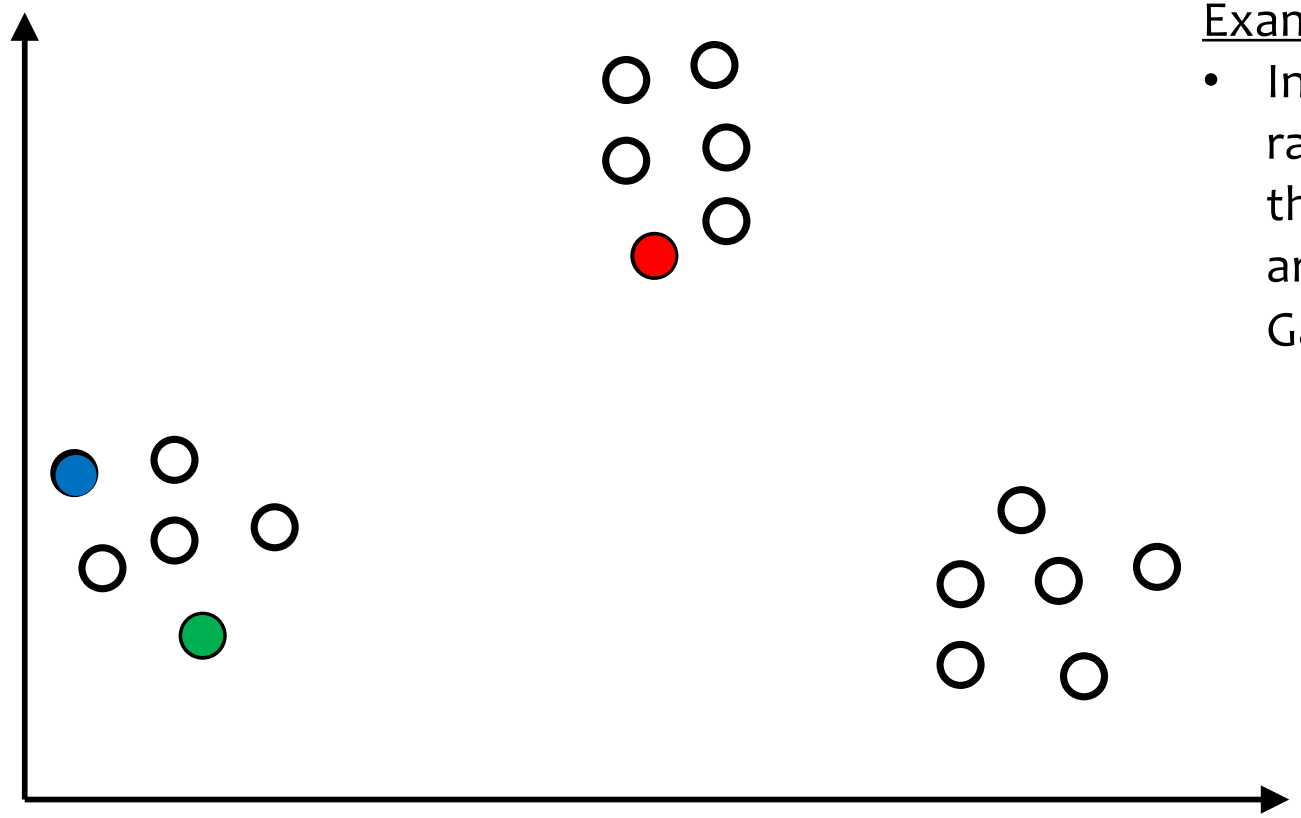

Example 2:
- Initialized randomly such that two centers are in the same Gaussian cluster

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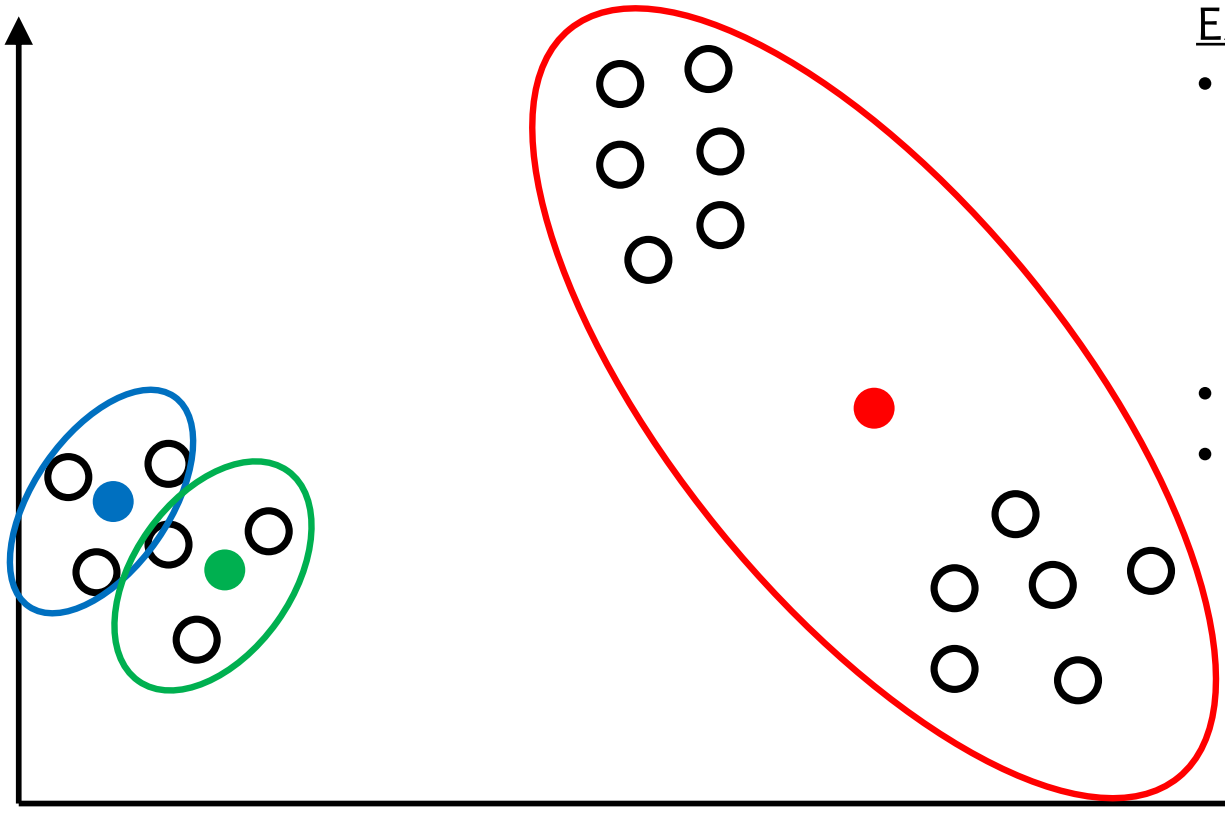


Example 2:
- Initialized randomly such that two centers are in the same Gaussian cluster
- Poor performance
- Can be **arbitrarily bad** (imagine the final red cluster points moving arbitrarily far away!)

Initialization for K-Means

K-Mean Performance (with Random Initialization)

If we do **random initialization**, as k increases, it becomes more likely we won't have perfectly picked one center per Gaussian in our initialization (so K-Means will output a bad solution).

- For k equal-sized Gaussians,

$$\Pr[\text{each initial center is in a different Gaussian}] \approx \frac{k!}{k^k} \approx \frac{1}{e^k}$$

- Becomes unlikely as k gets large.

