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Fourier Transformation Methods in the Field of Gamma Spectrometry

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Abstract

The basic principles of a new version of Fourier transformation is presented. This new version was applied to solve some main problems such as smoothing, and denoising in gamma spectroscopy. The mathematical procedures were tested firstly by simulated data and then by actual experimental data.

Introduction

Fourier Transform (FT) is a tool for processing signals in both, time domain and frequency domains. Fourier analysis is based on the idea of decomposing periodic signals into their harmonic components. Many years after Fourier had discovered this remarkable property of (periodic) functions, his ideas were generalized first to non-periodic functions, and then to periodic or non-periodic discrete time signals. It is after this generalization that it became a very suitable tool for automatic calculations. In 1965, a new algorithm called Fast Fourier Transform (FFT) was developed and FT became even more popular.

The application of FT to nuclear-radiation spectra analysis, and in particular to gamma-ray spectroscopy was first proposed by Inouye [1]. His work opened a new field in data analysis to nuclear spectroscopy, but only a few papers can be found in the literature concerning the application of Fourier-Transform methods to practical cases in α, β or γ-ray spectroscopy [2-5]. There wa a restriction for using FT in searching peaks especially in the presence of peak multiplets. FT requires Lorentzian peak shapess and transformation of Gaussian into Lorentzian peak shapess is a difficult problem [6]. This is why we will present a new version of FT namely, Modified Fourier Transform (MFT) technique to handel gamma ray spectra. analysis.

Theory And Algorithm

The discrete Fourier Transform (DFT) of a set (X_j) of N points is defined as[7]

$$C_r = \sum_{k=0}^{N-1} X_K \exp(-2\pi irk/N),\ \ r = 0,1,...N-1 \tag{1}$$

and its inverse

$$X_r = \sum_{k=0}^{N-1} C_K \ \ / \ \ N \exp(2\pi irk/N) \tag{2}$$

where $\{C_r\}$ are the complex coefficients obtained in the DFT of $\{X_j\}$ and $i = \sqrt{-1}$.

It is clear that in the FT there is a resolution problem that we cannot know exactly the number of oscilations in aperiodic signal at certain time. What gives the perfect resolution in the FT is the fact that the window used in the FT is its kernel, the $\exp\{2\pi irk\}$function, which lasts at all times from 0 to number of points minus one. Now, we will make a modification that, our window is very narrow and compact.

The window, which was used, is constructed as a basis function $\Psi_{a,b}(x)$ which is derived from the main function through the following dilation and translation (varied positions) processes $\Psi(x)$ [8]:

$$\Psi_{a,b}(x) = a^{-1/2}\Psi(\frac{x-b}{a}) \quad a,b \in R, a \neq 0 \tag{3}$$

where a and b are the scale and position parameters respectively,, with a>0 and b having arbitrary values. The MFT of a signal f (x) is given by:

$$MFT_{\Psi}(a,b)f = \frac{1}{\sqrt{C_{\Psi}}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{|a|}} \Psi_{a,b}(x) f(x)\, dx \tag{4}$$

In practical uses, the resolution algorithm of multi signals decomposition proposed by Mallat is generally used [9,10]. Once a certain wave has been chosen, one can use its coefficients to define two filters, namely approximations filter and the details filter. Both types of filters use the same set of wave filter coefficients, but with alternating sign and in reversed order. These filters are used to construct the filter matrices, denoted as L and H. For example L and H matrices have the following structure:

$$L = \begin{bmatrix} C_0 & C_1 & C_2 & C_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & C_0 & C_1 & C_2 & C_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_0 & C_1 & C_2 & C_3 \\ C_2 & C_3 & 0 & 0 & 0 & 0 & C_0 & C_1 \end{bmatrix}$$

$$H = \begin{bmatrix} C_3 & -C_2 & C_1 & -C_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & C_3 & -C_2 & C_1 & -C_0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_3 & -C_2 & C_1 & -C_0 \\ C_1 & -C_0 & 0 & 0 & 0 & 0 & C_3 & -C_2 \end{bmatrix}$$

