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"Detection of Single Isotopes in Composite Gamma-ray Spectrum" An Application of Wavelet Theory to Gamma-ray Spectra Analysis

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ABSTRACT

Some of the difficulties with analyzing radioisotope spectra are the large amount of data, the detector sensitivity, and a high signal-to-noise ratio. Wavelet analysis is a relatively new technique that is useful for denoising data and localizing behavior in complex data sets. Yet, wavelet analysis has not been widely applied to the field of spectroscopy. This paper investigates the potential use of signature recognition for gamma-ray spectra analysis. Using Wavelet MultiResolution Analysis, a method for constructing signatures for gamma-ray spectra was developed. A test for detection of the isotopes was developed using the signatures. These methods provided useful results and warrant further testing.

1. INTRODUCTION

The objective of this paper is to explore the possible uses of Wavelet Theory, specifically, Wavelet transforms and Wavelet MultiResolution Analysis (MRA), to improve performance and/or accuracy of software codes currently used to analyze gamma-ray spectra.

The structure of the existing software applications for spectra analysis can be described by the following four steps (Debertin,1988):

1. Preprocess (calibration)
2. Peak finding and fitting
3. Peak analysis (calculation of areas under peaks)
4. Peak verification (calculation of activities)

Generally, the output of the applications includes information on possible detected isotopes, their activities, and statistical confidence intervals. Based on this information, a decision can be made on what isotopes are present in the composite spectrum.

This paper presents a method for detecting a particular isotope in a composite gamma-ray spectrum based on signature recognition. The method can be described in two main phases. Phase I: construction and storage of the signatures. Phase II: Detection of isotopes in composite gamma-ray spectrum.

Since the basic assumption for the development of this method is that each gamma-ray spectrum has a unique signature, and wavelet theory is the basic tool in the construction of the signatures, a section on wavelet theory will be presented followed by a section on each of the phases.

2. WAVELET THEORY

Any gamma-ray spectrum, a function whose domain is the channel numbers and whose range is the number of counts per channel, can be considered as an element $S \in L^2(\Re)$, meaning it has finite energy content Hence, it can be represented using a wavelet basis. The construction of the a wavelet basis begins with a clever choice of a function Φ (call it scaling function) such that (Kaiser, 1995) and (Chui, 1992):

$$\{\Phi(x-k),\ x \in \Re,\ k \in \mathrm{Z}\}$$

forms an orthonormal basis for a reference space $V_0 \subset L^2(\Re)$. Now build an increasing sequence of closed subspaces $\{V_i\}_{i \in \mathrm{Z}}$ such that:

1. $\cdots\cdots\cdots \subset V_{-1} \subset V_0 \subset V_1 \subset \cdots\cdots\cdots$

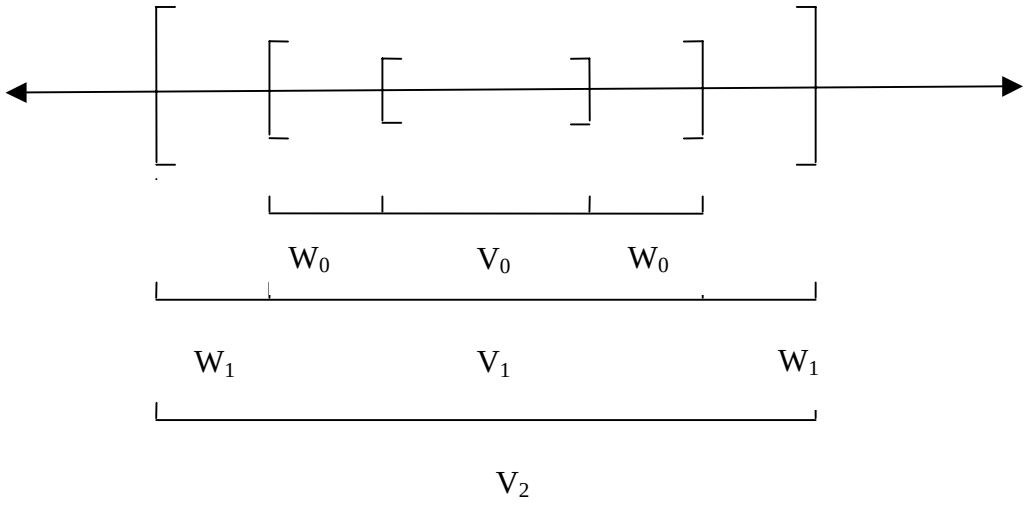
2. $\overline{\bigcup_{i \in \mathrm{Z}} V_i} = L^2(\Re)$ (dense)

3. $f(x) \in V_i \leftrightarrow f(2x) \in V_{i+1} \quad i \in \mathrm{Z}$.