Slide courtesy of Nina Balcan

Initialization for K-Means

Algorithm #2: Furthest Point Heuristic

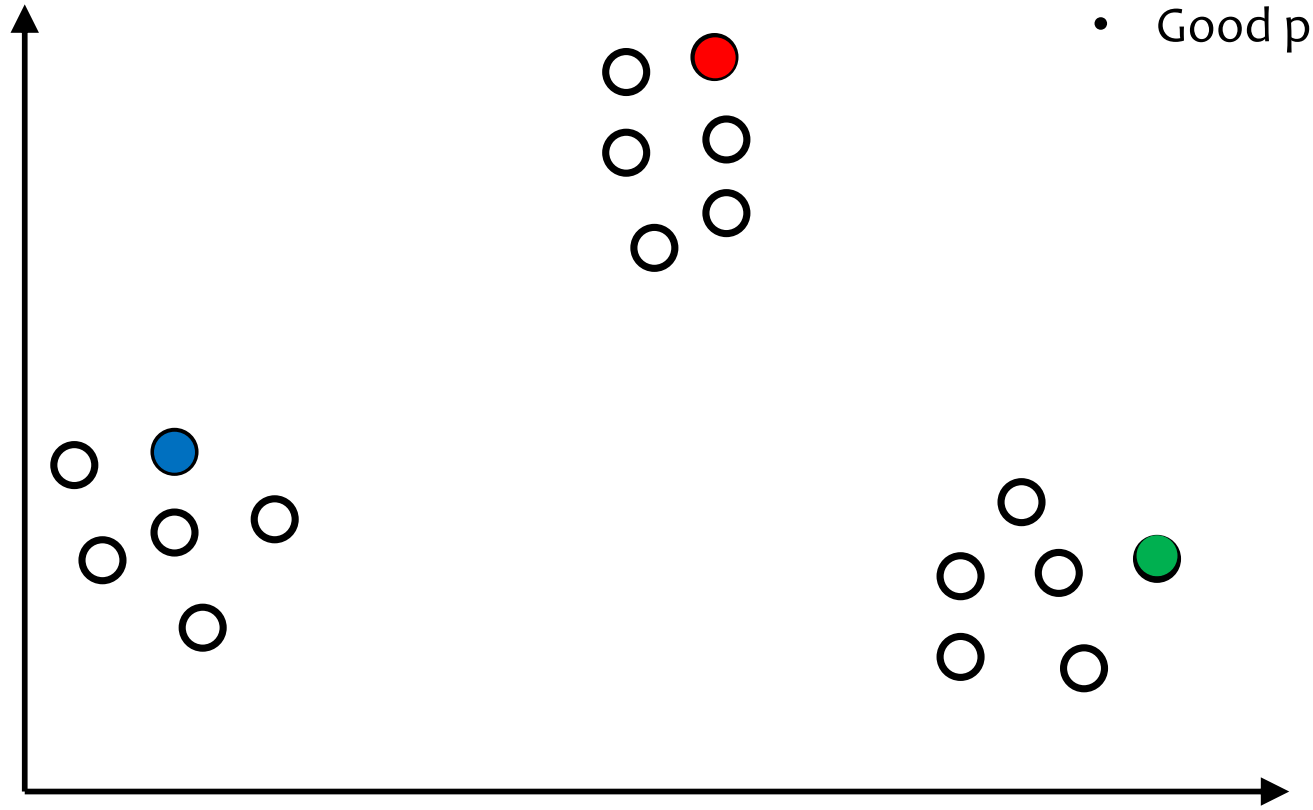
1. Pick the first cluster center $\mathbf{c}_1$ **randomly**
2. Pick each subsequent center $\mathbf{c}_j$ so that it is **as far as possible** from the previously chosen centers $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_{j-1}$

Observations:

- Solves the problem with Gaussian data
- But outliers pose a new problem!

Example 1:

- No outliers
- Good performance



Initialization for K-Means

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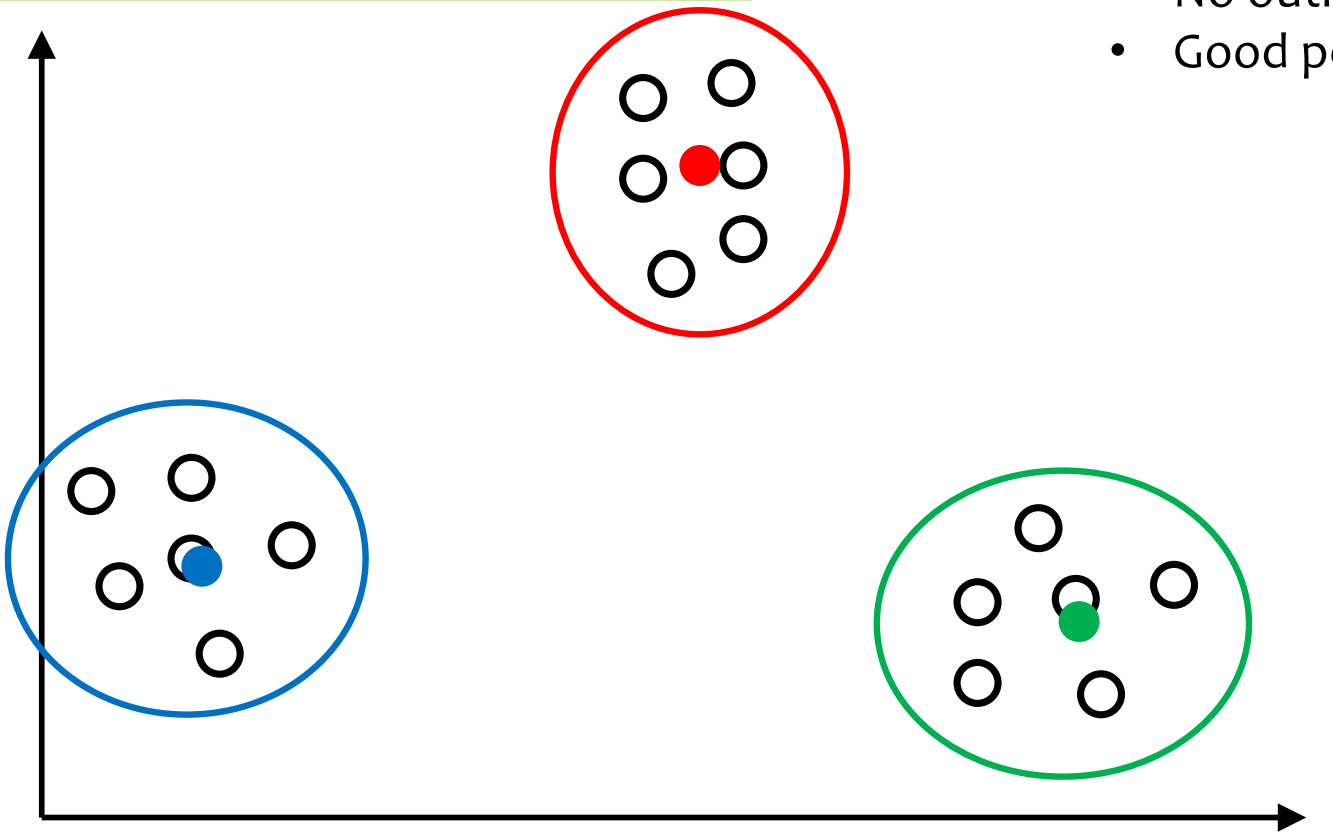


