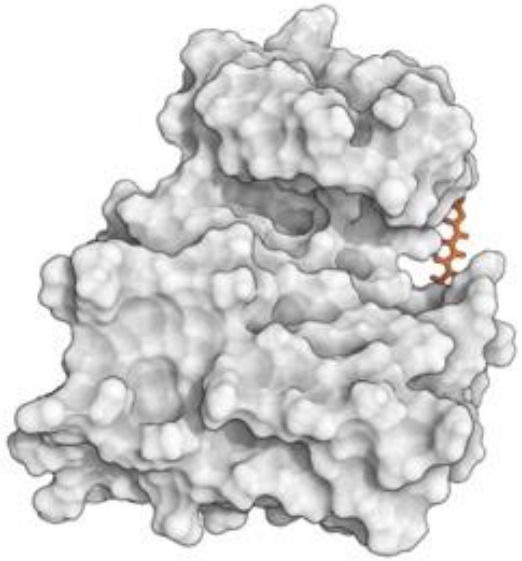
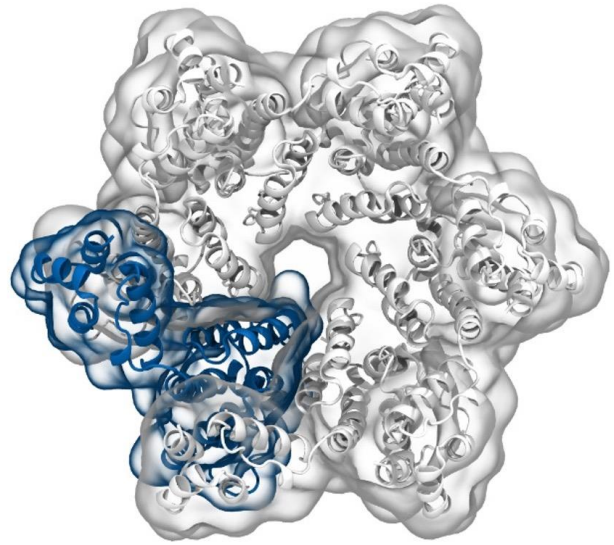
Simulation of Biomolecules



