10-301/601: Introduction to Machine Learning Lecture 19: Clustering & Bagging

Henry Chai & Matt Gormley

11/27/23

Front Matter

- Announcements
  - HW8 released 11/20, due 12/1 (Friday) at 11:59 PM

Clustering

- Goal: split an *unlabeled* data set into groups or clusters of "similar" data points
- Use cases:
  - Organizing data
  - Discovering patterns or structure
  - Preprocessing for downstream machine learning tasks
- Applications:

Recall: Similarity for kNN

- Intuition: ~~predict the label of a data point to be the label of the "most similar" training point~~ two points are "similar" if the distance between them is small
- Euclidean distance: $d(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_2$

Partition-Based Clustering

- Given a desired number of clusters, K, return a partition of the data set into K groups or clusters, $\{C_1, \dots, C_K\}$, that optimize some objective function

1. What objective function should we optimize?

2. How can we perform optimization in this setting?

Example Clusterings

Option A

Option B

Example Clusterings

Recipe for K-means

- Define a model and model parameters

- Write down an objective function

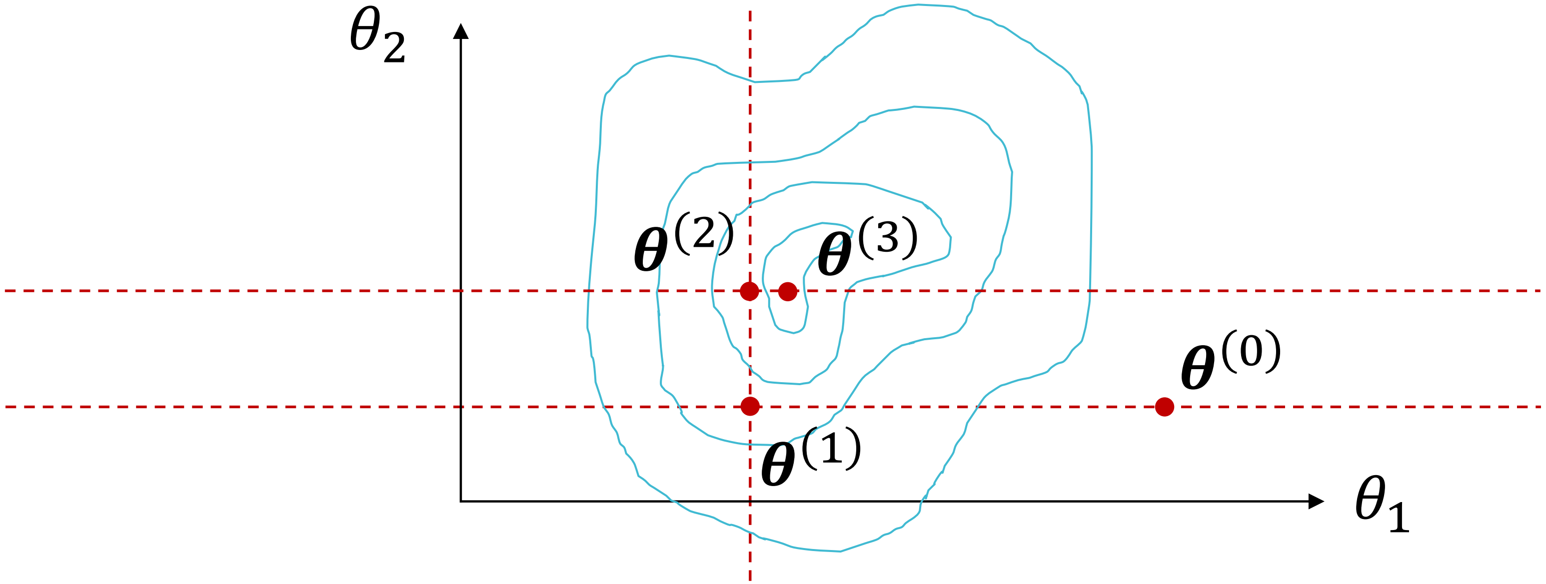
- Optimize the objective w.r.t. the model parameters

Coordinate Descent

- Goal: minimize some objective

$$\hat{\boldsymbol{\theta}} = \text{argmin } J(\boldsymbol{\theta})$$

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



Block Coordinate Descent

- Goal: minimize some objective

$$\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}} = \operatorname{argmin}\ J(\boldsymbol{\alpha}, \boldsymbol{\beta})$$

- Idea: iteratively pick one *block* of variables ($\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$) and minimize the objective w.r.t. that block, keeping the other(s) fixed.
  - Ideally, blocks should be the largest possible set of variables *that can be efficiently optimized simultaneously*

Optimizing the K-means objective

$$\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_K, z^{(1)}, \dots, z^{(\mathrm{N})} = \operatorname{argmin} \sum_{n=1}^{N} \left\| \boldsymbol{x}^{(n)} - \boldsymbol{\mu}_{z^{(n)}} \right\|_2$$

- If $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K$ are fixed
- If $z^{(1)}, \dots, z^{(N)}$ are fixed

K-means Algorithm

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}\right)\right\}_{n=1}^{N}, K$

1. Initialize cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
2. While NOT CONVERGED
   a. Assign each data point to the cluster with the nearest cluster center:
   $$z^{(n)} = \underset{k}{\operatorname{argmin}} \left\| \boldsymbol{x}^{(n)} - \boldsymbol{\mu}_k \right\|_2$$
   b. Recompute the cluster centers:
   $$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n\, : z^{(n)} = k} \boldsymbol{x}^{(n)}$$
   where N_k is the number of data points in cluster k

- Output: cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ and cluster assignments $z^{(1)}, \ldots, z^{(N)}$

K-means: Example ($K = 3$)

