Clustering big data

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1 Rationale

Telescopes surveying the Universe in search of exoplanets, DNA sequencers decoding our genes, governments monitoring cities, and people all over the world exchanging messages, images, videos produce across the Internet produce exabytes of data every day.

Researchers, businesses and governments all over the world are trying to make sense of the ever-increasing collection of data they have access to.

It needs to be stored, searched through, processed and analyzed to extract valuable information. Such a large volume of data comes with its own set of challenges and in the past few years, novel programming paradigms have emerged that make analyzing this data a lot more accessible. There are many systems that are designed to handle "big data". Out of these, the most famous one is MapReduce [**?**] from Google, for batch processing and more recently Storm [**?**] originally from Backtype, now acquired by Twitter.

Many applications that have previously been impossible are now a reality thanks to massive data sets. For example, quality statistical machine Translation can only work at very large scale. While the accuracy of currently available commerical fails to capture more subtle nuances, it is certainly good enough to convey the general meaning.

Large scale data analysis is a broad field with many overlapping disciplines like machine learning, data mining, data science etc.

Analyzing big data is challening. The complexity of many algorithms makes them difficult to parallelize and even when this is possible, because of the scale of the data, clusters of many machines are needed to process the data in reasonable time.

The mainframe era of the 80s, displaced by the affordable personal computer is making a comeback under the guise of "cloud computing" precisely because the complexity of maintaining a large enough cluster of machines to process "big data" makes it a ripe target for outsourcing.

Companies now offer "clouds", clusters of virtual machines that support MapReduce style processing through open-source Hadoop distributions like Amazon (Amazon Web Services), Google (Google Compute Engine), Microsoft (Windows Azure) have vast data centers at their disposal and offer infrastructure as a service to be billed by the hour (or minute).

Time is quite literally money in this market which makes fast processing even more critical. When processing data at terrabye scale and beyond especially in pipelines, the first priority is usually to reduce the data through some aggregation such that the resulting size is much smaller, for example storing statistics instead of the raw data.

One of the most useful algorithms to analyze data with is clustering. Intuitively the aim of clustering is to find clumps of data that are more similar to one another than the others.

The traditional use of clustering is for revealing interesting patterns in the data — for example, if n good quality clusters do form, this could mean there are n types of users in the system.

It's also especially useful for getting a good representative sample of the data that should behave similarly to the original distribution. This is important because sometimes there are no obvious ways of aggregating the data being processed directly to reduce its size. If the data is clustered however, the resulting clusters' centroids can be used as input for the next stage of processing.

2 Clustering

There are many kinds of clustering which vary significantly in their approach in building the clusters. The kind of clustering we'll be discussing in this paper is "centroid" based.

To apply any clustering, or machine learning for that matter, the data needs to be transformed from its raw representation to "feature vectors". The corresponding feature vector for a data item should capture plausibly relevant characteristics of the item in a numeric form. For example, when working with text documents, feature vectors containing frequencies a given word in a document compared to the corpus are useful.

This paper doesn't attempt to further describe the various ways used to encode data into feature vectors or assess the usefulness of a subset of features. This is requires domain-specific knowledge and is the goal of feature engineering. It's assumed the data is already available as feature vectors and so now the clustering problem can be formalized.

Given n vectors (also referred to as a points) in $\mathbf{R}^d$ and an integer k, and a distance measure, *dist*, group the n points into k disjoint sets X_1 through X_k. The mean of the points in cluster i (or, disjoint set X_i) is called the "centroid" of that cluster, which we call c_i.

The clustering needs to be good in some sense, so define a measure of quality to optimize for. For this, *dist*, a distance measure is needed, making the combined vector space and measure a metric space.

T_c, is what gets optimized for — the total cost of the clustering, which is the sum of the distances from each point to the centroid of the cluter it is assigned to.

$$T_c = \sum_{i=1}^{k} \left(\sum_{\mathbf{x_{ij}} \in \mathbf{X_i}} dist(\mathbf{x_{ij}}, \mathbf{c_i}) \right) \tag{1}$$

In this formulation, the number of clusters, k is fixed, but this problem is related to the facility placement problem, which essentially identical except in that the number of cluster can vary.

