CLUEstering: a high-performance density-based clustering library for scientific computing

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Co-supervisors: Francesco Giacomini, INFN-CNAF
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Alma Mater Studiorum – Università di Bologna

20 September 2024

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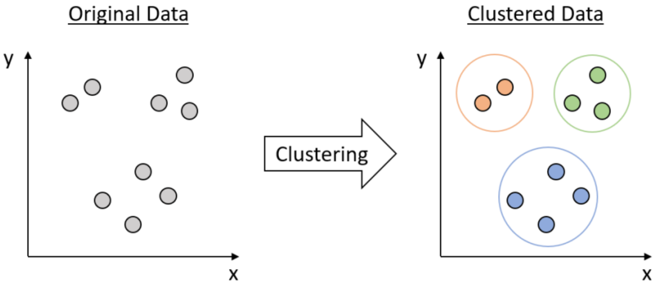
- Achieve performance portability using the Alpaka library
- Benchmark the library and assess the quality of the results
- Apply the library to several problems regarding different branches of science, in order to show its generality

Clustering

- Clustering is used to group data based on some measure of proximity or similarity



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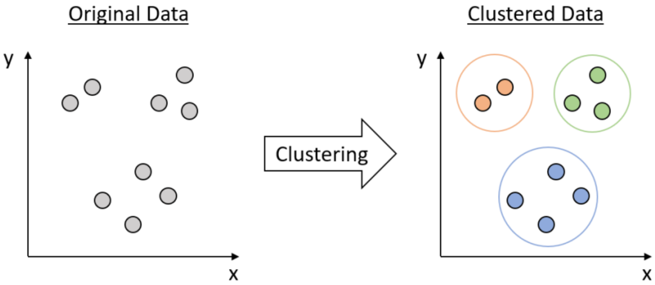

- It's a widely used technique because it allows to reconstruct classes of objects when there is no truth information available

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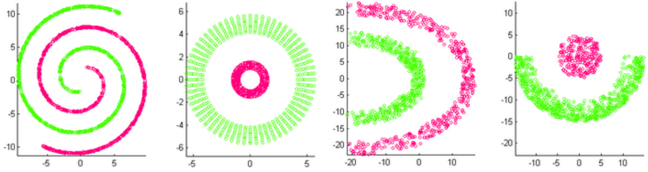

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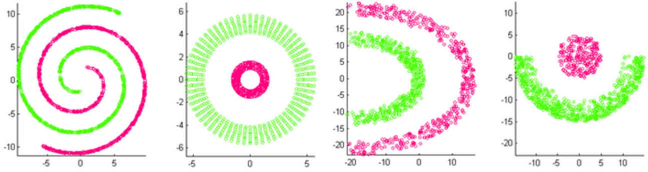

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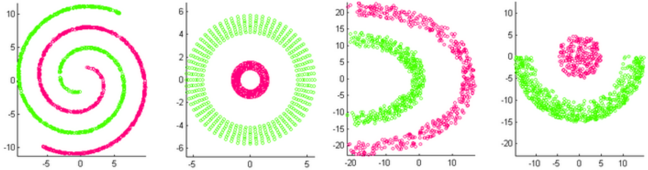

- it doesn't require a-priori knowledge of the number of clusters
- it works well with data full of noise and outliers

The importance of weighted clustering

- In weighted clustering each point is assigned a weight
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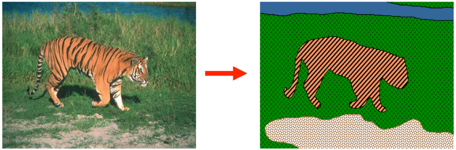
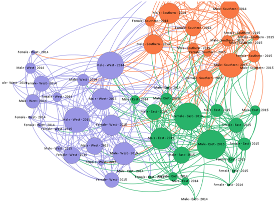
- Weights can be used to represent: signal measures, prior knowledge
- Widely used in many applications: customer segmentation, image segmentation, social network analysis, anomaly detection, biological analysis





