Fitting multiple alpha peaks using neural network techniques

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***Abstract*— Despite the sophistication of today's radiochemical separation techniques, it often occurs that the peaks in the spectra of α-emitting radioactive samples partially overlap. We here demonstrate the usefulness of a procedure based on a neural network, a multilayer perceptron with backpropagation training method, trained with isolated alpha peaks of environmental samples in resolving such partially overlapping alpha peaks and in predicting the activities of the α-emitters detected.**

I. INTRODUCTION

In nature, there are a number of radionuclides that disintegrate emitting radiation. One form of this radiation consists of alpha particles, which are helium nuclei (2 protons and 2 neutrons) with a high kinetic energy, of the order of MeV (mega-electron-volts). The emission energies are discrete and characteristic of each alpha emitting radionuclide, which allows their identification. Because of the great mass of these charged particles, they interact strongly as they pass through matter. Indeed, they are completely stopped by the thickness of a sheet of paper. For their measurement, it is necessary to use a radiochemical separation process to isolate the radionuclides, which are then deposited onto a planchet, forming a layer as thin as possible. The alpha particles are usually detected using PIPS (Passivated Implanted Planar Silicon) detectors in which the energy of the alpha particle is deposited. Due to the strong interaction of alpha particles with matter, the distance between sample and detector must be as short as possible, typically a few millimetres, to avoid losing energy in the detection. A certain degree of vacuum is also needed in the detection chamber. Despite these precautions, however, it is impossible that all the alpha particles emitted will reach the detector with their complete energy, and low-energy tails are commonly observed in the spectra. These spectra consist of plots of the number of alpha particles detected, called counts, at defined energy intervals, called channels. The resolution of the detectors used is of the order of 0.025 MeV. The low-energy tails usually pose no problem if the alpha peaks are well separated, i.e., their energies are so different that they do not overlap. Unfortunately, that is not always possible, as in the case of Fig. 1.

A. *Existing solutions*

To resolve this problem, deconvolution processes are often used based on the semi-empirical functions of the shape of a mono-energetic alpha peak with a large number of fitting parameters. Functions based on the convolution of several components have been proposed by Bortels and Collaers [1] and Westemeier and Van Aarle [2]. The parameters of these models are determined by optimizing the fit of the corresponding function to the real spectrum. The more parameters the function contains, the better the fit, although the optimization procedure is more complicated and several types of ambiguities arise. There are similar applications of the neural networks on chemical problems [3], but the main difference is the asymmetric shape of the alpha peaks.

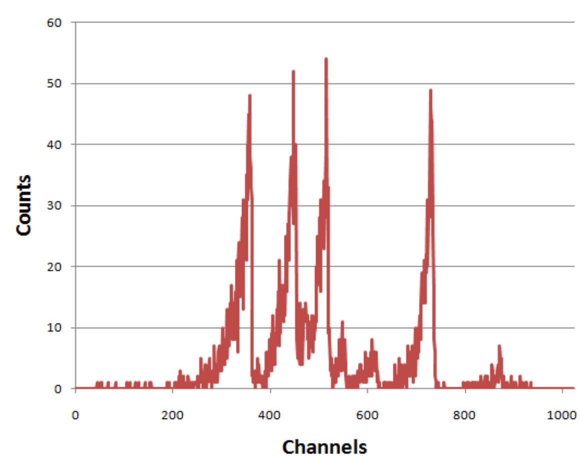

Figure 1. Radium alpha spectrum with multiple, partially overlapping peaks.

B. *Proposed solution*

The present communication describes a different approach to the problem. Using the trained neural network of a previous work [4], we developed a procedure based on the reconstruction of alpha peaks and their subtraction from the original spectrum, obtaining the individual contributions of

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each of the overlapped peaks. Instead of generating certain parameterized model functions to fit the peaks, a generalization based on the shape of peaks taken from real alpha spectra is used. The purpose of this work is thus the application of neural network techniques to the fitting analysis of two partially overlapping peaks in alpha spectra.

II. Method

A. *The neural network*

In the previous work, we designed a neural network for singlet alpha-peak fitting. That network (see Fig. 2) consists of a multilayer perceptron (MLP) feed-forward neural network using a back-propagation training algorithm, trained on several energetically isolated peaks of polonium. The inputs are 7 characteristics of a peak (see Fig. 3) sufficiently descriptive to allow the network to determine the peak shape. The outputs are the 21 channel values of the alpha-peak integral, as shown in Fig. 4.

