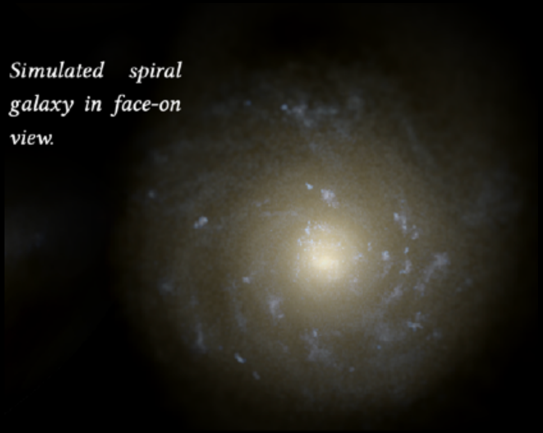
ASTR4004

COMPUTATIONAL ASTRONOMY

Week 8 https://github.com/svenbuder/astr4004_2024_week9

Spiral galaxy M74 in face-on view. ***Figure credit:*** *Gemini Observatory, GMOS Team*



Simulated spiral galaxy in face-on view.

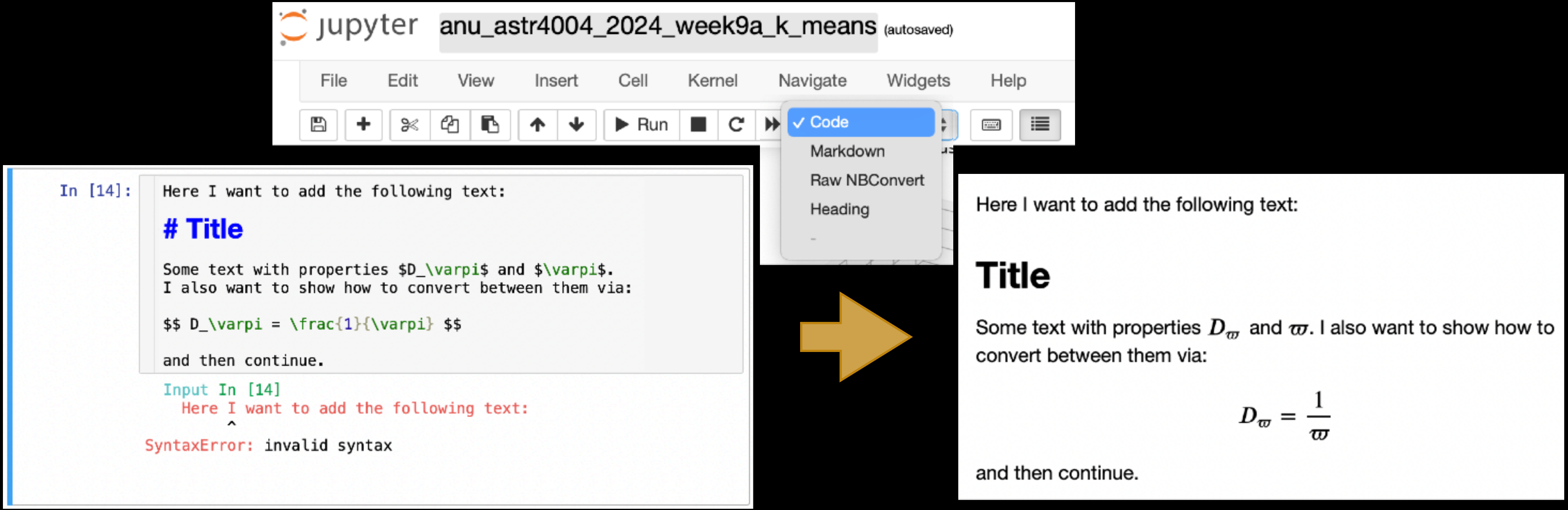
Figure credit: *Tobias Buck*

Australian National University

Adding description in Jupyter notebooks (.ipynb)

Markdown (.md) is an often used hybrid format between text, latex, and html.

It comes in very handy for adding text between code, e.g. for "discussion" tasks of an assignment.



```
In [14]: Here I want to add the following text:

         # Title

         Some text with properties $D_\varpi$ and $\varpi$.
         I also want to show how to convert between them via:

         $$ D_\varpi = \frac{1}{\varpi} $$

         and then continue.

  Input In [14]
    Here I want to add the following text:
         ^
SyntaxError: invalid syntax
```

Here I want to add the following text:

Title

Some text with properties D_ϖ and ϖ. I also want to show how to convert between them via:

$$D_\varpi = \frac{1}{\varpi}$$

and then continue.