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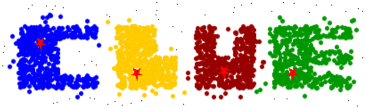
- Most density-based algorithms don't support weighted clustering out-of-the-box
  - ➙ They need hand-made modifications to the dataset or to the distance matrix
- There is a need for an alternative solution that combines the power of **density-based** algorithms with the generality of **weighted** clustering

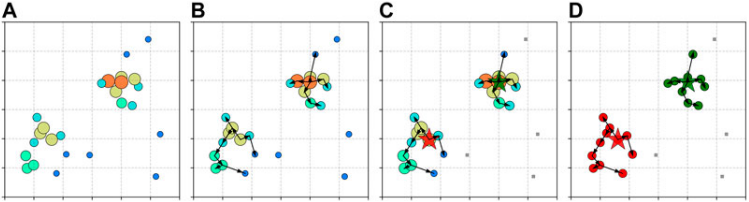
The CLUE algorithm



- CLUE (CLUstering of Energy) is a density-based clustering algorithm used in the CMS experiment at LHC
- It was originally designed for the clustering of hits in the calorimeters
- Each point has a weight which is used when calculating the densities
- The weights are the energy deposit measurements of the detector layer sensors

Reference: https://www.frontiersin.org/journals/big-data/articles/10.3389/fdata.2020.591315/full#B16

Description of the algorithm



a → Computation of the local density for each point

b → Selection of the *nearest highers*

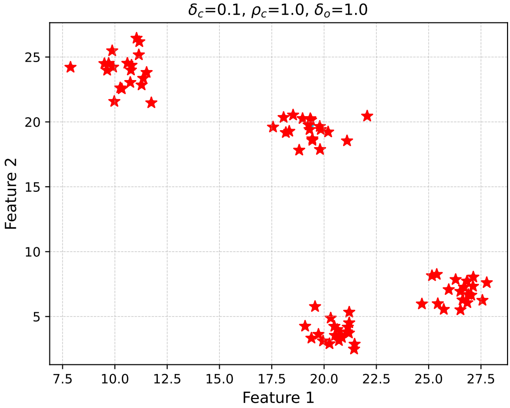
c → Finding clusters and outliers

d → Assigning clusters

The parameters of CLUE

3 parameters:

- δ_c, size of query range for computation of local density
- ρ_c, density cut-off for promotion to cluster seed
- δ_o, size of query range for cluster extension



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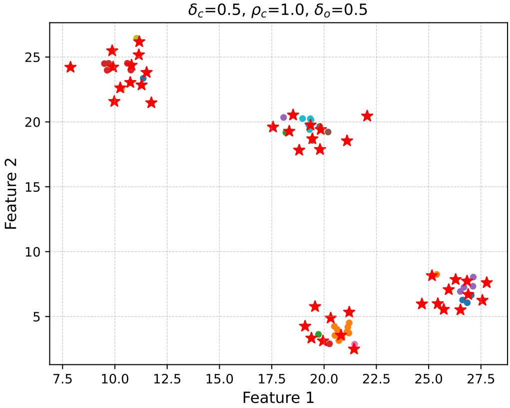

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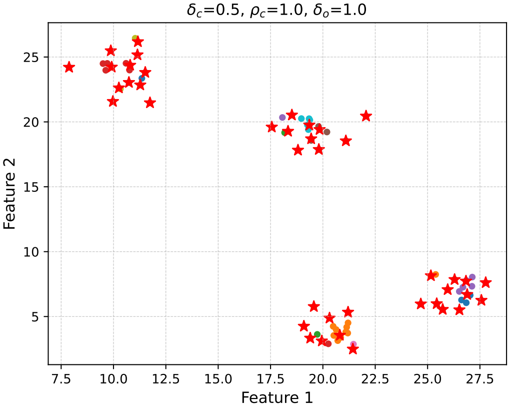

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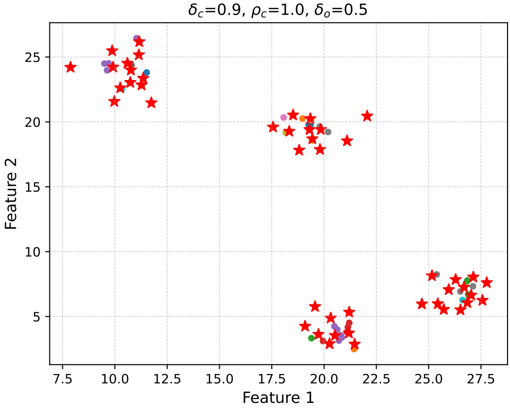

