

Application of neural network techniques in gamma spectroscopy *

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The usual methods of automatic radiation spectra analysis, based on fittings of peaks and background to exact mathematical curves, are valid for high resolution detectors. However, these methods are less successful for lower resolution detectors, such as the common scintillators or new room temperature semiconductors. Trying to solve some of the problems inherent in the application of complex fittings to the response of these detectors, we test here a new and less strict approach, based on the use of a neural network algorithm known as “associative memory”. This method appears useful in those cases in which a simple operation and a fast response are needed, together with a reasonable (and not extreme) accuracy. Furthermore, as the pattern recognition is carried out through the rough shape of the whole spectrum, instead of each individual peak, it can be used with advantage for low resolution detectors. With the idea of comparing the behavior of this method with the “classical” ones, the response of the network in the analysis of several spectra, taken with a NaI spectrometer, is presented.

1. Introduction

The problem of the identification and quantification of radioisotopes through the analysis of the spectrum yielded by a MCA, has been extensively treated in the literature since the early sixties [1]. These spectra consist of several photopeaks (or “sharp” maxima), rising over a background due to electronic noises, Compton scattering and other physical processes. The positions and intensities of these peaks are characteristic of each radioisotope, this being a suitable way for identifying the substances present in the source under study. A computer code that performs a systematic search for peak positions and, according to these, assigns the corresponding intensities to each substance, can be a good tool for routine measurements of spectra at laboratory level.

If the photopeaks are well resolved, their identification becomes a relatively simple task. However, the situation is rather more complicated when overlapping of peaks occurs as a consequence of lack of resolution. This is the case for common scintillator detectors, that offer worse resolution than Ge spectrometers but with the advantage of their easier operation, and for the less popular (but increasingly in use) room temperature

semiconductor detectors, CdTe and HgI₂ [2,3]. The difficulties encountered in the reliable identification and exact quantification of isotopes from the spectra formed by spectrometers based on these detectors, are so great that most of the codes usually employed can not deal properly with inputs produced by mixtures of relatively low complexity.

The need for an operative method that allows one to perform routine automatic analysis of spectra produced not only by high resolution cooled Ge detectors, but also by other spectrometers of inferior resolution, has led us to face the problem from an alternative point of view. This makes use of modern techniques of pattern recognition, that yield a reliable identification with an acceptable quantification of the isotopes present in an unknown mixture. The description of the method, its features, a comparison with standard automatic spectrum analysis techniques and several typical tests will be described here.

2. Description of the method

2.1. Theoretical background

“Classical” solutions to the automatic spectrum analysis problem make use of complex mathematical algorithms, generally based on the separation of a given curve (the spectrum) into a combination of individual curves, associated to each individual peak, plus

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a background [4,5]. The latter does not contribute additional information but, on the contrary, is usually considered as a rather negative element that detracts from the quality of the analysis. Thus, only the position of the centroids of the clear peaks are valid parameters for isotope identification, the area contained inside them being a true measurement of the received intensity. Other refinements refer to the subtraction of spurious background and separation of peaks by fitting them to exact mathematical functions and perform well only with good quality data from high resolution detectors.

The alternative approach takes into account the shape of the whole spectrum to perform the analysis, instead of each individual peak. In this schema, the spectrum is represented by a vector x of dimension n , equal to the number of energy channels, the component x_i giving the intensity (or events) detected in the energy bin i ; n is typically a number between 1024 and 4096. The method is based on the following two assumptions:

- (i) For a given spectrometer, and under the same experimental conditions, two spectra x_1 and x_2 produced by the same source, the second one taken during an interval t times greater than the first one (or during the same time, but being t times more intense), have the same shape, the number of events in each channel being in the ratio 1 to t , i.e. $x_2 = t \times x_1$. Statistical fluctuations inherent in the detection process will be commented upon later.
- (ii) The rough shape of a linear combination of spectra,

$$y = \sum_{j=1}^m c_j x_j \quad (1)$$

(meant as the usual vectorial expansion, i.e., each channel in y being the addition, weighted by c_j , of each channel of spectra x_j), is equal to the pattern that would be obtained by an exposure to a source containing a cocktail of the isotopes corresponding to x_j , with activity ratios defined by c_j .

