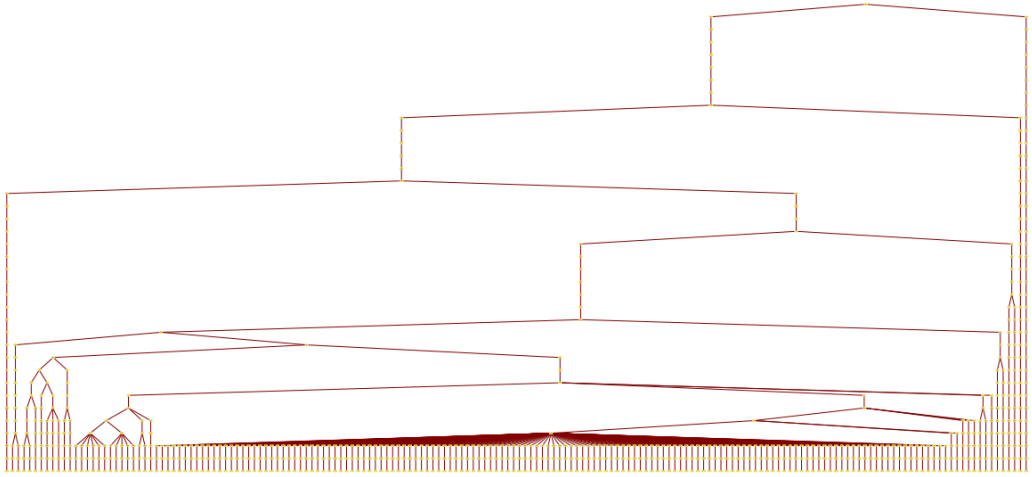
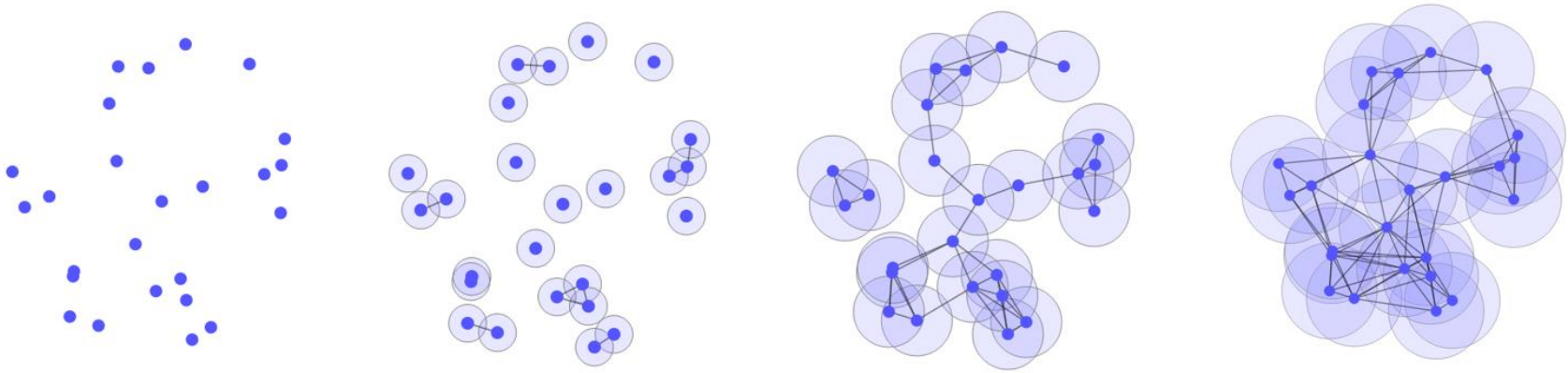
Where can we use graph algorithms we learned in ML?

Mustafa Hajij



Hierarchical Clustering



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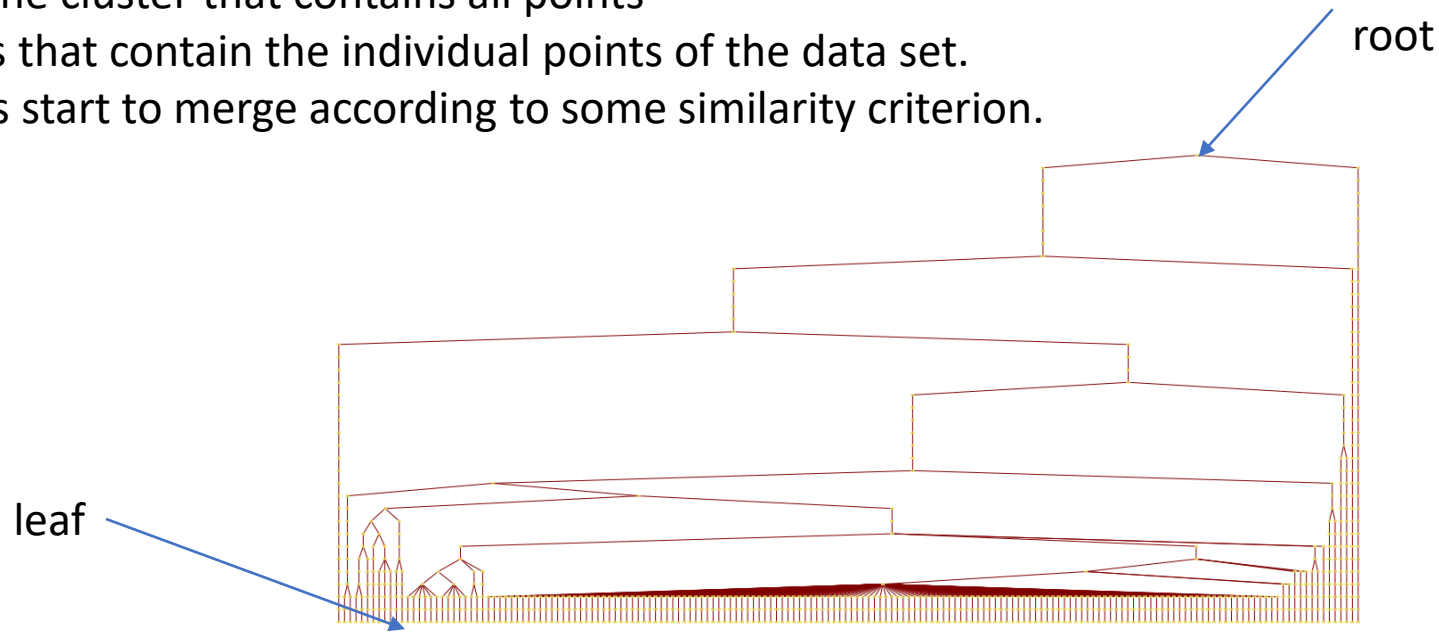
Hierarchical clustering is usually represented by a tree called the dendrogram that represents the clusterings at all levels.

Each node in the tree represents a cluster

- In particular the root of the tree represents the cluster that contains all points
- The leaves of the tree represents the clusters that contain the individual points of the data set.
- As we go from the leaves to the root, clusters start to merge according to some similarity criterion.

There are two types of Hierarchical clustering
Agglomerative : bottom up (Merge).
Divisive : Top down (Split).



General Steps

General Steps in a standard hierarchical agglomerative clustering algorithm:

1. Compute the distance matrix, or the dissimilarity, between all points in the input data. Choosing the metric will impact the results largely.

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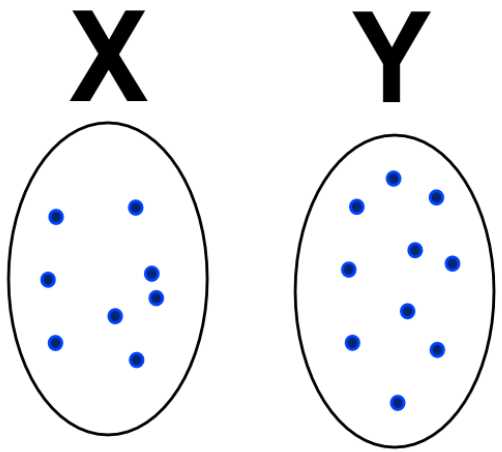
Question : how do we measure the distance between two clusters ?