The N input data is passed through the scaling and the modified FT filters. The output of the filters consists of two sets of N/2 coefficients. The high-pass and low-pass filtered data are detail d1 and approximation coefficients a1 at first level of resolution. The approximation coefficients a1 can be used as the data input for the MRSD to generate sets of N/4 of detail d2 and approximation coefficients a2 at the second level of resolution. This process is iterated as many times as wanted. If the original signals were taken as the approximation of signals at the lowest resolution level 0, i.e.

$$a_0 = f(t) \tag{5}$$

then a^j and d^j are computed via the following decomposition equation:

$$a^j = La^{j-1} \tag{6}$$

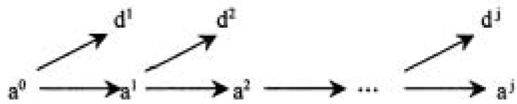
$$d^j = Hd^{j-1} \tag{7}$$

where j denotes the resolution level .

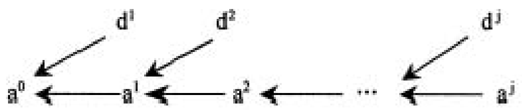
To reconstruct the signal from its decomposition is just to run the recursion algorithm in the reverse with conjugates of H and L. The reconstruction algorithm is therefore of type of a pyramid algorithm using the same filter coefficients as the decomposition. Signal reconstruction can be presented as follows:

$$a^{j-1} = L^* a^j + H^* d^j \tag{8}$$

where L* and H* represent the conjugates of the L and H matrices. Schematically, the decomposition can be represented by:



and the reconstruction can be represented by:



The algorithm of our program is not exactly the same as of Mallat, because the we don't need the data points number to be exactly 2^N. We doubled the number of data points of the filters by inserting zeros into the every adjacent item of the filters.

Smoothing and Denoising

Various methods have been proposed for smoothing and denoising data sets, but a distinction is seldom made between the two procedures. Here, we distinguish between them in the signal domain and its transformed domain.

Smoothing removes components (of the transformed signal) occurring in the high end of the transformed domain regardless of amplitude while denoising removes all small-amplitude components occurring in the transformed domain regardless of position. A distinction can be drawn between the two types of filters. A direct filter acts on the transformed signal in the frequency domain. The observed signal is transformed from the time to the frequency domain by an orthogonal transform such as the Fourier transform (FT), filter. It works by taking the Fourier transform of a signal and cutting off all of the frequencies above a specified limit (frequency cutoff). Afterward, the signal is back-transformed in the time domain. The assumption is made that the frequency components of the signal are mainly present at low frequencies and those of the noise at high frequencies. The frequency cutoff was computed on the basis of the power spectrum so that a maximum of noise is eliminated with a minimal distortion of the signal. An indirect filter smooth or denoise of the observed signal in the time domain; no transformation to the frequency domain is required. Numerous methods exist for this type of filtering. Windowed smoothing algorithms such as Savitzky-Golay [11] is often employed.

