10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Clustering (K-Means)

Clustering Readings:
Murphy 25.5
Bishop 12.1, 12.3
HTF 14.3.0
Mitchell --

Matt Gormley
Lecture 15
March 8, 2017

Reminders

- **Homework 5: Readings / Application of ML**
  - **Release: Wed, Mar. 08**
  - **Due: Wed, Mar. 22 at 11:59pm**

Outline

- **Clustering: Motivation / Applications**
- **Optimization Background**
  - Coordinate Descent
  - Block Coordinate Descent
- **Clustering**
  - Inputs and Outputs
  - Objective-based Clustering
- **K-Means**
  - K-Means Objective
  - Computational Complexity
  - K-Means Algorithm / Lloyd's Method
- **K-Means Initialization**
  - Random
  - Farthest Point
  - K-Means++

Clustering, Informal Goals

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

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

Useful for:

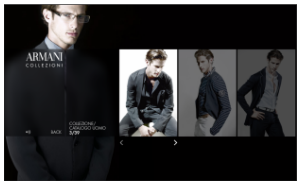
- Automatically organizing data.
- Understanding hidden structure in data.
- Preprocessing for further analysis.
    - Representing high-dimensional data in a low-dimensional space (e.g., for visualization purposes).

Slide courtesy of Nina Balcan

Applications (Clustering comes up everywhere…)

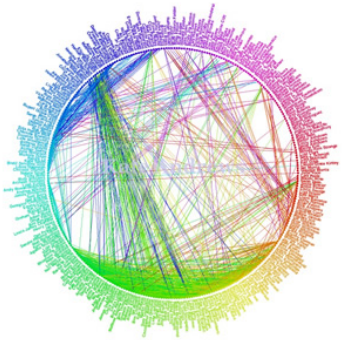
- Cluster news articles or web pages or search results by topic.



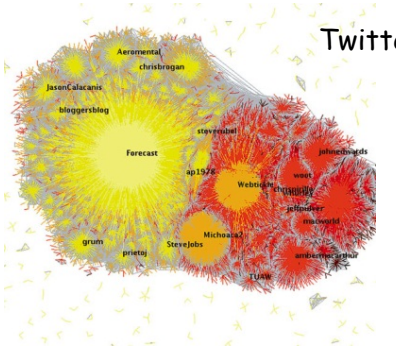


- Cluster protein sequences by function or genes according to expression profile.


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



Facebook network



Twitter Network

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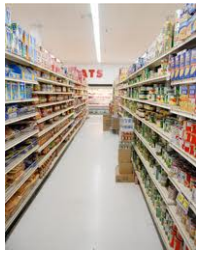
Applications (Clustering comes up everywhere…)

- Cluster customers according to purchase history.



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

- And many many more applications….

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Optimization Background

Whiteboard:

- Coordinate Descent
- Block Coordinate Descent

Clustering

Whiteboard:

- Inputs and Outputs
- Objective-based Clustering

K-Means

Whiteboard:

- K-Means Objective
- Computational Complexity
- K-Means Algorithm / Lloyd's Method

K-Means Initialization

Whiteboard:

- Random
- Furthest Traversal
- K-Means++

Lloyd's method: Random Initialization

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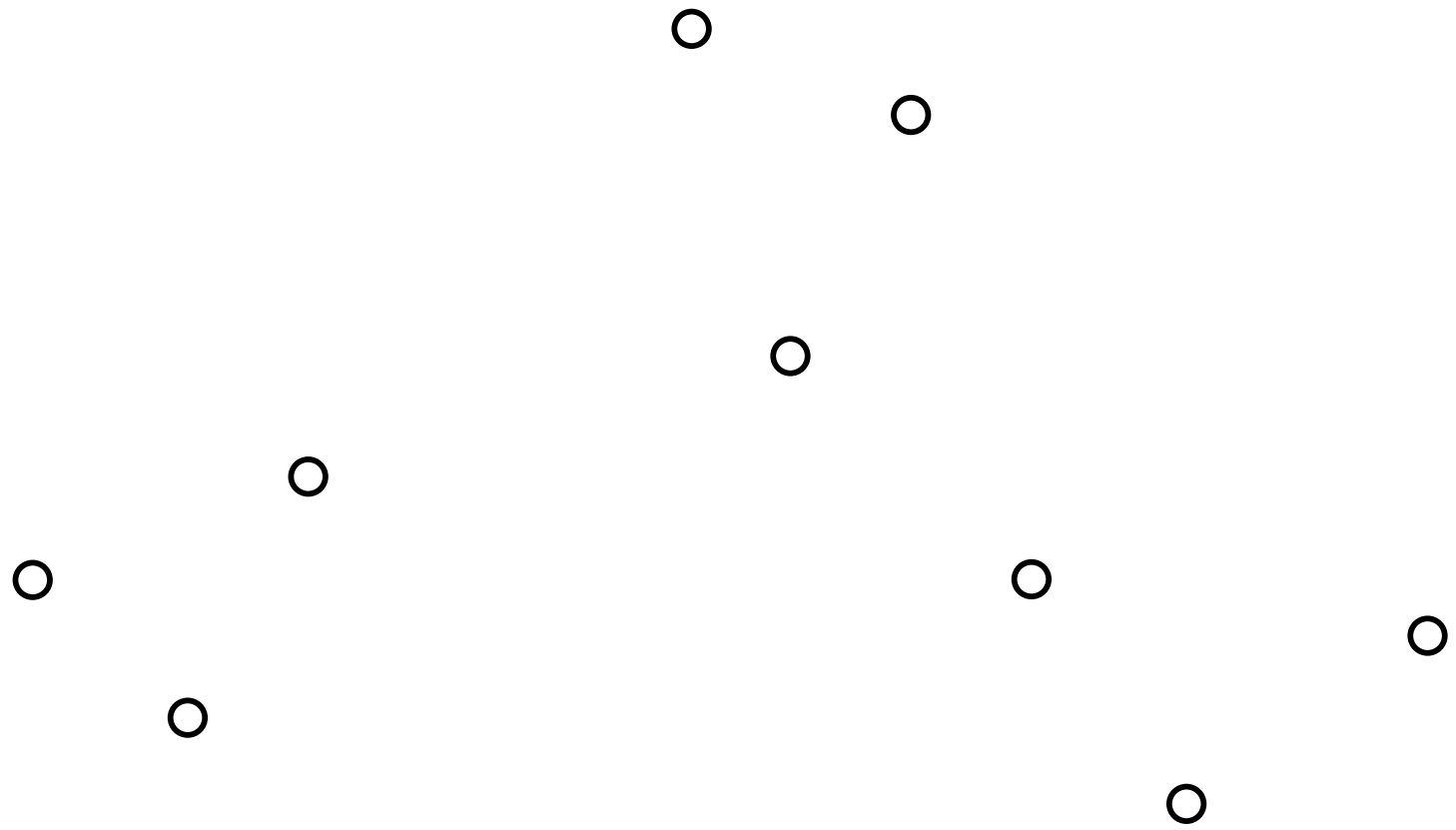
Lloyd's method: Random Initialization