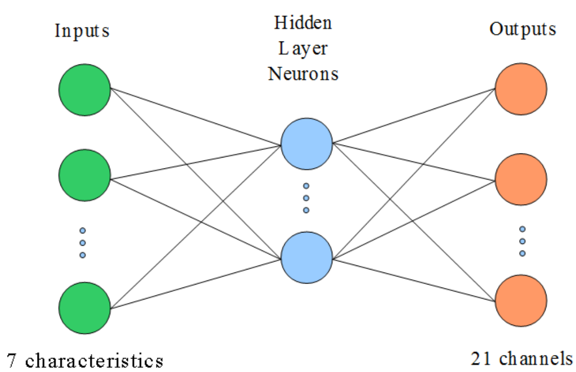

Figure 2. The neural network scheme.

The network was trained on 102 different alpha peaks of polonium, using a cross-validation method with Mean Squared Error (MSE) cost function to determine the training level. The trained network obtained is used in the procedure explained in this work.

B. *The procedure*

In order to study the results of the fitting process when there are multiple alpha-peaks, we artificially constructed some spectra by adding integrals of individual peaks of real alpha spectra. These peaks were obtained from the measurement of real polonium sources of environmental samples. From these spectra are possible to generate artificially overlapped peaks at will to share a given percentage of channels. This is illustrated in Fig. 5, with the overlap being the ratio between areas 3 and 1 expressed as percentages. For example, we consider the overlap to be 10% when the integral of the right peak adds 10% to the left peak integral.

To resolve the two partially overlapped peaks of a spectrum, we proceed as follows. The first step is to extract the characteristics of the higher energy peak, located on the right side in the spectrum. This information is then fed to the neural network. We use the neural network output to fit that peak and subtract it from the original two peaks spectrum. The result is the isolated left peak, which can then be analyzed using the single peak fitting procedure again.

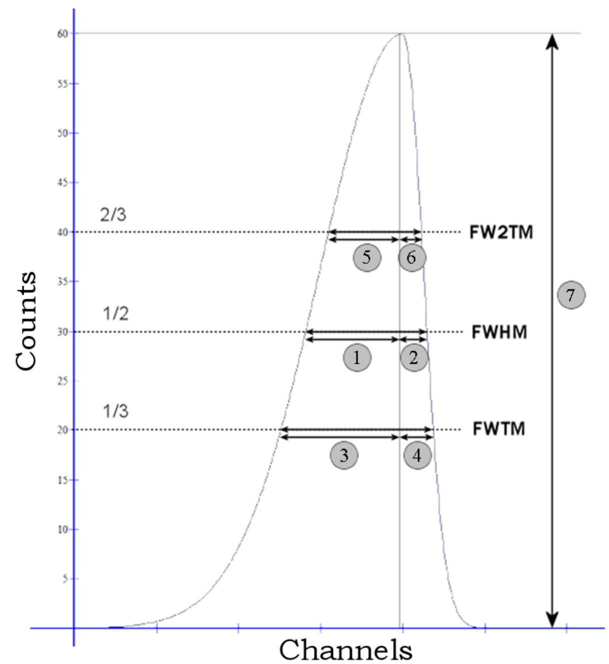

Figure 3. Characteristics of a peak. (1) first half of FWHM; (2) second half of FWHM; (3) first half of FWTM; (4) second half of FWTM; (5) first half of FW2TM; (6) second half of FW2TM; (7) maximum number of counts of the peak in a channel.

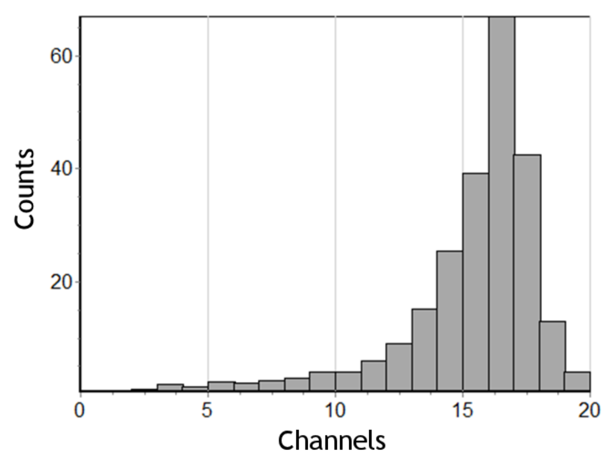

Figure 4. Neural network output example (21 values).