Note that the V_i space is therefore spanned by: $\{\Phi_{ik}(x),\ x \in \Re,\ i \in Z,\ k \in \mathrm{Z}\}$

Where: $\Phi_{ik}(x) = 2^{i/2}\Phi(2^i x - k)$

Now, the wavelets enter into the picture. Consider the orthogonal complement W_i of V_i in V_{i+1}: $V_{i+1} = V_i \oplus W_i$



Since $V_0 \subset V_1$ and $\Phi(x) \in V_0$ then: $\Phi(x) = \sum_k h(k)\sqrt{2}\Phi(2x-k)$

where: $h(x) = \langle \Phi(x), \sqrt{2}\Phi(2x-k) \rangle$. Define $\Psi(x)$ as follows:

$\Psi(x) = \sqrt{2}\sum (-1)^k h(-k+1)\Phi(2x-1)$ then:

1. $\{\sqrt{2}\Psi(2x-k), \quad k \in \mathrm{Z}\}$ is an orthonormal basis for W_1

2. $\{2^{i/2}\Psi(2^i x-k), \quad k \in \mathrm{Z}\}$ is a basis for W_i

3. $\overline{\bigcup_{i \in \mathrm{Z}} W_i} = L^2(\Re)$ and W_i is orthogonal to W_{i+1}

Given all the properties above we have:

$$\begin{aligned} V_N &= V_{N-1} \oplus W_{N-1} \\ V_N &= V_{N-2} \oplus W_{N-2} \oplus W_{N-1} \\ &\vdots \quad \vdots \qquad \vdots \qquad \vdots \\ V_N &= V_0 \oplus W_0 \oplus \cdots\cdots W_{N-1} \end{aligned}$$

So, if $S(x) \in V_N$ then, $S(x) = f_0(x) + \sum_{k=0}^{N-1} f_k(x)$, where $f_0 \in V_0$ (the approximation space) and $f_k \in W_k$ (each is a wavelet space).

Given the construction and properties of the wavelet representation of S, the MRA can be constructed (see below) and used for the study of the behavior of the function (spectrum signal).

MultiResolution Analysis (MRA)

$$
\begin{array}{ll}
\vdots & \oplus \quad W \\
V_N & \oplus \ \vdots \\
\vdots & \qquad \perp \\
\vdots & \qquad \vdots \\
\cap & \\
V_{-1} & \oplus W_{-1} \\
\cap & \quad \perp \\
V_0 & \oplus W_0 \\
\cap & \quad \perp \\
V_1 & \oplus W_1 \\
\vdots & \vdots \quad \vdots
\end{array}
$$

The following are properties of an MRA:

1. V_i's are nested
2. $L^2(\Re) = \overline{\bigcup_{i \in \mathrm{Z}} V_i}$
3. $S(x) \in V_i \leftrightarrow S(2x) \in V_{i+1} \quad i \in \mathrm{Z}$
4. $V_{i+1} = V_i \oplus W_i$

Since the function S has a representation in each of the direct sums, the MRA provides us with a tool to represent the function at different resolutions (Benedetto, 1994).

3 PHASE I

In this phase, the signatures of the single isotopes of interest are constructed and stored. Starting with the gamma-ray spectrum for each isotope, which is preferably collected with the same detector that will be used to collect the composite gamma-ray spectrum, and which is calibrated as often as needed to keep the data stable, the following steps are taken:

1. Construction of the wavelet approximation (de-noising of the signal)
2. Construction of the non-parametric local smooth
3. Detection of *significant* peaks (peaks needed to identify a given isotope)

3.1 Construction of the wavelet approximation

Let S be the gamma-ray spectrum of a single isotope. The coefficients of the wavelet decomposition were obtained using the wavelet toolbox in Matlab. The family of wavelet functions used in the construction of the signatures is "Daubechies-one" wavelets (db1) and the selected resolution (level) of decomposition is three. Figure 1 is a

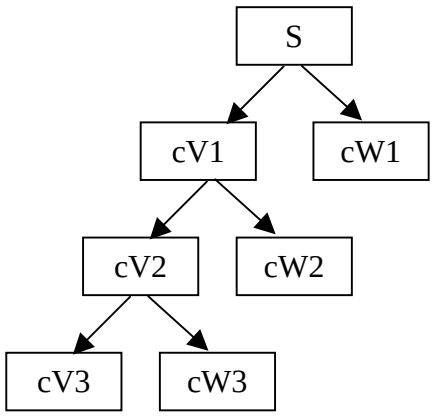


Figure 1. Tree view of the coefficient vectors of wavelet decomposition.

