STEPS TOWARD A CLASSIFIER FOR THE VIRTUAL OBSERVATORY. I. CLASSIFYING THE SDSS PHOTOMETRIC ARCHIVE.

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Modern photometric multiband digital surveys produce large amounts of data that, in order to be effectively exploited, need automatic tools capable to extract from photometric data an objective classification.

We present here a new method for classifying objects in large multiparametric photometric data bases, consisting of a combination of a clustering algorithm and a cluster agglomeration tool. The generalization capabilities and the potentialities of this approach are tested against the complexity of the Sloan Digital Sky Survey archive, for which an example of application is reported.

1. Introduction

In the last few years the astronomical community is experiencing a tremendous growth in the size, quality and accessibility of databases. This trend will accelerate in the coming years due to the advent of large dedicated survey telescopes and to the implementation of the International Virtual Observatory infrastructure. There
is the practical fact that the extraction of useful information from such datasets cannot be effectively performed with traditional tools, and from the methodological point of view, the wealth of information contained in such huge data sets imposes to abandon old conceptual schemes largely based on the 3-D visualization capability of human minds and to adopt "ad hoc" statistical pattern recognition, classification and visualization methods. The application of such algorithms to the astronomical case is all but trivial, due to the complexity of astronomical data which usually present strong non-linear correlations among parameters and are highly degenerate. Among the other tools, especially relevant to the astronomical case are those which deal with the identification and visualization of groups of objects sharing the same physical properties.

2. The methods

The method outlined here follows a hierarchical approach which, starting from a preliminary clustering performed using a clustering algorithm, the "Probabilistic Principal Surfaces", followed by a second phase that uses the Negative Entropy concept and a dendrogram structure to agglomerate the clusters found in the first phase.

2.1. PPS - Principal Probabilistic Surfaces

Probabilistic Principal Surfaces (PPS) are a nonlinear extension of principal components, in that each node on the PPS is the average of all data points that projects near/onto it. PPS define a non-linear, parametric mapping $y(x; W)$ from a $Q$-dimensional latent space ($x \in \mathbb{R}^Q$) to a $D$-dimensional data space ($t \in \mathbb{R}^D$), where normally $Q \ll D$. The function $y(x; W)$ (defined continuous and differentiable) maps every point in the latent space to a point into the data space. Since the latent space is $Q$-dimensional, these points will be confined to a $Q$-dimensional manifold non-linearly embedded into the $D$-dimensional data space. In our method, the points belonging to the parameter space will be projected on the surface of 2-dimensional sphere. The visualization capabilities of the PPS can prove very useful in several aspects of the data interpretation phase such as, for instance, the localization of data points lying far away from the more dense areas (outlayers), or of those lying in the overlapping regions between clusters, or to identify data points for which a specific latent variable is responsible.

2.2. NEC - Negentropy Clustering

Most unsupervised methods require the number of clusters to be provided a priori, a serious problem when exploring large complex data sets where the number of clusters can be very high or unpredictable. A simple threshold criterion is not satisfactory in most astronomical applications due to the high degeneracy and the noisiness of the data which lead to erroneous agglomeration, while a different approach based on the
combination of a similarity criterium based on the concept of Negative Entropy and the use of a dendrogram as agglomerative algorithm is achievable. We implement the Fisher’s linear discriminant which is a classification method that first projects high-dimensional data onto a line, and then performs a classification in the projected one-dimensional space \(^2\). On the other hand, we define the differential entropy \(H\) of a random vector \(y = (y_1, \ldots, y_n)^T\) with density \(f(.)\) as \(H(y) = \int f(y) \log f(y) dy\) so that negentropy \(J\) can be defined as \(J(y) = J(y_{\text{Gauss}}) - H(y)\), where \(y_{\text{Gauss}}\) is a Gaussian random vector of the same covariance matrix as \(y\). The Negentropy can be interpreted as a measure of non-Gaussianity and, since it is invariant for invertible linear transformations, it is obvious that finding an invertible transformation that minimizes the mutual information is roughly equivalent to finding directions in which the Negentropy is maximized. Our implementation of the method use approximations of Negentropy that give a very good compromise between the properties of the two classic non-Gaussianity measures given by kurtosis and Negentropy. Negentropy can be used to agglomerate with an unsupervised method the clusters (regions) found by the PPS approach. The only \textit{a priori} information is a dissimilarity threshold \(T\). We suppose to have \(c\) multi-dimensional regions \(X_i\) with \(i = 1, \ldots, c\) that have been defined by the PPS approach, then passing these regions to the Negentropy Clustering algorithms which, in practice, measures whether two clusters could or could not be modeled by one single Gaussian or, in other words, if the two regions can be considered to be aligned or as part of a greater data set.