Example: Given a set of datapoints



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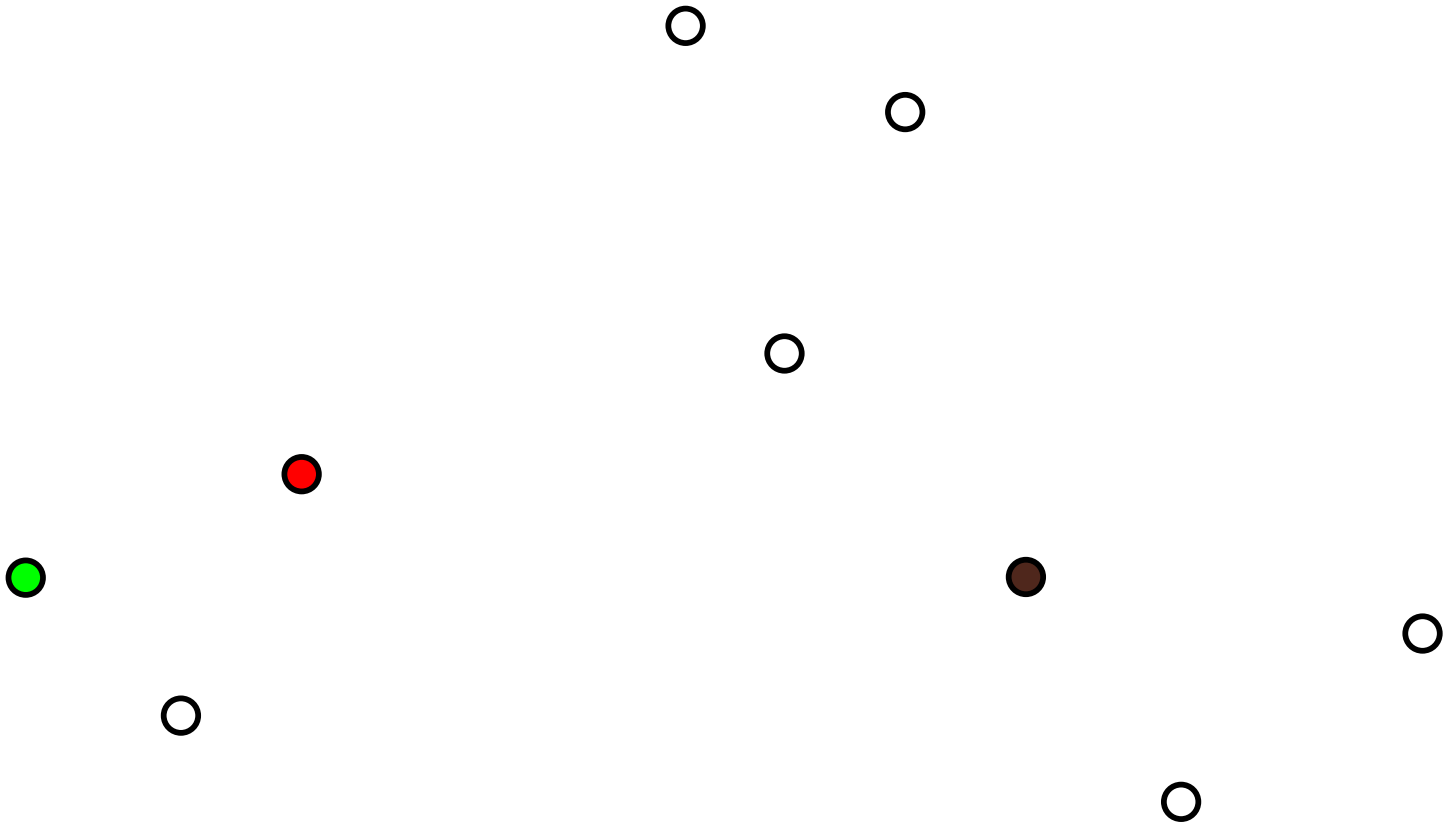
Lloyd's method: Random Initialization

Select initial centers at random



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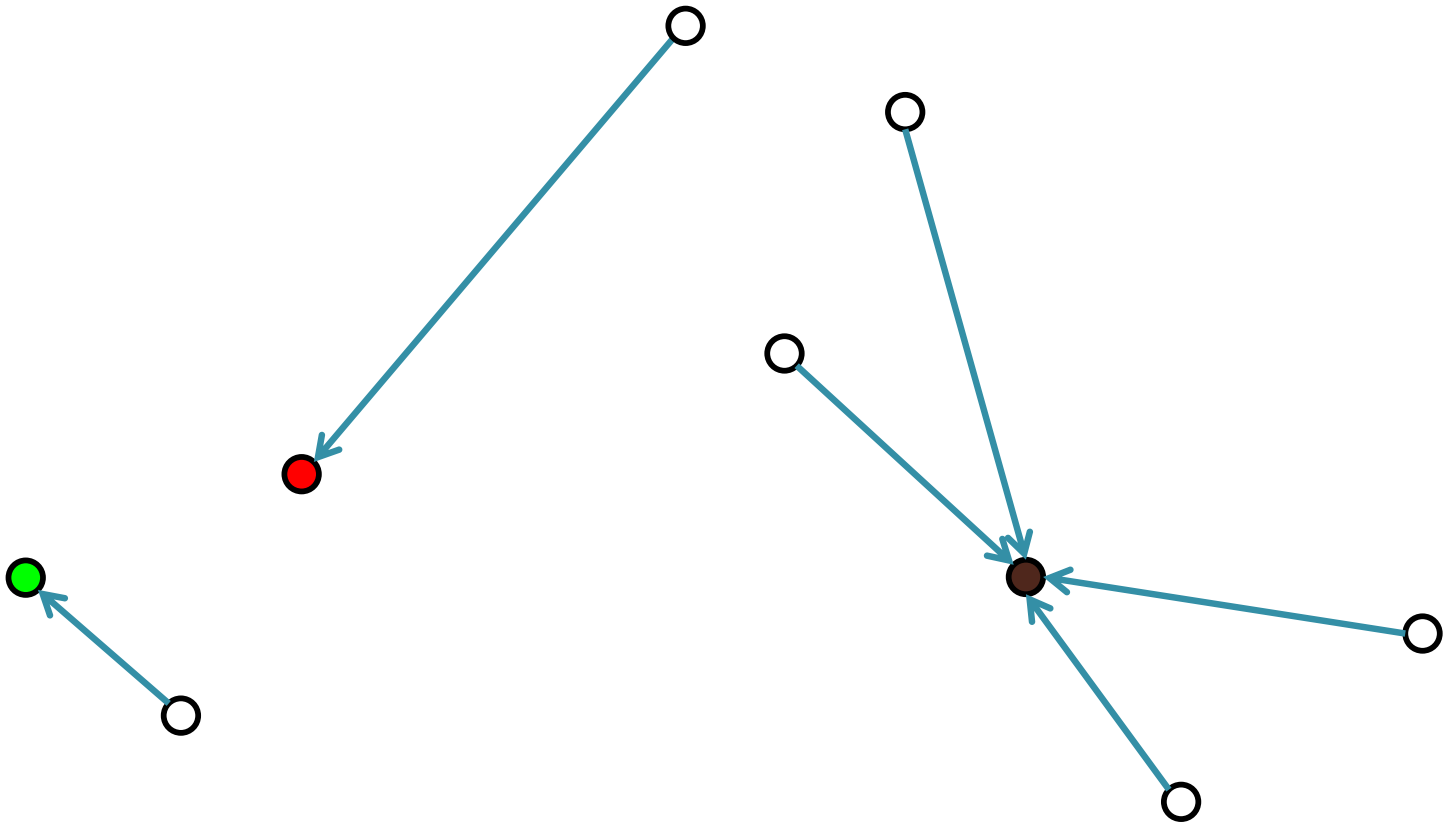
Lloyd's method: Random Initialization

