Reliability Checks on the Indo-US Stellar Spectral Library Using Artificial Neural Networks and Principal Component Analysis

Harinder P. SINGH

Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India hpsingh@physics.du.ac.in

Manabu YUASA and Nawo YAMAMOTO

Research Institute for Science and Technology, Kinki University, Higashi-Osaka, Osaka 577-8502 yuasa@rist.kindai.ac.jp

and

Ranjan GUPTA

Inter-University Center for Astronomy and Astrophysics, Ganeshkhind, Pune 411007, India rag@iucaa.ernet.in

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Abstract

The Indo-US coudé feed stellar spectral library (CFLIB) made available to the astronomical community recently by Valdes et al. (2004, ApJS, 152, 251) contains spectra of 1273 stars in the spectral region 3460 to 9464 Å at a high resolution of 1 Å (FWHM) and a wide range of spectral types. Cross-checking the reliability of this database is an important and desirable exercise since a number of stars in this database have no known spectral types and a considerable fraction of stars has not so complete coverage in the full wavelength region of 3460–9464 Å resulting in gaps ranging from a few Å to several tens of Å. We use an automated classification scheme based on Artificial Neural Networks (ANN) to classify all 1273 stars in the database. In addition, principal component analysis (PCA) is carried out to reduce the dimensionality of the data set before the spectra are classified by the ANN. Most importantly, we have successfully demonstrated employment of a variation of the PCA technique to restore the missing data in a sample of 300 stars out of the CFLIB.

Key words: catalogs — methods: data analysis — stars: general

1. Introduction

Automated schemes of data validation and analysis have assumed added significance recently as larger databases are increasingly becoming available in almost all areas of observational astronomy. With the advent of bigger CCD detectors in spectroscopy, the need for having large libraries of stellar spectra at high spectral resolution is also getting fulfilled. Jacoby, Hunter, and Christian (1984, hereafter JHC) made 158 spectra available in the range of 3510-7427 Å at 4.5 Å resolution. Prugniel and Soubiran (2001) published a library of 708 stars using the ELODIE eschelle spectrograph at the Observatoire de Haute-Province that covers a wavelength band of 4100–6800 Å at a resolution of R = 42000. Cenarro et al. (2001) have provided a database of 706 stellar spectra in the wavelength region 8350-9020 Å at 1.5 Å resolution and Le Borgne et al. (2003, hereafter STELIB) with 247 spectra in the range of 3200–9500 Å at 3 Å resolution. Moultaka et al. (2004, hereafter ELODIE) compiled 1959 spectra in the range of 4000–6800 Å at a resolution of 0.55 Å.

More recently, Valdes et al. (2004) observed more than 1200 stars with emphasis on broad wavelength coverage (3400–9500 Å) at a resolution of \sim 1 Å (FWHM) at an original dispersion of 0.44 Å per pixel. Their coudé feed stellar spectral library (CFLIB) provides a resolution sufficient to resolve numerous diagnostic spectral features that can be used in the automated parameterization of spectra.

Neural networks are a form of multiprocessor computing system, with simple processing elements with a high degree of inter-connection, simple scalar messaging, and adaptive interaction between elements. In a supervised back propagation algorithm, the network topology is constrained to be feedforward, i.e., connections are generally allowed from the input layer to the first (and mostly only) hidden layer; from the first hidden layer to the second, ..., and from the last hidden layer to the output layer. The hidden layer learns to recode (or to provide a representation for) the inputs. More than one hidden layer can be used. The architecture is more powerful than single-layer networks: it can be shown that any mapping can be learned, given two hidden layers (of units).

