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Unsupervised classification of CIGALE galaxy spectra

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ABSTRACT

Aims. The present study aims at providing a deeper insight into the power and limitation of an unsupervised classification algorithm (called Fisher-EM) on spectra of galaxies. This algorithm uses a Gaussian mixture in a discriminative latent subspace. To this end, we investigate the capacity of this algorithm to segregate the physical parameters used to generate mock spectra and the influence of the noise on the classification.

Methods. With the code CIGALE and different values for nine input parameters characterising the stellar population, we have simulated a sample of 11 475 optical spectra of galaxies containing 496 monochromatic fluxes. The statistical model and the optimum number of clusters are given in Fisher-EM by the integrated completed likelihood (ICL) criterion. We repeated the analyses several times to assess the robustness of the results.

Results. Two distinct classifications can be distinguished in the case of the noiseless spectra. The one above 13 clusters disappears when noise is added, while the classification with 12 clusters is very robust against noise down to a signal to noise ratio (SNR) of 3. At SNR=1, the optimum is 5 clusters, but the classification is still compatible with the previous one. The distribution of the parameters used for the simulation shows an excellent discrimination between classes. A higher dispersion, both in the spectra within each class and in the parameter distribution, leads us to conclude that despite a much higher ICL, the classification with more than 13 clusters in the noiseless case is not physically relevant.

Conclusions. This study yields two conclusions valid at least for the Fisher-EM algorithm. Firstly, the unsupervised classification of spectra of galaxies is both reliable and robust to noise. Secondly, such analyses are able to extract the useful physical information contained in the spectra and to build highly meaningful classifications. In an epoch of data-driven astrophysics, it is important to trust unsupervised machine learning approaches that do not require training samples which are unavoidably biased.

Key words. Methods: data analysis – Methods: statistical – Galaxies: statistics – Galaxies: general – Techniques: spectroscopic

1. Introduction

Machine learning is becoming increasingly popular in astrophysics, mainly through the supervised approach, which consists in training the algorithm with whatever relevant information we already know. This is for instance the case of the classification of astronomical objects, where the observations are matched against representative data of previously established classes (Fraix-Burnet et al. 2015).

Supervised classification has two appealing advantages. The first one is that it can be very fast and well adapted to the very large databases produced by new telescopes. The second one is its immediate usefulness since a new observation is assigned to a class with supposedly known physical properties.

Supervised classification has however several limitations. It depends much on the quality of the reference classification and this relies on important prerequisites: large enough data samples, good quality of the data and a proper understanding of the physics underlying the studied objects. Moreover, a careful visual inspection may be needed in many cases. Hence, rarer objects might not be well represented, inducing biases in the learning process (e.g. Cavuoti et al. 2014). Supervised classification is also obviously not suited to characterise or identify new kinds of objects.

Conversely, unsupervised classification consists in pattern recognition in the data space to establish a reference classification. Cleared from human subjectivity, this approach can be expected to be more suited for subsequent supervised classification since it is entirely data-driven.

Among clustering techniques, model-based approaches (Fraley & Raftery 2002; McLachlan & Peel 2000) are popular. They are renowned for their probabilistic foundations and their flexibility. One of the main advantages of these approaches is the fact that their models and results can be interpreted from both the statistical and practical points of view. In addition, it turns out that many of the other heuristic approaches (mostly based on similarity measures) correspond approximately to particular clustering models (Bouveyron et al. 2019). One of the simplest and wellknown algorithm is the k-means approach, which considers a mixture of identical Gaussian. A more powerful tool is the Gaussian mixture model (GMM, Bouveyron et al. 2019) approach, which fits a multivariate Gaussian to each cluster (e.g. de Souza et al. 2017). The GMM allows for more adaptability to the distribution of points and clusters in the data space, but that may not be sufficient. Two solutions are possible : merging of Gaussian components (e.g. Hennig 2010) and use of non-Gaussian components (see a comprehensive review in Bouveyron et al. 2019).

However, the choice of the merging criterion and of the models rises philosophical issues (e.g. Hennig 2015). In our experience, if the data do not fit the model, the algorithm fails to find the optimum number of clusters as in De et al. (2016). We never met this problem with GMM on astrophysical data.

Unfortunately, model-based methods usually show a disappointing behaviour in high-dimensional spaces (e.g. De et al. 2016). They suffer from the well-known curse of dimensionality (Bellman 2010), which is mainly due to the fact that modelbased techniques are over-parametrised in high-dimensional spaces. For this reason, dimension reduction methods are frequently used in practice to reduce the dimension of the data before the clustering step. Feature extraction methods, such as principal component analysis (PCA), or feature selection methods are very popular. In astrophysics, PCA is used to separate some big classes of spectra or even remove some noise (Marchetti et al. 2013). However, dimension reduction usually does not consider the clustering task and provides a suboptimal data representation for the classification step. For instance, the variance axes of PCA are not necessarily the discriminant axes (Chang 1983). Indeed, dimension reduction methods usually imply an information loss which could have been discriminative. To avoid the drawbacks of dimension reduction, several approaches have been proposed in the last decade to allow model-based methods to efficiently classify high-dimensional data. Subspace clustering techniques are one of them. They are mostly based on probabilistic versions of the factor analysis model and allow to classify the data in low-dimensional subspaces without reducing the dimension (Bouveyron 2016).

The main drawback of unsupervised classification is that the classes are built from a statistical point of view. Statistical criteria (and this is the advantage of model-based methods) provide objective ways to find the "best" solution and assess their robustness. But there is no real "good" classification in the sense that only the physical interpretation and the goal of the study constitute the metric assessing the usefulness of the classification (e.g. Hennig 2015). Nevertheless, several works have proven the relevance of this approach in astrophysics (see a review for the extragalactic domain in Fraix-Burnet et al. 2015). For instance, de Souza et al. (2017) used a Gaussian Mixture Model (GMM, e.g. Bouveyron et al. 2019) approach to classify emission line galaxies using, as observables, the two line ratios log[OIII]/H β and log[NII]/H α and the equivalent width of the H α line (logEW(H α)). They find a statistical optimum of four classes that revised slightly the separation between active galactic nuclei (AGNs), Seyfert galaxies, low-ionization nuclear emission-line regions (LINERs) and star forming regions. With a larger sample of 362923 galaxies and 47 observables (including emission lines, Lick indices, morphologies and photometric observables), Chattopadhyay et al. (2019) applied an Independent Component Analysis (Jutten & Herault 1991) to reduce the dimensionality, followed by a k-means (MacQueen 1967) analysis. They obtain 10 classes that correspond to the classical known classes of galaxies.

A significant step forward in both the sample size and the number of features has been performed by Fraix-Burnet et al. (2021) on a sample of 702248 optical spectra (1437 monochromatic fluxes each) of galaxies from the Sloan Digital Sky Survey (SDSS) using an unsupervised clustering discriminative latent mixture model algorithm called Fisher-EM (Bouveyron & Brunet 2012). They obtained 86 robust and very homogeneous classes that a preliminary analysis shows they can be easily given a physical interpretation.

Table 1: Table of parameter linear correlation coefficients. The parameters are not intrinsically correlated in CIGALE, but the combinations of values used to generate the sample for this study may show underlying involuntary correlations between some parameters.

	T _{main}	$ au_{main}$	f _{burst}	T _{burst}	τ_{burst}	Metallicity
$ au_{main}$	0.17					
f _{burst}	-0.42	0.01				
T _{burst}	0.21	0.18	-0.28			
$ au_{burst}$	-0.06	0.38	-0.11	0.20		
Metal.	0.33	-0.20	-0.39	0.11	-0.02	
E(B-V) _{cont}	-0.22	0.10	0.27	-0.10	-0.01	-0.28

In the present paper, we aim at bringing some insight into the power and limitation of the use of the algorithm Fisher-EM on a simple mock sample of spectra. This is a follow-up of the above study (Fraix-Burnet et al. 2021) but its results can be helpful for many unsupervised approaches. It is well known that the many degeneracies present in spectra cause the derivation of the properties of galaxies to be somewhat difficult (Marchetti et al. 2013). We are particularly interested in the way the classification obtained through Fisher-EM is able or not to segregate the physical properties and in its sensitivity to noise.