Assign each point to its nearest center



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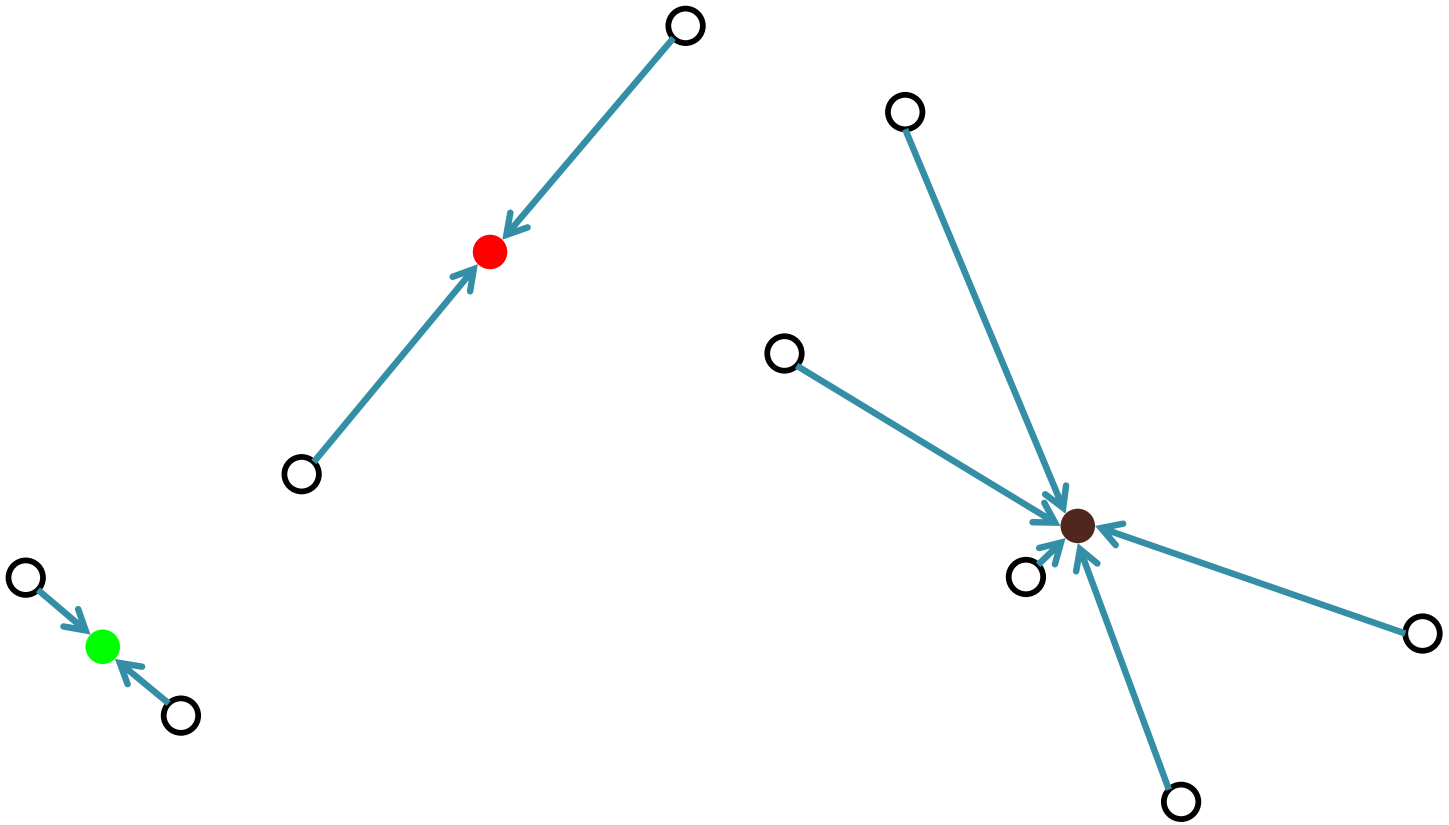
Lloyd's method: Random Initialization

