

# The power (and caveats) of

## clustering algorithms

with examples from use on Gaia data

NAM 2022 // Techniques2 // 13.07.22

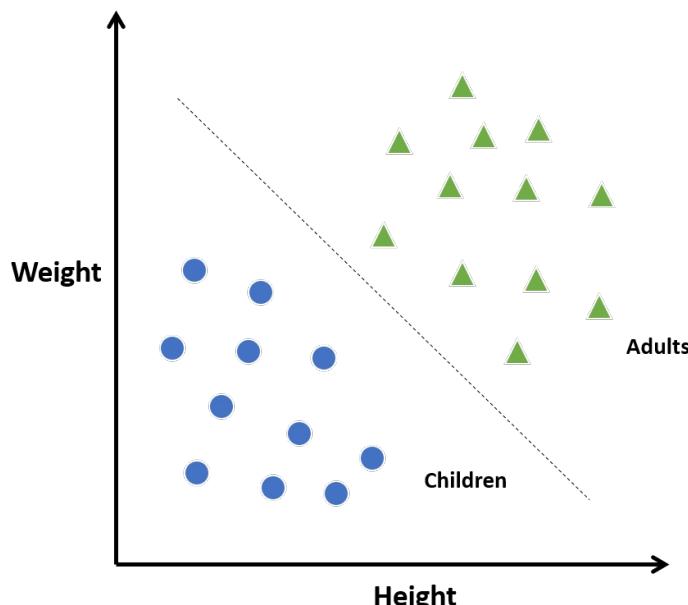
**Emily L. Hunt<sup>1,2</sup> & Sabine Reffert<sup>1</sup>**

1. LSW, Universität Heidelberg // 2. IMPRS-HD Fellow

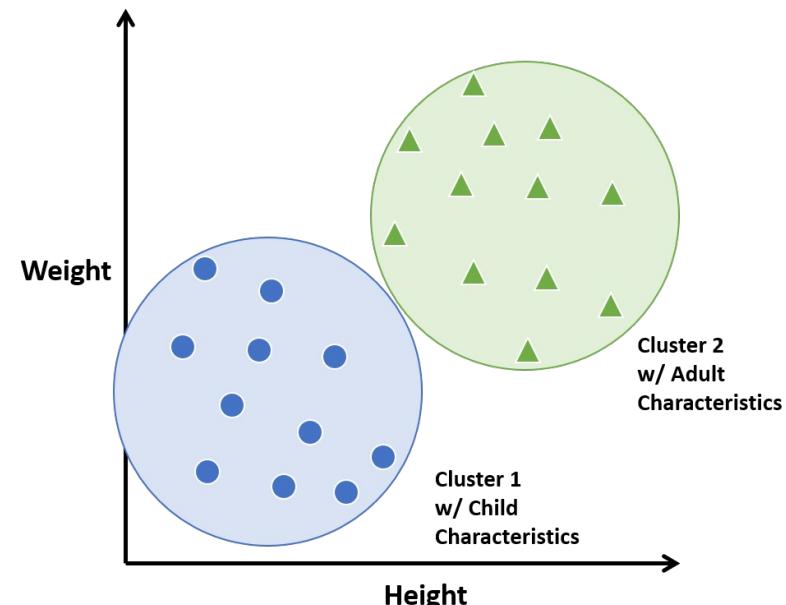
Background image: scikit-learn

# what is *unsupervised* ML?

**Classification** in supervised ML is about making a **decision boundary** between different regions



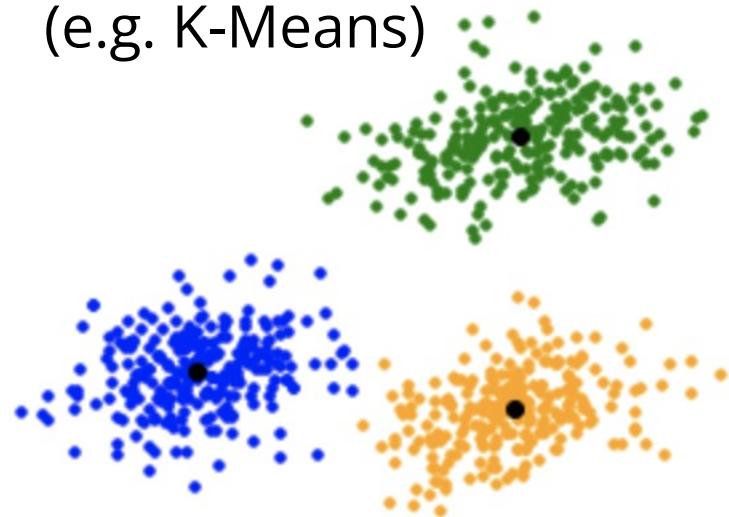
**Clustering algorithms** (a type of unsupervised ML) do this using **properties of the data itself**



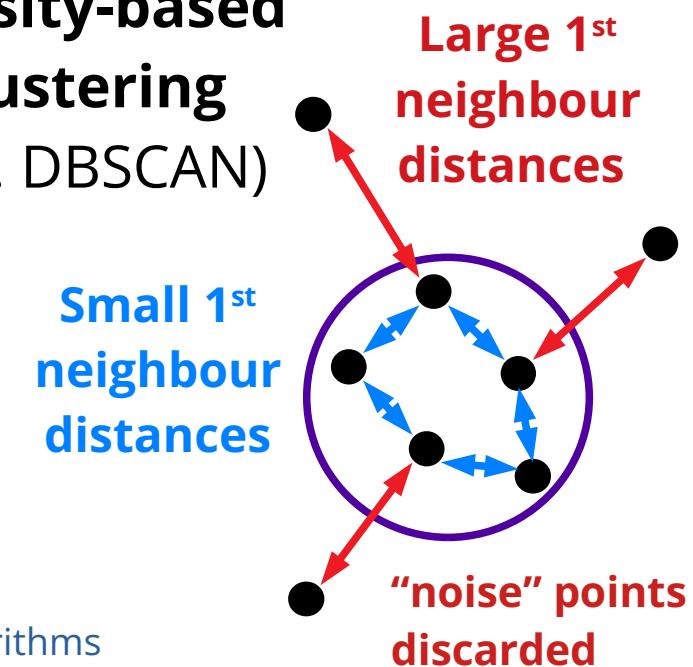
# the many, many algorithms...

There are many different types, each suited to different problems

## Partitioning (e.g. K-Means)



## Density-based clustering (e.g. DBSCAN)



Link: [Overview of various algorithms](#)

# play around with this in a notebook!

[github.com/emilyhunt/nam\\_2022\\_talk](https://github.com/emilyhunt/nam_2022_talk)  
(also includes these slides)

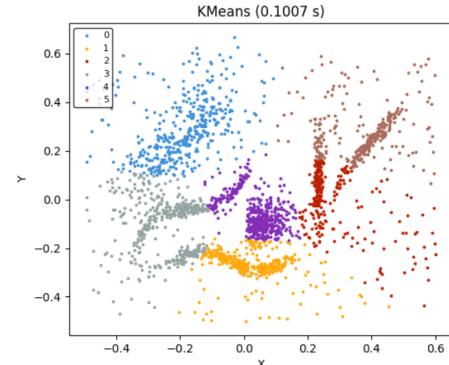
## 4. The clustering algorithms

Let's try various algorithms! Feel free to play around with the parameters.