To this end, we simulated a sample of galaxy spectra with the spectral energy distribution (SED) fitting code CIGALE (Boquien et al. 2019) using a number of input physical parameters. Then we performed the clustering with Fisher-EM on the spectra. Finally, we analysed the resulting classes in terms of these input parameters. We also study the influence of the noise on the results.

This paper is organised as follows. The simulations and the data are presented in Sect. 2. The algorithm Fisher-EM is briefly described in Sect. 3 together with the method to select the optimum number of clusters. In Sect. 4 we describe the classifications obtained on the noiseless spectra, and show the distribution of the physical parameters of the simulations and determine the most discriminant ones. In Sect. 5, the influence of different levels of noise on the classification and on the associated physical properties of the classes is presented. After a discussion in Sect. 6 we conclude this paper in Sect. 7.

2. Data

2.1. Generation of the spectra

The spectra used in this study have been simulated with the code CIGALE (Code Investigating GALaxy Emission), a software that extends the work of Burgarella et al. (2005) and Noll et al. (2009).

The code CIGALE creates spectra from the UV to the far-IR. In the present work, we consider the optical part of the spectra (496 fluxes between 380.66-737.00 nm) to be able to make a later comparison with observed data such as those from the SDSS (see for example Fraix-Burnet et al. 2021). Each simulated spectrum requires a set of input parameters characterising the galaxy. In our simulations, we assumed a Chabrier (2003) Initial Mass Function (IMF). We limited the star formation history (SFH) to a main population and, in some cases, a later burst of same metallicity. With these assumptions, the optical part of the spectra is affected by nine parameters in CIGALE. We simulated spectra with bursts of varying strength (f_{burst}): none, medium and large. For each burst strength, we considered populations of different ages and time scales (T_{main} , τ_{main} , T_{burst} , τ_{burst}), metallicity, reddening ($E_{(B-V)lines}$, $E_{(B-V)factor}$), and redshift. See Sect. 2.2 for the description of the input parameters. The combinations of the values chosen for the input parameters yield 11475 spectra. All spectra were normalised by their mean values between 505 and 581 nm, a region where the spectra have no emission lines.

2.2. Description of the input parameters

The optical part of the spectra is affected by nine CIGALE input parameters. The values taken in this work are listed in Table A.1 and their distribution shown in Fig. 1. These nine parameters are reduced to seven, as explained in the following:

- T_{main} is the age (in Myr) of the main stellar population in the galaxy. It is varied from 2000 to 13000 Myr.
- τ_{main} is the e-folding time (in Myr) of the main stellar population and characterises the SFR of the main population together with T_{main} (module *sfhdelayed* of CIGALE) :

$$\text{SFR}_{main}(t) \propto \frac{t}{\tau_{main}^2} \exp(-t/\tau_{main})$$
 (1)

In the sample, τ_{main} varies from 500 to 10500 Myr.

- f_{burst} is the mass fraction of stars produced during a burst of star formation, and ranges from 0 to 0.5. When $f_{burst} = 0$, no burst is considered in the history of the galaxy.
- T_{burst} is the age (in Myr) of the burst of star formation, and ranges from 5 to 100 Myr. When $f_{burst} = 0$, T_{burst} is fixed to 0.
- τ_{burst} is the e-folding time (in Myr) of the burst of star formation and characterises the SFR of the burst event together with T_{burst} :

$$\text{SFR}_{burst}(t) \propto \frac{t}{\tau_{burst}^2} \exp\left(\frac{-t}{\tau_{burst}}\right) \quad \text{for } t > T_{main} - T_{burst} \quad (2)$$

It varies from 4500 to 50000 Myr. These values are of the same order of $T_{main}-T_{burst}$, and much larger than T_{burst} , so that the SFR is essentially constant during the second burst of star formation. When $f_{burst} = 0$, no burst is considered in the history of the galaxy, and τ_{burst} is therefore fixed to 0.

- Metallicity is assumed to be identical for the main and burst stellar populations as well as for the interstellar medium, and takes three possible values: 0.008, 0.02 and 0.05.
- E(B-V)_{cont}: the reddening of the continuum that intervenes in the computation of the attenuation due to the dust inside the galaxy. For the lines, we have E(B-V)_{lines} =E(B-V)_{cont}/E(B-V)_{factor} where E(B-V)_{factor} is a normalising factor given as an input parameter. We choose to discuss only E(B-V)_{cont} throughout this paper for its physical relevance. In the simulated spectra, E(B-V)_{cont} takes a wide variety of values from 0.000125 to 0.44.
- Redshift was varied from 0 to 1 to include the effect of the intergalactic medium (IGM) on the spectra. For the classification process, we shifted the spectra to the same redshift of 0. As a consequence, the spectra that differ only by redshift end up being very similar because the effect of the IGM happens to be very small. We will thus not discuss the redshift any more in the rest of this paper.

As defined previously, the T_{main} , τ_{main} , f_{burst} , T_{burst} and Metallicity parameters are actually the building blocks of the stellar populations composing a galaxy. It is thus natural that

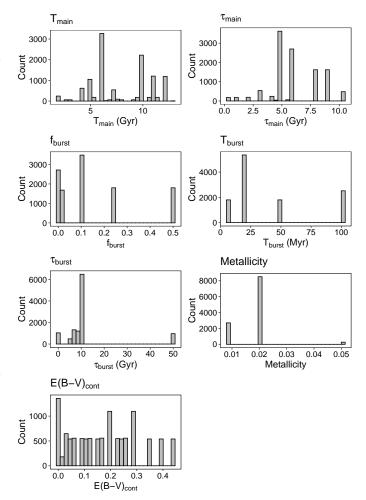


Fig. 1: Histograms of CIGALE parameters input values in the study sample. This sample was not created to fit some specific parameter distribution, but rather cover the parameter space as much as CIGALE allowed it while keeping the spectra realistic.

varying the values of these parameters would directly influence the continuum and the absorption lines of a galaxy spectrum (e.g. a high value of T_{main} would redden the spectrum and deepen molecular lines, etc.). Also, E(B-V)_{cont} translates the presence of dust in the interstellar medium by reddening the spectrum. On the other hand, the emission lines in a galaxy spectrum are the signature of a recent star forming event in the history of that galaxy. Therefore, the same parameters T_{main} , τ_{main} , f_{burst} , T_{burst} are also responsible for the presence and the height of these lines. Moreover, since the interstellar medium, in CIGALE, has the same metallicity as the stars, the Metallicity parameter will also affect the emission lines in addition to the stellar component. Finally, because the chosen values of τ_{burst} are much larger than those of T_{burst} (see Table A.1), τ_{burst} only weakly affects our spectra.

Most CIGALE parameters only take discrete and predetermined values, making it impossible to fully cover the parameter space. Some parameters such as $E(B-V)_{cont}$ allow for a decent sampling, while some others such as Metallicity only take very few values. The sampling density of a parameter may affect somewhat its discriminant power, but in a very indirect way since the clustering is performed with the spectra and not with the input parameters. Moreover, while the parameters are not intrinsically correlated in CIGALE, some of them may be slightly correlated due to our parameter sampling. Such correlations have to be kept in mind when analysing the discriminative properties of the classification method, as one parameter may deceptively appear well discriminated due to its correlation with another discriminated parameter. However, for our sample the Pearson correlation coefficients remain small (see Table 1), and reach at most -0.42 (f_{burst} vs T_{main}).

We wish to insist that our mock sample is not intended to represent a complete diversity of spectra of real galaxies. Rather, it must be considered as a realistic sample with selection biases. These biases are here not observational, instrumental or catalogue-based, but are due to the necessarily limited choice for the values of the input parameters.

The simulated spectra are noiseless, and their analysis is presented in Sect. 4. To study the influence of the level of noise on the clustering result, we generated different signal-to-noise ratio (SNR) set of spectra by adding a Gaussian noise to each monochromatic flux. The analysis of these noisy spectra is described in Sect. 5.