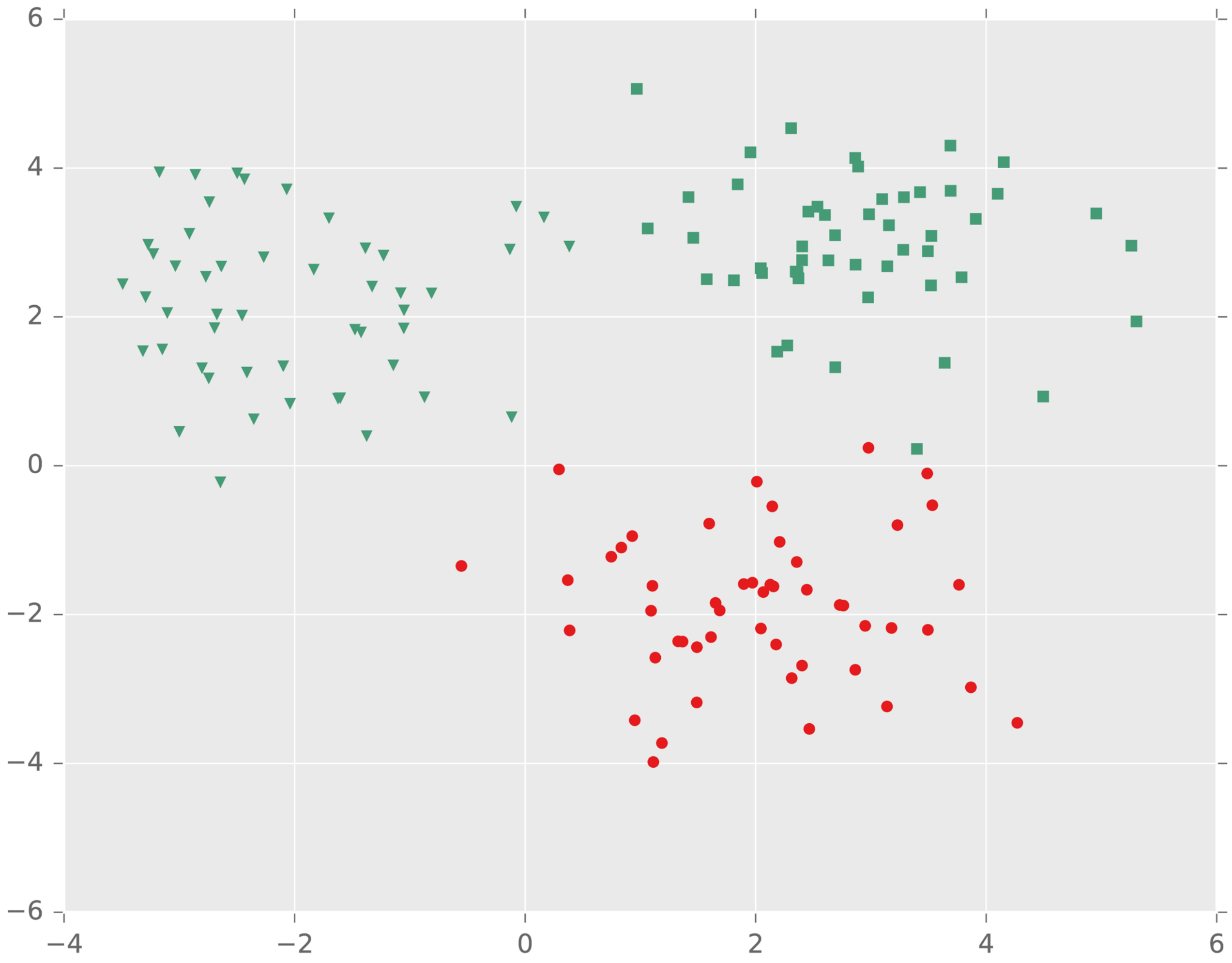


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

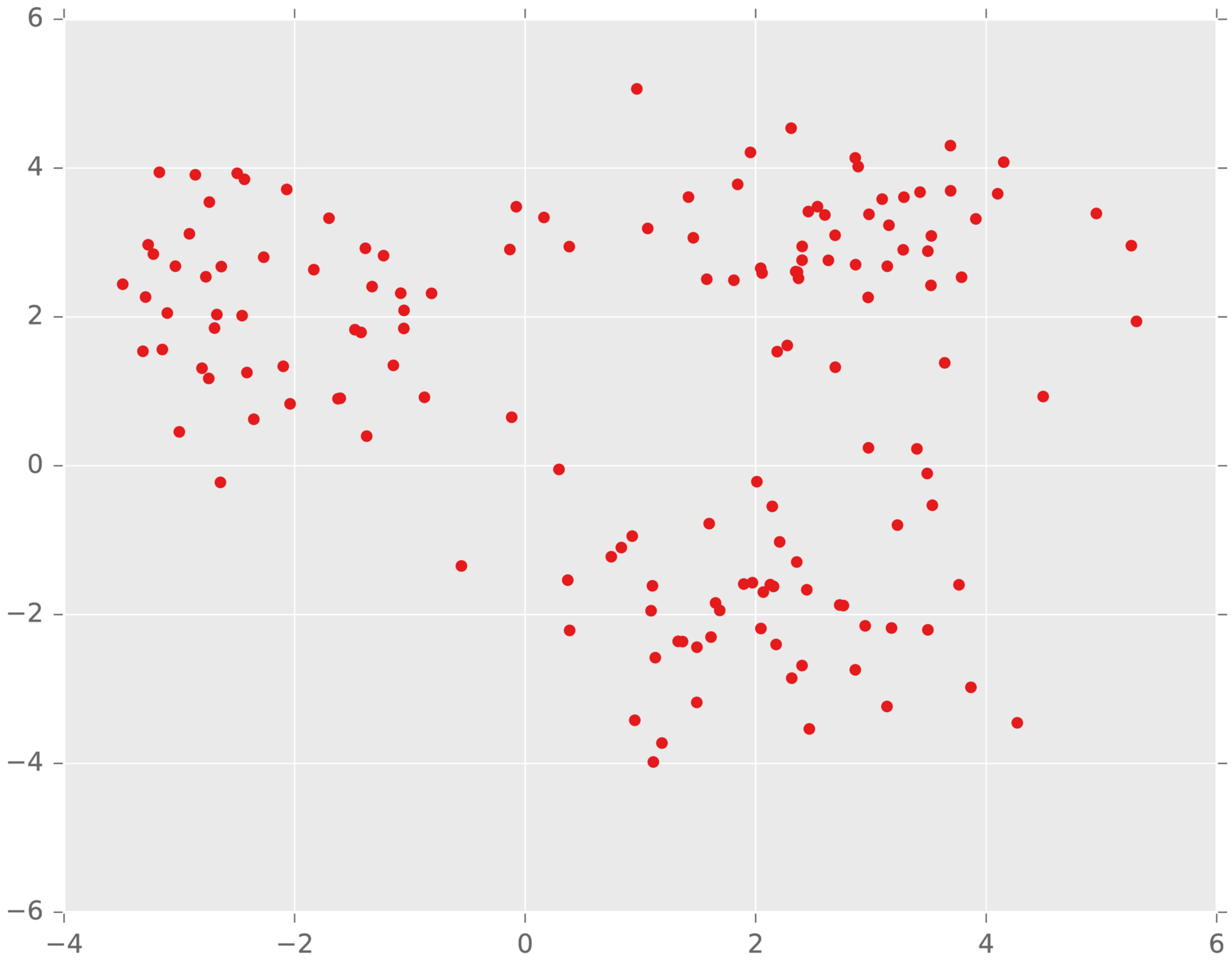


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

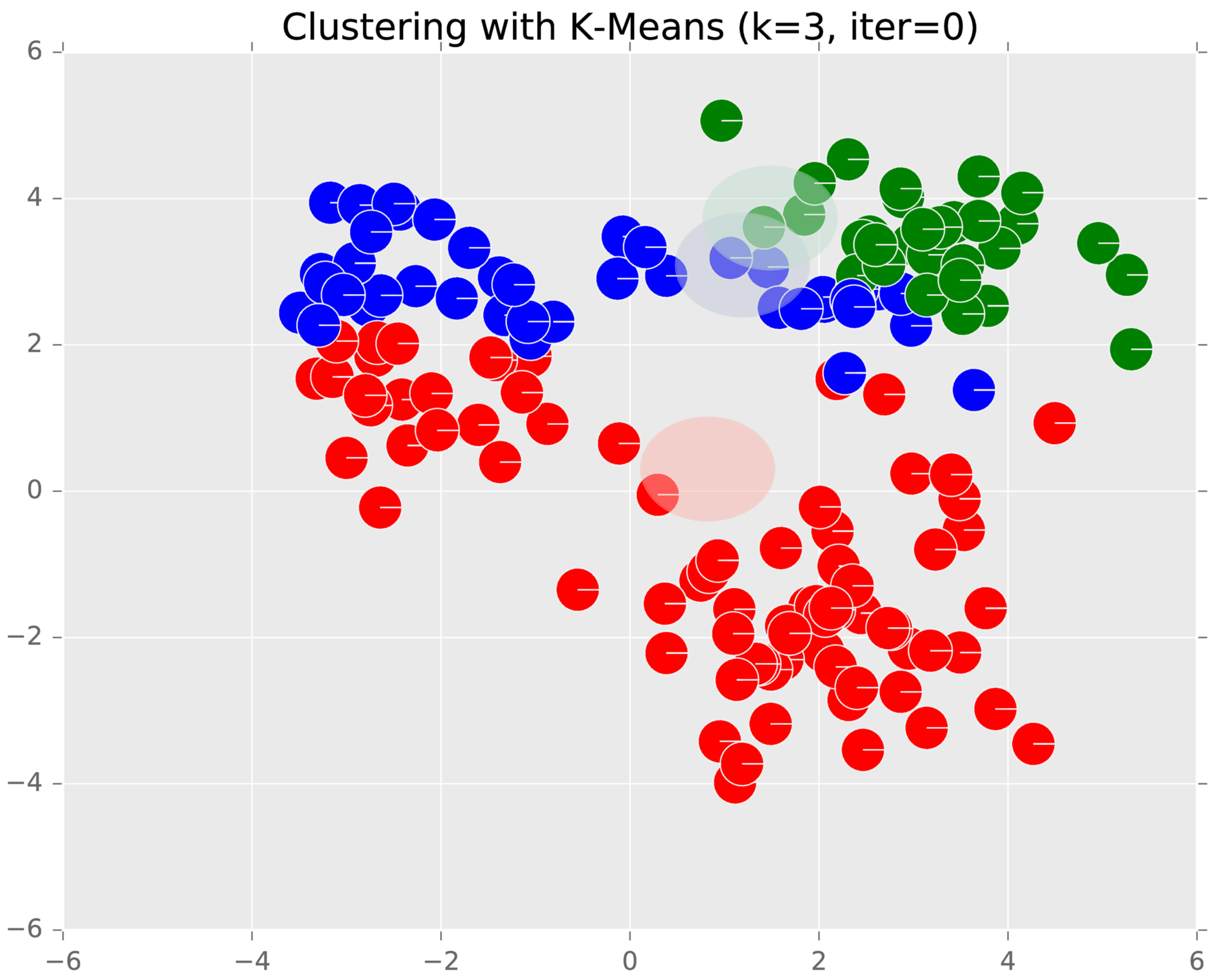


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

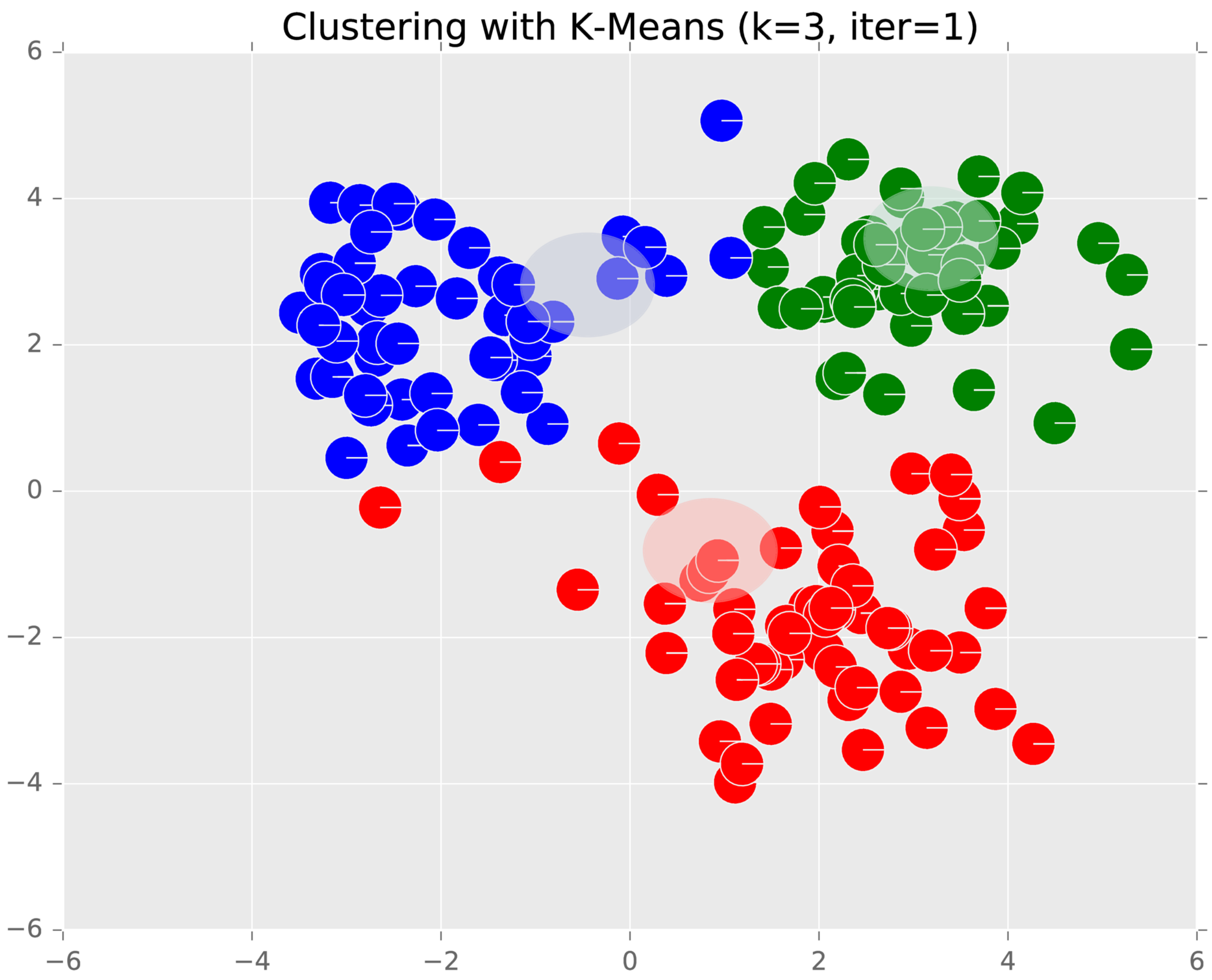