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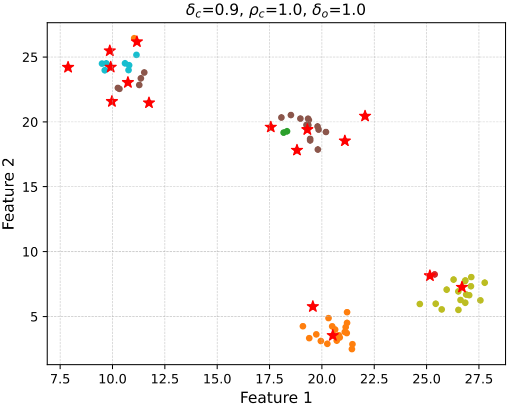

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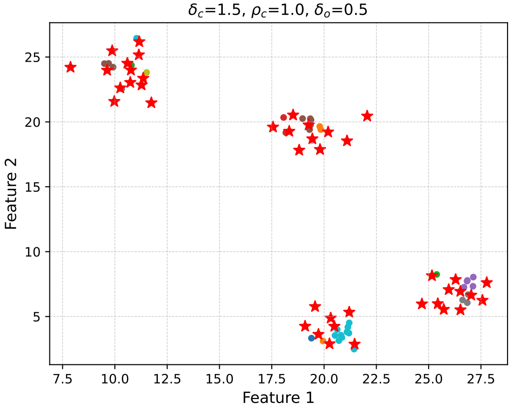

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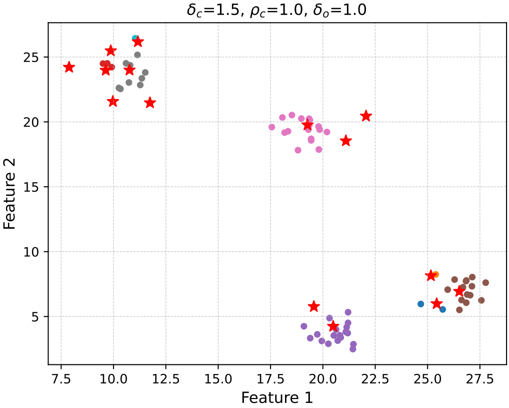

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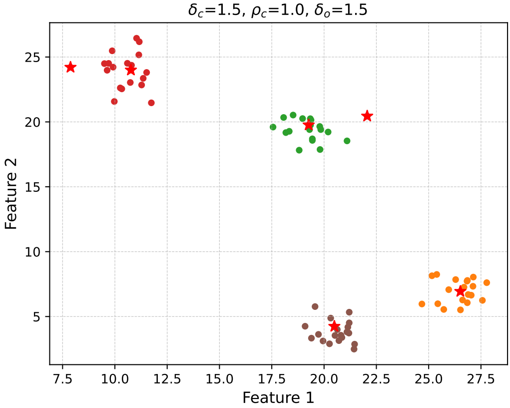

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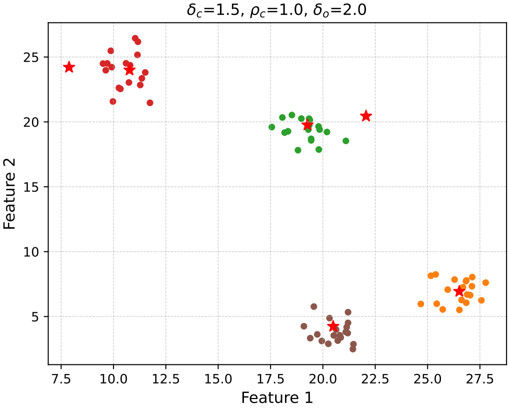