The main issue with this formulation is that the optimization problem we're trying to solve is NP-hard in the general case. This has the very important implication that it is infeasible to find an optimal solution to this problem. Any polynomial-time algorithm we can devise will at best be an approximation scheme. This turns out to not be as dire as it first sounds, because "good

enough" is fine for virtually all applications and also because real data tends to have additional properties that results in stronger quality guarantees.

2.0.1 Distance measure

One difference users used to clustering literature might have noticed in this formulation is that our choice of distance measure is not fixed. Normally most papers on clustering work with $||\mathbf{x} - \mathbf{y}||_2^2$, the squared Euclidean distance (or squared $L2$-norm). We acknowledge this and indeed some results we use for our implementations have this assumption. As implementors of a machine learning library however, we need to support user extensibility and we feel that other than providing documentation to our users, we shouldn't enforce other kinds of restrictions. It turns out that most distances used in practice are variants of this distance measure (for example the $L2$-norm and the cosine distance), in which case the results likely the same. If some completely different distance measure is used, we can't provide any guarantees.

2.1 Quality

When it comes to the quality of the clusters generated by any algorithm, it is often said that "clustering is in the eye of the beholder". In unsupervised learning, which this problem is a part of, there is no known "right answer". Compare this with classification or regression where an example is either correctly clasified or predicted, or it isn't.

Things are not so clear-cut in this case. While the total cost is certainly what we optimize for, multiple measure have been devised over the years that attempt to formalize the degree a clustering is "good". Intuitively, we want clusters that are:

- compact, meaning that the points in a cluster are close together (the intra-cluster distances are small between any two points)
- well separated, meaning that two different clusters will be relatively far apart (the inter-cluster distances are large between any two clusters)

The Dunn Index and Davies-Bouldin Index try to express compactness and separability in one score. These are called "internal" scores because they only at one clustering.

Additionally, it is often useful to compare two different clusterings and to see how similar they are. This is useful especially when comparing different clusteirng algorithms. A widely used score for this is the Adjusted Rand Index based off the "confusion matrix" (same idea as with classification).

2.1.1 Dunn Index

The Dunn Index, was invented in 1974 by J. Dunn. A higher Dunn Index indicates a better clustering. It combines Δ_i, a distance score for cluster i

(called intracluster distance) and the distance between two clusters, $dist(\mathbf{c}_i, \mathbf{c}_j)$ (intercluster distance).

Δ_i can have different expressions. For cluster X_i it could be:

- the maximum distance between any two points

$$\Delta_i = \max_{\mathbf{x},\mathbf{y} \in X_i} dist(\mathbf{x}, \mathbf{y}) \tag{2}$$

- the mean distance between any two points

$$\Delta_i = \frac{1}{|X_i|(|X_i| - 1)} \sum_{\mathbf{x},\mathbf{y} \in X_i, \mathbf{x} \neq \mathbf{y}} dist(\mathbf{x}, \mathbf{y}) \tag{3}$$

- the mean distance between any point and the centroid

$$\Delta_i = \frac{\sum_{\mathbf{x} \in X_i} dist(\mathbf{x}, \mathbf{c}_i)}{|X_i|} \tag{4}$$

- the median distance between any point and the centroid. This is the one we use in the implementation. The reasoning is that the median is much more roubst to outliers than the mean or max. Additionally, computing distances between all pairs of points is simply not feasible for large datasets.

Having defined Δ_i, the Dunn Index is:

$$D = \min_{1 \leq i \leq k} \left\{ \min_{1 \leq j \leq k, j \neq i} \left\{ \frac{dist(\mathbf{c}_i, \mathbf{c}_j)}{\max_{1 \leq l \leq k} \Delta_l} \right\} \right\} \tag{5}$$

2.1.2 Davies-Bouldin Index

The Davies-Bouldin Index was invented in 1979 by D. Davies and D. Bouldin. Like the Dunn Index, it is an internal evaluation scheme. A lower Davies-Bouldin Index indicates a better clustering.

Defining a cluster-specific measure, exactly like for the Dunn Index, Δ_i, the index is:

$$DB = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} \left(\frac{\Delta_i + \Delta_j}{dist(\mathbf{c}_i, \mathbf{c}_j)} \right) \tag{6}$$

2.1.3 Adjusted Rand Index

The Rand Index was invented by W. Rand in 1971. It measures how similar two clusterings are to one another. When the index is adjusted for change grouping of elements it is known as the Adjusted Rand Index.