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

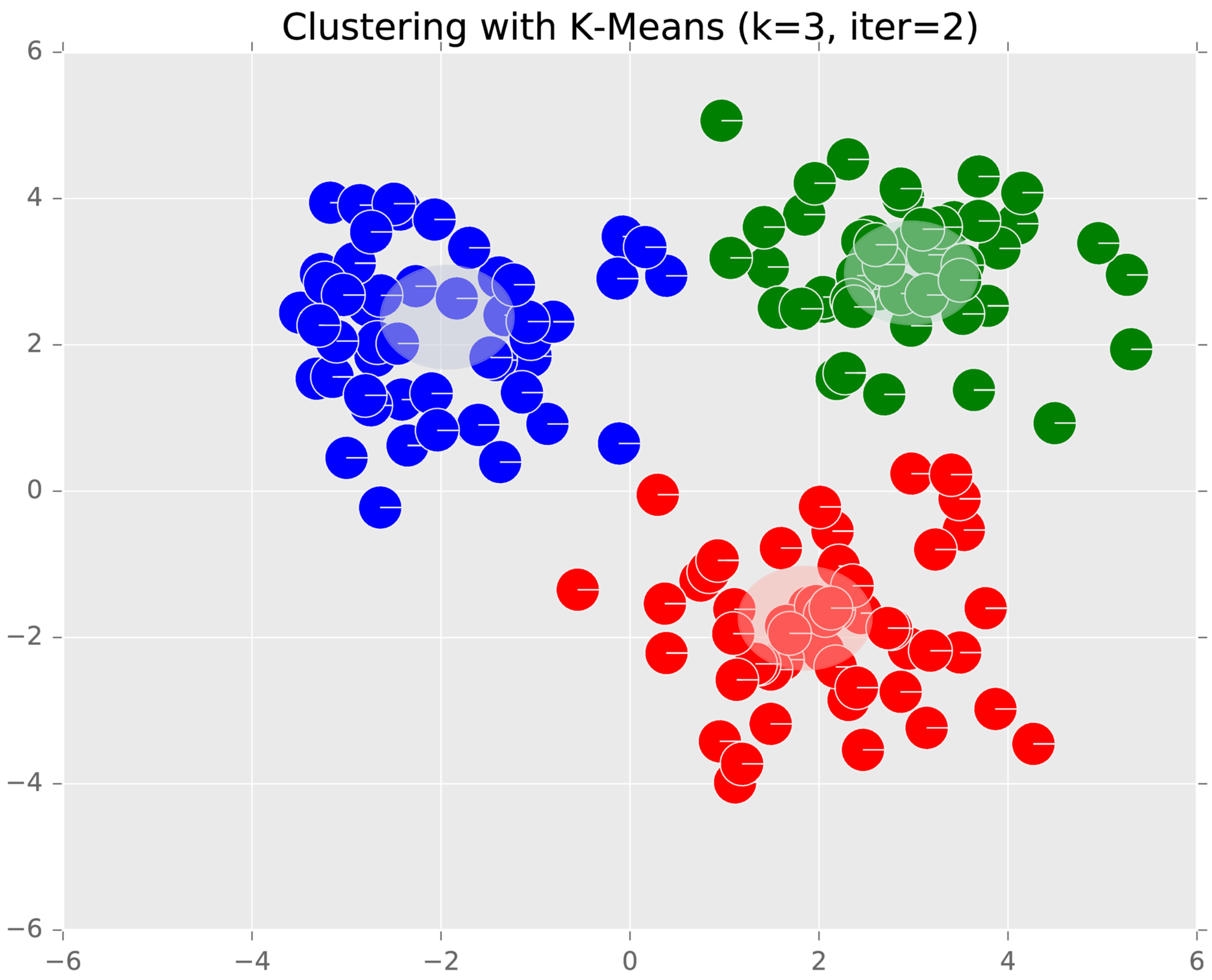


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

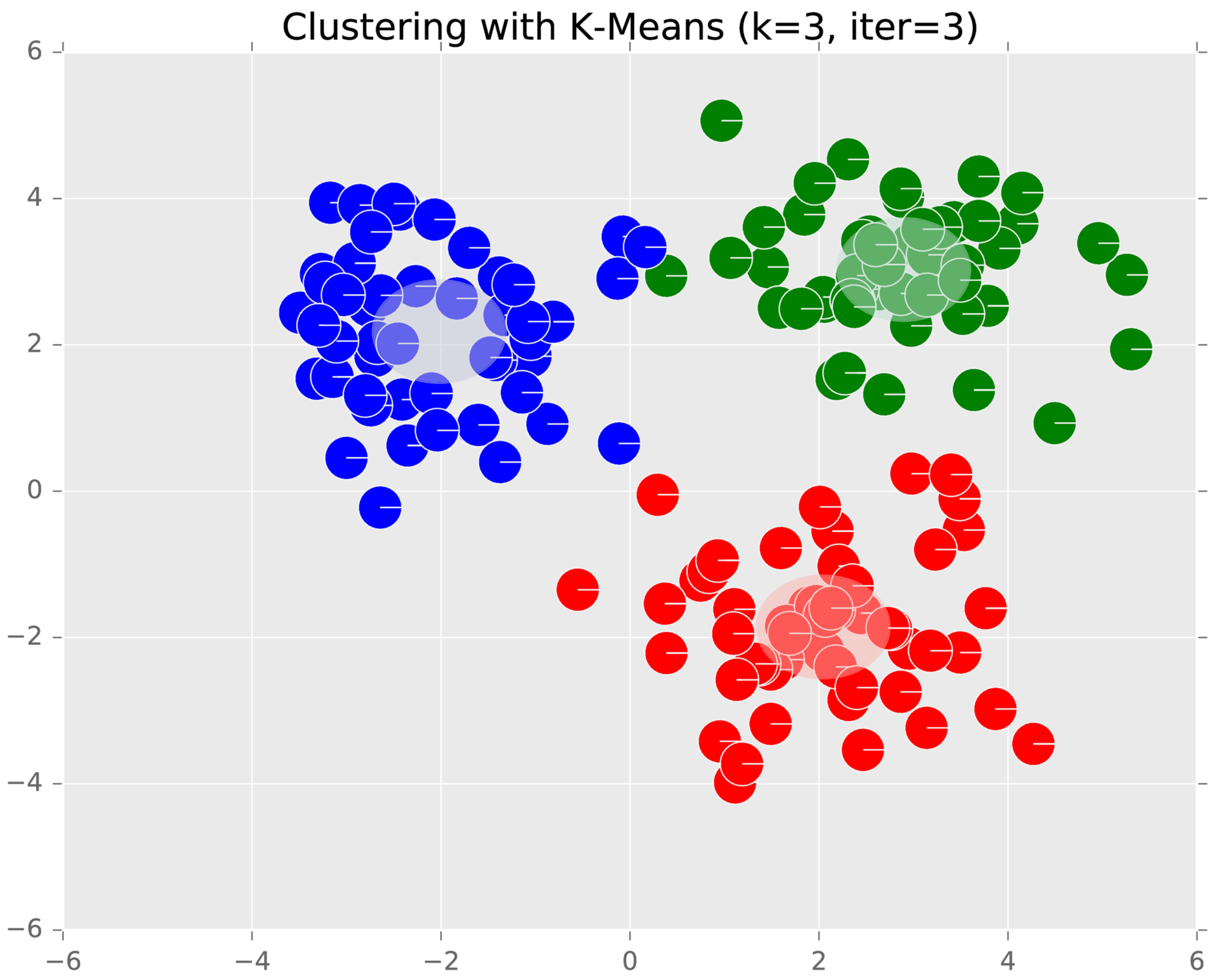


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

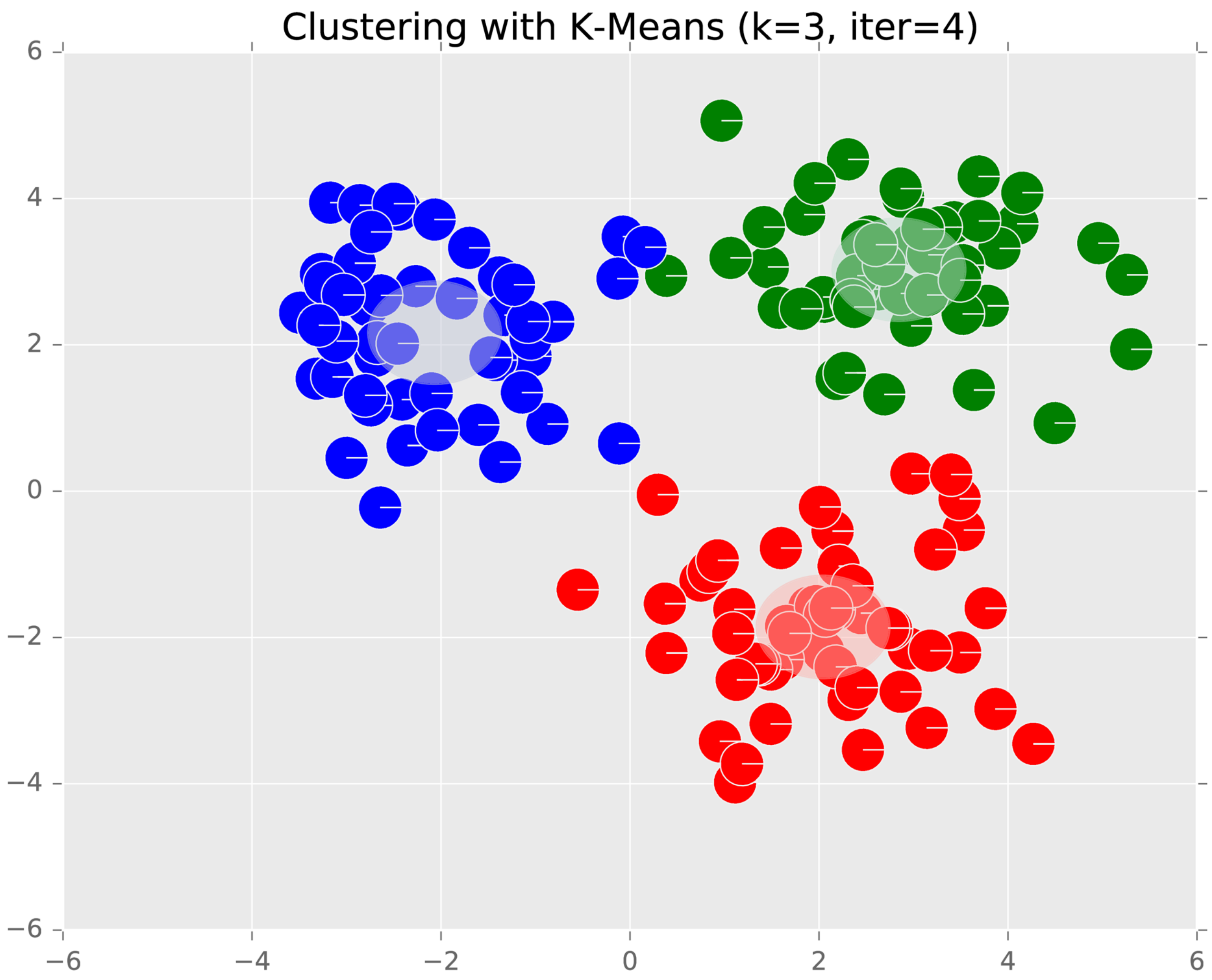


Figure courtesy of Matt Gormley

K-means: Example ($K = 3$)