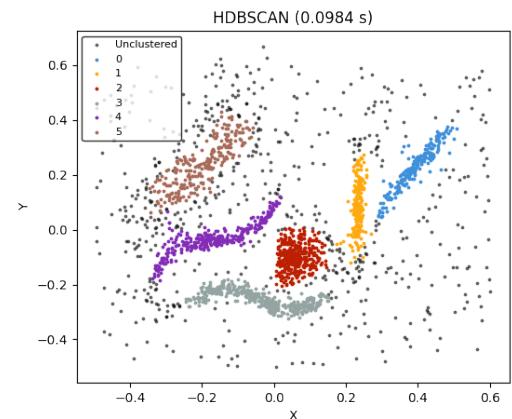
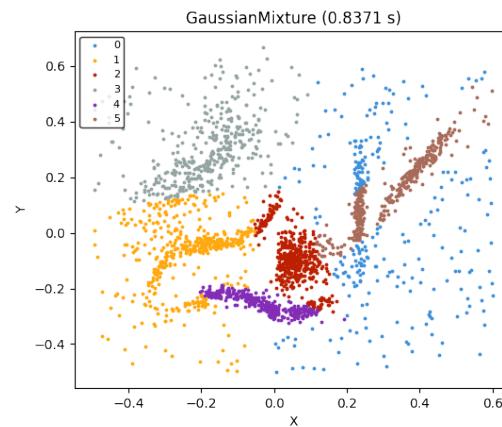
### 4.1. K-Means

The archetypal (and most simple) clustering algorithm...

```
[118]: run_clustering_algorithm(data, sklearn.cluster.KMeans, n_clusters=6, savename='KMeans')
Running clustering algorithm!
clustering took 0.1007 seconds
Plotting results!
```



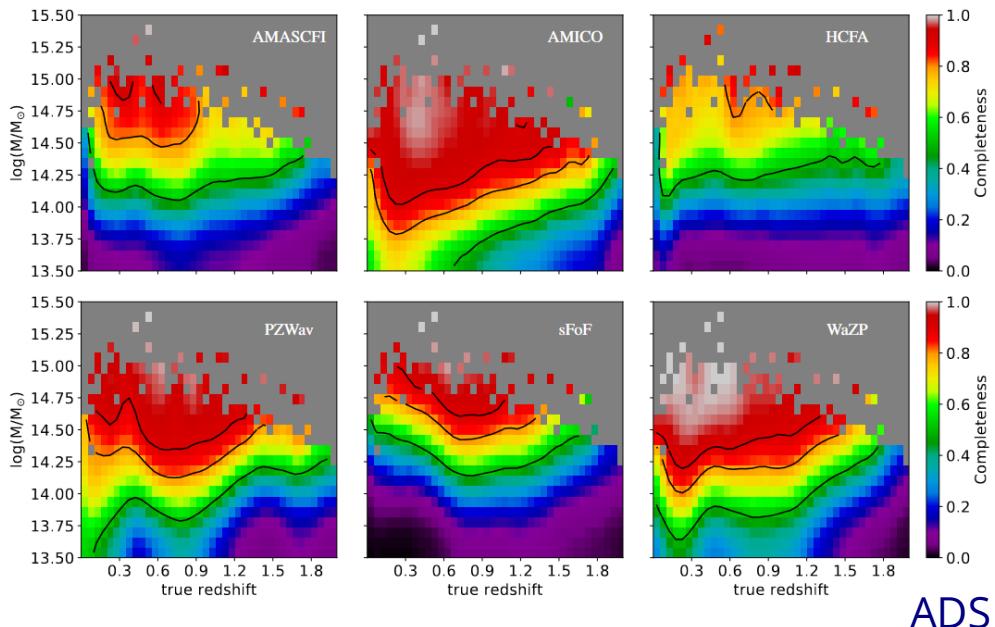
Basic algorithm; some things are roughly separated, but not so well.



# many astro problems come in clusters.

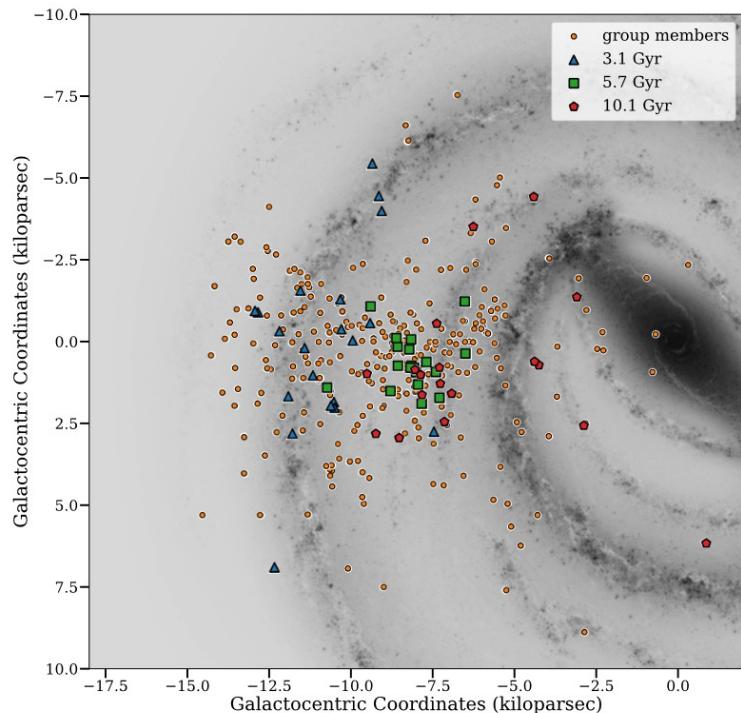
## *Euclid preparation III. Galaxy cluster detection in the wide photometric survey, performance and algorithm selection*

Euclid Collaboration, R. Adam<sup>1,2,3\*</sup>, M. Vannier<sup>2</sup>, S. Maurogordato<sup>2</sup>, A. Biviano<sup>4</sup>, C. Adami<sup>5</sup>, B. Ascaso<sup>6</sup>,



## Strong chemical tagging with APOGEE: 21 candidate star clusters that have dissolved across the Milky Way disc

Natalie Price-Jones<sup>1,2\*</sup>, Jo Bovy<sup>1,2</sup>, Jeremy J. Webb<sup>1</sup>, Carlos Allende Prieto<sup>3,4</sup>,



# our problem: open clusters of stars.

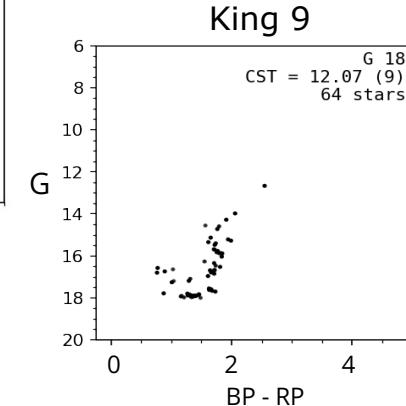
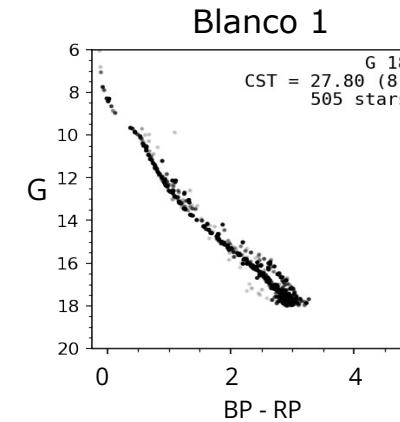
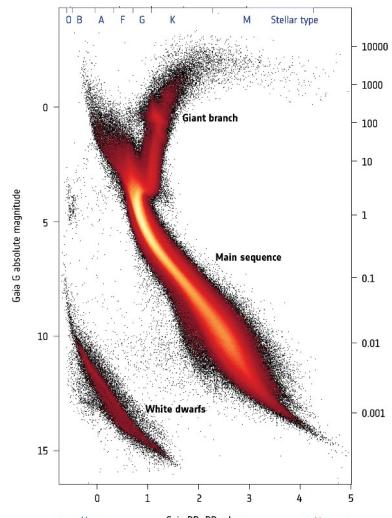
The Pleiades, age: ~100 Myr