To compute the index, one must first construct a contingency table (also known as a confusion matrix). Assuming the clusterings are $X = \{X_1, X_2, \ldots X_k\}$

and $Y = \{Y_1, Y_2, \ldots Y_k\}$, the overlap between cluster i of X, and cluster j of Y, n_{ij} is the number of points that are closest to cluster i in clustering X and cluster j in clustering Y. That is $n_{ij} = X_i \cap Y_j$.

	Y_1	Y_2	$\ldots$	Y_k	Sums
X_1	n_{11}	n_{12}	$\ldots$	n_{1k}	a_1
X_2	n_{21}	n_{22}	$\ldots$	n_{2k}	a_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
X_k	n_{k1}	n_{k2}	$\ldots$	n_{kk}	a_k
Sums	b_1	b_2	$\ldots$	b_k	

The Adjusted Rand Index is:

$$AR = \frac{\sum_{ij}\binom{n_{ij}}{2} - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}\right] - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}} \tag{7}$$

3 k-means

The most famous, simple and quite venerable clustering algorithm, known since the 50s is k-means and later Lloyd's method.

It first starts by chosing k point out of the n as seeds. These will be the first centroids (they're not "really" centroids since they are not the means of the points). The algorithm then proceeds by doing some number of iterations of the following steps:

1. assign each point to the cluster whose centroid is closest to it
2. recompute the existing centroids

The following 6 figures illustrates how this works in a toy example with 2D points we want to cluster into 3 clusters.

Figure 1: These are some example points we'll cluster in 3 groups

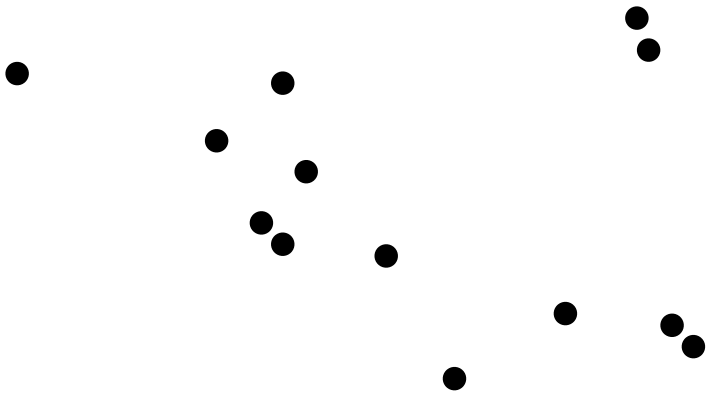


Figure 2: Here we selected 3 points as the initial centroids

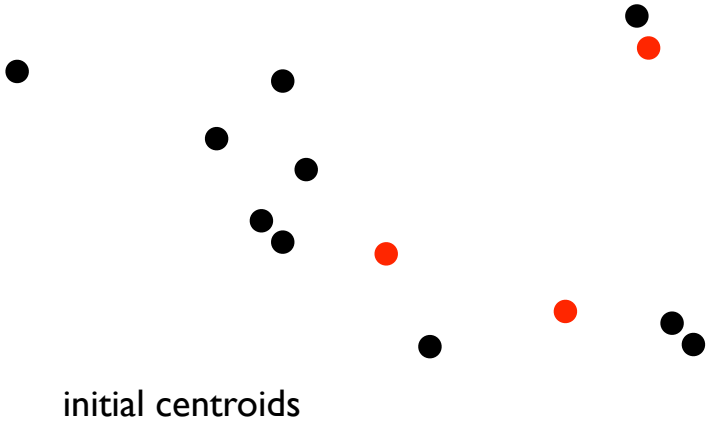


Figure 3: Here we assign each point to the cluster whose centroid it's closest to