Recompute optimal centers given a fixed clustering



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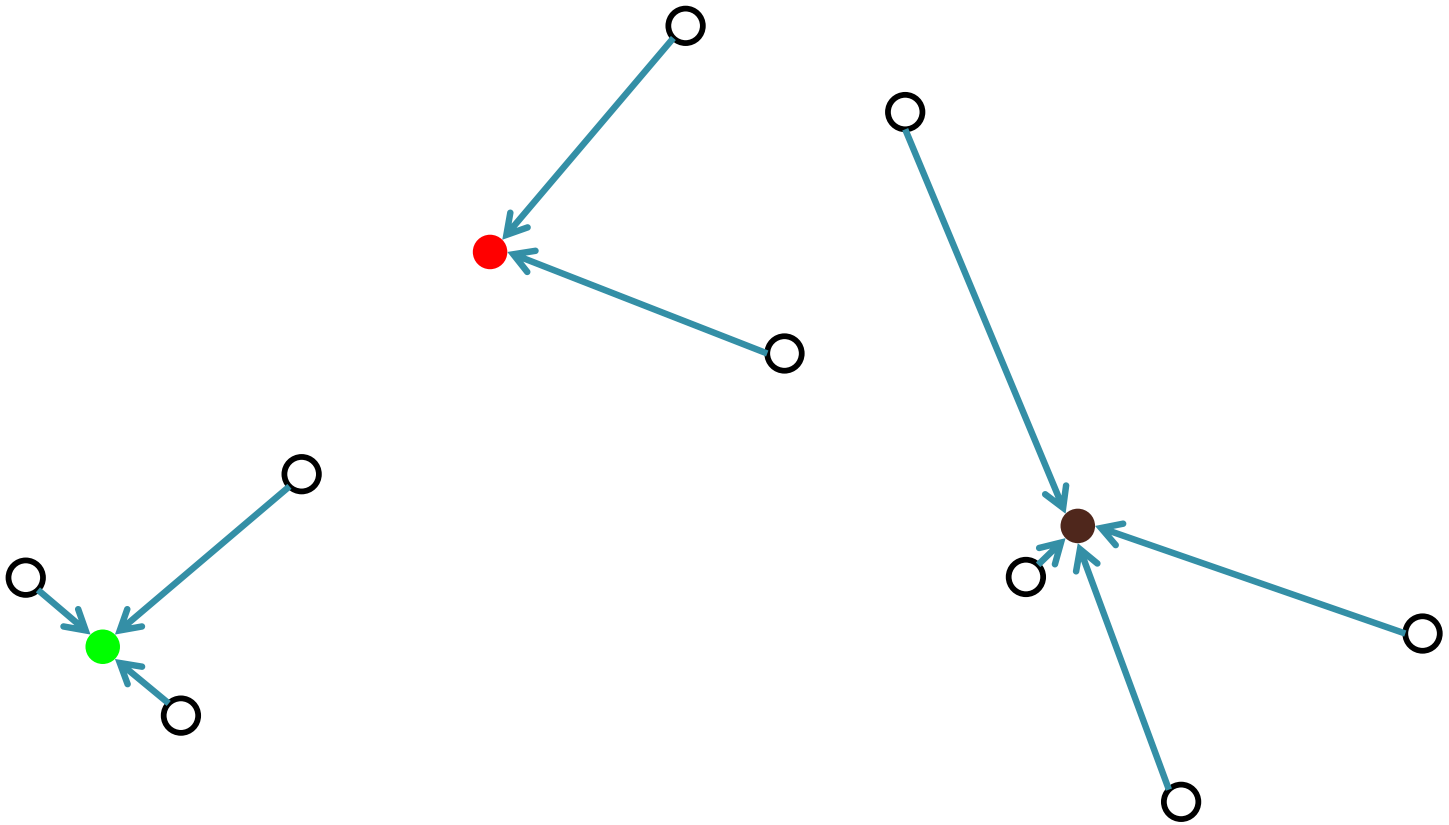

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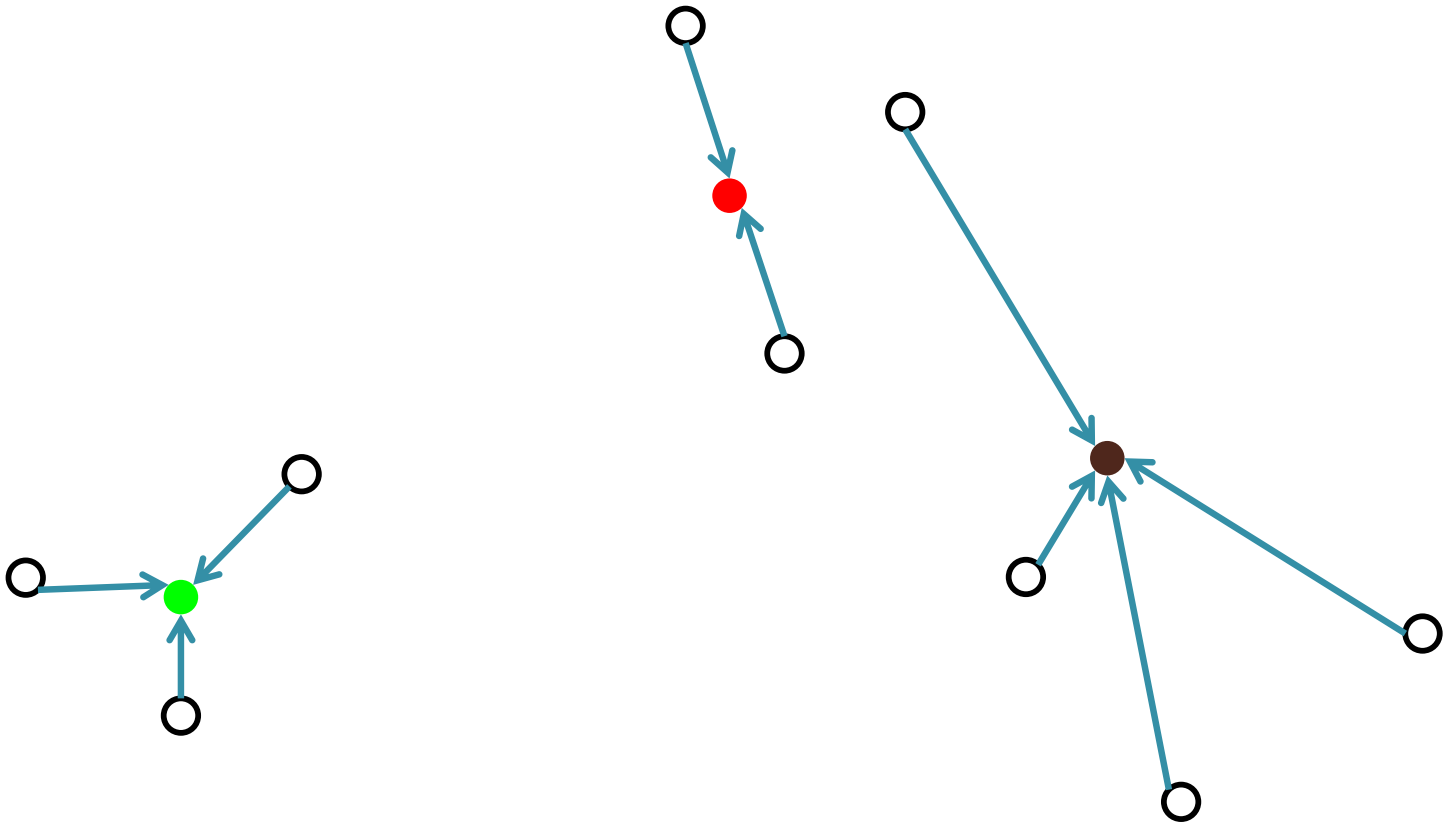

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Lloyd's method: Random Initialization