representation of the digital decomposition into coefficient vectors (cVi's and cWi's) at each level. Paired filters (low-pass and high-pass), together with a down-sampling process, are used to obtain the coefficient vectors. Each vector is approximately 2^{-i} the size of the original spectrum. Due to the data down-sampling, complementary filters must be used to reconstruct the approximation (Vi) and the detail (Wi), and hence the spectrum (S) (Misiti, 1996) (Fig 2).

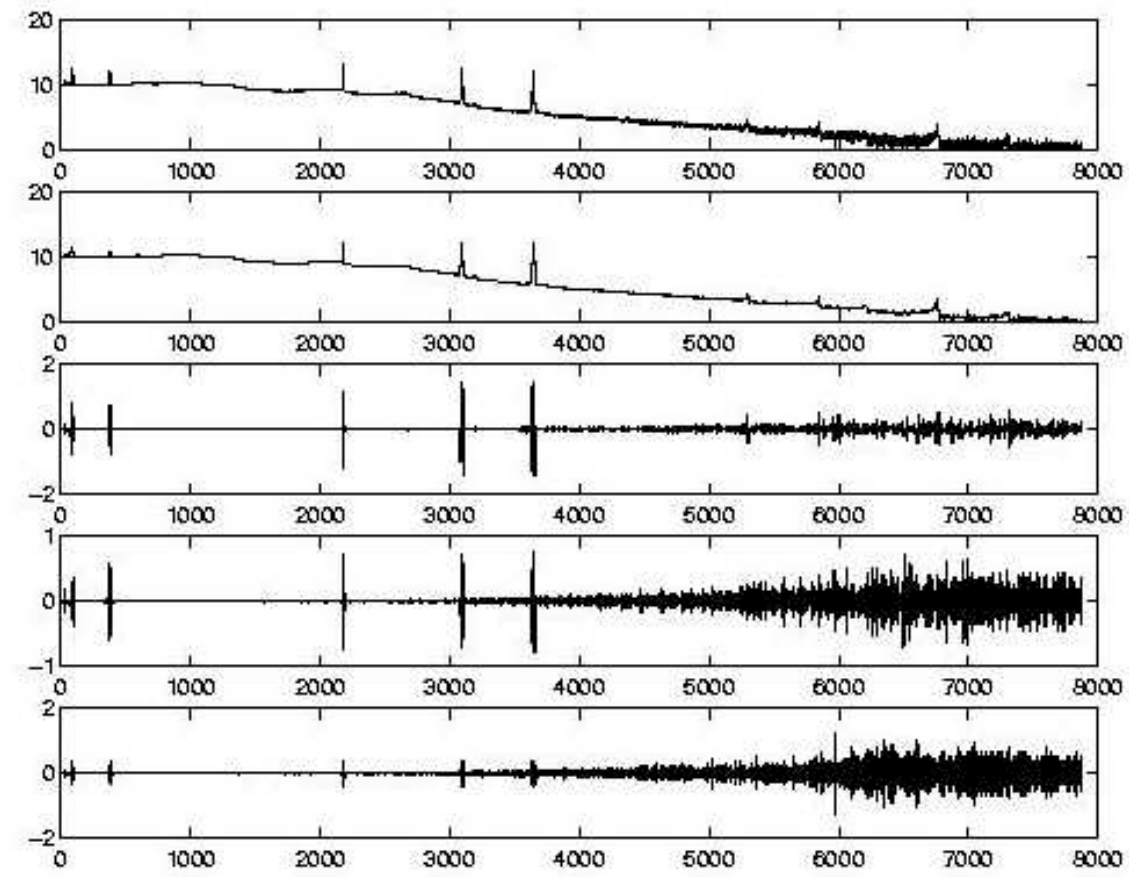


Figure 2. From top to bottom, the plots are: gamma-ray spectrum of Ag108m (S), wavelet reconstruction of the approximation (V3), wavelet reconstruction level 3 (W3), wavelet reconstruction level 2 (W2), wavelet reconstruction level 1 (W1). Note: S=V3+W3+W2+W1.