3. Method

3.1. The Fisher-EM algorithm

In this work, we have applied the unsupervised classification method named Fisher-EM (Bouveyron & Brunet 2012) on the sample of optical galaxy spectra simulated with CIGALE (see Sect. 2).

Fisher-EM is a subspace Gaussian mixture algorithm that relies on a statistical model, named the discriminative latent mixture (DLM) model. It uses a modified version of the expectationmaximisation (EM) algorithm by inserting a Fisher-step to optimise the ratio of the sum of the between-class variance over the sum of the within-class variance for a better clustering.

Formally, we may define the observation vector $\mathbf{Y} = {\mathbf{y_1}, ..., \mathbf{y_n}}$ such that $y_i \in \mathbb{R}^p$ describes spectrum number *i*. The dimension *p* is the *p* fluxes at the *p* wavelengths of the spectra.

Classifying the observations into K classes mathematically translates into finding the vector $\mathbf{Z} = {\mathbf{z}_1, ..., \mathbf{z}_n}$ which assigns each spectrum y_i to a given class $z_i \in [\![1, K]\!]$. In the case of Fisher-EM, the clustering process occurs in a subspace $\mathbb{E} \subset \mathbb{R}^p$ of dimension d = K - 1 < p. Therefore, the Gaussian mixture model is applied to the projected data **X** rather than the observed data **Y**:

$$\mathbf{Y} = \mathbf{U}\mathbf{X} + \boldsymbol{\epsilon} \tag{3}$$

where $\mathbf{U} \in \mathcal{M}_{\mathbf{p},\mathbf{d}}(\mathbb{R})$ is the projection matrix and ϵ is a noise vector of dimension *p* following a Gaussian distribution centred around 0 and of covariance matrix $\Psi(\varepsilon_k \sim \mathcal{N}(0, \Psi_k))$. The multivariate Gaussian probability distribution **X** describing the class *k* in the subspace is parameterised by a mean vector $\mu_{\mathbf{k}}$ and a covariance matrix $\Sigma_{\mathbf{k}}$:

$$X|_{Z=k} \sim \mathcal{N}(\mu_k, \Sigma_k) \tag{4}$$

Combining Eqs. 3 and 4, we obtain:

$$Y_{|X,Z=k} \sim \mathcal{N}(UX, \Psi_k) \tag{5}$$

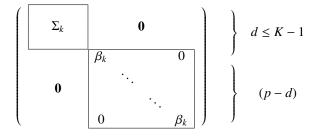
The observed data is thus modelled by a marginal distribution $f(\mathbf{y})$ that is the sum of K multivariate Gaussian density functions

Article number, page 4 of 18

 ϕ of mean $U\mu_k$ and covariance $U\Sigma_k U^t + \Psi$, each weighted by the corresponding mixing proportion π_k :

$$f(\mathbf{y}) = \sum_{k=1}^{K} \pi_k \phi(\mathbf{y}; \mathbf{U}\mu_k, \mathbf{U}\boldsymbol{\Sigma}_k \mathbf{U}^t + \boldsymbol{\Psi})$$
(6)

By further assuming that the noise covariance matrix Ψ_k satisfies the conditions $V^t \Psi_k V = \beta_k \mathbf{I}_{p-d}$ where V is the orthogonal complement of U, and $U^t \Psi_k U = \mathbf{0}_d$, the whole statistical model denoted by $DLM_{[\Sigma_k \beta_k]}$ can be shown to take the following form:



These last conditions imply that the discriminative and the nondiscriminative subspaces are orthogonal, which suggests in practice that all the relevant clustering information remains in the latent subspace. From a practical point of view, β_k models the variance of the non-discriminative noise of the data.

Several other models can be obtained from the $DLM_{[\Sigma_k\beta_k]}$ model by relaxing or adding constraints on model parameters. It can, for example, be assumed that the noise parameter β_k differs from class to class, or that the covariance matrices Σ_k are the same for all *K* classes. A thorough description of the DLM model, its 12 declinations, as well as the algorithm itself can be found in Bouveyron & Brunet (2012).

The Fisher-EM algorithm requires the number of groups K and the DLM model as input. After undergoing an initialisation obtained from multiple k-means runs, the algorithm proceeds as follows:

- E-step: the posterior probabilities that the *n* observations y_i belong to each of the K classes are computed.
- Fisher-step: The projection matrix U is computed to maximise the Fisher criterion.
- M-step: the DLM model parameters are adjusted to maximise the likelihood.

The Fisher-EM algorithm is implemented in the eponym package for R.

3.2. Choice of the model and number of classes

The choice of the best statistical DLM model and the optimum number of clusters depends on the data and are estimated in this study with the integrated completed likelihood (ICL) criterion. This criterion penalises the likelihood by the number of parameters of the statistical model, the number of observations, and favours well separated clusters (Biernacki et al. 2000; Girard & Saracco 2016).

The best statistical model was found to be $A_{kj}B_k$ in all the cases studied in this paper. This model is such that in each group, the covariance matrix Σ_k is assumed to be diagonal: $\Sigma_k = \text{diag}(\alpha_{k_1}, ..., \alpha_{k_d})$.

The optimum number of clusters K is also given by the maximum ICL value, and depends on each data set.

In order to characterise the stability of the algorithm, several classifications were generated for each number of clusters

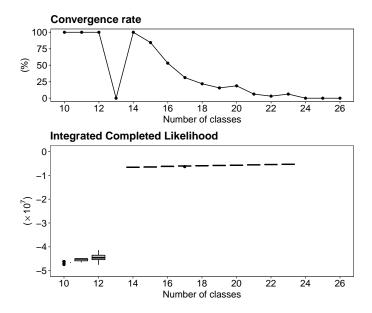


Fig. 2: Clustering analysis of noiseless spectra with Fisher-EM. *Top:* the convergence rate as a function K. For every K value considered, 32 classifications were calculated. *Bottom:* boxplots of the ICL is as a function of the number of clusters K. The horizontal bars show the median value, the boxes represent the two quartile values, the whiskers extend to points that lie within 1.5 times the interquartile range of the lower and upper quartile and data beyond are shown individually with dots.

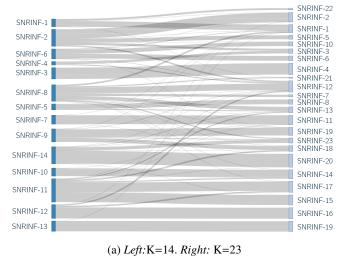
K yielding a distribution of ICL values for each. This dispersion is found to be generally low, and is shown as boxplots in the ICL-vs-K figures presented throughout this paper.

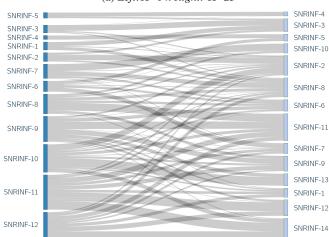
The EM algorithm is known to sometimes find an empty cluster (i.e. a null π_k in Eq. 6). This results in an undefined log-likelihood that stops Fisher-EM. In this paper, we call this the non-convergence of the algorithm.

4. Analysis of the noiseless spectra

4.1. Optimal number of clusters

In this section, we apply the Fisher-EM algorithm on the simulated noiseless spectra, described in Sect. 2. There is a remarkable jump in ICL values at K = 14 (Fig. 2). In addition, the algorithm does not converge for K = 13 while there is a 100% convergence rate at K = 12 and K = 14. Henceforth, K = 13appears as a frontier between two very distinct regimes. For K < 13, the algorithm always converges, and the ICL is maximum at K=12. In the K > 13 regime, the convergence rate decreases as the number of clusters increases, and no convergence is obtained for any K > 23. Strictly speaking, the ICL is the greatest for K = 23 and from a statistical standpoint, K = 23 is therefore the best result but has a low convergence rate. Besides, the classification at K = 14, on top of having no convergence issue, matches very well the one at K = 23 in that they share a lot of classes containing the same galaxies (i.e. they have similar class composition, see Fig. 3a). Undeniably, the latter having 9 more clusters and a slightly better ICL makes it more refined. Nonetheless, the K = 14 classification seems to be a good compromise between reproducibility and goodness-of-fit, and is therefore chosen to represent the K > 13 regime.





