Multidimensional Data Driven Classification of Active Galaxies

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Outline

1. The Classification Problem
   - The Scientific Problem
   - The Dataset
   - Existing Classification methods
   - Inefficiency of Existing Methods

2. Clustering Methodology
   - Introduction
   - Finite Mixture Models
   - Stylized Facts of the Dataset
   - Proposed Approach
   - Comparing the Classification Schemes

3. Multidimensional Decision Boundaries

4. Discussion
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The Scientific Problem

- **Spectroscopy** is the study of the measurement of radiation intensity as a function of wavelength.
- Spectroscopy has been utilised in identifying the main power source in active galaxies.
The Scientific Problem

Survey: boss Program: boss Target: GAL_LOZ  
RA=235.65078, Dec=0.67420, Plate=4055, Fiber=408, MJD=55359  
z=0.40793±0.00008 Class=GALAXY  
No warnings.

Figure: A selected spectrum from the DR10 BOSS data, showing absorption (red) and emission (blue) lines (http://www.sdss.org).
Based on the different mechanisms that excite the gas inside the galaxies (and which, as a result of those mechanisms, glows in different wavelengths), the Galaxies may be separated, according to Kewley et al (2001):

- **H\textsubscript{II}** region-like galaxies (star forming galaxies, SFG).
- **AGN** (Active Galactic Nuclei) which can be divided further to LINER and Seyferts.
- **Composite** galaxies which exhibit characteristics from both AGNs and SFGs.
The Dataset

- Sloan Digital Sky Survey (SDSS).
- The SDSS is a major multi-filter imaging and spectroscopic redshift survey.
- The latest Data Release (DR 10) the from SDSS-III's Baryon Oscillation Spectroscopic Survey (BOSS) contains 1,848,851 Optical Galaxy spectra.
From early on (see Alloin et al. (1978)), intensity ratios, such as $O_{\text{III}}/H\beta$, have been utilised as means to classify the emission line spectra of galactic $H_{\text{II}}$ region.

Baldwin et al. (1981) proposed three diagnostic diagrams based on four emissions intensities ratios; $\log(N_{\text{II}}/H\alpha)$, $\log(S_{\text{II}}/H\alpha)$, $\log(O_{I}/H\alpha)$ and $\log(O_{\text{III}}/H\beta)$.

Those three diagrams, known as \textbf{Baldwin-Phillips-Terlevich (BPT)} diagrams, were introduced in order to classify the dominant energy source in emission-line galaxies.
Figure: Example diagnostic (BPT) diagram based on observational data from the DR10 BOSS data.
In the **first diagnostic:**

- There are two different loci of sources; a stream moving from the bottom middle to the top left and another fuzzier stream moving from the bottom middle to the top right.
- The first stream corresponds to the star-forming galaxies and the latter to the AGN.

The **second and third diagnostics** verify that the AGN are made up of two groups, the Seyfert and the LINER.
Kewley et al. (2001) introduced a maximum ‘starburst’ line on the BPT diagrams. This line (red line in the next slide) defines the upper limit of the star-forming galaxies and was developed using theoretical models.

Kauffmann et al. (2003) presented an empirical line to distinguish the pure SFGs from Seyfert- SFG composite objects (cyan dashed line in the next slide).

The spectra of those composite galaxies contain significant contributions from both AGN and star-formation according to Kewley et al. (2006).
Existing Classification methods

**Figure:** Diagnostic (BPT) diagram based on observational data from the DR10 BOSS data with the maximum ‘starburst’ line (red) and composite line (cyan) plotted.
The theoretical model of Kewley et al. (2001) fails to distinguish the AGN from the star-forming galaxies. The use of the three diagnostics independently of each other often gives contradicting classification for the same source. In Kewley et al. (2006), 8 percent of the galaxies in their sample are characterized as ambiguous galaxies.

We propose a new soft clustering scheme, the soft allocation data driven method (SoDDA), for classifying galaxies using emission-line ratios.
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Introduction

Cluster analysis is a statistical method that aims to partition a dataset into subgroups so that the members within each subgroup are more homogeneous (according to some criterion) than the population as a whole.

The Probabilistic (model-based) algorithms assume that the data is an i.i.d. sample from a population described by a density function, which is taken to be a mixture of component density functions.

It is common to assume that the mixture components are all from the same parametric family, such as the normal.
Finite Mixture Models

Given data $x$ ($n \times p$) with independent multivariate observations $x_1, \ldots, x_n$, the joint density for a Finite Mixture model with $K$ components:

$$p(x|\theta, \pi) = \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k f_k(x_i|\theta_k), \quad (1)$$

where $f_k$ and $\theta_k$ are the density and parameters of the component $k$ in the mixture model and $\pi_k$ is the probability that an observation comes from the component $k$. Furthermore, $\pi_k \geq 0$ and $\sum_{i=1}^{K} \pi_k = 1$. 
Dempster et al. (1977) proposed a framework for computing the maximum likelihood estimators in finite mixture models for a general specification of the component density functions $f_k$ using the Expectation-Maximization (EM) algorithm.