This is important because step 3 we need to measure the distance between clusters rather than points.

Distance between clusters

Given two clusters X and Y. How do we measure the distance between them ?



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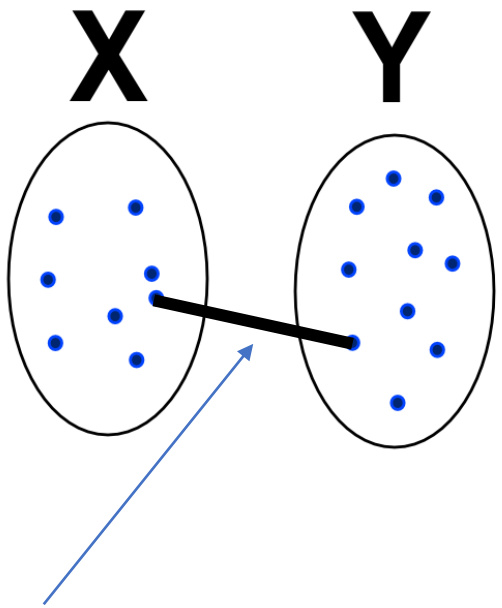

$$D(X,Y) := \min_{x \text{ in } X, y \text{ in } Y} d(x,y)$$

One way is to measure the minimal distance between all points of X and Y.
This distance induce single linkage clustering.

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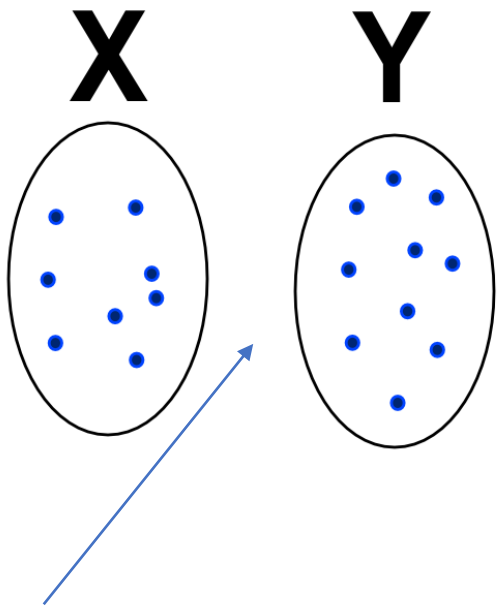

$$D(X,Y) := \frac{1}{|X||Y|} \sum_{x\ in\ X, y\ in Y}^{n} d(x,y)$$

We could also consider the mean distance between the points of the clusters

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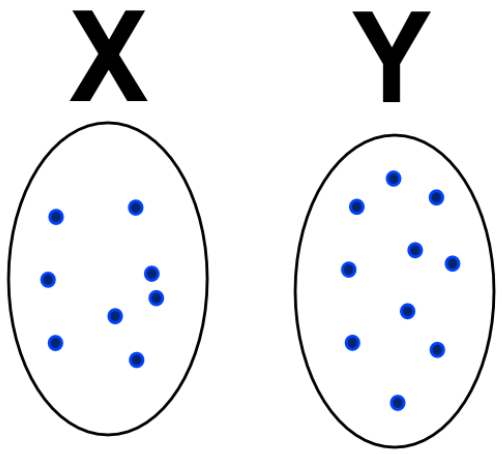

There are other measures as well : The minimal energy criterion , the distance between the centroids of the clusters

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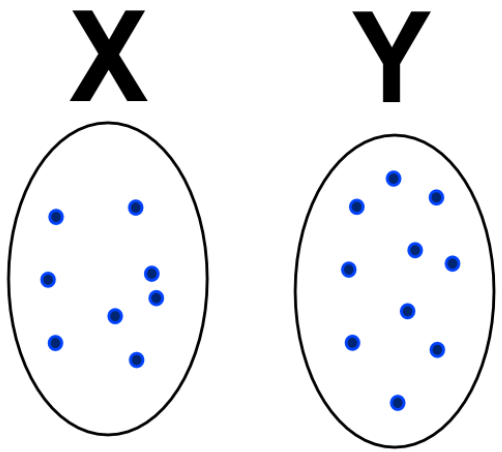


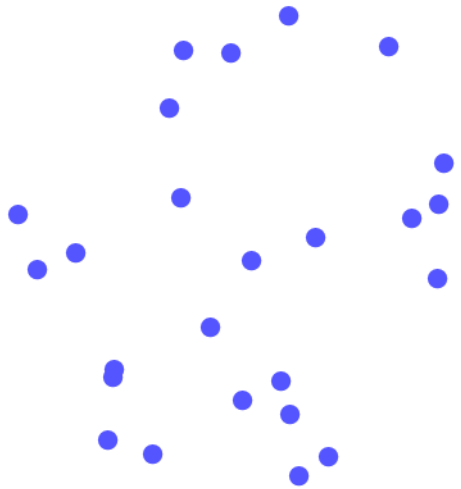
For efficient calculations we usually require the following condition:
Knowing the distance D(A,C), D(B,C)
Implies we can calculate in constant time the distance D(A+B,C)

There are other measures as well : The minimal energy criterion , the distance between the centroids of the clusters

Single Linkage Hierarchical Clustering and the ε- Neighborhood Graph

Suppose that we are given a set of points $X = \{p_1, p_2, \dots, p_n\}$ in R^d with a distance function d defined one them.

Consider the connected components of the ε-neighborhood graph as we continuously increase ε from zero to infinity.



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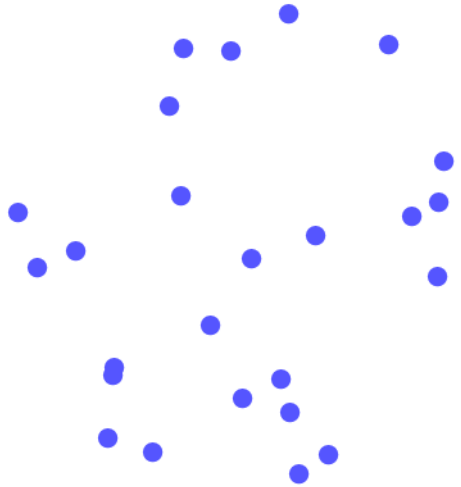

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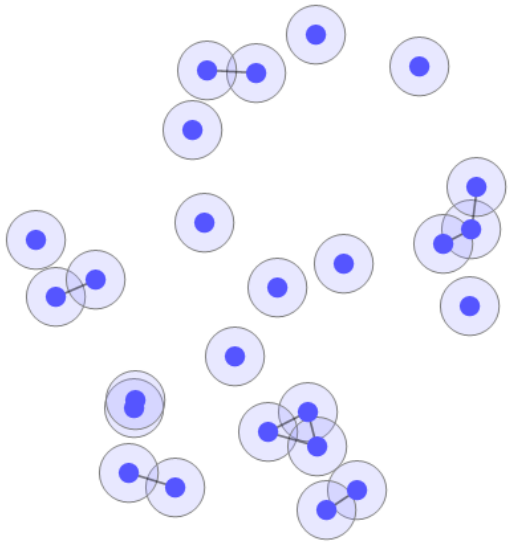

When ε is a little larger we start some clusters starts to get form

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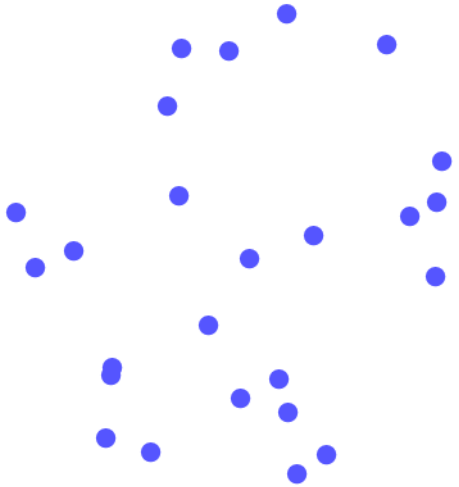