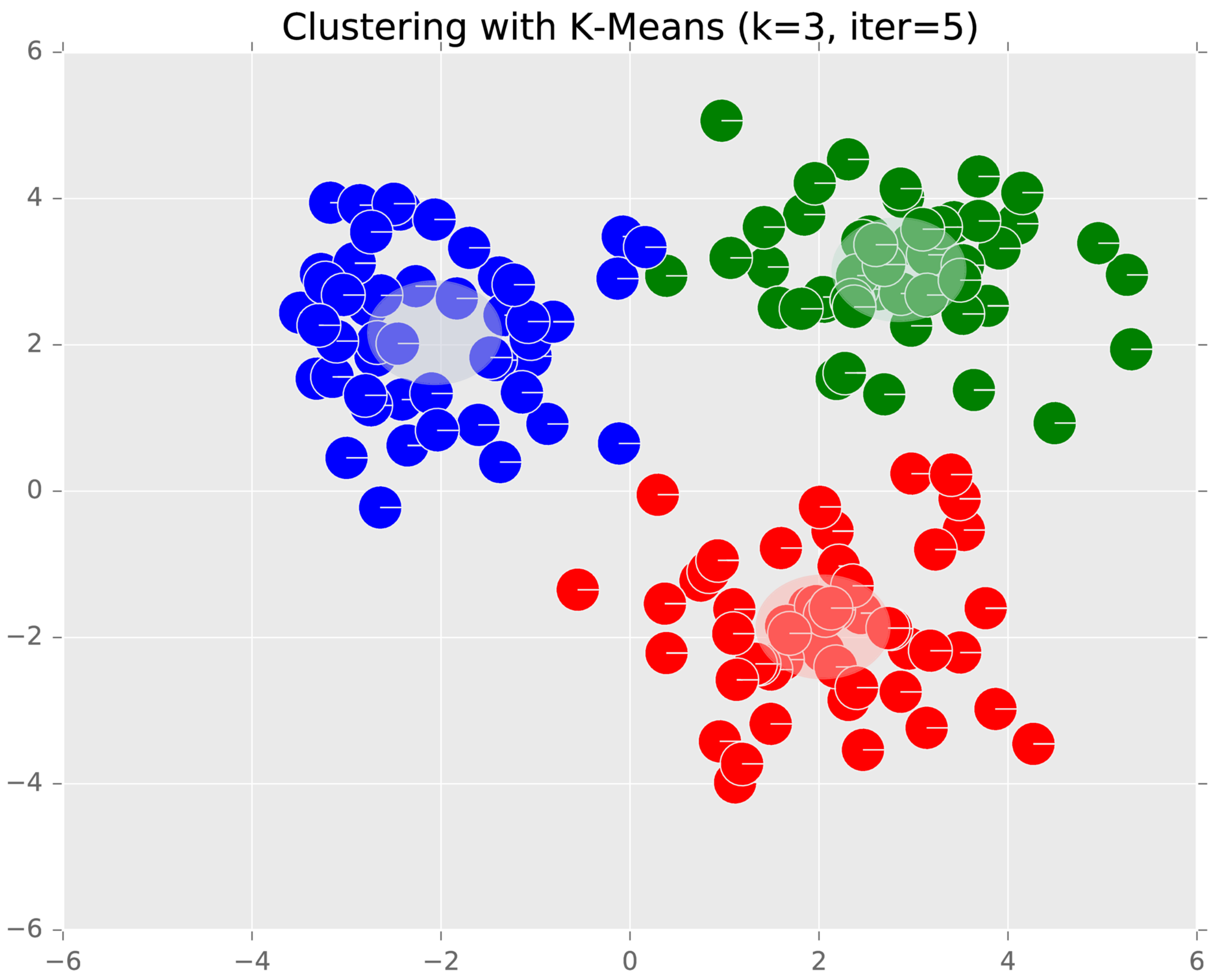


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

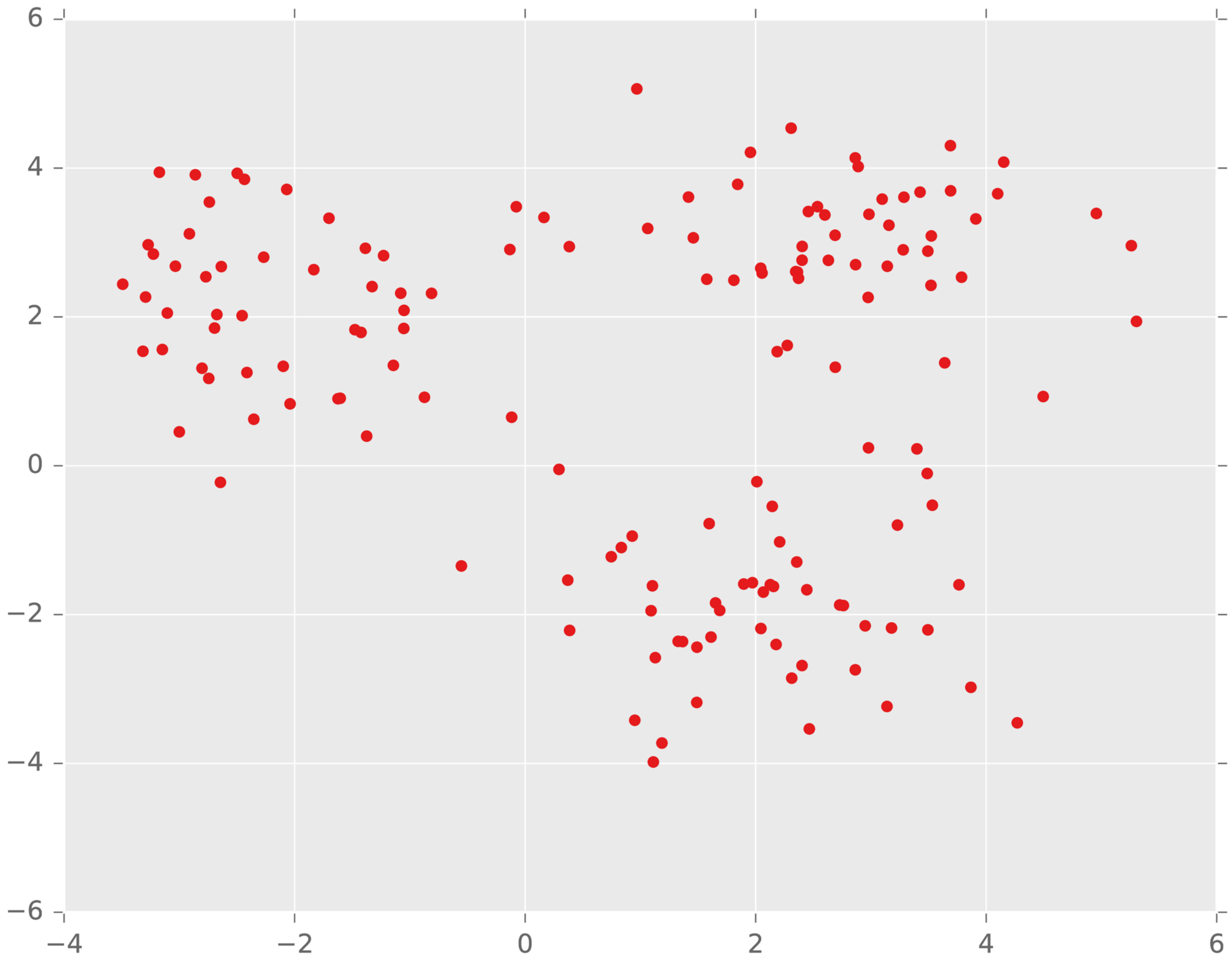


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

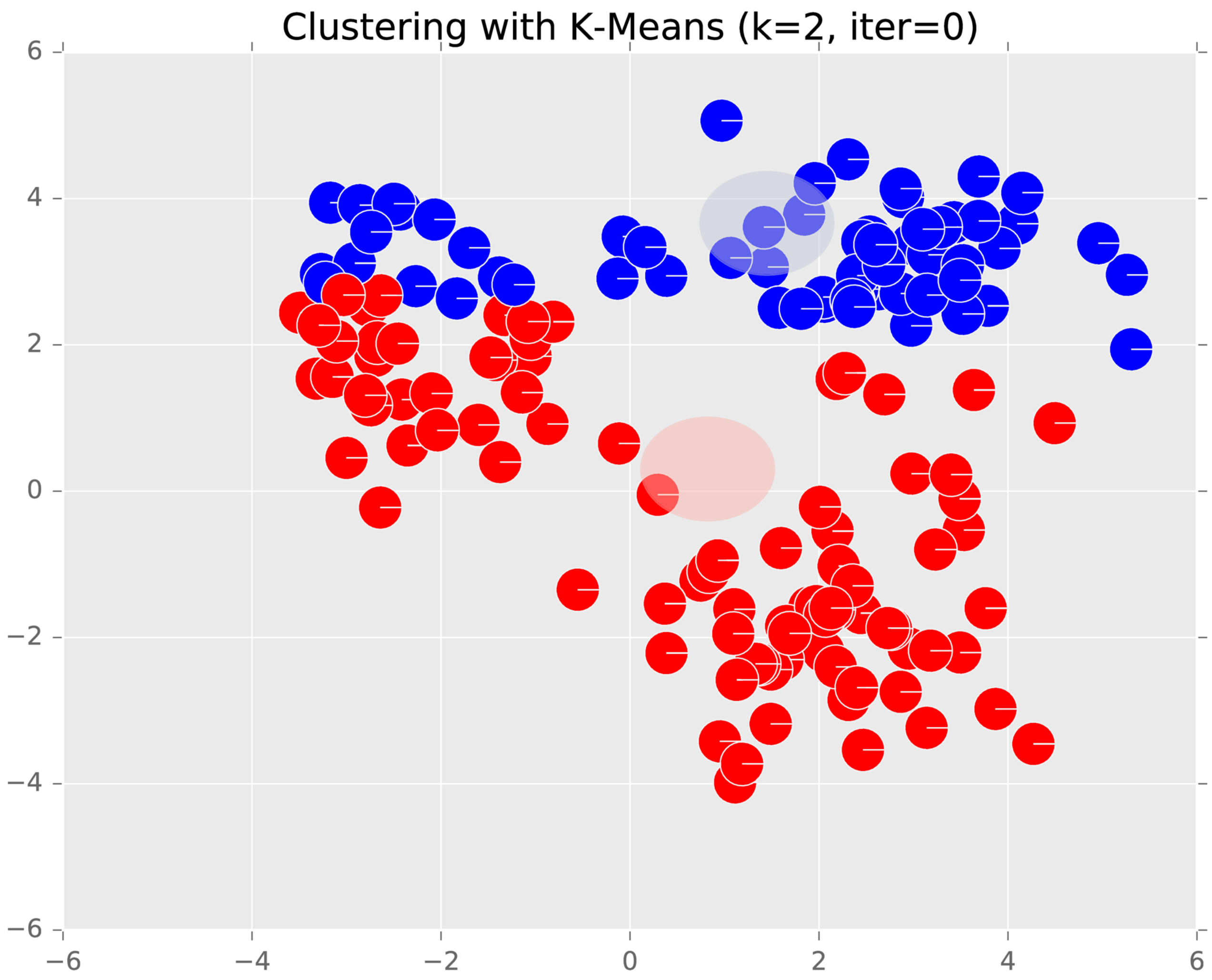


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

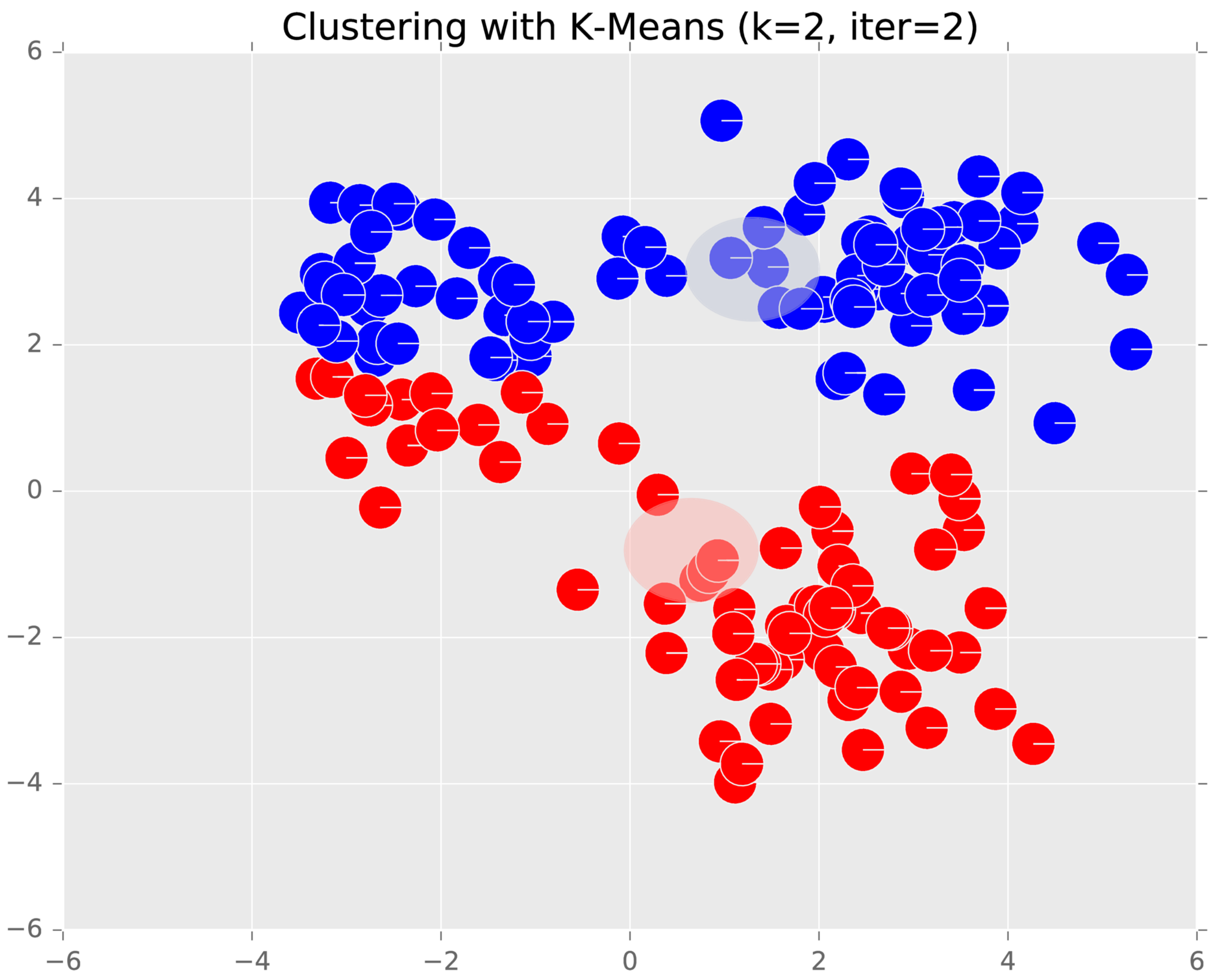


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

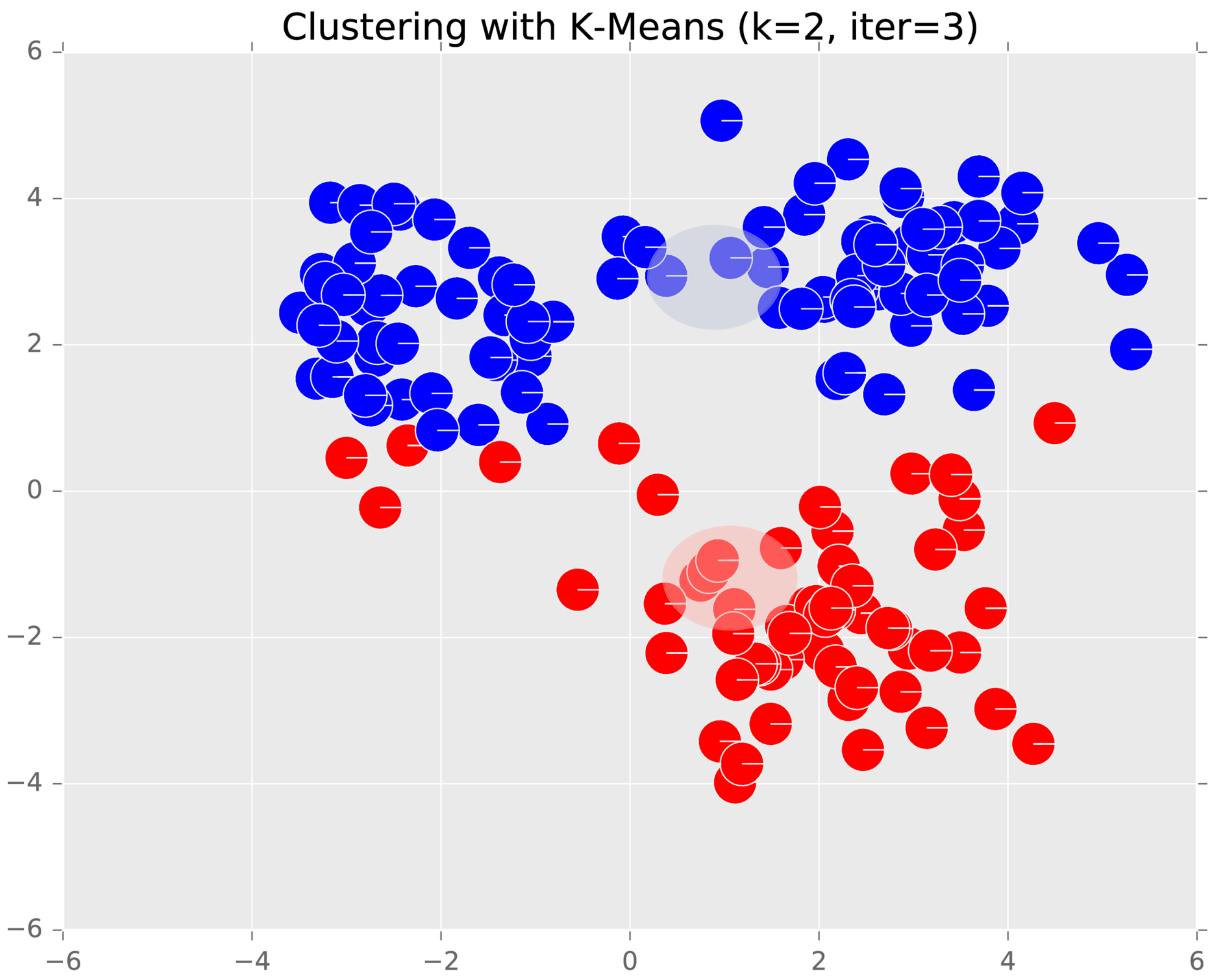


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

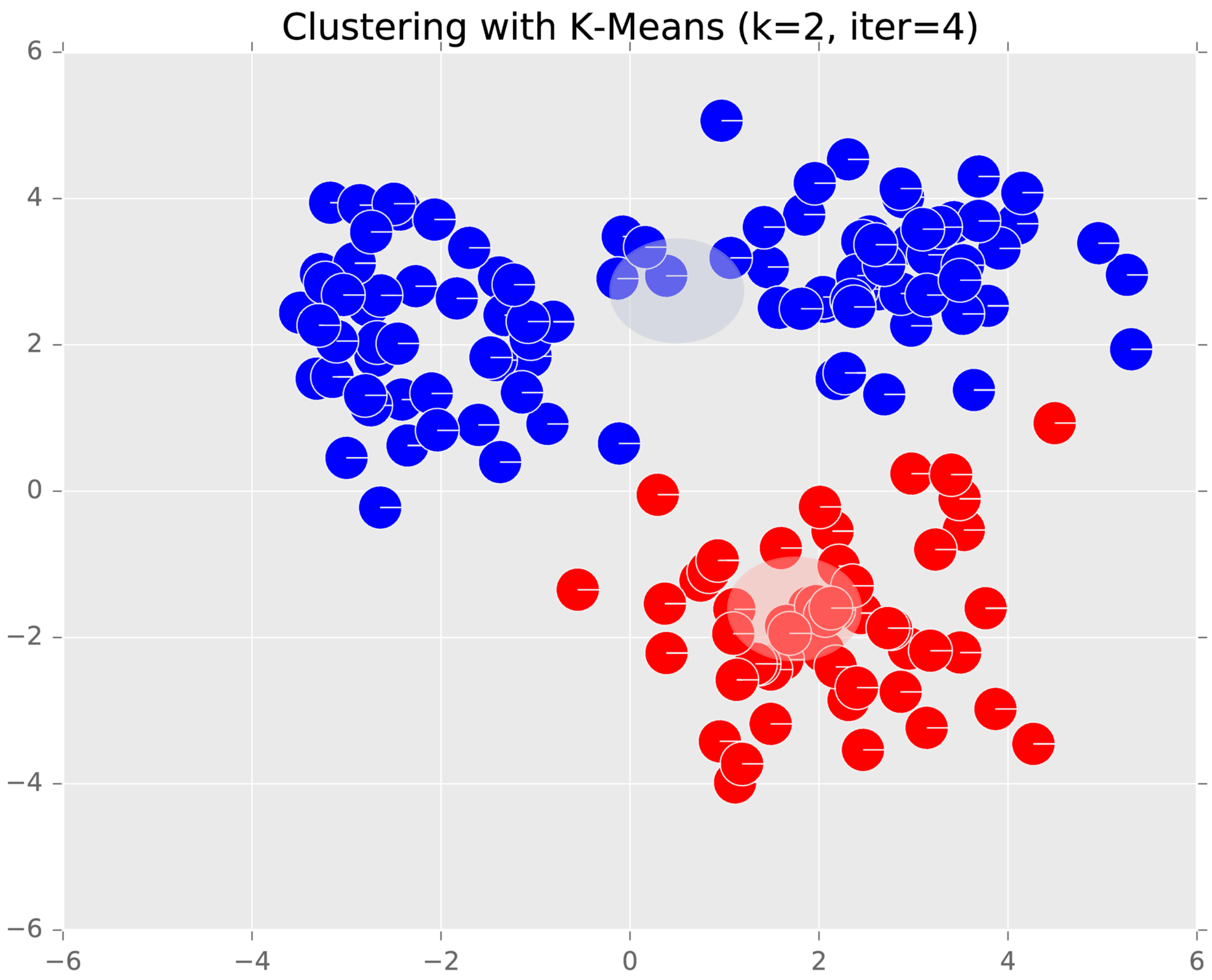


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)