- The EM algorithm is an iterative method for posterior mode finding.
- Given a statistical model consisting of a set $x$ of observed data, a set of unobserved latent data or missing values $z$, and a vector of unknown parameters $\theta$, the EM alternates between performing an expectation (E) step and a maximization (M) step.
In the context of **Finite Mixture models** Dempster et al. (1977):

- Introduced an unobserved vector $z (n \times K)$, where $z_i$ is the indicator vector of length $K$ with $z_{ik} = 1$ if the observation $x_i$ belongs to cluster $k$ and 0 otherwise.
- The $z$’s are latent variables that specify from which component each observation is drawn.
The joint distribution $p(x, z|\theta, \pi) = p(z|\theta, \pi)p(x|z, \theta, \pi)$.

- $p(z|\theta, \pi)$ is multinomial distribution $p(z|\theta, \pi) = \prod_{k=1}^{K} \pi_{zk}$, $\theta = (\theta_1, ..., \theta_K)$ and $\pi = (\pi_1, ..., \pi_K)$.
- Conditional on $z_{ik} = 1$, $x_i \sim f_{k}(x_i|z_{ik} = 1, \theta_k)$.

The resulting complete-data log-likelihood (the likelihood of both the observed and missing data) is:

$$
\ell(\theta, \pi|x, z) = \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} \log[\pi_{k} f_{k}(x_i|\theta_k)]
$$
The Multivariate Gaussian mixture model has been used with success for many clustering problems. Multivariate normal mixtures can be used for data with varying structures due to the flexibility in how we define the covariance matrices.

The Multivariate Normal distribution is defined as:

\[
f(x_1, \ldots, x_p) = \frac{1}{\sqrt{(2\pi)^p|\Sigma|}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu)\right)
\]
Fraley et al. (2002) pointed out that data generated by mixtures of multivariate normal distributions are characterized by clusters centered at the means $\mu_k$ with increased density for points closer to the means.

The practical use of multivariate mixture models is limited for data that exhibit non-normal features, including asymmetry, multi-modality and heavy tails as in the SDSS dataset.
Non Gaussian Features of the Dataset

- The distribution of the Star forming Galaxies (the HII-region) is clearly highly skewed and not-linear (curve-shaped).
- In the LINER and Seyfert clusters, the mass doesn’t seem to be concentrated at the centers.
- There seems to be a big overlap between the 4 different clusters.
Fitting $K$ Multivariate Normal Distributions

- We use a mixture of MG distributions with $K$ considerably larger than the actual number of galaxy classes.
- This allows a great deal of flexibility in the class-specific distributions of emission line ratios.
- Then we perform hyper-clustering of the $K$ MG distributions so as to concatenate them into subpopulations representing the four desired galaxy classes.
The number \((K \gg 4)\) of MG distributions that we fit to our data is chosen using the Bayesian Information Criterion (BIC).

**Figure:** The Bayesian Information Criterion (BIC) computed over a grid of values of \(K\) (using increments of 5) using the data of the SDSS DR 10.
Fitting 20 Multivariate Normal Distributions

Figure: The BPT diagnostic diagrams for the SDSS DR10 sample; each datapoint is coloured according to its most probable allocation to one of the 20 multivariate Gaussian Distributions.
SoDDA accomplishes the hyper-clustering of the $K$ subpopulations into the four galaxy classes using the classification scheme of Kewley et al. (2006).

We treat the fitted subpopulations means $(\mu_1^*, ... , \mu_K^*)$ as a dataset and classify them into the four galaxy classes.

Thus, we define the distribution of the emission line ratios for each galaxy class as a finite mixture of MG distributions.
Combining the 20 Multivariate Normal Distributions

**Table**: The suggested classification of the 19 subpopulations means.

<table>
<thead>
<tr>
<th>Class</th>
<th>Subpopulation ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>SFG</td>
<td>1,2,5,6,7,8,11,13,14,15,17,18</td>
</tr>
<tr>
<td>Seyferts</td>
<td>3,10,20</td>
</tr>
<tr>
<td>LINER</td>
<td>9</td>
</tr>
<tr>
<td>Composites</td>
<td>12,16,19</td>
</tr>
</tbody>
</table>

We opted to discard cluster 4. It is located in a different region on each one of the three diagnostic diagrams and inspection of the optical spectra of several of the sources allocated to this cluster, shows that they have very broad emission lines with complex structure, resulting in unreadable line measurements.
The Classification Problem
Clustering Methodology
Multidimensional Decision Boundaries
Discussion

