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Biased clustering for selecting representative samples in chemical databases

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Motivation

Provide a faster method of **materials screening**, so that experts have access to large-scale analysis of material properties.

How?

Using **Machine Learning** methods, specifically **biased clustering**, to obtain molecules that represent a larger set. Only these molecules will need to be analyzed using costly methods like **Density Functional Theory**, instead of all the others.

Supervised Clustering?

For a biased clustering system, two algorithms working together are needed:

- Clustering algorithm
- Optimization algorithm

For the purposes of this presentation, it will be shown how **K-Means** and **Simulated Annealing** work together to bias the clustering process, in order to satisfy the needs of the specialist.

K-Means

Clusters dataset’s items based on similarity.

1. Choose k centroids to match k random elements from the database

2. Assign each element to the nearest (most similar) centroid

3. Recalculate the centroid of each cluster as the center of mass of its members

4. While the convergence criterion isn’t met, repeat from step 2

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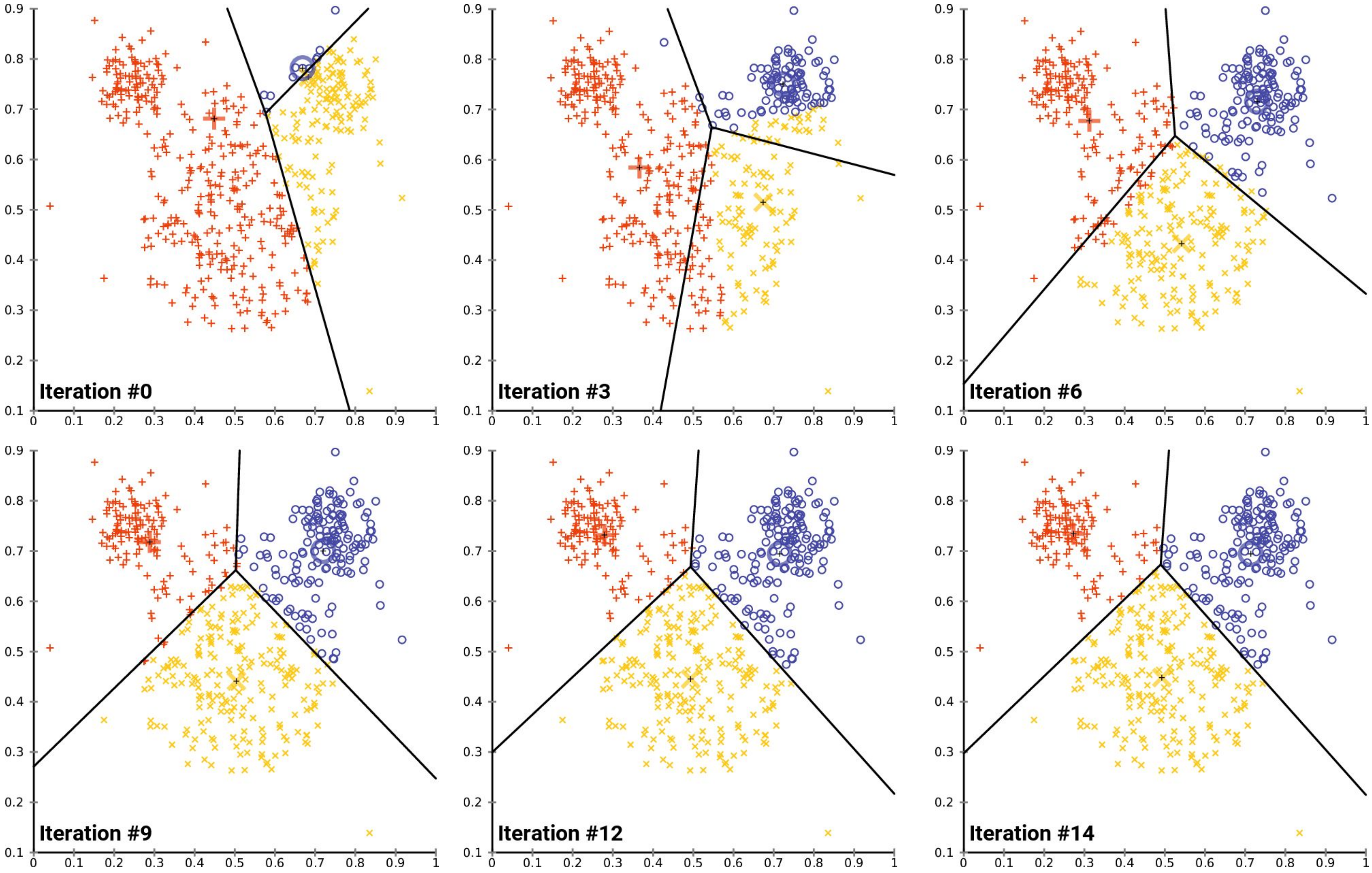
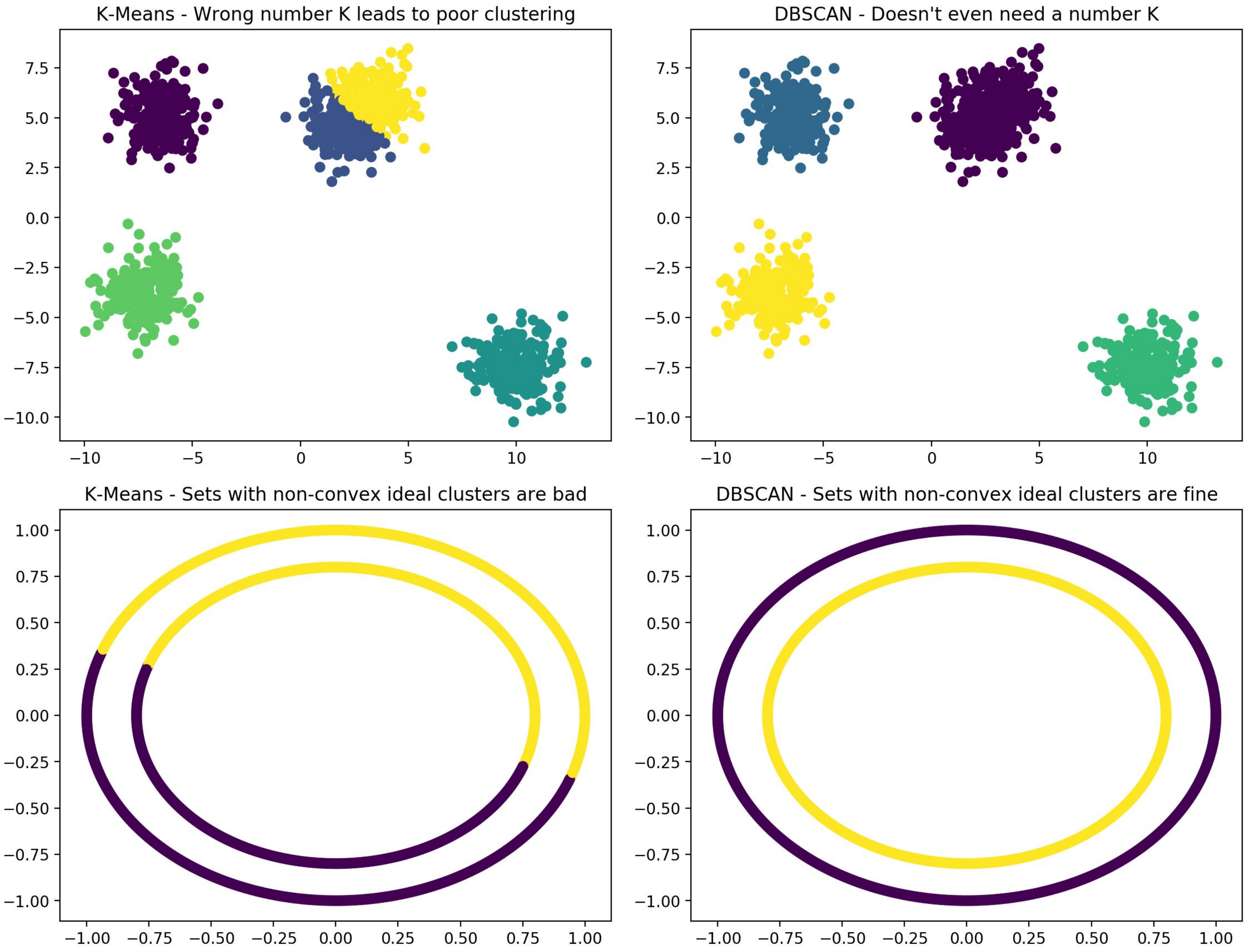