Automated schemes like the Artificial Neural Networks (ANN) have been used in Astronomy for a number of data analysis tasks like scheduling observations (Johnston, Adorf 1992), adaptive optics (Angel et al. 1990), stellar spectral classification (Gulati et al. 1994; von Hippel et al. 1994), and star–galaxy separation studies (Odewahn et al. 1992). In addition Gulati, Gupta, and Rao (1997a) extended the ANN analysis to compare synthetic and observed spectra of G and K dwarfs. Gulati, Gupta, and Singh (1997b) estimated interstellar extinction E(B-V) using ANN from low-dispersion ultraviolet spectra for O and B stars. Bailer-Jones, Gupta, and Singh (2002) provide a review of the ANN applications in astronomical spectroscopy.

Another powerful statistical tool for data analysis is the

Table 1.	ANN	training	and	test	cases.	*
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Case	Training (Library, number of spectra)	Testing (Library, number of spectra)	λ Region	Resolution	Classification error
A1	JHC, 158	CFLIB, 1273	4100–5500 Å	4.5 Å	674.3
A2	JHC, 158	ELODIE, 1959	4100–5500 Å	4.5 Å	514.8
A3	JHC, 158	STELIB, 247	3600–7400 Å	4.5 Å	861.2
B1	ELODIE, 174	ELODIE, 1959	4000–5500 Å	1 Å	496.4
B2	ELODIE, 174	ELODIE, 1959	4000–6800 Å	1 Å	576.0
В3	ELODIE, 174	CFLIB, 1272	4000–5500 Å	1 Å	742.7
B4	ELODIE, 174	CFLIB, 1273	4000–6800 Å	1 Å	848.5
C1	STELIB, 247	CFLIB, 1273	4000–6800 Å	3 Å	643.9
C2	STELIB, 247	CFLIB, 1273	3500–9400 Å	3 Å	670.6
C3	STELIB, 247	ELODIE, 1959	4000–6800 Å	3 Å	501.8

^{*} Two hidden layers were used for all the cases.

principal component analysis (PCA). It involves a mathematical procedure that transforms a number of (possibly) correlated variables into a (smaller) number of uncorrelated variables called principal components. The first principal component accounts for as much of the variability in the data as possible, and each succeeding component accounts for as much of the remaining variability as possible. Objectives of principal component analysis are to discover or to reduce the dimensionality of a data set and to identify new meaningful underlying variables. The technique has been used widely for a number of applications in Astronomy, viz., for stellar classification by Murtagh and Heck (1987), Storrie-Lombardi et al. (1994), and Singh et al. (1998), by Francis et al. (1992) for QSO spectra, and for galaxy spectra by Sodré and Cuevas (1994), Connolly et al. (1995), Lahav et al. (1996), and Folkes, Lahav, and Maddox (1996).

Another important application was developed by Unno and Yuasa (1992, 2000) for supplementing missing observational data using a generalized PCA technique. Subsequently, Yuasa, Unno, and Magono (1999) made use of this technique to determine distances of 183 mass-losing red giants.

The primary aim of this paper is to perform validity checks on the CFLIB by running the ANN code on various inter library sets like JHC, ELODIE, and STELIB. In the next section we describe the ANN analysis. In section 3, we demonstrate the possibility of using PCA for filling the gaps in the spectra of CFLIB. In section 4, we summarize important conclusions of the study.

2. ANN Analysis

A classification scheme using ANN involves two stages: a training stage and a testing stage. In the training stage, the input patterns and the desired output patterns are defined before the learning process of the ANN is carried out. During training, the network output and the desired output are compared and the network weights are adjusted. We employ a back propagation algorithm (Rumelhart et al. 1986) to achieve this. The learning is stopped when the desired error threshold is reached

and the network weights are frozen for use with the test set. In the testing stage, the test patterns are used by the network and classified in terms of the training classes.

