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How to understand the drawbacks of K-means

K-means is a widely used method in cluster analysis. In my understanding, this method does NOT require ANY assumptions, i.e., give me a dataset and a pre-specified number of clusters, k, and I just apply this algorithm which minimizes the SSE, the within cluster squared error.

So k-means is essentially an optimization problem.

I read some material about the drawbacks of k-means. Most of them say that:

- k-means assumes the variance of the distribution of each attribute (variable) is spherical;
- all variables have the same variance;
- the prior probability for all k clusters is the same, i.e., each cluster has roughly equal number of observations;

If any one of these 3 assumptions are violated, then k-means will fail.

I could not understand the logic behind this statement. I think the k-means method makes essentially no assumptions, it just minimizes the SSE, so I cannot see the link between minimizing the SSE and those 3 "assumptions".

machine-learning clustering data-mining k-means

edited Jan 13 at 12:05

Anony-Mousse
18.8k 3 23 50

asked Jan 16 '15 at 4:38

KevinKim
1,558 3 6 18

29 I would say that the number of clusters is already quite an assumption. – njzk2 Jan 16 '15 at 16:58

16 The key assumptions of k-means are: 1. there *are* k clusters. 2. SSE is the *right objective* to minimize. 3. all clusters have the *same* SSE. 4. all variables have the same importance for every clusters. These are pretty strong assumptions... – Anony-Mousse Jan 17 '15 at 14:12

2 To your second question (posted as answer, then deleted): if you want to understand k-means as optimization problem similar to linear regression, understand it as **quantization**. It tries to find the least squares approximation of the data using k instances. I.e. if you actually *replaced* every point by the nearest centroid. – Anony-Mousse Jan 19 '15 at 9:48

1 I added an illustration to my answer below of a data set where one might assume k-means works really well (all clusters of same shape) yet it still gets stuck in local minima; and even 1000 iterations did not find the optimum result. – Anony-Mousse Jan 19 '15 at 21:58

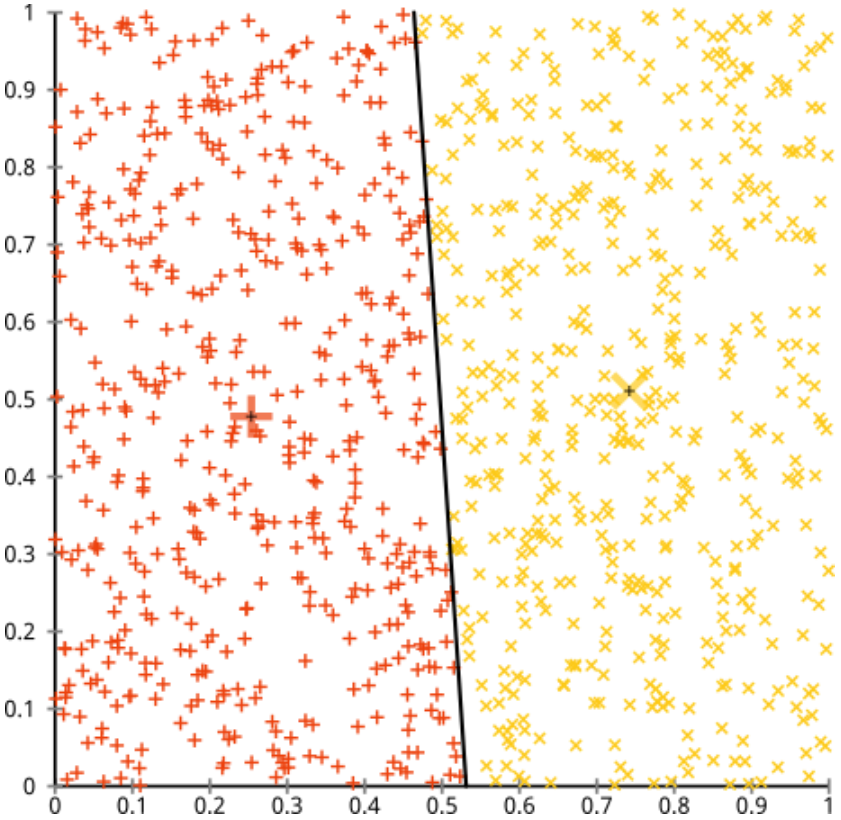
3 May I suggest that you accept the best answer below? – Aaron Hall Apr 24 '15 at 20:27

2 Answers

While I like David Robinsons answer above a lot, here's some additional critique of k-means.

Clustering non-clustered data

Run k-means on uniform data, and you will *still* get clusters! It doesn't tell you when the data just does *not* cluster, and can take your research into a dead end this way.