K-Means Convergence By Chire - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=59409335


K-Means - Wrong number K leads to poor clustering

DBSCAN - Doesn't even need a number K

K-Means - Sets with non-convex ideal clusters are bad

DBSCAN - Sets with non-convex ideal clusters are fine

Simulated Annealing

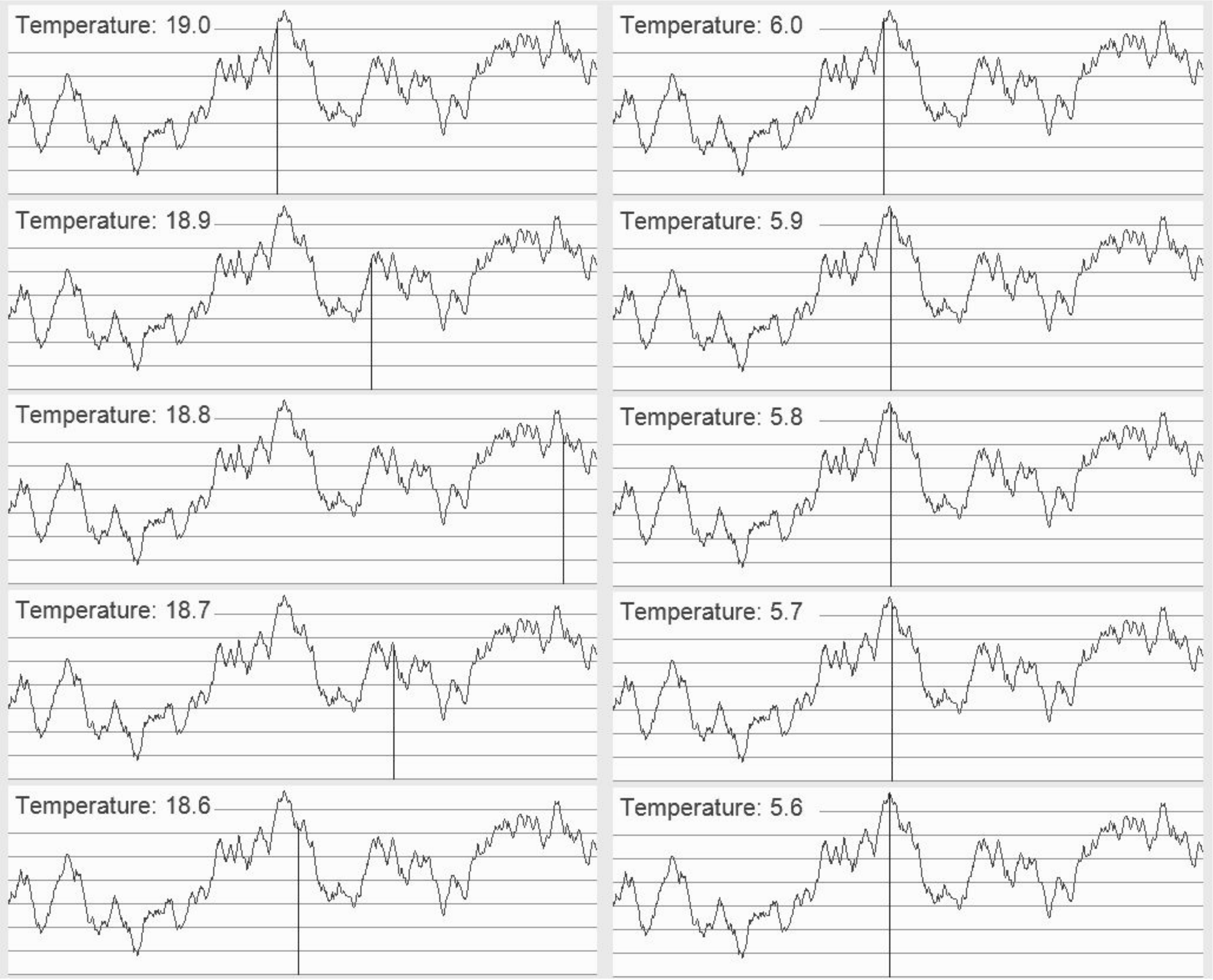
Aims to find global optima of functions

```
1.  Initialize the temperature t as a high value
    and the current state c0 as a set of random
    values

2.  Select a new state c1 from a neighbor of the
    current state and calculate $\Delta C = c1 - c0$

3.  If $\Delta C \leq 0$ or $\exp(-\Delta C / t) > \text{random}(0, 1)$ then
       current_state <- new_state
    Else
       do nothing

4.  Decrement t. If there is still no convergence,
    repeat the second step
```