Clustering



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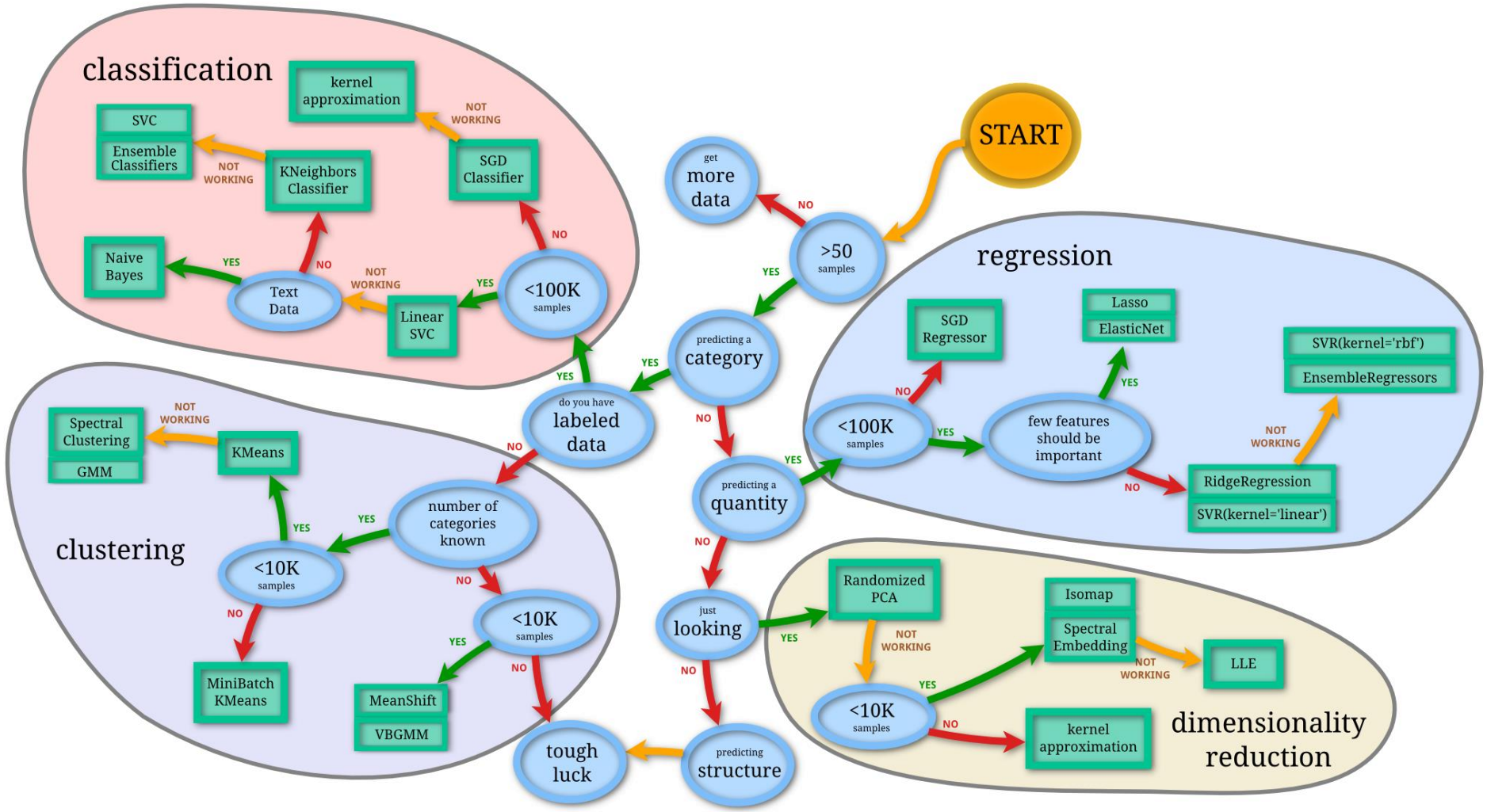
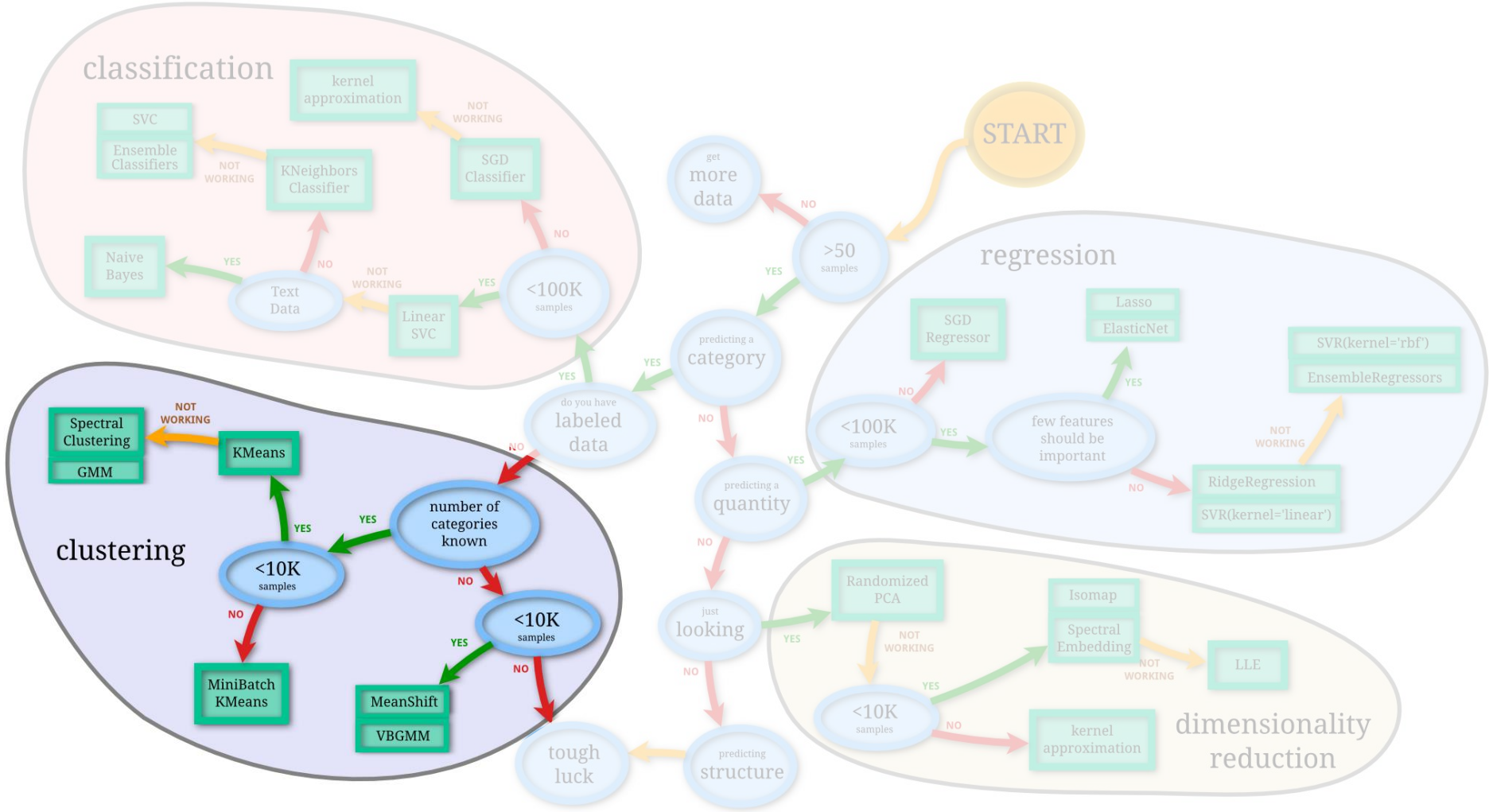
The Data Mining world