Initialization for K-Means

Algorithm #2: Furthest Point Heuristic

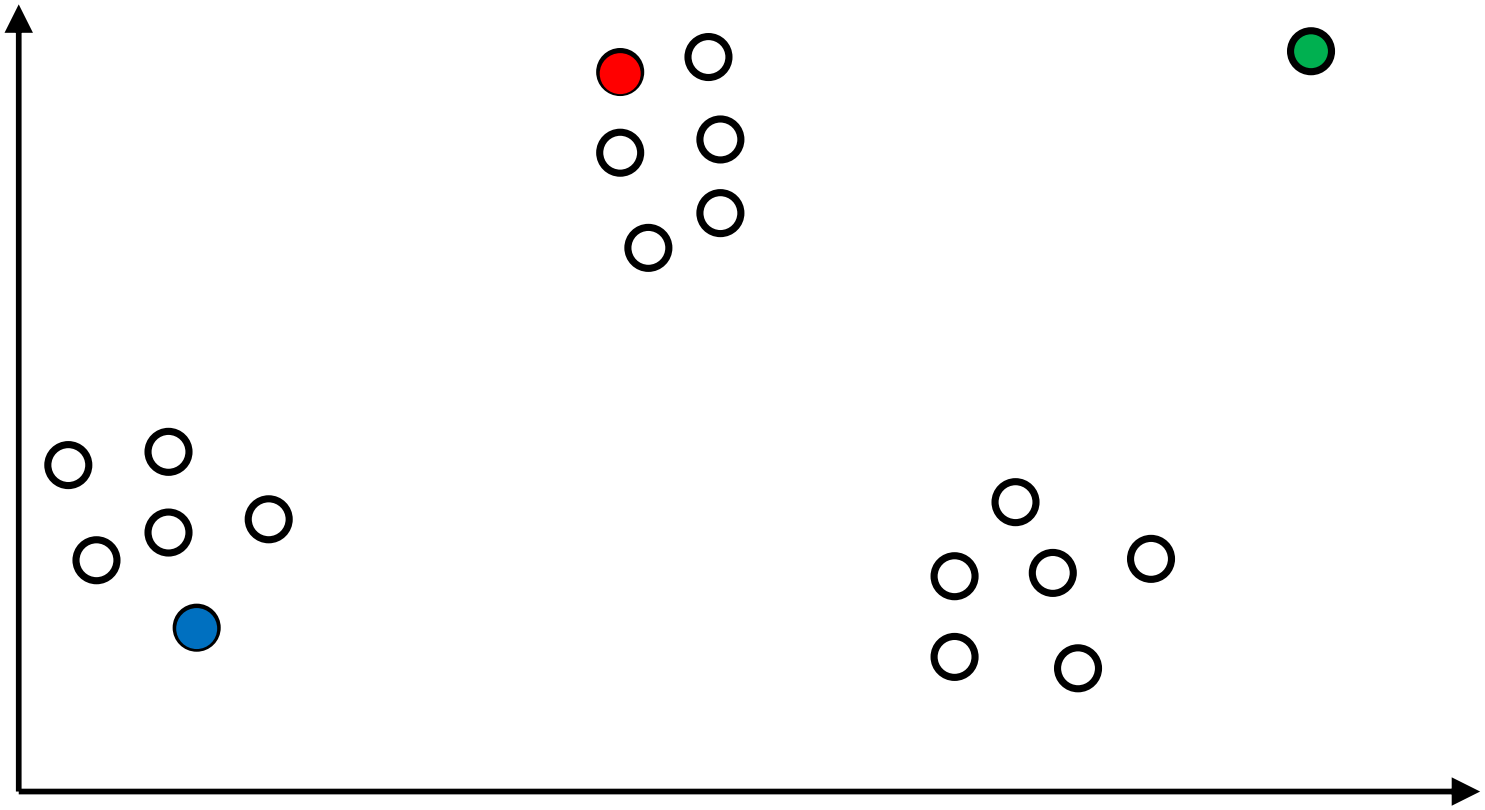
1. Pick the first cluster center $\mathbf{c}_1$ **randomly**
2. Pick each subsequent center $\mathbf{c}_j$ so that it is **as far as possible** from the previously chosen centers $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_{j-1}$

Observations:

- Solves the problem with Gaussian data
- But outliers pose a new problem!

Example 2:

- One outlier throws off the algorithm
- Poor performance



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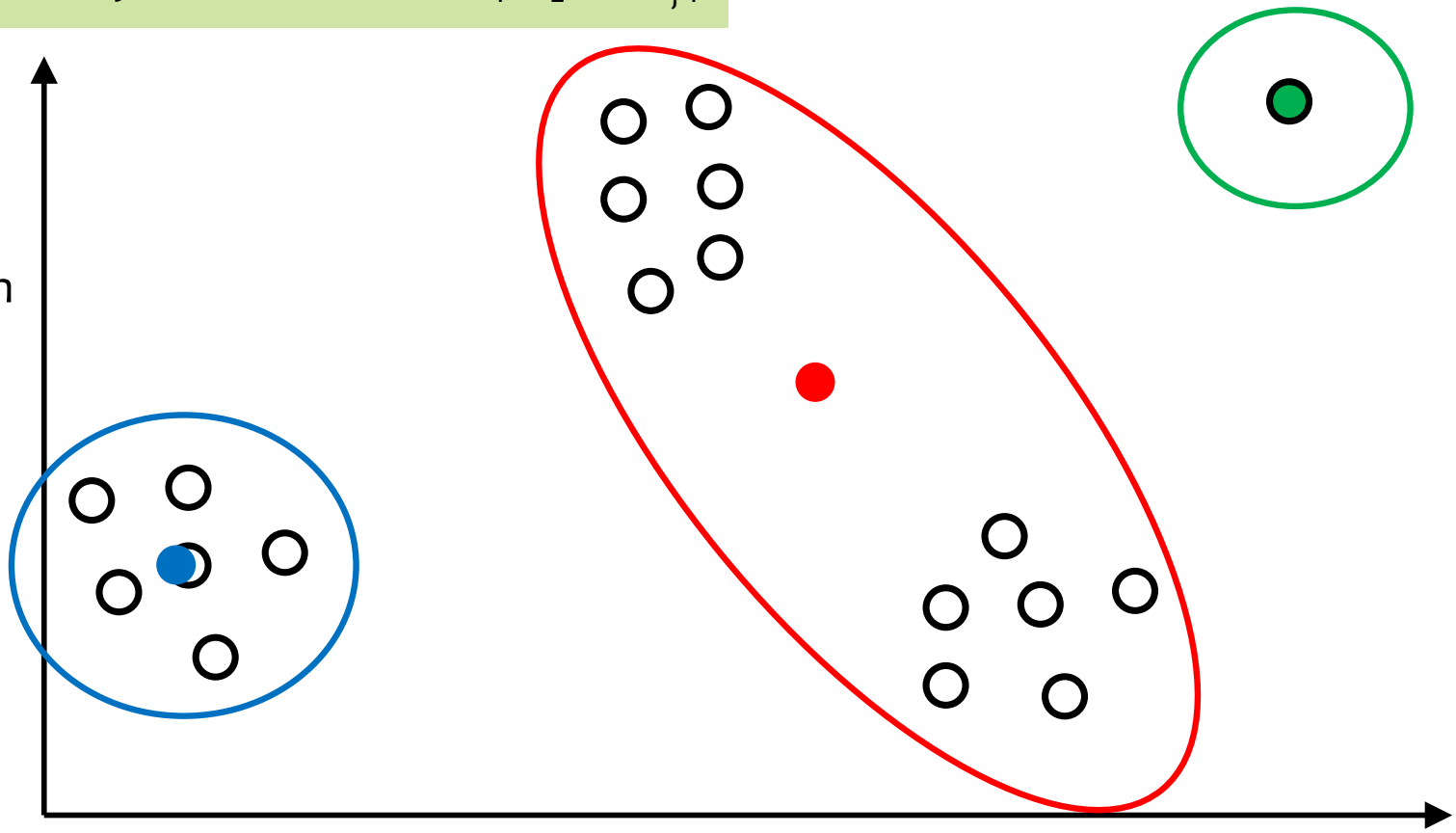
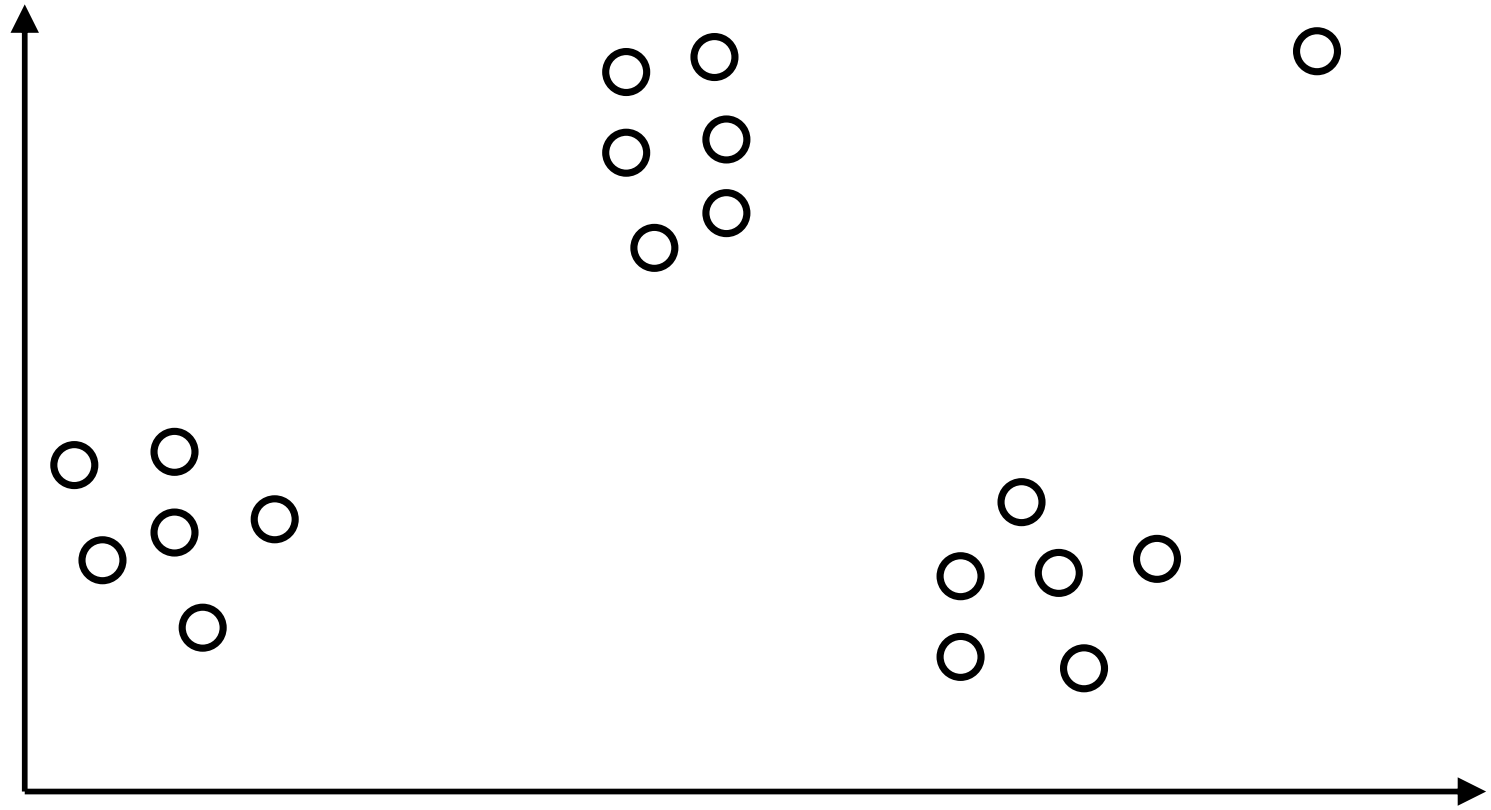


