Gamma Ray Spectrum Unfolding Using Derivative Kernels

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Abstract
The unfolding of a gamma ray spectrum experience many difficulties due to noise in the recorded data, that is based mainly on the change of photon energy due to scattering mechanisms (either in the detector or the medium), the accumulation of recorded counts in a fixed energy interval (the channel width of the detector) and finally the statistical fluctuation inside the detector. In order to deal with these problems, a new method is developed which interpolates the ideal spectrum with the use of special designed derivative kernels. Preliminary simulation results are presented and show that this approach is very effective even in spectra with low statistics.

Key words: Spectrum unfolding, Derivative kernels
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1. Introduction

Response function calculation of NaI based scintillators has many applications like process control tasks in manufacturing industry, in oil detection, in safety and alarm systems, in Prompt Gamma Neutron Activation Analysis (PGNAA) and others (see for example [1], [2], [3] and references there in). In general, Monte Carlo techniques are used to calculate the interactions of source photons with the detector ([4], [5], [6]) and thus the response function.

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Also both analytical ([7], [8]) and statistical ([9]) techniques have been used too.

On the other hand, during the detection of gamma rays, several problems are encountered, i.e., the efficiency vs. resolution of semiconductor or scintillation detectors used, the geometry, which causes in turn uncertainties in the solid-angle determination, etc. Also the form of the spectrum becomes more complex due to the following properties: (i) the scintillation detectors have a lower energy resolution compared to Ge detectors, (ii) the environment and/or shielding play an important role because of the scattering of high energy x-rays into the detector, (iii) the first and second escape peaks become important at high energies and (iv) a significant tail develops towards the low-energy continuum due to Compton scattering and escape of bremsstrahlung from the detector. These effects reduce the detection efficiency in the full-energy peak, and have also other serious consequences. If the spectrum is complex, with a continuous $\gamma$-yield (e.g. due to statistical $\gamma$-rays following the decay of highly excited nuclei), the large superimposing continuous tails of the high-energy $\gamma$-rays may hamper an accurate evaluation of the continuous $\gamma$-yield.

To improve these drawbacks several attempts have been made in the past. In the experiments a combination of different detectors (Ge and BaF, anti-Compton shields, etc.) has been used. However, these techniques either reduce the overall efficiency by rejecting a large part of the detected events (anti-Compton), or hamper a precise determination of the overall efficiency (addition of coincident signals from different types of detectors). In the data analysis the generally used forward method fits the measured spectrum using appropriate physical models (input information): a master-spectrum is generated using e.g. statistical model calculations (some model parameters are to be adjusted later), which is then folded with the detector response function and the resulting spectrum is compared with observation. Finally, the model parameters are adjusted, until an acceptable agreement is found. Problems arise here from peaks in the experimental spectrum due to contaminants in the target creating discrete lines, which cannot be simulated easily. The remaining problem is the choice of the physical model and the appropriate model parameters. If several physical processes compete, the generation of the master spectrum can often be ambiguous [10]. On the other hand, even if the model spectrum is accurate, the accuracy of the unfolding process is reduced due to two main reasons: (i) the noise in the measuring spectrum and (ii) the fact that the measuring spectrum represents the total counts recorder
in a finite energy interval, which is the channel width of the detector.

The purpose of this work is to present a new method which can improve
the unfolding procedure of a given measured spectrum. The method interpo-
lates the ideal spectrum with the use of special designed derivative kernels.
Preliminary simulation results are presented which show that this approach
is very effective even in spectra with low statistics.

2. Derivative kernels in unfolding procedure

Consider the case where a radioactive source emits photons in a uniform
medium and at a given point a photon detector has been placed. Photons,
after their emission and before they reach the detector, interact with the
atoms of the uniform medium and can change their energy due to Compton
scattering or pair production, or disappear due to the photoelectric effect.
The effect of the interaction of photons with the medium can be formulated
as follows. Let $S(E)$ be the source spectrum and $M(E)$ the measured one.