These two premises are strictly valid in practical spectroscopy, if the same equipment is used to acquire all the spectra, subject to the statistical fluctuations introduced by the detection process (and assuming that no drift affects the measurements), which can be considered as random numbers added to each channel, with zero mean and a rms value equal to the square root of the events detected in that channel. Therefore, setting aside the effect of such fluctuations, an unknown spectrum can be considered as a vector formed by a linear combination of a set of vectors, their coefficients being a measure of the intensity of each

component relative to the intensity of the reference vector taken as the unity.

In these conditions, the problem has been reduced to a typical example of pattern recognition, well treated in specific literature of information technology. It has been found that the application of neural network structures [6] is a suitable choice for a reliable and versatile spectrum analysis. In particular, a type of neural network known as "associative memory" has been selected, implemented by means of the Greville's algorithm [7], which will be summarized as follows.

Let $\{x_j\}$ ($j = 1, \dots, m$) be the set of reference radioisotopes, whose rough patterns are desired to be found in an unknown mixture and whose intensities are taken as unity. A spectrum y to be analyzed can therefore be expanded as expressed in eq. (1), the problem being reduced to find the quantities c_j , given y and x_j . This is practically accomplished by means of the pseudoinverse matrix W in such a way that

$$c_j = \sum_{i=1}^n w_{ji} y_i, \quad (2)$$

w_{ji} being the elements of the $(n \times m)$ matrix W , which is formed of the reference vectors, x_j , following the Greville's technique. A detailed theoretical description of the method can be found in ref. [8].

One of the features of this approach, that constitutes an advantage for handling radiation spectra, is its lower sensitivity to random statistical fluctuations, as a logical consequence of the scalar product implied in eq. (2). This fact, that can be considered as a low-pass filtering, helps to avoid the additional complications introduced by statistical fluctuations, this being a unique feature of the pseudoinverse matrix that is fulfilled whenever $m < n$. This condition is always encountered in a practical situation, where n is of the order of 1000 and m usually never exceeds 50. We should not forget that this method is intended for performing automatic routine measurements involving few and well known common isotopes. In this sense, it can be considered as an alternative for conventional algorithms developed for low resolution and strong background detectors (too complicated to be easily implemented in low level computers) able to work in autonomous and small size field equipments.

2.2. Confidence level of the analysis

Any automatic method that performs an analysis of a given input should supply, in addition to the desired output, a coefficient that indicates how good the analysis was. In this approach, this is related to the presence in the source of nuclides whose spectra are not contained in the reference set. This fact, due to the particular nature of the identification process, would

lead to erroneous concentrations of other isotopes, thus spoiling the measurement.

The confidence level can be defined by making use of the projection of the unknown vector (spectrum) on a vector normal to the vectorial subspace formed by the spectra of the reference radioisotopes. When this value is low enough, there will not exist an additional component in the mixture, different from the reference nuclides used to train the network. On the contrary, the presence of extra components implies a non-negligible projection outside of the vectorial reference subspace and a high value of this coefficients results. This criterion has been tested in ref. [8] and a threshold of 0.15 was fixed for considering a given analysis as valid. Values higher than this limit indicate the presence of elements for which the network was not trained.

3. Experimental results

Although the good identification and quantification capabilities of the network have been demonstrated in a previous work [9], here we will examine its performances when dealing with situations of certain complexity, although encountered in practical spectroscopy. To do this, we have used a high efficiency (7.5 cm \times 7.5 cm) NaI detector, associated with a Canberra MCA (series 35 PLUS). The scale has been divided in 1024 channels, making all the electronic adjustments in order to obtain a resolution of 2 keV per channel. In these conditions, the network was trained with standard point sources (^{133}Ba , ^{137}Cs , ^{60}Co , ^{57}Mn , ^{22}Na and ^{109}Cd), placed at 18 cm in front of the detector; their activities had values around 0.4 MBq. Reference spectra were formed by exposing the detec-

tor to all the isotopes, plus an additional background pattern, during 250 s.

The aim of these experiments was to test the behavior of the method in the analysis of difficult cases involving spectra having components with close, or even superposed, peaks and intensity ratios differing greatly from unity. In this context, they can be understood as a continuation of the first analysis reported in ref. [9]. So, a group of combinations has been chosen in such a way that it was sometimes very difficult to appreciate the contributions of some isotope, hence testing the method in extreme situations. These mixtures, formed by placing some point sources at the same position and exposing the detector to them during different times, are summarized in table 1. The spectrum in table 1 marked with * is plotted in fig. 1, together with the spectra of the individual nuclides contained in it. It is seen that no clear identification can be done "by the eye", the peak corresponding to ^{109}Cd being masked by the low energy peak of ^{133}Ba . Other combinations present similar difficulties, that make the identification of their components a nontrivial task.

