k-Means Clustering

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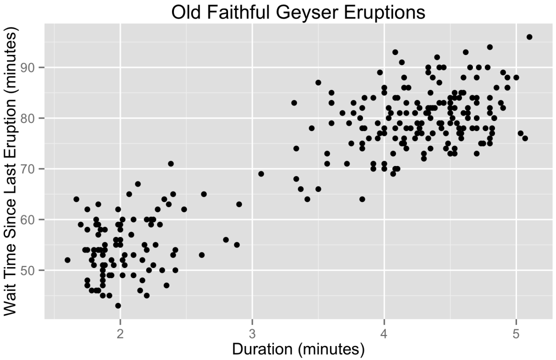
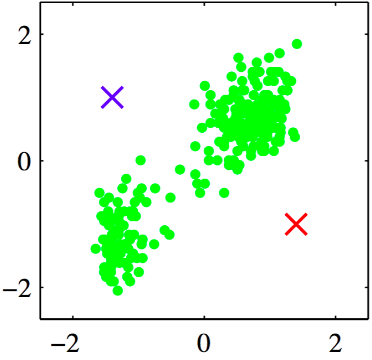
Example: Old Faithful Geyser



- Looks like two clusters.
- How to find these clusters algorithmically?

k-Means: By Example

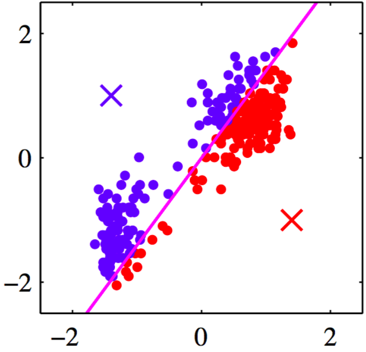
- Standardize the data.
- Choose two cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(a).

k-means: by example

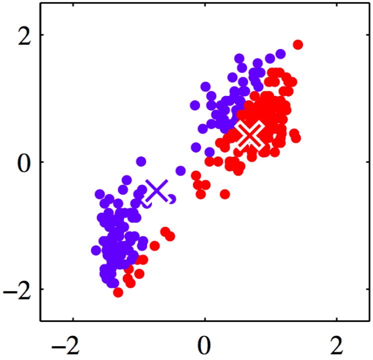
- Assign each point to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(b).

k-means: by example

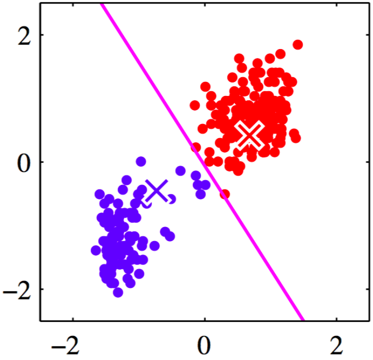
- Compute new class centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(c).

k-means: by example

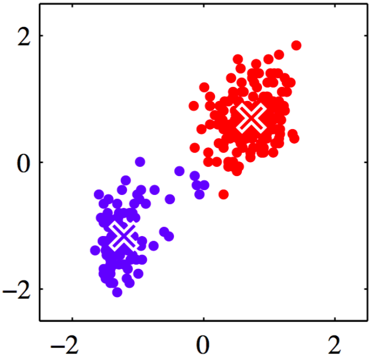
- Assign points to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(d).

k-means: by example

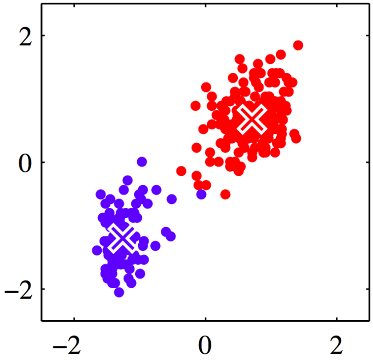
- Compute cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(e).

k-means: by example

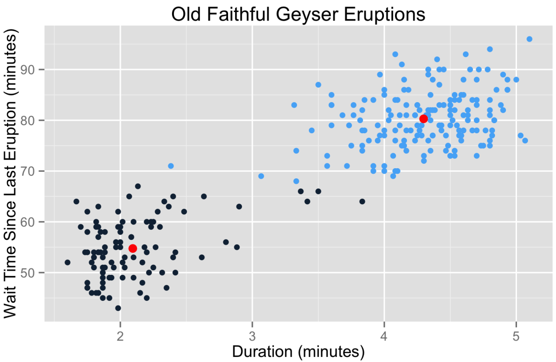
- Iterate until convergence.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(i).

k-Means Algorithm: Standardizing the data

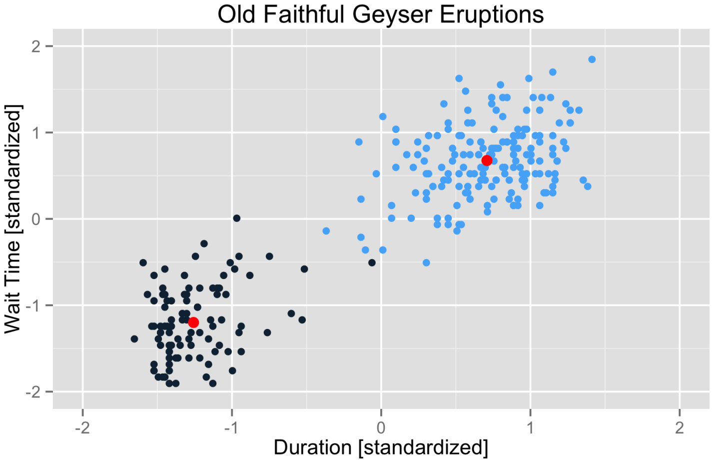
- Without standardizing:



- Blue and black show results of k-means clustering
- Wait time dominates the distance metric

k-Means Algorithm: Standardizing the data

- With standardizing:

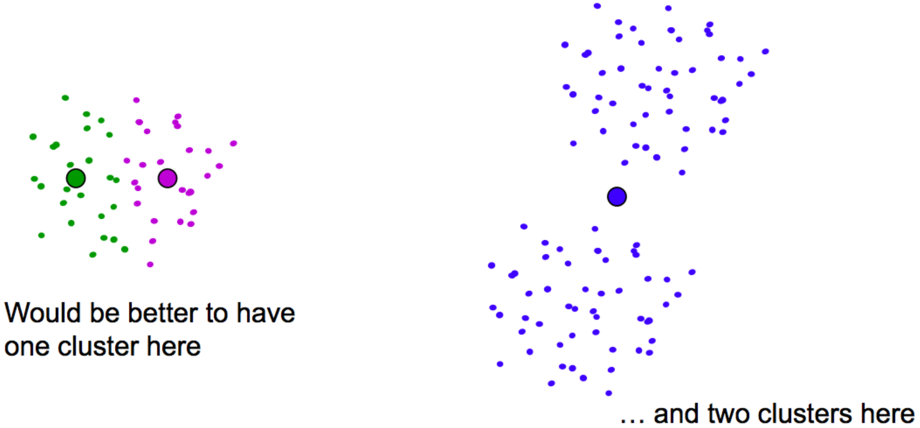


- Note several points have been reassigned from black to blue cluster.

k-Means: Failure Cases

k-Means: Suboptimal Local Minimum

- The clustering for $k = 3$ below is a local minimum, but suboptimal:



From Sontag's DS-GA 1003, 2014, Lecture 8.

k-means Formalized

k-Means: Setting

- Let $\mathcal{X}$ be a space with some distance metric d.
  - Most commonly, $\mathcal{X} = \mathbf{R}^d$ and $d(x, x') = \|x - x'\|$.
- Dataset $\mathcal{D} = \{x_1, \dots, x_n\} \subset \mathcal{X}$.
- Goal: Partition data $\mathcal{D}$ into k disjoint sets $C_1, \dots, C_k$.
- The **centroid** of C_i is defined to be

$$\mu_i = \mu(C_i) = \operatorname*{arg\,min}_{\mu \in \mathcal{X}} \sum_{x \in C_i} d(x, \mu)^2.$$

- Note: For Euclidean distance on $\mathbf{R}^d$, $\mu(C_i)$ is the mean of C_i.

Based on Shalev-Shwartz and Ben-David's book *Understanding Machine Learning*, Ch 22.

k-Means: Objective function

- The k-means objective is

$$
\begin{aligned}
J_{k\text{-means}}(C_1,\ldots,C_k) &= \sum_{i=1}^{k}\sum_{x\in C_i} d(x,\mu(C_i))^2 \\
&= \min_{\mu_1,\ldots,\mu_k\in\mathcal{X}} \sum_{i=1}^{k}\sum_{x\in C_i} d(x,\mu_i)^2
\end{aligned}
$$

- In **vector quantization**, we represent each $x \in C_i$ by the centroid μ_i.
- We can think of this as lossy data compression,
  - the k-means objective can be viewed as the reconstruction error.
- How many bits does it take to represent each point with vector quantization?
  - If $k = 2^d$, then d bits. (Fewer on average if the clusters have unequal sizes.)

k-Means: Algorithm

- input: $\mathcal{D} = \{x_1, \ldots, x_d\} \subset \mathcal{X}$
- initialize: Randomly choose initial centroids $\mu_1, \ldots, \mu_k \subset \mathcal{D}$.
- repeat until convergence (i.e. until the centroids or clusters repeat):
    - $\forall i$, let $C_i = \left\{x \in \mathcal{D} : i = \arg\min_j d(x, \mu_j)\right\}$. (break ties in some arbitrary manner)
    - $\forall i$, let $\mu_i = \arg\min_{\mu \in \mathcal{X}} \sum_{x \in C_i} d(x, \mu)^2$. (For Euclidean distance, $\mu_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$)

k-Means++

- In k-means, objective never increases, but no guarantee to find minimizer.
- General recommendation is to re-run with several random starting initial centroids.
- k-means++ is a way to randomly initialize the centroids with some guarantees:
  - Randomly choose first centroid from the data points $\mathcal{D}$.
  - For each of the remaining $k-1$ centroids:
    - Compute distance from each x_i to the closest already chosen centroid.
    - Randomly choose next centroid with probability proportional to the computed distance squared.
- If we let $J^*_{k\text{-means}}$ be the minimizer of the k-means objective, then using k-means++ for initialization guarantees that

$$\mathbb{E}\left[J_{k\text{-means}}(C_1, \ldots, C_k)\right] \leqslant 8\left(\log k + 2\right) J^*_{k\text{-means}}.$$