In what follows, we have trained the ANN on three libraries with a view to run validity checks on the CFLIB. Three libraries that we used for training are:

- 1. JHC (Jacoby et al. 1984) with 158 spectra available in the range of 3510–7427 Å at 4.5 Å resolution
- ELODIE (Moultaka et al. 2004) with 1959 spectra in the range of 4000–6800 Å at a resolution of 0.55 Å
- 3. STELIB (Le Borgne et al. 2003) with 247 spectra in the range of 3200–9500 Å at 3 Å resolution

A total of 10 test cases were run and are summarized in table 1. We also give the wavelength region used in each case, resolution, and the resulting classification error. Cases A1–A3 involved training of the ANN by JHC and testing on, respectively, the CFLIB, ELODIE, and STELIB. Cases B1–B4 involved training the ANN with 174 individual classes of ELODIE and testing on ELODIE (4000–5500 Å, Case B1), ELODIE (4000–6800 Å, Case B2), CFLIB (4000–5500 Å, Case B3), and CFLIB (4000–6800 Å, Case B4). The last three cases C1–C3 involved training on STELIB and testing on CFLIB (4000–6800 Å, Case C1), CFLIB (3500–9400 Å, Case C2), and ELODIE (4000–6800 Å, Case C3).

The resolution used for training and testing for cases A1–A3 is 4.5 Å which is the resolution of JHC, 1 Å for cases B1–B4 which is the resolution of CFLIB, and 3 Å for cases C1–C3 which is the resolution of STELIB. The higher resolutions of some of the testing cases were degraded to match the resolution of the training library by Gaussian convolution. The testing is done on the complete libraries, i.e., for 247 stars of STELIB, 1959 stars of ELODIE, and 1273 stars of CFLIB.

The classification scatter plots from these analyses are shown in figures 1–3. The MK spectral types have been coded numerically for use by the ANN. The MK alphabetic type O is given a numeric code of 1000, B is 2000, A is 3000, and so on with M being 7000. The subclasses are multiplied by 100 and added in, thus an F5 star is coded as 4500. The luminosity

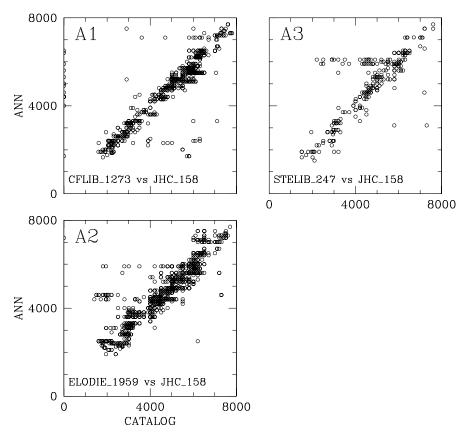


Fig. 1. Classification scatter plots for Cases A1-A3. Expression by numbers in axes for classification is referred to the text.

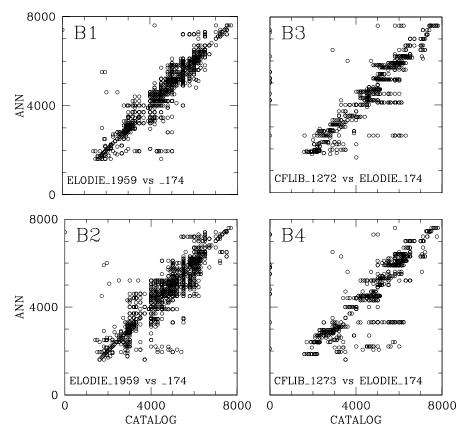


Fig. 2. Classification scatter plots for Case B1–B4.

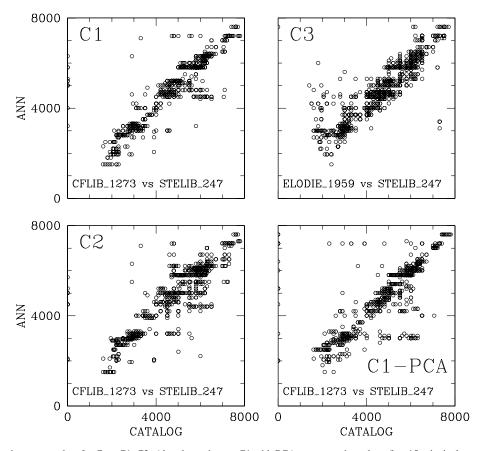


Fig. 3. Classification scatter plots for Case C1–C3. Also shown is case C1 with PCA preprocessing where first 15 principal components were used.

classes I, II, III, IV, and V are coded as 1.5, 3.5, 5.5, 7.5, and 9.5, respectively. An F5 V star is thus coded as 4509.5. In the present scheme, the luminosity class is given a low weight and the main emphasis on classification of the spectral types.