Sim. Annealing Convergence By Kingpin13 - Own work, CC0, https://commons.wikimedia.org/w/index.php?curid=25010763

K-Means + Simulated Annealing

K-Means receives an array of features, where each feature has a weight **w**, so that clustering can be done. From the configuration generated by K-Means, a result **v** is extracted. This result is precisely what will be optimized by Simulated Annealing. The optimization algorithm control the weights **w** given the value **v**.

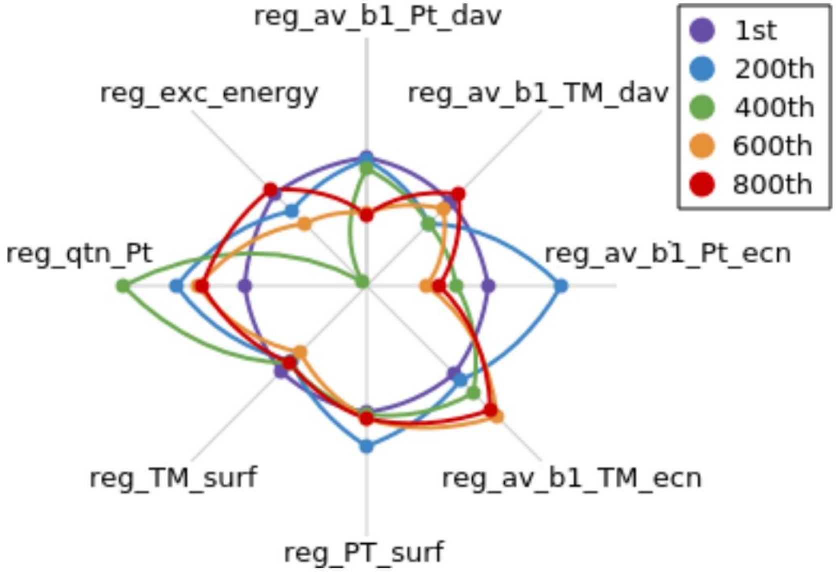
$$Simulated\ Annealing$$

$$f\left(K\text{–}Means\left(\left(\begin{bmatrix} v_{11}\overset{\Downarrow}{w_1} & v_{12}\overset{\Downarrow}{w_2} \\ v_{21}w_1 & v_{22}w_2 \\ v_{31}w_1 & v_{32}w_2 \end{bmatrix}\right)\right)\right) = \overset{\Uparrow}{v}$$

K-Means + Simulated Annealing

Thus, it is possible to bias the clusters following an objective. For example: minimize the maximum variance in the number of elements per cluster.