3.2 Non-Parametric Smoothing

Given the decomposition S=V3+W3+W2+W1, where cV3 contains the coefficients of the approximation V3 of S, the vector cV3 is smoothed using lomesmo (lomesmo is an acronym for our "local median smoother"). Lomesmo generates the smooth, SM, by taking a large enough neighborhood about each point of the approximation and calculating the median of the signal on this neighborhood to use as the smooth at that point. This smoothing technique will allow us to separate the peaks on the signal from the smooth trend (see Fig 3).

```
function sm=lomesmo(y,n)
% This function is a Locally Median Smoother
%
% sm=lomesmo(y,n)
% Takes a vector y and fits a smooth to it by
% calculating the median of a local neighborhood
% about each point of y.
% y data input
% n neighborhood radius input
% sm smooth calculated output
%
len=length(y);
for i=1:len,
     x(1)=y(i);
     j=i+1;
     for k=2:n+1,
          if j>len
          x(k)=y(2*len-j);
          j=j+1;
          else
          x(k)=y(j);
          j=j+1;
          end
     end
     j=i-1;
     for l=0:n-1,
          if j==0
          j=j-1;
          end
          k=k+1;
          x(k)=y(abs(j));
          j=j-1;
     end
     sm(i)=median(x);
end
```

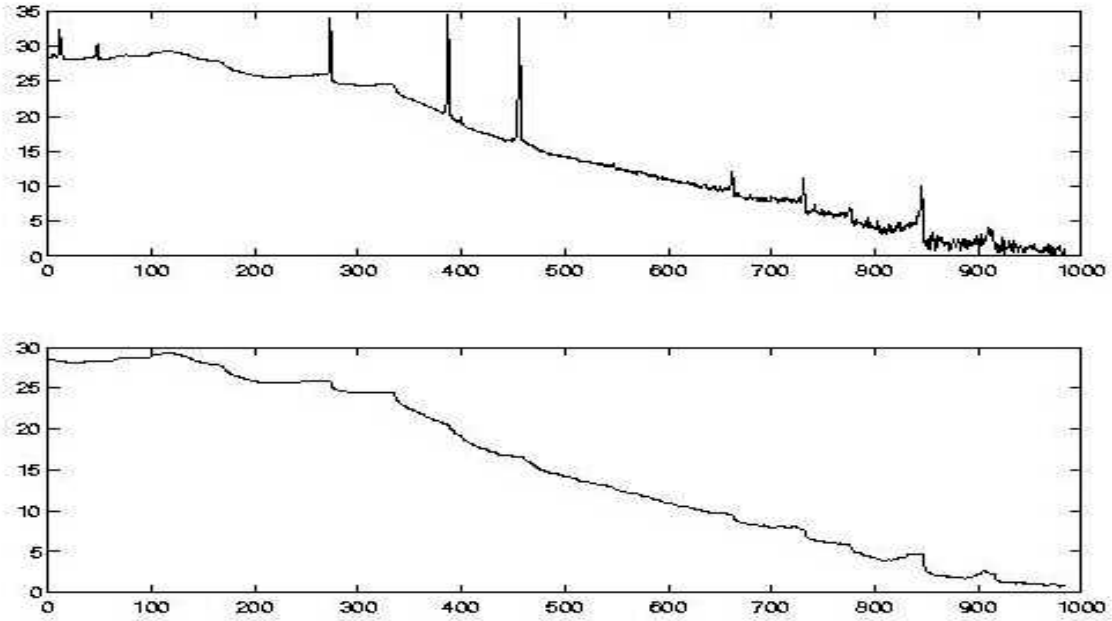


Figure 3. Approximation coefficients of Ag108m (cV3) (top) and non-parametric local smooth (SM)(bottom).

3.3 Detection of the *significant* peaks

To detect the *significant* peaks, which are the heart of the signature of the isotopes, define the following error function: $error(x) = |cV3(x) - SM(x)|$. Recall $cV3(x)$ are the coefficients of the wavelet approximation and $SM(x)$ are the values of the non-parametric local median smooth (Fig. 5). It is clear that the smooth trend of the wavelet approximation has been removed from the signal and the peaks have been isolated (see Fig. 4). But more importantly, since the smooth trend has been removed from the approximation, all the peaks can now be compared using the same base line (Fig. 5). Physicists would recognize the smooth, SM, as the intrinsic efficiency of the gamma ray detector.