Initialization for K-Means

Algorithm #3: K-Means++

- Let $D(\mathbf{x})$ be the distance between a point x and its nearest center. Chose the next center proportional to $D^2(\mathbf{x})$.



Initialization for K-M

i	D(x)	$D^2(x)$	$P(c_2 = x^{(i)})$
1	3	9	9/137
2	2	4	4/137
…			
7	4	16	16/137
…			
N	3	9	9/137
	Sum:	137	1.0

Algorithm #3: K-Means++

- Let $D(\mathbf{x})$ be the distance between a point x and its nearest center. Chose the next center proportional to $D^2(\mathbf{x})$.

- Choose $\mathbf{c_1}$ at random.
- For $j = 2, \ldots, K$
  - Pick $\mathbf{c_j}$ among $\mathbf{x^{(1)}}, \mathbf{x^{(2)}}, \ldots, \mathbf{x^{(n)}}$ according to the distribution

$$\mathbf{P(c_j = x^{(i)}) \propto \min_{j'<j} \left|\left|x^{(i)} - c_{j'}\right|\right|^2} \; D^2(\mathbf{x^i})$$

Theorem: K-Means++ always attains an $O(\log k)$ approximation to optimal K-Means solution in expectation.

Slide adapted from Nina Balcan

Initialization for K-M

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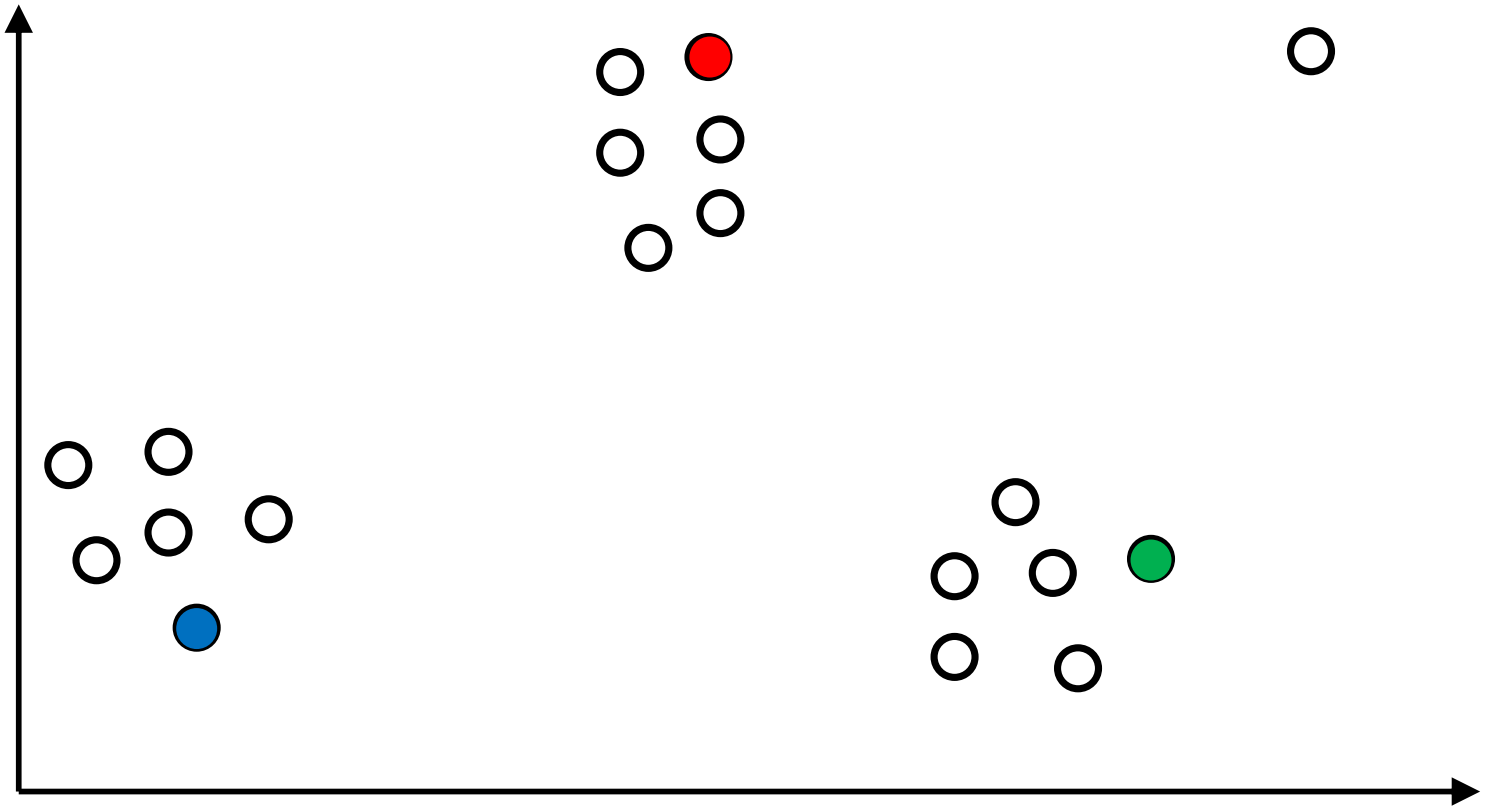