Credit: ESO

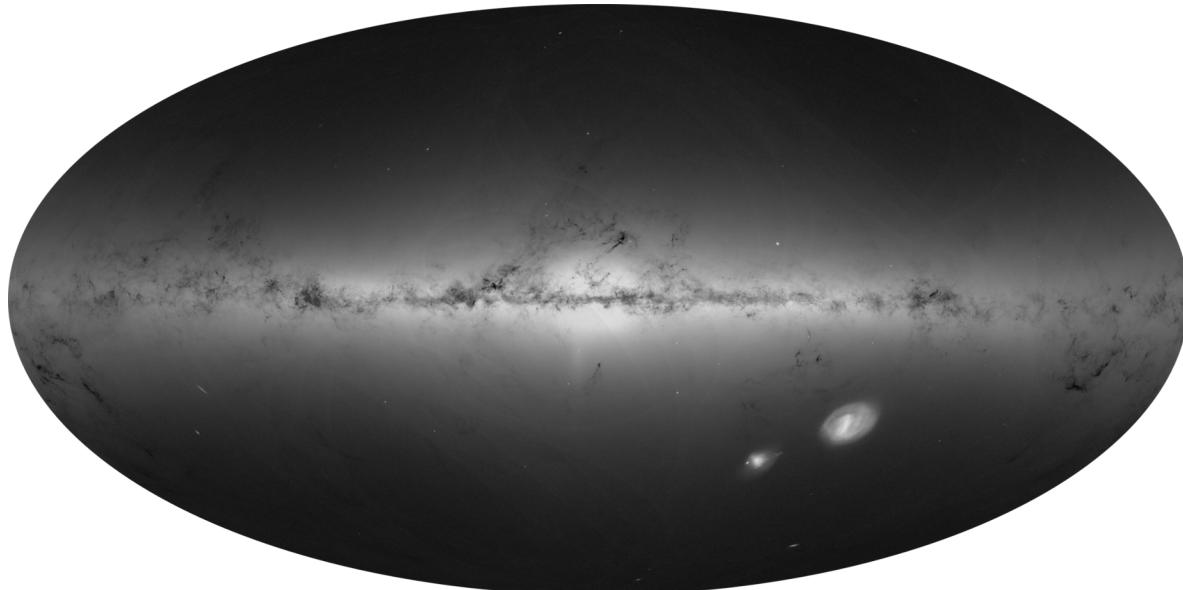
Open clusters are **homogenous** and **bound** groups of **coeval** stars

**Highly useful** to stellar & galactic science!



# Gaia data is a challenge.

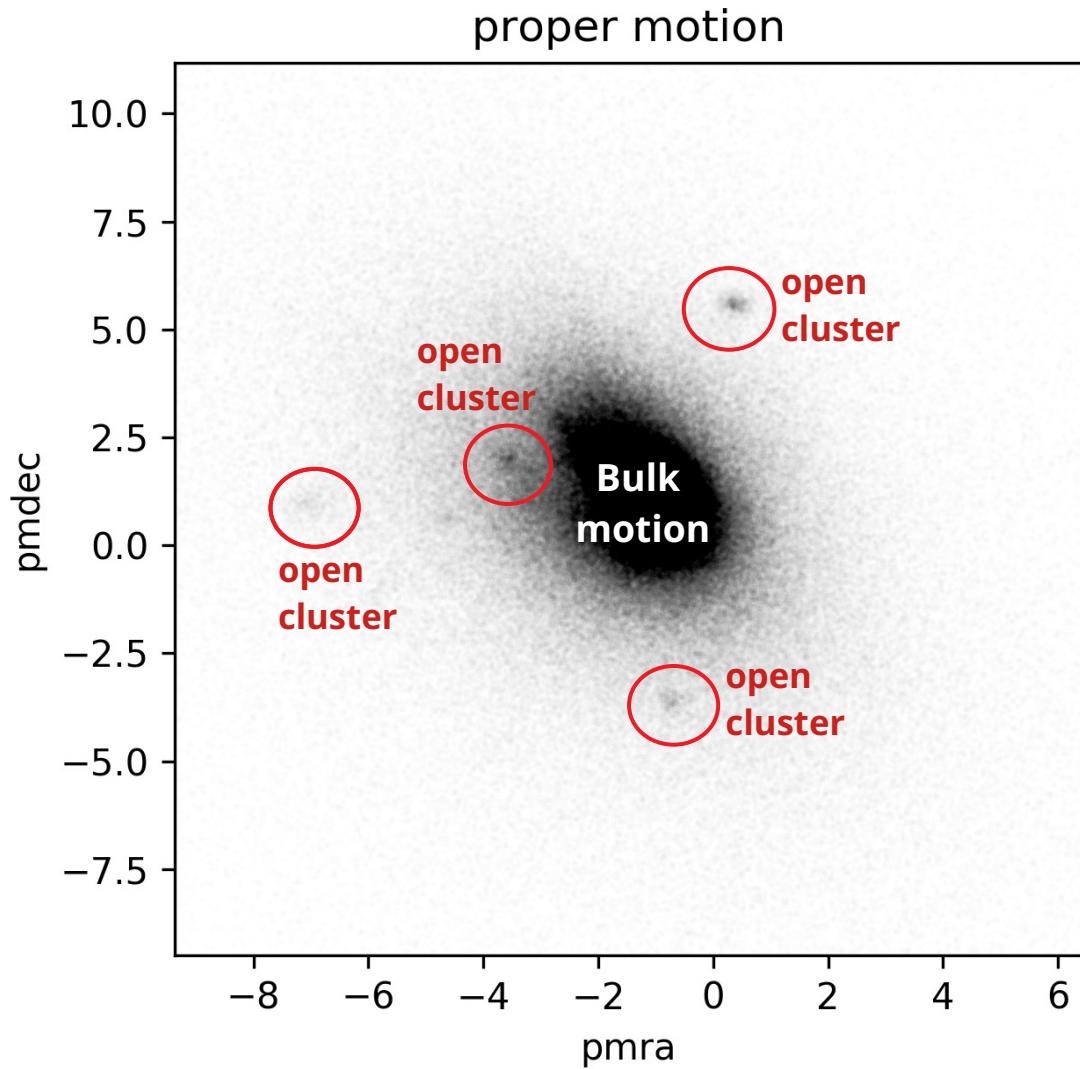
*Gaia* satellite has reliable astrometry for **~1 billion** stars  
=> **~0.1%** of which in **open clusters**



*Gaia* source density skymap. Credit: ESA

- Some challenges:*
- **So many sources...**
  - **~99.9%** of which must be discarded!
  - Open clusters vary from **~0.1°** to **~10°** in size

**but... Gaia is still  
perfect for open  
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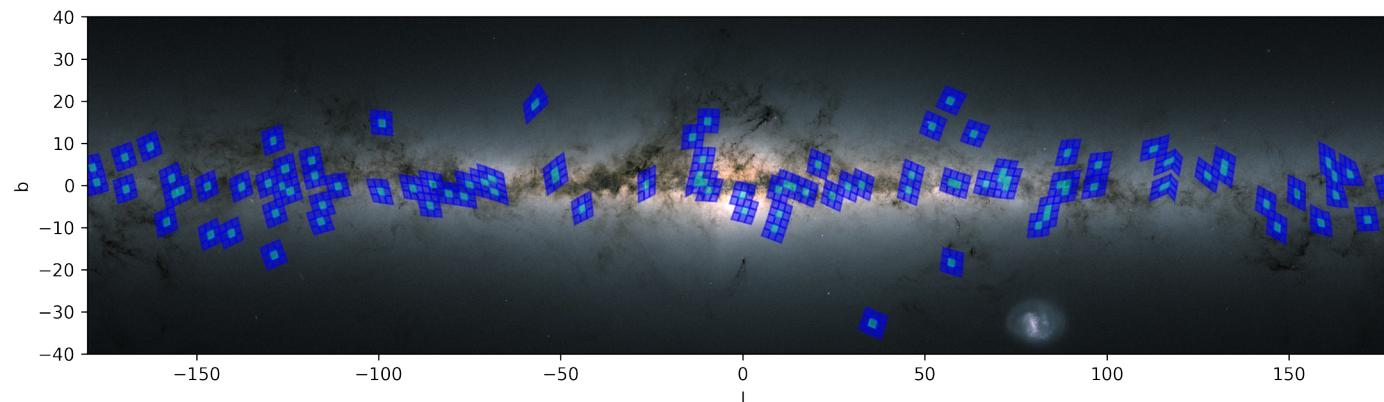


# testing different algorithms.

Hunt & Reffert (2021): search for literature clusters in randomly selected fields

After initial trials of what worked best...

