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PREPROCESSOR

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Spectral Recognition with a PCNN Preprocessor

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Abstract

This is a report on work in progress. Spectral recognition is central to many areas of science and technology. Classical spectral recognition analysis techniques (least squares, partial least squares, etc.) are sensitive to offset and gain drifts and errors. This sensitivity can cause excessive costs for spectrometer resources and calibrations. Neural techniques relieve some of this sensitivity but none approach human competence. It is desirable to mimic human spectral analysis not only to improve the results but to minimize detector constraints and costs. We suggest that the first step in human analysis is peak detection. We are exploring the one dimensional PCNN as a peak segmenter for spectral peak finding in the presence of noise and drifts in gain and offset. We present results of one dimensional pulse coded neural network peak detection with both simulated and actual static spectra. We also use the PCNN to form a scale and translation invariant feature vector that may be decomposed using classical techniques such as least squares. Finally, we propose using a PCNN to exploit the temporal aspects of spectral acquisition.

Keywords: pulse coded neural networks, spectral recognition

1. Introduction

A spectrum is a one dimensional function. It is a specification of the dependence of a single independent variable on a dependent variable. Nuclear spectra are often cast as event rate vs. energy. Chemical spectra of absorbance or reflectance vs. wavelength are ubiquitous. Many other forms of spectra exist. The dependent variable is sometimes constrained to fixed values (e.g., measurements stimulated by lasers with frequencies fixed by quantum mechanics) but often it is not. If not fixed, the dependent variable must also be measured, with associated errors, or "calibrated", with associated constraints on long term drifts and errors. A spectrum is typically but not necessarily time invariant. Spectra also usually contain peaks, although this is also not a requirement. When peaks exist, the functional dependence is contained in the relative spacing and magnitudes of the spectral peaks.

Spectral recognition is the decomposition of spectra from composite sources into estimates of the number and fraction of constituents. In pattern recognition nomenclature, a spectrum is a feature vector. Each constituent has a feature vector. The composite spectrum is the linear sum of the constituent spectra or, alternatively, the composite feature vector is the linear combination of the constituent feature vectors, weighted by the fractions of the constituents present. If spectral peaks are present, and if the peaks for each constituent have no overlap, the spectral feature vectors are linearly independent. Typically, the constituent spectral peaks have overlaps and are not linearly independent.

Spectral recognition is central to many areas of science and technology. Least squares and partial least squares decompositions are typically used when the constituent spectra are not linearly independent, or when other requirements such as weight, size, and power result in degraded sensor resolution and associated spectral overlap¹. These techniques are sensitive to noise and to offset and gain drifts and errors. This sensitivity often causes excessive costs for spectrometer resources and calibration procedures. Even when the constituent spectra are linearly independent, peak rule-based approaches are still sensitive to these same uncertainties and errors.

Current "standard" neural techniques such as feedforward backpropagation and counterpropagation neural networks relieve some of this sensitivity but none approach human competence. The absence of robust spectral recognition algorithms can result in excessive requirements on spectrometer noise, offset, and gain specifications. It is desirable to mimic human spectral analysis not only to improve the results but to minimize detector constraints and costs.

We suggest that the first step in human analysis is peak detection. This is problematic using existing techniques. The pulse coupled neural network ², or PCNN, has proven to be a versatile and robust segmentation preprocessor for images. We investigate the use of a PCNN as a peak segmentation tool for static spectra. We also investigate using a PCNN preprocessor to transform the spectra into scale and translation invariant feature vectors for subsequent processing by classical least squares decomposition. Finally, we propose the use of a PCNN for peak segmentation using motion queues from dynamic spectra forming during the acquisition process.

2. PCNN Preprocessing

Our present research is on static spectral processing; i.e., the spectra are not changing with time. A primary goal is to use a PCNN to segment the spectral peaks from the background. The 1D PCNN has 512 neurons that receive feeding inputs from the spectra. The linking field consists of the feeding neuron and its three nearest neighbors on each side. We used sigmoidal linking ($\beta = 1$). The linking decay time is 1, the threshold decay time is 5, the linking gain is 0.2, and the threshold gain is 20. Each PCNN run is 10000 iterations.

Synthetic spectra were constructed for initial testing. The synthetic spectra have 512 channels. Spectrum A has three peaks superimposed on a background of random noise with a mean of 0 and a variance of 0.1. The first peak has 1024 counts at channel 100 and a Gaussian half width at half maximum of 10. The second peak has 512 counts at channel 250 and a Gaussian half width at half maximum of 2. The third peak has 800 counts at channel 400 and a Gaussian half width at half maximum of 6. Figure 1 shows spectrum A and the accumulated pulses from the PCNN. The peaks have clearly been segmented.

Figure 1. Synthetic spectrum A and accumulated PCNN pulses.