Combining the 20 Multivariate Normal Distributions

Figure: Combining the 20 multivariate Normals in the SDSS dataset as explained above and plotting each datapoint with different color according to the most probable allocation.
Figure: A 3-dimensional projection of the SDSS DR10 sample on the \( \log(N_{\text{II}}/H\alpha), \log(S_{\text{II}}/H\alpha), \) and \( \log(O_{\text{III}}/H\beta) \) volume, in which each datapoint is plotted with different colour according to the allocation from SoDDA.
The theoretical Classification

**Figure**: The SDSS dataset in which each datapoint is plotted with different color according to the classification scheme of Kewley et al. (2006).
Table: A 3-way classification table that compares the SoDDA classification with the standard, 2-dimensional classification scheme Kewley et al. (2006). Each cell has 3 values: the number of galaxies with (i) $\rho_{ic} \geq 75\%$, (ii) $50\% \leq \rho_{ic} < 75\%$, and (iii) $\rho_{ic} < 50\%$, where $\rho_{ic}$ is the posterior probability that galaxy $i$ belongs to galaxy class $c$ under SoDDA.
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4-dimensional Linear Decision Boundaries

- The multidimensional decision boundaries implied by SoDDA can be obtained using support vector machine (SVM).
- A SVM is a discriminative classifier formally defined by a separating hyperplane.
- Given classified galaxies, the algorithm outputs an optimal hyperplane which can be used to categorise new unlabelled galaxies.
### 4-dimensional Linear Decision Boundaries

**Table:** Comparing the classifications of SoDDA with that of the 4-dimensional SVM.

<table>
<thead>
<tr>
<th></th>
<th>SVM</th>
<th>SoDDA</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SFGs</td>
<td>Seyferts</td>
<td>LINERs</td>
<td>Composites</td>
<td>Total</td>
</tr>
<tr>
<td>SFGs</td>
<td>69794</td>
<td>0</td>
<td>0</td>
<td>573</td>
<td>70367</td>
</tr>
<tr>
<td>Seyferts</td>
<td>3</td>
<td>7033</td>
<td>59</td>
<td>273</td>
<td>7368</td>
</tr>
<tr>
<td>LINERs</td>
<td>0</td>
<td>20</td>
<td>2703</td>
<td>143</td>
<td>2866</td>
</tr>
<tr>
<td>Composites</td>
<td>391</td>
<td>253</td>
<td>132</td>
<td>7478</td>
<td>8254</td>
</tr>
<tr>
<td>Total</td>
<td>70188</td>
<td>7306</td>
<td>2894</td>
<td>8467</td>
<td></td>
</tr>
</tbody>
</table>
3-dimensional Linear Decision Boundaries

- The $[O_1]$ line is generally hard to observe.
- Thus, we fit the SVM algorithm to the SDSS DR10 dataset using the classifications from SoDDA and only the 3 emission line ratios $\log(N_{II}/H\alpha)$, $\log(S_{II}/H\alpha)$, and $\log(O_{III}/H\beta)$
3-dimensional Linear Decision Boundaries

Table: Comparing the classifications of SoDDA with that of the 3-dimensional SVM.

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<tr>
<td></td>
<td>SFGs</td>
<td>SFGs</td>
</tr>
<tr>
<td></td>
<td>Seyfert</td>
<td>Seyferts</td>
</tr>
<tr>
<td></td>
<td>LINERs</td>
<td>LINERs</td>
</tr>
<tr>
<td></td>
<td>Composites</td>
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</tr>
<tr>
<td></td>
<td>Total</td>
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</tr>
<tr>
<td>SFGs</td>
<td>70188</td>
<td>69746</td>
</tr>
<tr>
<td>Seyferts</td>
<td>7306</td>
<td>0</td>
</tr>
<tr>
<td>LINERs</td>
<td>2894</td>
<td>7</td>
</tr>
<tr>
<td>Composites</td>
<td>8467</td>
<td>808</td>
</tr>
<tr>
<td>Total</td>
<td>8108</td>
<td>70561</td>
</tr>
</tbody>
</table>
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- We propose a new soft clustering scheme, the soft allocation data driven method (SoDDA), for classifying galaxies using emission-line ratios.
- The main advantages of this method are the use of all four optical-line ratios simultaneously.
Further Research Direction

- Extend to include **additional diagnostic lines** (e.g. OII or IR lines PAH, OIV, NeII) information in other wavamebds (e.g. combination of optical line ratios with IR colours such as the Stern or Donley diagnostics, or flux ratios in different wavelengths (e.g. X-ray to optical ratio).

- Use SoDDA in order to create log $N$ – log $S$ **diagrams** for AGNs and star-forming Galaxies.
Thank you!

Many Thanks to:

David van Dyk
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Vinay Kashyap
Bibliography