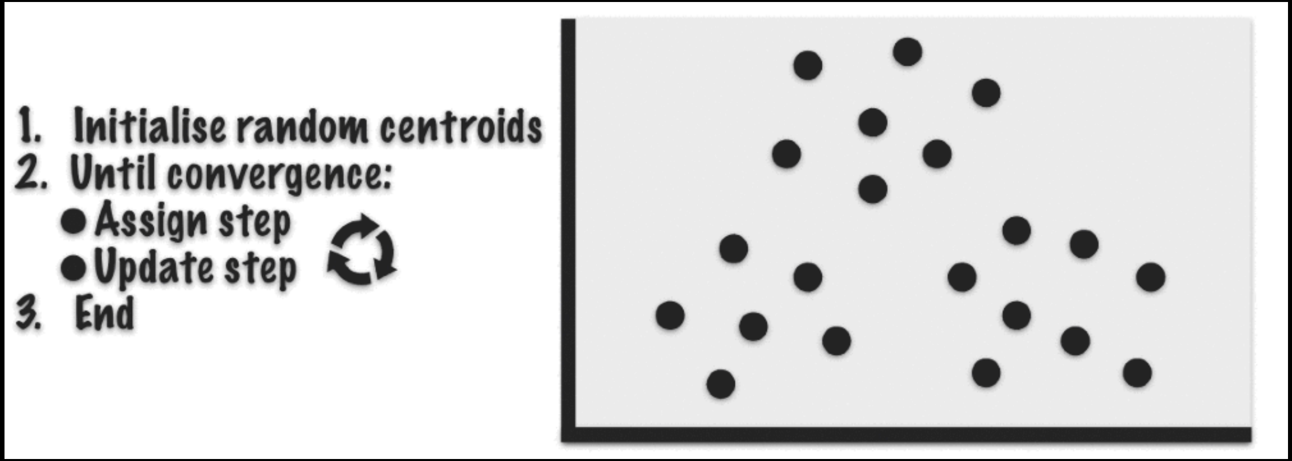
Most GitHub repository and code documentation (e.g. README.md) is written in markdown.

My idea for our 3 weeks:

Assignment 3
due in Week 10a
(October 8)

Week	Summary	What I actually plan to talk about
7	Data Processing	git, csv/FITS Files, ADQL/SQL, joining & cleaning catalogues, ...
	Statistics	Fantastic Uncertainties and how to calculate/report them, ...
	Plot Clinic	How to plot well & better - with my (and hopefully your) examples, ...
8	Regression	how to fit y = f(x), if y (and even x) have uncertainties, python fitting packages and when to apply them how to which function, ...
	Dimensionality Reduction	Principal Component Analysis (PCA), tSNE, ...
9	Clustering	k-means, HDBSCAN, Gaussian Mixture Models (GMM), ...
	Model Selection	AIC & BIC, train/test sets, ...
	Interdisciplinary Thinking	How to think abstract or creative and bridge barriers/gaps: How your expertise can help other researchers/industry, ...

CLUSTERING:

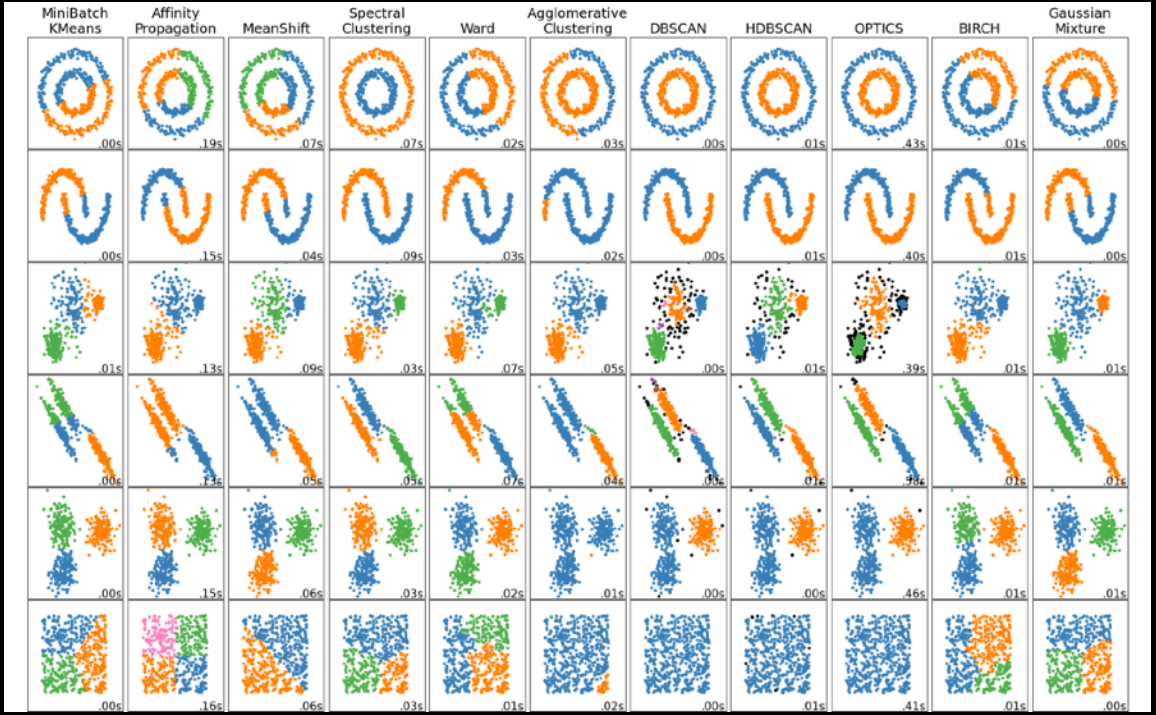


```
1. Initialise random centroids
2. Until convergence:
    ● Assign step
    ● Update step
3. End
```