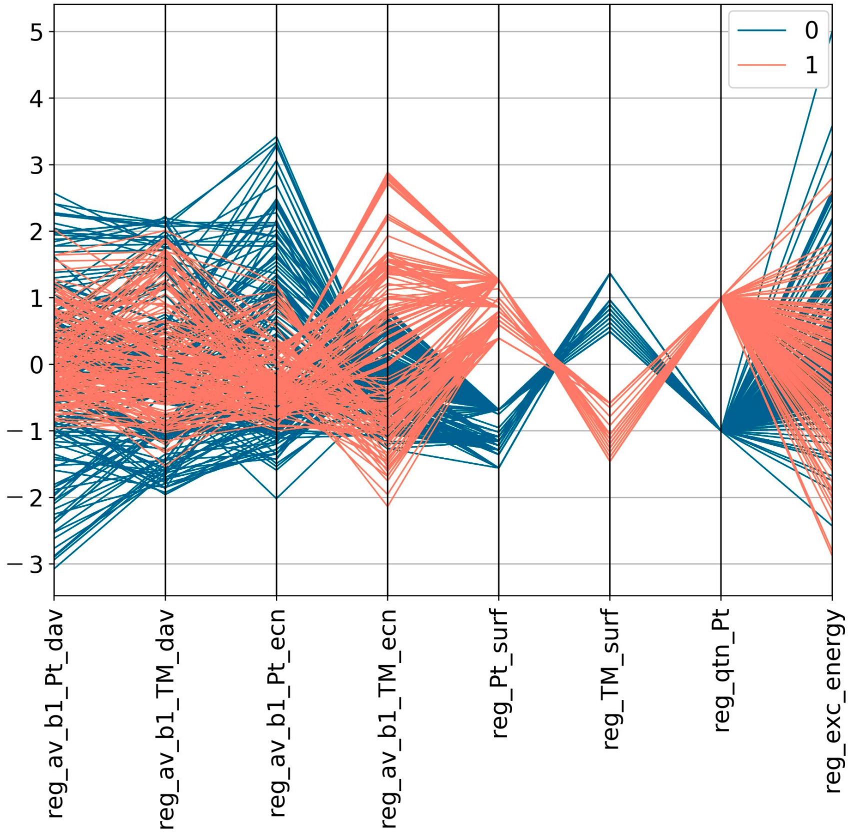
The figure to the side shows the convergence of the weights of the features along the iterations.



Notice how, in the beginning, all features had the same weight and these weights were transformed until they converged.

