

A Comparative Study of KBS, ANN and Statistical Clustering Techniques for Unattended Stellar Classification

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Abstract. The purpose of this work is to present a comparative analysis of knowledge-based systems, artificial neural networks and statistical clustering algorithms applied to the classification of low resolution stellar spectra. These techniques were used to classify a sample of approximately 258 optical spectra from public catalogues using the standard MK system. At present, we already dispose of a hybrid system that carries out this task, applying the most appropriate classification method to each spectrum with a success rate that is similar to that of human experts.

1 Introduction

This work is part of a global project devoted to the study of the last phases of stellar evolution. Our main purpose is the development of an automatic system for the determination of physical and chemical stellar parameters by means of optical spectroscopy and artificial intelligence techniques. This system can contribute to evolutionary studies in Astrophysics that discover and follow the temporal changes of the physical and chemical conditions of stars.

Spectroscopy is a fundamental tool in the analysis of a star's physical conditions (temperature, pressure, density, etc.) and chemical components (H, He, Ca, K, etc.). In general terms, a stellar spectrum consists of a black body continuum light distribution, distorted by the interstellar absorption and reemission of light, and by the presence of absorption lines, emission lines and molecular bands [1].

We have collected a sample of approximately 400 stellar spectra from astronomical observations carried out by several telescopes. The stellar spectra are collected from telescopes with appropriate spectrographs and detectors. Observers collect the flux distribution of each object and reduce these data to obtain a one-dimensional spectrum calibrated in energy flux ($\text{erg-cms}^{-2}\text{-}\text{\AA}^{-1}$) and wavelength (\AA).

In order to extract useful information from the individual spectra and to study the stellar evolution in the whole sample, we must complete a solid and systematic spectral classification in the current Morgan-Keenan system (MK).

The MK classification system was firstly proposed in 1943 by Morgan, Keenan & Kellman, and has experienced many revisions ever since [2]. This two-dimensional system is the only one that is widely used for stellar classification. One of its main advantages is that MK classifications are often static, because they are based on the visual study of the spectra and on a set of standard criteria. However, the same spectra can be classified differently by different experts and even differently by the same person at different times. This classification system quantifies stellar temperatures and levels of luminosity. Stars are divided into groups, i.e. spectral types, that are mainly based on the strength of the hydrogen absorption lines and on the presence or absence of some significant lines of Ca, He, Fe, and molecular bands. The temperature of the stars is divided into a sequence called OBAFGKM, ranging from the hottest (type O) to the coolest (type M) stars. These spectral types are further subdivided by a decimal system, ranging from 0 (hottest) to 9.5 (coolest). In addition, a luminosity class (from I to V) is assigned to the star, which depends on the intrinsic stellar brightness.

Table 1 illustrates the main properties of each spectral type in the MK standard classification system.

Table 1. Main spectral features in the MK system

Type	Color	Prominent Lines
O	Bluest	Ionized He
B	Bluish	Neutral He, Neutral H
A	Blue-white	Neutral H
F	White	Neutral H, Ionized Ca
G	Yellow-white	Neutral H, Strongest Ionized Ca
K	Orange	Neutral Metals (Ca, Fe), Ionized Ca
M	Red	Molecules and Neutral Metals

The estimation of the stellar parameters is often carried out by human experts, who analyse the spectra by hand, with no more help than their own experience. These manual analyses usually lead to a MK classification of the spectra. The manual classification techniques are often based on the visual study of the spectra and on a set of standard criteria [1]. Although this manual method of classification has been used by the researchers and the astrophysicists widely and successfully along the years, it is no longer viable because of the spectacular advance of the objects collection technologies, which allow us to obtain a huge amount of spectral data in a relatively short time. Since the manual classification of all the spectra that are currently available would involve a considerable increase in human resources, it is highly advisable to optimise the manual procedure by means of automatic, fast and efficient computational techniques.

In the course of the last 10 years, research in the field of spectral classification has been focused on either the need for the development of automatic tools, or on the revision and improvement of the manual techniques.

As for the application of artificial intelligence techniques to the design of automatic classification systems, some well-known previous works have also applied artificial neural networks to the problem of stellar classification [3], obtaining

classifications with diverse resolution grades. Our research team has contributed to this research line with the development of various fuzzy experts systems for the classification of super giant, giant and dwarf stars. A complete description of our previous works can be found in [4].