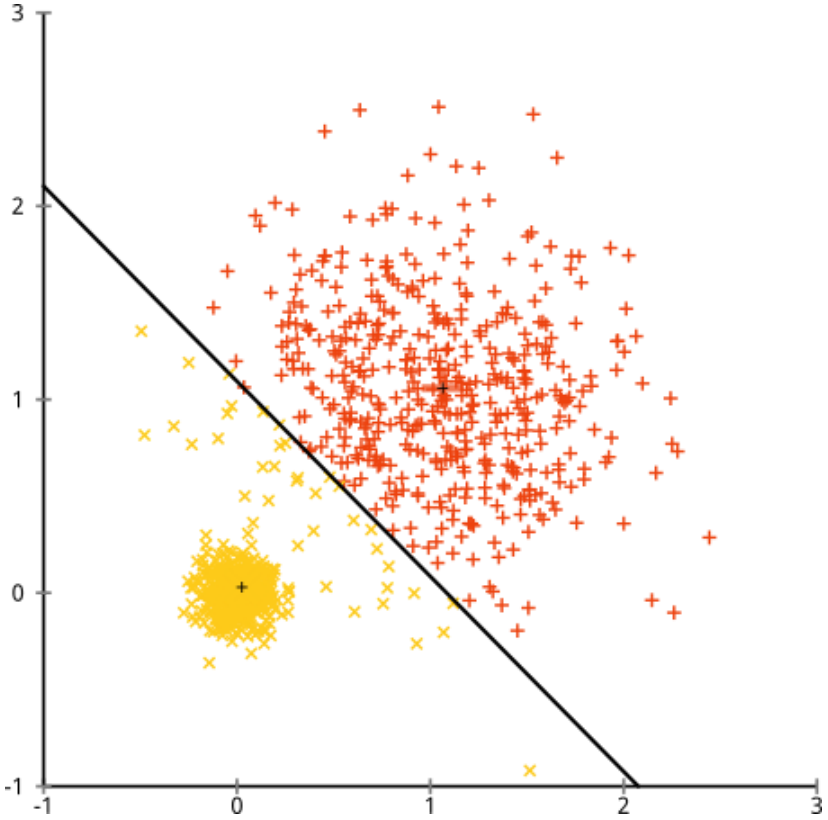
Sensitive to scale

Rescaling your datasets will completely change results. While this itself is not bad, not realizing that *you have to spend extra attention to scaling your data* is bad. Scaling factors are extra d hidden parameters in k-means that "default" to 1 and thus are easily overlooked, yet have a major impact (but of course this applies to many other algorithms, too).

This is probably what you referred to as "all variables have the same variance". Except that ideally, you would also consider non-linear scaling when appropriate.

Also be aware that **it is only a heuristic to scale every axis to have unit variance**. This doesn't ensure that k-means works. Scaling depends on the meaning of your data set. And if you have more than one cluster, you would want every cluster (independently) to have the same variance in every variable, too.

Here is a classic counterexample of data sets that k-means *cannot* cluster. Both axes are i.i.d. in each cluster, so it would be sufficient to do this in 1 dimension. But the clusters have varying variances, and k-means thus splits them incorrectly.



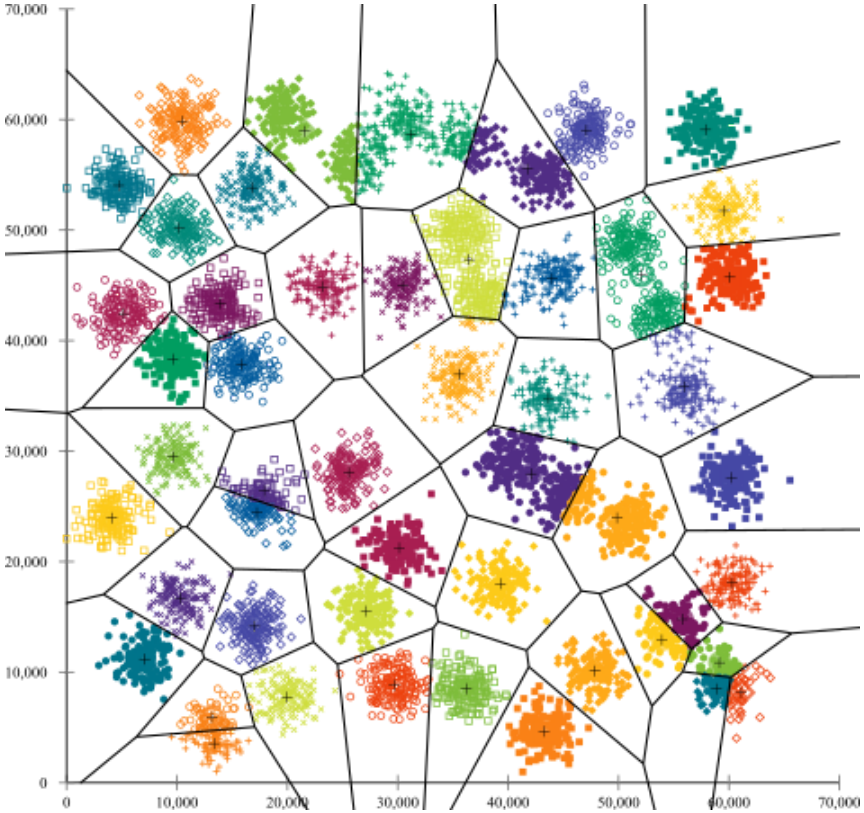
I don't think this counterexample for k-means is covered by your points:

- All clusters are spherical (i.i.d. Gaussian).
- All axes have the same distribution and thus variance.
- Both clusters have 500 elements each.

