Neural Networks and the Classification of Active Galactic Nucleus Spectra

Daya M. Rawson¹, Jeremy Bailey² & Paul J. Francis³
¹Mount Stromlo and Siding Springs Observatory, Australian National University, Private Bag, Weston Creek, ACT, 2611, Australia.
E-mail: daya@merlin.anu.edu.au
²Anglo-Australian Observatory, PO Box 296, Epping, NSW 2121, Australia.
E-mail: jab@aaoepp.aao.gov.au
³School of Physics, University of Melbourne, Parkville, Victoria 3052, Australia. E-mail: pfrancis@physics.unimelb.edu.au

Abstract: The use of Artificial Neural Networks (ANNs) as a classifier of digital spectra is investigated. Using both simulated and real data, it is shown that neural networks can be trained to discriminate between the spectra of different classes of active galactic nucleus (AGN) with realistic sample sizes and signal-to-noise ratios. By working in the Fourier domain, neural nets can classify objects without knowledge of their redshifts.

Keywords: galaxies: nuclei, galaxies: quasars: general, galaxies: seyferts, methods: data analysis

1. Introduction

The advent of current generation spectrographs, such as the 2dF system on the AAT (Taylor, 1995) is leading to order-of-magnitude increases in the number of spectra that can be obtained in a given amount of observing time. This in turn has stimulated research into computer algorithms capable of handling large samples of spectra (eg. Francis et al. 1992).

One family of such algorithms are artificial neural networks. These algorithms, inspired by a model of the workings of the human brain, have recently found application in fields as diverse as sonar signal processing (Gorman & Sejnowski 1988), and medical diagnostics (Rayburn et al. 1991). Neural networks are increasingly being used in astronomy (eg. Storrie-Lombardi et al., 1992, Lahav et al., 1994, von Hippel et al. 1994, and 14 papers in a special issue of Vistas in Astronomy, 1994, 38, 251).
In their most common application, artificial neural networks function as classification algorithms. They have one unique feature that sets them apart from most classification algorithms: they can be trained. The procedure is known as supervised learning. To train a neural network to divide some large dataset up into different classes of object, one would classify some subset of the whole sample manually. The neural net is then trained using this subset to identify the various classes of object in the data. It can then be used to automatically classify the remainder of the dataset. Unlike most classification algorithms, this trainability allows neural networks to duplicate the subjectivity so common in astronomical classification.

The aim of this paper is to determine if neural networks can be usefully applied to data sets of realistic astronomical spectra, with typical sample sizes, redshift ranges and signal-to-noise ratios. This is tested using both real and simulated spectra of active galactic nuclei (AGN).

2. Method

The simplest and most widely used type of neural network algorithm is backpropagation, and this is the algorithm used in this paper. Excellent descriptions of neural networks and the backpropagation algorithm can be found in Hertz, Krogh & Palmer (1991), Maren, Harston & Pap (1990), Hinton (1992), van Camp (1992), and Lahav et al. (1995). A neural network is defined by a series of variables known as weights. The process of training consists of choosing the weights such that the network duplicates the known classifications of some training set of data. Once the weights are chosen, the neural network can then be applied to other, previously unclassified data sets. The backpropagation algorithm is one of many iterative techniques for choosing the weights.

In this paper, a modified version of the code of Rao & Rao (1993) was used; the code (in C or C++) is available on request from DMR. Any backpropagation code using Sigmoid transfer functions will work equally well. A full technical description of the algorithm used can be found in Rawson (1994).

Many classification schemes for AGN spectra use derived quantities as their input variables, such as emission-line fluxes and continuum slopes (eg. Boroson & Green 1992). Unfortunately, the measurement of these derived quantities
from spectra introduces an inevitable subjectivity into the classification (Francis et al. 1992). In this paper, a different approach was tried; the spectra are used directly, with the flux in each wavelength bin an input variable. This is more objective, but greatly increases the computational load.

3. Simulations

The neural network was first tested with a synthetic data set, to investigate its sensitivity to noise, sample size and redshift. The classification of AGN spectra into Seyfert I and Seyfert II galaxies (Osterbrock 1989) was chosen as a test of our neural network. Seyfert I and II galaxies differ primarily in the velocity width of their permitted emission lines.

The synthetic spectra covered the rest-frame wavelength region 4800–5100 Å. Three emission-lines were included; H-β and the [O III] doublet. No continuum emission was included. The peak fluxes of the lines were fixed for the H-β and [OIII] doublet in the ratio 2 : 3 : 9 respectively. The [O III] lines were assigned velocity widths of 800 km s$^{-1}$ (Full Width at Half Maximum Height, FWHM). The velocity width of H-β was randomly assigned a value in the range 100 < FWHM < 4500 km s$^{-1}$, the widths being drawn from a uniform distribution. Peak flux was conserved with a magnitude of 10 as the width was changed. Objects with H-β FWHM > 1500 km s$^{-1}$ were considered to be Seyfert I galaxies; all others were Seyfert II galaxies. The sample was divided equally between the two classes. Random noise was added to the spectra; the noise being drawn from a Gaussian distribution, with a standard deviation independent of wavelength. The signal-to-noise ratio in the emission-lines, for a noise standard deviation of 1, is comparable to that of a typical AGN spectrum with a continuum signal-to-noise ratio of ∼ 10 (Francis et al. 1991), i.e. typical of spectral surveys.