Synthetic spectrum B has four peaks superimposed on a background of random noise with a mean of 0 and a variance of 0.1. The first peak has 512 counts at channel 100 (directly overlapping with the first peak of spectrum A) and a Gaussian half width at half maximum of 6. The second peak has 1024 counts at channel 200 and a Gaussian half width at half maximum of 8. The third peak has 1024 counts at channel 300 and a Gaussian half width at half maximum of 6. The fourth peak has 1024 counts at channel 420 and a Gaussian half width at half maximum of 10 (partially overlapping with the third peak of spectrum A). Figure 2 shows spectrum B and the accumulated pulses from the PCNN. Again, the peaks have clearly been segmented.

Figure 2. Synthetic spectrum B and accumulated PCNN pulses.

Figure 3 shows the results of PCNN preprocessing of a Yt^{88} calibration spectrum from the Lunar Prospector gamma ray detector. The major peaks are segmented. The minor peaks are not as clearly segmented.

Figure 3. Gamma ray detector Yt88 calibration spectrum and accumulated PCNN pulses.

It is possible to extract even more useful information from the PCNN preprocessing. The time series of the total number of neuron firings summed over the spectrum is a feature vector that encodes the spectral information into a repetitive signature of a given spectrum. This feature vector is invariant to rescaling and translation of the input spectrum, that might be readily decomposed using conventional techniques such as least squares. Figure 4 shows a portion of the time series at the end of the spectrum B run. The unbiased and normalized autocorrelation is also shown. It is not obvious from the top panel that the signal is repetitive but the 90% autocorrelation is indicative that it indeed is cyclic.

Figure 4. - PCNN summed pulse time series and its autocorrelation.

To illustrate the translation invariance of the total number of neuron firings summed over the spectrum, we shifted spectrum B to the left by 50 channels and repeated the PCNN preprocessing. The normalized unbiased correlation was unity at zero lag and had correlation peaks of 98% approximately every 18 or 19 channels, just as in both the unshifted and shifted summed pulse time series. This is a strong indicator that the summed pulse time series is indeed translation invariant.

3. Postprocessing

Once the peaks have been segmented, if each constituent spectrum has at least one peak that is distinct and non-overlapping with other constituent peaks, peak processing with a rule-based system is the simplest procedure. The standard technique is to identify a unique peak, determine the fraction of the associated constituent present, subtract the constituent contribution from the entire spectrum, and repeat for the remaining unique peaks. Unfortunately, this process currently relies on knowledge of the exact channels for the unique peaks and is therefore not translation invariant. Using the PCNN to segment peaks, much as humans do, rules such as "if there are three peaks with amplitudes in the ratio 1:5:2 and with relative separations of 1:1.4:2, then Mg must be present" are possible. Although still sensitive to scale (gain) changes, even this simple step is an important advance in our ability to do spectral decomposition.

Typical spectra contain enough overlap between constituent peaks that procedures such as least squares and partial least squares are required. It should be possible to do least squares decomposition on the summed firing time series in order to get translation and scale invariant decomposition. As a test, we constructed a synthetic spectrum containing 65% of constituent A and 35% of constituent B. Figure 5 shows the resulting time series of total number of neuron firings summed over the spectrum.

Figure 5. Summed pulse time series for a mixture of 65% A and 35% B.

Let the time series in figure 5 be a column vector of length 100 called Y . Construct another matrix with two columns of length 100 called M . The first column of M is the summed pulse time series for spectrum A and the second column is the summed pulse time series for spectrum B. Finally, construct a single column vector with two rows, called X . The first row of X is the fraction of component A in the mixture and the second row is the fraction of component B in the mixture. The resulting equation $Y = MX$ can be solved for X using least square decomposition. For our test case, the decomposition produced an estimate of 50% for each component. At this point, it is not clear whether this incorrect result means the technique is incorrect or whether we are not operating the PCNN preprocessor incorrectly. The research continues.

4. Conclusions

We have shown that it is possible to segment the peaks in static spectra using the PCNN preprocessor. We have not quantified how well this works. We further believe it is possible to use the motion queues present during spectrum accumulation to enhance this segmentation; i.e., since the peaks grow linearly with time while the noise grows like the square root of time, the peaks appear to grow more quickly than the noise. The PCNN can readily process this additional information.

We have shown that the time series of neuron pulses summed over the spectrum is a feature vector that is invariant to translation (offset). Other work [2] indicates that this feature vector is also invariant to scale (gain). Such a feature vector should be more amenable to standard decompositions like least squares. However, we did not find this to be true. It is not clear if the technique is incorrect or if our operation of the PCNN is flawed.

We conclude that the use of a PCNN preprocessor for spectral recognition has exciting possibilities for significantly easing system requirements but that further research is required to demonstrate this.

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