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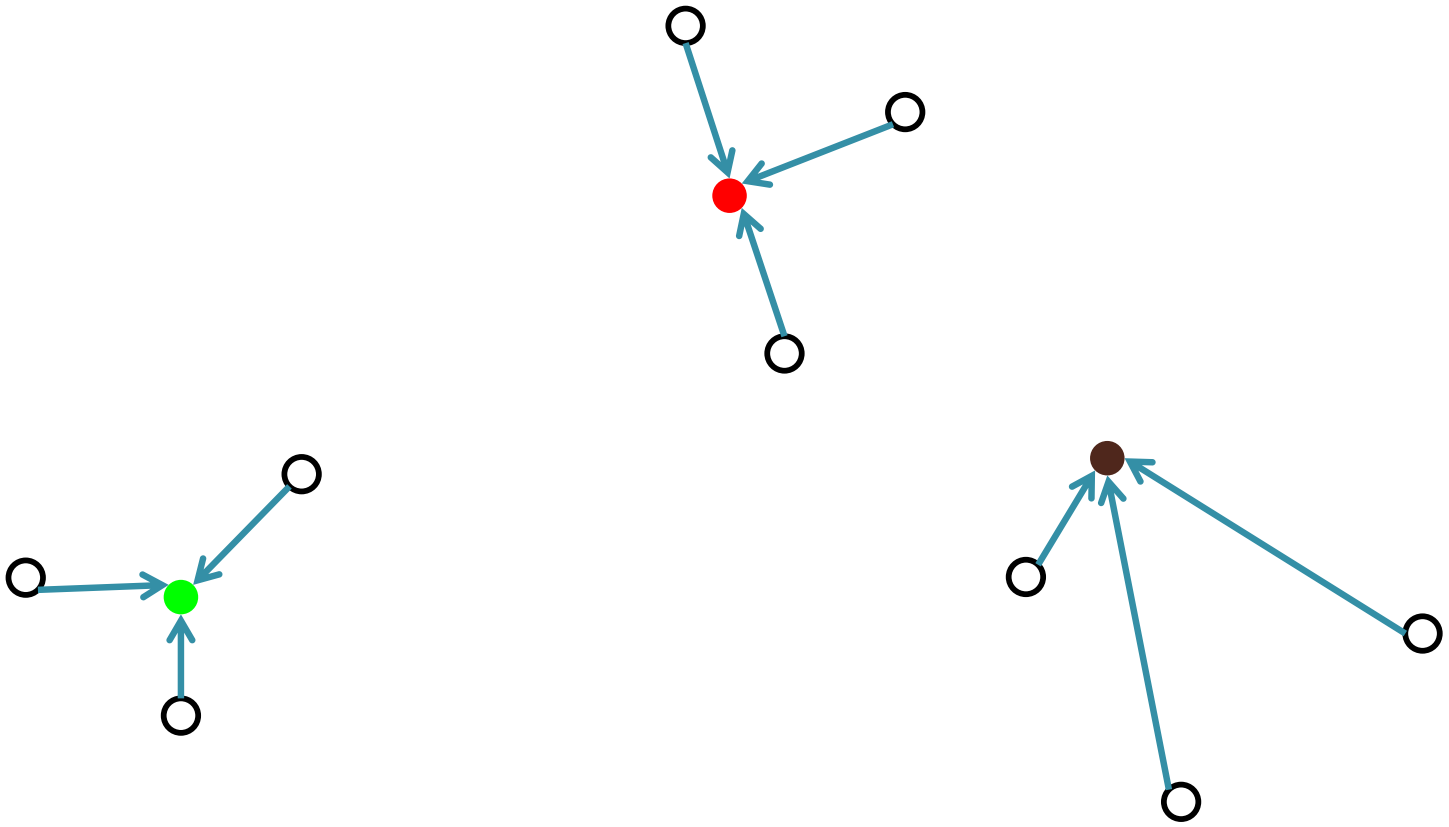

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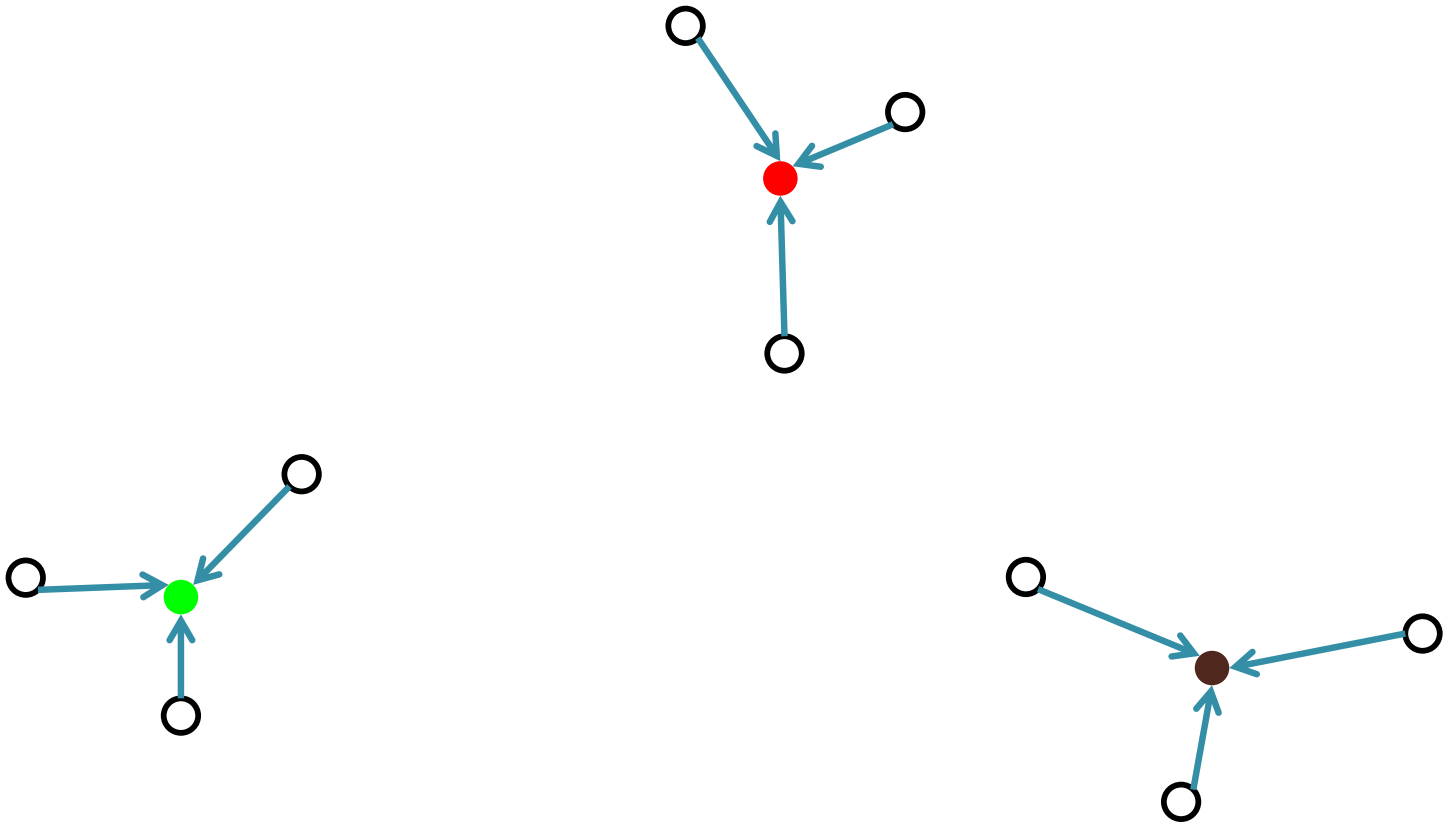
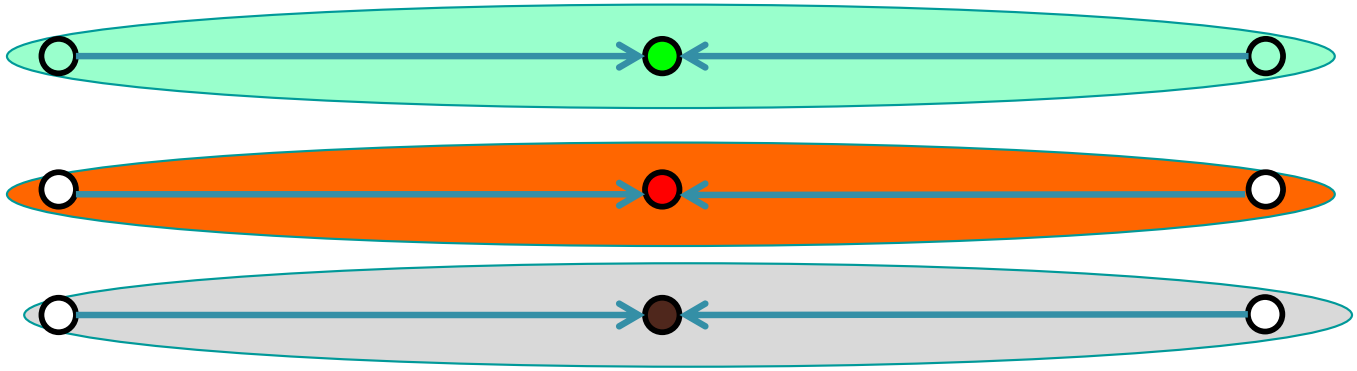
Lloyd's method: Random Initialization