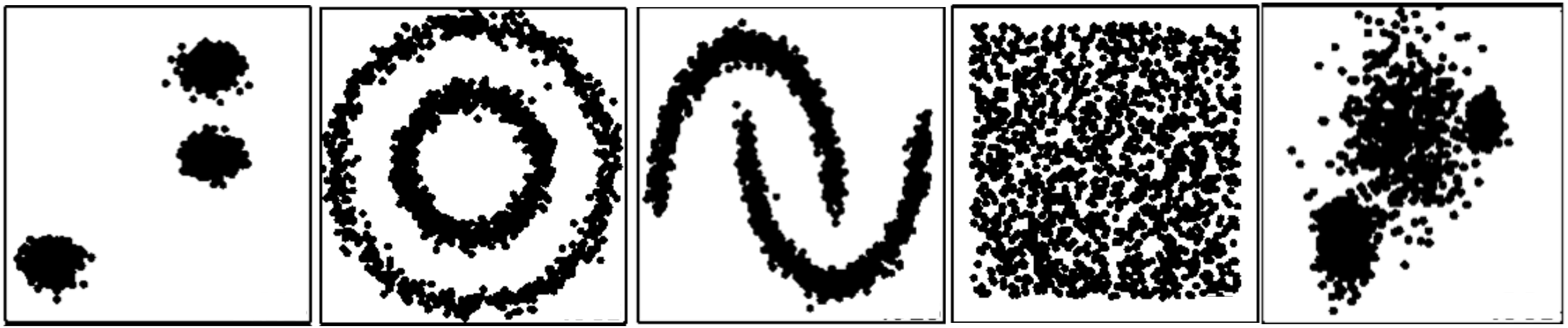
From **scikit-learn.org**

The Data Mining world



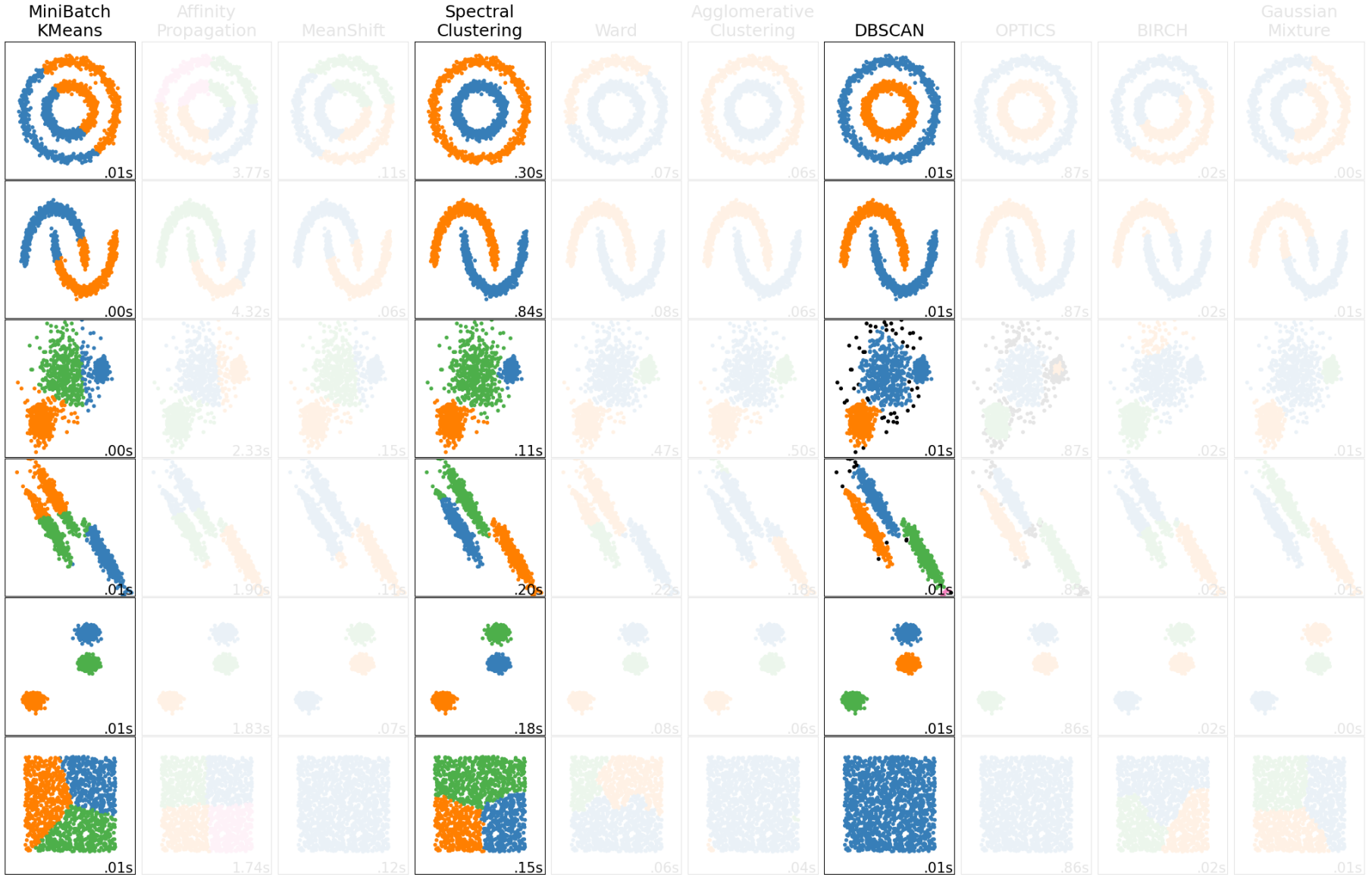
From **scikit-learn.org**

Clustering (i.e., unsupervised learning)



Known number of clusters? Flat geometry?
Even cluster size? Outliers? Centroids needed?