Our intention is not to test models or techniques that have already demonstrated their suitability in this problem, but rather to integrate several models of artificial neural networks and clustering algorithms with our previous expert systems. Combining all the techniques, we intend to formalise a hybrid system able to determine the most appropriate method for each spectrum type and to obtain on-line MK classifications through an Internet Stellar Database (<http://starmind.tic.udc.es>).

2 Classification Techniques

The following sections start by describing the spectral data that were used to train and test the automatic classification techniques. Secondly, we describe the morphological analysis algorithms that were applied to the spectra before presenting them to the automatic techniques. Finally, we present the different neural networks and clustering algorithms that were tested and we contrast their results.

2.1 Astrophysical Data

We have chosen a complete and consistent set of spectra in order to design and test the neural networks and clustering algorithms that will be applied to the problem of stellar classification.

The 258 selected spectra proceed from the public catalogues of Silva [4] (28 spectra sampled in the range of 3500 to 8900 Å with 5 Å of spectral resolution), Pickles [1] (97 spectra sampled in the range of 1150 to 25000 Å with 5 Å of spectral resolution) and Jacoby [5] (133 spectra sampled in the range of 3510 to 7426 Å with 1.4 Å of spectral resolution). The selected spectra cover all the types and luminosities of the MK system and are sufficiently representative, because they offer a continuous transition of the spectral features between each spectral type and its adjacent types. These spectra were previously analyzed and corrected by human experts that collaborate in the project.

In order to guarantee the generalization of the designed networks and algorithms, we have built the training set with approximately 50% of the spectra of each spectral type, leaving around 15% of them to validate the training and the remaining 35% to evaluate the classification capability of each model.

The neural networks and the clustering techniques of this experimentation have been designed and tested so as to consider both full spectra and spectral parameters as input patterns. Before presenting the spectra to the automatic techniques, we carry out a morphological analysis of all the spectra in order to obtain the values of the parameters that characterize each spectrum separately.

2.2 Morphological Analysis

The patterns that are presented to both neural networks and clustering algorithms were obtained automatically by using signal processing techniques to measure the

spectral peculiarities (absorption and emission lines, spectral energy, molecular bands, etc.).

In particular, we measure the 25 spectral features that are described in Table 2. These spectral parameters can be grouped into three general types:

- Absorption and emission lines: including hydrogen, helium and metallic lines (Ca, K).
- Molecular bands: hydrogen and carbon absorption bands.
- Rates between lines: CH-K rates, He-H rates, etc.

Table 2. Spectral classification parameters

Parameter	Description	Parameter	Description
Band 1	$5005 \pm 055 \text{ \AA}$	Line H Iδ	4102 \AA
Band 2	$6225 \pm 150 \text{ \AA}$	Line He I	4026 \AA
Band 3	$4435 \pm 070 \text{ \AA}$	Line He II	4471 \AA
Band 4	$5622 \pm 180 \text{ \AA}$	Line H Iβ	4861 \AA
Band 5	$5940 \pm 135 \text{ \AA}$	Line H Iα	6563 \AA
Band 6	$6245 \pm 040 \text{ \AA}$	Main Bands	$\sum_{i=1}^{i=2} Band_i$
Band 7	$6262 \pm 130 \text{ \AA}$	Secondary Bands	$\sum_{i=3}^{i=9} Band_i$
Band 8	$6745 \pm 100 \text{ \AA}$	Rate K-H	Ca II K / Ca II H
Band 9	$7100 \pm 050 \text{ \AA}$	Rate CH- H Iγ	CH band / H I γ
Line Ca II (K)	3933 \AA	Rate H Iδ - HeI	H I δ / He I
Line Ca II (H)	3968 \AA	Rate H Iδ - HeII	H I δ / He II
Line CH band	4300 \AA	Energy	Flux Integral
Line H Iγ	4340 \AA	Line H Iδ	4102 \AA

The signal processing algorithms used to obtain the spectral parameters are mainly based on the spectral continuum estimation and the energy measurement.