Recompute optimal centers given a fixed clustering



Get a good quality solution in this example.

Lloyd's method: Performance



It always converges, but it may converge at a local optimum that is different from the global optimum, and in fact could be arbitrarily worse in terms of its score.

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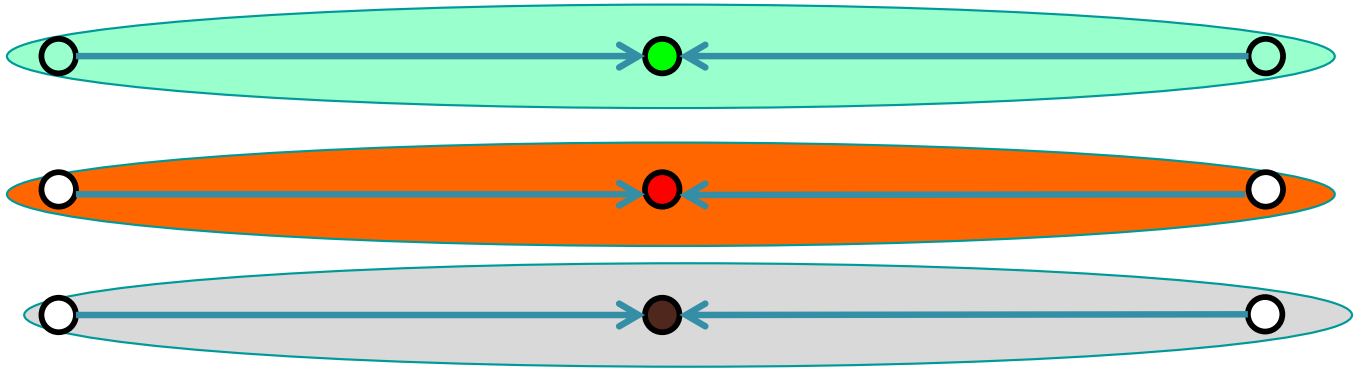
Lloyd's method: Performance



Local optimum: every point is assigned to its nearest center and every center is the mean value of its points.

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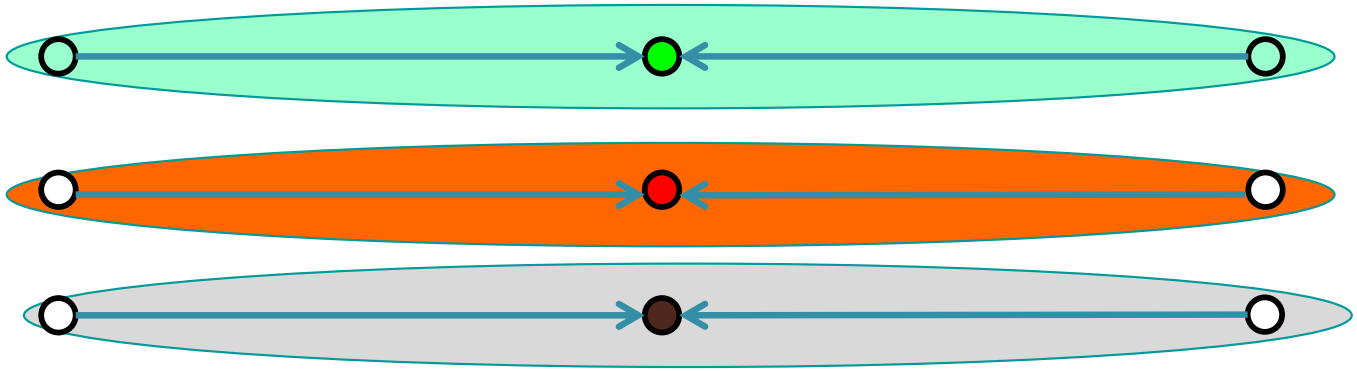
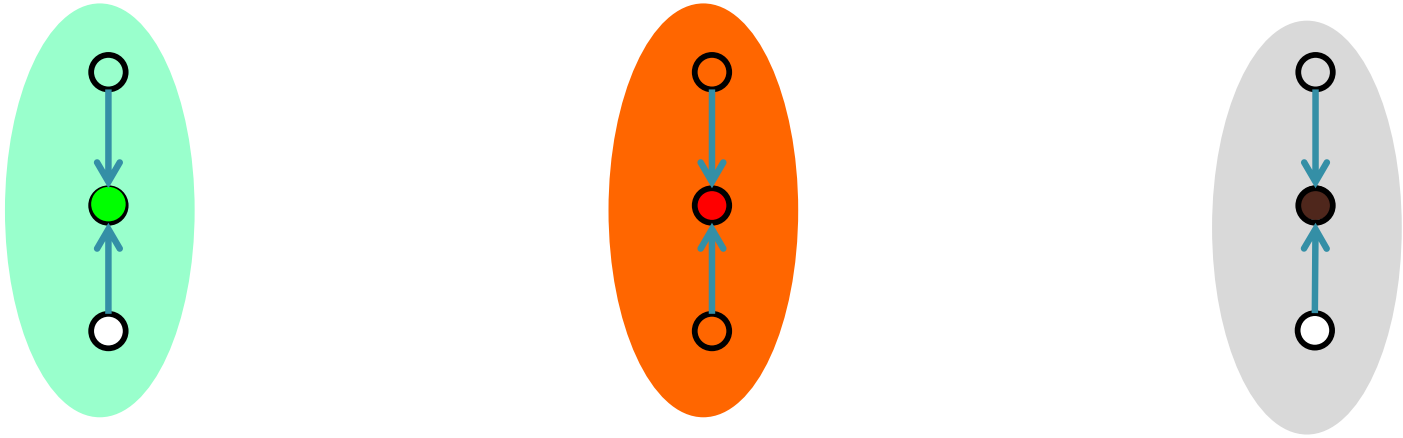
Lloyd's method: Performance