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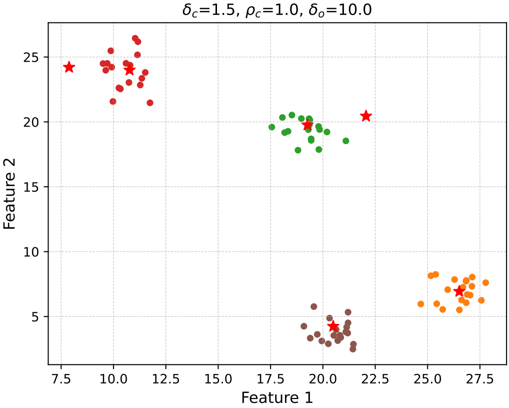

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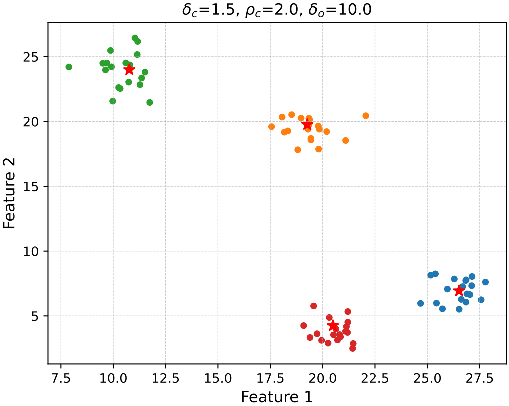

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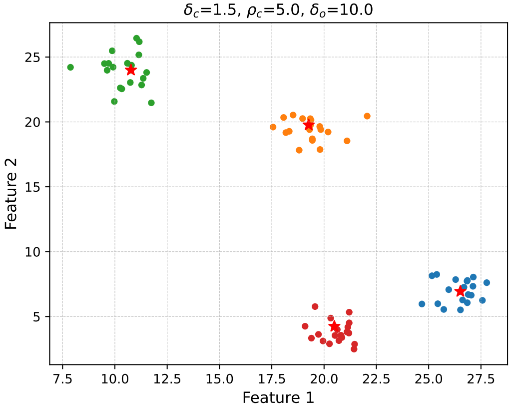

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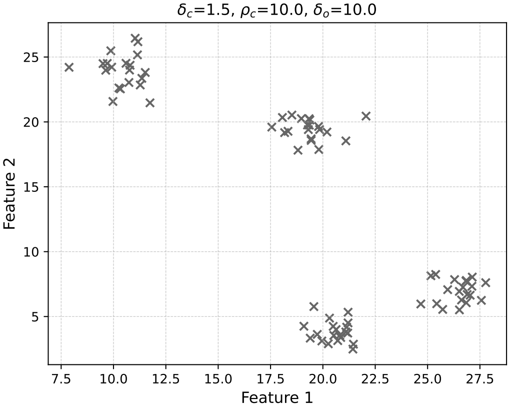

From CLUE ...

- CLUE was specifically tailored to work in the CMS detector
- 2-dimensional clustering for each of the layers
- Could not be used on a general dataset

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- CLUEstering provides a generalization of CLUE
  - ➙ It's a general-purpose library
  - ➙ Applicable to any number of dimensions

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- CLUEstering provides a generalization of CLUE
  - ➙ It's a general-purpose library
  - ➙ Applicable to any number of dimensions
- Provides a Python interface to the C++ backend, which makes it easily usable by the machine learning community

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- It can be applied to a large variety of problems that use clustering
  - ➞ in particular density-based clustering
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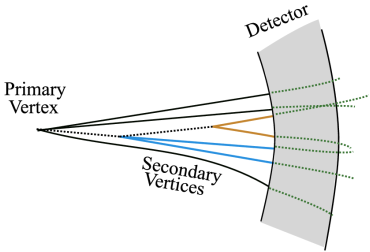
- Two examples:
  - ➞ vertex reconstruction in particle physics
  - ➞ star detection in astronomy

Example 1: Vertex reconstruction (vertexing)



