k-means continued

Rebecca C. Steorts

October 18, 2024

Optional reading: ISL 10.3, ESL 14.3

Announcements

1. Exam 2: Released Monday, November 18. Due Monday, November 25.
2. Exam 3: Released Monday, December 2. Due Friday, December 6.

Dissimilarity and within-cluster scatter

Assume observations $X_1, \dots X_n$, and dissimilarites $d(X_i, X_j)$.

Let K be the number of clusters (fixed).

A clustering of data points $X_1, \dots X_n$ is a function C that assigns each observation X_i to a group (or cluster) $k \in \{1, \dots K\}$

Dissimilarity and within-cluster scatter

Let $C(i) = k$ denote that X_i is assigned to group (or cluster) k.
Let n_k be the number of data points in the group (or cluster) k.
Let $d_{ij} = d(X_i, X_j)$.

Dissimilarity and within-cluster scatter

Let $C(i) = k$ denote that X_i is assigned to group (or cluster) k.
Let n_k be the number of data points in the group (or cluster) k.
Let $d_{ij} = d(X_i, X_j)$.

The within-cluster scatter is defined as

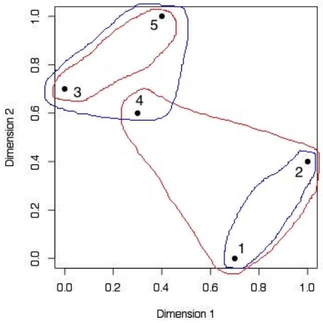
$$W = \frac{1}{2} \sum_{k=1}^{K} \frac{1}{n_k} \sum_{C(i)=k,\, C(j)=k} d_{ij}$$

Smaller W is better

Simple example

Here $n = 5$ and $K = 2$,
$X_i \in \mathbb{R}^2$ and $d_{ij} = \|X_i - X_j\|_2^2$

	1	2	3	4	5
1	0	0.25	0.98	0.52	1.09
2	0.25	0	1.09	0.53	0.72
3	0.98	1.09	0	0.10	0.25
4	0.52	0.53	0.10	0	0.17
5	1.09	0.72	0.25	0.17	0



- Red clustering:
  $W_{\text{red}} = (0.25 + 0.53 + 0.52)/3 + 0.25/2 = 0.56$
- Blue clustering:
  $W_{\text{blue}} = 0.25/2 + (0.10 + 0.17 + 0.25)/3 = 0.30$

(Tip: `dist` function in R)

Finding the best group assignments

Smaller W is better, so why don't we just directly find the clustering C that minimizes W?

Problem: doing so requires trying all possible assignments of the n points into K groups. The number of possible assignments is

$$A(n,K) = \frac{1}{K!}\sum_{k=1}^{K}(-1)^{K-k}\binom{K}{k}k^n$$

Note that $A(10,4) = 34,105$, and $A(25,4) \approx 5 \times 10^{13}$ ... huge

Most problems we look at are going to have way more than $n = 25$ observations, and potentially more than $K = 4$ clusters too!

So we'll have to settle for an approximation

Rewriting the within-cluster scatter

Focus on Euclidean space: now $X_i \in \mathbb{R}^p$ and dissimilarities are $d(X_i, X_j) = \|X_i - X_j\|_2^2$

Fact: within-cluster scatter can be rewritten as

$$\frac{1}{2}\sum_{k=1}^{K} \frac{1}{n_k} \sum_{C(i)=k} \sum_{C(j)=k} \|X_i - X_j\|_2^2 = \sum_{k=1}^{K} \sum_{C(i)=k} \|X_i - \bar{X}_k\|_2^2$$

with $\bar{X}_k$ the average of points in group k, $\bar{X}_k = \frac{1}{n_k}\sum_{C(i)=k} X_i$. The right-hand side above is called within-cluster variation

Hence, equivalently we seek a clustering C that minimizes the within-cluster variation (approximately so)

Rewriting the minimization

Remember: we want to choose C to minimize

$$\sum_{k=1}^{K} \sum_{C(i)=k} \|X_i - \bar{X}_k\|_2^2$$

Another fact: for any $Z_1, \ldots Z_m \in \mathbb{R}^p$, the quantity $\sum_{i=1}^m \|Z_i - c\|_2^2$ is minimized by taking $c = \bar{Z} = \frac{1}{m}\sum_{i=1}^m Z_i$, the average of the Z_i's