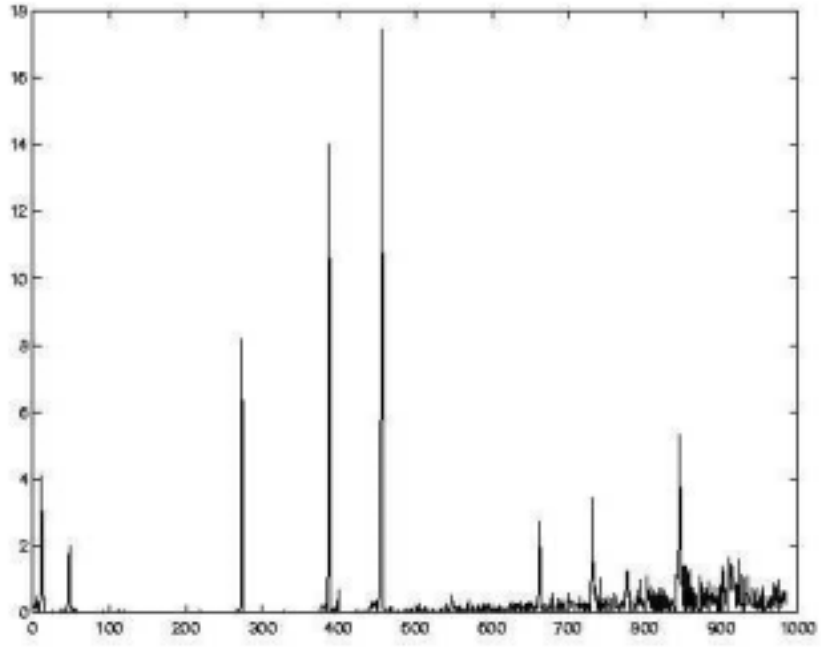


Figure 5. Error function $error(x)$ using the approximation vector for Ag108m.

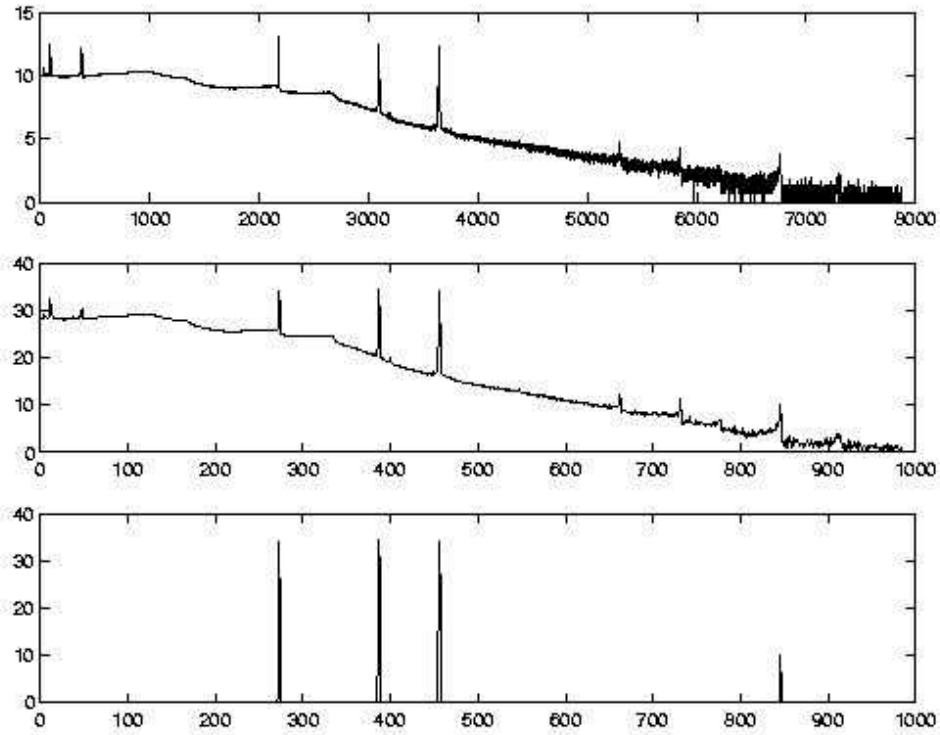


Figure 6. Ag108m gamma-ray spectrum (S) (top), Ag108m approximation coefficients (cV3) (middle), Ag108m signature (bottom).

For the selection of the *significant* peaks, the error function was thresholded by $\mu + 4*\sigma$, where μ and σ are the mean and the standard deviation of the *error* function,

respectively. The remaining coefficients will produce the "signature" of the isotope. The fine tuning of the thresholding parameter σ is important for finding the *significant* peaks and can be changed depending on the number of *significant* peaks desired on the signature of the isotope. The threshold *error* function is the signature of the given isotope's gamma-ray spectrum. Figure 6, in order from top to bottom, shows the plots for the gamma-ray spectrum (S), the coefficient vector of the wavelet approximation (cV3), and the signature for Ag108m.