Yet, k-means still fails badly (and it gets worse if I increase the variance beyond 0.5 for the larger cluster) But: **it is not the algorithm that failed. It's the assumptions, which don't hold**. K-means is working perfectly, it's just optimizing the wrong criterion.

Even on perfect data sets, it can get stuck in a local minimum

Below is the *best* of 10 runs of k-means on the classic A3 data set. This is a synthetic data set, *designed for k-means*. 50 clusters, each of Gaussian shape, reasonably well separated. Yet, it only with k-means++ and 100 iterations I did get the expected result... (below is 10 iterations of regular k-means, for illustration).



You'll quickly find many clusters in this data set, where k-means failed to find the correct structure. For example in the bottom right, a cluster was broken into three parts. But there is no way, k-means is going to move one of these centroids to an entirely different place of the data set - it's trapped in a local minimum (and this already was the *best* of 10 runs!)

And there are *many* of such local minima in this data set. Very often when you get two samples from the same cluster, it will get stuck in a minimum where this cluster remains split, and two other clusters merged instead. Not always, but very often. So you need a lot of iterations to have a lucky pick. With 100 iterations of k-means, I still counted 6 errors, and with 1000 iterations I got this down to 4 errors. K-means++ by the way it weights the random samples, works much better on this data set.

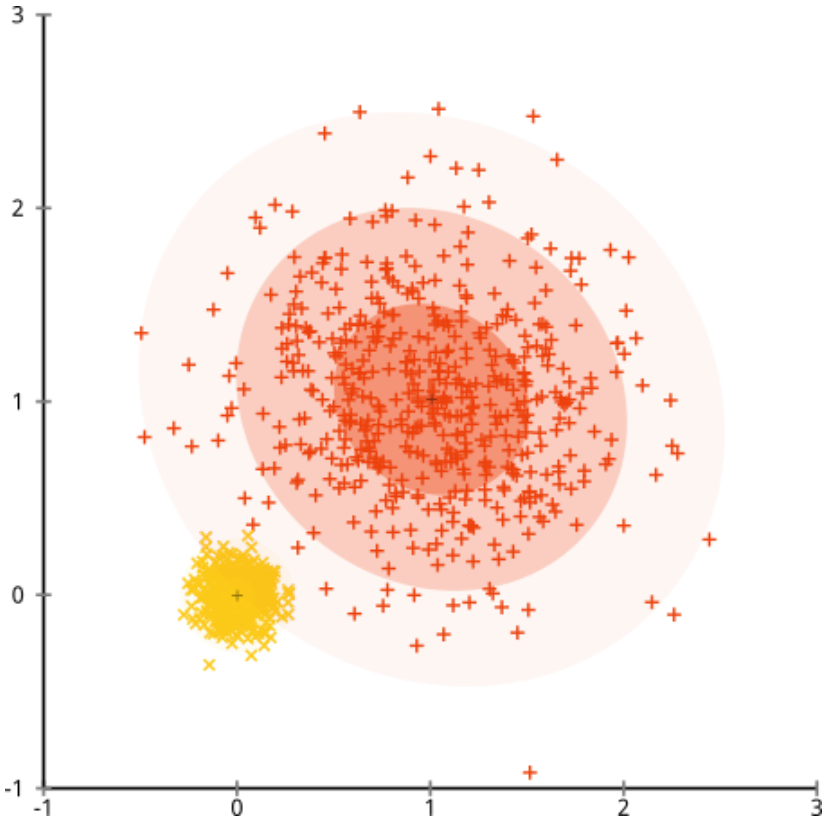
Means are continuous

While you can run k-means on binary data (or one-hot encoded categorial data) the results will not be binary anymore. So you do get a result out, but you may be unable to iterpret it in the end, because it has a different data type than your original data.

Hidden assumption: SSE is *worth* minimizing

This is essentially already present in above answer, nicely demonstrated with linear regression. There are some use cases where k-means makes perfect sense. When Lloyd had to decode PCM signals, he did know the number of different tones, and least squared error minimizes the chance of decoding errors. And in color quantization of imaged, you do minimize color error when reducing the palette, too. But on your data, is the sum of squared deviations a meaningful criterion to minimize?

In above counterexample, the variance is *not* worth minimizing, because it depends on the cluster. Instead, a Gaussian Mixture Model should be fit to the data, as in the figure below:



(But this is *not* the ultimate method either. It's just as easy to construct data that does not satisfy the "mixture of k Gaussian distributions" assumptions, e.g. by adding a lot of background noise)

Too easy to use badly

All in all, it's too easy to throw k-means on your data, and nevertheless get a result out (that is pretty much random, but you won't notice). I think it would be better to have a metod which can fail if you haven't understood your data...

K-means as quantization

If you want a theoretical model of what k-means does, consider it a *quantization* approach, not a clustering algorithm.

The objective of k-means - minimizing the squared error - is a reasonable choice *if* you replace every object by its nearest centroid. (It makes a lot less sense if you inspect the groups original data IMHO.)