Once the network has been trained with the reference isotopes, the spectra resulting from exposures to the mixed sources were analyzed by it. The response consists, as was mentioned before, of a set of coefficients indicating the number of times that a reference pattern is contained in the unknown spectra or, what is the same, the detection intensity of a given identified radioisotope with respect to that of the calibration spectrum. In addition, the confidence level of the analysis is also obtained. These results are presented in tables 2 and 3. Table 2 shows those cases for which a good response was obtained, while in table 3 severe

Table 1

Description of the mixtures prepared for testing the network. Sources were placed at 18 cm in front of the detector during the indicated times

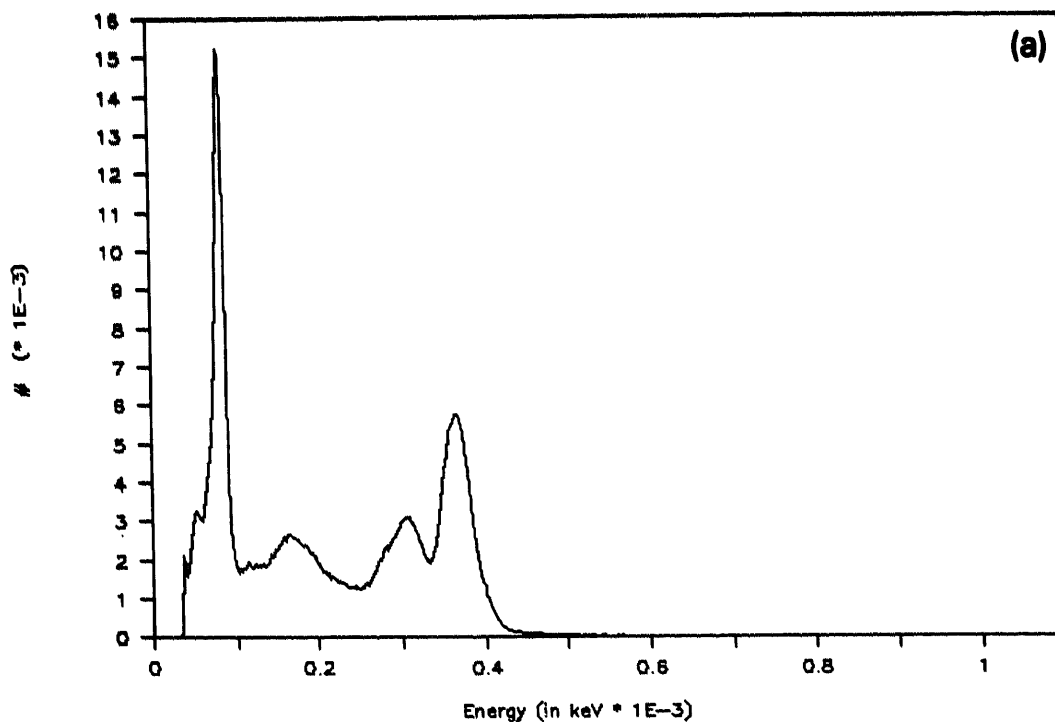
Sample	Exposure time [s]						
	^{22}Na	^{60}Co	^{133}Ba	^{109}Cd	^{54}Mn	^{137}Cs	^{57}Co
0.4 ^{22}Na + 0.4 ^{60}Co	100	100	0	0	0	0	0
0.4 ^{22}Na + 2 ^{60}Co	100	500	0	0	0	0	
2 ^{22}Na + 0.08 ^{60}Co	500	20	0	0	0	0	0
4 ^{22}Na + 0.02 ^{60}Co	1000	5	0	0	0	0	0
20 ^{22}Na + 0.08 ^{60}Co	5000	20	0	0	0	0	0
0.24 ^{54}Mn + 0.24 ^{137}Cs	0	0	0	0	60	60	0
1 ^{54}Mn + 0.08 ^{137}Cs	0	0	0	0	250	20	0
0.24 ^{54}Mn + 2 ^{137}Cs	0	0	0	0	60	500	0
(*) 0.4 ^{109}Cd + 0.4 ^{133}Ba	0	0	100	100	0	0	0
1 ^{109}Cd + 0.4 ^{133}Ba	0	0	100	250	0	0	0
0.24 ^{109}Cd + 0.24 ^{133}Ba	0	0	60	60	0	0	0
0.08 ^{109}Cd + 0.24 ^{133}Ba	0	0	60	20	0	0	0
60 ^{22}Na + 60 ^{60}Co + 60 ^{57}Co + 60 ^{54}Mn	15 000	15 000	0	0	15 000	0	15 000

deviations, corresponding to a less accurate analysis, can be appreciated.