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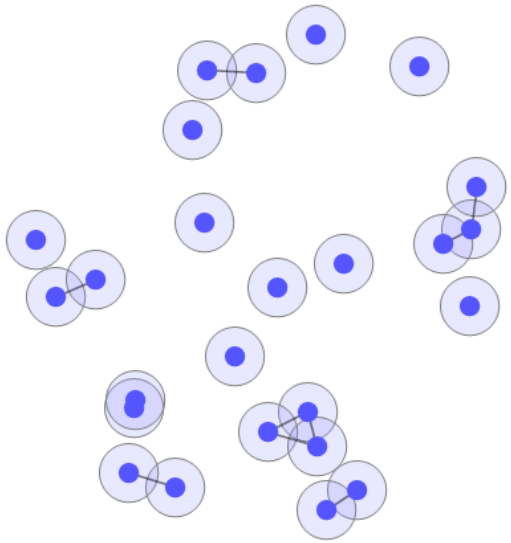

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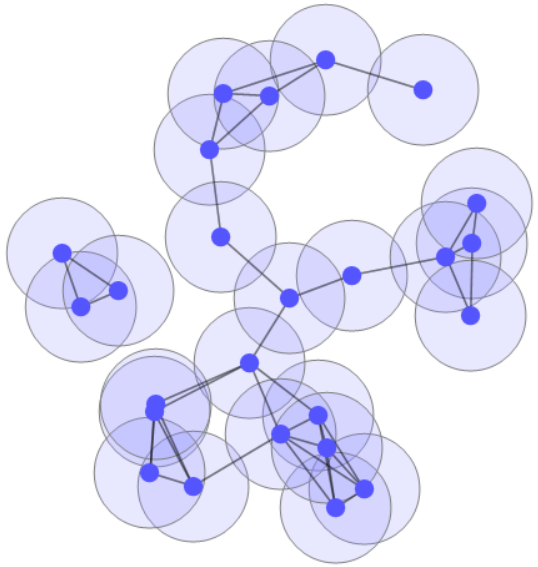

When ε is even larger we have few clusters
As the clusters get larger and larger

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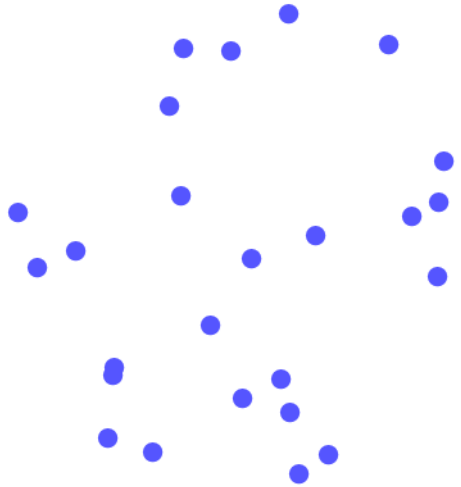

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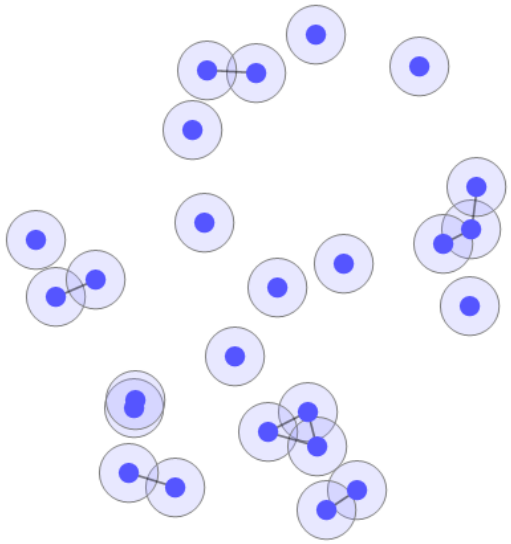

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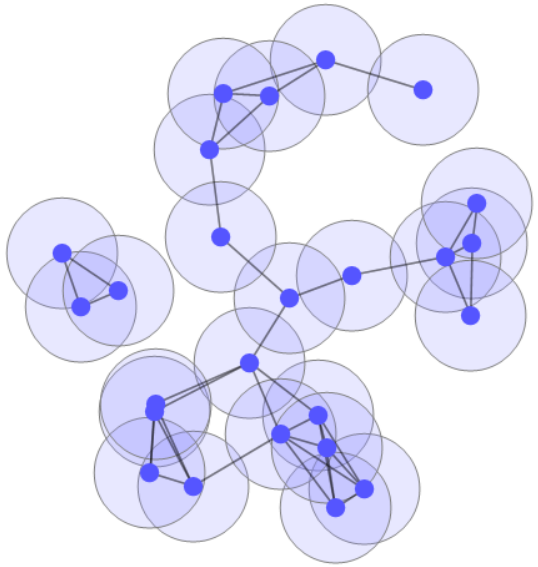

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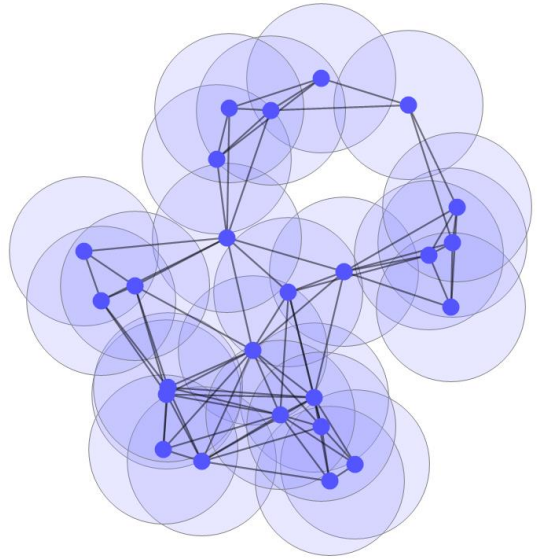


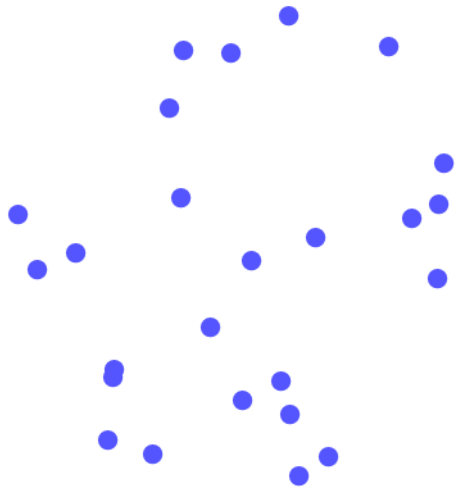
At some point all points become a par to of a single cluster

Single Linkage Hierarchical Clustering and the ε- Neighborhood Graph

Remark : Observe that the growing of this epsilon corresponds exactly to the idea of **Hierarchical Clustering!**

Question : How can we implement this effectively ?

Question : Does the minimal spanning tree of this graph give any information about the clustering?