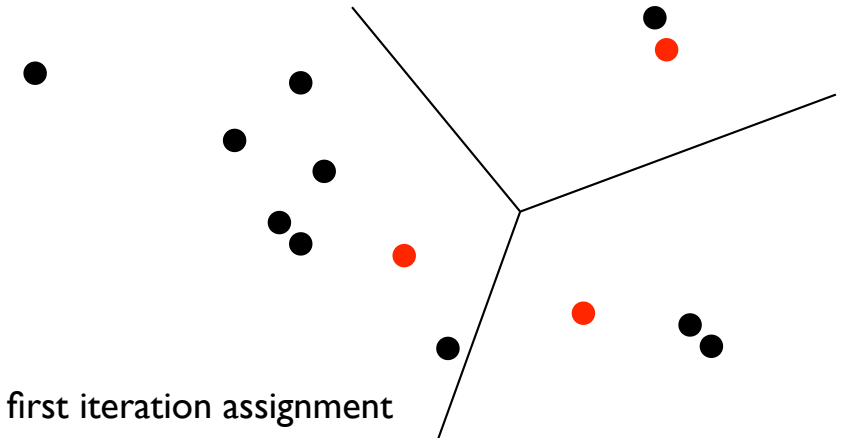


Figure 4: After asigning each point to a cluster, we compute the centroids of those clusters as the mean of the points in that cluster

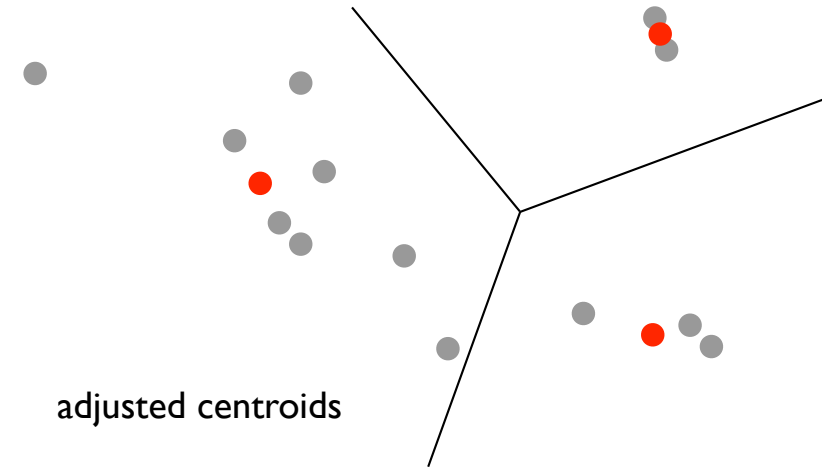


Figure 5: Second iteration assignment

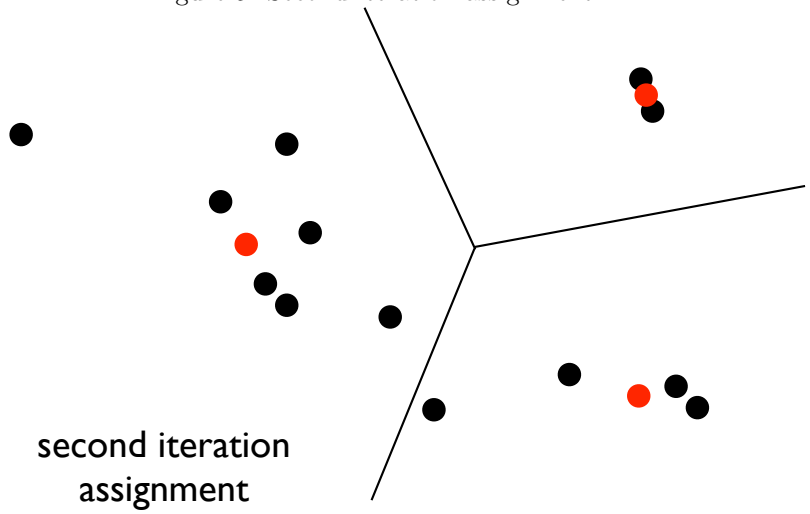
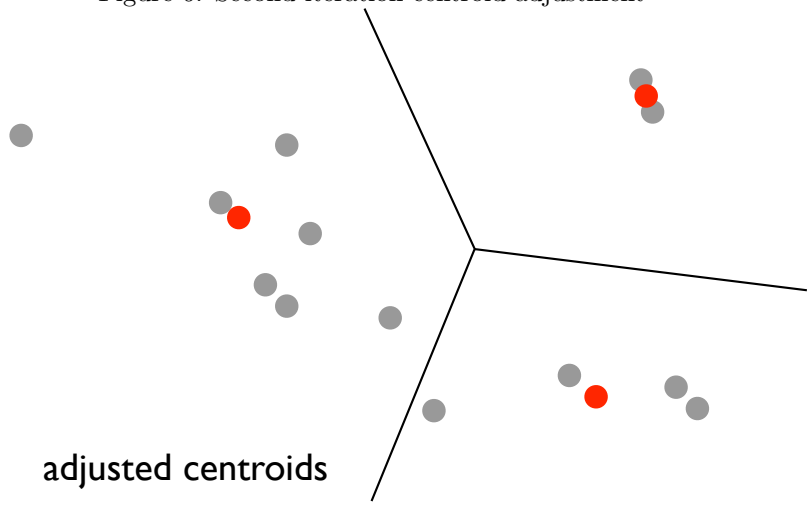