The concentrations are expressed, for clarity pur-

poses, as the relative error in the quantification of well identified isotopes (marked with P) and the output concentrations of spurious substances (marked with N).

0.4 x ^{109}Cd + 0.4 x ^{133}Ba SPECTRUM



^{133}Ba SPECTRUM USED FOR TRAINING

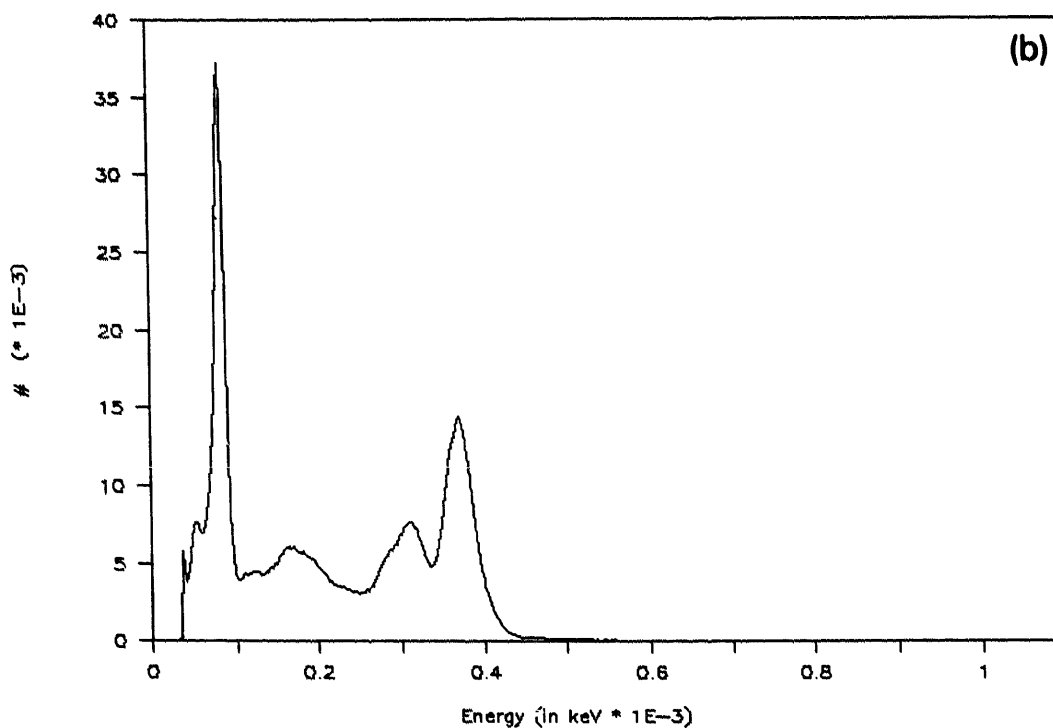


Fig. 1. (a) Typical composite spectrum. (b) and (c) Spectra of the isotopes present in the mixture (a), used for the training of the network.