.It is arbitrarily worse than optimum solution….



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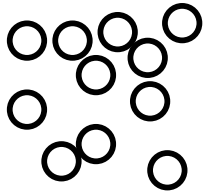
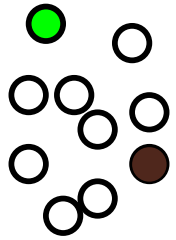
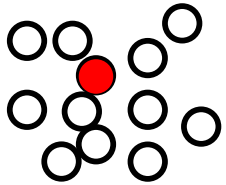
Lloyd's method: Performance







This bad performance, can happen even with well separated Gaussian clusters.

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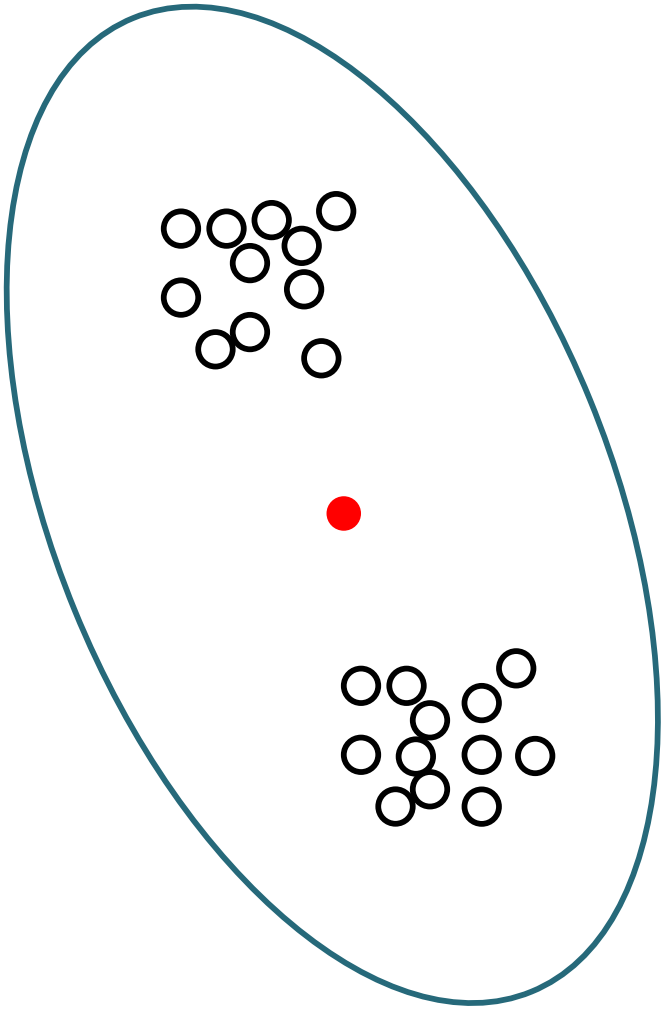
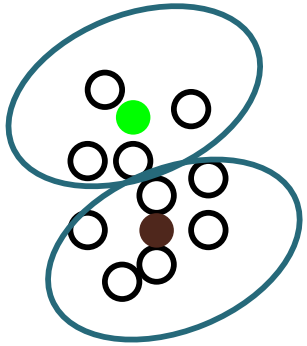
Lloyd's method: Performance





This bad performance, can happen even with well separated Gaussian clusters.

Some Gaussian are combined…..

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Lloyd's method: Performance

- 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 Lloyd's method will output a bad solution).

  - For k equal-sized Gaussians, Pr[each initial center is in a different Gaussian] $\approx \frac{k!}{k^k} \approx \frac{1}{e^k}$

  - Becomes unlikely as k gets large.

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Another Initialization Idea: Furthest Point Heuristic

Choose $\mathbf{c_1}$ arbitrarily (or at random).

- For $\mathrm{j} = 2, \ldots, \mathrm{k}$
  - Pick $\mathbf{c_j}$ among datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ that is farthest from previously chosen $\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_{j-1}}$

Fixes the Gaussian problem. But it can be thrown off by outliers….

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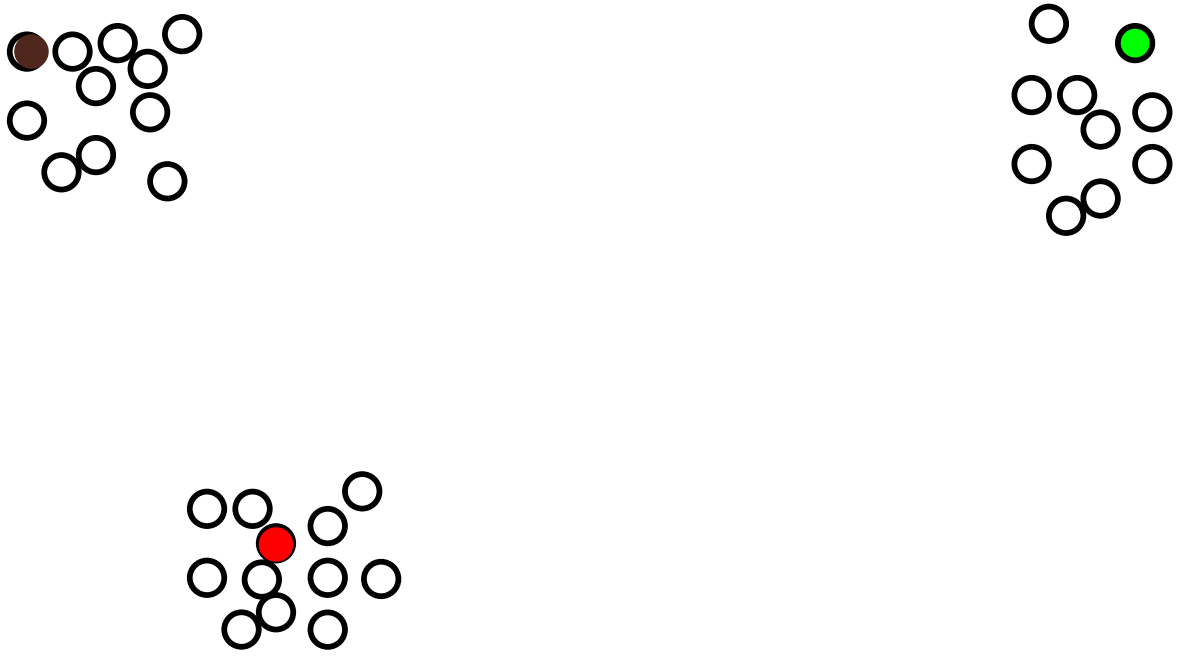
Furthest point heuristic does well on previous example