In the following we provide a discussion on the classification accuracy of the three sets of cases:

Cases A1-A3

The Cases A1–A3 use JHC as the training set with A1 and A2 in the wavelength region 4100–5500Å, i.e., in the blue part of the spectrum. In the case A3, JHC was trained for the full span i.e. 3600–7400 Å and tested on STELIB in the same band. The blue region classification error is lowest for ELODIE and somewhat inferior for CFLIB. However, the full span classification of STELIB deteriorates the error to about 861, i.e., 8.6 sub-spectral-type.

Cases B1-B4

In Case B1–B4, ELODIE was used as the training set and was tested on both ELODIE and CFLIB in the blue and full span. The training set of 174 spectra was preselected from amongst the 1959 ELODIE full set with one example spectra per spectro–luminosity class. The best classification is obtained for the case B1 with blue region of ELODIE. For the same region of CFLIB, i.e., case B2, the classification is somewhat inferior. The full span classification case B3 for ELODIE and case B4 for CFLIB are consequently with higher classification errors.

Cases C1-C3

Cases C1–C3 use STELIB as the training set and the test sets are CFLIB limited span C1, ELODIE limited span C3, and CFLIB full span case C2. The limited span cases of C1 and C3 show errors of 6.43 and 5.01 sub-spectral types but remarkably the case C2 with full span shows an error of only 6.7.

The most useful result as far as CFLIB is concerned, is the case C2 since the largest wavelength span is used for this case. It may be noted that except JHC, all other spectral libraries have gaps in them and this contributes greatly into the classification errors. Further, we also used a PCA based preprocessor for all the cases to reduce the dimensionality of the train—test sets as described in Singh et al. (1998). The resulting classification errors using first 15 principal components are only marginally poorer than the ones listed in the last column of table 1. Last panel in figure 3 shows the scatter plot of case C1 with PCA.

Figure 4 displays some example learning curves of the ANN training sessions for Cases A3, B2–B4, C1–C3, and a PCA version of C1–C3. The B2–B4 (and C1–C3) are same training sessions. All the learning curves fall to a low rms learning error at the level on number of iterations of 30000. The PCA version however requires much less number on iterations (~10000) to bring down these errors.

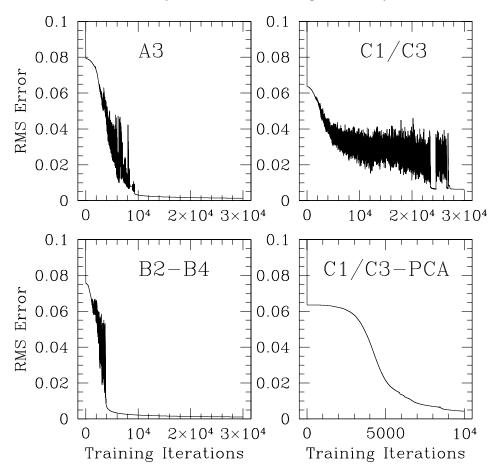


Fig. 4. ANN training session learning curves for some selected cases.

3. Restoration of Missing Data Using PCA

To fill the gaps in the spectra one can use the data from a similar type star which doesn't have a gap at the same wavelength. However, we present here a preliminary study of an automated method for restoration of missing data for a set of spectra of 300 stars in the wavelength region 4000–4300 Å selected from the CFLIB. The list of stars with their spectral types is given in table 3 in Appendix. The method of restoration is adopted from Unno and Yuasa (1992) and is briefly described here for the present data set.