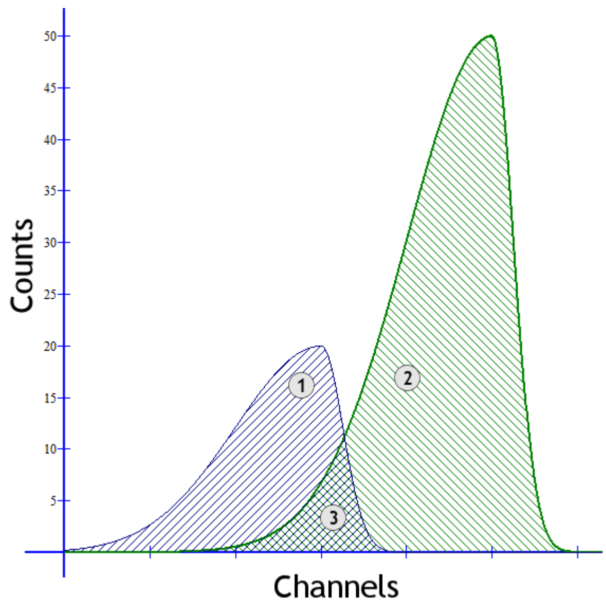

Figure 5. Overlapping peaks. (1) Left peak integral; (2) right peak integral; (3) overlapping area.

Figure 6 illustrates the process followed on the experiments. The continuous line represents the original artificially constructed spectrum. The dashed line, number 2 in the figure, is the first neural network output, i.e., the isolated right peak's contribution to the spectrum. The dotted line, number 3 in the figure, is the result of subtracting that output from the initial spectrum, i.e., the isolated left peak's contribution, which is then analyzed by the network again.

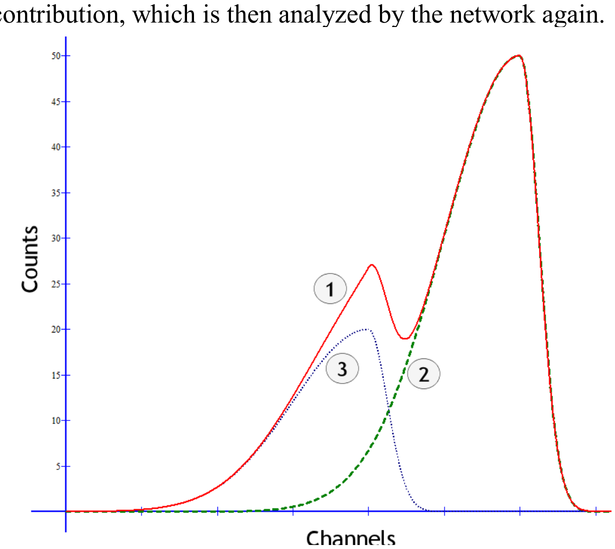

Figure 6. Peak overlap decomposition. (1) Continuous line; (2) dashed line; (3) dotted line.

III. RESULTS

The spectra we used in this work were constructed with two isolated alpha-peaks obtained from the measurement of environmental samples. These peaks are unknown by the neural network. To construct the test spectra, we selected by way of example a 590-count ^{208}Po alpha peak, with a measurement uncertainty of 23.4 counts (4.26 %), and a 127-count ^{210}Po alpha peak, with a measurement uncertainty of 11.2 counts (8.92 %). These compositions contain two peaks that overlap by a determined percentage in the range 1% – 95%.

In order to study the quality of the procedure's results, we tested three different configurations of the artificially constructed spectra: (1) the integrals of both peaks are equal, (2) the left peak is smaller, and (3) the right peak is smaller.

In the first case (see Fig. 7), we used the same 590-count alpha peak of ^{208}Po in both the right and left positions. In the second and third cases, we used the 127-count ^{208}Po alpha peak as the smaller, and the 590-count ^{210}Po peak as the larger (see Figs. 8 and 9, respectively).

We tested the procedure on each of the three configurations, varying the percentage overlap in the aforementioned range of 1% – 34%. Figures 7–9 present the results. To facilitate the visual appraisal of the resulting percentage deviations, the values are represented overlain on top of the intrinsic error of measurement (the "measurement uncertainty") of each alpha spectrum (shaded zones in the figures).