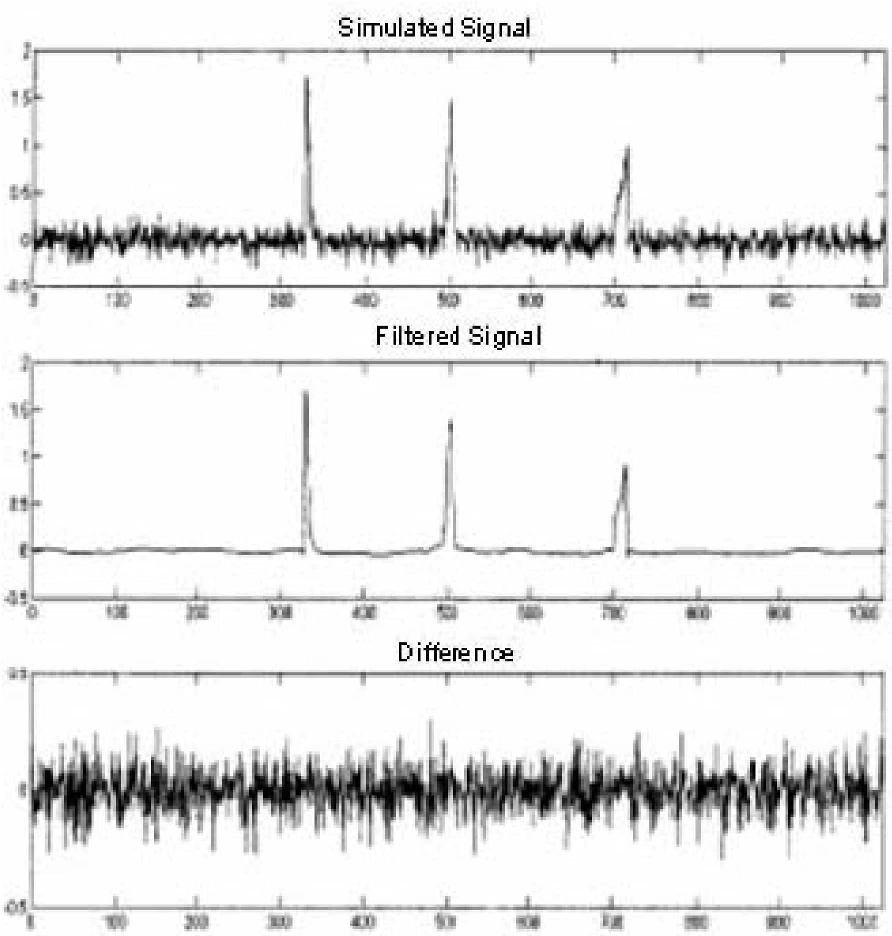


Figure 1: Modified FT denoising of simulated signals: top fig., simulated signals;, middle fig., filtered signals; bottom fig., vector of differences between the filtered and original signals.

The general procedure of denoising and smoothing with this modification is summarized as follows:

• Applying the MFT to a noisy spectrum and obtaining MFT coefficients,

• Suppresing these coefficients by the thresholding methods of smoothing and denoising.

• Applying the inverse transform to the suppressed modified FT coefficients, to obtain the denoised or smoothed spectrum.

Reconstruction of a signal after filtering in the transformed domain can produce artifacts near discontinuities. These artifacts can be attributed mainly to an inappropriate modified FT shape or to a non alignment between a sharp change in the signal and features of the modified FT. To reduce such artifacts, the signal is shifted N times to obtain N signals. Each of them is filtered in the transformed domain. The final reconstructed signal is obtained by averaging the N filtered signals.