(b) *Left*:K=12. *Right*: K=14

Fig. 3: Comparisons between three classifications of the noiseless spectra (SNRINF): K=12, K=14 and K=23. In (a), the composition of the classes of K=14 (left) and K=23 (right) are compared, and of K=12 (left) and K=14 (right) in (b). The colour boxes represent the classes, the grey lines represent galaxies that are shared by the two classes they link, and the height of the colour boxes is proportional to the number of galaxies in a given class.

The classifications at K = 14 and K = 12 are arranged in a significantly different way (Fig. 3b), showing that the two regimes in fact correspond to two distinct classifications.

The mean spectra and dispersion of each class of the retained classifications (i.e. K = 14 and K = 12) are shown in Fig. 4 and Fig. 5 (the vertical scale is arbitrary but the same for all plots of spectra in this paper). Despite its better ICL, the K = 14 classification shows a higher dispersion than K = 12 for most of the classes besides a few exceptions (classes 4, 10 and 14), and in some cases, blue and red continua are even mixed together (classes 2, 3, 6, 9). On the other hand, the dispersion within most classes of the K = 12 classification is rather small, indicating a decent homogeneity of the classes.

The distribution of the spectra among the 14 and 12 classes, is relatively well-balanced (Figs. 6 and 7), although arguably more even for the 14 classes. It varies from about 200 to 2000 spectra with an average of circa 500.

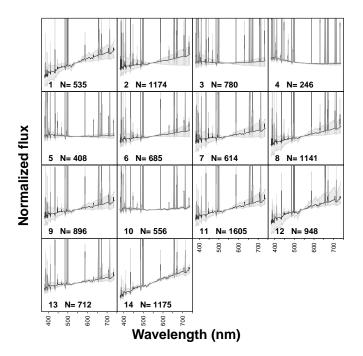


Fig. 4: 14-cluster classification of the noiseless spectra, with the mean spectra (in black) and their dispersion (in grey) for every class. N is the number of members in each class. All the spectra were normalised by their mean values between 505 and 581 nm, a region where the spectra have no emission lines. The scale is the same for all panels and all other figures of spectra throughout this paper. The dispersion corresponds to the 10% and 90% quantiles for each monochromatic flux. The classes are sorted by ascending average T_{main} .

In both cases, there is no mean spectrum without emission lines. This is because several spectra with intense lines are present in all classes. In particular, in our sample, emission lines are present in spectra with $f_{burst}=0$ that have a high τ_{main} (e.g. 5000).

4.2. Parameter distribution among classes

As mentioned is section 2, the simulated spectra are associated each with a set of parameter values. As explained in Sect. 2, the relevant ones are T_{main} , T_{burst} , τ_{main} , τ_{burst} , f_{burst} , metallicity and $E(B-V)_{cont}$.

A parameter-by-parameter analysis and class-by-class analysis of the classifications is made possible by visualising the parameters' distribution among the 12 and 14 classes (Fig. 7 and Fig. 6).

4.2.1. Classification at K=14

Let us first consider the parameter-by-parameter approach. f_{burst} is mostly separated into two categories in this classification: higher values (classes 2, 3, 4, 5, 6, 10 and 13) and lower values (classes 1, 7, 8, 9, 11, 12 and 14). The separation is, however, not very sharp, especially for some lower f_{burst} classes.

The metallicity is not well sampled as it only takes three discrete values (0.008, 0.02 and 0.05), but is rather well segregated in the classes. Half of the classes gather one single metallicity value, two of them being the lower one (classes 4 and 5), and five being the medium one (classes 7, 10, 11, 13 and 14). The

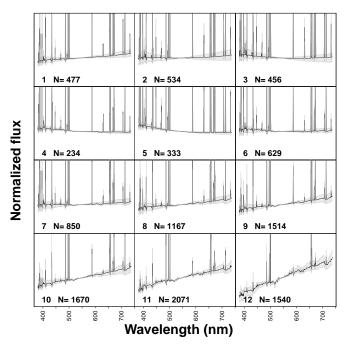


Fig. 5: 12-cluster classification of the noiseless spectra (see Fig. 4).

other half contain a mixture of usually two values: lower and medium (classes 1, 3 and 6) or medium and higher (classes 10 and 12) with the exception of classes 2 and 8 which mix all three values. The higher metallicity value is not as well separated as the medium and lower values.

The classes have been sorted by ascending age T_{main} . There is a clear distinction made in the classification between younger and older galaxies. Three categories can be drawn: classes containing the youngest galaxies (1 to 6), classes containing an equivalent mixture of young and old galaxies (7 to 12), and classes of older galaxies (13 and 14).

 τ_{main} has a high dispersion in the classes, although the lower values happen to be concentrated in the classes with lower f_{burst} .

The T_{burst} values are well isolated among the classes with high f_{burst} , with the exception of class 2 which also contains a fraction of low f_{burst} galaxies. In the other classes, where the burst of star formation is less prominent, no distinction is made between T_{burst} values.

 τ_{burst} is quite dispersed in most of the classes with lower f_{burst} classes. It is slightly less the case for higher f_{burst} classes, but τ_{burst} remains a parameter that is not well discriminated in the classification.

 $E(B-V)_{cont}$ does not appear to be well separated. Apart from a few classes (4, 10, and 14), high and low $E(B-V)_{cont}$ values are mixed together in this classification.

All things considered, the classification at K = 14 is essentially explained by four parameters (f_{burst} , T_{main} , T_{burst} , metallicity), while the other three (τ_{main} , τ_{burst} , E(B-V)_{cont}) show similar distributions among most of the classes with a few exceptions.

The properties of the classes can be summarized as follows. Classes 1 to 6 are made of galaxies of younger ages (T_{main}) and a rather significant burst of star formation (f_{burst}). Those classes, except for classes 1 and 2, nearly only have one value of T_{burst} : classes 3 and 4 contain galaxies that have had their burst hap-

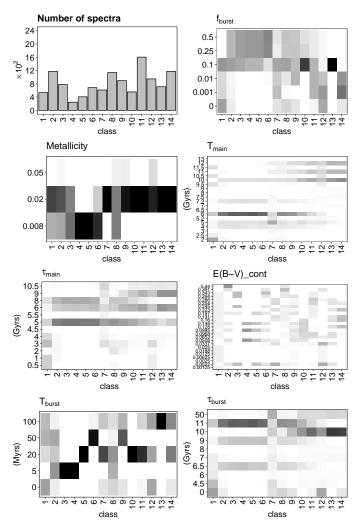


Fig. 6: 14-cluster classification of the noiseless spectra. *Top left:* number of spectra contained in each class. *All others:* heatmaps of the relevant CIGALE input parameters among the 14 classes on noiseless spectra. All possible parameter values (see Table A.1) are represented on the y-axis, and the class index on the x-axis. The within-class densities of the parameter values are illustrated in the form of a heatmap, where a dark square equates to a density of 1, and white of 0. The classes are sorted by ascending average T_{main}

pen very recently in the star formation history (5 Myr), class 6 contains galaxies of older bursts (50 to 100 Myr), and class 5 of medium age (20 Myr). Metallicity values are also fairly well separated in those classes. Galaxies of classes 2, 3 and 6 have metallicities of 0.008 and 0.02, while classes 4 and 5 only contain galaxies with a metallicity of 0.008.

Classes 7 to 12 mostly contain two populations of galaxies: older galaxies with a significant burst of star formation, and younger galaxies. Apart from class 8, they all gather galaxies of medium to high metallicity. In this category, class 10 stands out as the galaxies it is made of all have a 20 Myrs old prominent burst of star formation, while the other classes do not differentiate T_{burst} .

Finally, classes 13 and 14 gather old galaxies with a faint burst of star formation. More exactly, galaxies of class 14 have had little to no burst in their star formation history, while galaxies of class 13 did, but a long time prior to observation (old T_{burst}).