Clustering algorithms



scikit-learn.org/stable/modules/clustering.html

How does k-means work?

Input: K, set of points $x_1 \ldots x_n$ (can be in N-dimensional)

Place centroids, $c_1 \ldots$, c_n at random locations

Repeat until convergence:

For each point x_i:

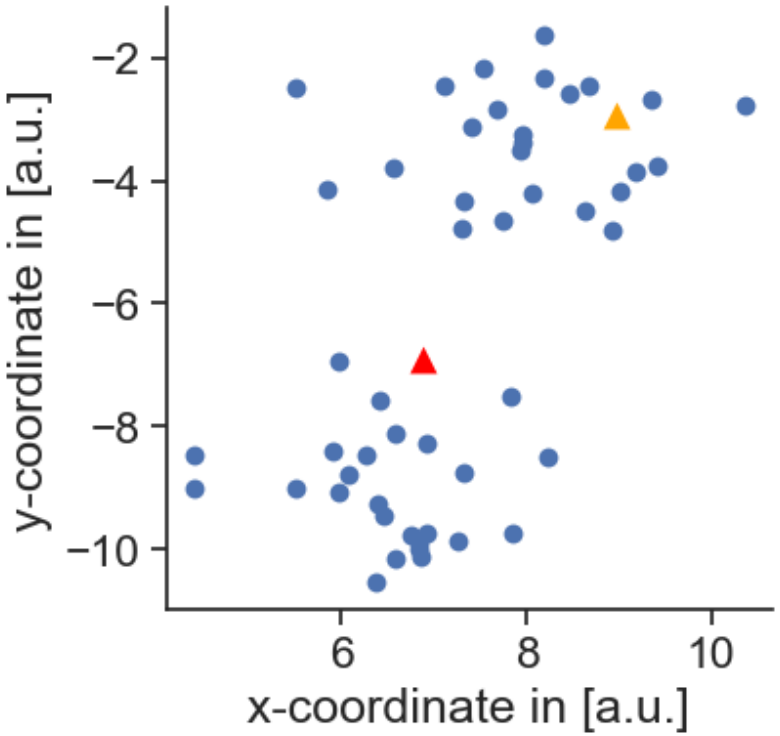
Find nearest centroid $c_j = \arg\min_j D(x_i, c_j)$

Assign the point x_i to cluster j

For each cluster j = 1…K:

Compute the centroid mean for all points in one cluster and update the centroid

$$c_j(a) = \frac{1}{n_j} \sum_{x_i \to c_j} x_i(a)$$



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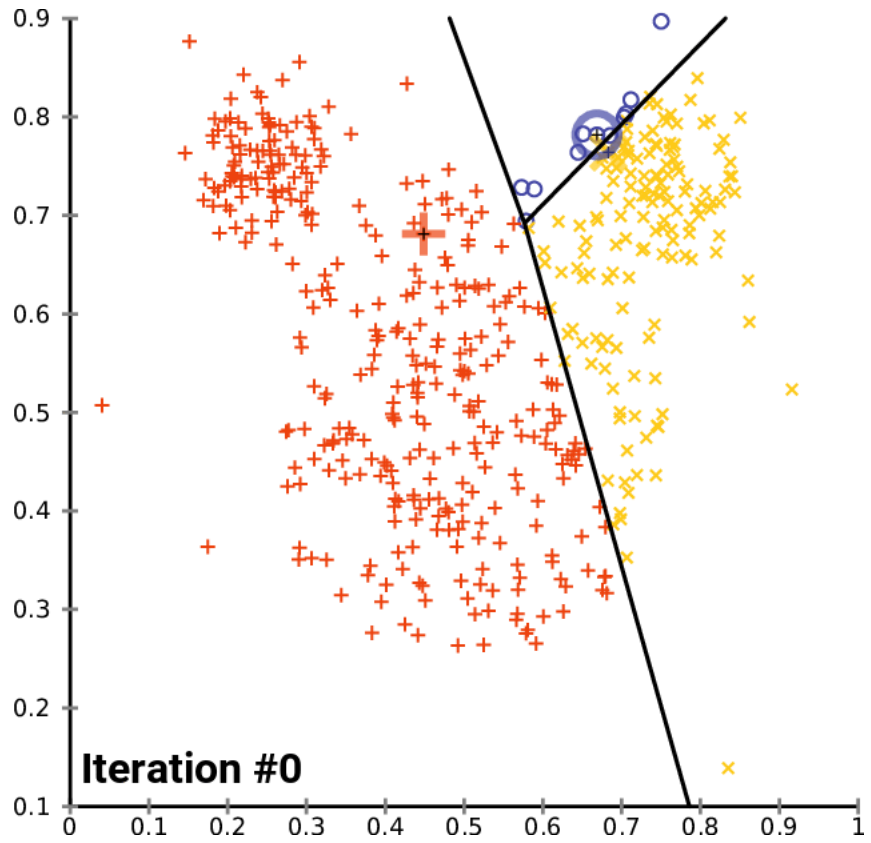
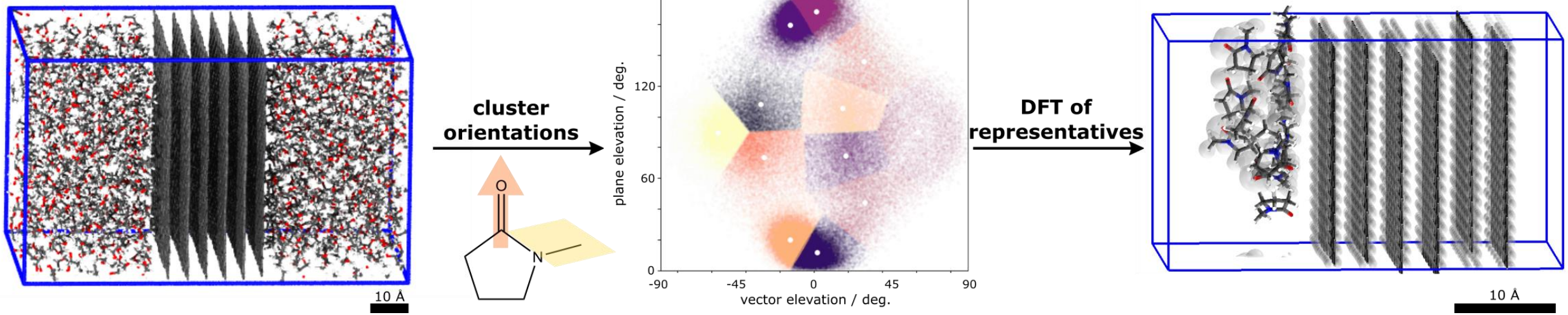


[Example] k-means vs solvent-graphite interactions

- k-means useful when number of clusters can be estimated, and cluster are approximately circular. Useful if cluster centres are required.