So our problem is the same as minimizing the enlarged criterion

$$\sum_{k=1}^{K} \sum_{C(i)=k} \|X_i - c_k\|_2^2,$$

over both clusterings C and $c_1, \ldots c_K \in \mathbb{R}^p$

K-means algorithm

1. Cluster (label) each point based the closest center
2. Replace each center by the average of points in its cluster

K-means algorithm

The K-means clustering algorithm approximately minimizes the enlarged criterion by alternately minimizing over C and $c_1, \ldots c_K$

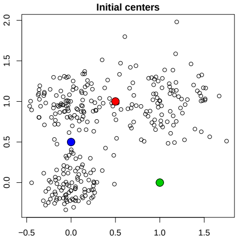
We start with an initial guess for $c_1, \ldots c_K$ (e.g., pick K points at random over the range of $X_1, \ldots X_n$), then repeat:

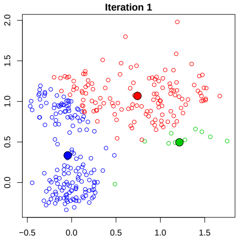
1. Minimize over C: for each $i = 1, \ldots n$, find the cluster center c_k closest to X_i, and let $C(i) = k$
2. Minimize over $c_1, \ldots c_K$: for each $k = 1, \ldots K$, let $c_k = \bar{X}_k$, the average of points in group k

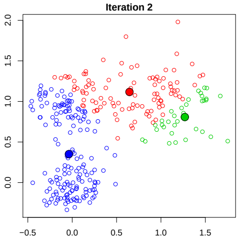
Stop when within-cluster variation doesn't change

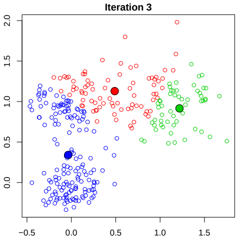
K-means example

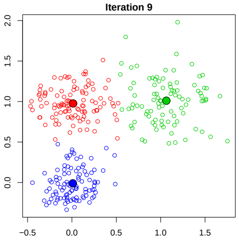
Here $X_i \in \mathbb{R}^2$, $n = 300$, and $K = 3$









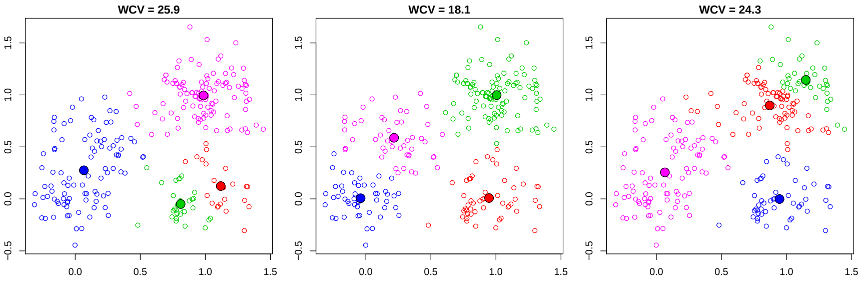


Properties of K-means

- Within-cluster variation decreases with each iteration of the algorithm. I.e., if W_t is the within-cluster variation at iteration t, then $W_{t+1} \leq W_t$
- The algorithm always converges, no matter the initial cluster centers. In fact, it takes $\leq K^n$ iterations (why?)
- The final clustering depends on the initial cluster centers. Sometimes, different initial centers lead to very different final outputs. So we typically run K-means multiple times (e.g., 10 times), randomly initializing cluster centers for each run, then choose among from collection of centers based on which one gives the smallest within-cluster variation
- The algorithm is not guaranteed to deliver the clustering that globally minimizes within-cluster variation (recall: this would require looking through all possible assignments!)