© Alan Jeffares

Clustering

You can imagine a lot of examples of easy or difficult clustering problems



Overview from https://scikit-learn.org/stable/modules/clustering.html

Clustering Checklist

- Why am I clustering these data? What do I want to learn or infer from the data?

- Since the clustering algorithm I choose is almost guaranteed not to be representative of the generative model that produced the data, what artefacts in the clustering outputs do I need to be worried about?

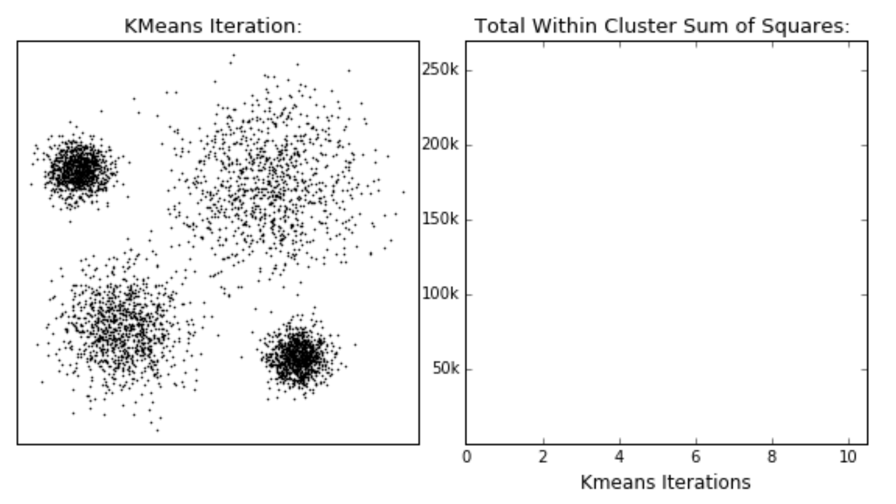
- How much can I believe the clustering results? What things can I cross-check to make sure they look sensible?

- Even though you may disbelieve the clustering results, are they **sufficient for my purpose**? That is to say: even if the model is wrong, does it still have utility?

K-means

clusters data by trying to separate samples in n groups of equal variance, minimizing a criterion known as the *inertia (within-cluster sum-of-squares):*

$$\sum_{i=0}^{n} \min_{\mu_j \in C}(||x_i - \mu_j||^2)$$



Initialise cluster centres $\boldsymbol{\mu}_j$

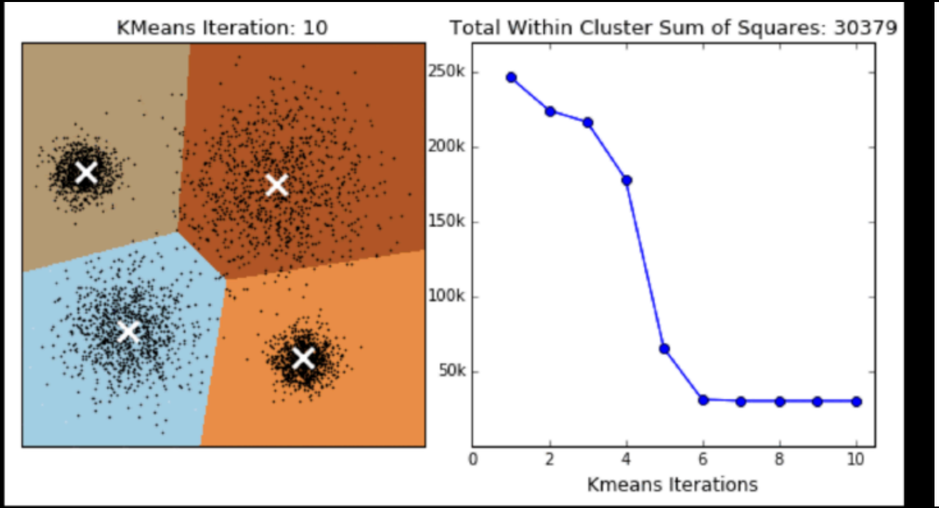
Iteratively reassign data points x_i to the closest centroid