To begin with, we have 301 flux values at 1 Å interval in the range for 4000–4300 Å for 300 stars. A sample of seven spectra are shown in figure 5. For the i-th star, let F_j^i and w_j^i be the j-th observed flux value and its weight respectively, where $j=1,\ldots,n$ (n=301) and $i=1,\ldots,N$ (N=300). If a particular flux value F_j^i for a particular star is missing, its weight is equal to zero.

For applying the PCA, the normalized data f_i^i is defined as

$$f_j^i = \frac{\left[F_j^i - \langle F_j \rangle\right]}{\sigma_i},\tag{1}$$

where $\langle F_j \rangle$ and σ_j are the mean and the standard deviation of F_j respectively and are given by

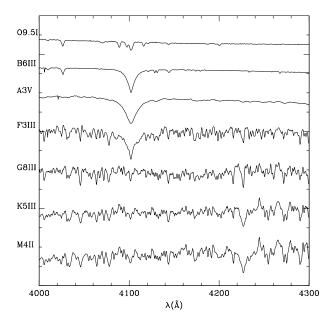


Fig. 5. Representative spectra of seven stars out of the total of 300 stars. The spectral types are listed on the vertical axis.

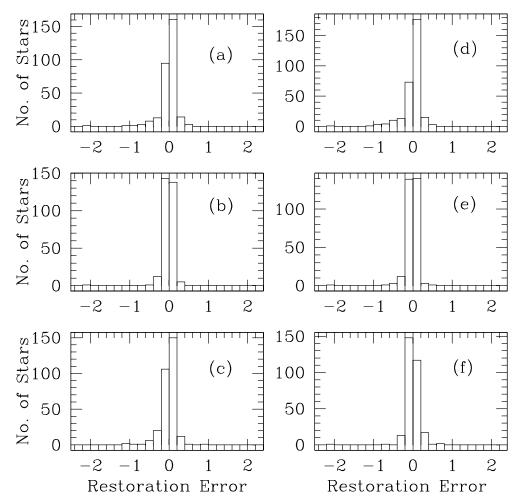


Fig. 6. Histogram of restoration error and the number of stars for the six cases. All stars with restoration errors greater than ± 0.2 are binned together.

$$\langle F_j \rangle = \frac{\sum_{i=1}^{N} w_j^i F_j^i}{\sum_{i=1}^{N} w_j^i}, \tag{2}$$

and

$$\sigma_j^2 = \frac{\sum_{i=1}^N w_j^i \left[F_j^i - \langle F_j \rangle \right]^2}{\sum_{i=1}^N w_j^i}.$$
 (3)

Following Unno and Yuasa (1992), we define virtual data x_j^i and their corresponding weight v_j^i for each observed flux value f_j^i for each star as

$$v_j^i = 1 - w_j^i, \tag{4}$$

$$\sum_{i=1}^{N} v_{j}^{i} x_{j}^{i} = 0, \qquad \sum_{i=1}^{N} v_{j}^{i} (x_{j}^{i})^{2} = \sum_{i=1}^{N} v_{j}^{i}.$$
 (5)

Equation (5) represents the statistical constraint that the mean value of the virtual data is zero and the standard deviation is unity. For such a case, the correlation coefficient between the j-th quantity and the k-th quantity is defined by

$$C_{jk} = \frac{1}{N} \sum_{i=1}^{N} (w_j^i f_j^i + v_j^i x_j^i) (w_k^i f_k^i + v_k^i x_k^i).$$
 (6)