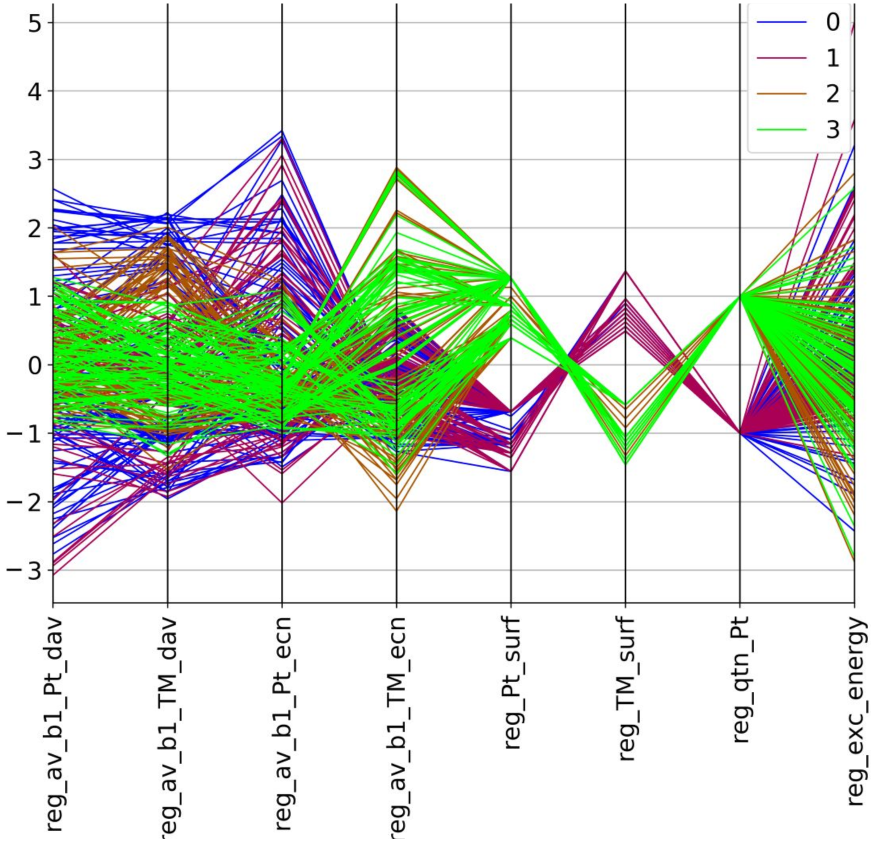
Example Result 1

In the graph we can see a disparity in **reg_qtb_Pt** (amount of platinum), **reg_TM_surf** (amount of transition metals on the surface) and **reg_Pt_surf** (amount of platinum on the surface). That is, the molecules were grouped taking into account mainly the amount of platinum and transition metals.



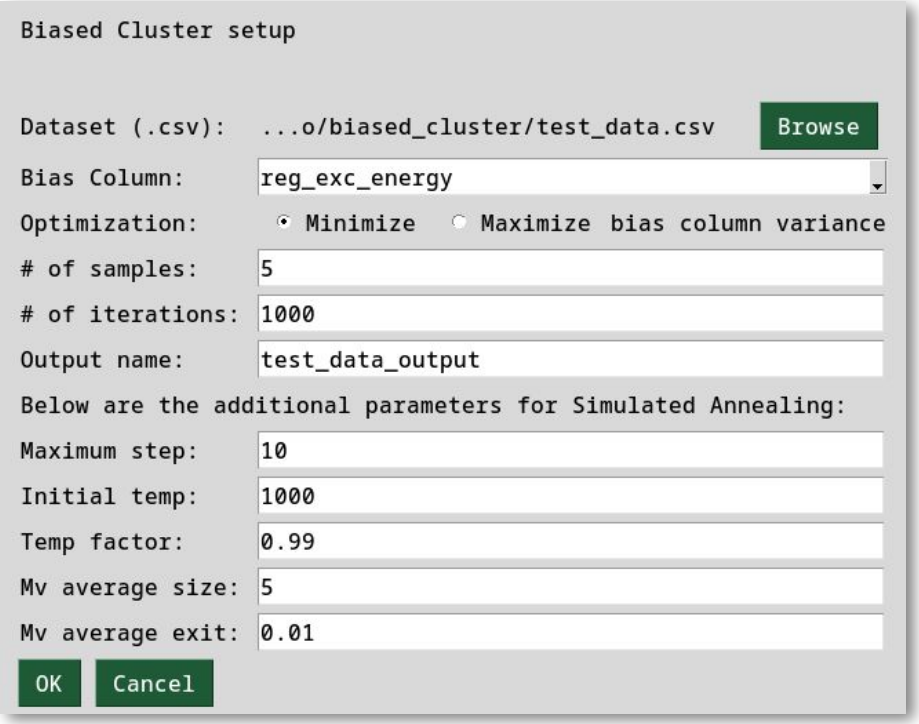
Example Result 2

Increasing the number of clusters causes subdivisions into groups given by less prevalent characteristics such as **reg_av_b1_Pt_ecn** and **reg_av_b1_TM_ecn** (average number of neighbors of Pt or TM in the molecule).



Toolbox in development

A toolbox for executing the supervised/biased clustering algorithm from graphical or command line interfaces is being developed.



Biased Cluster setup

Dataset (.csv): ...o/biased_cluster/test_data.csv

Bias Column: reg_exc_energy

Optimization: ● Minimize ○ Maximize bias column variance

# of samples: 5

# of iterations: 1000

Output name: test_data_output

Below are the additional parameters for Simulated Annealing:

Maximum step: 10

Initial temp: 1000

Temp factor: 0.99

Mv average size: 5

Mv average exit: 0.01

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Remarks

1. The toolbox will support not only K-Means, but other clustering algorithms too.

2. This tool can be used in many different situations where the specialist wants to look for specific groups, highlighting some property.

Acknowledgements

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CINE
CENTER FOR INNOVATION ON NEW ENERGIES

CMSC
Computational Materials Science and Chemistry

QTNano

IQSC USP

PIBIC
CNPq

Thank you!

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