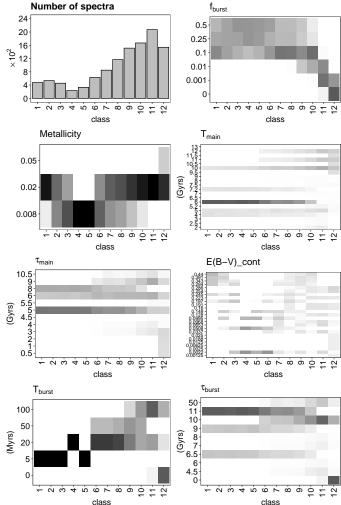


Fig. 7: 12-cluster classification of the noiseless spectra. *Top left:* number of spectra contained in each class. *All others:* heatmaps of the relevant CIGALE input parameters among the 12 classes on noiseless spectra. All possible parameter values (see Table A.1) are represented on the y-axis, and the class index on the x-axis. The in-class densities of the parameter values are illustrated in the form of a heatmap, where a dark square equates to a density of 1, and white of 0. The classes are sorted by ascending average T_{main}

Overall, each class shows its own specificity in regard to the physics of the galaxies it contains. Three groups of classes can be distinguished (1-6, 7-12, 13-14) which essentially categorise the galaxies as young and active, less active, and inactive and old.

4.2.2. Classification at K=12

As shown in Fig. 3b, the classification at K = 12 is significantly different from the one at K = 14 in terms of spectrum distribution. However, from a physical standpoint, they show very similar characteristics (Fig. 7).

They are in fact both mostly driven by f_{burst} , metallicity, T_{main} and T_{burst} . Nonetheless, their distribution among the classes show significantly less dispersion for K = 12 despite the lower ICL. This is specifically striking for lower values of f_{burst} which

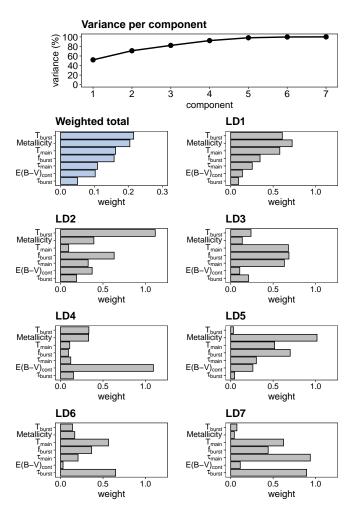


Fig. 8: Linear discriminant analysis on the classification of noiseless spectra at K = 14. *Top:* cumulative data variance described by the linear discriminant analysis components. *LD1 to LD7:* weight of each parameter for components 1 to 7 of the linear discriminant analysis. *Weighted total:* cumulative weight of each parameter among the 7 components weighted by the percentage of data variance described by each component.

are scattered around a lot of classes and mixed with higher values for K = 14, while they are extremely well separated for K = 12.

Class-wise, a similar categorisation as in K = 14 can be made, with classes 1-5 corresponding to the young active galaxies, classes 6-10 to a mixture of old active galaxies, and younger ones, and classes 11-12 to the old and mostly inactive ones. In addition, class 12 gathers almost all galaxies that did not undergo an additional period of star formation, while that information was not retrieved at K = 14.

As a whole, the classification at K=12 is more discriminative that the one at K=14, but they both are sensitive to the same physical parameters. As such, despite the statistical superiority of K=14, K=12 appears to be a better version of K=14 in terms of their physical discriminative properties.

4.3. Linear Discriminant Analysis

Linear discriminant analysis (LDA) was applied to the classified data in order to identify the influence of each parameter in the classification process. As a matter of fact, the LDA analysis returns a set of components that are essentially the projection vectors that best separates the classes, and while the classification was done based on the information of the spectra, LDA analysis uses the information of the parameters, therefore highlighting the links between them and the classification. The results are shown in Fig. 8 and Fig. 9.

4.3.1. Classification at K=14

The analysis at K = 14 resulted in seven components labelled LD1 to LD7 (Fig. 8). The first one explains almost half of the data variance, and adding the next three brings it up to close to 90%.

An overall weight attributed to each parameter by the LDA is obtained by summing the seven components weighted by their relative variance explained. This overall weight quantifies how discriminated the parameters are by the classification. The results agree well with the conclusion obtained in Sect. 4.2, namely, the parameters that are best discriminated, are T_{burst} , metallicity, T_{main} and f_{burst} . The e-folding time of the burst of star formation is by far the least discriminated parameter, followed by the reddening and the e-folding time of the main stellar population.

The first component allocates most of its weight equally to T_{burst} , metallicity and T_{main} . The second one is dominated by the age of the burst of star formation (T_{burst}) and to a lesser extent the stellar mass fraction of the burst (f_{burst}) . The third component equally distributes most of its weight to three parameters, namely T_{main} , τ_{main} and f_{burst} . The fourth component is completely dominated by the reddening $(E(B-V)_{cont})$ which was mostly ignored by the previous component. The final three components are mostly dominated by parameters that are already greatly taken into account in the first three components, but they also allocate some of their weight to the e-folding times of the SFR of the main stellar population and the burst event (τ_{main} , τ_{burst}), which were totally insignificant in the previous components.

4.3.2. Classification at K=12

As expected given their similarities, the LDA analysis at K = 12 shows similar results than K = 14 (Fig. 9).

There is, however, a significant difference between LD4 and LD6. But because the explained variance of those components is so small, they have little to no impact on the overall weight of the parameters.

5. Analysis of the noisy spectra

In this section, we study the effect of noise on the classification of the spectra for different values of SNR. As such, a Gaussian noise of constant SNR was added to the 11 475 spectra. We used seven of values for the SNR: 1, 3, 5, 10, 20, 100, and 500.

5.1. Optimal number of clusters

The very characteristic break of the ICL curve observed at K=13 for the noiseless spectra disappears as soon as a noise as small as SNR=500 is added. The ICL curves obtained have an optimum independently of the noise level (Fig. 10), as opposed to the ever-increasing ICL on noiseless spectra.

For SNR ≤ 100 and below, the ICL reaches its maximum for K=11 to 13. Besides, convergence is reached every single time for any K smaller than 30-40, depending on the noise

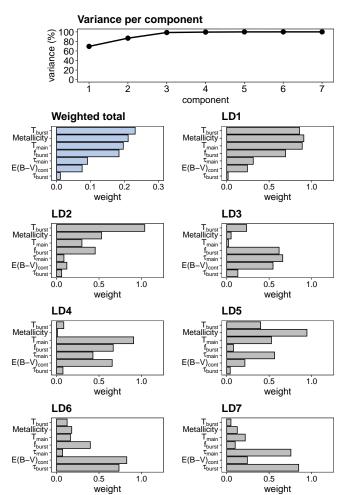
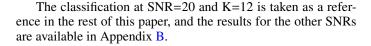


Fig. 9: Linear discriminant analysis on the classification of noiseless spectra at K = 12. *Top:* cumulative data variance described by the linear discriminant analysis components. *LD1 to LD7:* weight of each parameter for components 1 to 7 of the linear discriminant analysis. *Weighted total:* cumulative weight of each parameter among the 7 components weighted by the percentage of data variance described by each component.

level. At SNR=500, the ICL sometimes shows another behaviour that fully depends on the random generation of the noise. At SNR=500, the noise may be insufficient to blur out the data sparsity, which is likely responsible for the ICL break and convergence issues on noiseless spectra. Therefore, while for most generated noise the ICL showed an optimum, one particular noise vector lead to an ever-increasing ICL curve (until loss of convergence) that resembles that of the noiseless spectra.

Our study of the noise shows that the ICL curves at different SNR differ from that of the noiseless case, but they all agree and yield the same optimal number of clusters around K=12. Furthermore, we show that the optimal classifications on the spectra with added noise closely resembles the K = 12 one on noiseless spectra, whether it be based on the composition of the classes (Fig. 11) or their median spectrum (Fig. 12).