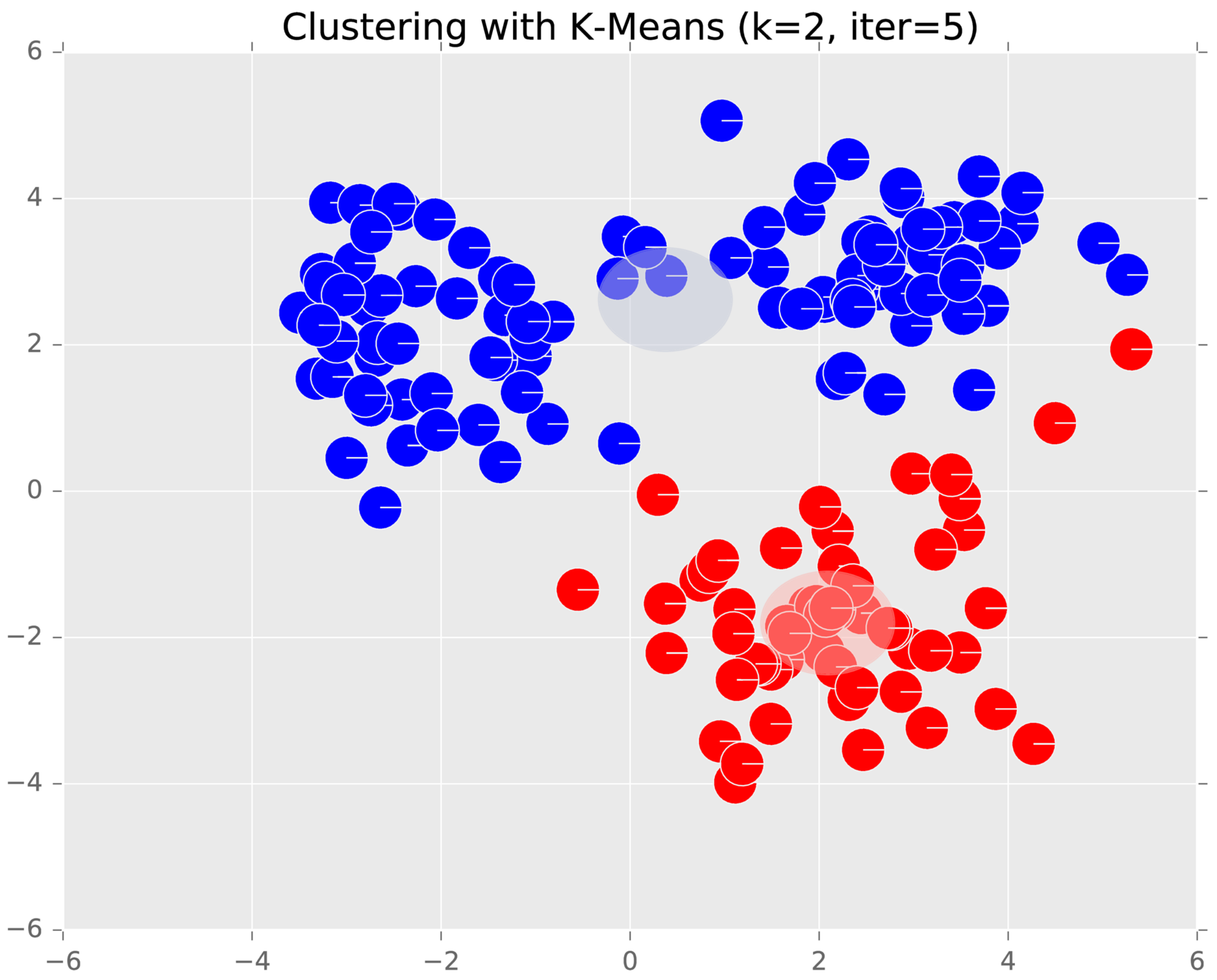
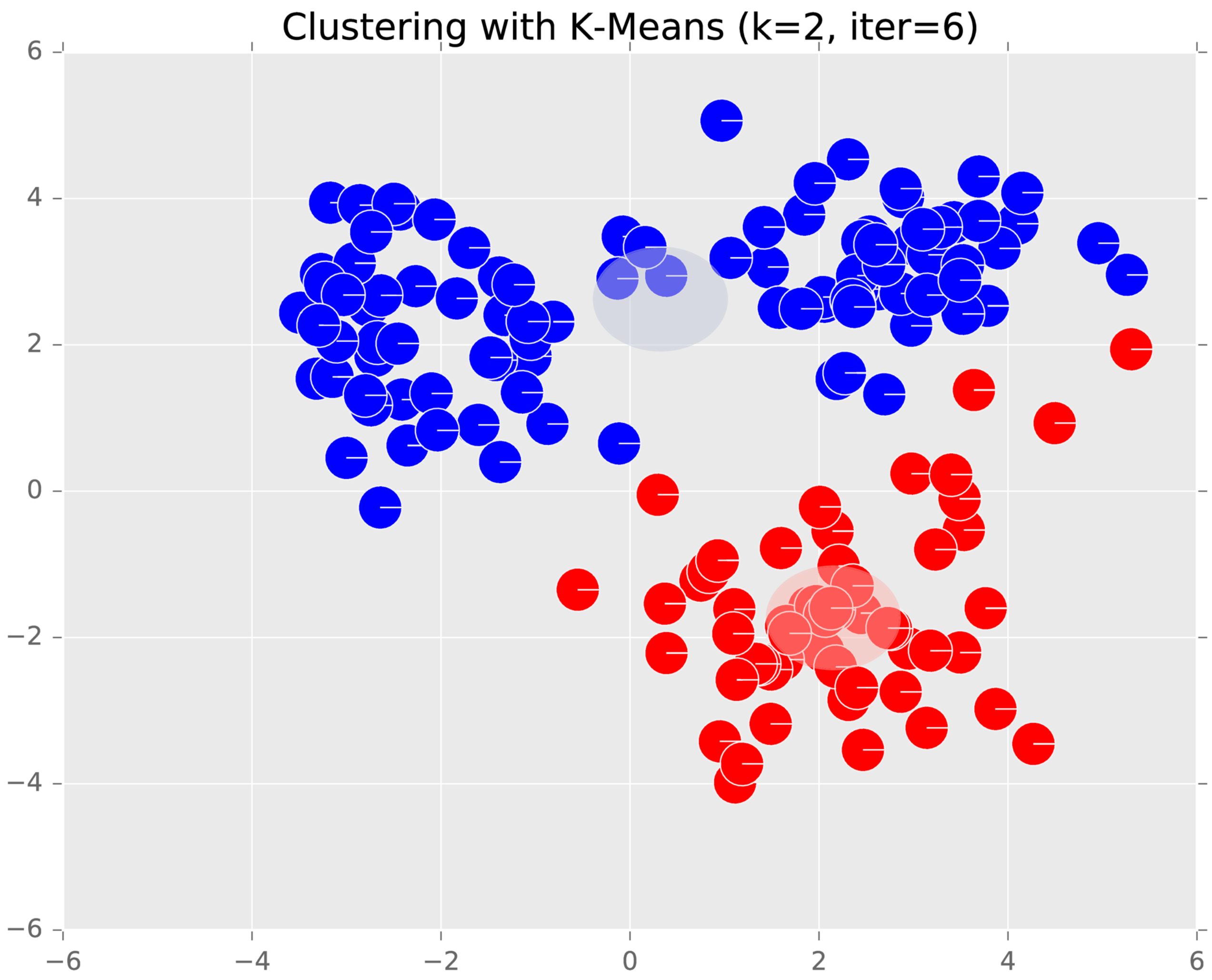


Figure courtesy of Matt Gormley

K-means: Example ($K = 2$)



K-means: Example ($K = 2$)

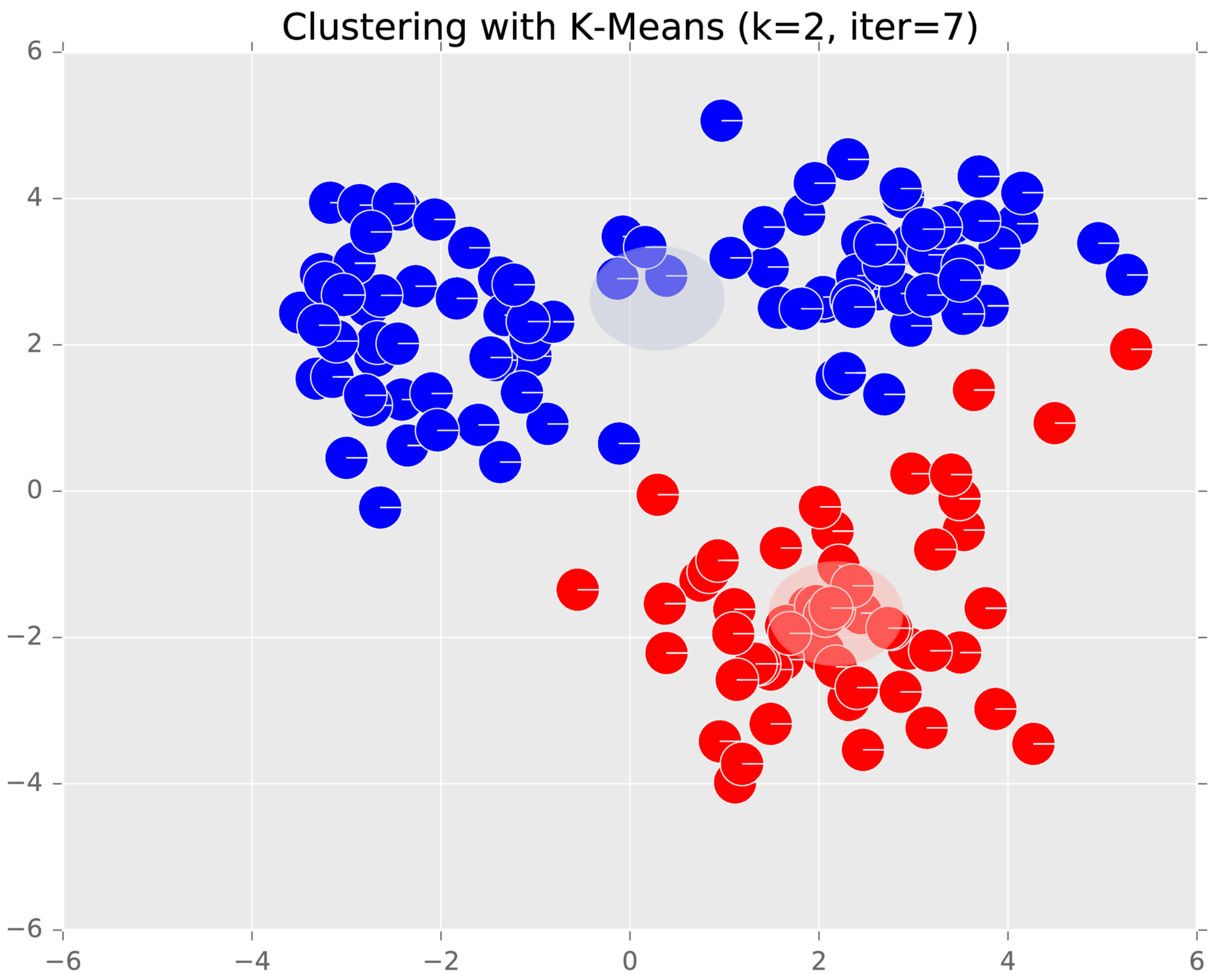


Figure courtesy of Matt Gormley

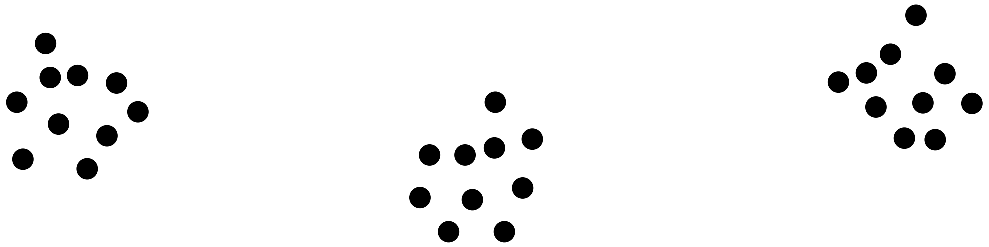
Setting K

- Idea: choose the value of K that minimizes the objective function

- Better Idea: look for the characteristic "elbow" or largest decrease when going from $K-1$ to K

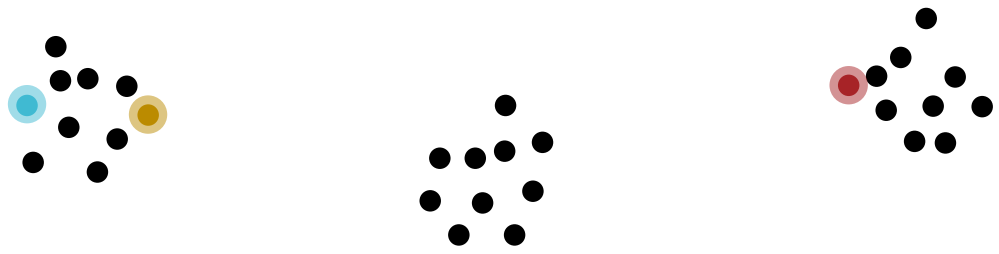
Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



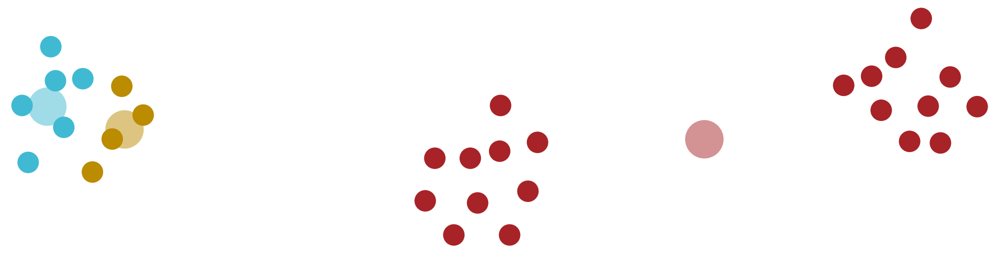
Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



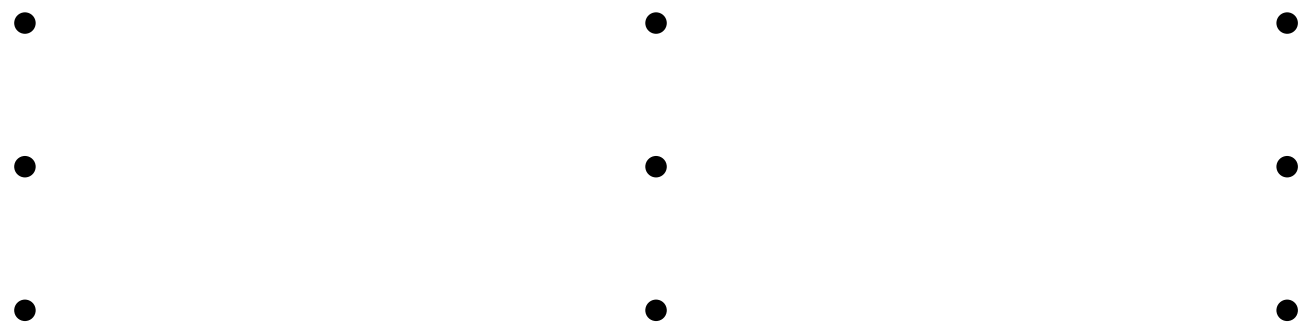
Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