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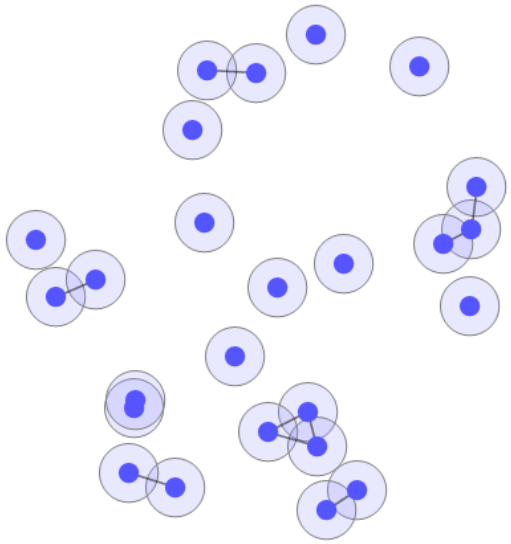

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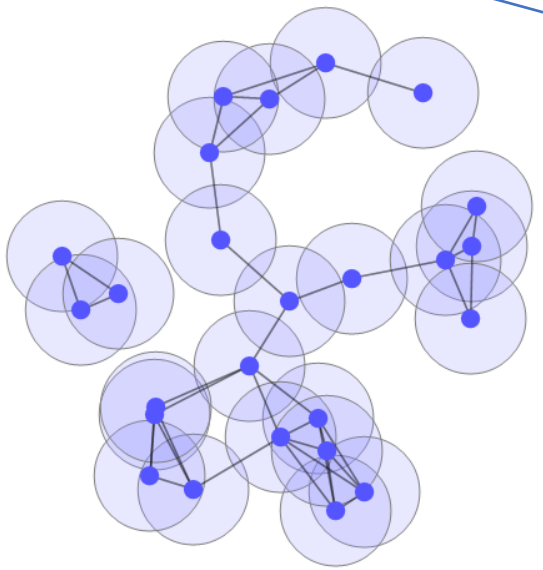

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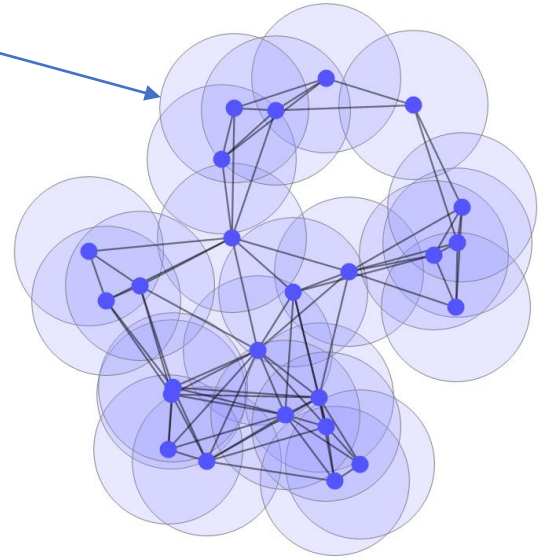

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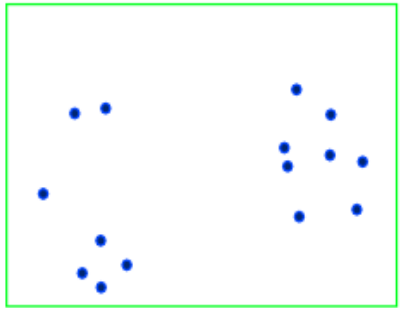
Single Linkage Hierarchical Clustering and the and Kruskal's algorithm



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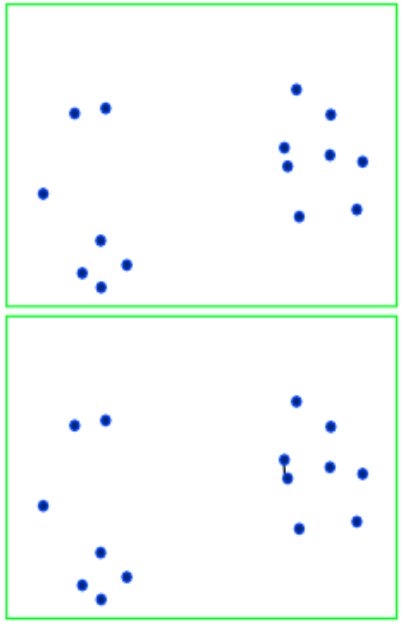

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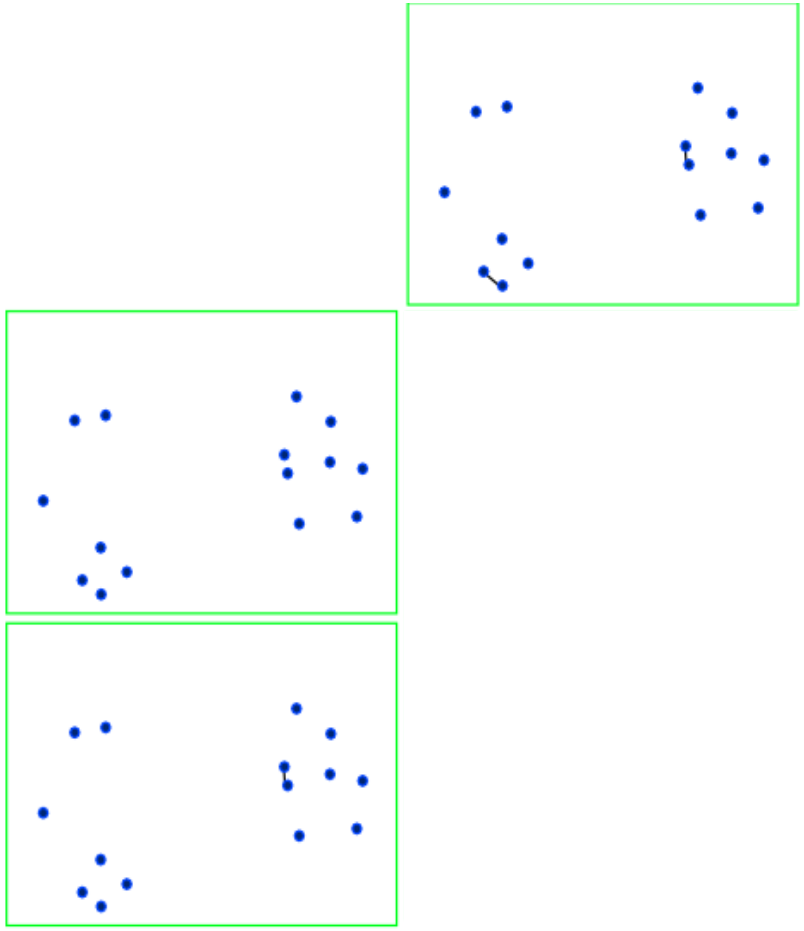

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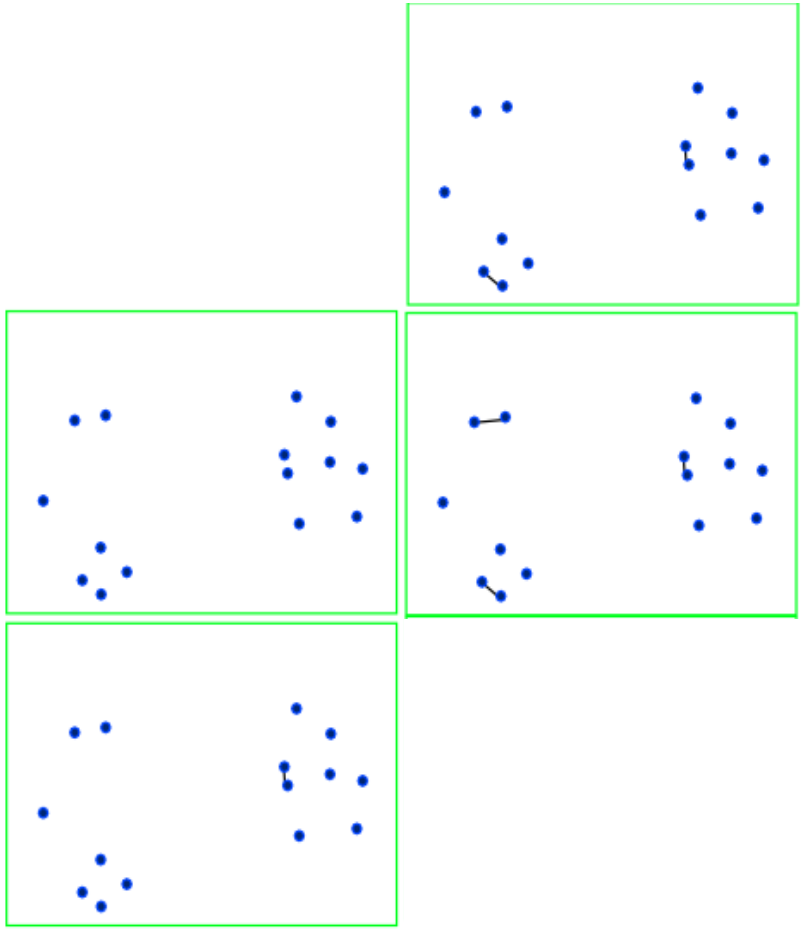