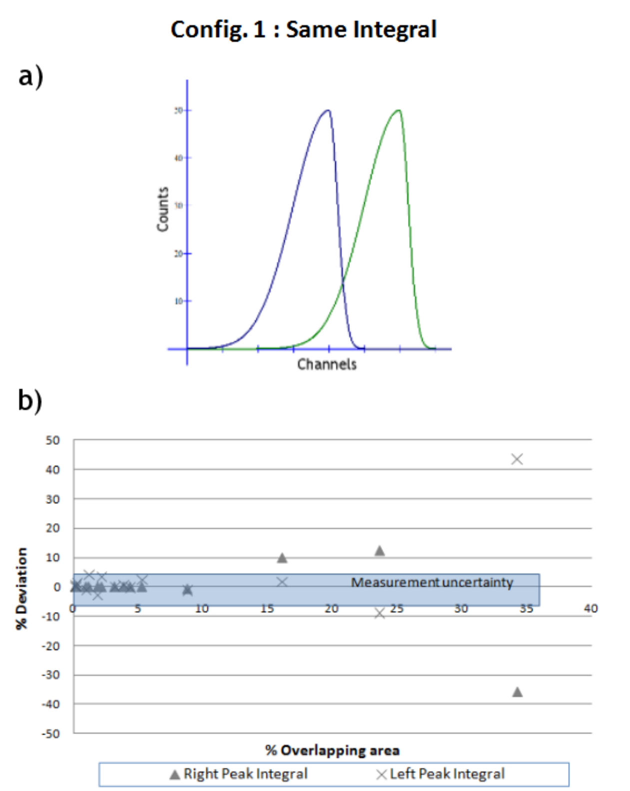

Figure 7. Configuration 1. (a) Example of the two partially overlapping peaks (8% in the figure). (b) Percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peaks versus the integrals predicted by the network for the same two isolated peaks.

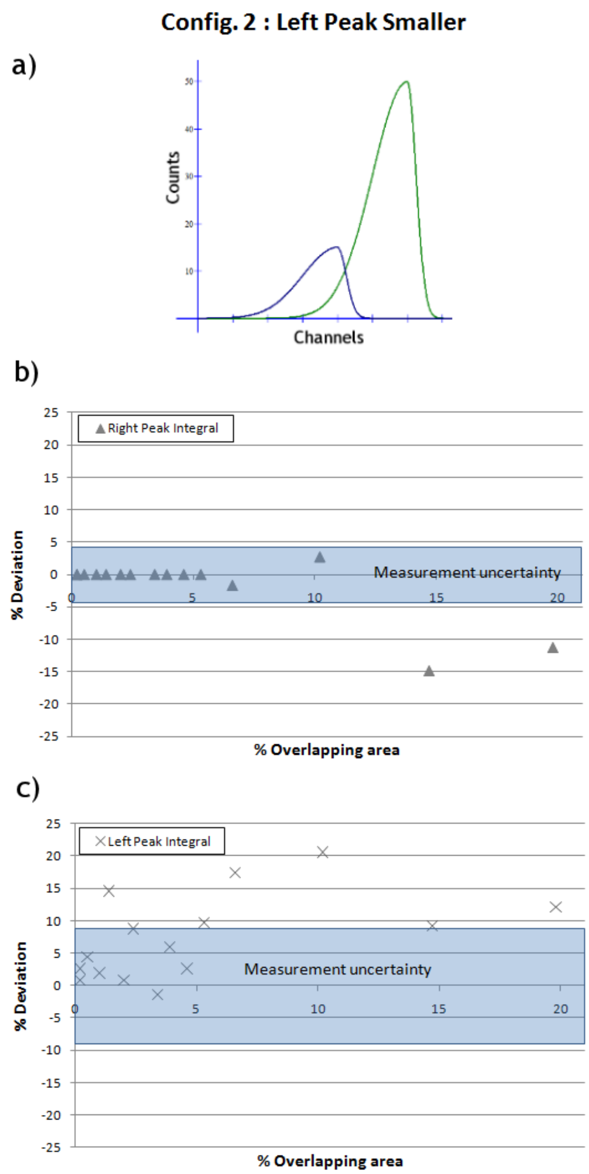

Figure 8. Configuration 2. (a) Example of the two partially overlapping peaks (35% in the figure). (b) Percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peak on the right (larger) versus the integrals predicted by the network for the same isolated peak. (c) Percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peak on the left (smaller) versus the integrals predicted by the network for the same isolated peak.