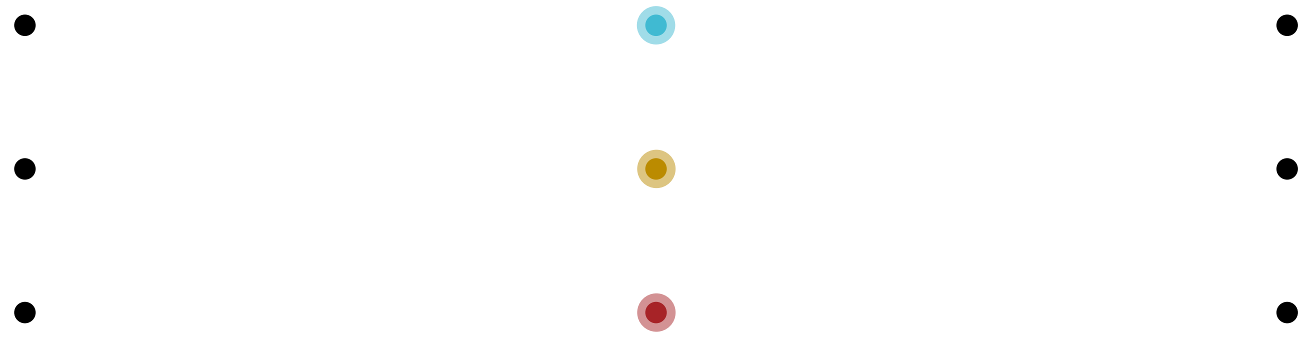
Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



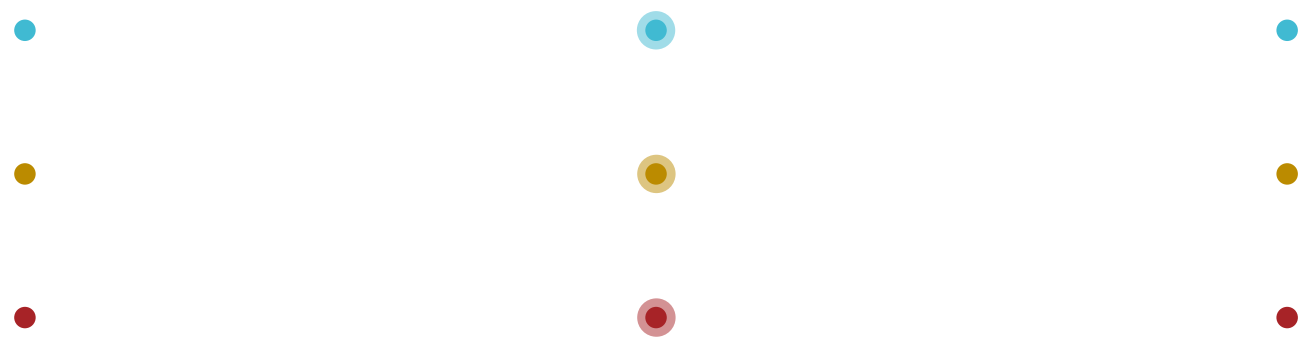
Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



Initializing K-means

- Common choice: choose K data points at random to be the initial cluster centers (Lloyd's method)



- Lloyd's method converges to a local minimum and that local minimum can be arbitrarily bad (relative to the optimal clusters)
  - This is because the K-means objective is nonconvex!
- Intuition: want initial cluster centers to be far apart from one another

K-means++ (Arthur and Vassilvitskii, 2007)

1. Choose the first cluster center randomly from the data points.
2. For each other data point $\boldsymbol{x}$, compute $D(\boldsymbol{x})$, the distance between $\boldsymbol{x}$ and the nearest cluster center.
3. Select the next cluster center proportional to $D(\boldsymbol{x})^2$.
4. Repeat 2 and 3 $K-1$ times.

- K-means++ achieves a $O(\log K)$ approximation to the optimal clustering in expectation
- Both Lloyd's method and K-means++ can benefit from multiple random restarts.

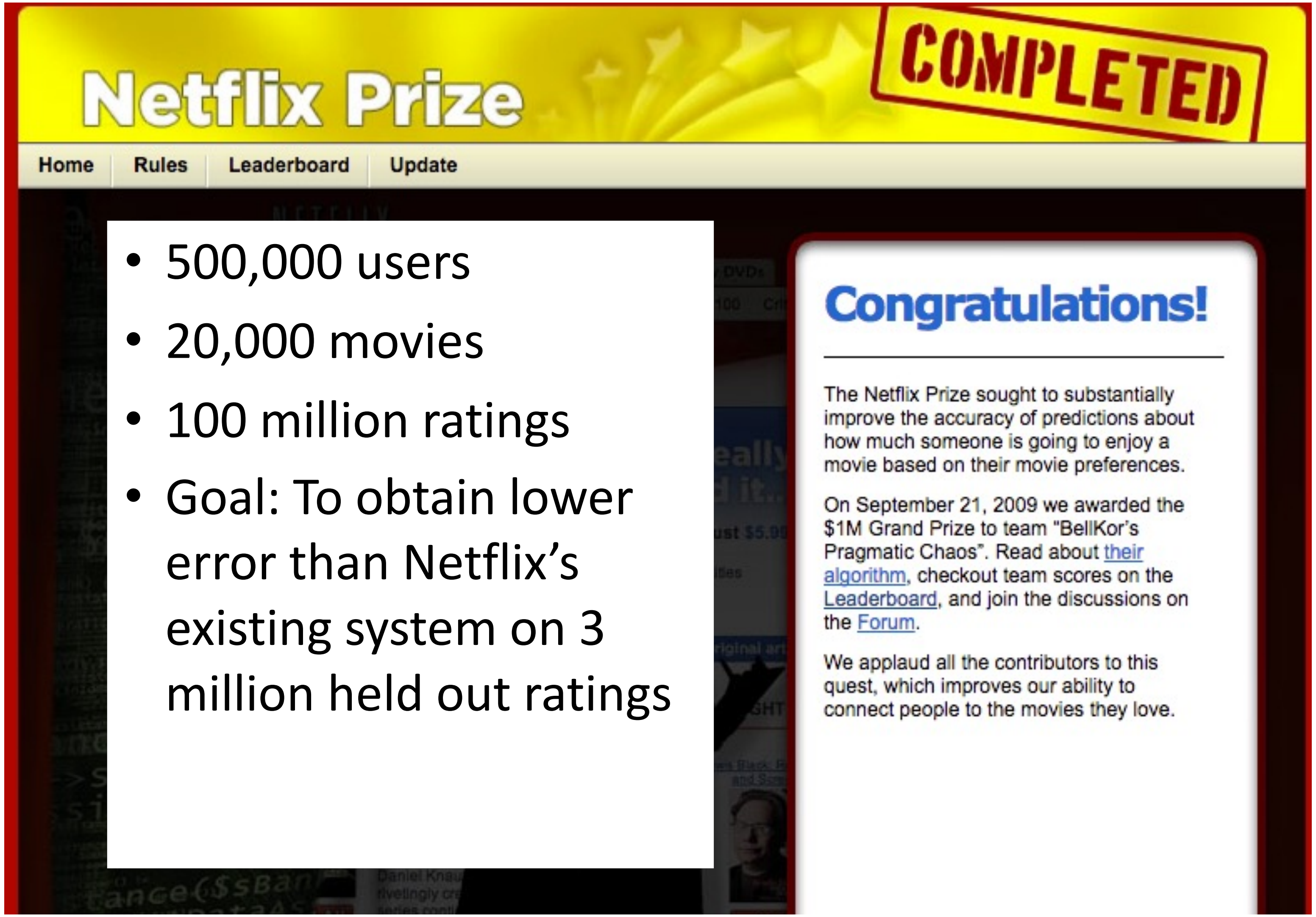
K-means Learning Objectives

- 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

The Netflix Prize

- 500,000 users
- 20,000 movies
- 100 million ratings
- Goal: To obtain lower error than Netflix's existing system on 3 million held out ratings



The Netflix Prize

Netflix Prize COMPLETED

Home Rules Leaderboard Update Download

Leaderboard

Showing Test Score. Click here to show quiz score

Display top 20 **leaders.**

Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace_	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
11	Opera Solutions	0.8623	9.47	2009-07-24 00:34:07
12	BellKor	0.8624	9.46	2009-07-26 17:19:11

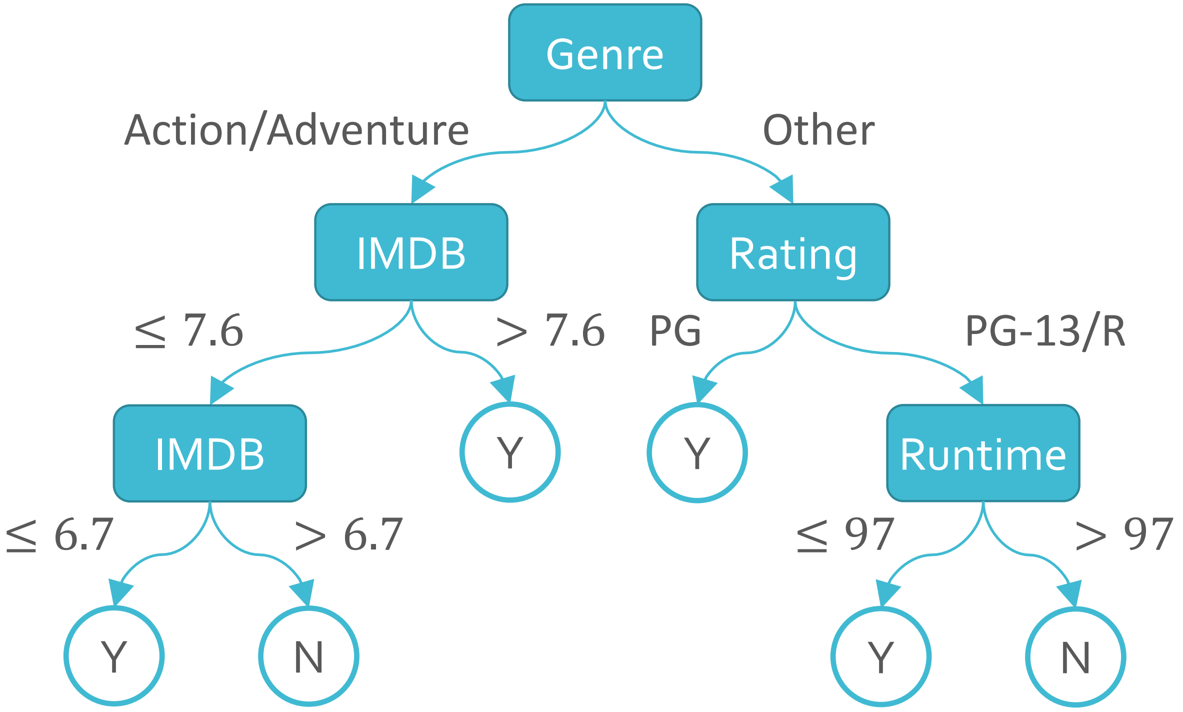
Source: https://web.archive.org/web/20090926213457/http://www.netflixprize.com/leaderboard

MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Y
2	105	Action	30M	1984	7.8	PG	Y
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Y
5	128	Comedy	16.4M	1989	8.1	PG	Y
6	120	Comedy	11M	1992	7.6	R	N
7	120	Drama	14.5M	1996	6.7	PG-13	N
8	136	Action	115M	1999	6.5	PG	Y
9	90	Action	90M	2001	6.6	PG-13	Y
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Y
12	94	Comedy	26M	2004	7.2	PG-13	Y
13	157	Biography	100M	2007	7.8	R	N
14	128	Action	110M	2007	7.1	PG-13	N
15	107	Drama	39M	2009	7.1	PG-13	N
16	158	Drama	61M	2012	7.6	PG-13	N
17	169	Adventure	165M	2014	8.6	PG-13	Y
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Y
20	141	Action	275M	2019	6.5	PG-13	Y

Movie Recommendations

Source: https://www.kaggle.com/datasets/danielgrijalvas/movies

MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Y
2	105	Action	30M	1984	7.8	PG	Y
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Y
5	128	Comedy	16.4M	1989	8.1	PG	Y
6	120	Comedy	11M	1992	7.6	R	N
7	120	Drama	14.5M	1996	6.7	PG-13	N
8	136	Action	115M	1999	6.5	PG	Y
9	90	Action	90M	2001	6.6	PG-13	Y
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Y
12	94	Comedy	26M	2004	7.2	PG-13	Y
13	157	Biography	100M	2007	7.8	R	N
14	128	Action	110M	2007	7.1	PG-13	N
15	107	Drama	39M	2009	7.1	PG-13	N
16	158	Drama	61M	2012	7.6	PG-13	N
17	169	Adventure	165M	2014	8.6	PG-13	Y
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Y
20	141	Action	275M	2019	6.5	PG-13	Y



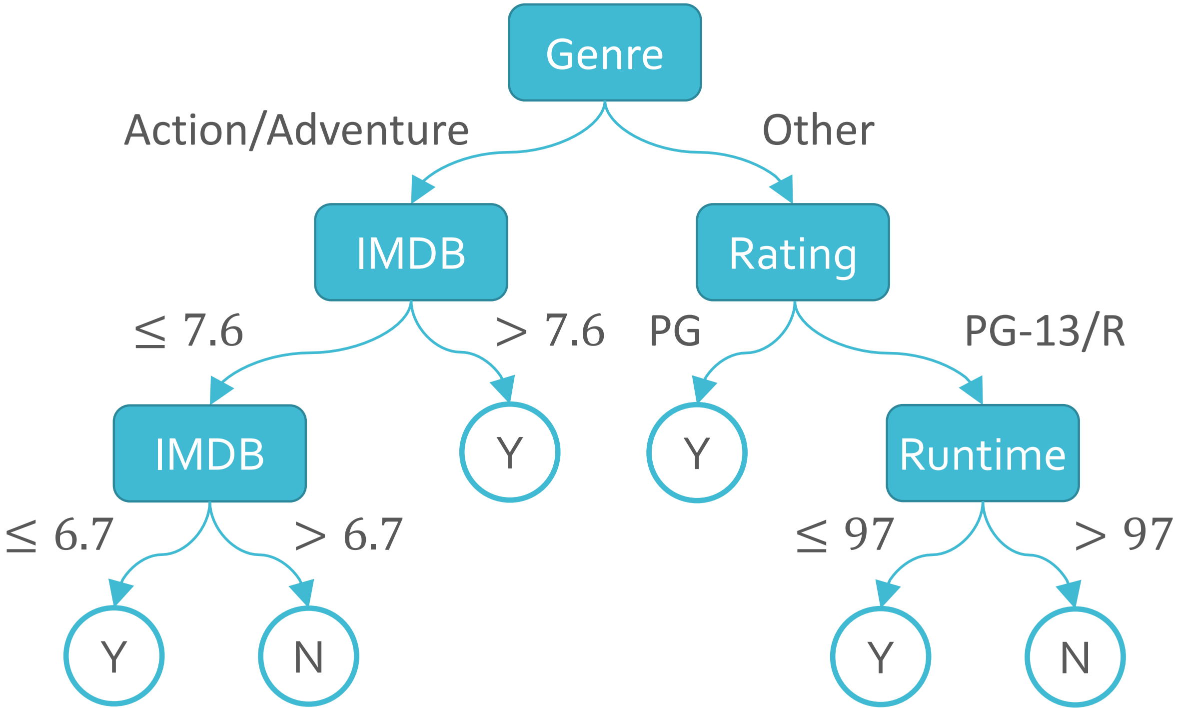
Decision Trees

Source: https://www.kaggle.com/datasets/danielgrijalvas/movies

Recall: Decision Tree Pros & Cons

- Pros
  - Interpretable
  - Efficient (computational cost and storage)
  - Can be used for classification and regression tasks
  - Compatible with categorical and real-valued features
- Cons
  - Learned greedily: each split only considers the immediate impact on the splitting criterion
    - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
  - Prone to overfit
  - High variance