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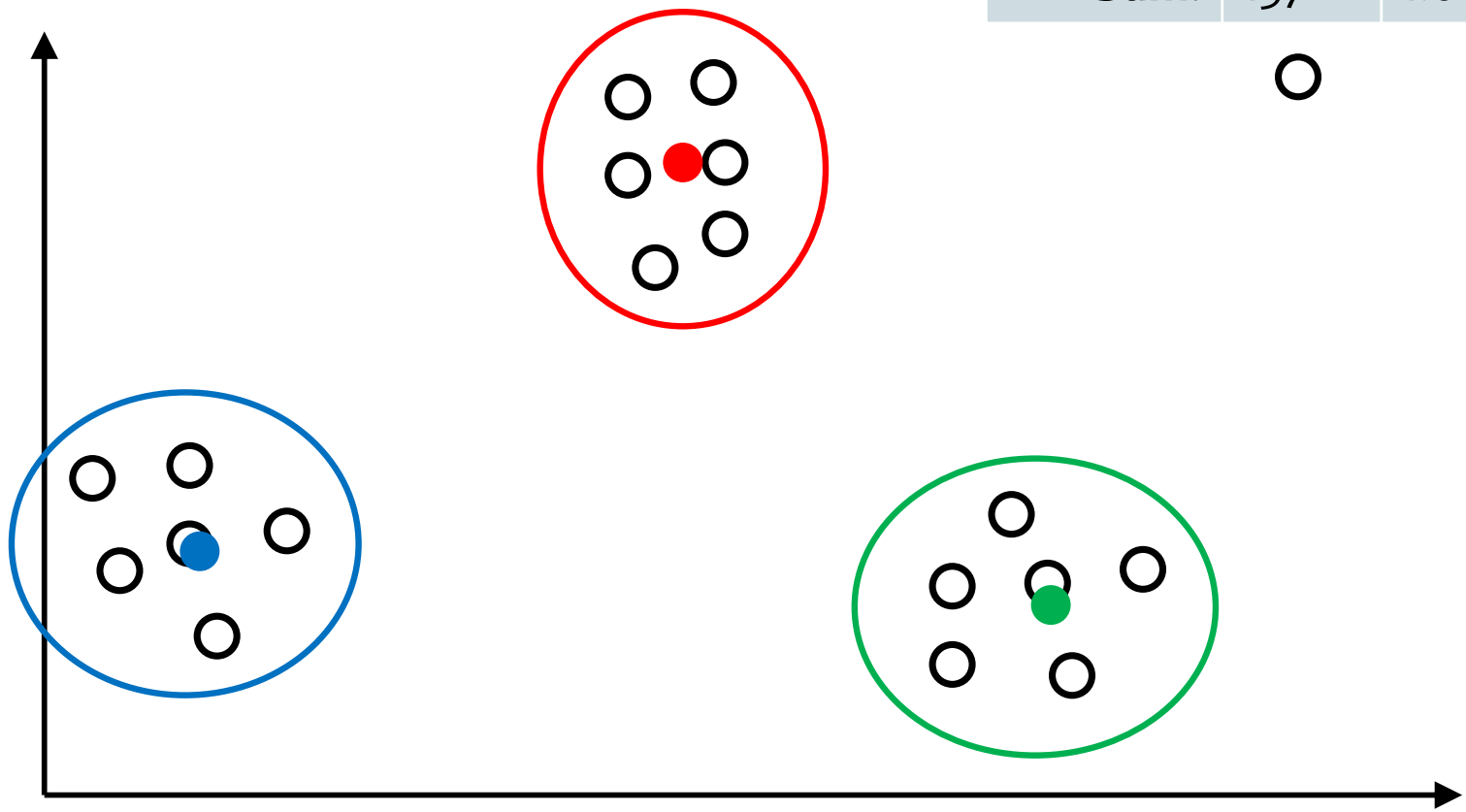


Initialization for K-Means

Algorithm #3: K-Means++

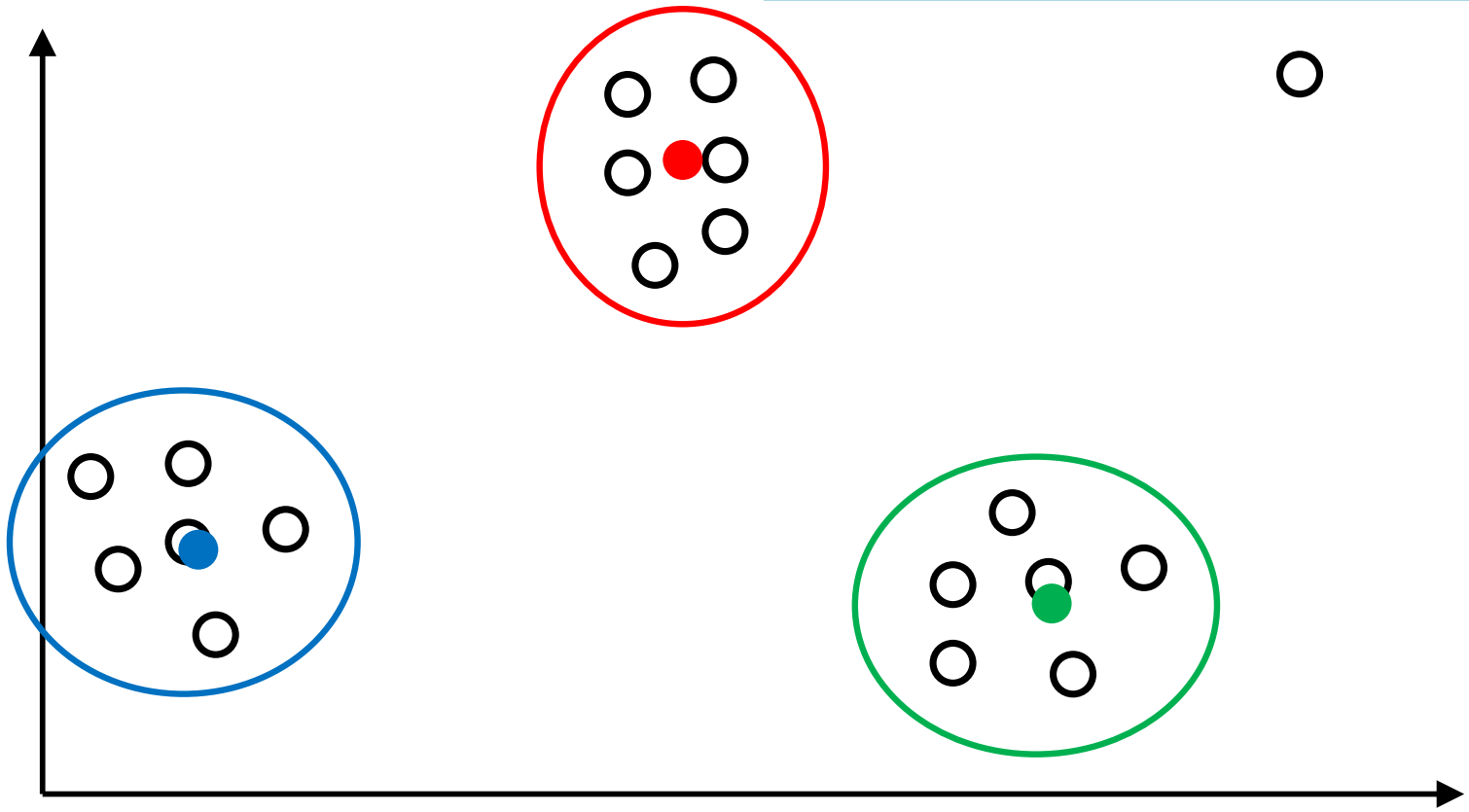
- Let $D(\mathbf{x})$ be the distance between a point x and its nearest center. Chose the next center proportional to $D^2(\mathbf{x})$.