In vacuum,

$$M(E) = \int_0^\infty R(E, V) \cdot S(V) \cdot dV$$  \hspace{1cm} (1)

where $R(E, V)$ is equal to the number of photons that will be recorded at
energy $E$ when one photon is emitted with energy $V$. The function $R(E, V)$
is known as the transfer function of the detector. In the uniform medium, this
relation is more complicated. If a photon with initial energy $U$ is emitted,
then there is a probability $P(V, U)$ that the photon will reach the detector
surface with a final energy $V$. Thus, the measured spectrum now will be
given by:

$$M(E) = \int_0^\infty R(E, V) \cdot \left( \int_0^\infty P(V, U) \cdot S(U) \cdot dU \right) \cdot dV$$  \hspace{1cm} (2)

Changing the order of integration, the function

$$\hat{R}(E, V) = \int_0^\infty R(E, U) \cdot P(U, V) \cdot dU$$  \hspace{1cm} (3)

can be regarded now as the modified transfer function of the detector, for
operation inside the uniform medium [11]. The measured spectrum can now
be expressed as:

$$M(E) = \int_0^\infty \hat{R}(E, V) \cdot S(V) \cdot dV$$  \hspace{1cm} (4)
But instead of the function $M(E)$ the detector integrates this function in small energy intervals, called channels. Thus, the detector output $\bar{M}(E)$ is given:

$$\bar{M}(E) = \int_{E}^{E+\epsilon} M(V) \cdot dV$$

where $\epsilon$ is the channel width. Consider now the function

$$m(E, E') = \int_{E}^{E+E'} M(V) \cdot dV$$

Since $\bar{M}(E)$ is equal to $m(E, \epsilon)$, the 2-dimensional function $m(E, E')$ is known on the grid $(n_1 \cdot \epsilon, n_2 \cdot \epsilon)$, $n_1, n_2 = 0(1)N$. Our purpose now is to find optimal derivative kernels in order to calculate derivatives of the function $m(E, E')$. Then, we can calculate $M(E)$:

$$\lim_{E' \to 0} \frac{\partial m(E, E')}{\partial E'} = M(E)$$

An important property of $m(E, E')$ which allows for the application of equation (7) is that:

$$m(E, -E') = -m(E - E', E')$$

Figure 1 shows the measured spectrum from a NaI detector in an underwater experiment, described in [12]. Both $\bar{M}(E)$ and the calculated from equation (7) $M(E)$ are shown in Figure 2.

The unfolding of the gamma ray spectrum $M(E)$ can now be easily obtained in the case where radioactive sources emit photons in discrete energies and the counting rate is low enough to avoid additive effects in the detector. In this case and based on the linearity of the folding mechanism, we assume that

$$S(E) = \sum_{n=0}^{k} a_n \delta(E - E_n)$$

and we want to calculate both $a_n$ and $E_n$. Then, it is easily found that

$$M(E) = \sum_{n=1}^{k} a_n \hat{R}(E, E_n)$$

Finally, consider a continuous function $g : R^2 \to R$ and its discrete version

$$g_s = \sum_{n_1, n_2 = -\infty}^{\infty} g(x, y) \delta(x - n_1 T) \cdot \delta(y - n_2 T)$$
where $\delta$ is the Dirac delta function. The knowledge of the discrete version $g_s$ can lead to the reconstruction of the continuous function $\bar{g}$ with the aid of a kernel $K$ such that

$$\bar{g}(x, y) = \sum_{n_1, n_2 = -\infty}^{\infty} g_s(n_1, n_2)K(x - n_1T, y - n_2T) \quad (12)$$

The ideal interpolation where $\bar{g} = g$ is achieved if $K(x, y) = s_T(x) \cdot s_T(y)$, where

$$s_T(x) = \frac{\sin(\pi x / T)}{\pi x / T} \quad (13)$$

and $T$ is the Nyquist rate. For practical reason, we assume that

$$K(x, y) = d_0(x) \cdot d_0(y) \quad (14)$$

and

$$d^n d_0(x) = d_n(x) \quad (15)$$

Then, the expression for the derivative with respect to $x$ of the reconstructed function $\bar{g}$ becomes:

$$D_x\{\bar{g}\}(x, y) = \sum_{n_1, n_2 = -\infty}^{\infty} g_s(n_1, n_2)d_1(x - n_1T)d_0(y - n_2T) \quad (16)$$

In order to construct an efficient kernel, it is not necessary that $d_1(x) = d'_0(x)$. Although this seems controversial consider the following example: it is common to use a sampled Gaussian and its derivative. However, because the Gaussian is not strictly bandlimited, sampling introduces artifacts, thus destroying the derivative relationship between the resulting kernels. So, instead we choose to simultaneously design a pair of discrete kernels that optimally preserve the required derivative relationship. If

$$D_0(\omega) = \sum_n d_0(nT)e^{-i\omega n}, \quad D_1(\omega) = \sum_n d_1(nT)e^{-i\omega n} \quad (17)$$

with $\omega = 2\pi / T$ are the discrete Fourier transforms of $d_0, d_1$, we can demand that

$$i\omega D_0(\omega) = D_1(\omega) \quad (18)$$

in the case of one dimensional signals $g$. In the case of two dimensional signals, we can demand for example that the pair of kernels preserve the derivative relationship in all directions [13].
3. Simulation results