The most probable value of x_j^i are thus given by the following set of n simultaneous linear algebraic equations:

$$\sum_{l=1}^{n} \frac{1}{\lambda_{l}} \left[\mu_{lj}^{2} x_{j}^{i} + \sum_{k \neq j} \mu_{lj} \mu_{lk} (w_{k}^{i} f_{k}^{i} + v_{k}^{i} x_{k}^{i}) \right] = 0, \tag{7}$$

where λ_l is the *l*-th eigenvalue and μ_l^j represent the *j*-th component of the *l*-th eigenvector in the PCA. The final adjusted value for the normalized *j*-th flux value for the *i*-th star is given by

$$w_j^i f_j^i + v_j^i x_j^i. (8)$$

To check the veracity of this procedure let us assume that from the data set only one flux value F_1^s is missing. This means

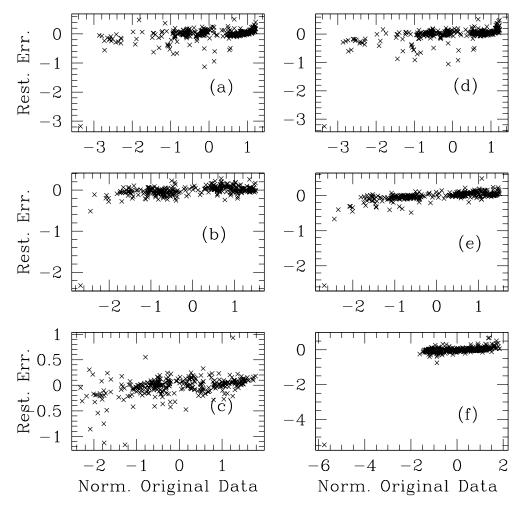


Fig. 7. Restoration error plotted against the normalized original data for all the six cases. The outlier at the bottom left of most of the plots is HD 31996.

Table 2. Cases studied for flux restoration analysis using PCA.

Case	Reconstructed flux	Number of principal components	λ region
(a)	4000 Å	10	4000–4009 Å
(b)	4077 Å	10	4077–4086 Å
(c)	4291 Å	10	4291–4300 Å
(d)	4000 Å	20	4000–4019 Å
(e)	4077 Å	20	4077–4096 Å
(f)	4281 Å	20	4281–4300 Å

that $w_1^s = 0$ and all the other weights w_j^i except w_1^s are equal to unity. In this simplified situation, equations (7) reduce to

$$\left(\sum_{l=1}^{n} \frac{\mu_{l1}^{2}}{\lambda_{l}}\right) x_{1}^{s} + \sum_{l=1}^{n} \frac{\mu_{l1}}{\lambda_{l}} \left(\sum_{k=2}^{n} \mu_{lk} f_{k}^{s}\right) = 0,$$

$$(s = 1, \dots, N).$$
(9)

Equation (9) can be easily solved to get x_1^s for the missing flux f_1^s . By exchanging the columns, one can compute x_2^s , x_3^s , and so on for the missing flux for any wavelength and for any

star. Six separate cases were studied and are listed in table 2. The results of our preliminary analysis are shown in figures 6 and 7.

Case (a) uses a flux region of 10 Å starting from 4000 Å and thus 10 principal components to reconstruct the fluxes at 4000 Å for all the 300 stars. From figure 6a we see that 256 stars have restoration error $(f_1^i - x_1^i)$ within ± 0.1 . Figure 7a shows the restored error vs. original value of the normalized flux f_1^i (with mean zero). It is clear that for most of the stars the reconstruction is good. Case (d) uses 20 principal components

and the reconstruction of flux at 4000 Å is comparable, maybe slightly worse as is clear from figure 6d and figure 7d.

We also tested the validity of this flux reconstruction method by attempting to reproduce a strong absorption feature, namely the 4077 Å Sr II feature, visible in the representative spectra in figure 5. Case (b) attempts to achieve this using 10 principal components rather successfully as is clear from figure 6b and figure 7b respectively. The flux at 4077 Å was reconstructed to within ± 0.1 for a total of 281 stars out of 300. The case (e) with 20 principal components also reproduces the flux at 4077 Å well although no better than case (b) (279 stars within ± 0.1) suggesting that the 10 PC's are enough for the data reconstruction in this data set. Lastly, cases (c) and (f) show similar behavior in reconstructing towards the end of the wavelength interval and the results are plotted in figure 6c and f, and figure 7c and f.