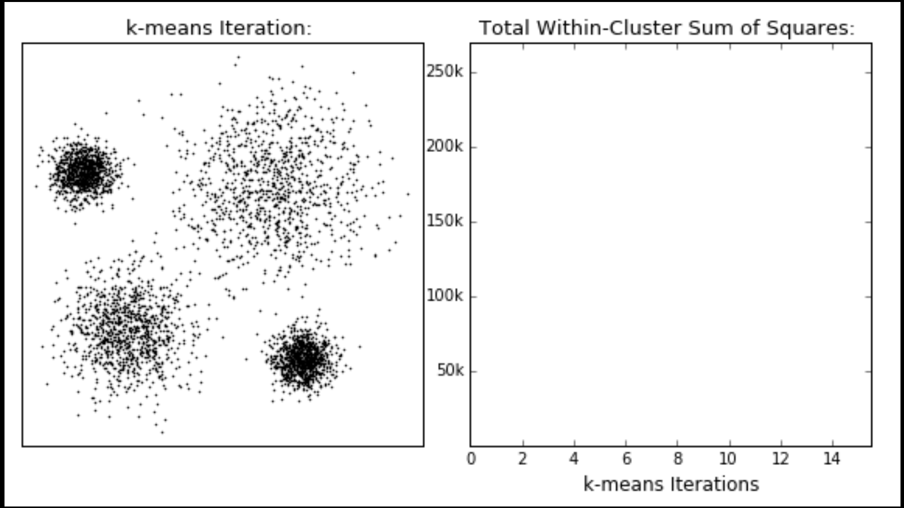
Move the centroids to the centre of their assigned points

Iterate towards more compact & separated clusters until little to no improvement

K-means

k-means algorithms are sensitive to the starting position of the cluster centres, as each method converges to local optima





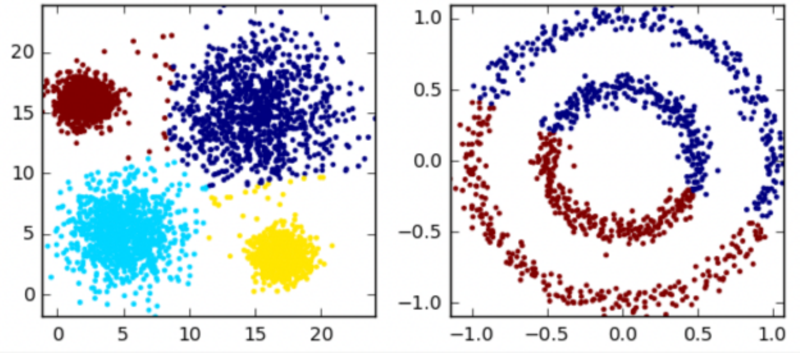
sklearn allows you to initialise "smarter" than random (init='k-means++') and multiple times (**n_init)

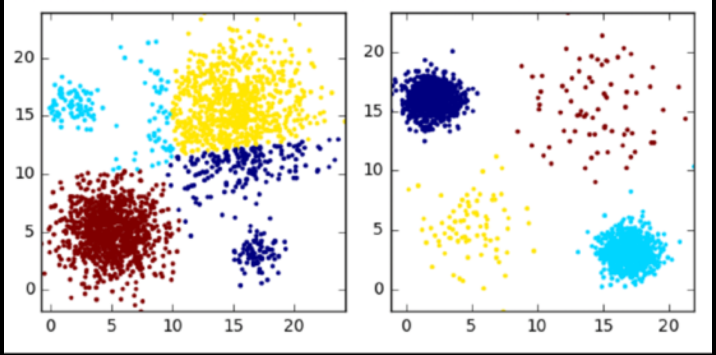
© David Sheehan

K-means

The algorithm seeks and identifies globular (essentially spherical) clusters.

If this assumption doesn't hold,
the model output may be inadequate (or just really bad).





k-means can also underperform with clusters of different size and density.

But: k-means is one of the least complex and thus fastest algorithms!