Figure 6: Second iteration centroid adjustment



3.1 Algorithm

The pseudocode for the algorithm described above is:

```
1: Centroids ← select k points ∈ Points
2: while not done do
3:     for c ∈ Centroids do
4:         Clusters[c] ← ∅
5:     end for
6:     for p ∈ Points do
7:         d_min ← ∞
8:         for c ∈ Centroids do
9:             d ← dist(p, c)
10:            if d < d_min then
11:                d_min ← d
12:                c_min ← c
13:            end if
14:        end for
15:        Clusters[c_min] ← Clusters[c_min] ∪ {p}
16:    end for
17:    Centroids ← ∅
18:    for C ∈ Clusters do
19:        Centroids ← Centroids ∪ {mean(C)}
20:    end for
21: end while
```

The crucial details in the algorithm are:

1. centroid initialization: how are the k points selected to become centroids at the beginning?

2. stopping condition: how long do we need to do the point assignment and centroid adjustment?

These two questions have a variety of solutions each of them resulting in a slightly different version of the algorithm, but with mostly similary results.

3.2 Initialization

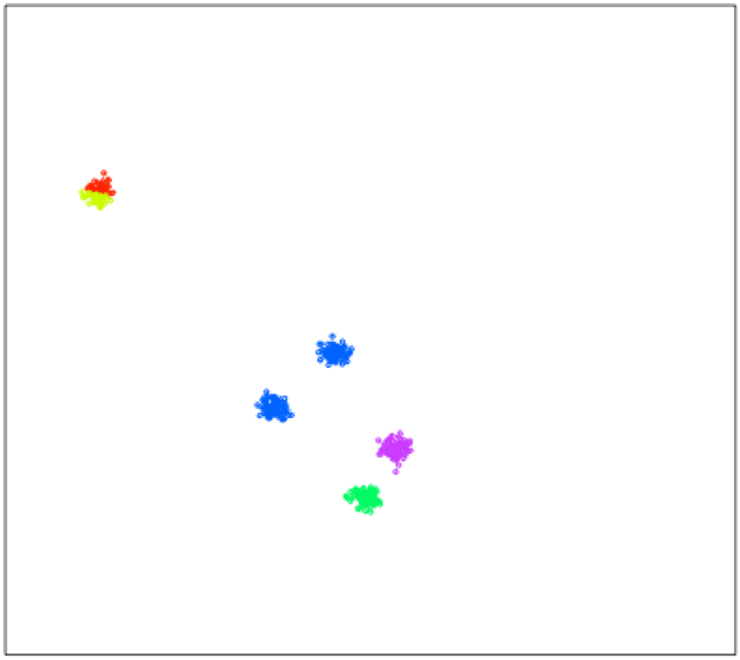
Selecting the first k points to become centroids, or "seeding" as it is also known is the single most important factor in getting a high-quality clustering.

3.2.1 Random selection

The simplest solution is to simply select k points of the n randomly. This produces a seed but has no real guarantees about what these points are. For a good quality clustering, assuming there are k real clusters and we wish to identify them, the seeds should ideally come from the k clusters and no two seeds should come from the same clusters. If this is true, because we assumed

the clusters really do exist in the data, the cluster assignment will set nearly all the points in the right cluster in just a few steps. The downside of this approach is illustrated in the figure below. There, two seeds are selected from the same real cluster, causing it to be split among the two k-means clusters (red and yellow). This means, another cluster (the blue one) will have to contain points from two real clusters.