Another interesting offshoot of this analysis was in picking outliers, stars which have either no known MK spectral types or have noisy spectra. Figure 7a,b,d,e,f clearly show one outlier for which our scheme is unable to restore or reconstruct the fluxes. The star is HD 31996 and it indeed has no MK spectral class assigned to it (table 3) as was verified from the CFLIB and the SIMBAD database. Another star, HD 46687, also has no known spectral type but its spectrum resembles an M type star. For this star, our analysis was able to reconstruct the fluxes. The spectra of these two stars obtained from the CFLIB are plotted in figure 8.

4. Conclusions

We have performed an extensive analysis based on artificial neural networks to classify stars in an automated manner in the Indo-US CFLIB using three databases viz., JHC, STELIB, and ELODIE. The main aim of this exercise was two-fold. One was to perform the reliability checks on CFLIB to see how the gaps in the library affect the classification accuracy. We find that the despite the presence of gaps, we have achieved classification accuracy of less than one main class. The second aim was to evolve and test automated procedures of classifying stellar spectra. This was achieved by trying our ANN scheme on ten different cases of training and testing on different pairs of libraries. The schemes are numerically intensive, with the ANN training stage requiring several hours of CPU time on the fastest of workstations. A PCA analysis was employed successfully to reduce the dimensionality of the data set and hence faster training without appreciable loss in classification accuracy.

Both STELIB and ELODIE libraries have variable spans of wavelength gaps where the fluxes are filled with zeros (similar to CFLIB). Such gaps lead to classification errors in the PCA and ANN schemes. However, we have carried out some preliminary analysis with the basic χ^2 minimization scheme on

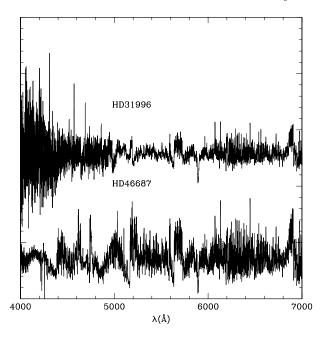


Fig. 8. Spectrum of the two stars HD 31996 and HD 46687 which have no known spectral types. Star HD 31996 is the outlier in the flux restoration analysis.

these libraries wherein the gap portions were omitted in both train and test sets. This lead to a remarkable improvements in the classification accuracy.

We have also employed a generalized principal component analysis to first create and then fill the gaps in a sample of 300 stars out of the CFLIB in the blue region. At present, we have used a simplified system to reconstruct flux values at one wavelength bin at a time for these 300 stars. We hope to exploit the full potential of the scheme and attempt to fill larger gaps in stellar spectra in a subsequent study.

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Appendix. List of Stars for Data Restoration Analysis

The list of 300 stars with their HD numbers and the spectral types is given in table 3. Two stars HD 31996 and HD 46687 have no known spectral types.

Table 3. Sample of 300 stars used for data restoration analysis.