From a morphological point of view, an absorption line is a descending (ascending for emission) deep peak that appears in an established wavelength zone. As mentioned, the absorption/emission lines are supposed to appear in a fixed wavelength, but due to the spectrum displacement caused by the measuring instruments, they can be found in the previous or next sample. To accurately calculate the intensity of each line, we carry out an estimation of the local spectral continuum. We smoothen the signal with a low pass filter, excluding the peaks in an interval around the sample where the line was detected. This filter is implemented by a five-point moving average method that selects the five more stable fluxes. That is

$$C_j = \left(\frac{\sum_{i=j-n}^{j+n} E_i * X_i}{N} \right) \quad (1)$$

where C_j is the estimation of the continuum for sample j , E_i is the flux in sample i , N is the number of values used in the moving average method to calculate the local spectral continuum, and X is a binary vector that indicates the representative fluxes of the spectral continuum in the zone. This means that $X_i = 1$ if E_i is a flux value representative of the local spectral continuum, and $X_i = 0$ if E_i is a peak. The intensity is positive for the absorption lines and negative for the emission lines.

A molecular band is a spectral zone where the flux suddenly decreases from the local continuum during a wide λ interval. For the molecular bands this means that we only have to measure their energy to decide if they are significant enough. In this case, the upper threshold line for each band is calculated by means of linear interpolation between the fluxes in the limits of the interval defined for each band. Then, the area between this line and the axis of abscissas is calculated with discrete integral; the area that surrounds each band is calculated by integrating the flux signal between the extremes of the band. Finally, the flux of the band is obtained by subtracting both calculated energies. That is

$$B_{lr} = \int_l^r L(\lambda_i) - \int_l^r E(\lambda_i) \quad (2)$$

where B_{lr} is the flux of the band between the samples l and r , L is the projection line, E is the flux function, λ the wavelength, l the left limit of the band and r the right limit. Since the obtained value becomes more negative as the band becomes deeper and wider, positive or negative values close to zero are not considered as bands.

The sampling frequency of the input spectra is not limited because we developed a simple algorithm that automatically resamples them; this increases the flexibility and avoids losing spectral resolution because of format reasons.

Although most of the spectra are uniformly sampled, some of them have zones where there is no flux. This lack of information is generally due to the atmospheric effects and to the resolution of the measuring instruments. With the purpose of correcting the spectra and covering all the spectral ranges, we have elaborated an algorithm that reproduces the experts' behaviour in this specific situation. It is based on the interpolation of the energy flux in the wavelengths that belong to void zones.

After having scaled and adapted the spectra, the system carries out an exhaustive analysis of the most relevant spectral features, i.e., molecular bands and absorption/emission lines, using the signal processing algorithms described above. These algorithms have been implemented in a software module, the spectral analyzer, that is equipped with signal processing techniques to extract and measure the main spectral features of each spectrum. It is developed in C++ and integrates ad hoc ActiveX components for the visualization of spectra.

In this module we have also elaborated other algorithms to estimate the flux of some additional spectral features that are not directly considered in the manual process, e.g. the spectral energy. These features have been examined to find out their capacity to classify spectra.

We use both the spectral parameters obtained by the spectral analyzer module and the full spectral data to build the input patterns of the neural networks and clustering techniques.

In order to implement the neural networks we used the Stuttgart Neural Network Simulator (SNNS v.4.1), and we developed the clustering algorithms by using MATLAB v.6.5.1. After analyzing the performance of both techniques, we implemented the best models in C++ by integrating them with the spectral analyzer, which allow us to obtain a unique tool for processing and classifying the optical spectra of stars.

2.3 Knowledge Based Systems

This first approach proposes the implementation of a knowledge-based system that provides the user with a comfortable tool for the processing of stellar spectra. We have integrated signal processing, knowledge-based and fuzzy techniques, obtaining a very satisfactory emulation of the current manual process. This approach results in two classification modalities: spectra with no given luminosity class, and spectra of stars with a well-known luminosity level.