Figure 7: Here is a case where the random initialization failed and a single real cluster was split between the yellow and red k-means clusters



Additionally, like many machine learning algorithms that only result in locally optimal solutions, k-means benefits from multiple restarts. Multiple restarts are even more important as this makes it nearly impossible to not have a good set of initial centroids.

3.2.2 k-means++

There are ways of improving the selection of centroids through the intuitive idea that we want to have seeds that are as far apart to each other as possible. This effectively eliminates the problem of having two seeds in the same cluster. While there are multiple ways of doing this, the most widely used one probably being [1]. The approach I implemented is described in [2] and is summarized below. In [2], Ostrovsky et. all introduce a new condition, called ϵ-*separability* that formalizes what data should look like for a good clustering to exist and give an new way of sampling the initial centroids with provably-good guarantees. This sampling is fairly similar to k-means++ and they show how it can produce a constant-factor approximation of the optimal clustering with just one Lloyd step provided the data is ϵ-separable.

From an implementor's perspective, checking if the data is indeed ϵ-separable is of little interest. We would need to know the optimum clustering cost for k clusters and $k-1$ clusters and if we could compute those, we'd just do it directly. The new sampling method however, is useful and we describe it below (based on section 4.1.1 in [2]).

First, we select two centroids, c_1 and c_2 with probability proportional to $dist(c_1, c_2)$. [2] uses $dist(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}||_2^2$ as the distance measure, but as explained above, we generalize this in the implemetation to any user supplied function. We now have the first 2 centroids.

Then, to select the $(i+1)$-th centroid, call the i already selected centers, $\mathbf{c}_1 \dots \mathbf{c}_i$. The new point is selected randomly with probability proportional to $\min_{j \in \{1 \dots i\}} dist(\mathbf{x}, \mathbf{c}_j)$.

3.3 Convergence

As with most iterative machine learning algorithms, the main k-means step is performed multiple times. We stop the algorithm after:

- a fixed number of iterations, this is usually an upper bound
- a quality metric plateaus (in this case, total cost), meaning that it stops decreasing after a few iterations
- no points change cluster assignment

3.4 Number of clusters

Clustering is a very broad and somewhat loosely defined problem in general. In fact, [3] jokingly remarks that "clustering is in the eye of the beholder". While we have formalized the problem in section 2, by explicitly stating that we are given n d-dimensional points and the distance measure $dist$, we also assume to be given k.

This might be true, but most of the time in practice it isn't. Typically however, this being an unsupervised learning problem, there is no ground truth.

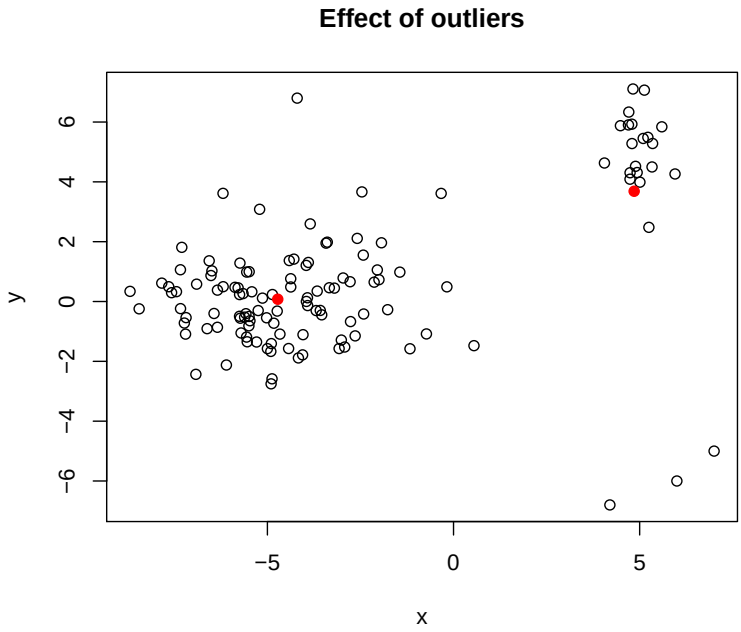
This implies that we can't know what the value of k actually is, and sometimes we don't particularly care (notably, when using clustering to sample our original data set). One well known way of addressing this is the "Elbow Method", where one tries clustering the points with different values of k and plots the total cost T_c as a function of k. The total cost should go down as more clusters are available, because "real" clusters in the data have too few clusters to properly represent them, until after reaching this point, the cost plateaus because more clusters fit the real clusters exactly.