- Algorithms given **rescaled** positions, proper motions and parallaxes (5 dimensions) + corrected for spherical distortions
- Paper used **DBSCAN**, **HDBSCAN** and **Gaussian mixture models**

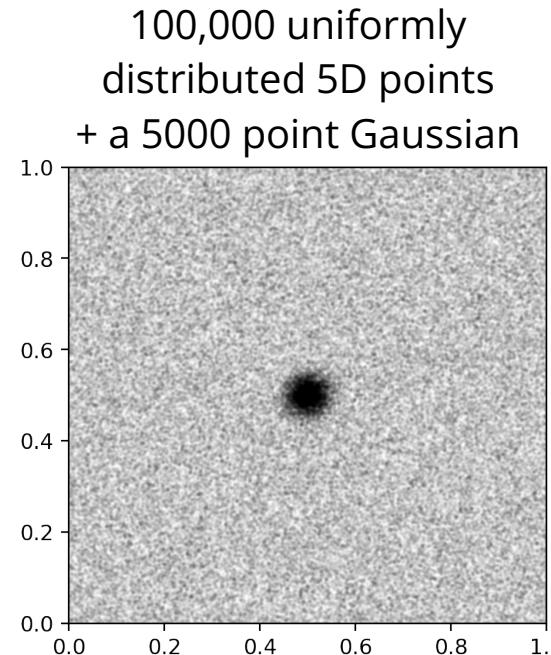


# which one is best?

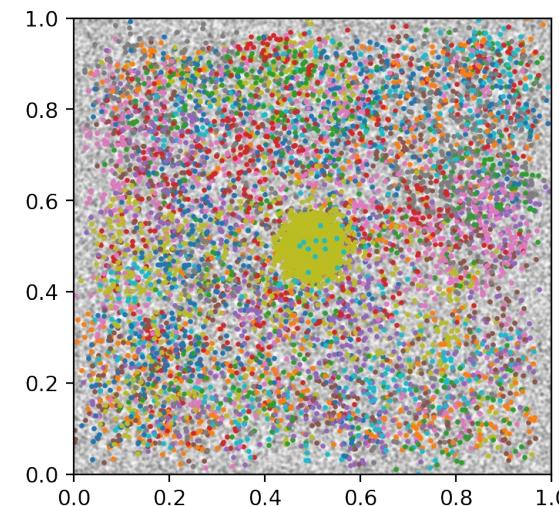
Algorithm	Speed	Sensitivity TP / (TP + FN)	Precision TP / (TP + FP)	
<b>DBSCAN</b> (Castro-Ginard+18 parameters)	Fast	0.53	1.00	← Main literature approach
<b>DBSCAN</b> (My parameters)	Fast	0.62	0.93	
<b>HDBSCAN</b>	Quite fast	0.82	0.82	← My favourite
<b>Gaussian Mixtures</b>	Slow	0.33	1.00	

# let's talk about false positives.

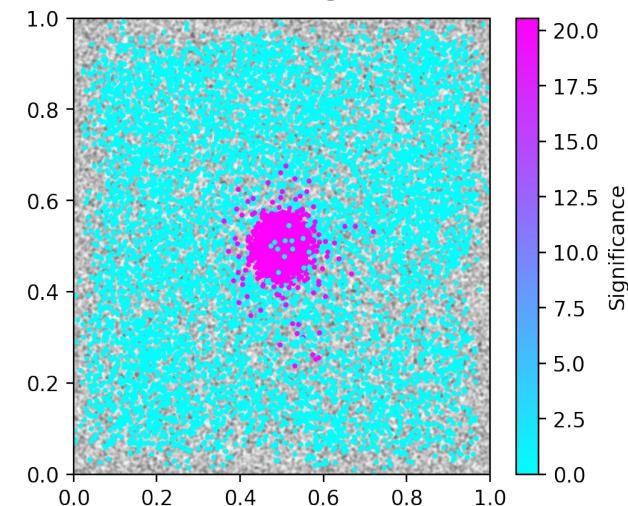
The **most sensitive** clustering methods can also produce **the most false positives**. Care **must** be taken when using "off-the-shelf" methods



**HDBSCAN**,  $m_{clSize} = 20$ ...  
151 clusters?!

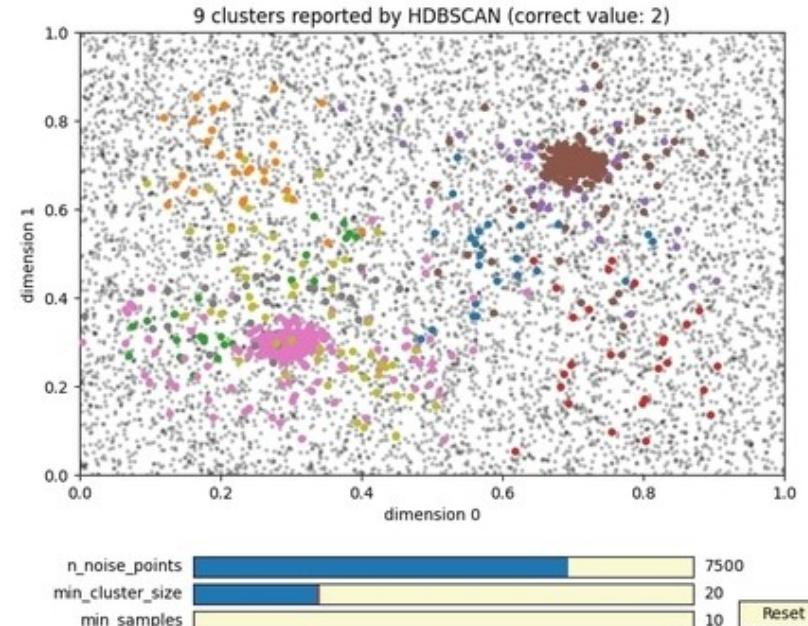
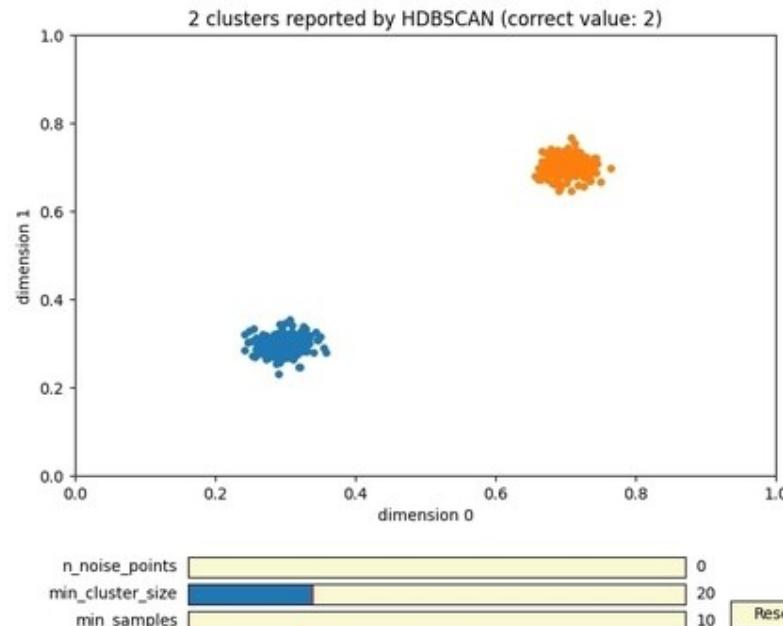