K-means example, multiple runs

Here $X_i \in \mathbb{R}^2$, $n = 250$, and $K = 4$, the points are not as well-separated



These are results of result of running the K-means algorithm with different initial centers (chosen randomly over the range of the X_i's). We choose the second collection of centers because it yields the smallest within-cluster variation

In K-means, cluster centers are averages

A cluster center is representative for all points in a cluster, also called a prototype

In K-means, we simply take a cluster center to be the average of points in the cluster. Great for computational purposes—but how does it lend to interpretation?

This would be fine if we were clustering, e.g., houses in Durham based on features like price, square footage, number of bedrooms, distance to nearest bus stop, etc.

We have to be careful as some applications may not be well suited to k-means. For instance, any applications where the data overlaps would not work well. Examples: entity resolution, network analysis, medical data, and others.

K-medoids algorithm

In some applications we want each center to be one of the points itself. This is where K-medoids comes in—an algorithm similar to the K-means algorithm, except when fitting the centers $c_1, \ldots c_K$, we restrict our attention to the points themselves

Initial guess for centers $c_1, \ldots c_K$ (e.g., randomly select K of the points $X_1, \ldots X_n$), then repeat:

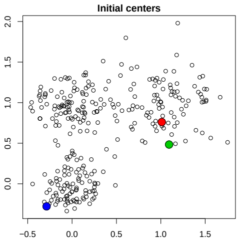
1. Minimize over C: for each $i = 1, \ldots n$, find the cluster center c_k closest to X_i, and let $C(i) = k$
2. Minimize over $c_1, \ldots c_K$: for each $k = 1, \ldots K$, let $c_k = X_k^*$, the medoid of points in cluster k, i.e., the point X_i in cluster k that minimizes $\sum_{C(j)=k} \|X_j - X_i\|_2^2$

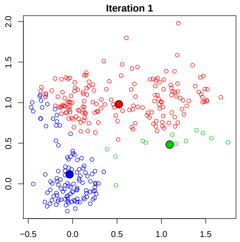
Stop when within-cluster variation doesn't change

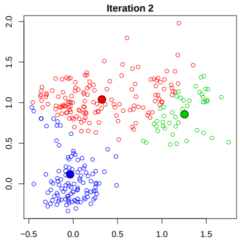
In words:

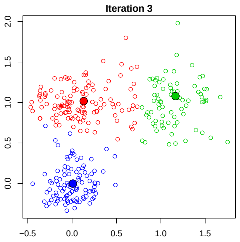
1. Cluster (label) each point based on the closest center
2. Replace each center by the medoid of points in its cluster

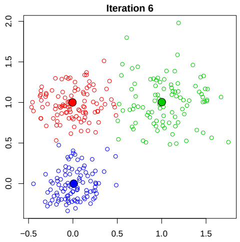
K-medoids example











Note: only 3 points had different labels under K-means

Properties of K-medoids

The K-medoids algorithm shares the properties of K-means that we discussed (each iteration decreases the criterion; the algorithm always converges; different starts gives different final answers; it does not achieve the global minimum)

K-medoids generally returns a higher value of

$$\sum_{k=1}^{K} \sum_{C(i)=k} \|X_i - c_k\|_2^2$$

than does K-means (why?). Also, K-medoids is computationally harder than K-means (because of step 2: computing the medoid is harder than computing the average)

Remember, K-medoids has the (potentially important) property that the centers are located among the data points themselves

K-means and K-medoids in R

The K-means algorithm is part of the base distribution in R, given by the `kmeans` function (use `algorithm="Lloyd"`)

E.g.,

```
km = kmeans(x, centers=k, nstart=10, algorithm="Lloyd")
```

The K-medoids algorithm is implemented by the function `pam` (stands “for partitioning around medoids”) in the package `cluster`

Recap: clustering

In clustering we divide up our data points into groups or clusters. We want points in any one group to be more similar to each other than to other points. All based on pairwise dissimilarities d_{ij}

Fixing the number of clusters K, the task of exactly minimizing the within-cluster variation (equivalently, within-cluster scatter) is not feasible. The K-means algorithm approximately minimizes this by iterating two simple steps

Though it always converges, the answer given by K-means depends on the initial centers. It also returns centers that are averages of data points. The K-medoids algorithm is an alternative where the centers are chosen among the points themselves. Its answer also depends on the starting configuration. Hence for either algorithm, one should run it several times with different starts