3.5 Outliers

Real data is often messy: it's put together from various data sources by (buggy) algorithms and (falible) humans and errors are likely. These errors look like outliers in the data where one of the dimensions is much different than the rest. In an unlucky case, these outliers migh even be fairly close together, warranting the question of whether they should be thought of as a cluster themeslves.

In the figure below, suppose we're convinced that the 3 points at the bottom right are outliers and that there are only 2 clusters in the data. Then, the reasonable thing to do, is discard them and not have them be part of any cluster.

Figure 8: Data set where outliers have skewed the centroids



That's not possible with standard k-means as every point is part of exactly one cluster and contributes to that cluster's mean. This is why in the figure, the centroid of the cluster in the top-right is skewed downwards towards the three outliers at the bottom-right. The only thing to do here is to manually remove the outliers which is plausible for a small data set, but impossible for even a medium-sized one.

The solution, lifted from [2] modifies the centroid update operation. Instead of taking all the points assigned to a cluster into account when computing the new centroid, onle points that are within a ball (in the topological sense) are averaged. The radius of this ball is fraction (user-configurable in practice) of the smallest inter-cluster distance within the clustering. This ensures that only points close to the cluster's "core" play a role in the adjustment of its centroid.

3.6 Algorithm Complexity

A major consideration not treated up until now in this paper is the complexity of the algorithm. While the number of iterations is highly-dependent on the initial centroid seeding and the particular shape of the data, for a given k-means step,

the two main operations take:

1. point to cluster assignment: for each of the n points, go through all k centroids and compute the distance between the d-dimensional vectors. This step is therefore $O(nkd)$.

2. centroid adjustment: the points are partitioned across k clusters, but they are essentially summed up and divided by their count in each cluster. Therefore, this step is $O(nd)$.

So, for a given step, the total cost is $O(nkd + nd) = O(nkd)$. Each of these variables could conceivable be reduced.

1. n: The data could be downsampled, thereby reducing n. Downsampling needs to take into account the particular distribution of the data and preserve it well-enough for the final clustering. This is the route taken indirectly by the streaming k-means approach described in section 9.

2. d: The vectors' dimensionality could be reduced through standard techniques like Principal Component Analysis.

3. k: Searching for the nearest neighbor among all the centroids is usually not a significant expense when k is small. For most "classical" clustering applications, k is less than 100. However, especially when using clustering as a way of approximating data, or when dealing with web-scale data, k can be much larger, potentially on the order of millions. And even if it isn't, being a multiplicative constant is reason enough to want to reduce it. This can be achieved through approximate nearest-neighbor searches.

3.6.1 Approximate nearest-nerighbor search

There are many approaches to this problem, some of which are surveyed by Riegger in [5]. The one we chose is based on the Johnson-Lindenstrauss Lemma by W. Johnson and J. Lindenstrauss in [6], for which an elementary proof is given by Dasgupta et. all in [7]. Citing directly from their abstract,

> A result of Johnson and Lindenstrauss shows that a set of n points in high dimensional Euclidean space can be mapped into an $O(\log \frac{n}{\epsilon})$-dimensional Euclidean space such that the distance between any two points changes by only a factor of $(1 \pm \epsilon)$.

The mapping can be obtained by simply sampling $O(\log \frac{n}{\epsilon})$ the components of d-dimensional vectors from $\mathcal{N}(0, 1)$ and then normalizing the results.

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[6] W. B. Johnson and J. Lindenstrauss, Extensions of Lipschitz maps into a Hilbert space, Contemp Math 26 (1984), 189206.

[7] Dasgupta, S., & Gupta, A. (2003). An elementary proof of a theorem of Johnson and Lindenstrauss. Random Structures and Algorithms, 22(1), 6065. doi:10.1002/rsa.10073