As a previous step towards the design of the expert system, we carried out a sensibility analysis of the classification parameters in order to define the different fuzzy sets, variables and membership functions. In this study, we have analysed the parameters of the spectra from the reference catalogue, using the aforementioned algorithms and determining the different spectral types that each parameter discriminates. Some parameters that seemed to be suitable were discarded, whereas others, which are not explicitly considered in the manual classification, were included, for example the additions of band fluxes: no molecular band, by itself, was found suitable to determine the global temperature (early, intermediate, late) for all the stars in the reference catalogue; however, we found a good discriminant between early, intermediate and late stars, which is the addition of several relevant bands. This new parameter can divide the stars from the catalogue into the three global temperature groups: since some stars that belong to the same group present a greater value in some bands, and in other stars the highest value corresponds to a different band, the addition solves these problems.

As a final result of this analysis, we have defined as many fuzzy variables as classification levels (global, type and subtype) for each luminosity class; we have also defined the fuzzy sets and membership functions determined by the values of the spectral features in the guiding catalogue spectra.

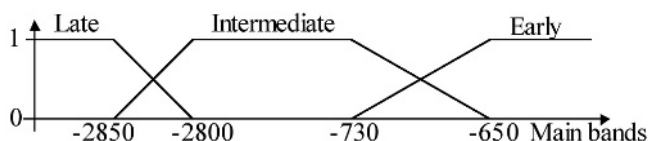


Fig. 1. Membership function for global classification in luminosity I

The developed expert system stores the information that is necessary to initiate the reasoning process in the facts base. This descriptive knowledge of the spectra is represented by means of frames [8], i.e. objects and properties structured by levels. This model was chosen because it is the simplest and most adequate to transfer the analysis data to the classification module and allows us to establish the equivalence

between analysis data and knowledge. The knowledge of the facts base includes general information, such as the names of the stars, and the results of the morphological analysis, i.e. the values of the classification parameters.

The real parameters of spectral classification and the limit values of each type and subtype were included in the expert system in the shape of fuzzy rules. The rules base is that part of the system where the human classification criteria are reproduced. We have adopted IF-THEN production rules for the implementation of this module, because they allow us to manage the uncertainty and imprecision that characterise human reasoning in this field.

The conditions of these rules refer to the values of the parameters stored in the current facts base (working memory). The conclusions allude to three levels of spectral classification: global (late, intermediate, early), spectral type and luminosity, and as such, the module communicates actively with the facts base.

To decide what rule to apply at each moment, we used the Means-End Analysis strategy (MEA) [9]: basically, among the rules that were incorporated last into the working memory, this strategy chooses the not executed rule that has the largest number of patterns. The production rules are linked in a forward reasoning, guided by objectives. The strategy used for the reasoning process combines guided reasoning methods with a method based on truth values. The rules also have associated credibility factors that were obtained from interviews with experts and from the bibliography of this field.

We used the Shortliffe and Buchanan methodology [10] to create an evolution that includes fuzzy sets and membership functions that are contextualized for each spectral type and allow superposition between them. The applied inference method is Max-product, which combines the influence of all the active rules and produces a smooth, continuous output. In our approach, the credibility factor of each rule has also been considered as another truth value. The defuzzification of the data into a crisp output was accomplished by the fuzzy-centroid method [11]. With this mixed strategy, we achieved a remarkable adaptation to human reasoning, able to successfully handle the imprecision and uncertainty implicit in the manual classification process. In addition, we obtained the spectral classification of stars with a probability value that indicates the grade of confidence.

This part of the spectral classifier was developed in OPS/R2 [12] and integrated with the analyzer by means of dynamic link libraries (DLL).

An additional research topic consisted in improving the implemented system by applying the results of the best neural models, and will be described in the next sections. The weights of the output layer units were analyzed so as to determine, for each spectral type, which input parameters have more influence on the output. The normalized values of the higher weights were included in the expert system in the shape of credibility factors of the rules that correspond to the most influential parameters for each spectral type. This modification of the reasoning rules (using the weights values of the trained neural networks) resulted in a slightly significant improvement of the performance of the original expert systems (around 2%).

2.4 Artificial Neural Networks

The neural networks of this approach are based on both supervised and non-supervised learning models. In particular we have implemented Backpropagation,

Kohonen and Radial Basis Functions (RBF) networks. The topologies, the learning functions and the results obtained by these networks are described below.

2.4.1 Backpropagation Networks

Backpropagation is a supervised learning algorithm that belongs to the general feed-forward model. This model is based on two stages of learning: forward propagation and backward propagation.