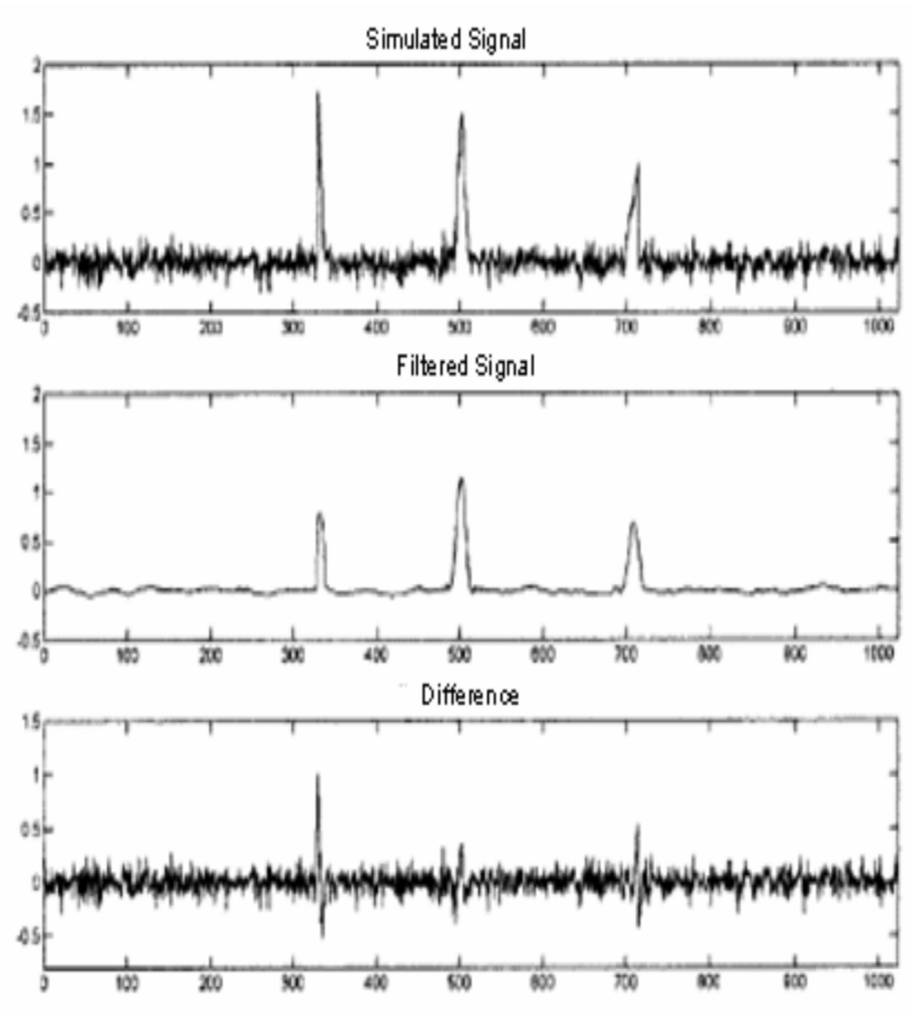


Figure 2: Savitzky-Golay smoothing of simulated signals: top, simulated signals, middle, filtered signals; bottom, vector of differences between the filtered and the original signals.

Applications

Simulated spectra

A simulated signal containing three peaks of different shapes was first used to evaluate the performance of the modified FT transform. Correlated noise was simulated according to

$$n_i = (n_{i-1} + a_i)\sqrt{0.5} \tag{9}$$

where n_i is the i-th point describing noise, and a_i is a random value between 0 and 1.