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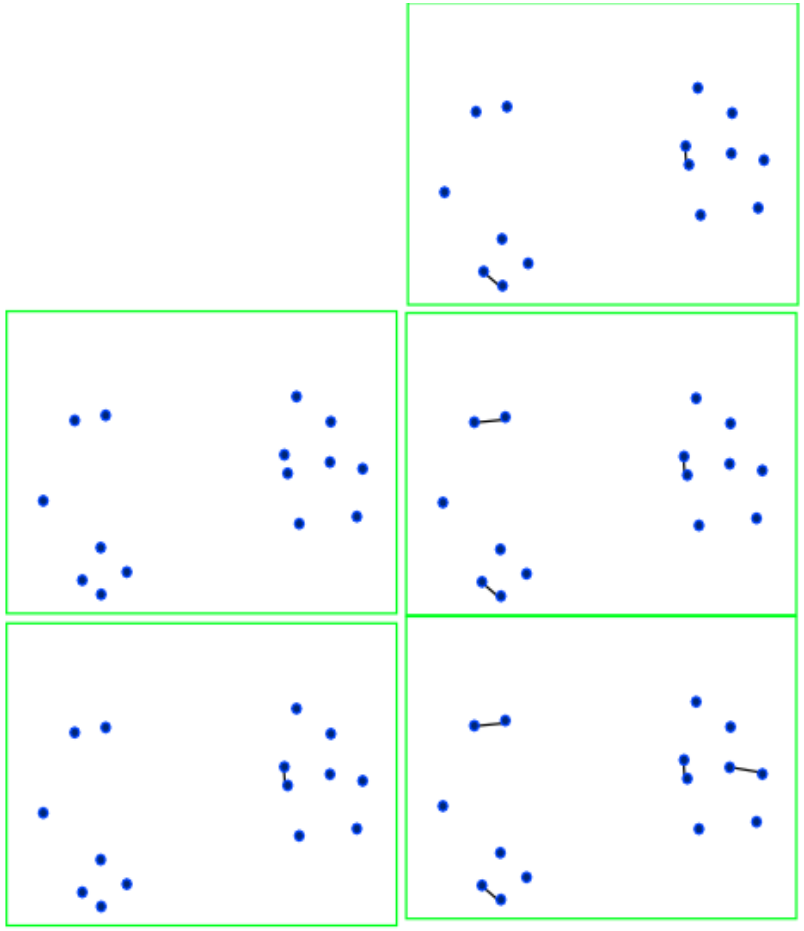

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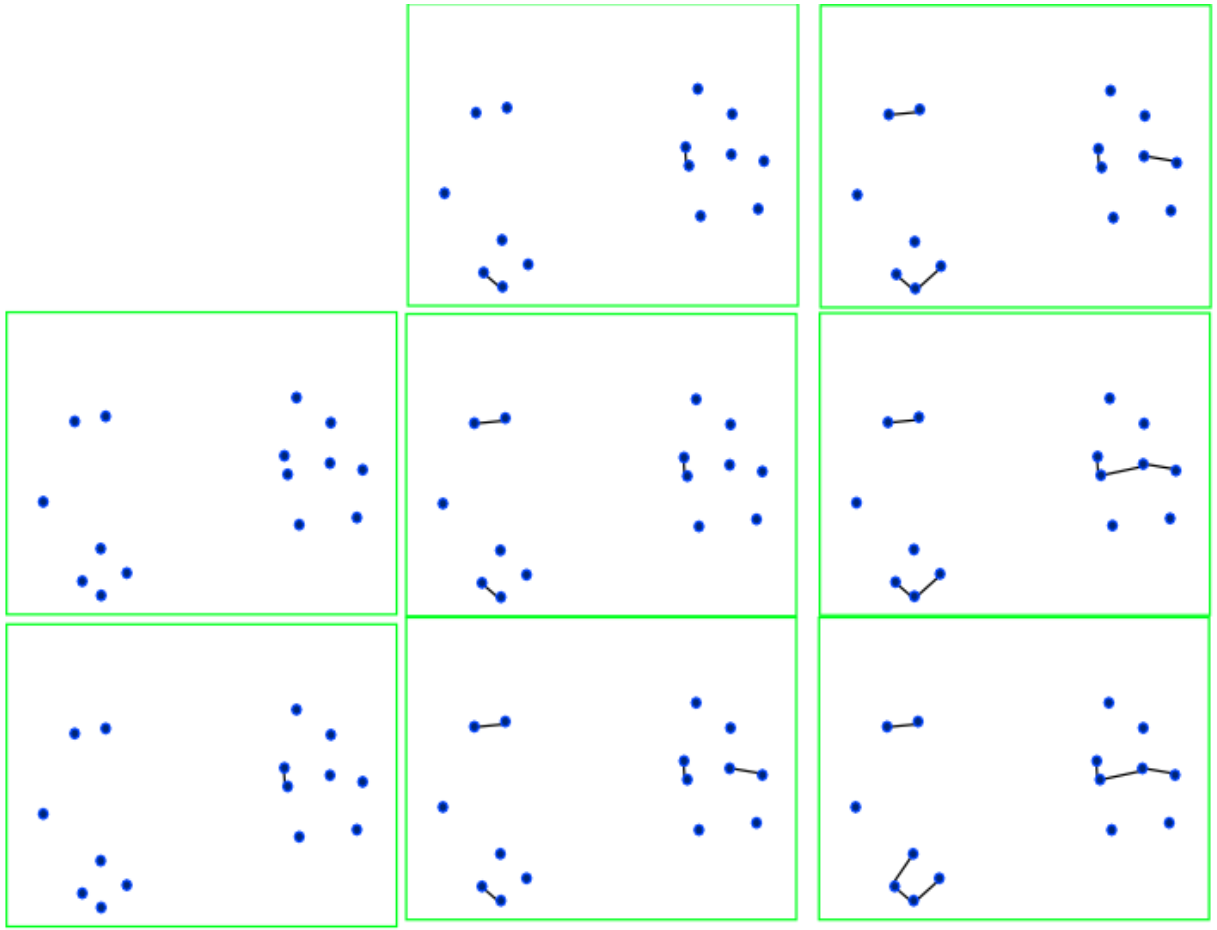