GAUSSIAN MIXTURE MODELS

Australian National University

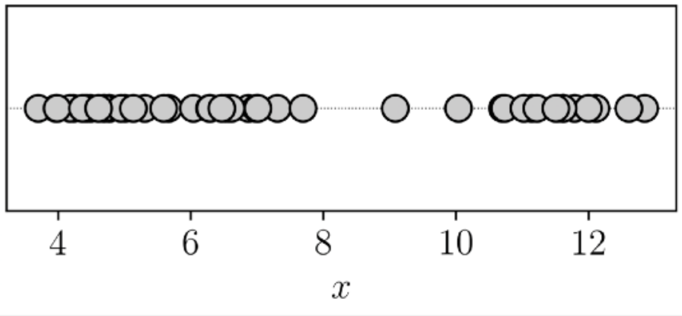
Gaussian Mixture Models

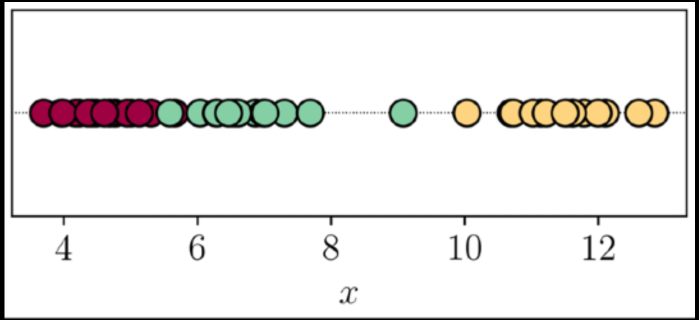
Let's consider the possibility that some data x is described by K components with model parameters Z_k:

$$p(x) = \sum_{k=1}^{K} \pi_k p(x|Z_k)$$

with weight values π_k

$$\sum_{k=1}^{K} \pi_k = 1$$





Simple case:

$Z_k = (\mu_k, \sigma_k)$

$$\mu_1 = \frac{1}{N_{\text{red}}} \sum_{i=1}^{N_{\text{red}}} x_i$$

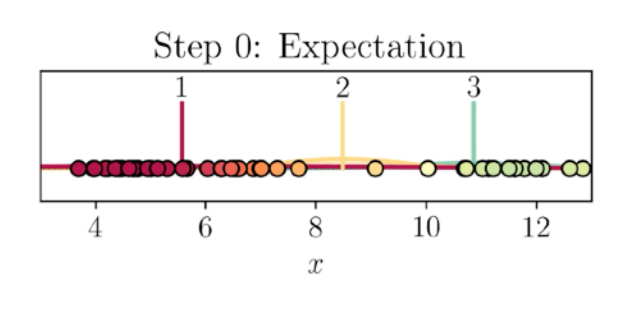
$$\sigma_1^2 = \frac{1}{N_{\text{red}}} \sum_{i=1}^{N_{\text{red}}} (x_i - \mu_1)^2$$

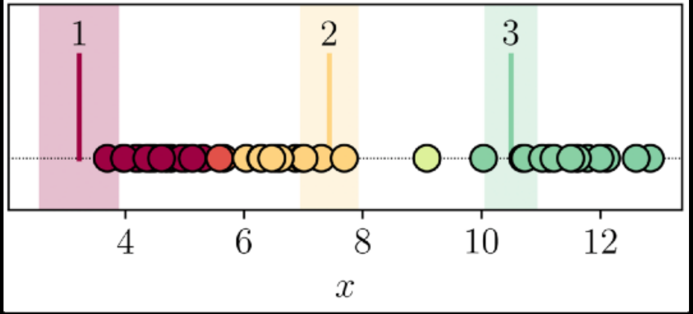
$$\pi_1 = \frac{N_{\text{red}}}{N}$$

Gaussian Mixture Models

$$p(\mathcal{M}_k|x_i) = \frac{p(x_i|\mathcal{M}_k)p(\mathcal{M}_k)}{\sum_{j=1}^{K} p(x_i|\mathcal{M}_j)p(\mathcal{M}_j)}$$

posterior probability of membership for belonging to one component, compared to all components





data points in between two components have a membership proportion that is split between the two components

Expectation Maximization (EM):
Alternate steps between expectation which component data point comes from and update of model parameter estimate

Gaussian Mixture Models (GMM)

GMM for N data points each of D dimensions, drawn from K Gaussian components

$$p(y|\theta) = \sum_{k=1}^{K} w_k p_k(y|z_k, \theta_k)$$

where $\sum^K w_k = 1$ and $\theta_k = \{\mu_k, \Sigma_k\}$

Iterative Expectation-Maximization (EM)

E-step (Expectation): Estimate which Gaussian each data point most likely belongs to.

$$w_{nk} = p(z_{nk} = 1|y_n, \theta) = \frac{w_k p_k(y_n|z_k, \theta_k)}{\sum_{m=1}^{K} w_m p_m(y_n|z_m, \theta_m)}$$

$$p_k(\mathbf{y}|\theta_k) = \frac{1}{(2\pi)^{D/2}|\Sigma_k|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{y} - \mu_k)^\top \mathbf{\Sigma}_k^{-1} (\mathbf{y} - \mu_k)\right]$$

M-step (Maximization): Update the parameters (means, variances, and mixing coefficients) based on the estimated membership from the E-step.