Observations:

- Interpolates between random and farthest point initialization
- Solves the problem with Gaussian data
- **And** solves the outlier problem

Example 1:

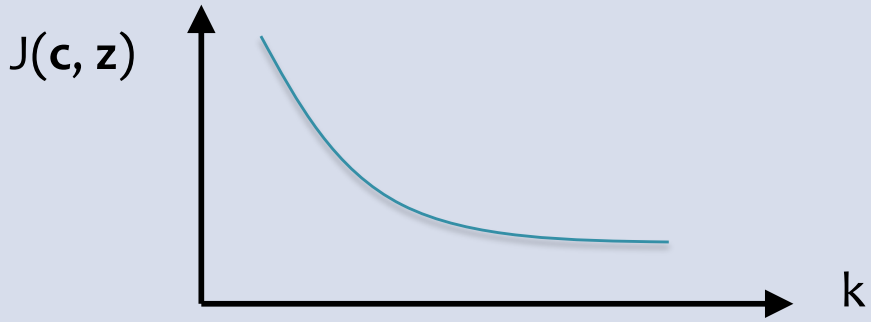
- One outlier
- Good performance



Q&A

Q: In k-Means, since we don't have a validation set, how do we pick k?

A: Look at the training objective function as a function of k and pick the value at the "elbo" of the curve.



Q: What if our random initialization for k-Means gives us poor performance?

A: Do **random restarts**: that is, run k-means from scratch, say, 10 times and pick the run that gives the lowest training objective function value.

The objective function is **nonconvex**, so we're just looking for the best local minimum.

Learning Objectives

K-Means

You should be able to…

1. Distinguish between coordinate descent and block coordinate descent
2. Define an objective function that gives rise to a "good" clustering
3. Apply block coordinate descent to an objective function preferring each point to be close to its nearest objective function to obtain the K-Means algorithm
4. Implement the K-Means algorithm
5. Connect the non-convexity of the K-Means objective function with the (possibly) poor performance of random initialization

Ensemble Methods

Ensemble methods learn a collection of models (i.e. the **ensemble**) and combine their predictions on a test instance.

We consider two types:

- **Bagging**: learns models in parallel by taking many subsets of the training data
- **Boosting**: learns models serially by reweighting the training data

Bagging

"BAGGing" is also called Boostrap AGGregretion

Bagging answers the question:
How can I obtain many classifiers/regressors to ensemble together?

We'll consider three possible answers:

1. **(sample) bagging**
2. **feature bagging** (aka. random subspace method)
3. **random forests** (which combine sample bagging and feature bagging to train a "forest" of decision trees)

BAGGING

(Sample) Bagging

Key idea: Repeatedly sample with replacement a collection of training examples and train a model on that sample.

Return an ensemble of the trained models; combine predictions by majority vote for classification and by averaging for regression.

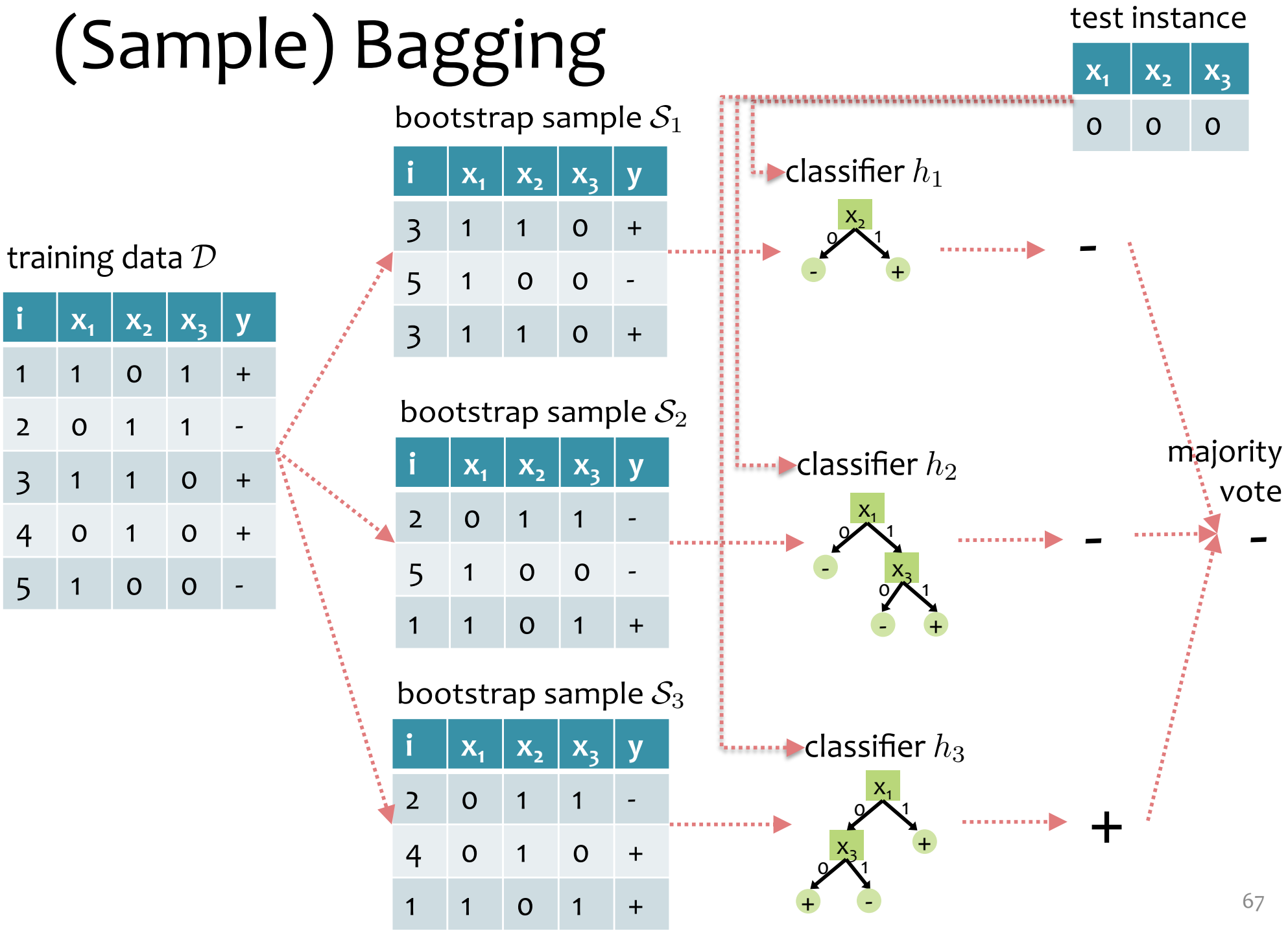
Algorithm 1 (Sample) Bagging

procedure SAMPLEBAGGING($\mathcal{D}$, T, S)
  for $t = 1, \ldots, T$ **do**
    for $s = 1, \ldots, S$ **do**
      $i_s \sim \text{Uniform}(1, \ldots, N)$
    $\mathcal{S}_t = \{(\mathbf{x}^{(i_s)}, y^{(i_s)})\}_{s=1}^{S}$ ▷ Bootstrap sample
    $h_t = \text{train}(\mathcal{S}_t)$ ▷ Classifier
  return $\hat{h}(\mathbf{x}) = \text{aggregate}(h_1, \ldots, h_T)$ ▷ Ensemble

for classification: $\hat{h}(\mathbf{x}) = \text{argmax}_{y \in \mathcal{Y}} \sum_{t=1}^{T} \mathbb{I}[y = h_t(\mathbf{x})]$ ▷ Majority vote

for regression: $\hat{h}(\mathbf{x}) = \frac{1}{T} \sum_{t=1}^{T} h_t(\mathbf{x})$ ▷ Average

(Sample) Bagging



Feature Bagging

Key idea: Repeatedly sample without replacement a subset of the features, create a copy of the training data with only those features, and train a model on the copy.

Return an ensemble of the trained models; combine predictions by majority vote for classification and by averaging for regression.