There are very good use cases for this. The original PCM use case of Lloyd comes to mind, or e.g. color quanization (Wikipedia). If you want to reduce an image to k colors, you *do* want to replace every pixel with the nearest centroid. Minimizing the squared color deviation then *does* measure L2 optimality in image approximation using k colors only.

This quantization is probably quite similar to the linear regression example. Linear regression finds the *best linear model*. And k-means finds (sometimes) the **best reduction to k values** of a multidimensional data set. Where "best" is the least squared error.

IMHO, k-means is a good *quantization* algorithm (see the first image in this post - if you want to approximate the data set to two points, this is a reasonable choice!). If you want to do cluster analysis as in *discover structure* then k-means is IMHO not the best choice. It tends to cluster when there are not clusters, and it cannot recognize various structures you do see a lot in data.

Fine print: all images were generated with ELKI. Data were generated using the `.xml` data generation format, but they are so basic it is not worth sharing them.

edited Mar 10 at 12:39

answered Jan 17 '15 at 12:25

Anony-Mousse
18.8k 3 23 50

9 (Just to note - it's probably not a good idea to talk about the "above answer", since the answer order that a reader sees can be variable. For instance, if they set the display order to "active", then your answer is actually the one above!) – Silverfish Jan 17 '15 at 23:18

@Anony-Mousse This answer is really awesome. But until now, I kind of forget what do we usually mean by saying "k-means will work under some conditions and will fail under other conditions." What do the word "work" or "fail" mean in this context? Does "work" means the solution generated by k-means will visually 'looks reasonable'? This is kind of vague. Or 'work' mean if k-means provide solution which is the same as the 'standard solution' i.e., we pre-generate a data set and use k-means. In this context 'work' makes sense, but in reality, data are not pre-generated by some distribution. – KevinKim Jan 23 '15 at 2:24

Usually people refer to some ground truth, i.e. how the data was generated or to some label hidden from the algorithm. Comparing to generated data will prefer algorithms that optimize the model that was used for generation (e.g. GMM and k-means for Gaussians). And even on real and labeled data this evaluation is about reproducing a

known result. When you consider the explorative / knowledge discovery aspect, where you want to learn something *new*. But it's all we've got. – Anony-Mousse Jan 23 '15 at 7:07

Would it work better on the A3 data set if k were adjusted to the number of effectively present clusters as determined a priori? – TMOTTM Sep 3 at 11:39

@TMOTTM this is with k chosen by prior knowledge. Best of 10 runs all with the "correct" k chosen a priori. – Anony-Mousse Sep 3 at 11:43

What a great question- it's a chance to show how one would inspect the drawbacks and assumptions of any statistical method. Namely: make up some data and try the algorithm on it!

We'll consider two of your assumptions, and we'll see what happens to the k-means algorithm when those assumptions are broken. We'll stick to 2-dimensional data since it's easy to visualize. (Thanks to the curse of dimensionality, adding additional dimensions is likely to make these problems more severe, not less). We'll work with the statistical programming language R: you can find the full code here (and the post in blog form here).

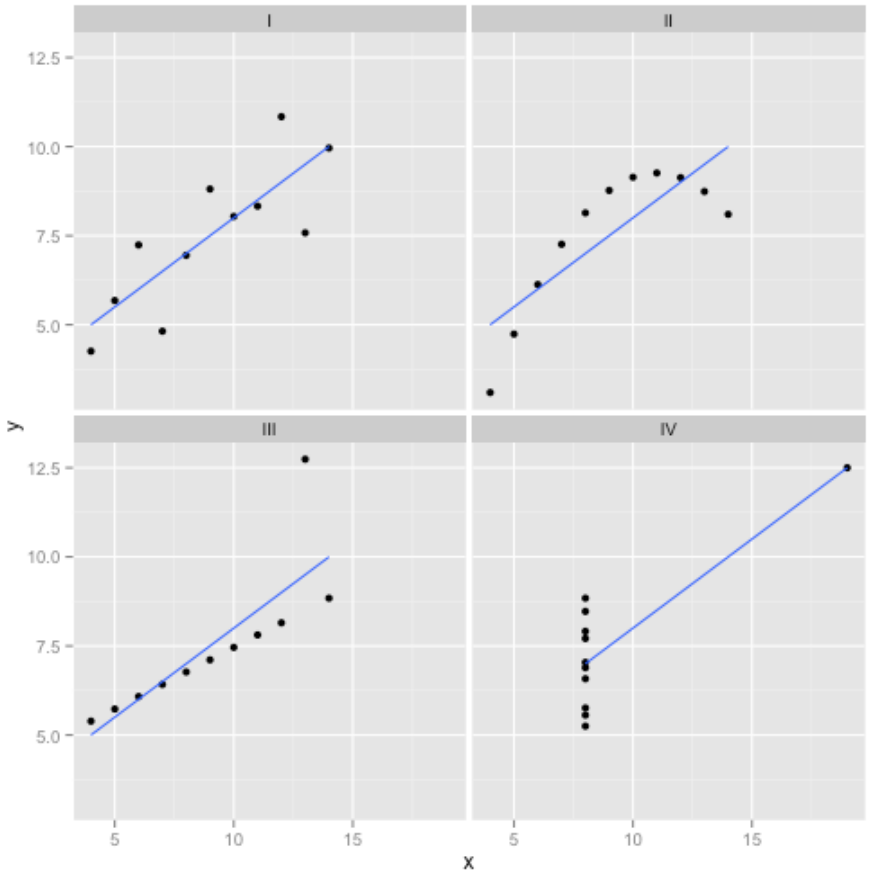
Diversion: Anscombe's Quartet

First, an analogy. Imagine someone argued the following:

> I read some material about the drawbacks of linear regression- that it expects a linear trend, that the residuals are normally distributed, and that there are no outliers. But all linear regression is doing is minimizing the sum of squared errors (SSE) from the predicted line. That's an optimization problem that can be solved no matter what the shape of the curve or the distribution of the residuals is. Thus, linear regression requires no assumptions to work.

Well, yes, linear regression works by minimizing the sum of squared residuals. But that by itself is not the goal of a regression: what we're *trying* to do is draw a line that serves as a reliable, unbiased predictor of *y* based on *x*. The Gauss-Markov theorem tells us that minimizing the SSE accomplishes that goal- but that theorem rests on some very specific assumptions. If those assumptions are broken, you can still minimize the SSE, but it might not *do* anything. Imagine saying "You drive a car by pushing the pedal: driving is essentially a 'pedal-pushing process.' The pedal can be pushed no matter how much gas in the tank. Therefore, even if the tank is empty, you can still push the pedal and drive the car."

But talk is cheap. Let's look at the cold, hard, data. Or actually, made-up data.



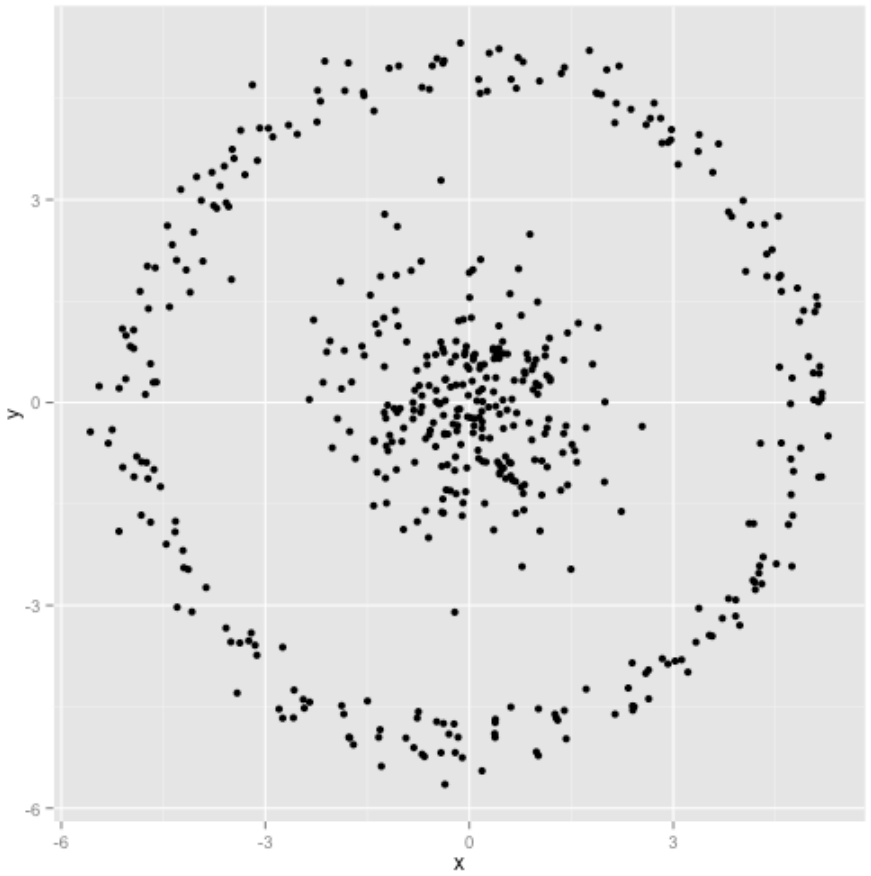
This is in fact my *favorite* made-up data: Anscombe's Quartet. Created in 1973 by statistician Francis Anscombe, this delightful concoction illustrates the folly of trusting statistical methods blindly. Each of the datasets has the same linear regression slope, intercept, p-value and R^2- and yet at a glance we can see that only one of them, **I**, is appropriate for linear regression. In **II** it suggests the wrong shape, in **III** it is skewed by a single outlier- and in **IV** there is clearly no trend at all!

One could say "Linear regression is still *working* in those cases, because it's minimizing the sum of squares of the residuals." But what a Pyrrhic victory! Linear regression will always draw a line, but if it's a meaningless line, who cares?