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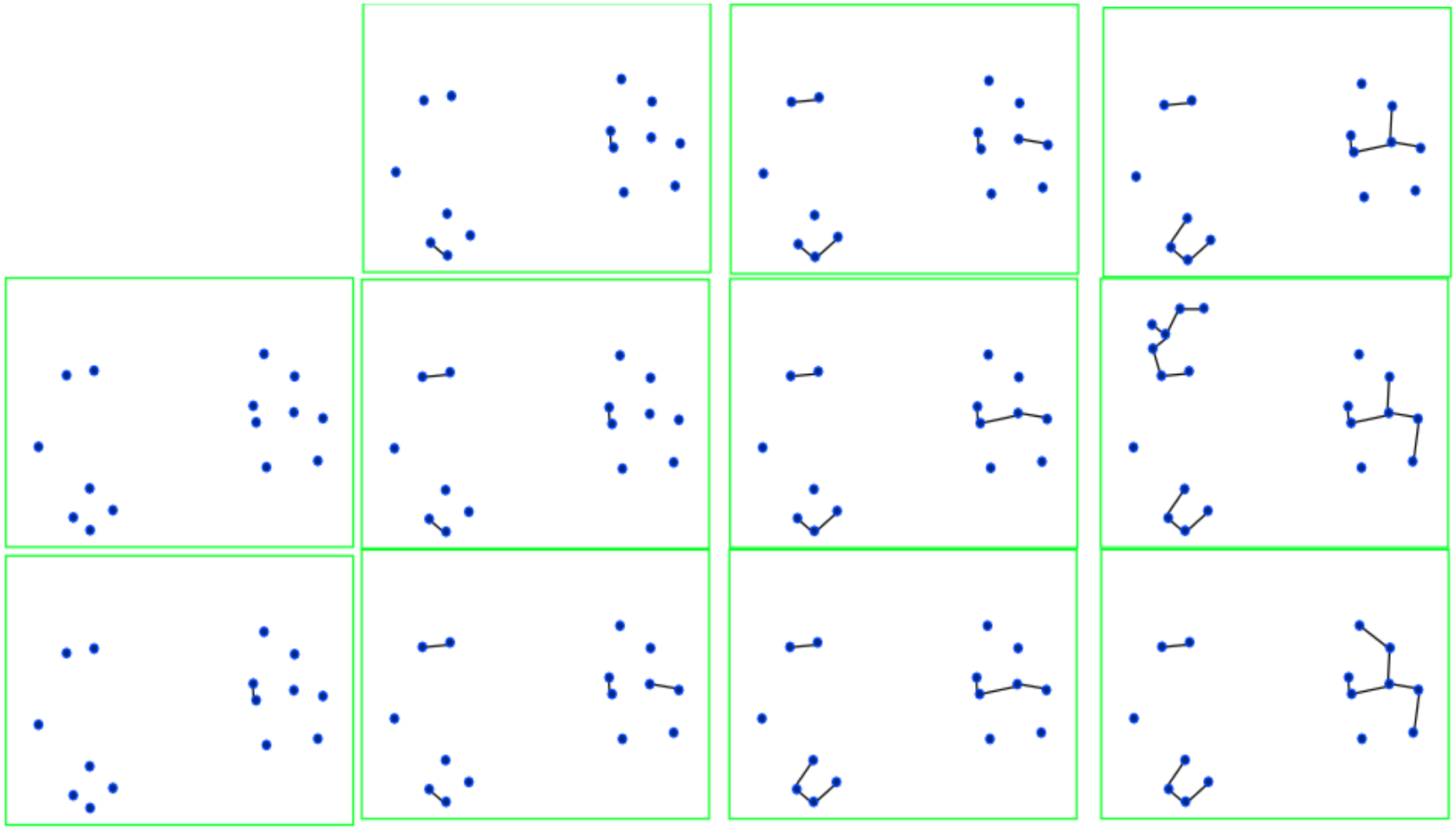

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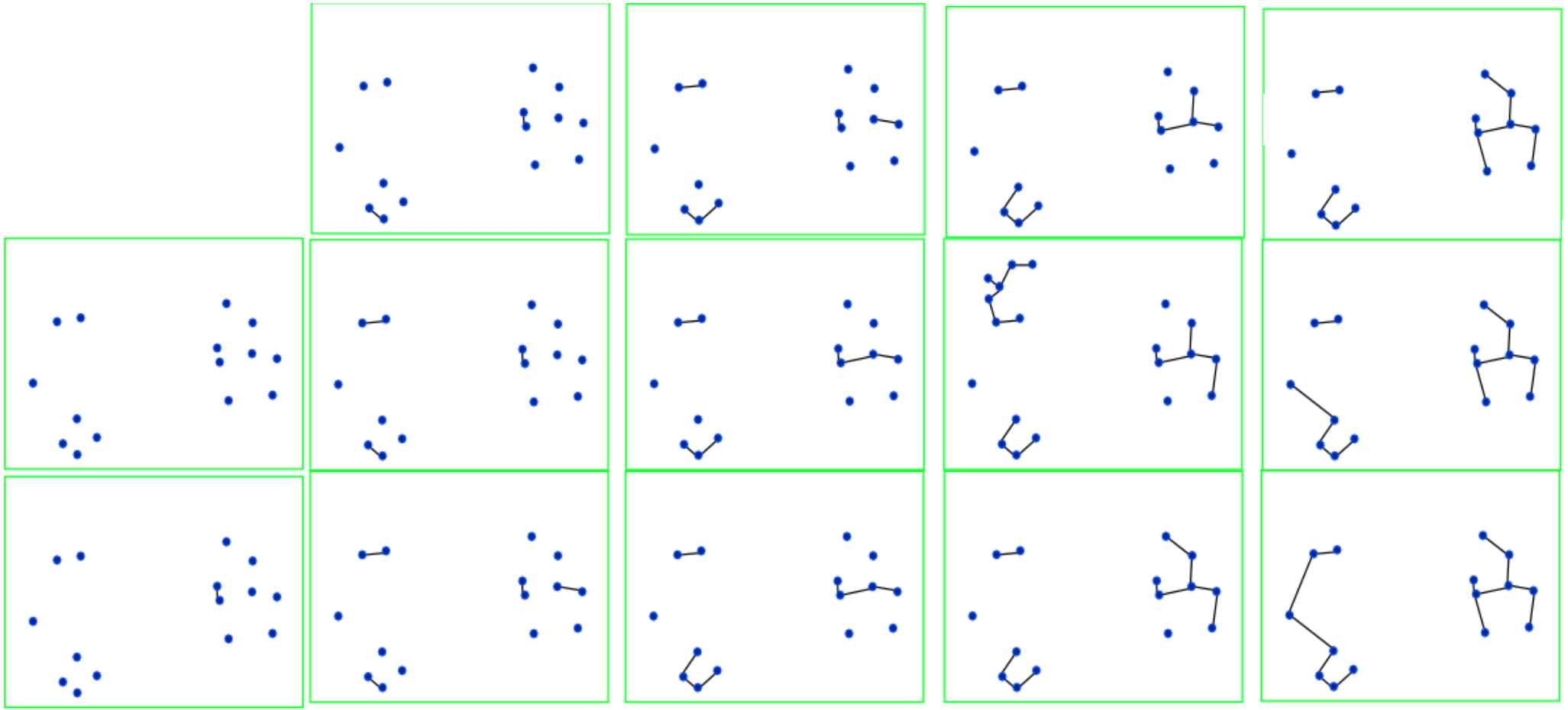

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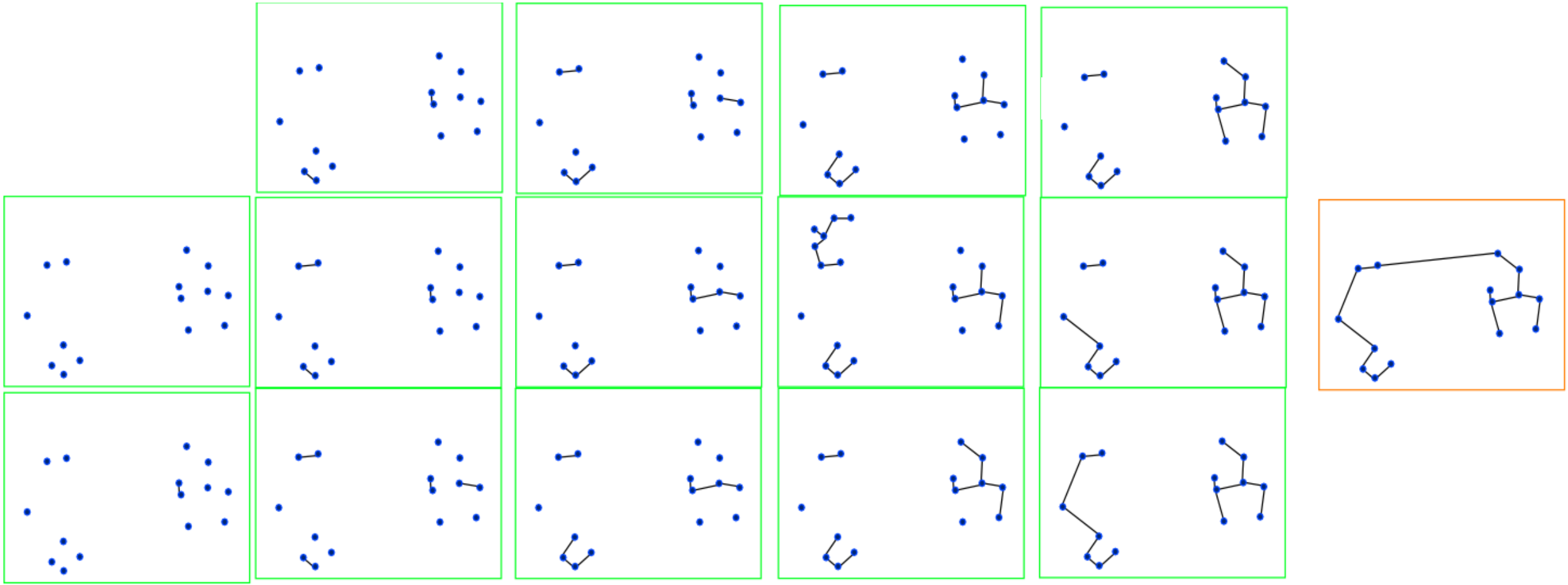

The minimal spanning tree obtained in this way provides exactly
the Single linkage hierarchical clustering that we talked about earlier

An Introduction to Multidimensional Scaling and ISOMAP

MDS

Let D=[d_{ij}] be an $N \times N$ dissimalrity matrix.