Algorithm 2 Feature Bagging

procedure SAMPLEBAGGING($\mathcal{D}$, T, S)
  for $t = 1, \ldots, T$ **do**
    for $s = 1, \ldots, S$ **do**
      $m_s \sim \text{Uniform}(1, \ldots, M)$
    for $i = 1, \ldots, N$ **do**
      $\tilde{\mathbf{x}}^{(i)} = [x_{m_1}^{(i)}, x_{m_2}^{(i)}, \ldots, x_{m_S}^{(i)}]^T$
    $\mathcal{D}_t = \{(\tilde{\mathbf{x}}^{(i)}, y^{(i)}\}_{i=1}^N$ ▷ Random subspace
    $h_t = \text{train}(\mathcal{D}_t)$ ▷ Classifier
  return $\hat{h}(\mathbf{x}) = \text{aggregate}(h_1, \ldots, h_T)$ ▷ Ensemble

Feature Bagging

training data $\mathcal{D}$

i	x_1	x_2	x_3	x_4	y
1	1	0	1	0	+
2	0	1	1	1	-
3	1	1	0	0	+

bootstrap sample $\mathcal{S}_1$

i	x_4	x_2	y
1	0	0	+
2	1	1	-
3	0	1	+

bootstrap sample $\mathcal{S}_2$

i	x_2	x_3	y
1	0	1	+
2	1	1	-
3	1	0	+

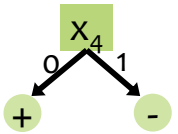
bootstrap sample $\mathcal{S}_3$

i	x_1	x_3	y
1	1	1	+
2	0	1	-
3	1	0	+

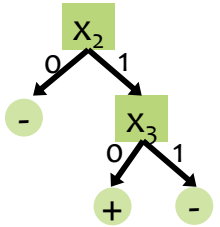
test instance

x_1	x_2	x_3	x_4
0	1	0	0

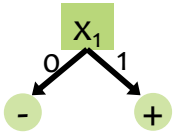
classifier h_1



classifier h_2



classifier h_3



majority vote

+

RANDOM FORESTS

Random Forests

- Combines the prediction of many diverse decision trees to reduce their variability
- If B independent random variables $x^{(1)}, x^{(2)}, \dots, x^{(B)}$ all have variance σ^2, then the variance of $\frac{1}{B}\sum_{b=1}^{B} x^{(b)}$ is $\frac{\sigma^2}{B}$
- Random forests

  = bagging + split-feature randomization

  = **b**ootstrap **agg**regat**ing** + split-feature randomization

Random Forests

Key idea: Combine (sample) bagging and a specific variant of feature bagging to train decision trees.

Repeat the following to train many decision trees:

- draw a sample with replacement from the training examples,
- recursively learn the decision tree
- but at each node when choosing a feature on which to split, first randomly sample a subset of the features, then pick the best feature from among that subset.

Return an ensemble of the trained decision trees.

Split-feature Randomization

- Issue: decision trees trained on bootstrapped samples still behave similarly
- Idea: in addition to sampling the data points (i.e., the rows), also sample the features (i.e., the columns)
- Each time a split is being considered, limit the possible features to a randomly sampled subset

Runtime	Genre	Budget	Year	IMDB	Rating

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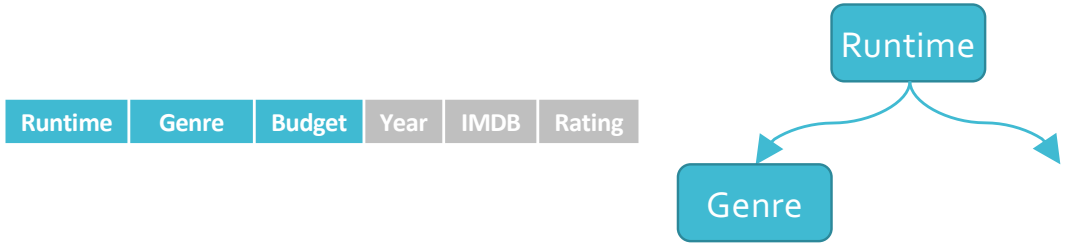

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Random Forests

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$, B, ρ
- For $b = 1, 2, \ldots, B$
  - Create a dataset, $\mathcal{D}_b$, by sampling N points from the original training data $\mathcal{D}$ ***with replacement***
  - Learn a decision tree, t_b, using $\mathcal{D}_b$ and the CART algorithm ***with split-feature randomization***, sampling ρ features for each split
- Output: $\bar{t} = f(t_1, \ldots, t_B)$, the aggregated hypothesis

How can we set B and ρ?

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$, B, ρ
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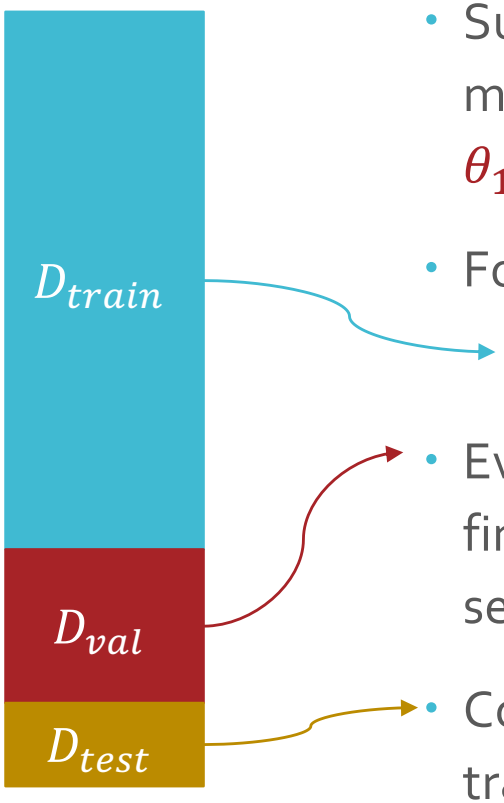
Recall: Validation Sets



- Suppose we want to compare multiple hyperparameter settings $\theta_1, \ldots, \theta_K$
- For $k = 1, 2, \ldots, K$
  - Train a model on D_{train} using θ_k
- Evaluate each model on D_{val} and find the best hyperparameter setting, θ_{k^*}
- Compute the error of a model trained with θ_{k^*} on D_{test}

Out-of-bag Error

- For each training point, $\boldsymbol{x}^{(n)}$, there are some decision trees which $\boldsymbol{x}^{(n)}$ was not used to train (roughly B/e trees or 37%)
  - Let these be $t^{(-n)} = \left\{t_1^{(-n)}, t_2^{(-n)}, \ldots, t_{N-n}^{(-n)}\right\}$
- Compute an aggregated prediction for each $\boldsymbol{x}^{(n)}$ using the trees in $t^{(-n)}$, $\bar{t}^{(-n)}\left(\boldsymbol{x}^{(n)}\right)$
- Compute the out-of-bag (OOB) error, e.g., for regression

$$E_{OOB} = \frac{1}{N}\sum_{n=1}^{N}\left(\bar{t}^{(-n)}\left(\boldsymbol{x}^{(n)}\right) - y^{(n)}\right)^2$$