Density test → only the real cluster is significant



# a way to try this in real time!

I made a script that shows this in real time! ([GitHub link](#))

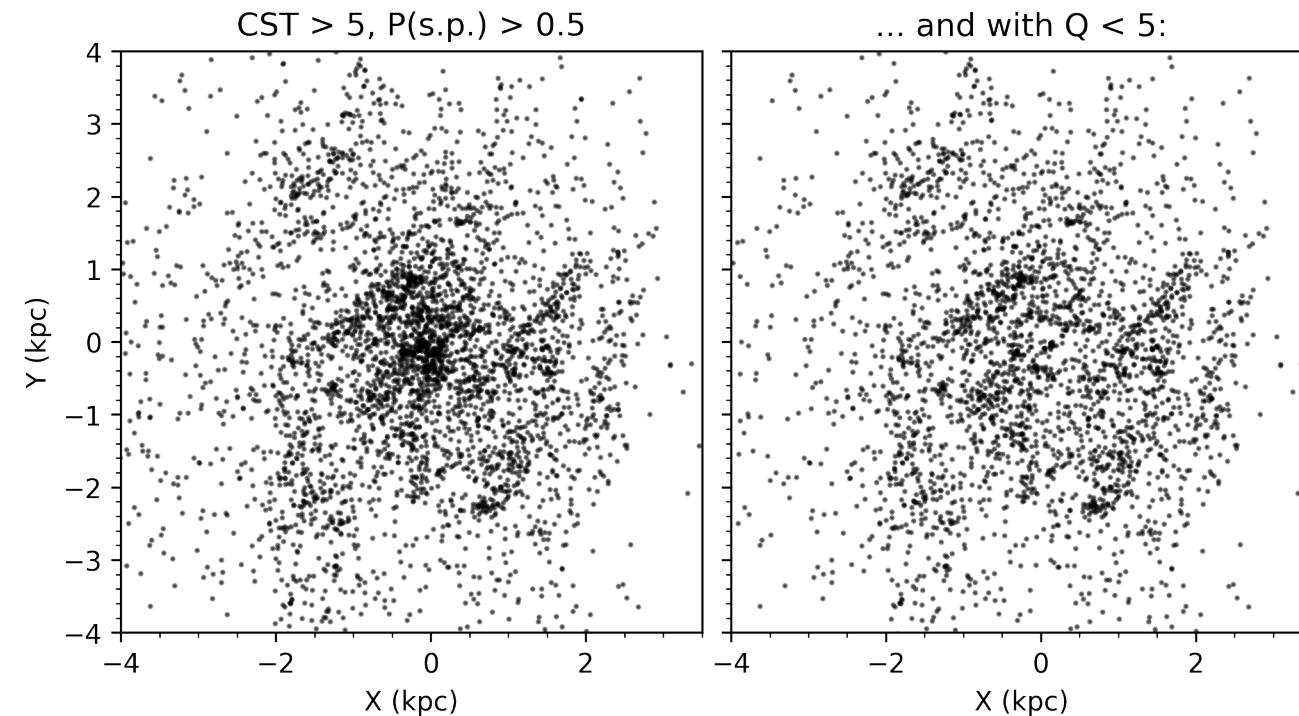


# clustering 729 million stars in Gaia EDR3.

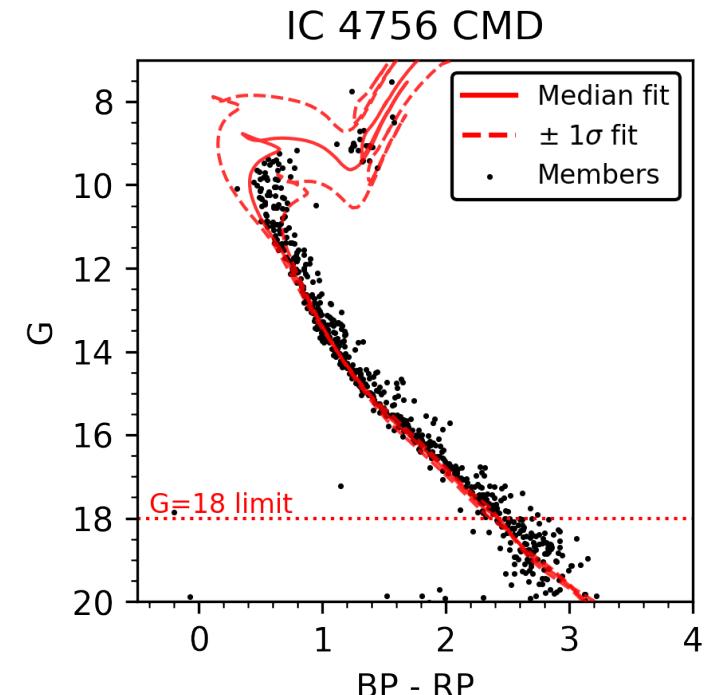
- Ran **HDBSCAN** on largest-ever sample of stars
- Used **HEALPix** tessellation scheme for regions
- About **8 days of wall time** on a powerful machine (actually not bad)

# after much work: results.

Distribution,  $|z| < 500$  pc:



Example CMD:



# and a cautionary tale on false positives...

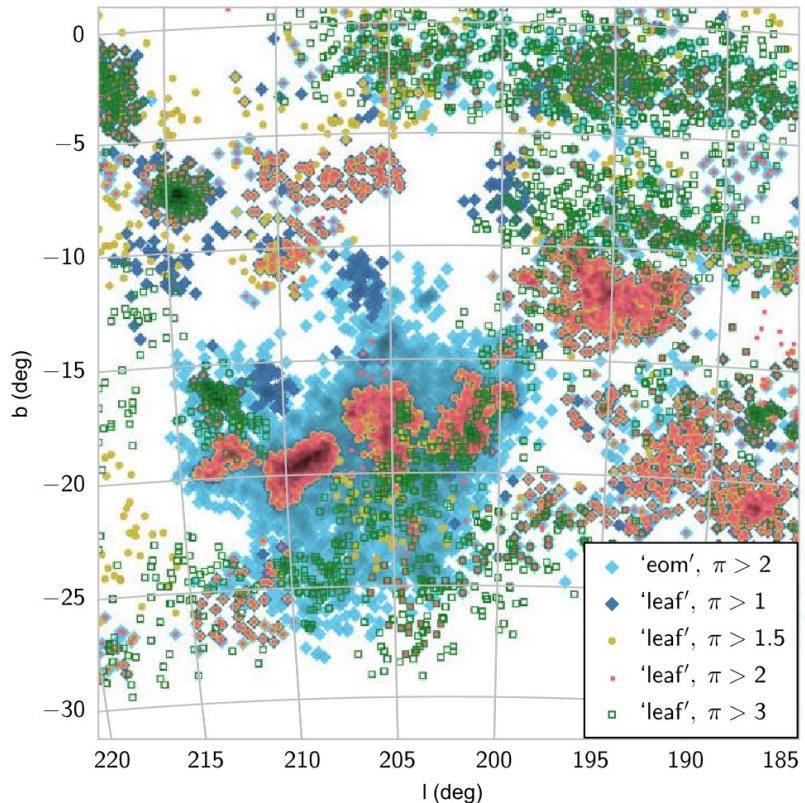
**Kounkel+19,20:** reported **thousands** of groups and ‘strings’ of stars using **HDBSCAN** on Gaia DR2 data (+ with no significance test)