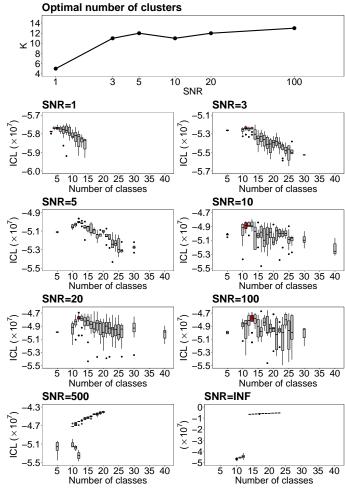


Fig. 10: *Top:* Optimal number of clusters across the different noise levels. *All others:* ICL as a function of K for different noise levels. In each of those panels, the red boxplot highlights the maximum median value of the ICL i.e. the associated best-fit K value. For the SNR of 500, two behaviours were observed depending on the randomly generated noise. They are both illustrated by the two sets of boxplots (black and grey) in the corresponding panel.

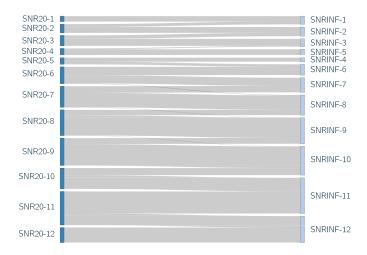


Fig. 11: Same as Fig. 3 between the K = 12 classification on noiseless spectra (right) and on spectra with an added noise of SNR=20 (left).

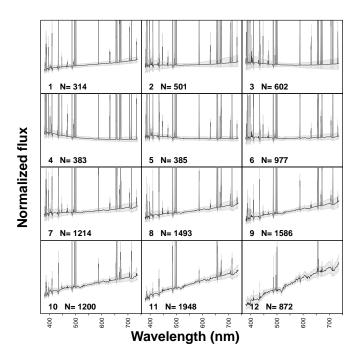


Fig. 12: 12-clusters classification obtained on the spectra with added noise of SNR=20 (see Fig. 4).

5.2. Parameter distribution among classes

The optimal classification at SNR=20 is essentially identical to that on the noiseless spectra presented in Sect. 4.2.2 in regard to the parameter distribution in the classes (Fig. 13). Slight differences appear nonetheless, highlighting the loss of information induced by the additional noise. For example, there is no longer a class isolating 20 Myr old star bursts. On the other hand, some specificities in the spectra appear to be retrieved more accurately with the addition of noise. There is, for instance, 5 classes containing a unique value of metallicity, as opposed to 3 on noiseless spectra. Lower values of f_{burst} are also more sharply separated.

At greater noise (Appendix B), this enhanced ability to discriminate some parameters fades out, and the dispersion in the classes increases for all parameters. At SNR=3, the method is still capable of making out burstless galaxies from burst-heavy ones, but lower non-zero values of f_{burst} become more erratically distributed around the classes. Metallicity is not as well discriminated either, as only a single class of unique value remains. T_{main} , and T_{burst} to a lesser extent, are still separated in a similar fashion despite the significant amount of noise.

At SNR=1, the optimum shifts from 12 to 5 classes, but the method is still capable of approximately separating old and inactive galaxies from young and active ones.

5.3. Linear Discriminant Analysis

The LDA applied on the noisy spectra with SNR=20 shows that the first three components completely dominate the analysis (60%, 20%, 10%), whereas five components were significant for the noiseless spectra. The first component is similar to that of the noiseless spectra, with a more heavily weighted f_{burst} parameter nonetheless. The second and third components, however, are distinctively different. It appears that the weight of the parameters have been shifted from one component to another: T_{burst} , f_{burst} and τ_{main} are less significant in the second component, but

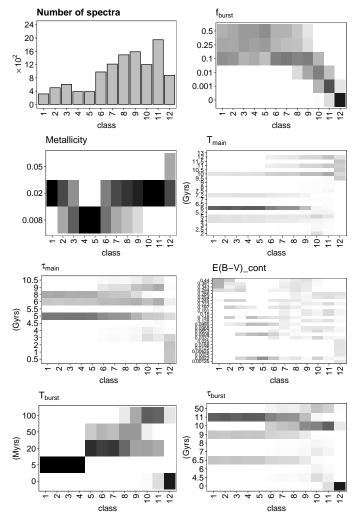


Fig. 13: 12-cluster classification on the spectra with an added noise of SNR=20. *Top left:* number of spectra contained in each class. *All others:* heatmaps of the relevant CIGALE input parameters among the 12 classes. All possible parameter values (see A.1) are represented on the y-axis, and the class index on the x-axis. The in-classes densities of the parameter values are illustrated in the form of a heatmap, where a dark pixel equates to a density of 1, and white of 0.

more important in the third one. Likewise, T_{main} , τ_{main} and E(B-V)_{cont} have higher weights in the second component, and lower weight in the third one. While some components are indeed different, the overall relevance of each parameter in regard to the classification remains close to unchanged.

6. Discussion

6.1. The origin of the $K \ge 13$ regime

The analysis on the noiseless spectra revealed an odd behaviour at $K \ge 13$: a lack of convergence at K=13, and a high plateau of the ICL for K from 14 to 23 (Fig. 2).

In an ideal world, the ICL curve as a function of the number K of clusters should show a clear peak, since this criterion takes into account the number of free parameters in the statistical models and the good separation of the clusters. But the ICL curve has not always this ideal behaviour, especially in high dimension (e.g. Fraix-Burnet et al. 2021). In particular, it often

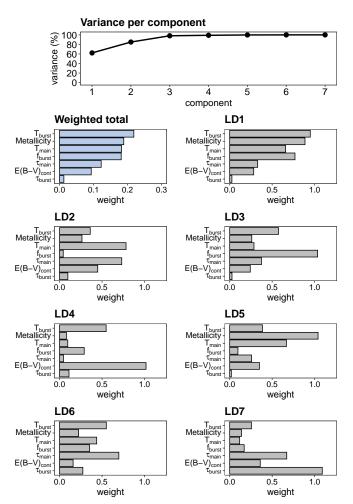


Fig. 14: Linear discriminant analysis on the classification of spectra with added noise of SNR=20. *Top:* cumulative data variance described by the linear discriminant analysis components. *LD1 to LD7:* weight of each parameter for components 1 to 7 of the linear discriminant analysis. *Weighted total:* cumulative weight of each parameter among the 7 components weighted by the percentage of data variance described by each component.

shows a plateau that ends when the algorithm fails to converge (i.e. encounters an empty cluster, see Sect. 4.1).

Since the classifications for K>13 differs from the classifications obtained for K=12 with and without noise, we suspected that this might be due to the fact that the data are simulated with a necessarily limited coverage of the parameter space.

To test this hypothesis, we devised a toy model at the lowest possible dimension to reproduce this behaviour. After trials and errors, we managed to find a data set that is described in Appendix C. The ICL curves show an optimum at K=4, with solutions at K=2 but no convergence at K=3. Remarkably, if we add a very small amount of noise to a part of one of the five variables, solutions are found in all cases, exactly as with our CIGALE data.

Even if this toy model cannot be considered as a proof, we conclude that the behaviour found in the noiseless data may be due to some peculiar distribution of the data in the parameter space, i.e. too small a dispersion and probably a significant level of sparsity. In addition, Jouvin et al. (2021) find a poor performance of the Fisher-EM results in the case of very little noise, a behaviour that they cannot explain but suspect it might be related

to insufficient constraints brought by the data set. Such problems are known to occur in EM-GMM based clustering (e.g. Kasa & Rajan 2020).

The case of $K \ge 13$ is therefore thought to be an artefact resulting from the simulated nature of the spectra, and is dismissed in the rest of this section. Instead, K=12 shall be seen as the representative classification of the noiseless spectra.

We stress that the noiseless situation cannot be encountered in reality.

6.2. The physical discrimination capacity of unsupervised classification

The classification at K=12 shows classes of spectra that are very homogeneous with little dispersion, demonstrating the ability of Fisher-EM to find structures in a high-dimensional data space. This was already noticed for the much larger SDSS sample (Fraix-Burnet et al. 2021).

