Distance in High Dimensions and Clustering

Chris Cornwell

April 29, 2025

Outline

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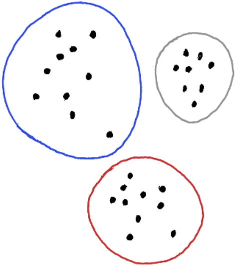
Clustering uses Distance

Aim of clustering: group the training data $\mathcal{S}$ into **clusters** $C_1, C_2, \ldots, C_k$, with every point in some cluster C_i (i.e., $\mathcal{S} = C_1 \cup C_2 \cup \ldots \cup C_k$) and clusters are disjoint.[a]



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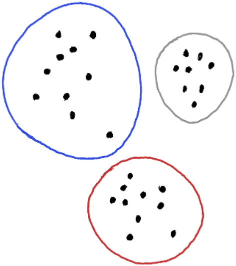

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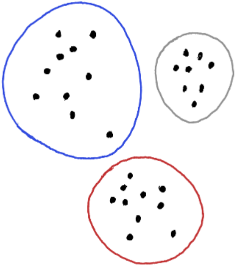

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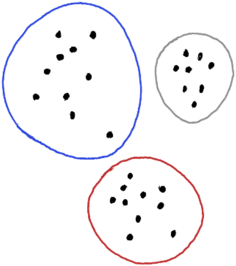

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- Makes a phenomenon called the **curse of dimensionality** especially relevant.

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- Strict interpretation: The amount of training data used needs to increase exponentially in the number of features, i.e., independent variables. (If the number of samples needed to see how position/value of one feature might affect y labeling is roughly constant over the features.)
- Broad interpretation: With large number of features (so, large d, where $\mathbf{x}_i \in \mathbb{R}^d$), our intuition for the way that the distance between points relates to properties we care about will break down.
  Distance in high dimensions is *weird*. (*Let's see how*.)

Spheres in $\mathbb{R}^d$, d large: weird

Often, work with those points that are within a given distance R from fixed point. These are points in a d-dimensional "ball" (that is, enclosed by a d-dimensional sphere):

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The volume of $B_R(\mathbf{p})$: $\frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}R^d$.

Γ is Euler's gamma function. If d is even, $\Gamma(\frac{d}{2}+1) = (\frac{d}{2})!$ and if d is odd, it's roughly similar: $(\frac{d}{2})(\frac{d}{2}-1)\ldots(\frac{1}{2})\pi^{1/2}$.

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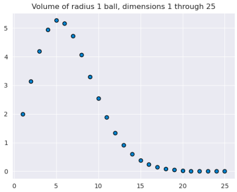

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Choose ε with $0 < \varepsilon < R$. What proportion of points in $B_R(\mathbf{p})$ are at least ε away from the boundary sphere? That is, how large is $B_{R-\varepsilon}(\mathbf{p})$ in comparison to $B_R(\mathbf{p})$?

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Since $1 - \frac{\varepsilon}{R} < 1$, this approaches 0 as $d \longrightarrow \infty$. Returning to $\varepsilon = 0.05$ and $R = 1$, the ratio is less than 0.05 if $d \geq 59$; so, more than 95% of the volume of $B_R(\mathbf{p})$ is contained in an outer shell, within 0.05 of the boundary.

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Increasingly likely, also, that none of these points are near each other: points below sampled with random coordinates (i.i.d., with a mean-zero normal distribution). Distances between all pairs of sampled points were calculated and plotted in a histogram.

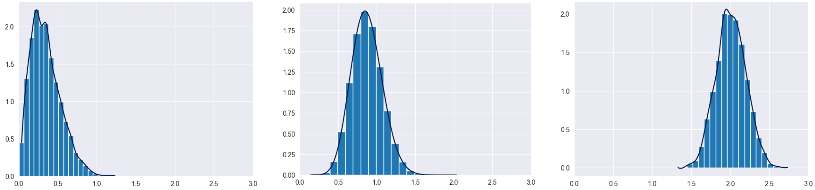
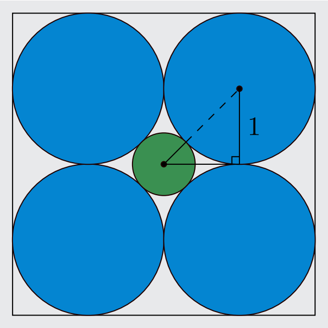


Figure: Left: points in $\mathbb{R}^2$; Middle: points in $\mathbb{R}^{10}$; Right: points in $\mathbb{R}^{50}$

Another example of high dimensional weirdness

In $\mathbb{R}^2$, consider the five depicted circles in the square $[-2, 2]^2$. The four “corner” circles are tangent to (two) edges of the square and tangent to each other. Each of them has radius 1. The “center” circle has center at the origin and is tangent to all four corner circles.