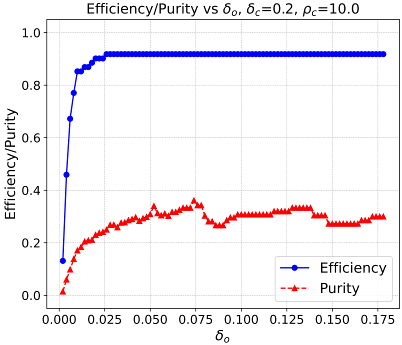
- Vertexing is the reconstruction of the interaction points (vertices) of the particle tracks
- The reconstructed vertices (recos) are compared to simulated vertices (sims)
- There is a match if recos and sims share at least 40% of the points (tracks)
- The relationship between recos and sims is a Many-To-Many

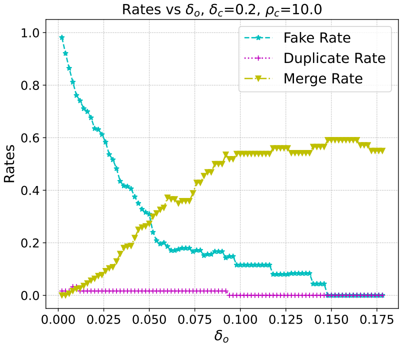
Useful definitions in vertexing

- **Efficiency**: fraction of sims associated to at least one reco
- **pure:** a reco where less than 20% of the points are noise
- **duplicate:** a sim associated to more than 1 reco
- **merged:** a reco associated to more than 1 sim
- **fake:** a reco associated to 0 sims

CLUEstering for vertexing

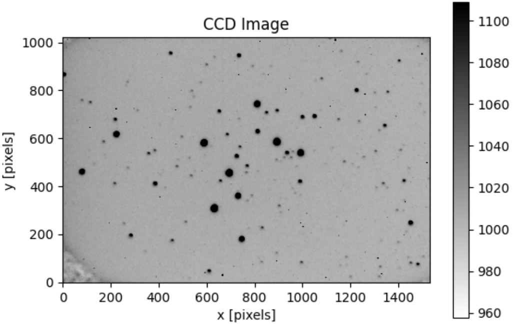
Simulation from an official sample of the CMS tracker community.
Clustering done using the z coordinate of the tracks and p_T as weight





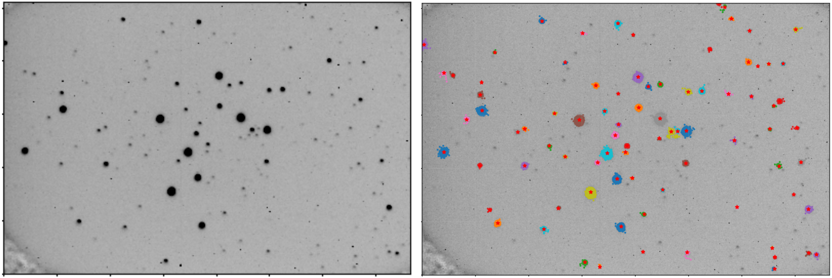
Reminder: δ_o indicates the size of query region used for cluster extension

Example 2: Star detection in astronomy



- Modern telescopes use CCDs (charge-coupled devices) to convert impinging photons into electrons
- Each pixel contains the number of electrons

Comparison of the PSF (Point Spread Function) image and the stars detected by CLUEstering



The advent of big data

- The amount of data being produced keeps increasing in every branch of science
- Software needs to continually improve in order to handle the increasing volume of data

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  - → Performance portability libraries

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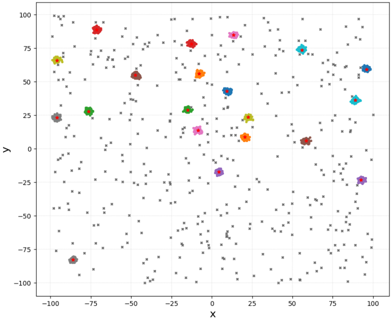
Performance portability in CLUEstering