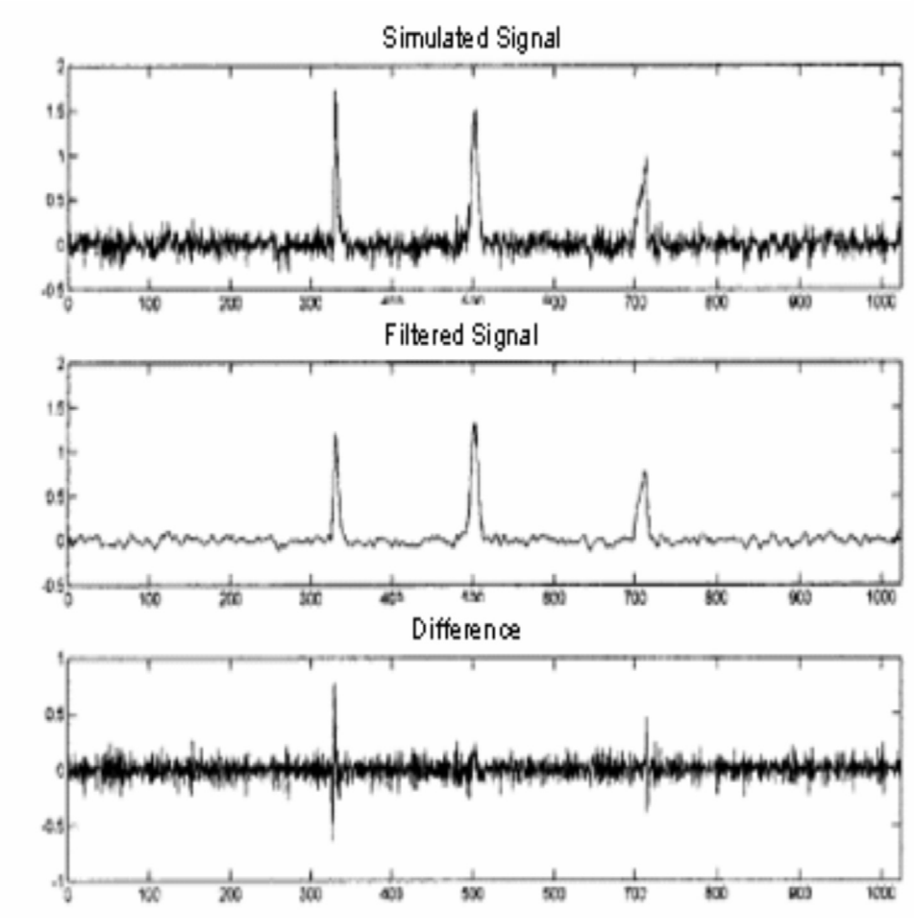


Figure (3): Fourier low pass filtering of simulated signals: top, simulated signals; middle, filtered signals; bottom, vector of differences between the filtered and the original signals.

Experimental spectra

Experimental spectra were taken from some irradiated samples with 14MeV neutron beam, and other IAEA test spectra.

Programming

All computations were performed using Borland C++, version 4.5, for Windows. All variances were calculated using a robust estimate of the variance, the median absolute deviation (MAD).

$$S^2 = median(\left|W_{coeff}\right| / 0.6745 \quad (10)$$

Results and Discussion

Denoising of simulated signals

The strategy for denoising of gamma spectra was first developed on simulated spectra and eventually applied to real ones as shown in Fig. (1).

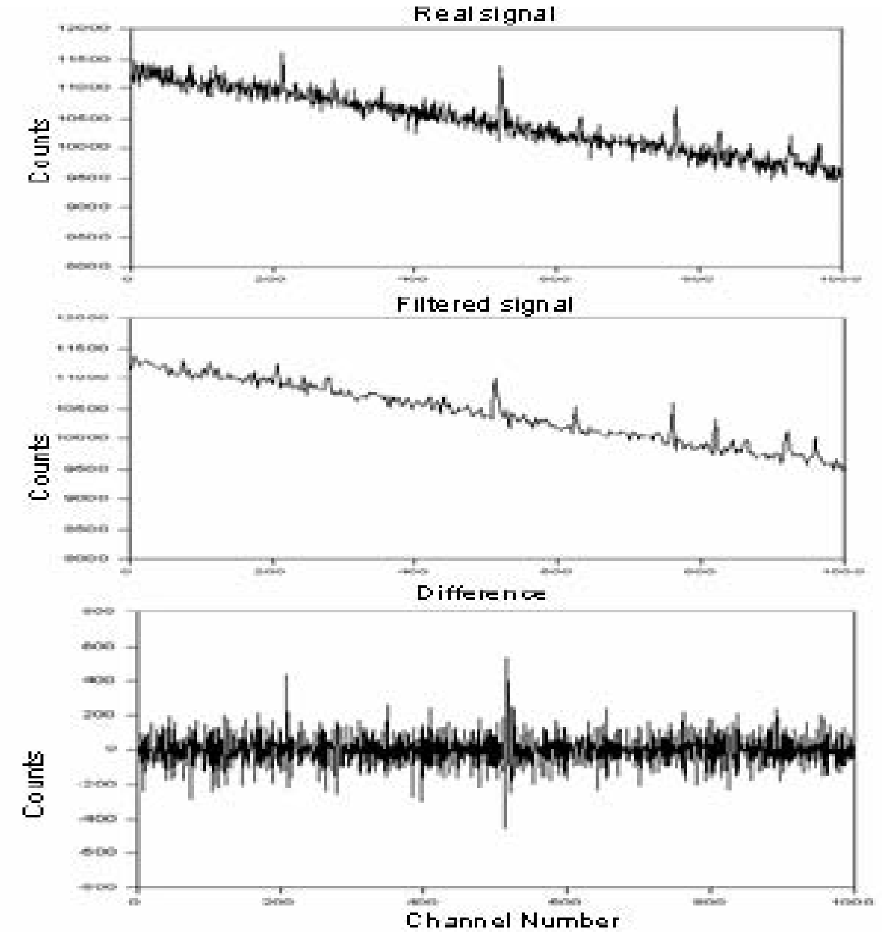


Figure 4: Modified FT filtering of IAEA test spectra: top, spectrum;, middle, filtered spectrum; bottom, vector of differences between the filtered and the original spectrum