109Cd SPECTRUM USED FOR TRAINING

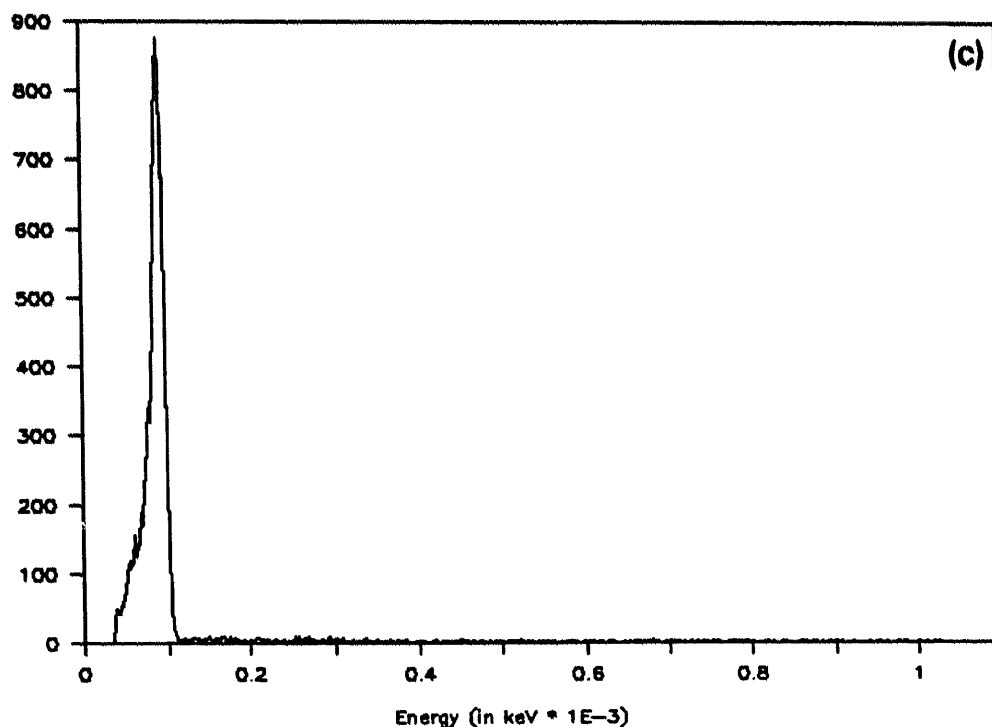


Fig. 1. (continued).

relative to the intensity of their calibration spectra; the term "spurious" refers to those isotopes not existing in the original cocktails. Table 2 shows a very good response, with an adequate identification in every case and accuracies better than 10%, which for this kind of detector is an excellent figure. Furthermore, those nuclides not present in the mixtures are rejected, indicating that their concentrations are lower than the 8% of the intensity detected during the network training; note that most of these (spurious) values are around 2%, while the confidence level is never greater than 0.13.

The results presented in table 3 are, however, worse, being some of the errors in the concentrations of P-substances greater than 100%; at the same time, excessive quantities were assigned to the N-isotopes. The first two mixtures contained in the table consist of combinations of ^{133}Ba and ^{109}Cd , in which, as can be seen in fig. 1, the presence of the latter isotope is less significant (almost two orders of magnitude) than that of the former. Bearing this fact in mind, it is easy to realize that the error associated with the output concentrations of ^{109}Cd will be higher than that encountered by its partner, having a more serious effect when

Table 2
Results of the analysis performed by the network with good accuracy

Sample	^{22}Na	^{60}Co	^{133}Ba	^{109}Cd	^{54}Mn	^{137}Cs	^{57}Co	Conf. lev.
0.4 ^{22}Na + 0.4 ^{60}Co	P 6%	P 6%	N 0%	N 1%	N 5%	N 1%	N 0%	0.014
0.4 ^{22}Na + 2 ^{60}Co	P 6%	P 2%	N 0%	N 4%	N 8%	N 1%	N 0%	0.017
2 ^{22}Na + 0.08 ^{60}Co	P 1%	P 10%	N 1%	N 0%	N 0%	N 1%	N 3%	0.026
4 ^{22}Na + 0.02 ^{60}Co	P 2%	P 10%	N 1%	N 1%	N 0%	N 1%	N 5%	0.032
0.24 ^{54}Mn + 0.24 ^{137}Cs	N 0%	N 0%	N 0%	N 1%	P 2%	P 2%	N 1%	0.111
1 ^{54}Mn + 0.08 ^{137}Cs	N 0%	N 0%	N 0%	N 0%	P 1%	P 1%	N 0%	0.090
0.24 ^{54}Mn + 2 ^{137}Cs	N 1%	N 1%	N 0%	N 3%	P 2%	P 1%	N 5%	0.119
0.4 ^{109}Cd + 0.4 ^{133}Ba	N 0%	N 0%	P 1%	P 1%	N 3%	N 0%	N 1%	0.062
1 ^{109}Cd + 0.4 ^{133}Ba	N 1%	N 0%	P 1%	P 2%	N 3%	N 1%	N 2%	0.068