- CLUE is a highly-parallel algorithm
- It's designed to work well on heterogeneous platforms
- The backend of CLUEstering is implemented with Alpaka
- Users can run the clustering on any backend with a single command

alpaka

https://github.com/alpaka-group/alpaka

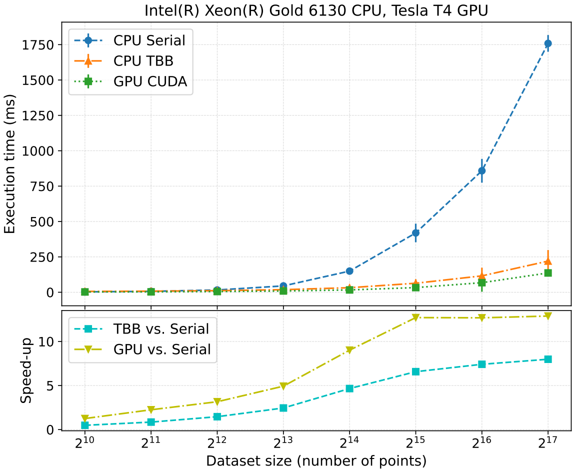
A representative dataset



- This dataset is representative of a common clustering ploblem
- The clusters are surrounded by noise, which mimics physical data
- CLUEstering reconstructs all the clusters correctly and the results are not affected by the noise

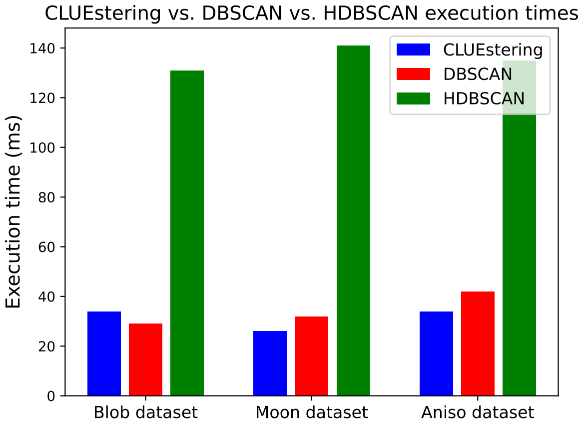
Scaling with dataset size

Parallel accelerators provide a 10× speed-up with respect to serial execution.



Comparison with other algorithms

Finally, how does CLUEstering compare with two of the most popular density-based algorithms against typical benchmarking datasets?



Note: The lower the better.

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  `https://github.com/cms-patatrack/CLUEstering`

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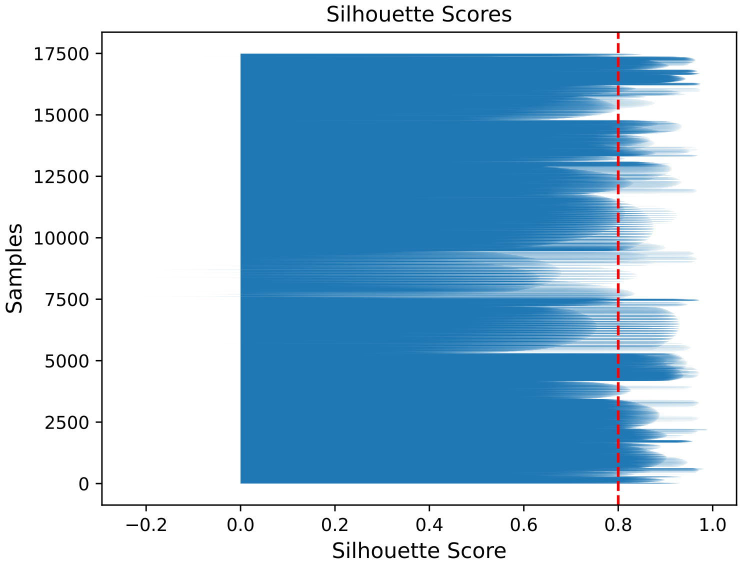
- Its use of heterogeneous platforms and its performance portability make it stand out from most other clustering libraries
- It's open source and available on github `https://github.com/cms-patatrack/CLUEstering`
- Can be easily installed with a simple `pip install` command

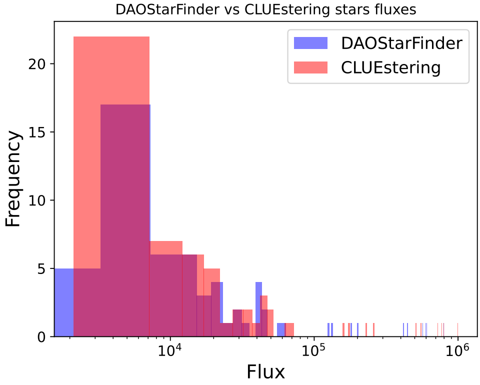
CLUEstering for star detection: silhouette scores