In EDR3: we re-detect just **18.1%** of their groups

Also echoes **Zucker+22:**

*“many Kounkel+ group members inconsistent with having common origin”*

**Clustering algorithms can make unrepeatable results!**



# where next for clustering algorithms?

- Clustering algorithms are **fantastic** tools for astronomy
- Many off-the-shelf algorithms available (e.g. scikit-learn)
- BUT: they aren't designed for astronomy problems, and can run into weird issues

**In the future:** astro must collaborate with computer scientists, mathematicians etc. to develop algorithms

# datasets to come...

**Gaia DR5** (~2030): 2 billion stars

**Euclid** (late 2020s): ~1 billion galaxies with redshifts

**LSST** (final data ~2035): 17 billion stars, 20 billion galaxies

**GaiaNIR** (~2050): 12 billion stars

+ many, many other uses across astronomy for clustering algorithms



Check out the slides on GitHub:



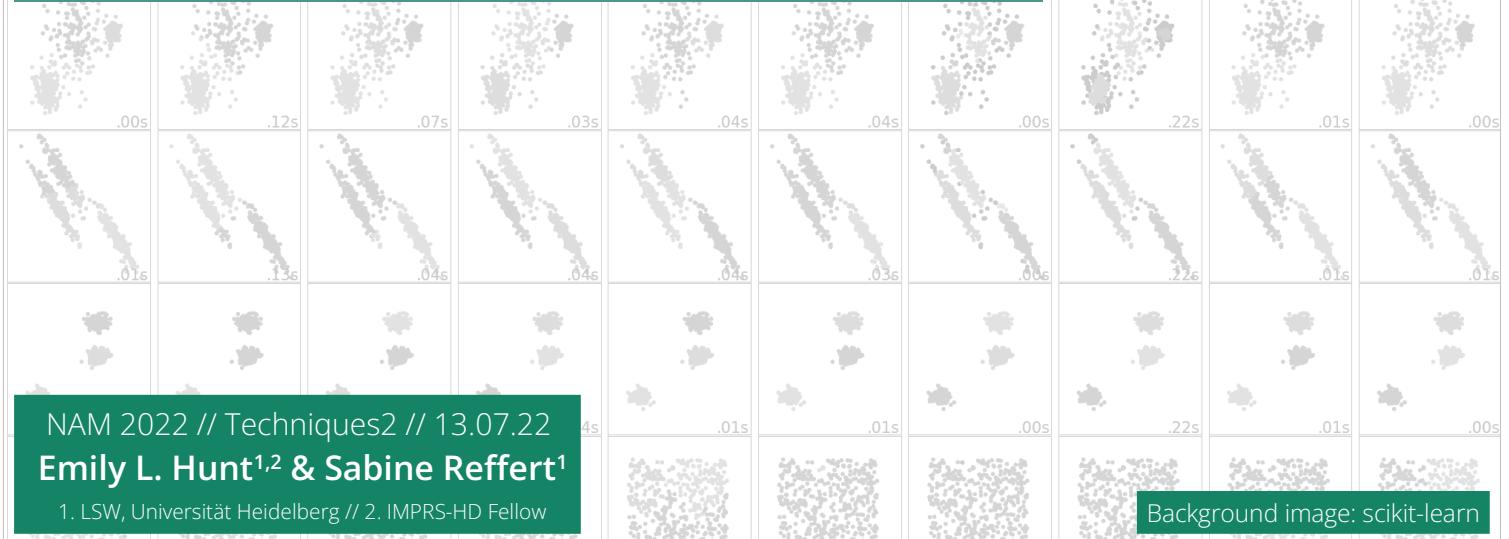
Direct link:  
[github.com/emilyhunt/nam\\_2022\\_talk](https://github.com/emilyhunt/nam_2022_talk)

## Key Takeaways:

- Clustering algorithms are great
- Many off-the-shelf solutions available
- BUT: be careful! They can be wrong (and not tell you)

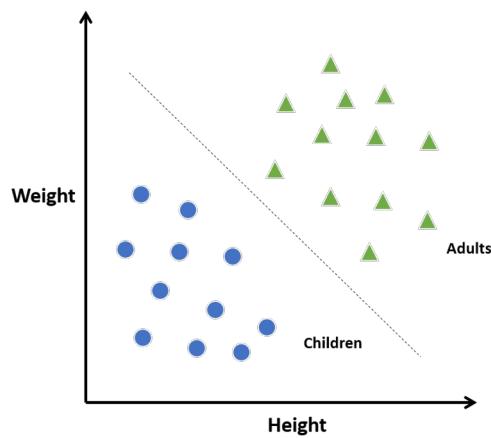
Background image: scikit-learn

# The power (and caveats) of clustering algorithms with examples from use on Gaia data

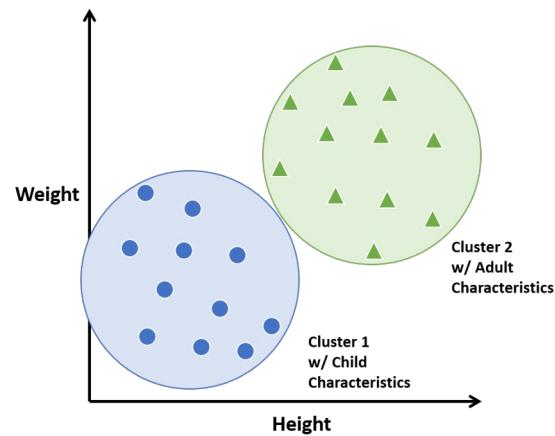


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Emily L. Hunt. *The power (and caveats) of clustering algorithms.*

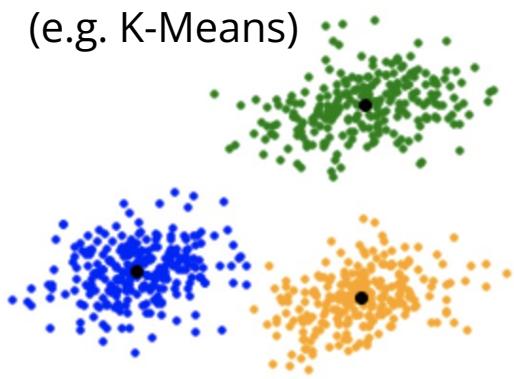
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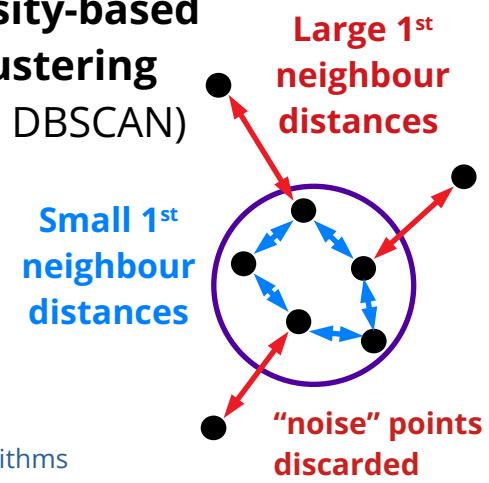
## Partitioning

(e.g. K-Means)



## Density-based clustering

(e.g. DBSCAN)



Link: [Overview of various algorithms](#)