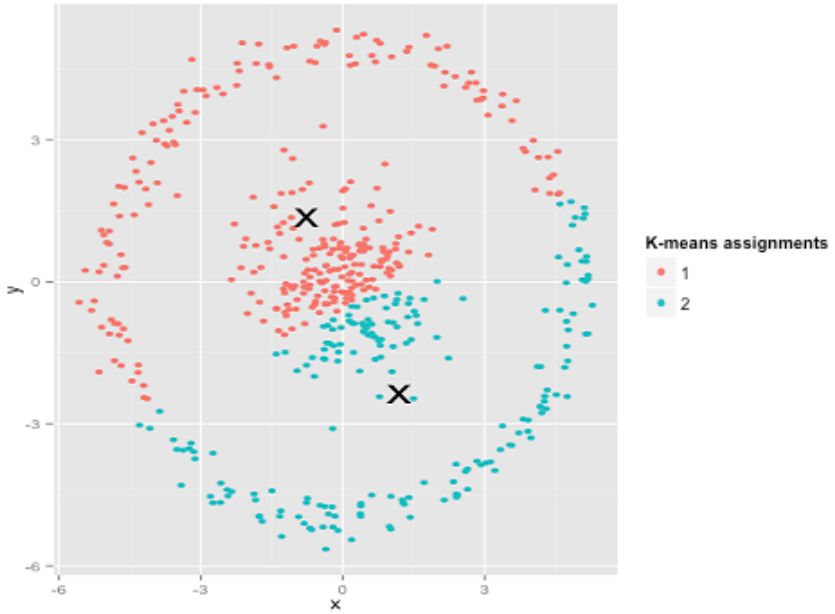
So now we see that just because an optimization can be performed doesn't mean we're accomplishing our goal. And we see that making up data, and visualizing it, is a good way to inspect the assumptions of a model. Hang on to that intuition, we're going to need it in a minute.

Broken Assumption: Non-Spherical Data

You argue that the k-means algorithm will work fine on non-spherical clusters. Non-spherical clusters like... these?

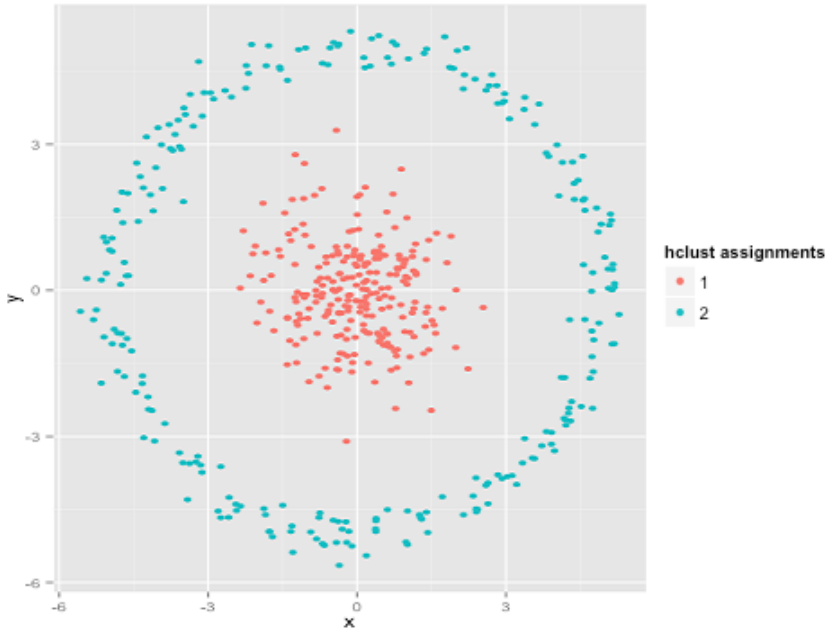


Maybe this isn't what you were expecting- but it's a perfectly reasonable way to construct clusters. Looking at this image, we humans *immediately* recognize two natural groups of points- there's no mistaking them. So let's see how k-means does: assignments are shown in color, imputed centers are shown as X's.



Well, *that*'s not right. K-means was trying to fit a square peg in a round hole- trying to find nice centers with neat spheres around them- and it failed. Yes, it's still minimizing the within-cluster sum of squares- but just like in Anscombe's Quartet above, it's a Pyrrhic victory!