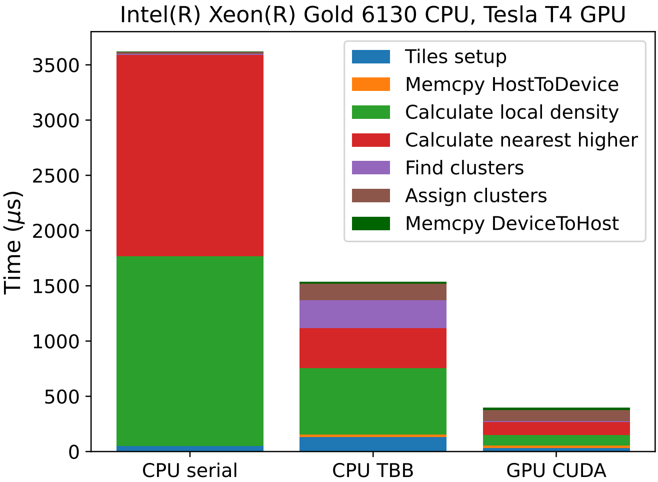
CLUEstering for star detection: comparison of fluxes

Compare the fluxes obtained using CLUEstering with DAOStarFinder and aperture photometry.

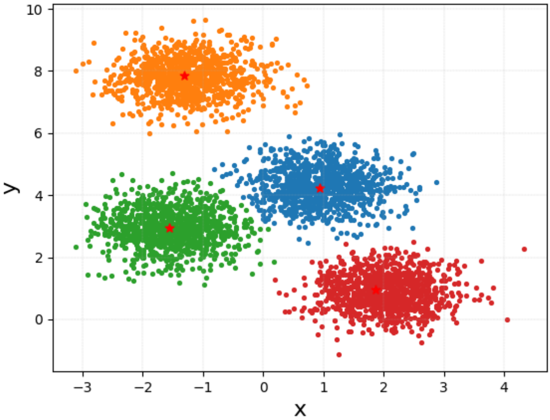
Execution time: $59 \pm 2\,ms$ for CLUE and $262 \pm 15\,ms$ for DAOStarFinder