The analysis of the distribution of the parameters used in the CIGALE simulations shows that this discriminative power among the spectra is also visible in the physical properties of the galaxies. Among the seven parameters, four are clearly well discriminated (T_{main} , T_{burst} , f_{burst} and Metallicity), and to a lesser extent τ_{main} and E(B-V)_{cont}. This is an important result which shows that Fisher-EM is capable of picking up the expected relevant physical parameters. The LDA analysis confirms these most influential parameters. The fact that the weights of T_{burst} and Metallicity appear stronger than that of T_{main} could be due to their small sampling density (respectively three and four values). However, f_{burst} has only six values and has a similar weight as T_{main}. Also, the latter has a higher weight than τ_{main} despite having a similar distribution. Lastly, the LDA analysis shows that τ_{burst} has a weak impact on the classification, but this is probably not due to its small sampling density since it was expected from the physics itself (Sect. 2.2).

As a conclusion, we have shown that each class has not only a specific spectral shape, but also its members have specific physical properties. Hence, in a real data set, a detailed analysis of the mean spectra of the classes should reveal these properties and transform an unsupervised classification into an objective and physical atlas of galaxy spectra.

6.3. The effect of the noise

The addition of noise raises two questions that we address in this section: i) does it change the classification itself, and, ii) does it change the physical interpretation.

6.3.1. Effect on the classification

Adding some noise to our spectra strongly modifies the ICL curve by revealing a clear maximum around K=12 (for SNR ≥ 3) with a quasi identical classification, the noiseless one included. At SNR=1, the optimum is K=5 so that a higher level of noise tends to smear out the classes and, as expected, lessens the discriminative capability of the analysis.

The presence of noise in the data also tends to facilitate the convergence of Fisher-EM. In fact, at the SNRs considered, the convergence issues that were encountered in the noiseless case were non-existent. Lack of convergence was still observed in the noisy case when a high number of classes was chosen, but this behaviour is usual and was seen on real data as well (Fraix-Burnet et al. 2021).

6.3.2. Effect on the physical meaning of the classes

The present study shows that our unsupervised classification and its physical meaning are essentially unchanged between SNR=3 and SNR=500 for our simulated data, demonstrating its robustness.

At SNR=1, most of the physical discriminative capacity of the method is lost, and only 5 classes are found. Nonetheless, those 5 classes are not meaningless, and remarkably separate rather well active galaxies from inactive ones. As a matter of fact, Jouvin et al. (2021) showed that in some cases, Fisher-EM could even prove itself capable of accurately classifying data with a SNR as low as -1dB.

7. Conclusion

The present study shows that the unsupervised classification algorithm Fisher-EM applied on thousands of CIGALE galaxy spectra yields a classification that is both robust against the initialisation of the algorithm and against the noise. Very importantly, the classification is very discriminating with respect to the physical properties of the galaxies.

Unsupervised classification in astrophysics is still in its infancy, and the first robust classification of spectra of galaxies have been published very recently (Fraix-Burnet et al. 2021). The aim of such an objective classification is to produce an atlas that is entirely data-driven, and that could be used later with supervised learning in big surveys. Even though the preliminary interpretation of the classes found in Fraix-Burnet et al. (2021) have shown their physical relevance, the present work confirms that unsupervised machine learning is able to yield not only a robust statistical classification but also a physical classification of the properties of the galaxies from the spectra.

The main advantage of the unsupervised classification is that we do not put any a priori physical information into the classification process but rely on the ability of the algorithm to detect the structures that it is really able to detect, not the ones we would wish. We are thus not limited by the representativeness of the training set, and we consequently avoid all the associated biases. In addition, as shown in Fraix-Burnet et al. (2021), the classification is characterised by the statistical model that we can use for further supervised classifications. This is performed through the E-step only, which is extremely fast. This means that the Fisher-EM algorithm has built its own training set (Fig. 5) that happens to be physically well characterised (Fig. 7).

Our result is a strong encouragement to analyse in more depth the atlas proposed in Fraix-Burnet et al. (2021) and extend it to larger samples. The exciting perspective is to include galaxies at higher redshifts in order to study the evolution of the classification with time through a fully data-driven procedure.

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Article number, page 12 of 18

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Appendix A: Spectra generation

T _{main} (Myr)	$ au_{main}$ (Myr)	f _{burst}	T _{burst} (Myr)	τ _{burst} (Myr)	metallicity	E_BV_lines	E_BV_factor	redshift
9500 10500 11500	500 1000 3000	0		-	0.02 0.05	0.0005 0.01 0.025 0.05 0.075 0.1	0.25	0.001 0.002 0.003 0.004 0.005
10000 11000 12000	2000 5000				0.02	0.005 0.077 0.148 0.220 0.363 0.435 0.507 0.578 0.650	0.44	$\begin{array}{c} 0.01 \\ 0.02 \\ 0.03 \\ 0.04 \\ 0.05 \\ 0.06 \\ 0.07 \\ 0.08 \\ 0.09 \end{array}$
6000 10000	5000							0.1 0.2 0.3
5000 7500	5500							0.4 0.5 0.6
4000 6500	4500							0.7 0.8
13000	5000							0
2000 5200	3000	0.001 0.01	20 100	4500				0.8 0.9 1
2000 7000	4000			6000				0.7
2500 7500	4000			7000				0.6
3000 8000	5000			7000				0.5
4000 9000		0.1		8000				0.4
5000 10000	5000 10500			50000				0.1 0.2 0.3
10000 11000 12000	6000 9000			10000				0.01 0.02 0.03 0.04 0.05
6000	5000 8000	0.1 0.25 0.5	5 20 50	11000	0.008 0.02	$\begin{array}{c} 0.005\\ 0.116\\ 0.226\\ 0.337\\ 0.447\\ 0.558\\ 0.668\\ 0.779\\ 0.889\\ 1.000\\ \end{array}$		$\begin{array}{c} 0.03 \\ 0.06 \\ 0.07 \\ 0.08 \\ 0.09 \end{array}$
4000 7200	5000			6500				0.4 0.5 0.6
5000 10000	6000			9000				0.1 0.2 0.3