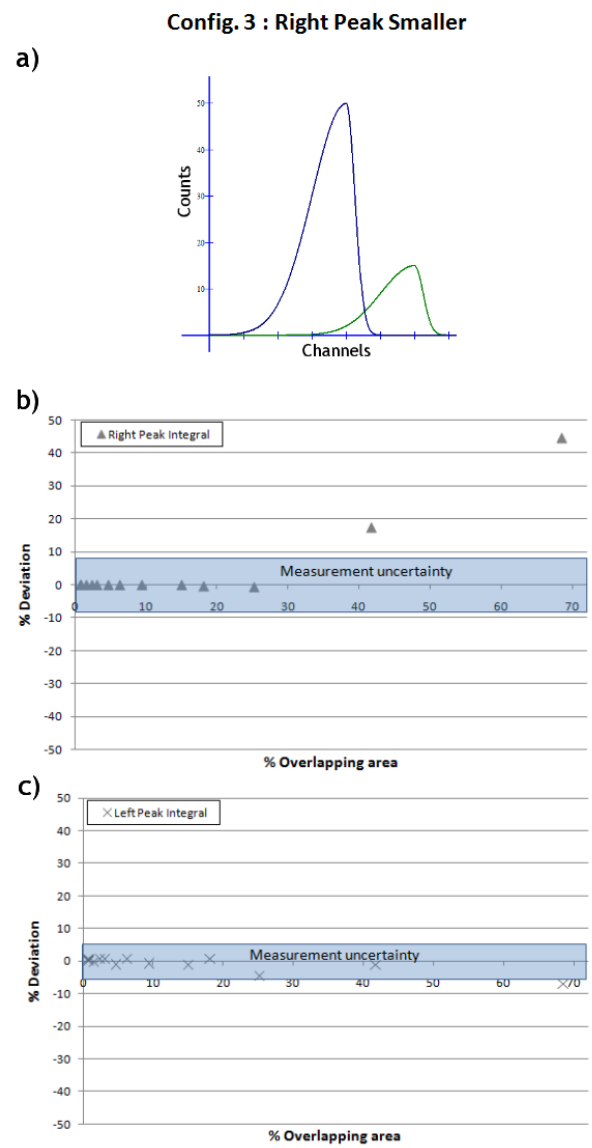

Figure 9. Configuration 3. (a) Example of the two partially overlapping peaks (10% in the figure). (b) Percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peak on the right (smaller) versus the integrals predicted by the network for the same isolated peak. (c) Percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peak on the left (larger) versus the integrals predicted by the network for the same isolated peak.

In the first configuration (Fig. 7), with peaks of equal integrals, the percentage deviation of the integrals predicted by the neural network for different degrees of overlap of the peaks versus the integrals predicted by the network for the same two isolated peaks is almost always less than the measurement uncertainty until 10% of overlapping area. Beyond this value, the shape of the spectra has only one visible peak, and the prediction become worst. Hence, for a wide range of overlap, the quality of the predicted integral is such that its uncertainty is even smaller than the intrinsic, and totally unavoidable, error of measurement.

In the second configuration (Fig. 8), the quality of the fit is the same as in the previous configuration when equal integral peaks overlapped. However, now the overlap affects more the smaller integral peak (on the left). Although the percentage deviation shows a greater dispersion, it is generally still less than the intrinsic error of measurement, when the overlapping area is less than 5%. In the other cases, the shape of the peak shape becomes single, and the prediction is worst again.

In the third configuration (Fig. 9), the quality of fit is the same as in the previous case, with percentage deviations less than the intrinsic error of measurement with overlapping area below the 25%, despite the smaller integral peak having a greater uncertainty.

IV. CONCLUSIONS

The present procedure allows one to solve the two overlapping peaks problem successfully, over a wide range of situations of overlap.

Nonetheless, notwithstanding the results described above, it is necessary to extend the work to test the procedure on multiplets of three or more overlapping alpha peaks as frequently occurs in real samples (as one observes in Fig. 1), in order to determine what are the potential limits, if any, of the application of this procedure.

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