In MDS, we want to find n vectors $x_1, \dots, x_N$ in R^d such that $||x_i - x_j|| \approx d_{ij}$

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- In this case the distance d above is the usual Euclidean distance.
- There are cases where the matrix D is valid distance matrix, but still there exists no set of vectors $x_1, \dots, x_N$ in any R^d with perfect $||x_i - x_j|| = d_{ij}$. Such a distance is called non-Euclidean distance.

Stress Majorization

In the classical MDS algorithm the cost function that we are trying to optimize is called the stress function and it is given by :

$$Stress_D(x_1, x_2, \ldots, x_N) = \left(\sum_{i \neq j = 1, \ldots, N} \left(d_{ij} - \|x_i - x_j\| \right)^2 \right)^{1/2}$$

In this function we try to find $x_1, \ldots, x_N$ in a certain dimension d such that Stress($x_1, \ldots, x_N$) is as small as possible

Stress Majorization

The stress function has a more general form as :

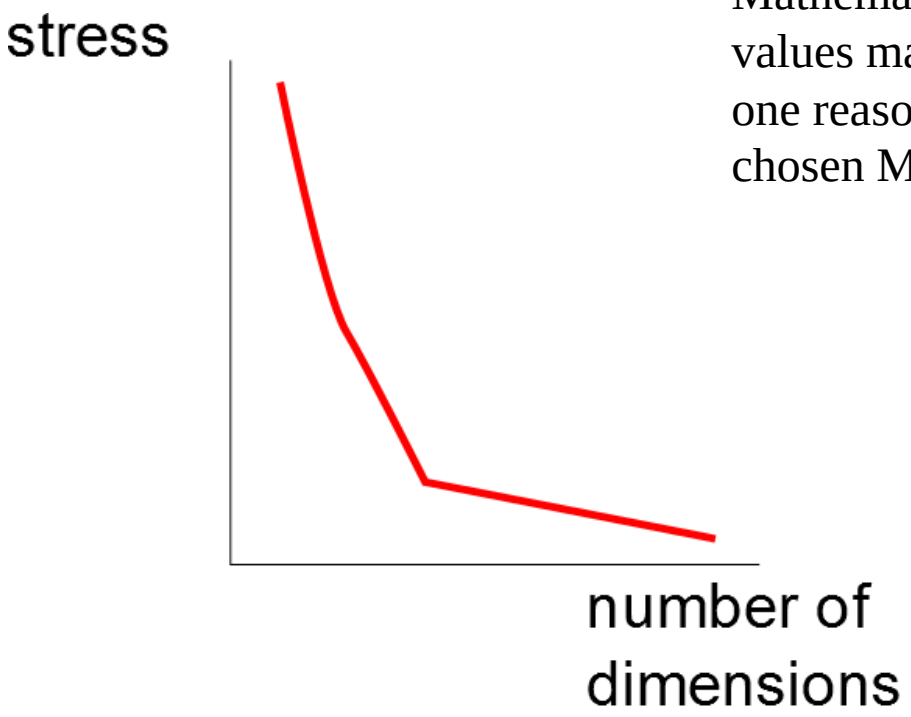
$$\sigma(X) = \sum_{i<j\leq n} w_{ij}(d_{ij}(X) - \delta_{ij})^2$$

Here wij weight between a pair of points (i,j) that represents the confidence in in the similarity between points (i,j) .

δ_{ij} the given distance between the points i,j

Stress Majorization

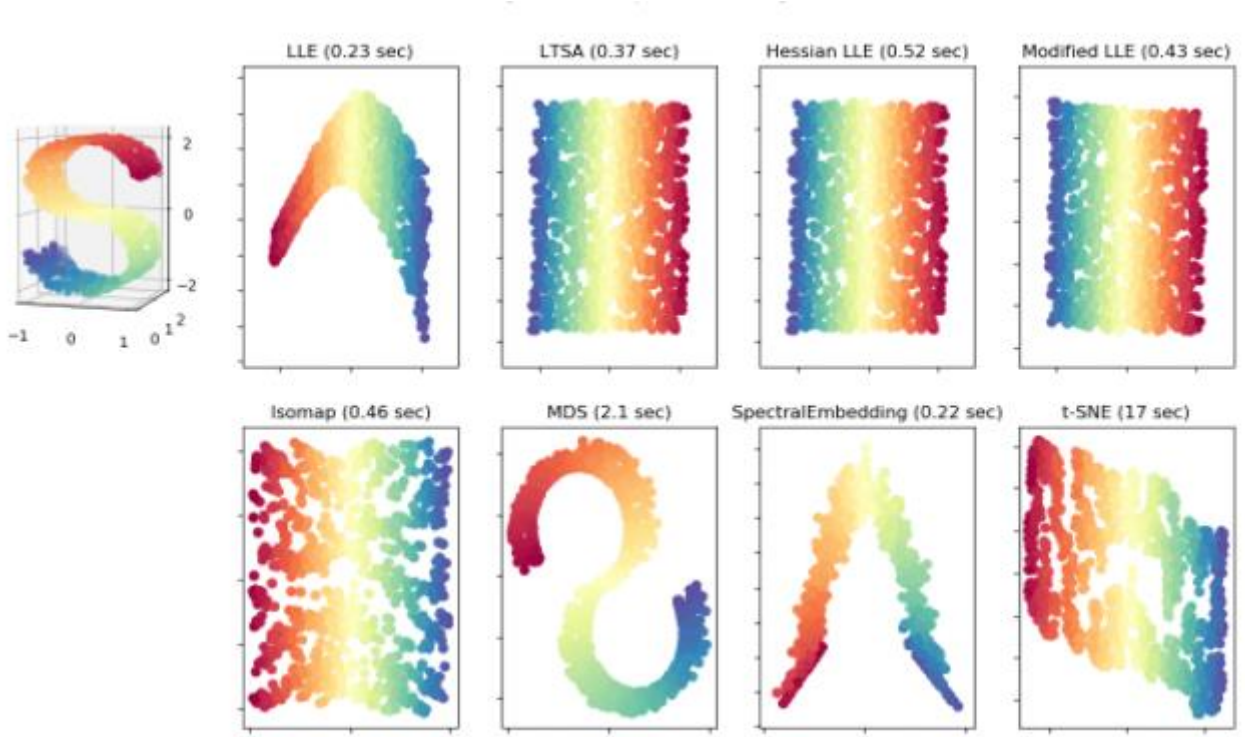
“Pressing” the data into 2 dimensions enables us to visualize the data. However, that comes with a price : high stress function value (which correlates wit distorted representation)



Mathematically non-zero stress values may occur only for only one reason: dimensionality of the chosen MDS projection is too low.