Denoising of simulated signals using the Haar modified FT and a level of decomposition of 6 was compared with Savitzky-Golay as shown in Fig. (2) and

Fourier denoising as shown in Fig.(3). A clearly better denoising of the signals by the modified FT process is obtained because an almost total removal of the noise was achieved without any damaging of the peaks. A similar denoising using Savitzky-Golay and Fourier approaches could not be achieved without dramatic damage to the peaks. Indeed, Fig. (2) shows that the vector of differences between the modified FT-filtered signal and the original signal is very homogeneous, meaning that only noise was removed. On the other hand, high-amplitude components were located in time at the same position as the peaks can be observed in the vectors of differences with Savitzky-Golay and Fourier denoising Fig. (2) and Fig. (3) show that the peaks are damaged.

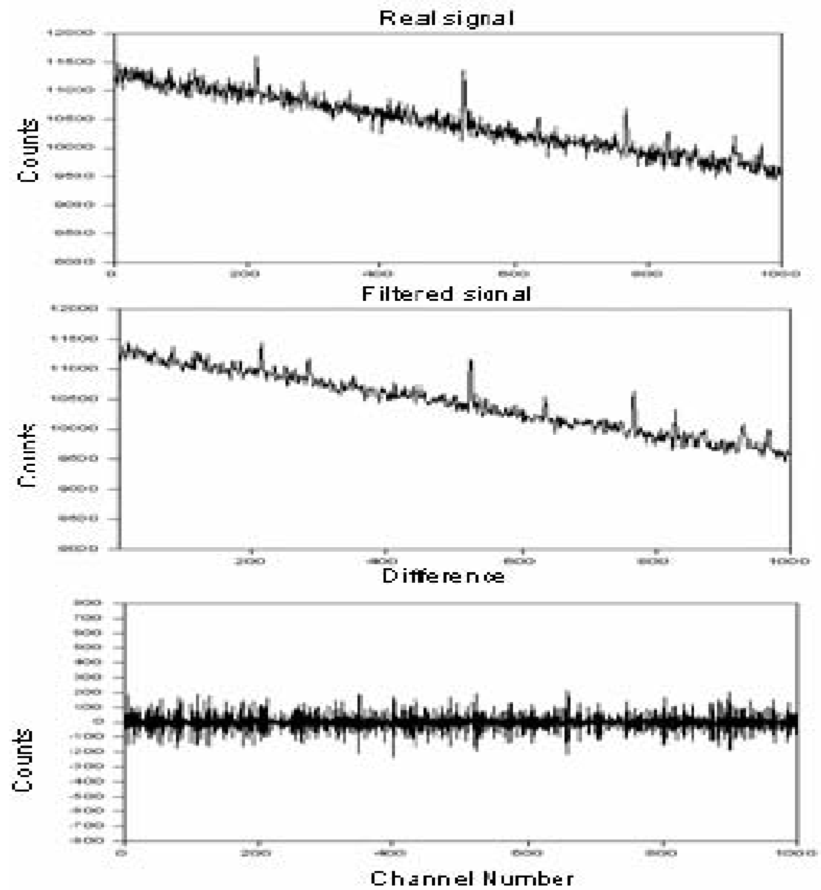


Figure 5: Savitzky-Golay smoothing of IAEA test spectra: top, spectrum;, middle, filtered spectrum; bottom, vector of differences between the filtered and the original spectrum.