Training a feed-forward neural network with supervised learning consists of presenting a set of input patterns that are propagated forward by the net until activation reaches the output layer. This constitutes the so-called forward propagation phase. When the activation reaches the output layer, the output is compared with the teaching input (provided in the input patterns). The error, or difference between the output and the teaching input of a target output unit, is then used together with the output of the source unit to compute the necessary changes of the link between both units. In this way the errors are propagated backwards, which is why this phase is called backward propagation [13].

We have tested the backpropagation learning algorithm for the spectral types and luminosity classes. We used both spectral parameters and full spectral data to train the networks.

Table 3. The topologies for backpropagation networks we implemented

Network	Input Patterns	Hidden Layer
Type	Spectral parameters	10
Type	Spectral parameters	5x5
Type	Spectral parameters	10x10
Type	Spectral parameters	10x5x3
Type	659 flux values	100x50x10x3
Luminosity	Spectral parameters	10x10
Luminosity	659 flux values	100x50x10x3

The backpropagation topology that has resulted in a better performance corresponds to a network trained with 25 spectral parameters as input layer and three hidden layers of 10, 5 and 3 units.

In the training phase, we used the topological order to update the weights: first the weights of units in the input layer are updated, then the units in the hidden layers and finally the units in the output layer. The weights are initiated randomly with values in the interval $[-1,1]$.

The number of training cycles, the frequency of validation and the values of the learning parameters were changed during the learning phase of the different implemented topologies. Our observations show that the implemented networks converge when MSE (Mean Square Error) is equal or inferior to 0.05 and the net becomes stable. If the training continues after having reached this rate of MSE, the net is over trained and its performance decreases. In the SNNS simulator, an output greater than 0.5 is equivalent to 1, otherwise to 0. In the analysis of the results, we have not considered the outputs near 0.5 as successes (from 0.45 to 0.55).

2.4.2 Kohonen Networks

The Self-Organizing Map (SOM) algorithm of Kohonen is based on non-supervised learning. SOMs are a unique class of neural networks, since they construct topology-preserving mappings of the training data where the location of a unit carries semantic information [14].

Self-Organising maps consist of two unit layers: a one-dimensional input layer and a two-dimensional competitive layer, organized as a 2D grid of units. Each unit in the competitive layer holds a weight vector that, after training, resembles a different input pattern. The learning algorithm for the SOM networks accomplishes two important goals: the clustering of the input data and the spatial ordering of the map, so that similar input patterns tend to produce a response in units that are close to each other in the grid. In the learning process, the input pattern vectors are presented to all the competitive units in parallel, and the best matching unit is chosen as a winner.

We have tested Kohonen networks for the spectral types and luminosity classes, using two-dimensional maps from 2x2 to 24x24 units. The best results for these networks were achieved by maps of 12x12 units.

2.4.3 RBF Networks

Networks based on Radial Basis Functions (RBF) combine non-supervised learning for hidden units and supervised learning in the output layer. The hidden neurons apply a radial function (generally Gaussian) to the distance that separates the input vector and the weight vector that each one stores, called centroid [13].

We have tested the RBF learning algorithm for the spectral types and luminosity classes. The RFB network that has resulted in a better performance corresponds to a network trained with 25 spectral parameters as input layer and 8 neurons in the hidden layer.

Table 4. The topologies for the implemented RBF networks

Network	Input Patterns	Hidden Layer
Type	Spectral parameters	16
Type	Spectral parameters	8
Type	Spectral parameters	4
Type	659 flux values	124
Luminosity	Spectral parameters	8
Luminosity	659 flux values	124

2.5 Clustering Techniques

In order to refine the classifications of the artificial neural networks, we implemented statistical clustering techniques and applied them to the problem of spectral classification, in particular the K-means, Max-Min and Isodata non-hierarchical clustering methods.

At the initial stage of non-hierarchical clustering, we selected an arbitrary number of clusters or groups. The members of each cluster are checked by means of selected parameters or distance measures, and relocated into the more appropriate clusters with higher separability [15]. The K-means algorithm is based on *k* cluster centers chosen

at random, assigning each data item to the closest cluster, recomputing the cluster center (e.g. the centroid of its data items), and looping back to the assignment step if the clusters have not converged. This technique has been applied to large-scale data sets because its time complexity is linear, once the number of clusters k and number of passes has been fixed [16]. The Isodata clustering method is a modification of k-means which adds splitting and merging; at each time step, clusters with variance above a fixed threshold are divided and pairs of clusters with centroids closer than another threshold are merged [15].