3. The data

All data used in this work are extracted from the Data Release 4 of the Sloan Digital Sky Survey \(^3\). This spectroscopic subsample will constitute the "knowledge base" on which we have founded the labelling of the unsupervised ones. The SDSS also provides, for each object in the SpS, a spectroscopic classification index called \textit{specClass}. All objects are classified in \textit{specClass} as either a quasar, high-redshift quasar (with \(z > 2.2\) ), galaxy, star, late-type star, or unknown (ranging in value of \textit{specClass} from 0 to 6) by matching emission lines found in the observed spectrum against a list of common galaxies and quasar emission lines. We have extracted from the SDSS-4 spectroscopic subsample a catalog containing \(\sim 600000\) objects, excluding from the query only the objects labelled as ‘SKY’ according to \textit{specClass}. The percentage distribution of the resulting sample respect to the \textit{specClass} index is the following: \textit{specClass} 0: 1.5\%, \textit{specClass} 1: 8.5\%, \textit{specClass} 2: 78.7\%, \textit{specClass} 3: 8\%, \textit{specClass} 4: 0.1\%, \textit{specClass} 6: 2.8\%. Furthermore we excluded from this sample drawn from the spectroscopical SDSS-DR4 data all objects fainter than \(r=18\), thus obtaining \(\sim 43000\) records.

4. The experiment

The unsupervised clustering method here presented is based on the combined use of PPS and NEC algorithms. We first applied the PPS algorithm to the sample of
spectroscopically selected SDSS DR-4 objects using as parameters for the clustering the 4 colors obtained from model magnitudes \((u-g, g-r, r-i, i-z)\) of SDSS archive. We fixed the number of latent variables and latent bases of the PPS to 614 and 51 respectively, so obtaining at the end of this step 614 clusters, each formed by objects which only respond to a certain latent variables. We chose a large number of latent variables in order to obtain an accurate separation of objects and to avoid that any group of distinct but near points in the parameter space could be projected in the same cluster by chance. The clusters so found by PPS algorithm are graphically represented by groups of points with the same color (a different color for each cluster) on the surface of a 2-d sphere embedded in the 3-dimensional latent space. These groups of objects are then input to the totally unsupervised agglomeration NEC algorithm, whose only free parameter is the dissimilarity threshold \(T\), as above mentioned. We performed a plateau analysis to determine the optimal value of this threshold: we performed different experiments with \(T\) varying over a wide range, then selected the central value of intervals of \(T\) for which the number of final clusters is constant. The number of clusters resulting from the NEC aggregation is 31. We present in table (1) a collection of the most interesting of these clusters after labelling each object with its \(\text{specClass}\) index.

| Cl. n | SP0 | SP1 | SP2 | SP3 | SP4 | SP6 |
|-------|-----|-----|-----|-----|-----|-----|
| 1     | 69  | 145 | 9362| 48  | 0   | 12  |
| 2     | 25  | 133 | 13370| 10  | 0   | 12  |
| 3     | 149 | 132 | 63  | 64  | 0   | 5   |
| 4     | 44  | 3396| 1530| 189 | 67  | 1   |
| 5     | 202 | 85  | 447 | 2428| 6   | 10  |
| 6     | 26  | 125 | 13728| 12  | 0   | 12  |
| 7     | 0   | 0   | 0   | 0   | 0   | 484 |
| 8     | 1   | 1   | 1   | 0   | 0   | 329 |
| 9     | 541 | 1507| 127 | 4750| 18  | 1   |
| 10    | 89  | 474 | 2117| 19  | 4   | 529 |

5. Conclusions

As can be seen from table (1), different groups of clusters, according to their \(\text{specClass}\) composition, are found. There is a significant fraction of clusters dominated by just one kind of \(\text{specClass}\) objects and contaminated by few objects flagged with different values of \(\text{specClass}\). Otherwise, other clusters show a quite homogeneous mixture of spectral type objects, with a prominence of stars\((\text{specClass}=1,6)\) - quasars\((\text{specClass}=3,4)\) and galaxy\((\text{specClass}=2)\) - unknown\((\text{specClass}=0)\) mixtures. Only few clusters show comparable proportions of all objects. A more profound analysis of these mixed clusters and the comparison between the colours and
other photometric and spectroscopic informations for the same objects will hopefully cast light upon the associations between objects with different values of $\text{specClass}$, and remove the degeneracy in the colour space.

References
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