As expected, the improvement is especially important in the case of the skewed peaks. Indeed, in such a case, few points describe that peaks and important errors are obtained using an averaging technique like Savitzky-Golay. In the case of Fourier denoising, because the frequency of sharp peaks is similar to the frequency of the noise, they are removed with the noise. By increasing the window size or the cutoff frequency, a better removal of the baseline can be achieved, but at the price of dramatic damage to the peak shapes and net peak areas. As a result of its specific properties, the modified FT can distinguish between the high-frequency components of the peaks and the high-frequency components of the noise. However, it must be noticed that low-frequency variations of the baseline are still present after the denoising with modified FTs.

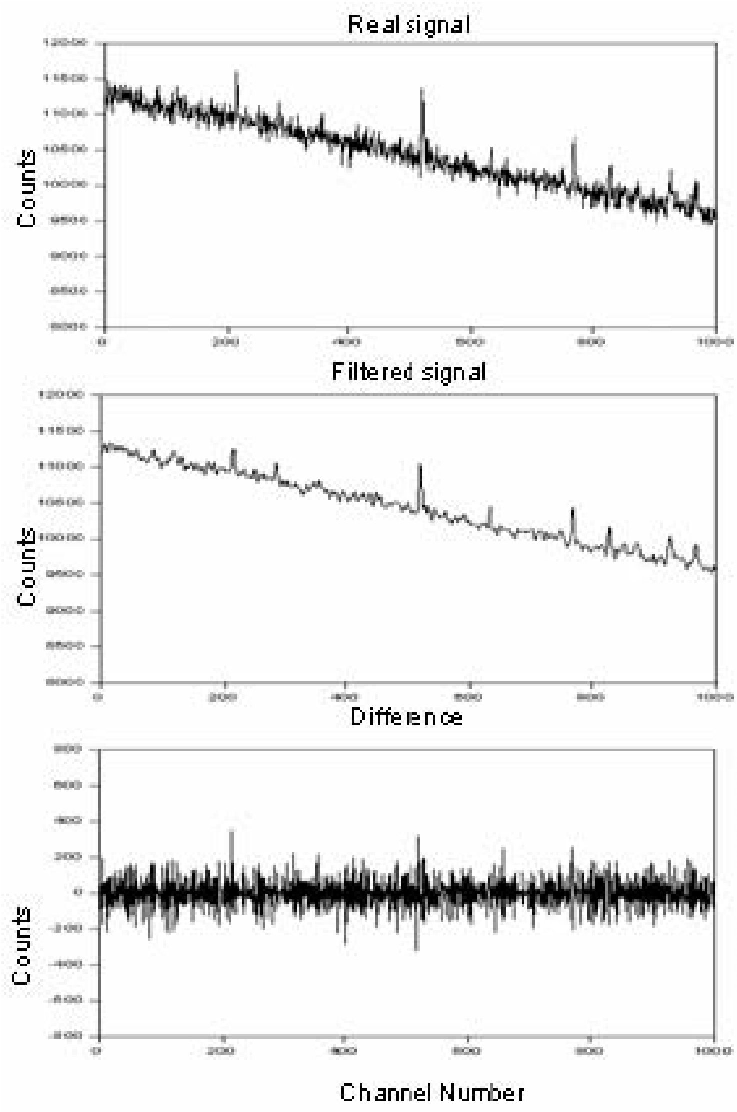


Figure 6: Fourier low pass filtering of IAEA test spectra: top, spectrum, middle, filtered spectrum; bottom, vector of differences between the filtered and the original spectrum.

Denoising of experimental gamma ray spectra

We have applied our method to a gamma spectrum of IAEA test spectra. This spectrum can be downloaded from the webpage http://www.nucleartraining.co.uk. The denoising of our method, Savitzky-Golay method and Fourier method are shown in Figs. (4- 6).

It is clear that the denoising of real data by the modified FT gives the best results in the comparison with FT and Savitzky-Golay method. Also it is clearly seen that Savitzky-Golay has less efficient denoising.

Conclusions

1. The potential of a modified Fourier transform for denoising of gamma spectra was evaluated.
2. It has shown that MFT is efficient technique for removal of the correlated noise present in the signals.
3. Because of their specific time-frequency localization properties, modified FT allows better denoising and peak shape preservation than classical denoising. methods, such as Savitzky-Golay and Fourier transform

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