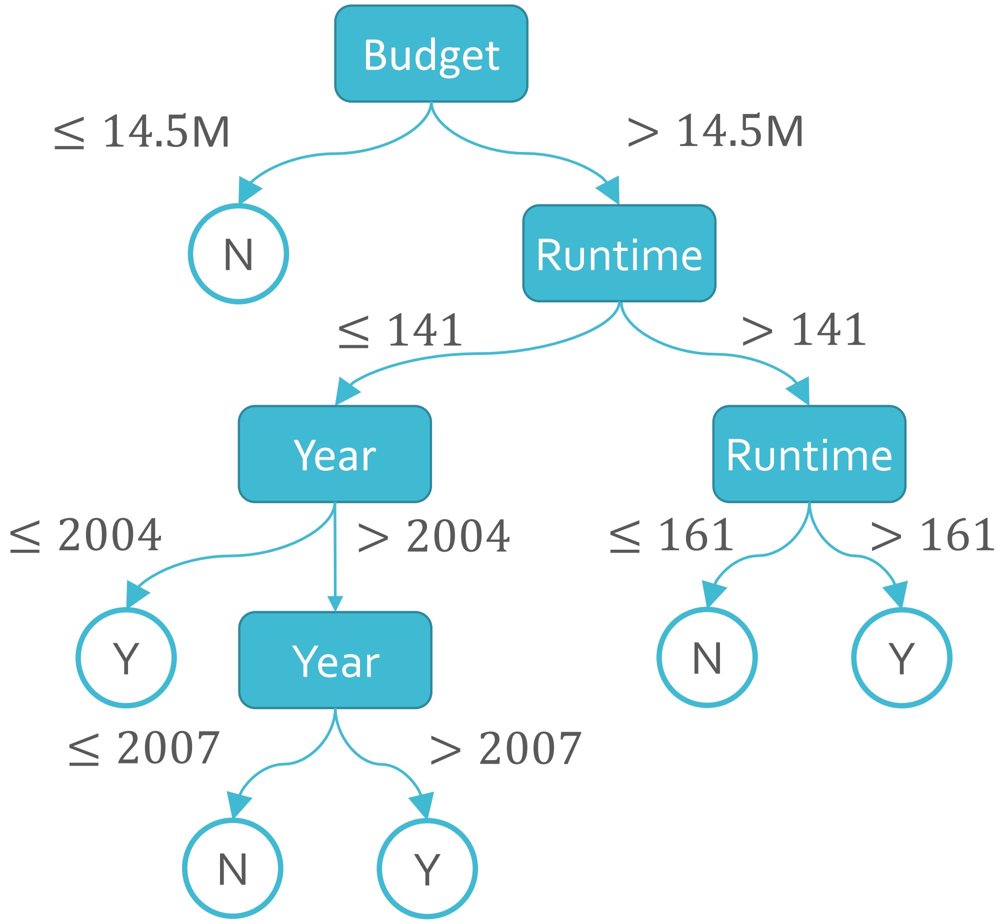
MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Y
2	105	Action	30M	1984	7.8	PG	Y
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Y
5	128	Comedy	16.4M	1989	8.1	PG	Y
6	120	Comedy	11M	1992	7.6	R	N
7	120	Drama	14.5M	1996	6.7	PG-13	N
8	136	Action	115M	1999	6.5	PG	Y
9	90	Action	90M	2001	6.6	PG-13	Y
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Y
12	94	Comedy	26M	2004	7.2	PG-13	Y
13	157	Biography	100M	2007	7.8	R	N
14	128	Action	110M	2007	7.1	PG-13	N
15	107	Drama	39M	2009	7.1	PG-13	N
16	158	Drama	61M	2012	7.6	PG-13	N
17	169	Adventure	165M	2014	8.6	PG-13	Y
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Y
20	141	Action	275M	2019	6.5	PG-13	Y



Decision Trees

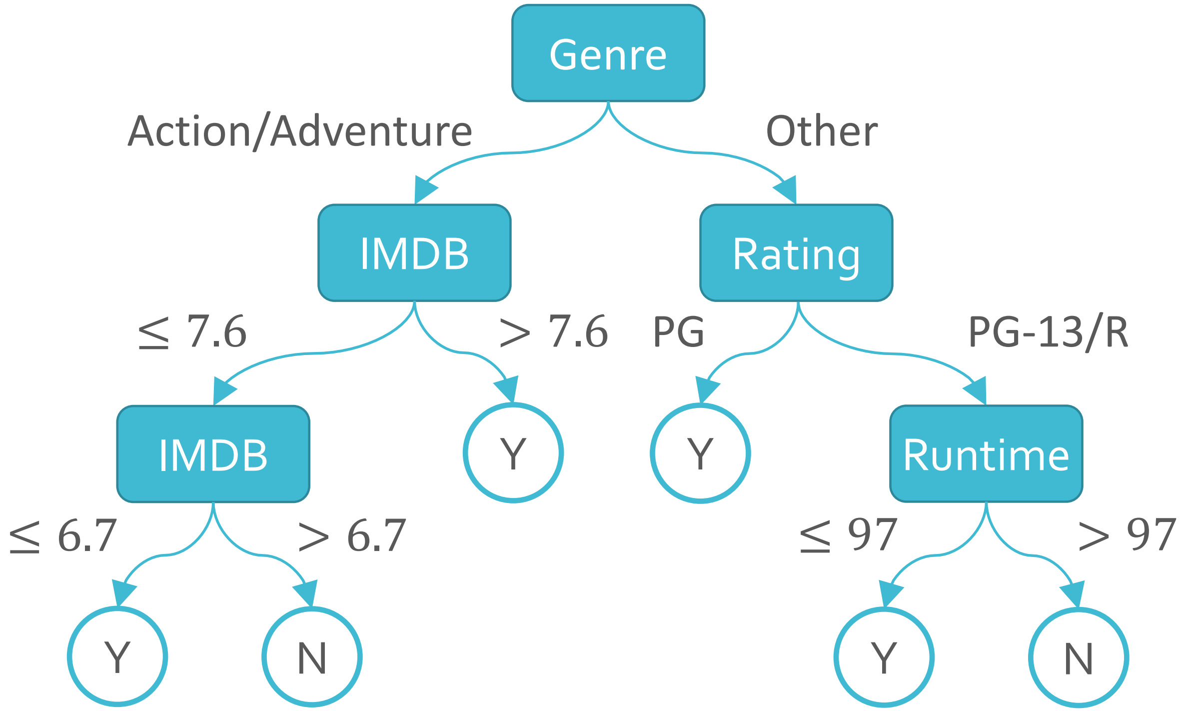
Source: https://www.kaggle.com/datasets/danielgrijalvas/movies

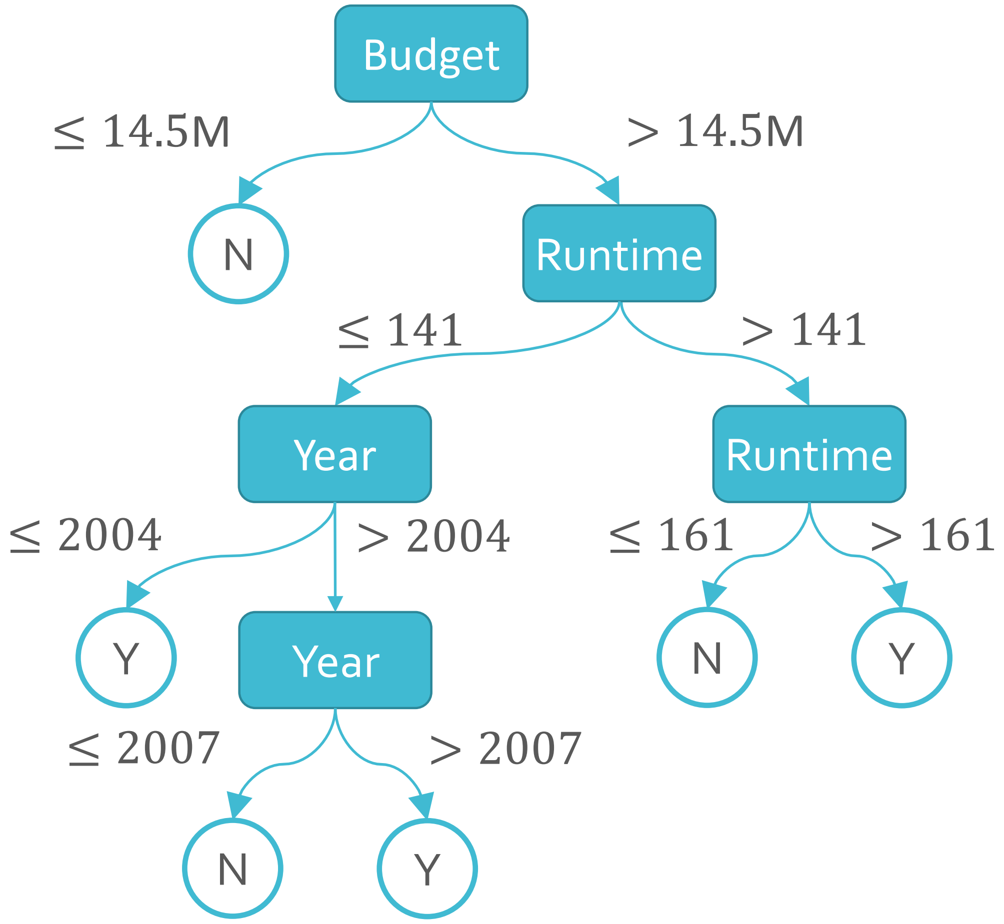
MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Y
2	105	Action	30M	1984	7.8	PG	Y
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Y
5	128	Comedy	16.4M	1989	8.1	PG	Y
6	120	Comedy	11M	1992	7.6	R	N
7	120	Drama	14.5M	1996	6.7	PG-13	N
8	136	Action	115M	1999	6.5	PG	Y
9	90	Action	90M	2001	6.6	PG-13	Y
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Y
12	94	Comedy	26M	2004	7.2	PG-13	Y
13	157	Biography	100M	2007	7.8	R	N
14	128	Action	110M	2007	7.1	PG-13	N
15	107	Drama	39M	2009	7.1	PG-13	N
16	158	Drama	61M	2012	7.6	PG-13	*Y*
17	169	Adventure	165M	2014	8.6	PG-13	Y
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Y
20	141	Action	275M	2019	6.5	PG-13	Y



Decision Trees

Source: https://www.kaggle.com/datasets/danielgrijalvas/movies





Decision Trees

Decision Trees: Pros & Cons

- Pros
  - Interpretable
  - Efficient (computational cost and storage)
  - Can be used for classification and regression tasks
  - Compatible with categorical and real-valued features
- Cons
  - Learned greedily: each split only considers the immediate impact on the splitting criterion
    - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
  - Prone to overfit
  - High variance
    - Can be addressed via ensembles → 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 = sample bagging + feature bagging

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

Random Forests

- Combines the prediction of many diverse decision trees to reduce their variability
- If B independent random variables $x^{(1)}, x^{(2)}, \ldots, x^{(B)}$ 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 = sample bagging + feature bagging

  = bootstrap aggregating + split-feature randomization

Aggregating

- How can we combine multiple decision trees, $\{t_1, t_2, \ldots, t_B\}$, to arrive at a single prediction?
- Regression - average the predictions:

$$\bar{t}(\boldsymbol{x}) = \frac{1}{B}\sum_{b=1}^{B} t_b(\boldsymbol{x})$$

- Classification - plurality (or majority) vote; for binary labels encoded as $\{-1, +1\}$:

$$\bar{t}(\boldsymbol{x}) = \operatorname{sign}\left(\frac{1}{B}\sum_{b=1}^{B} t_b(\boldsymbol{x})\right)$$

Random Forests

- Combines the prediction of many **diverse** decision trees to reduce their variability
- If B **independent** random variables $x^{(1)}, x^{(2)}, \ldots, x^{(B)}$ 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 = sample bagging + feature bagging

  = **bootstrap** aggregating + **split-feature randomization**

Bootstrapping

- Insight: one way of generating different decision trees is by changing the training data set
- Issue: often, we only have one fixed set of training data
- Idea: resample the data multiple times ***with replacement***

MovieID	…
1	…
2	…
3	…
⋮	⋮
19	…
20	…

Training data

MovieID	…
1	…
1	…
1	…
⋮	⋮
14	…
19	…

Bootstrapped Sample 1

MovieID	…
4	…
4	…
5	…
⋮	⋮
16	…
16	…

Bootstrapped Sample 2

…

…

Bootstrapping

- Idea: resample the data multiple times ***with replacement***
  - Each bootstrapped sample has the same number of data points as the original data set
  - Duplicated points cause different decision trees to focus on different parts of the input space