100 simulated spectra were generated for use as a training set; this size was chosen to match the typical sizes of many astronomical samples. Each spectrum was composed of 300 points at 1 Å intervals from 4800Å to 5100Å, with each point corresponding to the input to one neuron in the first layer.

A two-level neural network was initially used. This is only capable of linear classification; it defines a plane in the $n$-dimensional decision space defined by the input variables (in this case the fluxes in the 300 spectral bins), and
classifies objects as Seyfert I or Seyfert II galaxies depending upon which side of the plane they lie (a 300:1 perceptron network).

The network was trained on this set, using the backpropagation algorithm. Training continued until the network would reliably match the known classification. Approximate training times varied between 10 and 20 minutes on a Sun sparc10.

Once the neural network had been trained on the training set, it was applied to an additional set of 1000 simulated spectra (the testing set), to measure the success rate of the classification. Figure 1 shows the fraction of Seyferts classified correctly as a function of the noise added to the simulations. The results are encouraging; for noise levels of < 2 (signal-to-noise ratios of ~ 5 or better), the classification is more than 90% accurate. The classification is still 70% correct for noise standard deviations as large as 3.5 (signal-to-noise ratios ~ 3 per Å). This demonstrates that the simple neural network backpropagation algorithm is capable of classifying spectra with typical noise levels and sample sizes.

In these simulations, the noise level in the training set and in the testing set were identical. One possible strategy, however, would be to train the network upon data of better quality than that which it is to be used to classify. To simulate this, the neural network was trained on a noise-free training set (still of 100 objects). Remarkably, this was found to degrade the performance of the neural network at classifying noisy data. The likely explanation is as follows: in the N-dimensional space defined by the 300 input variables, a noise-free training set will be a curved line, along which the width of H-β increases. The training process chooses a plane which separates Seyfert-I and Seyfert-II galaxies, but in the absence of noise, this is a degenerate problem, as any plane cutting the curved line at the appropriate place will do equally well. Such a plane may not lie perpendicular to the line it bisects. When noise is added, the line becomes fuzzy, and if the classification plane is not parallel, many objects may be misclassified. Training the neural network on noisy data forces the classification plane to lie perpendicular to the line of sample points.
3a. Redshift Dependence

In the above simulations, it was tacitly assumed that the redshifts of the AGNs are known. In practice, we would like the classification algorithm to work without the need to be told a redshift.

As a first attempt to model this, the simulated spectra were randomly assigned redshifts in the range $0 < z < 0.1$, and the spectra were shifted appropriately. The neural network was once again trained on a training set of 100 spectra, and tested on a testing set of 1000 spectra. Even for noise-free data, the success-rate was only $\sim 45\text{—}55\%$, no better than random. This is because putting the spectra at a range of redshifts, thereby changing both the line-width and position, makes the boundary in decision space between Seyfert I and Seyfert II galaxies non-linear.

The standard solution to this problem is to add an additional layer (a hidden layer) of neurons to the neural network (Maren, Harston and Pap 1990). The extra layer of neurons is equivalent to combining several two-layer neural networks; instead of a single decision plane in the decision space defined by the 300 input variables, the classification can be done on a more complex surface, made up of several planes. This in principle allows the neural network to handle non-linear classification.

In practice, however, adding a hidden layer to the neural network did not significantly improve the classification success rate, regardless of the size of hidden layer employed. We hypothesise that this is due to the inadequate size of the training set; $\sim 100$ spectra is not sufficient to define the complex boundary between Seyfert I and Seyfert II spectra at a range of redshifts in the decision space.

As an alternative, the classification was attempted in the Fourier domain. A decision space made up of Fourier amplitudes should be invariant under changes in redshift. A Fast Fourier Transform routine from Press et al.(1992) was used, and the resulting 300 Fourier components were used as inputs into a two-layer neural network (a 300:1 perceptron).

This technique performed well; success rates as a function of noise level are shown in Figure 1. For signal-to-noise ratios $\sim 10$, success rates are comparable to those obtained when the redshift is known. The performance does, however,
decline for noiser data.

In real data, the continuum emission could complicate things. Unless removed or smoothed, edge effects will confuse the Fourier analysis. Standard techniques used in cross-correlation redshift measurement, such as cosine bell weighting, would introduce features into the Fourier transform on wavelength scales comparable to the emission-line widths which define the spectral classes. We therefore suggest that fitting and subtracting a continuum may be necessary.