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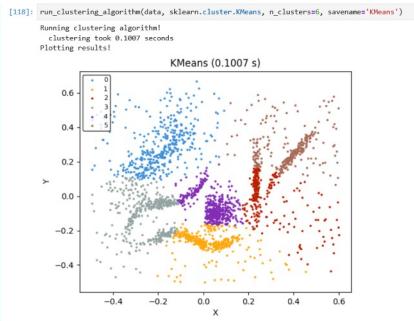
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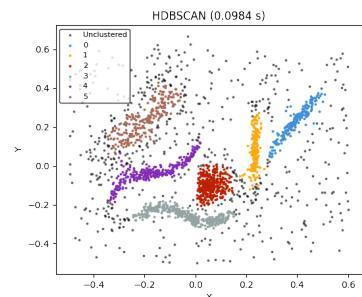
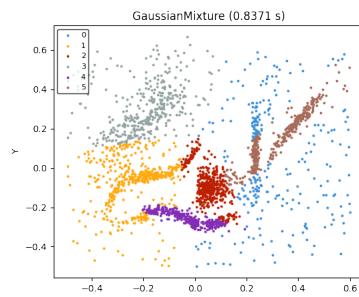
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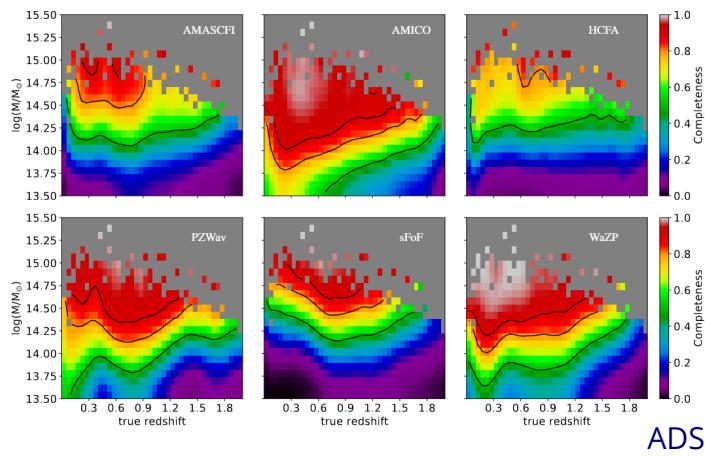
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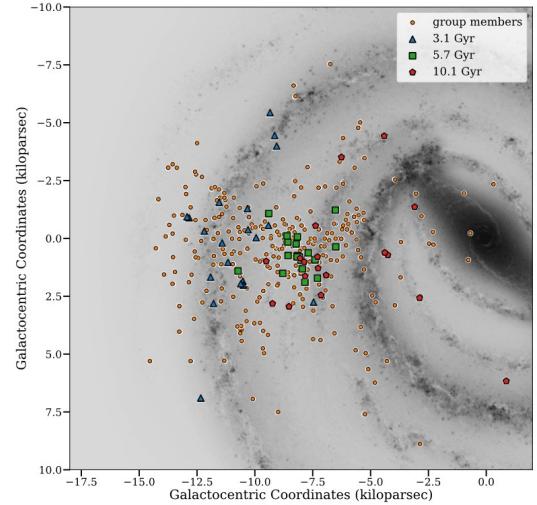
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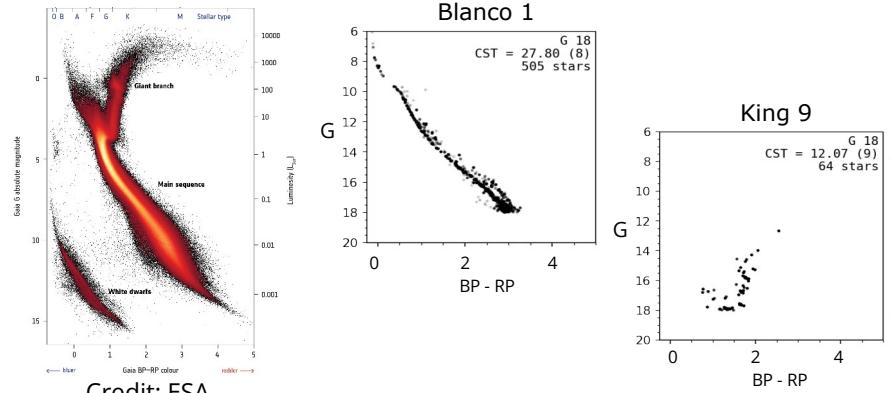
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**Highly useful** to stellar & galactic science!