MovieID	…
1	…
2	…
3	…
⋮	⋮
19	…
20	…

Training data

MovieID	…
1	…
1	…
1	…
⋮	⋮
14	…
19	…

Bootstrapped Sample 1

MovieID	…
4	…
4	…
5	…
⋮	⋮
16	…
16	…

Bootstrapped Sample 2

…

…

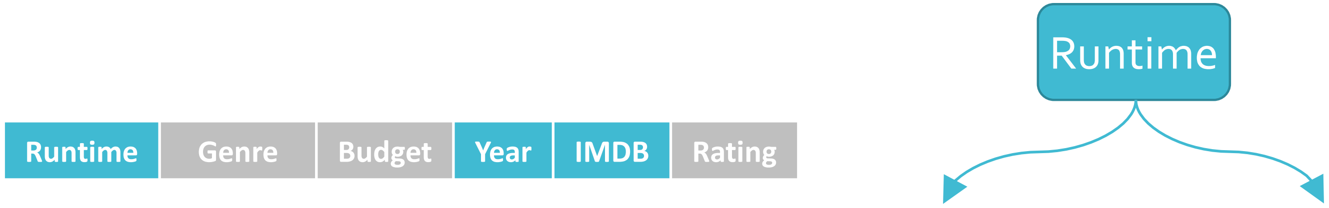
Split-feature Randomization

- 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

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

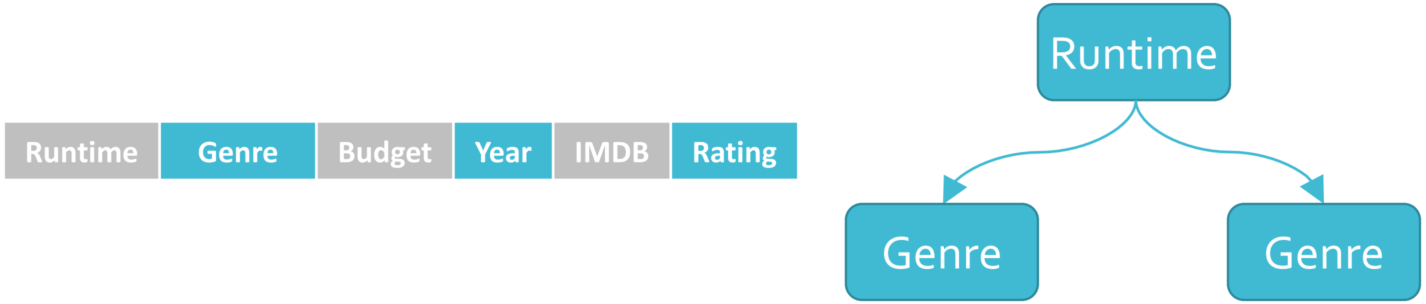


Split-feature Randomization

- 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

Split-feature Randomization

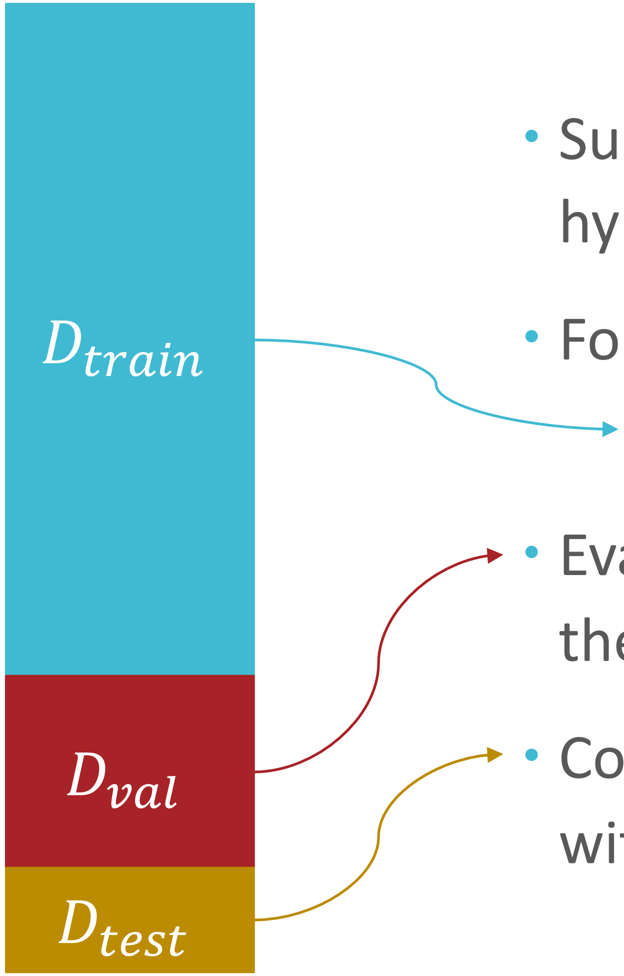
- Issue: decision trees trained on bootstrapped samples still behave similarly
- Idea: in addition to sampling the data points (i.e., the rows), also sample the features (i.e., the columns)
- Each time a split is being considered, limit the possible features to a randomly sampled subset



Random Forests

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}, B, \rho$
- 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 ID3 algorithm ***with split-feature randomization***, sampling ρ features for each split
- Output: $\bar{t} = f(t_1, \ldots, t_B)$, the aggregated hypothesis

Recall: Validation Sets



- Suppose we want to compare multiple hyperparameter settings $\theta_1, \dots, \theta_K$
- For $k = 1, 2, \dots, K$
  - 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 $t^{(-n)} = \left\{t_1^{(-n)}, t_2^{(-n)}, \dots, t_{N_{-n}}^{(-n)}\right\}$
- 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

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

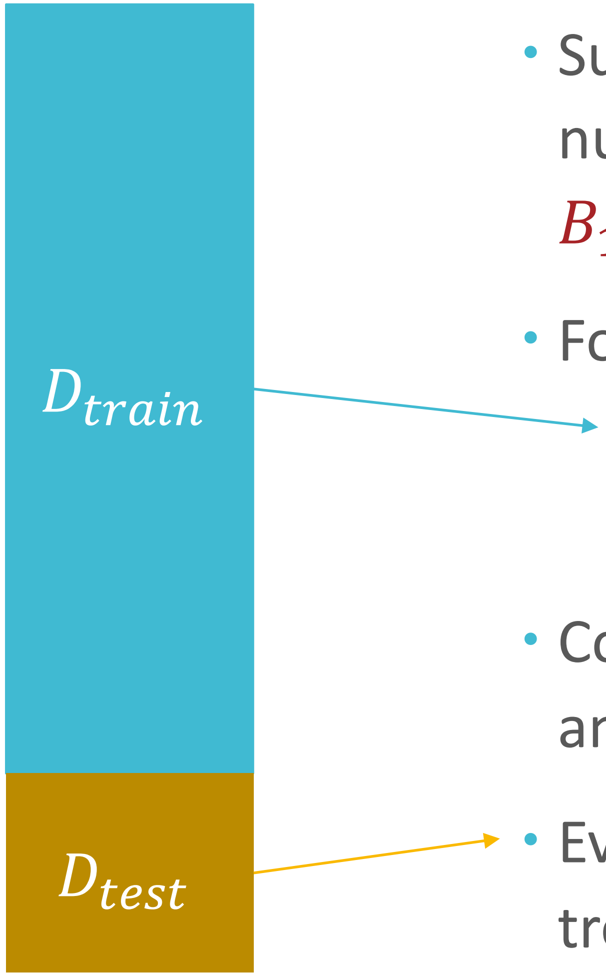
Out-of-bag Error

- 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 $t^{(-n)} = \left\{t_1^{(-n)}, t_2^{(-n)}, \dots, t_{N_{-n}}^{(-n)}\right\}$
- 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 classification

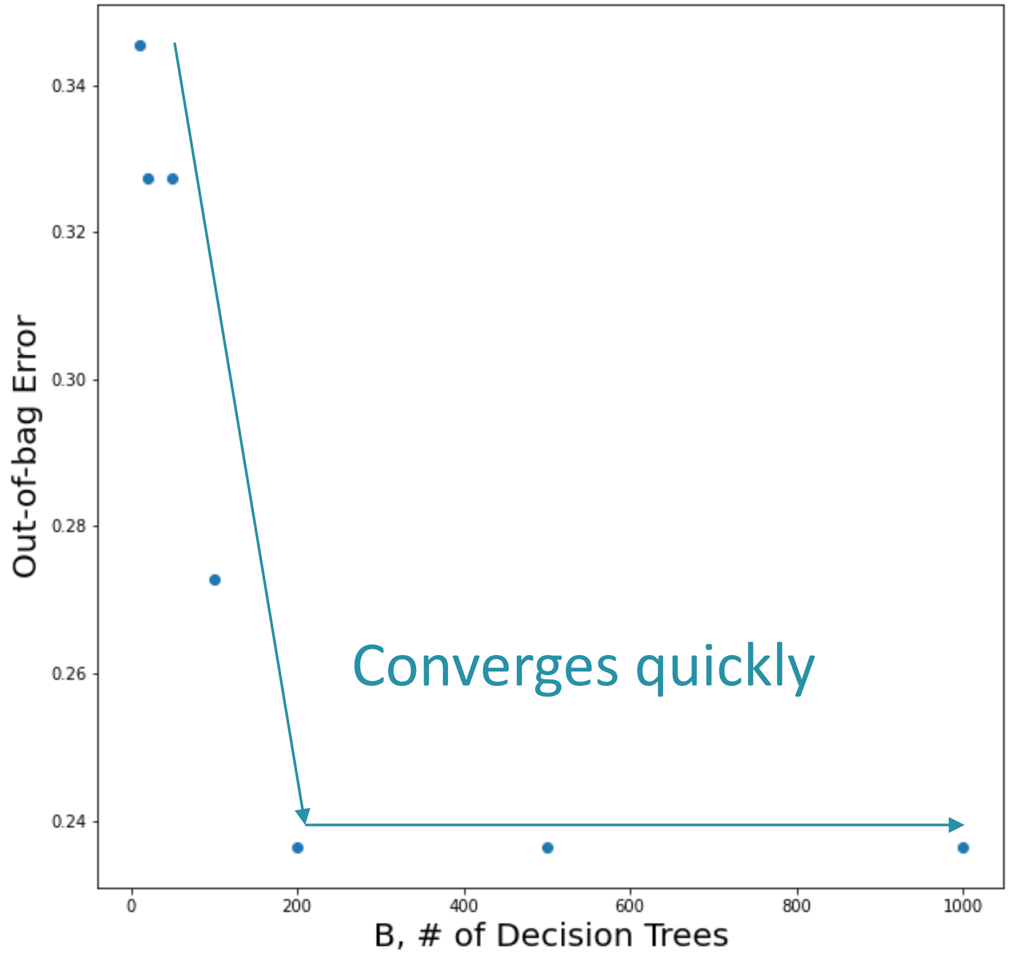
$$E_{OOB} = \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}\left(\bar{t}^{(-n)}\left(\boldsymbol{x}^{(n)}\right) \neq y^{(n)}\right)$$

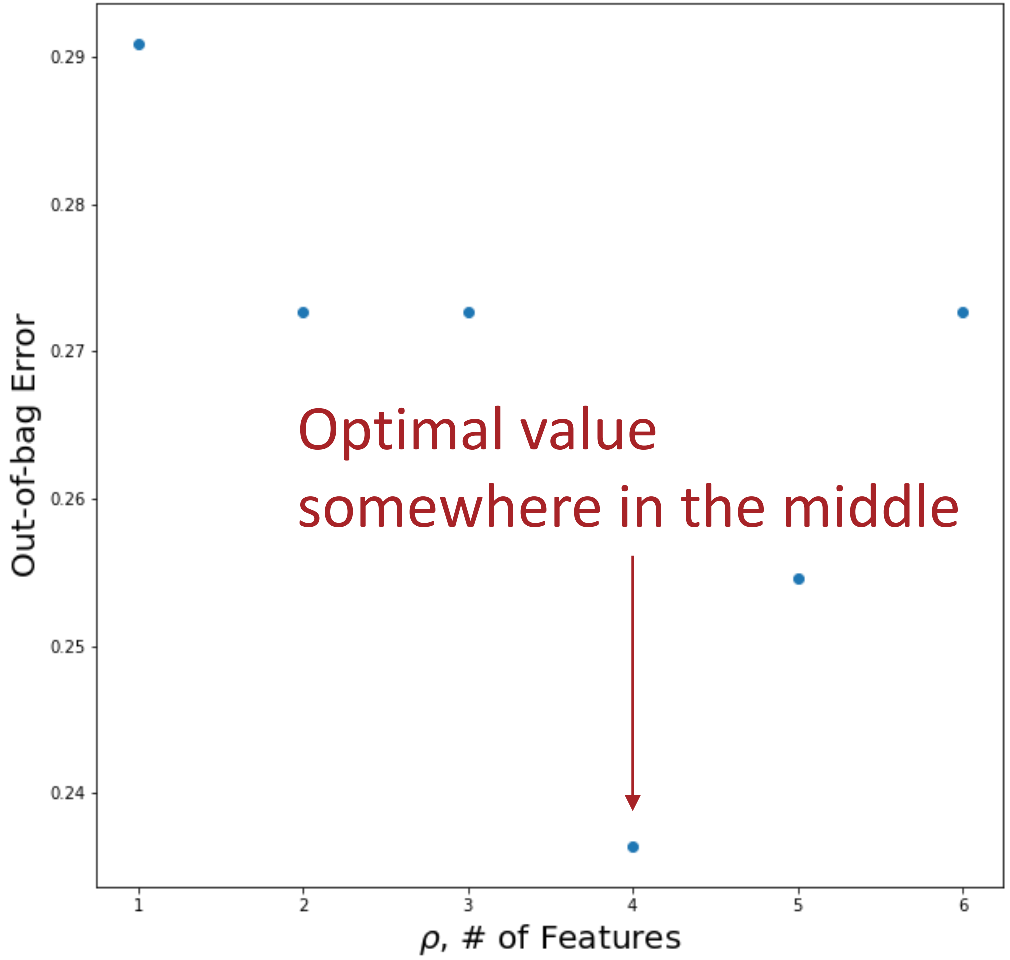
- E_{OOB} can be used for hyperparameter optimization!

Out-of-bag Error



- Suppose we want to compare different numbers of trees in our random forest $B_1, \dots, B_K$
- For $k = 1, 2, \dots, K$
  - 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 entropy (weighted by the number of data points in the split) to its importance

Feature Importance