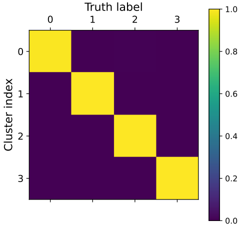
Profiling results

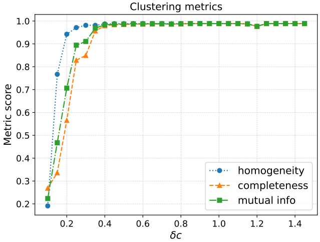


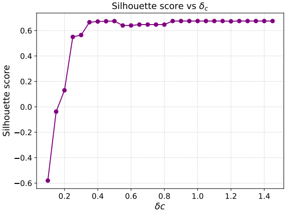
Blob datasets

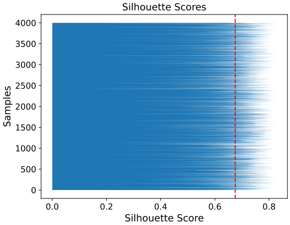


Results on the blob dataset

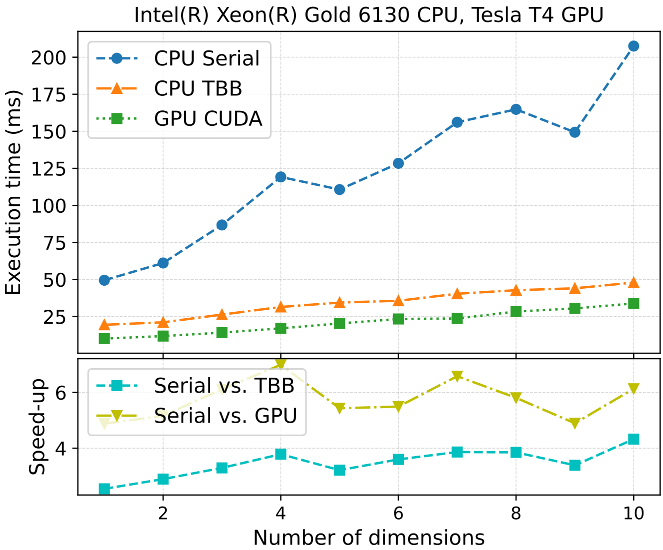




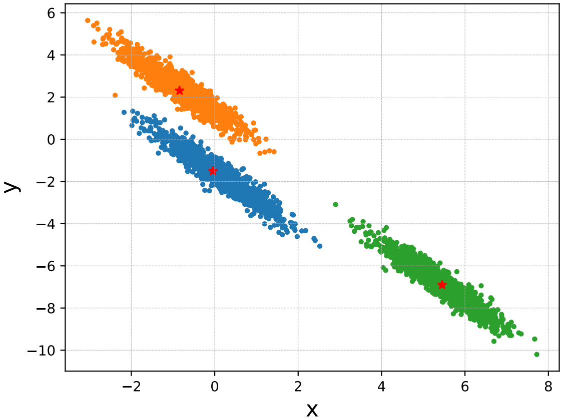




Scaling with number of dimensions



Aniso dataset



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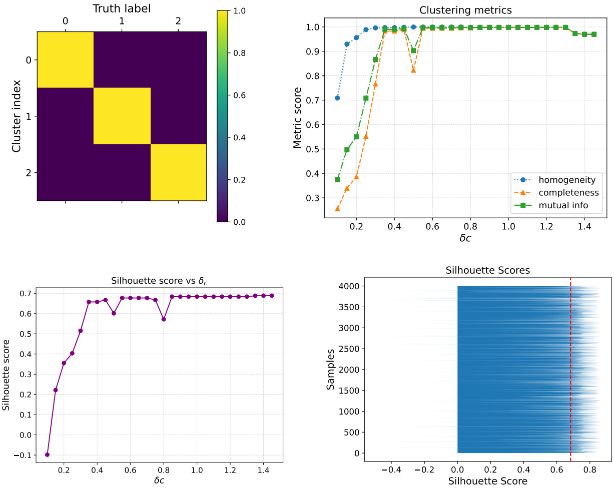
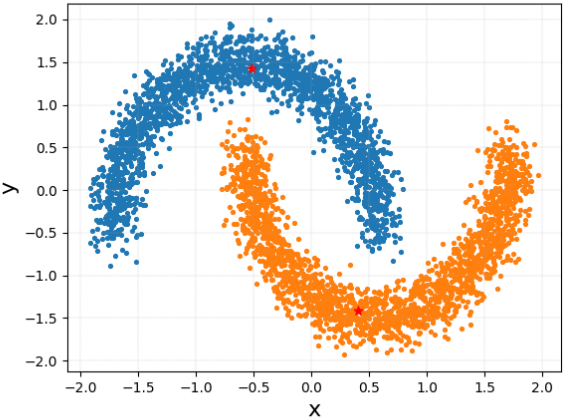


Moon dataset



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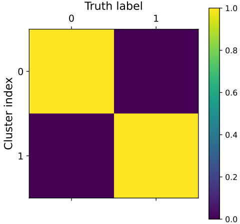

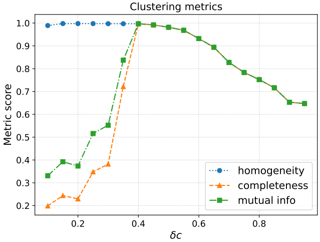

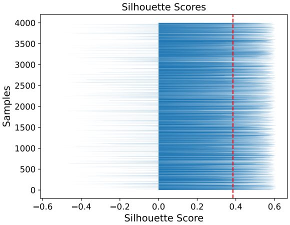

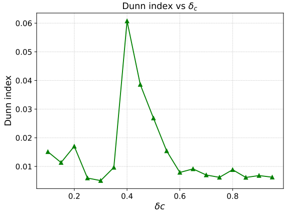

Backup: CLUEstering for vertexing (cont.)

Clustering done using the z coordinate of the tracks and p_T as weight