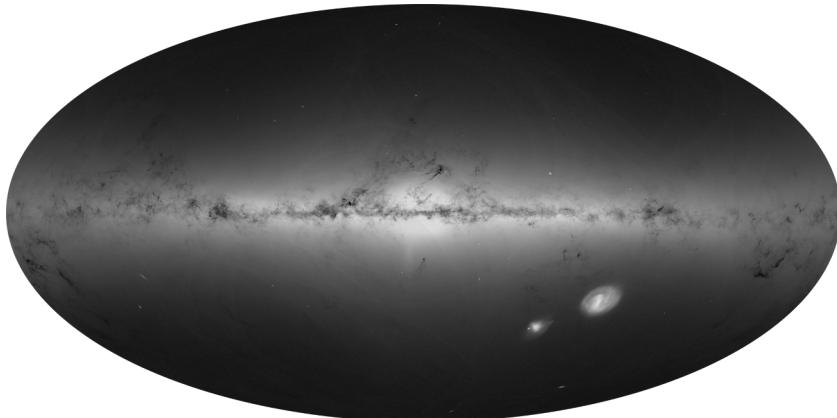


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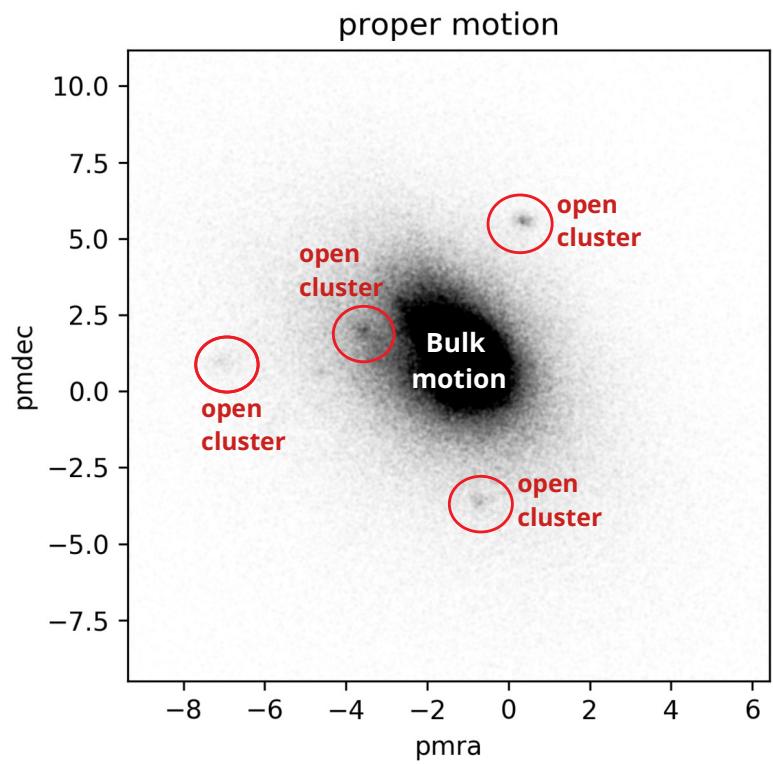
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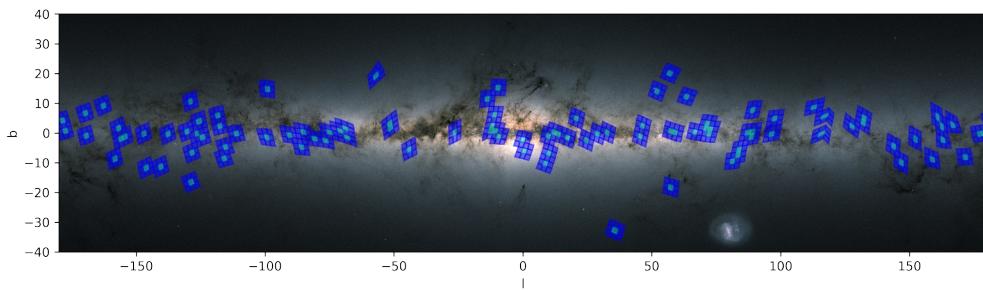
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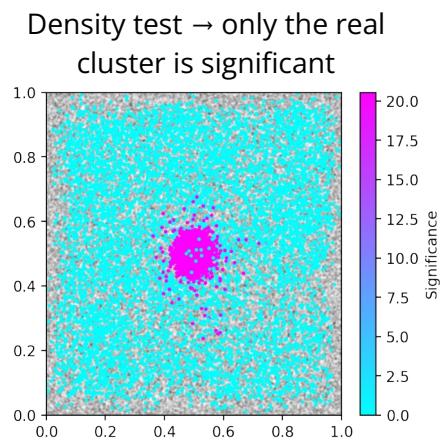
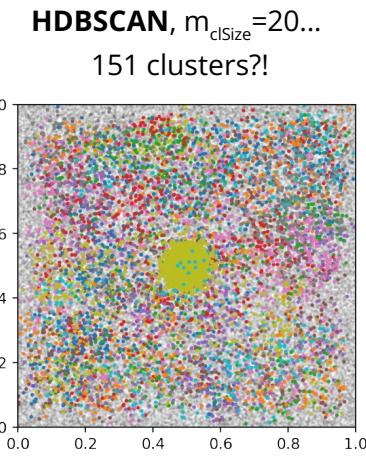
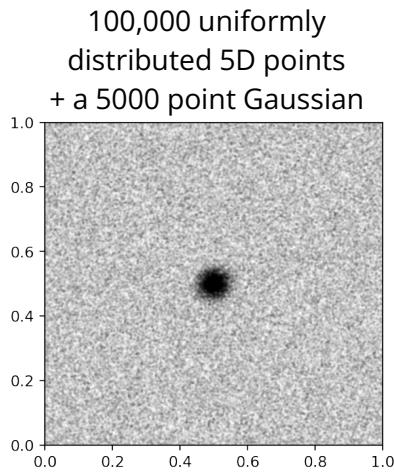
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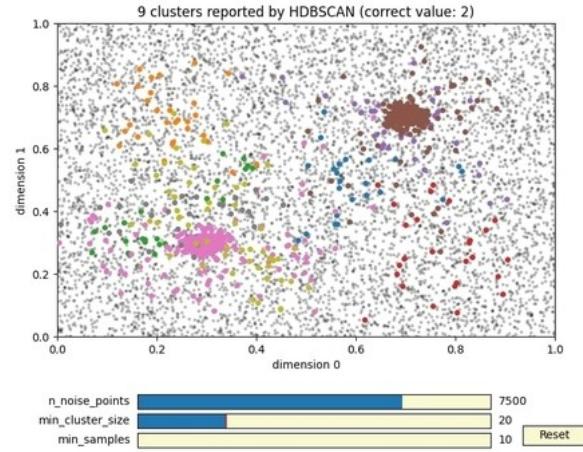
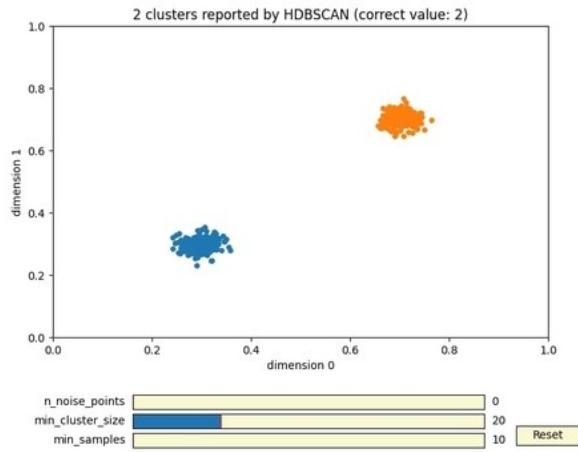


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# clustering 729 million stars in Gaia EDR3.

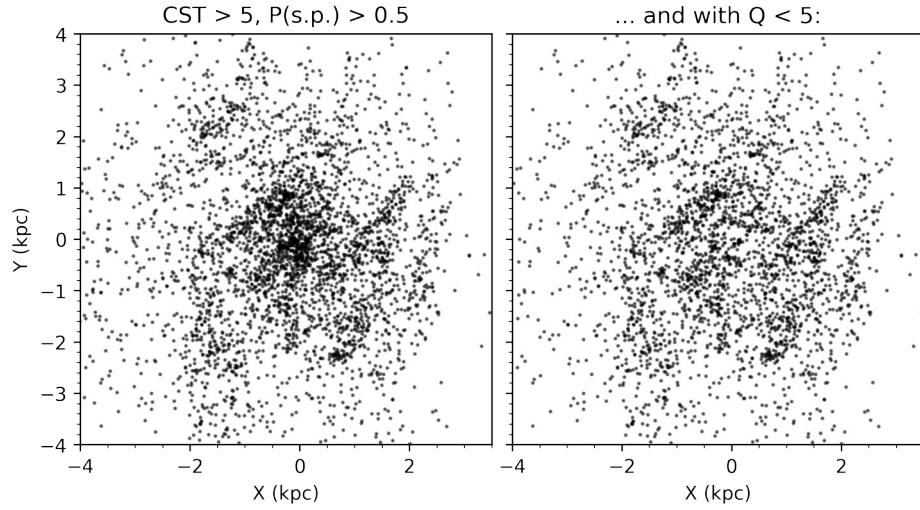
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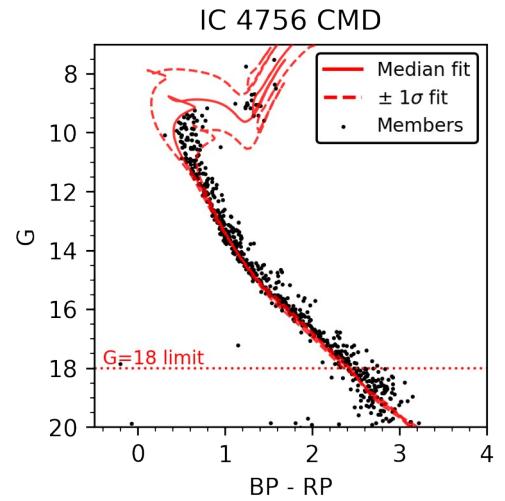
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Example CMD:



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# and a cautionary tale on false positives...

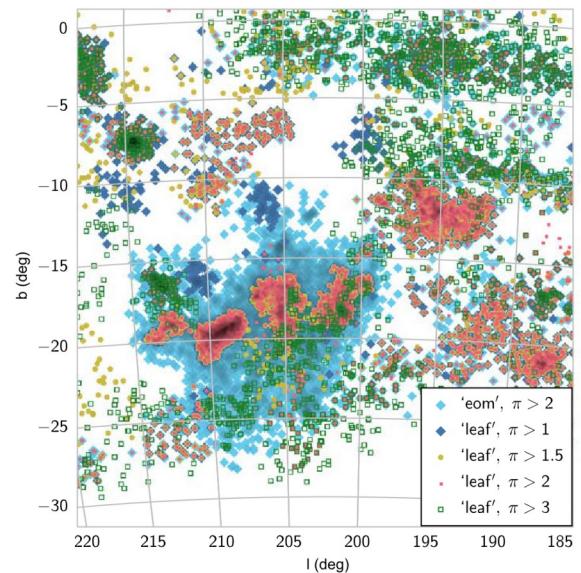
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emilydoesastro.com  
@emilydoesastro



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Background image: scikit-learn