Effective number of data points described by the k-th mixture: $N_k = \sum^{N} w_{nk}$ and $\sum^K w_{nk} = 1$ for every data point

New weights

New means

New covs.

$$w_k^{(\text{new})} = \frac{N_k}{N}$$

$$\mu_k^{(\text{new})} = \frac{1}{N_k} \sum_{n=1}^{N} w_{nk} \mathbf{y}_n$$

$$\mathbf{\Sigma}_k^{(\text{new})} = \frac{1}{N_k} \sum_{n=1}^{N} w_{nk} \left(\mathbf{y}_n - \mu_k^{(\text{new})}\right)\left(\mathbf{y}_n - \mu_k^{(\text{new})}\right)^\top$$

K-MEANS AND GAUSSIAN MIXTURE MODELS

IN PRACTICE

Australian
National
University

DENSITY-BASED SPATIAL CLUSTERING OF APPLICATIONS WITH NOISE (DBSCAN)

Australian
National
University

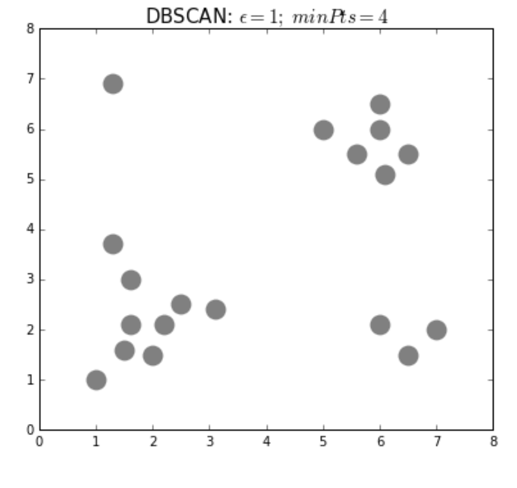
DENSITY-BASED SPATIAL CLUSTERING OF APPLICATIONS WITH NOISE (DBSCAN)

Clusters are considered zones that are sufficiently dense

Points that lack neighbours do not belong to any cluster and are thus classified as noise

Doesn’t require the user to specify the number of clusters; it works that out for you

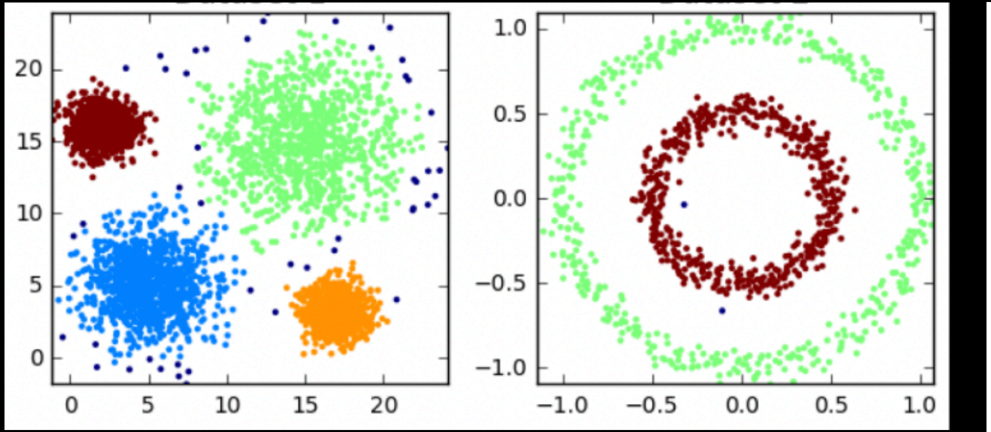
Needs minimum of points that constitutes a cluster (minPts) and the size of the neighbourhoods (epsilon)

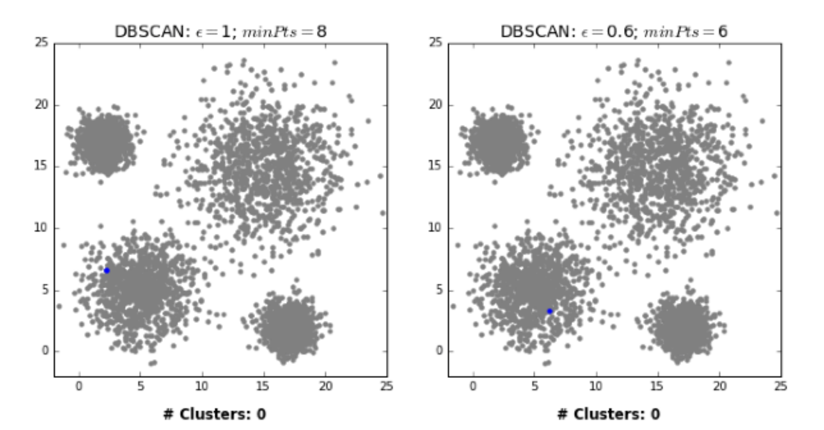


Identifies clusters and then expands clusters by scanning the neighbourhoods

Once all neighbourhoods have been exhausted, the process repeats with a new cluster, until all observations belong to a segment or have been classified as noise

DENSITY-BASED SPATIAL CLUSTERING OF APPLICATIONS WITH NOISE (DBSCAN)





Hierarchical DBSCAN (HDBSCAN), for example, is building a hierarchy of clusters and then condensing it into the most stable ones.