MDS in Sklearn

MDS is implemented in [Sklearn]



[Example]

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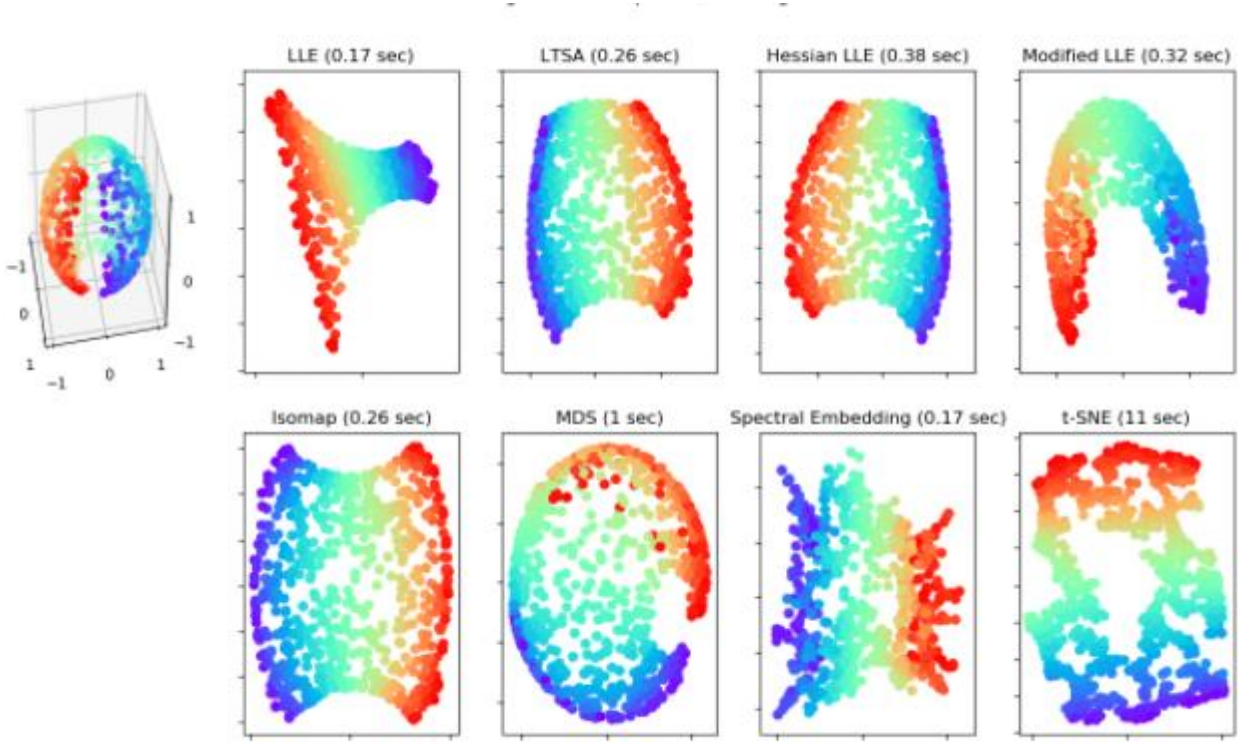

[Example]

MDS in Sklearn

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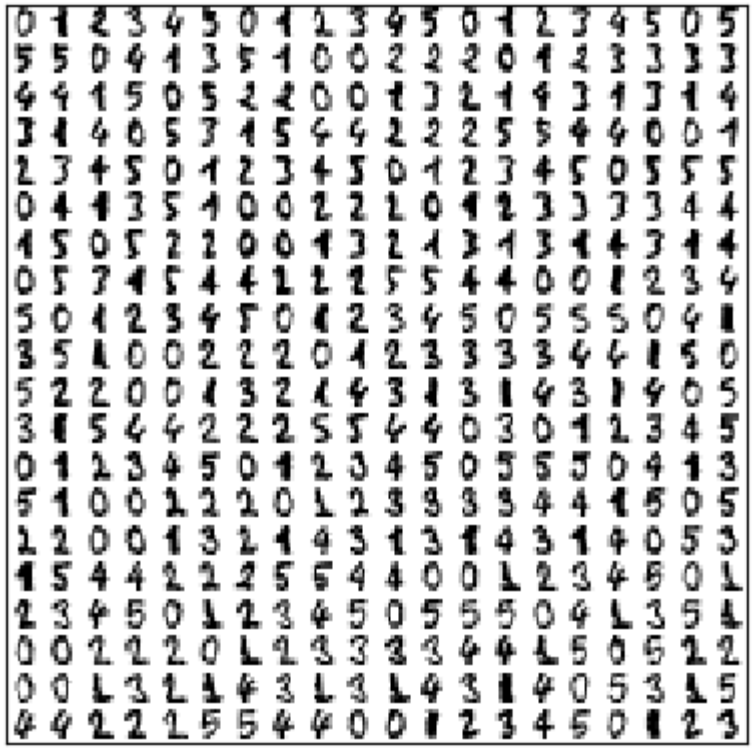
A selection from the 64-dimensional digits dataset



[Example]

ISOMAP

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- There is no essential difference between MDS and ISOMAP algorithm once we find the distance matrix induced by the neighborhood graph.

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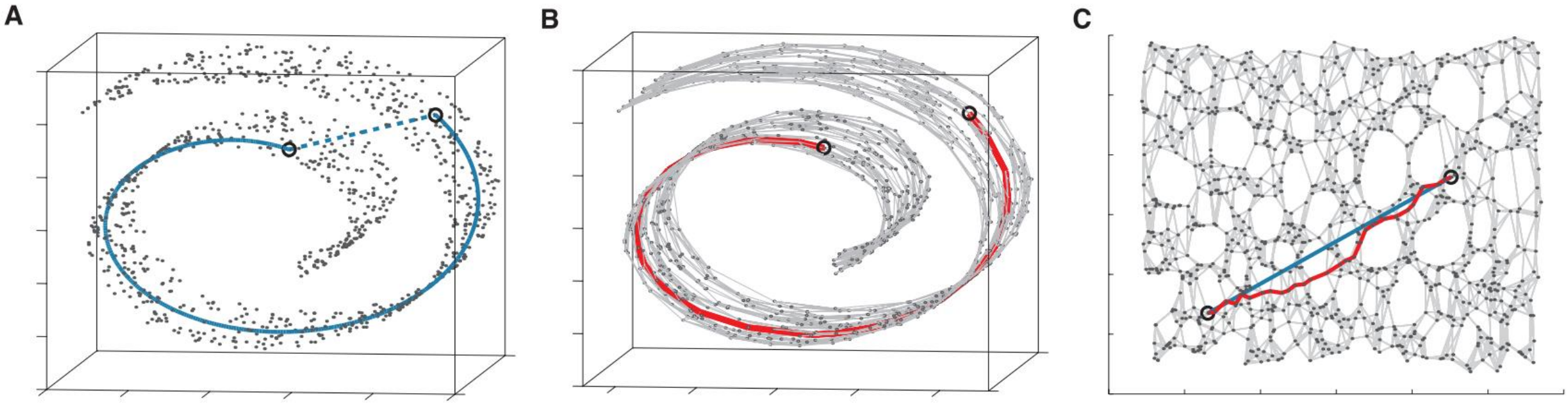
3- Apply MDS on the distance matrix above and extract the coordinates with the desired dimension

ISOMAP



A- Euclidian distance might not represent the actual distance between the points in the data.
B- We can construct the neighborhood graph of the data and then compute the geodesic distance between the points of the graph
C- Embedding the space we obtained in B into the plane.

Figure reference

Appendix : Floyd–Warshall algorithm

```
let dist be a |V| × |V| array of minimum distances
initialized to infinity

for each edge (u,v)
 dist[u][v] ← w(u,v)  // the weight of the edge (u,v)
for each vertex v
 dist[v][v] ← 0
for k from 1 to |V|
 for i from 1 to |V|
   for j from 1 to |V|
          if dist[i][j] > dist[i][k] + dist[k][j]
                     dist[i][j] ← dist[i][k] + dist[k][j]
           end if
```

Floyd algorithm is good to use when we want to compute the distance matrix on a dense graph.
When the graph G is sparse, Dijekstra algorithm is a better choice.