- Example: Molecular Dynamics simulation of graphite immersed in solvents. Centroids as representatives of >100k individual solvent-graphene interactions

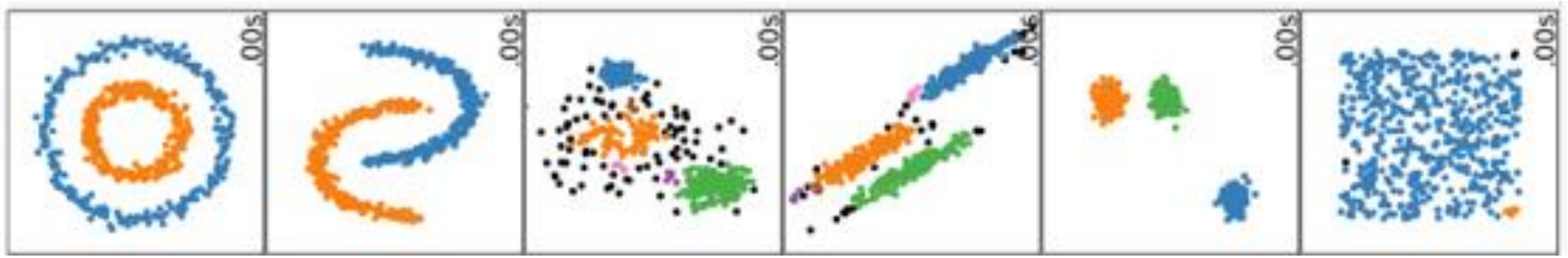


S. J. Goldie, M. T. Degiacomi, et al. *Identification of Graphene Dispersion Agents through Molecular Fingerprints*. ***ACS Nano***, 2022

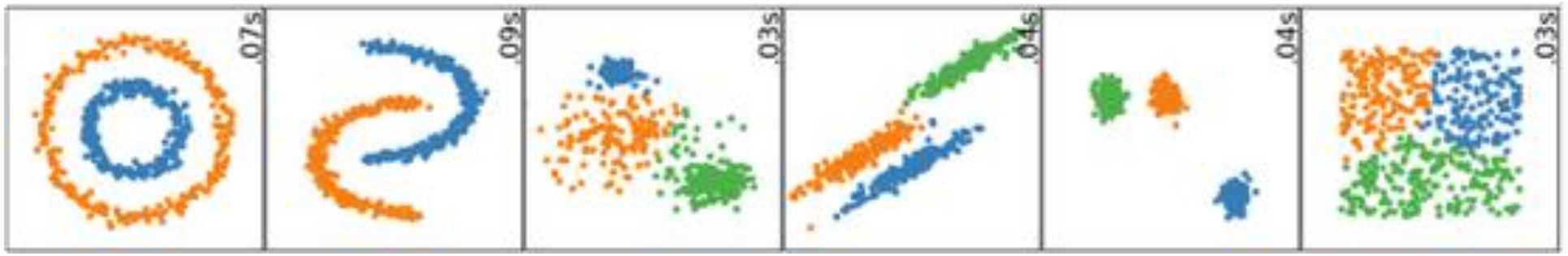
Density-based and spectral clustering

Useful when number of clusters is unknown, or clusters are not circular

DBSCAN



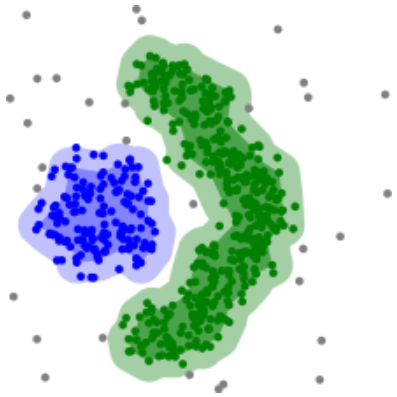
Spectral Clustering



Density-based and spectral clustering

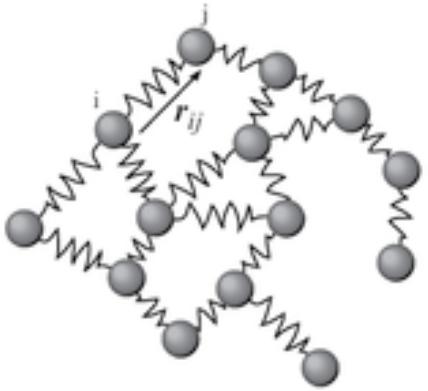
Useful when number of clusters is unknown, or clusters are not circular

DBSCAN



- Find points in the ε neighbourhood of every point, identify core points with more than n neighbours.
- Find the connected components of core points on the neighbour graph, ignoring all non-core points.
- Assign each non-core point to a nearby cluster if the cluster is an ε neighbour, otherwise assign to noise otherwise.