It is continuously varying the density parameter epsilon to detect clusters at multiple density levels (dense points of small clusters -> less dense and larger clusters)

There are millions of other clustering algorithms!

© David Sheehan

PLOT CLINIC

Australian
National
University

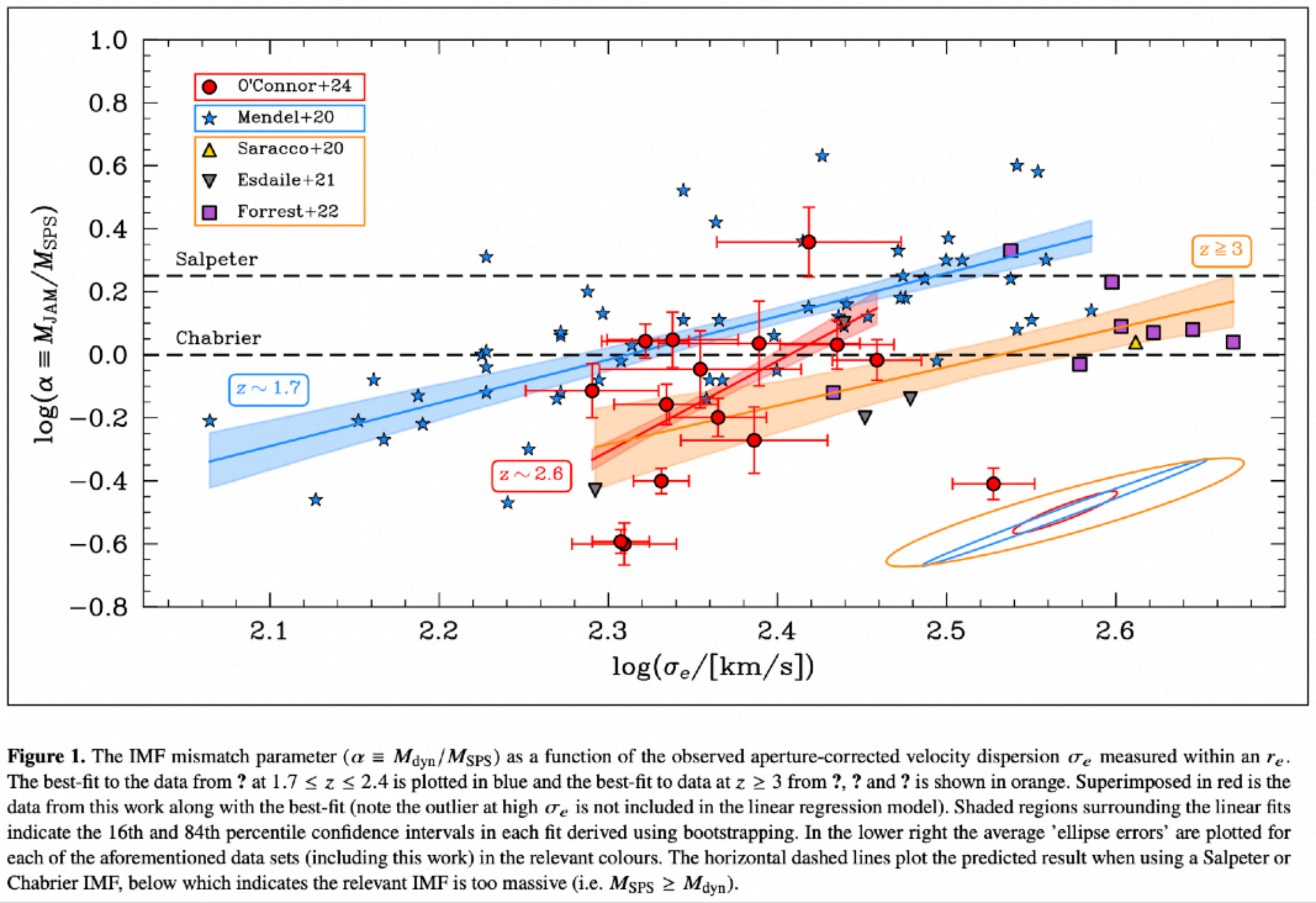


Figure 1. The IMF mismatch parameter ($\alpha \equiv M_{\rm dyn}/M_{\rm SPS}$) as a function of the observed aperture-corrected velocity dispersion σ_e measured within an r_e. The best-fit to the data from **?** at $1.7 \leq z \leq 2.4$ is plotted in blue and the best-fit to data at $z \geq 3$ from **?**, **?** and **?** is shown in orange. Superimposed in red is the data from this work along with the best-fit (note the outlier at high σ_e is not included in the linear regression model). Shaded regions surrounding the linear fits indicate the 16th and 84th percentile confidence intervals in each fit derived using bootstrapping. In the lower right the average 'ellipse errors' are plotted for each of the aforementioned data sets (including this work) in the relevant colours. The horizontal dashed lines plot the predicted result when using a Salpeter or Chabrier IMF, below which indicates the relevant IMF is too massive (i.e. $M_{\rm SPS} \geq M_{\rm dyn}$).