4. PHASE II

In this phase, the isotopes of interest are to be detected on a composite gamma-ray spectrum. Once the signatures of the isotopes are constructed and stored, the composite spectrum undergoes the following steps:

1 Construction of the signature for the composite gamma-ray spectrum
2 Ranking detection of the single isotopes
3 Verification of detection

4.1 Construction of the signature

The signature for the composite gamma-ray spectrum is constructed in exactly the same way that the signatures for the single isotopes were constructed. The assumption in this phase is: $Sigcomp(x) = \sum_j \alpha_j Sigiso_j$ where $sigcomp$ is the signature vector for the composite spectrum, $Sigiso_j$ is the signature vector for the jth single isotope, and the α_j are scalars which will be called mixing approximates. Note the mixing approximates are positive for all j i.e. $\alpha_j > 0 \quad \forall\, j$.

4.2 Detection of single isotopes

The testing for presence of a single isotope i is done by the use of the dot product as follows:

$$Sigcomp \bullet Sigiso_i = \sum \alpha_j Sigiso_j \bullet Sigiso_i$$

since:

$$Sigiso_j \bullet Sigiso_i = \begin{cases} 0 & if\ i \neq j \\ \left\| Sigiso_i \right\|_2^2 \end{cases}$$ (numerically nearly orthogonal)

then: $\alpha_i = \dfrac{Sigiso_i \bullet Sigcomp}{\left\| Sigiso_i \right\|_2^2}$

Each α_i gives us a numerical parameter for measuring the possibility of the presence of the ith isotope in the composite spectrum signature. The descending ranking in

magnitude of these mixing-approximates generates a list of possible detected isotopes, which is used in the verification stage.

4.3 Verification of Detection

The list of isotopes detected and ranked from step 4.2 is verified for confirmation in this stage. The verification stage is necessary because the error function was thresholded to obtained the signature composite spectrum. Due to this threshold, some of the peaks which are significant to the single isotope signatures might get lost in the construction of the composite spectrum signature.

To verify the detection of an isotope, the wavelet approximation of the composite spectrum decomposition is used to find the missing peaks, and hence improve the confidence on the detection of the isotope.

The mixing-approximates are used to build a weighted sum of signatures. The points, x_j at which $\sum_i \alpha_i Sigiso_i(x_j) > 0$ must also be points at which the $error(x_j) > 0$. So, a 95% confidence interval is constructed, which tests whether $\left|\sum_i \alpha_i Sigiso_i(x_j) - error(x_j)\right| \le 2 * \sigma$. Note that this confidence interval is for the entire mixture of isotopes and any individual isotope.

4. CONCLUSIONS

This detection method will be tested on experimental composite spectra containing up to eleven isotopes. Success ratios will be reported at the conference presentation. Note that the mixing approximates can only be used as indicators of the likely presence of a particular isotope. Further energy conservation computations must be performed to determine the actual proportion of that isotope in the mixture. The mixing-approximates should serve as a useful starting ratio for the above computations.

If a different gamma-ray detector is used within the same experiment, we expect problems with shifts in the isotope signatures due to the detector's intrinsic efficiency. Nonetheless, the detection of single isotopes can be performed by replacing the dot product in the computation of the mixing-approximates by a convolution. The mixing-approximates will then be taken as the largest component of the convolution resultant. This technique can be tested as well.

NOMENCLATURE

$\Re$	The Real number system
Z	The Integer number system
$L^2(\Re)$	The space of squared integrable functions defined on $\Re$
MRA	MultiResolution Analysis
Φ	Scaling function

V_i W_i subspaces of $L^2(\Re)$
cVi coefficient vector for the wavelet approximation at level ith
cWi coefficient vector for the wavelet detail at level ith
Vi reconstruction vector for the wavelet approximation at level ith
Wi reconstruction vector for the wavelet detail at level ith
lomesmo Matlab function (local median smoother)
SM smooth (out put of lomesmo)
σ thresholding parameter (standard deviation of the error function)
$sigcomp$ signature vector for the composite spectrum
$Sigiso_j$ signature vector for a single isotope spectrum
α_i mixing approximates
$\subset$ set contaiment
$\in$ is an element of
$\forall$ for all (universal qualifier)
$\oplus$ direct sum
$\bigcup$ set union

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