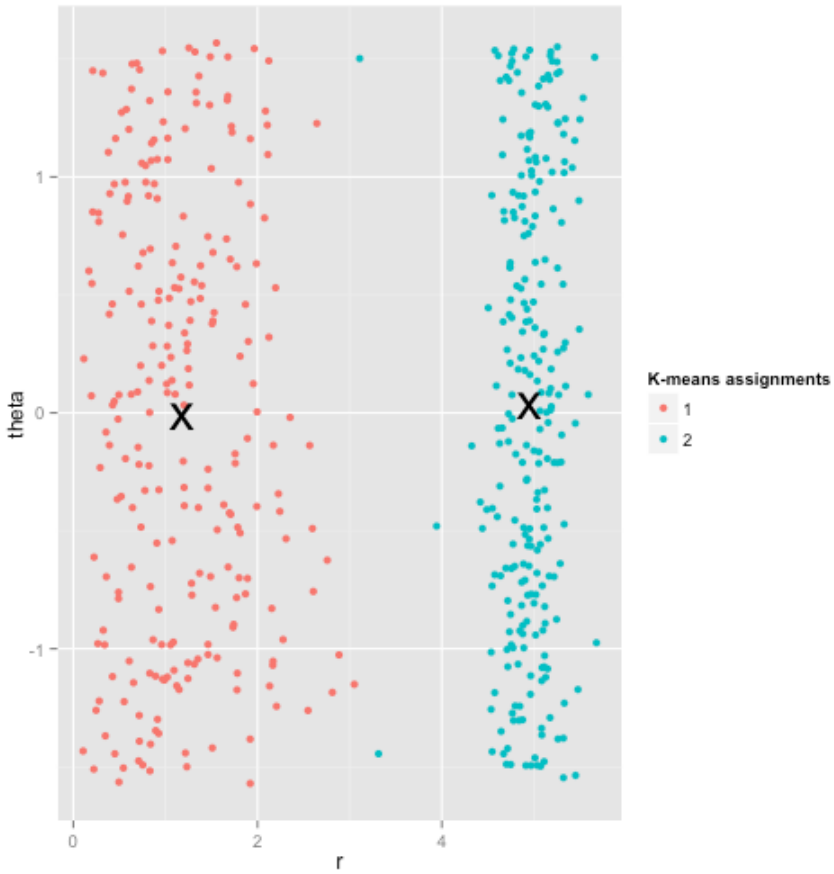
You might say "That's not a fair example... *no* clustering method could correctly find clusters that are that weird." Not true! Try single linkage hierachical clustering:



Nailed it! This is because single-linkage hierarchical clustering makes the *right* assumptions for this dataset. (There's a whole *other* class of situations where it fails).

You might say "That's a single, extreme, pathological case." But it's not! For instance, you can make the outer group a semi-circle instead of a circle, and you'll see k-means still does terribly (and hierarchical clustering still does well). I could come up with other problematic situations easily, and that's just in two dimensions. When you're clustering 16-dimensional data, there's all kinds of pathologies that could arise.

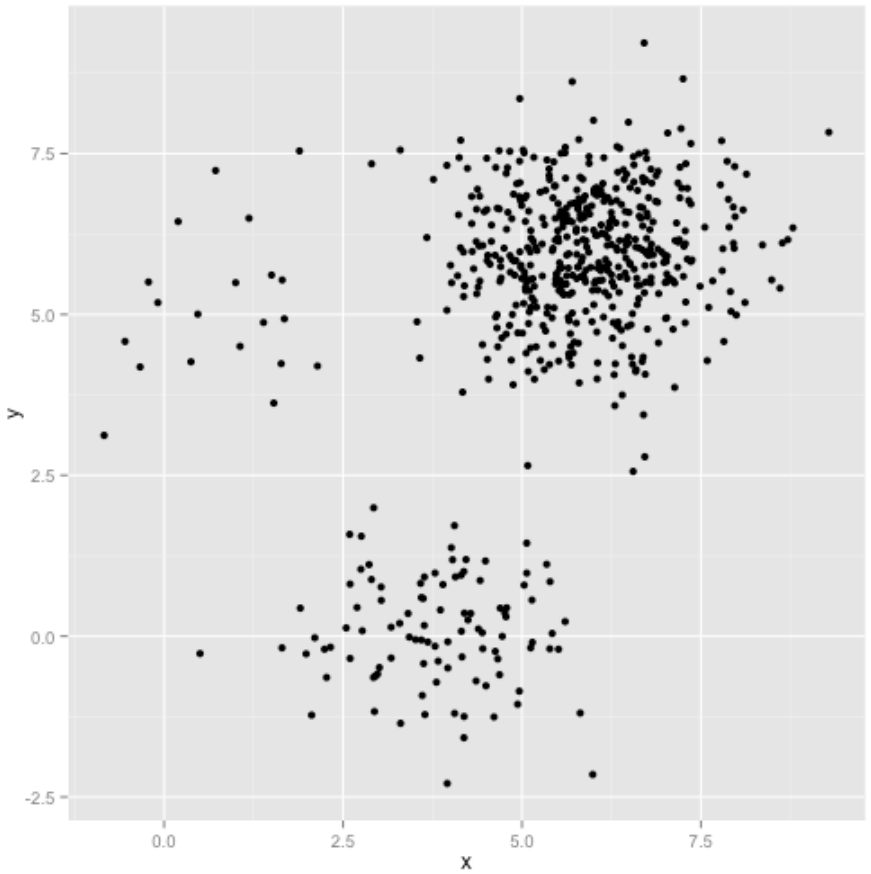
Lastly, I should note that k-means is still salvagable! If you start by transforming your data into polar coordinates, the clustering now works:



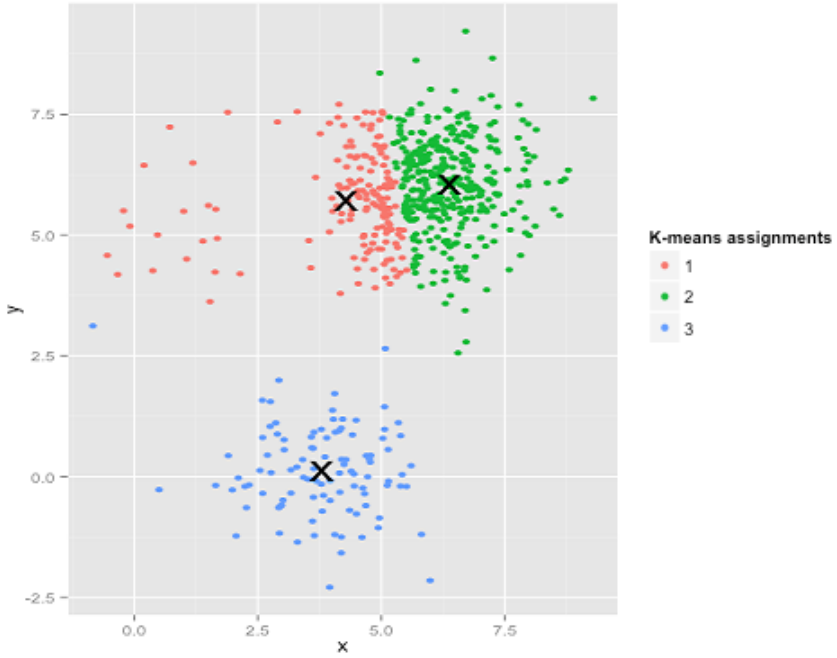
That's why understanding the assumptions underlying a method is essential: *it doesn't just tell you when a method has drawbacks, it tells you how to fix them.*

Broken Assumption: Unevenly Sized Clusters

What if the clusters have an uneven number of points- does that also break k-means clustering? Well, consider this set of clusters, of sizes 20, 100, 500. I've generated each from a multivariate Gaussian:



This looks like k-means could probably find those clusters, right? Everything seems to be generated into neat and tidy groups. So let's try k-means:



Ouch. What happened here is a bit subtler. In its quest to minimize the within-cluster sum of squares, the k-means algorithm gives more "weight" to larger clusters. In practice, that means it's happy to let that small cluster end up far away from any center, while it uses those centers to "split up" a much larger cluster.

If you play with these examples a little (R code here!), you'll see that you can construct far more scenarios where k-means gets it embarrassingly wrong.

Conclusion: No Free Lunch

There's a charming construction in mathematical folklore, formalized by Wolpert and Macready, called the "No Free Lunch Theorem." It's probably my favorite theorem in machine learning philosophy, and I relish any chance to bring it up (did I mention I love this question?) The basic idea is stated (non-rigorously) as this: **"When averaged across all possible situations, every algorithm performs equally well."**

Sound counterintuitive? Consider that for every case where an algorithm works, I could construct a situation where it fails terribly. Linear regression assumes your data falls along a line- but what if it follows a sinusoidal wave? A t-test assumes each sample comes from a normal distribution: what if you throw in an outlier? Any gradient ascent algorithm can get trapped in local maxima, and any supervised classification can be tricked into overfitting.

What does this mean? It means that assumptions *are where your power comes from!* When

Netflix recommends movies to you, it's assuming that if you like one movie, you'll like similar ones (and vice versa). Imagine a world where that wasn't true, and your tastes are perfectly random- scattered haphazardly across genres, actors and directors. Their recommendation algorithm would fail terribly. Would it make sense to say "Well, it's still minimizing some expected squared error, so the algorithm is still working"? You can't make a recommendation algorithm without making some assumptions about users' tastes- just like you can't make a clustering algorithm without making some assumptions about the nature of those clusters.

So don't just accept these drawbacks. Know them, so they can inform your choice of algorithms. Understand them, so you can tweak your algorithm and transform your data to solve them. And love them, because if your model could never be wrong, that means it will never be right.

edited Jan 16 '15 at 17:00

answered Jan 16 '15 at 9:56

David Robinson
7,713 3 13 28

29 +1 for this passionate answer. I particularly enjoyed the polar transformation example, those clever tricks never stop to amaze my mathematically ignorant brain. – mugen Jan 16 '15 at 11:16

12 + 1, this is an absolutely beautiful answer that does a great job of showing how the assumptions break down without getting bogged down in the details of the analysis. – LCialdella Jan 16 '15 at 15:05

7 +1 One of the common things people keep complaining to me is that theoretical things don't work in practice. But when I ask "does your data fit the assumptions of the model?" I simply get a blank look from their faces. Your answer and especially the final section made me really happy. – TenaliRaman Jan 17 '15 at 13:19

6 +1 Wow, I have been around for a while but I think I have *never* seen an answer to get 50+ upvotes in one day. This is a truly impressive achievement. – amoeba Jan 17 '15 at 15:15

4 The polar transform, as I see it, is mainly useful here as a first and jargon-free example towards kernel clustering techniques -- where this kind of pre-transformation is how to get linear learning methods to work. – Mikael Vejdemo-Johansson Jan 19 '15 at 7:55