Neural networks are thus capable of successfully classifying data for which redshifts are not known. For data with low signal-to-noise ratios, however, redshift information does improve the classification.

3b. Training Sample Size

Sensitivity of the performance of a neural network to the size the training set is particularly important because large samples of pre-classified spectra are difficult to obtain. The simulations described above were therefore run repeatedly, varying the number of spectra in the training set. Results are shown in Figure 2.

In all cases, a sample of \( \sim \) 100 spectra seems adequate; increasing the training set beyond this size does little to improve the success rate of the classification.

Using a larger training set does however give a more \textit{reproducible} classification. This was tested by repeating the classification using a different randomly generated training set of the same size. For training set sizes of \( \sim \) 50, \( \sim \) 5\% of objects in the testing set would change classification when different training sets were used. This fraction dropped to \( \sim \) 2\% for training set sizes \( \sim \) 1000. We hypothesise that the larger training set allows the decision space boundary to be better defined.

Thus for most purposes, a training set of \( \sim \) 100 spectra is adequate, unless high levels of reproducibility are required.

3c. Classifying Real Data

As a final test, the neural network was applied to a sample of real data; QSO spectra from the Large Bright QSO Survey (LBQS). The LBQS is a
large optically selected QSO sample, containing 1054 objects. References to the LBQS can be found Hewett, Foltz & Chaffee (1995). LBQS QSOs span the redshift range $0.2 < z < 3.4$; the spectra have resolutions of $\sim 10\,\text{Å}$ and uniform signal-to-noise ratios of $\sim 10$ per resolution element.

Roughly 10% of the QSOs in the LBQS belong to the sub-class of QSOs known as broad absorption-line QSOs (BALQSOs). This subset are characterised by P-Cygni type profiles to some of their high ionisation emission-lines, evidence for massive high velocity out-flowing winds. The properties of the BALQSOs in the LBQS are discussed by Weymann et al. (1991), and Francis, Hooper & Impey (1993). Broad absorption-lines are only seen in ultra-violet resonance lines, particularly C IV, which can only be seen in the spectra of higher redshift QSOs: we therefore restrict our analysis to QSOs with $z > 1.7$.

The aim of this test was to measure the robustness of the neural network algorithm when faced with real data, by training it to classify QSOs in the LBQS as BALQSOs or not on the basis of their spectra. The network was trained to reproduce the ‘by eye’ classification of a human expert (Craig Foltz).

Accurate redshifts are known for the LBQS QSOs, so the classification could be done in rest-frame wavelengths; the Fourier transform technique was not required. The spectra were shifted to the rest-frame, and rebinned into 16.3 Å bins to minimise the number of input variables. All spectra were normalised to unit mean flux, so that the analysis was sensitive only to the shape of the spectra, not their normalisation.

The imbalance in numbers between BALQSOs and non-BALQSOs was found to be a problem. It had the effect that the weights were trained to recognise only the more common non-BALQSOs type. All changes in the weights to facilitate the classification of the BALQSOs were overwhelmed by the number of times the weights were changed for the classification of non-BALQSOs, delaying or preventing convergence of the training. This was overcome by duplicating the BALQSOs in the training set, so that their numbers matched the non-BALQSOs. BALQSOs and non-BALQSOs were alternated in the training set.

Using a training set of $\sim 250$ QSOs, 33 of which were BALQSOs, the network was successfully trained. The trained neural network achieved a success
rate of $\sim 90\%$, comparable to that of the simulations described above with similar signal-to-noise levels. We therefore conclude that results derived from the simulations are valid for real data.

4. Conclusions

The major conclusion of this paper is that simple, two-layer backpropagation neural networks can be trained to perform useful binary classification on realistic samples of survey-quality spectral data. Training sets should contain $\sim 100$ spectra, with noise characteristics comparable to the data to be classified. Neural network classification of BALQSOs and Seyfert galaxies showed success rates of $\sim 90\%$ for signal-to-noise ratios $\sim 10$, and still does significantly better than randomly for signal-to-noise ratios as low as $\sim 3$.

It is not necessary to know redshifts for the spectra if the classification is done in the Fourier domain. If, however, redshift information is available, it improves the performance of the classification when signal-to-noise ratios are low.
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Figure Captions:

**Figure 1**—The success rate of the neural network classification, as a function of noise, for the simulated Seyfert spectra. 50% is the level expected by chance. The solid line is for the case when the redshift is known ($z = 0.0$), and the dashed line is for the case when the redshift is unknown ($0.0 < z < 0.1$), and the Fourier technique is applied.

**Figure 2**—The success rate of the neural network classification, as a function of the size of the training set. Line styles as in Fig 1; results are shown for two different noise levels.