The Max-min algorithm is based on the heuristic combination of minimum and maximum euclidean distances. At each iterative step, the algorithm verifies the viability of building a new class with an element sufficiently separated of the already existing classes.

As for the application of clustering techniques to the spectral classification of stars, we have used the spectral parameters obtained by means of the morphological analysis algorithms as well as the full spectra. In addition, we have implemented two different versions of each algorithm with 6 and 12 initial clusters.

Although the implemented clustering methods have achieved remarkable success rates in classifying stellar spectra, we have mainly applied this technique to carry out a sensibility analysis of the spectral parameters used to classify stellar spectra.

3 Results

The application of expert systems, clustering techniques and artificial neural networks has allowed us to elaborate a final comparison. We selected the neural models of each type with the best performance and classified, by means of the clustering algorithms and the expert systems, the 100 spectra that were used to test these networks. Figure 1 contrasts the behavior of the three techniques and that of two human experts who collaborated on this project.

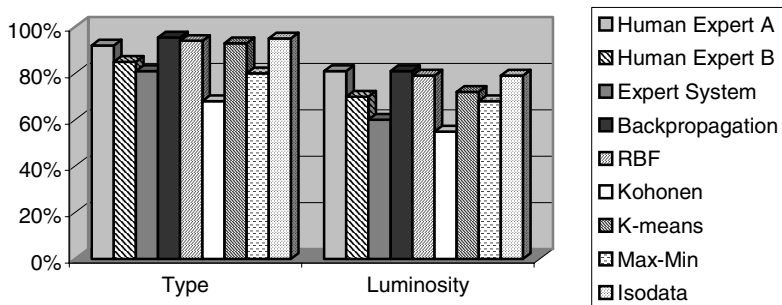


Fig. 2. Final performance for 100 testing spectra

The Backpropagation and RBF networks, as well as K-means and Isodata algorithms, obtained a high success rate of approximately 95%. The Kohonen model obtained a low success rate in all its implementations, which could be due to the size of the training set, since this kind of network has to cluster the data and therefore needs a training set that is big enough to extract similarities and group the data.

Although the final results for the three proposed classification methods seem to be very similar, an exhaustive study has revealed some interesting peculiarities; for example, we have observed that both techniques reached their worst results for B and M spectral types, i.e. the hottest and coolest stars respectively, and indeed, most of the grouping algorithms include these spectra in the same cluster. This fact led us to review the spectral parameters that were being used to train and test the networks and the algorithms: we discovered that B stars usually present great emission lines in zones where a molecular band is expected, so that the automatic techniques are unable to differentiate between them. Our hybrid approach tries to solve these problems by making a previous global classification of the star and then selecting the best method to classify it.

This hybrid strategy consists of choosing, among all the described techniques, those methods that present the best performance for each classification level. The final system is mainly based on an expert system that determines the global type of each star and that, according to the type, sends the spectra to different neural networks or clustering algorithms in order to obtain their spectral type as well as their luminosity level.

The implemented system includes two user-friendly interfaces: a web environment (STARMIND) and another environment under MS-Windows. Both allow the users to select the spectra, visualise them, carry out various analyses and classify as many spectra as they want in a fast, simple and reliable manner.

4 Conclusions

This work has analyzed the classification ability of artificial neural networks, expert system techniques, and statistical clustering techniques applied to stellar spectra. These approaches were integrated into a hybrid system that has resulted in a versatile and flexible automatic technique for the classification of stellar spectra.

Considering the fact that human experts reach an agreement percentage of approximately 87% of the spectra in the course of manual classifications, the success rate of approximately 95% for a sample of 100 testing spectra, obtained by the abovementioned techniques, corresponds to a performance increase of approximately 10%. The additional classification information provided by the clustering techniques refine the parameters used for automatic classifications, especially for cases of spectral types B and M; the implemented clustering techniques make it easier to analyze the sensibility of the spectral parameters used to classify stellar spectra in the neural networks approach.

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