Table 3
Results of the analysis performed by the network with bad accuracy

Sample	^{22}Na	^{60}Co	^{133}Ba	^{109}Cd	^{54}Mn	^{137}Cs	^{57}Co	Conf. lev.
0.24 ^{109}Cd + 0.24 ^{133}Ba	N 0%	N 0%	P 0%	P 20%	N 2%	N 0%	N 10%	0.060
0.08 ^{109}Cd + 0.24 ^{133}Ba	N 0%	N 0%	P 2%	P 125%	N 2%	N 0%	N 1%	0.066
20 ^{22}Na + 0.08 ^{60}Co	P 1%	P 73%	N 3%	N 28%	N 2%	N 16%	N 30%	0.097
60 ^{22}Na + 60 ^{60}Co + 60 ^{57}Co + 60 ^{54}Mn	P 12%	P 10%	N 150%	N 3700%	P 16%	N 290%	P 24%	0.130

the ratio is 1 to 3 in favour of ^{133}Ba . However, the errors are not relevant, if we take into account the small numbers involved, and the important point that the concentrations of ^{133}Ba and the spurious isotopes have been determined with their right values; note the very accurate output obtained for both isotopes in the 8th mixture of table 2. Thus, the mere fact of getting a reliable identification in such adverse conditions can be considered as a success of a method, that is able to find components not visible "by the eye" (see, for instance, how difficult it is to find the spectrum of fig. 1c inside the pattern of fig. 1a; obviously, this difficulty increases when the concentrations decrease).

The bad results suggested by the last two rows of table 3 reflect a very important point that should be taken into account when applying this kind of method. In effect, we see that the concentrations of some isotopes are several times higher than the calibration ones, which implies that their projections on the reference vectors are accordingly incremented by roughly the same factor. By comparing these values with those given in the 4th row of table 2, it is possible to deduce that the ratio of the isotope concentrations are not the primary cause of the bad behavior of the network.

Instead of this, we must put the blame on the excessively large projections on other spurious substances, which, for the last analyzed case, have a dramatic effect. Thus, a consequence should be deduced from this fact: the network will be able to analyze patterns whose intensity is of the same order of magnitude or lower than the calibration spectra, yielding in these cases very good results; however, when the concentrations are too high, the obtained quantities of undesired isotopes become large, even masking the values of small traces of other existing isotopes.

As a comparison with standard techniques of spectrum analysis, based on mathematical fitting, we have applied a commercial program [10] to several mixtures analyzed by the network. Table 4 summarizes the differences between the responses of both methods, from which we can conclude that better results are obtained when the shape of the whole spectrum is taken into account instead of the particular maxima positions. In effect, the peak width plays an important (almost crucial) role in the determination of the concentrations by computing the area contained under the photopeaks. Thus, either rather complicated programs must be used or the analysis is as not accurate as that obtained here.

Table 4
Comparison between the results obtained from pattern recognition methods and the classis program

Sample	Associative memory		Classical peak fitting	
	identification	quantification [% deviation]	identification	quantification [% deviation]
0.4 ^{22}Na + 0.4 ^{60}Co	yes	7	yes, but giving 10% of ^{133}Ba	12 in the best photopeak
1.0 ^{54}Mn + 0.08 ^{137}Cs	yes	1	yes, but giving 5% of ^{133}Ba	4 in ^{54}Mn 3 in ^{137}Cs
0.4 ^{109}Cd + 0.4 ^{133}Ba	yes	1	failed to find ^{109}Cd	13 in ^{133}Ba
0.24 ^{109}Cd + 0.24 ^{133}Ba	yes	2 in ^{133}Ba failed in ^{109}Cd	failed to find ^{109}Cd	8 in ^{133}Ba

On the contrary, the new identification method helps to avoid elegantly some of the limitations inherent in other algorithms.

4. Conclusions

A new automatic method for analyzing and quantifying the isotopes present in an unknown mixture, from the spectra produced by low resolution spectrometers, has been tested for several difficult cases. This method, based on a very simple application of neural network structures, has been demonstrated as a reliable tool for dealing with the response of low resolution detectors, working properly even in adverse situations. The good results obtained can be considered as a confirmation of the possibilities that a new approach, like this one, may offer in those situations in which the following features are more important than a very precise and accurate activity determination:

- (i) Portability: the network can be implemented in low level computers or even in ASIC (Application Specific Integrated Circuits).
- (ii) Reliable automatic performance.
- (iii) Indication of which substances are *not* present in the mixture, and to which extent.

The theoretical basis of the method is well understood. It is based on two premises that are approximated to the truth when the experimental conditions do not change, in particular the geometry of the source-detector positions. The results may be better than those obtained with standard methods in similar cases. A limitation of the method, when applied to complex cases, is the need of training the network with reference sources whose detected intensities are of the same order or greater than those expected during

operation. In this way, a good identification and quantification of existent (and nonexistent) isotopes is assured, even in adverse conditions. A more serious limitation, for some applications, is that for accurate results it is necessary, but not sufficient, that the set of radionuclides used to train the network must include all those present in the sample to analyze.

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