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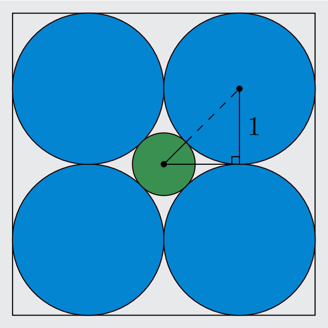

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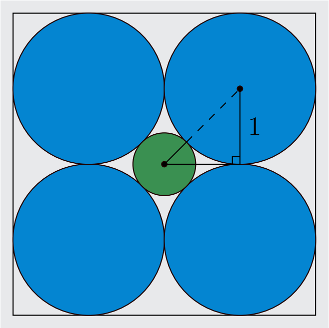
Generalize this: the (hyper)cube $[-2, 2]^d$ in $\mathbb{R}^d$. In general, there are 2^d corner spheres, each with radius 1. There is one center sphere, with the origin as its center (same as the hypercube) and which is tangent to all corner spheres.



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- For $d \geq 10$, the center sphere contains points that are *outside of* the hypercube. (Despite still being tangent to all 2^d corner spheres, which "surround" it and are *entirely contained* within the hypercube.

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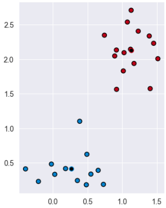

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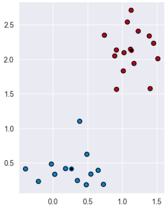
You choose k, the number of clusters and randomly initialize k centroids $\mu_1, \mu_2, \ldots \mu_k$, each $\mu_i \in \mathbb{R}^d$. Clusters $C_1, C_2, \ldots, C_k$ are determined as follows.



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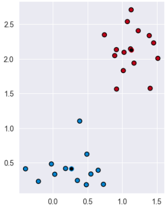

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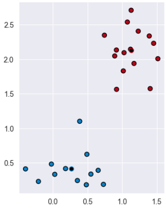

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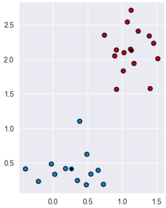

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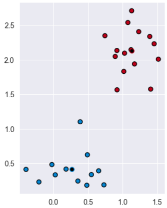

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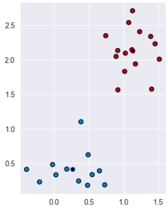

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In any iteration of 1, for $\mathbf{x}_i$ to change its cluster, it is necessary that $|\mathbf{x}_i - \mu_{j(i)}|$ decreases, so $\sum_{i=1}^{n} |\mathbf{x}_i - \mu_{j(i)}|^2$ decreases. In any iteration of 2, setting $\mu_j = \frac{1}{|C_j|} \sum_{\mathbf{x}_i \in C_j} \mathbf{x}_i$ will minimize $\sum_{\mathbf{x}_i \in C_j} |\mathbf{x}_i - \mu_j|^2$, and so $\sum_{i=1}^{n} |\mathbf{x}_i - \mu_{j(i)}|^2$ decreases (or stays the same) on this step.
Thus, the algorithm terminates: there are finitely many points in $\mathcal{S}$, so there are only a finite number of possibilities for the list $\mu_1, \mu_2, \ldots, \mu_k$.

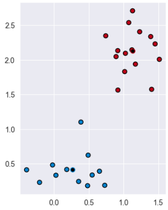

Figure: Result of k-means, 2 centroids in black

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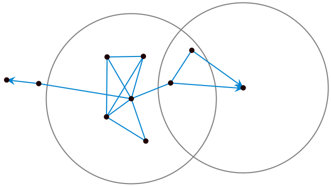

Figure: Points reachable from core point, `minPts`$= 4$

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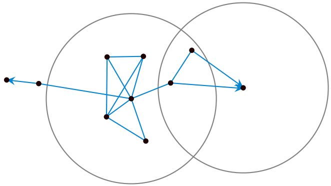
Describing how clusters are formed requires some terminology.
As with k-means, the distance function (metric) that is used is a central part of the process. Unlike the centroids used in k-means, though, a different metric would not require a change to the procedure (other than different distance computations).



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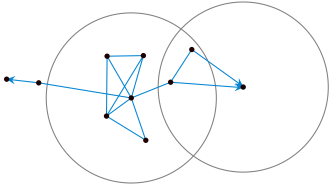
With this terminology, let $\mathbf{p} \in \mathcal{S}$ be a core point. The cluster, $C_{\mathbf{p}}$ say, is the set of all points in $\mathcal{S}$ (including $\mathbf{p}$) that are reachable from $\mathbf{p}$.



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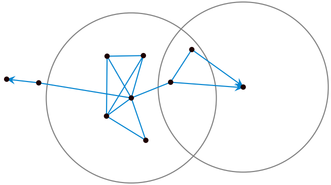

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