HD	Sp. type	HD	Sp. type	HD	Sp. type	HD	Sp. type	HD	Sp. type	HD	Sp. type
100889	B9.5 V	141680	G8 III	191615	G8 IV	117818	K0 III	163917	G9 III	43042	F6 V
102212	M1 III	141714	G3.5 III	195324	A1 I	117876		163989	F6 IV	43232	K1.5 III
102224	K0.5 III	142091	K1 IV	196867	B9 IV	118055	K0	164259	F2 IV	43247	B9 II
102328	K3 III	142198	K0 III	198001	A1 V	118266	K1 III	164284	B2 V	43318	F6 V
102870	F9 V	142373	F8 V	25329	K1 V	120136	F6 IV	164353	B5 I	43380	K2 III
103047		143107		28978	A2 V	120164	K0 III	165029	A0 V	43827	K1 III
103287	A0V	143666	G8 III	29613	K0 III			165358	A2 V	43947	F8 V
104985	G9 III	143761	G0V	29645	G0V	120452		165401	G0V	44007	G5 IV
105043	K2 III	145328	K1 III	30562	F8 V	121146		165645		44033	K3 I
105262			G9.5 III	30614	O9.5 I	121370		165687		44478	M3 III
106365		147677		30652	F6 V	122563		165760		44537	MOI
106714		148387		30739	A1 V		M4.5 III	165908		44769	A5 IV
107113		148783	M6 III	30743	F5 V	123977			B9.5 V	44951	K3 III
107213		148786		30812	K1 III	124570		166046		45282	G0
107383	G8 III		K4III	31295	A0 V	124850		166207		45410	K0 III
107418		149630		31421	K2 III		K1.5 III	167042		45412	F8 I
107950	G6 III	149661 149757		31996	0.0	125451		168151		46184	K1 III
108225 108954	G9 III	149737		32147	K3 V	125454 126141		168656 168723		46687	0.0 A0 IV
108934	K0 III	150112		33111 33256	A3 III F2 V	126141	K4III	169191	K0 III K3 III	47105 47205	K1 III
109317		150100		35468	B2 III	126868	G2 IV	169191		47203	G5 I
109343	G0 V	150449		35497	B7 III	127334			K2 III K1.5 III	47731	03 I
110281	K5	150449		36673	F0 I	127334		170093		48329	G8 I
110201		150680		36861	O8 III	128750		171301		48432	K0 III
	K5 III		G7.5 III	37043	O9 III	129312		172569		48433	K1 III
111591	K0 III	151431		37160	K0 III	129336		173087		48737	F5 IV
111765		151613		37984	K1 III		B9.5 V	173399		48781	K1 III
111812		151769		38656	G8 III		G8.5 III	175317		50420	A9 III
	M3 III	151862		38899	B9 IV		K2 III	175535		51309	B3 I
113226	G8 III	152569		39003	G9.5 III	130948	G1 V	175545		54662	O7 III
113436		152614		39283	A2 V	131111	K0 III	175588	M4 II	54719	K2 III
113848		152815		39587	G0 V	131156	G8 V	175640	B9 III	55280	K2 III
113996	K5 III	15318	B9 III	39801	M1	132132	K1 III	175743	K1 III	55575	G0V
114038	K1 III	153597	F6 V	39853	K5 III	132345	K3 III	175751	K2 III	57264	G8 III
114092	K4 III	153653	A7 V	39866	A2 II	133165	K0.5 III	176301	B7 III	57669	K0 III
114330	A1 IV	153808	A0V	40035	K0 III	133208	G8 III	176318	B7 IV	57727	G8 III
114357	K3 III	154278	K1 III	40111	B0.5 II	134083	F5 V	176582	B5 IV	58207	G9 III
114642	F6 V	154431		40136	F1 V		G7.5 III	176819		58343	B2 V
114710		154445		40183	A2 IV	135742		177724		58551	F6 V
115004		154660		40239	M3 II	136064		177817		59881	F0 III
115136		155763		40536	A6	136202		178125		60179	A1 V
115202		157741		40801	K0 II	136512		178329		61064	F6 III
115383		157910		41117	B2 I	136726		180006		61295	F6 II
115539		158716		41330	G0 V	137052		180711		62509	K0 III
115604		158899		41597	G8 III	138716		182293		63302	K3 I
115617		159332		41636	G9 III	139195		182568		65714	G8 III
116292		160765		41692	B5 IV	139446		183144		65900	A1 V
116656			B1.5 V	42475	M1 I		G7.5 III		B0.5 III	67228	G1 IV
117176		161868		42543	M1I	140027		188350		69897	F6 V
117243	GUIII	163588	K2III	43039	G8.5 III	141004	GU V	191243	DJI	70110	F9 V

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