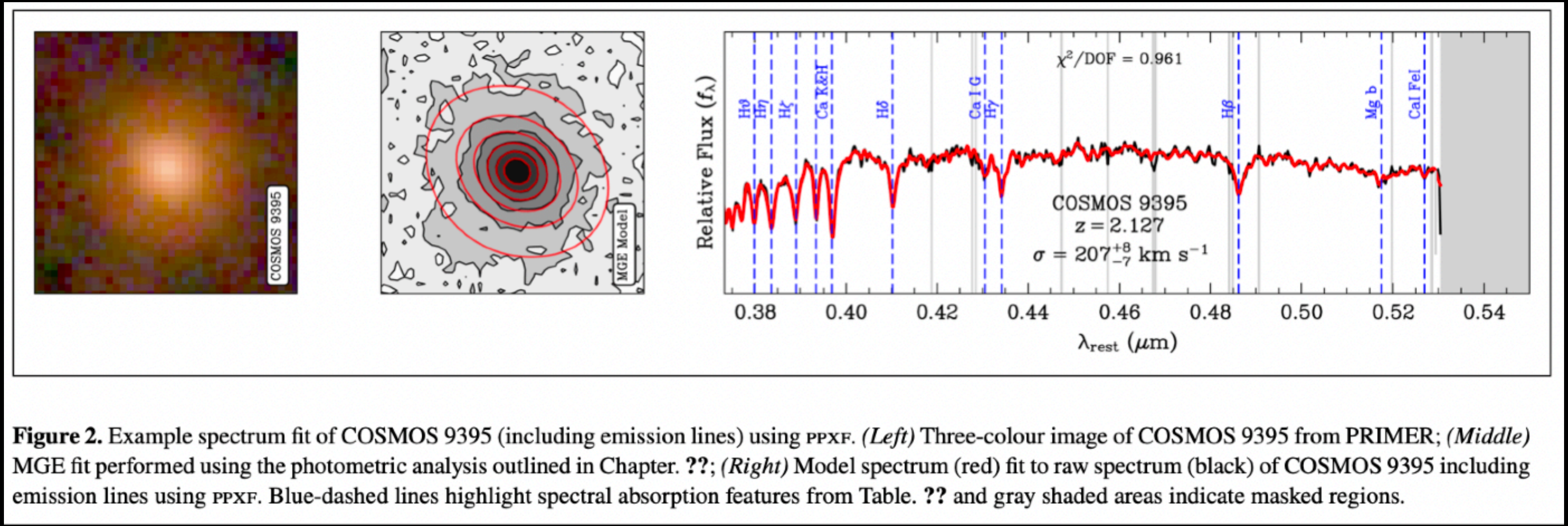


Figure 2. Example spectrum fit of COSMOS 9395 (including emission lines) using PPXF. *(Left)* Three-colour image of COSMOS 9395 from PRIMER; *(Middle)* MGE fit performed using the photometric analysis outlined in Chapter. **??**; *(Right)* Model spectrum (red) fit to raw spectrum (black) of COSMOS 9395 including emission lines using PPXF. Blue-dashed lines highlight spectral absorption features from Table. **??** and gray shaded areas indicate masked regions.

CAN YOU BEAT THE COMPUTER (PROGRAMMER)?

Australian
National
University

Can you solve the problem quicker by hand?

Solve the following equations:

AB + CD + EF = GH and GH + J == 100 and A < C < E and B < D < F

Digits are between 1 and 9. Each digit is used only once

One of you: actually try to solve it by hand. The other one: solve it with python. Once you have a winner (or 10 minutes have passed): use ChatGPT to optimise

Can you solve the problem quicker by hand?

Solve the following equation:

((4-1) * (a - b) + c) * (d + e + f) = 90

Consider the solution must use all of the digits 0-9 once and once only (including those already filled in)

Whoever did not solve problem 1 by hand: solve it by hand. The other one: solve it with python. Once you have a winner: use ChatGPT to optimise