Table A.1: CIGALE parameters used to generate the data

Appendix B: Results on spectra with added noise

B.1. Parameter distribution

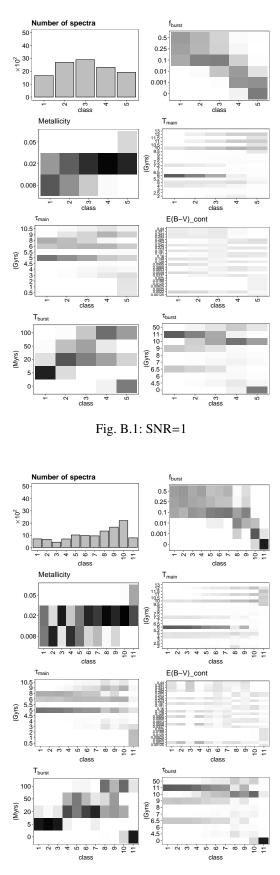


Fig. B.2: SNR=3

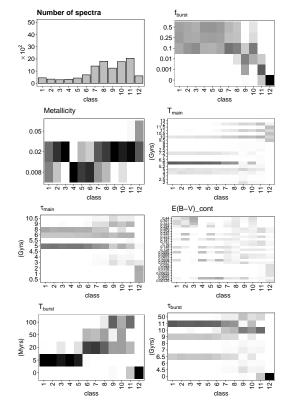


Fig. B.3: SNR=5

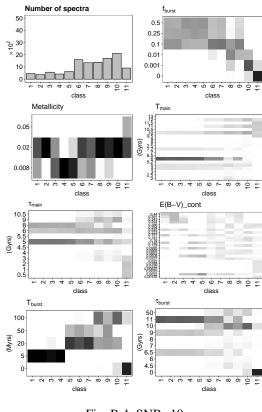


Fig. B.4: SNR=10

Article number, page 14 of 18

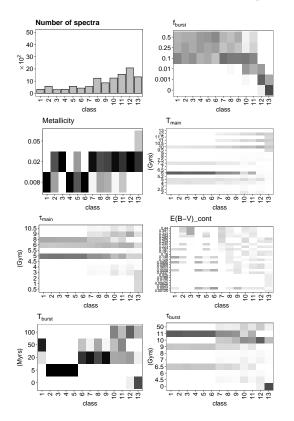


Fig. B.5: SNR=100

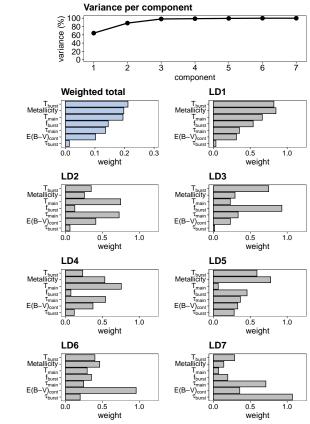


Fig. B.7: SNR=3

B.2. LDA analysis

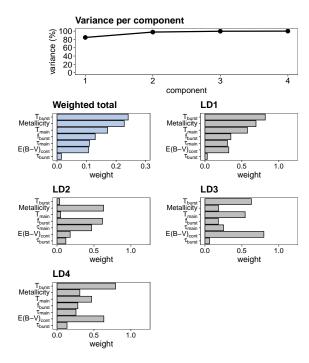


Fig. B.6: SNR=1

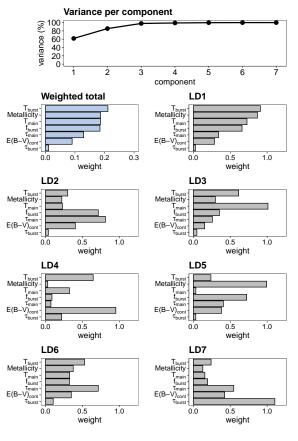
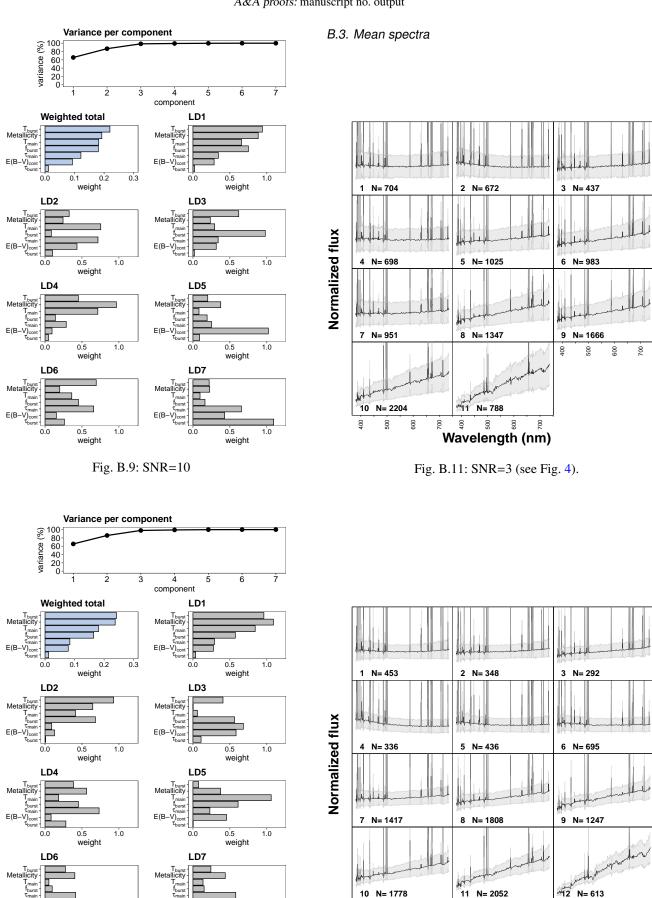


Fig. B.8: SNR=5

Article number, page 15 of 18

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6 200

Fig. B.10: SNR=100

1.0

0.5

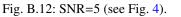
weight

E(B-

0.0

0.5 weight

1.0



8

Wavelength (nm)

8 202 8 200 600 200

200 64

800

Article number, page 16 of 18

0.0

E(B-V)c

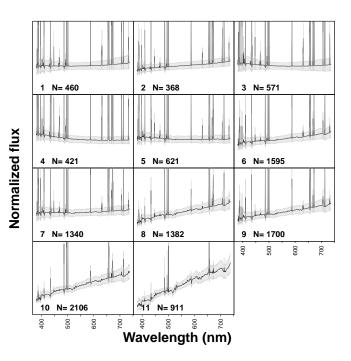
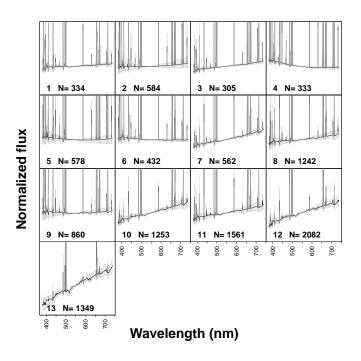
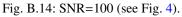


Fig. B.13: SNR=10 (see Fig. 4).





Appendix C: Toy model

To try visualise the conditions for the gap at K=13 in the ICL curve for the noiseless case (Sect. 4.1 and Fig. 2), we constructed a toy model by trials and errors. The simplest sample one can build to reproduce this behaviour is a sample of five variables, and 1000 observations to ensure a perfect reproducibility.

Let us consider the following matrix made with the following five variables:

where VarX[*i* : *j*] designates the indices from *i* to *j* of variable VarX, and $\mathcal{N}(\mu, \sigma^2)$ means that the values are drawn from a normal distribution of mean μ and standard deviation σ .

This sample (Fig C.2) yields a ICL curve Fig C.1 with a gap at K=3 (*Fisher-EM* never converges) and a much higher value at K=4 than at K=2. This behaviour is identical to the one at K=13 in Fig. 2.

Adding a little bit of dispersion in Var2 by increasing σ^2 from 0.01 to 0.05:

Var2[1:300] = N(10, 0.05) Var2[301:1000] = N(15, 0.05)

as represented by the red points in Fig C.2, the *Fisher-EM* analysis always yields a solution (Fig C.3).

This behaviour is thus very similar to the one obtained on the CIGALE sample, and is thus explained by the very peculiar distribution of the observations in the multivariate data space.

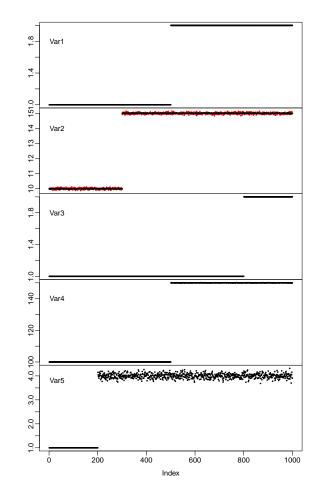
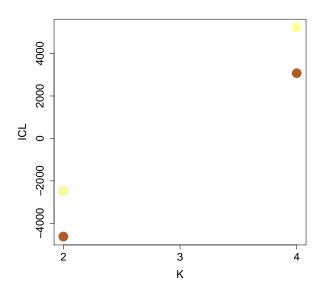


Fig. C.2: The values of the 5 variables for the toymodel with 1000 observations that yield the ICL curve in Fig C.1. The points in red in the second panel (Var2) are the ones with a slightly increased dispersion that yield the ICL curve in Fig C.3.



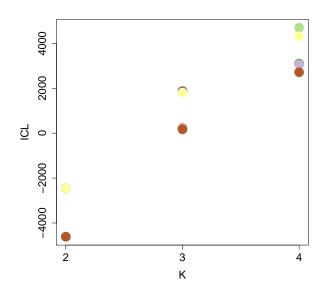


Fig. C.1: All the ICL values as a function of the number of cluster K obtained for the toymodel. Each points correspond to a successful run of *Fisher-EM* for one of the twelve statistical models. This figure should be compared with Fig. 2.

Fig. C.3: Same as Fig. C.1 with the slightly mode dispersed variable Var2.

Article number, page 18 of 18