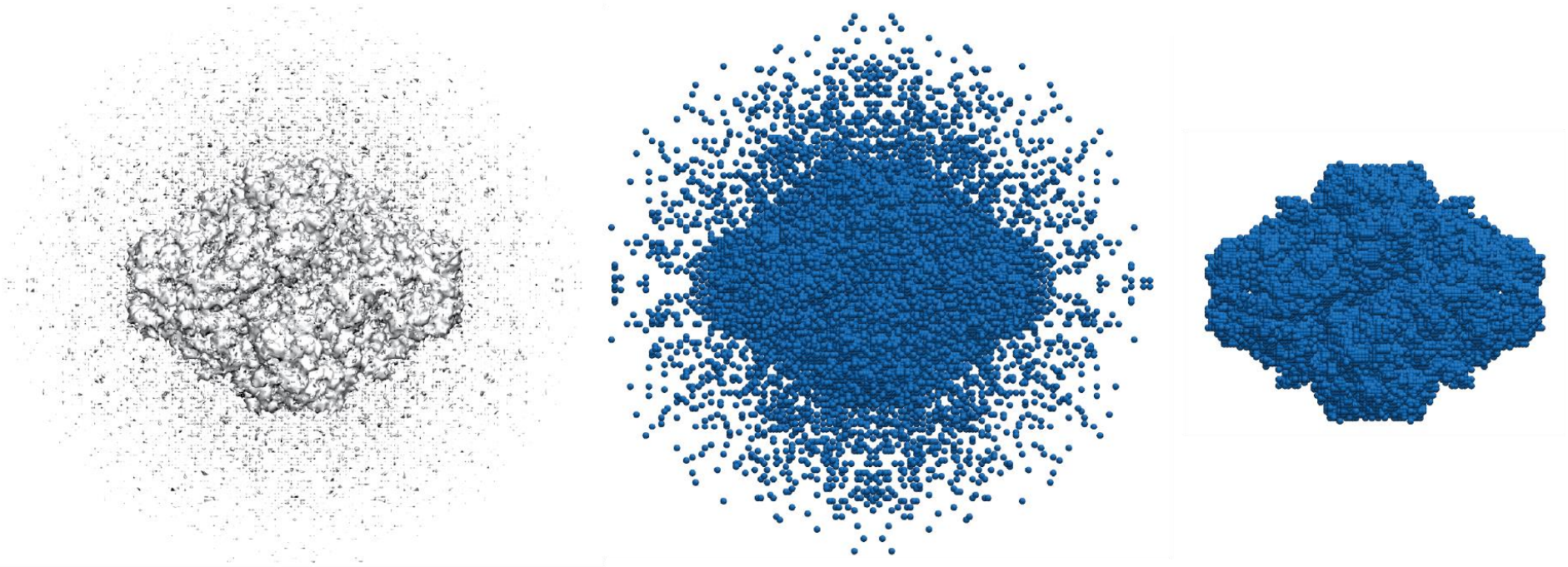
Spectral Clustering



- Calculate the Laplacian
- Calculate the first k eigenvectors
- Consider the matrix formed by the first k-eigenvectors
- Cluster the graph nodes based on these features (e.g., k-means)

[Example] DBSCAN for noise detection in EM maps

- Load electron density map and chose a threshold *t*
- Place pseudoatoms where intensity > *t*
- Cluster beads and delete small clusters (<1% of total beads



M.T.Degiacomi and J.L.P. Benesch, *EM∩IM: software for relating ion mobility mass spectrometry and electron microscopy data*, ***Analyst***, 2015