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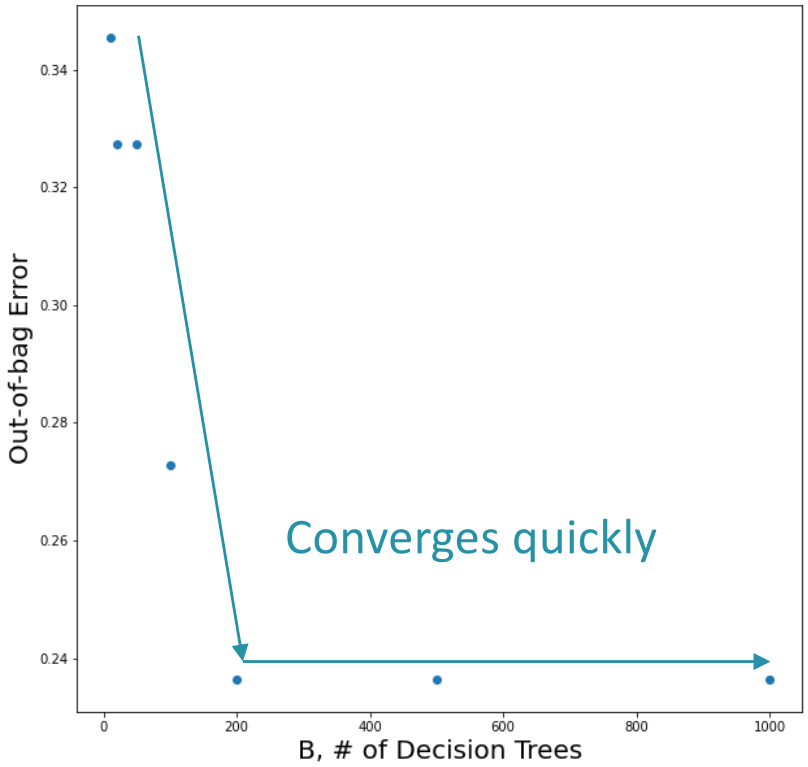
- Compute the out-of-bag (OOB) error, e.g., for classification

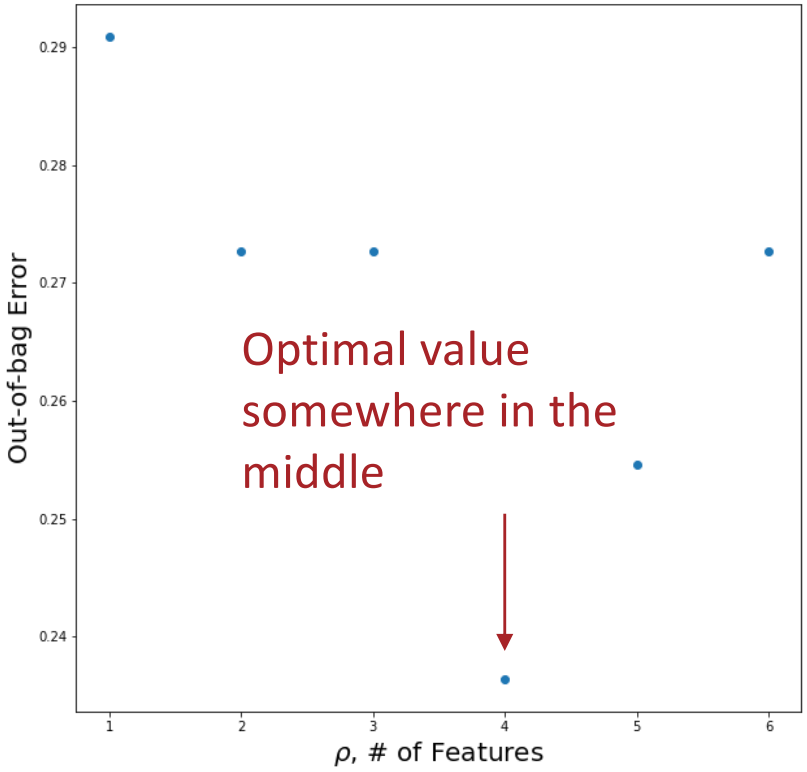
$$E_{OOB} = \frac{1}{N}\sum_{n=1}^{N}\left[\!\left[\bar{t}^{(-n)}\left(\boldsymbol{x}^{(n)}\right) \neq y^{(n)}\right]\!\right]$$

- E_{OOB} can be used for hyperparameter optimization!

Out-of-bag Error

- Suppose we want to compare different numbers of trees in our random forest $B_1, \ldots, B_K$
- For $k = 1, 2, \ldots, K$
  - Train a random forest on D_{train} with B_k trees
- Compute E_{OOB} for each random forest and find the best number of trees, B_{k^*}
- Evaluate the random forest with B_{k^*} trees on D_{test}



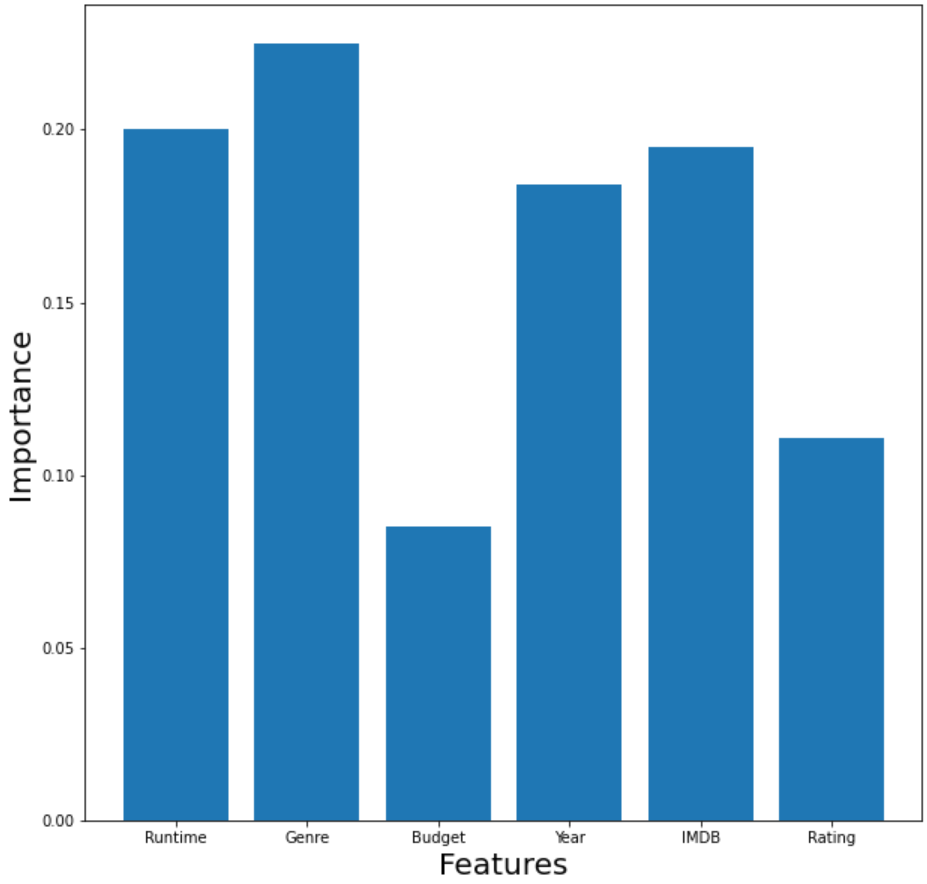


Setting Hyperparameters

Feature Importance

- Some of the interpretability of decision trees gets lost when switching to random forests
- Random forests allow for the computation of "feature importance", a way of ranking features based on how useful they are at predicting the target
- Initialize each feature's importance to zero
- Each time a feature is chosen to be split on, add the reduction in Gini impurity (weighted by the number of data points in the split) to its importance

Feature Importance



Key Takeaways

- Ensemble methods employ a "wisdom of crowds" philosophy
  - Can reduce the variance of high variance methods
- Random forests = bagging + split-feature randomization
  - Aggregate multiple decision trees together
  - Bootstrapping and split-feature randomization increase diversity in the decision trees
  - Use out-of-bag errors for hyperparameter optimization
  - Use feature importance to identify useful attributes

Learning Objectives

Ensemble Methods: Bagging

You should be able to…

1. Distinguish between (sample) bagging, the random subspace method, and random forests.
2. Implement (sample) bagging for an arbitrary base classifier/regressor.
3. Implement the random subspace method for an arbitrary base classifier/ regressor.
4. Implement random forests.
5. Contrast out-of-bag error with cross-validation error.
6. Differentiate boosting from bagging.
7. Compare and contrast weighted and unweighted majority vote of a collection of classifiers.
8. Discuss the relation in bagging between the sample size and variance of the base classifier/regressor.
9. Bound the generalization error of a random forest classifier.