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Furthest point initialization heuristic sensitive to outliers

Assume k=3

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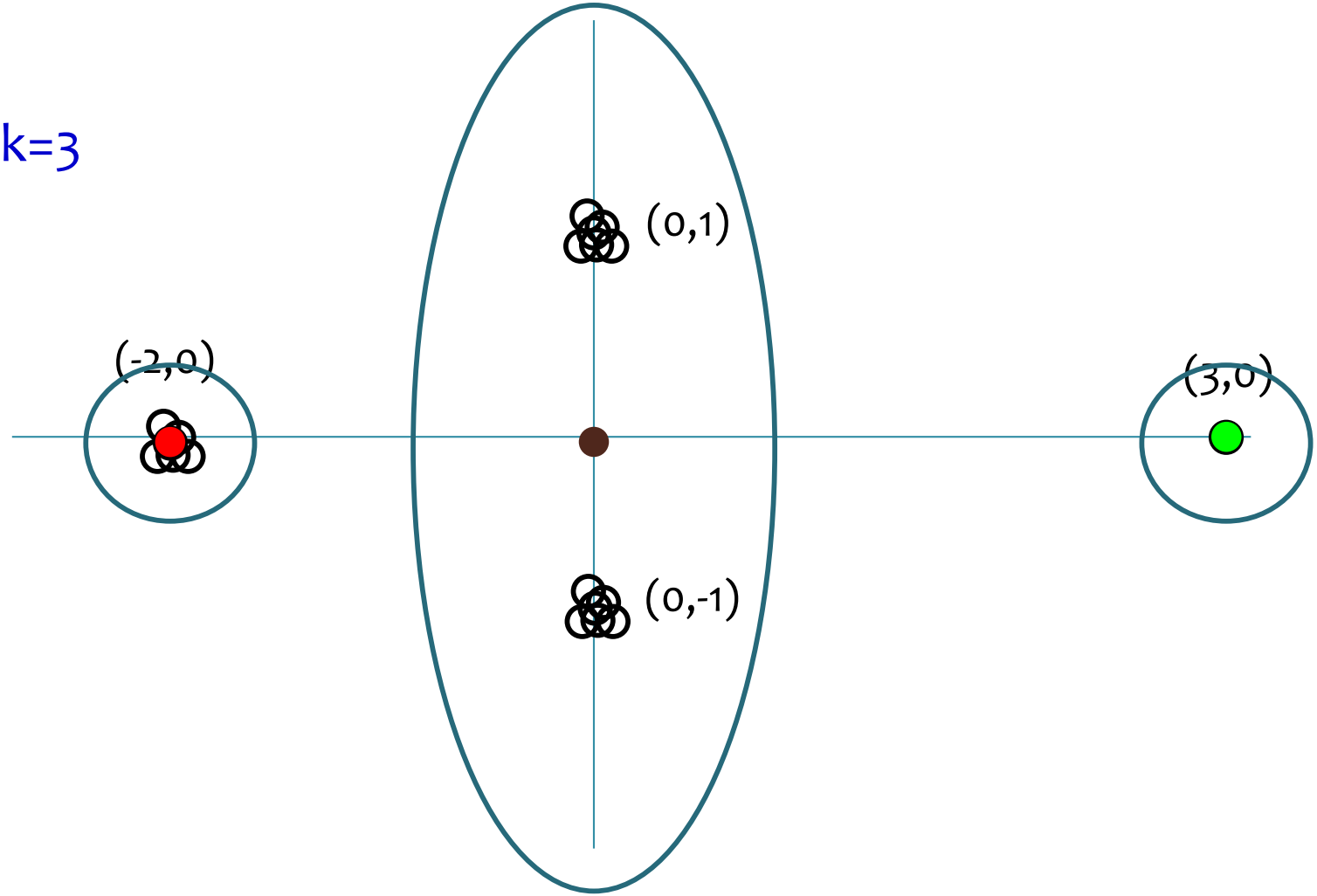
Furthest point initialization heuristic sensitive to outliers

Assume k=3



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K-means++ Initialization: D^2 sampling [AV07]

- Interpolate between random and furthest point initialization
- 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

$$\mathbf{Pr}(\mathbf{c_j} = \mathbf{x^i}) \propto \mathbf{min}_{j'<j} \left|\left|\mathbf{x^i} - \mathbf{c_{j'}}\right|\right|^2 \quad D^2(\mathbf{x^i})$$

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

Running Lloyd's can only further improve the cost.

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K-means++ Idea: D^2 sampling

- Interpolate between random and furthest point initialization
- Let $D(\mathbf{x})$ be the distance between a point x and its nearest center. Chose the next center proportional to $D^{\alpha}(\mathbf{x})$.
  - $\alpha = 0$, random sampling
  - $\alpha = \infty$, furthest point (Side note: it actually works well for k-center)
  - $\alpha = 2$, k-means++

Side note: $\alpha = 1$, works well for k-median

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K-means ++ Fix

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K-means++/ Lloyd's Running Time

- K-means ++ initialization: O(nd) and one pass over data to select next center. So O(nkd) time in total.

- Lloyd's method

Repeat until there is no change in the cost.

- For each j: $C_j \leftarrow \{x \in S$ whose closest center is $\mathbf{c_j}\}$
  - For each j: $\mathbf{c_j} \leftarrow$ mean of C_j

Each round takes time O(nkd).

- Exponential # of rounds in the worst case [AV07].

- Expected polynomial time in the smoothed analysis (non worst-case) model!

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K-means++/ Lloyd's Summary

- Running Lloyd's can only further improve the cost.
- Exponential # of rounds in the worst case [AV07].
- Expected polynomial time in the smoothed analysis model!
- Does well in practice.
- K-means++ always attains an O(log k) approximation to optimal k-means solution in expectation.

Slide courtesy of Nina Balcan

What value of k???

- Heuristic: Find large gap between k -1-means cost and k-means cost.
- Hold-out validation/cross-validation on auxiliary task (e.g., supervised learning task).
- Try hierarchical clustering.

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