In order to test the new method, a simulation experiment was performed. A folded spectrum is produced using the transfer function for a NaI based measuring system calculated in [14]. The spectrum is folded again using the method presented in [15] in order to simulate an underwater measuring system. Several simulated spectra were produced, with different number of photo-peaks and different number of total recorded counts in order to account for the spectrum statistics. Figure 3 shows the overall error in the unfolded spectrum, using a Gaussian derivative kernel (○) and three derivative kernels DK3 (□), DK4 (×) and DK5 (○) with 3, 4 and 5 points respectively calculated in [13]. Furthermore, in Figure 4 the dependence of the error in the unfolded spectrum on spectrum statistics is shown for the Gaussian (○) and DK5 (×) derivative kernel. It is clear that the new method is very promising even in cases with low statistics. A special experimental setup is under construction to test the new method in real spectrums. Moreover, new derivative kernels are designed in order to optimize their behavior.

4. Conclusions

Preliminary results on interpolation of a measured spectrum with derivative kernels, show that the unfolding procedure becomes more accurate even in cases of low statistics. The use of derivative kernels facilitate the numerical differentiation which is of high importance in both peak detection and spectrum unfolding.

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References

[1] H. Hakimabad, H. Panjeh, A. Noghreiyian, Evaluation the nonlinear response function of a 3x3 in NaI scintillation detector for PGNAA applications, Applied Radiation and Isotopes 65 (2007) 918.
[2] J. Tickner, Determination of the spatial response of neutron based analyzers using Monte Carlo based method, Applied Radiation and Isotopes 53 (2000) 507.

[3] S. Nafee, M. Abbas, A theoretical approach to calibrate radiation portal monitor (RPM) systems, Applied Radiation and Isotopes xx (2008) xx.

[4] M. Mitra, P. Sarkar, Monte Carlo simulations to estimate the background spectrum in a shielded NaI(Tl) gamma-spectrometric system, Applied Radiation and Isotopes 63 (2005) 415.

[5] S. Yalcin, O. Gurler, G. Jaynak, O. Gundogdu, Calculation of total counting efficiency of a NaI(Tl) detector by hybrid Monte-Carlo method for point and disk sources, Applied Radiation and Isotopes 65 (2007) 1179.

[6] A. Cengiz, An approximation for response function to gamma-rays of NaI(Tl) detectors up to 1.5 MeV, Applied Radiation and Isotopes xx (2008) xx.

[7] M. Abbas, Analytical formulae for well-type NaI(Tl) and HpGe detectors efficiency computation, Applied Radiation and Isotopes 55 (2001) 245.

[8] M. Abbas, S. Nafee, Y. Selim, Calibration of cylindrical detectors using a simplified theoretical approach, Applied Radiation and Isotopes 64 (2006) 1057.

[9] A. Sabharwal, M. Singh, B. Singh, B. Sandhu, Response function of NaI(Tl) detectors and multiple backscattering of gamma rays in aluminum, Applied Radiation and Isotopes xx (2008) xx.

[10] C. Sukosd, W. Galster, I. Licot, M. P. Simonart, Nuclear instruments and Methods in Physics Research A 355 (1995) 552.

[11] D. S. Vlachos, Self-Calibration Techniques of Underwater Gamma Ray Spectrometers, Journal of Environmental Radioactivity 82 (2005) 21.

[12] C. Tsabaris, D. Vlachos, C. Papadopoulos, R. Vlastou, C. Kalfas, Setup and Application of an Underwater gamma-ray Spectrometer for Radioactivity Measurements, Mediterranean Marine Science 6 (1) (2005) 35.
Figure 1: Two dimensional representation of measured spectrum obtained from [12].

[13] H. Farid, E. P. Simoncelli, Optimally rotation-equivariant directional derivative kernels, in: 7th Int’l Conf Computer Analysis of Images and Patterns, Kiel, Germany, 1997.

[14] D. S. Vlachos, C. Tsabaris, Response Function Calculation of an Underwater Gamma Ray NaI(Tl) Spectrometer, Nuclear Instruments and Methods in Physics Research A 539 (2005) 414.

[15] D. S. Vlachos, T. E. Simos, PDSW: A program for the calculation of the photon energy distribution in seawater, Computer Physics Communications 174 (2006) 391.
Figure 2: Measured (◦) and calculated spectrum (solid line) obtained from [12].
Figure 3: Unfolding of simulated spectra generated with the method in [14]. DK3 uses the 3-point kernel couple, DK4 the 4-point one and DK5 the 5-point kernel. The Gaussian curve is produced using a sampled Gaussian and its derivative. Gaussian derivative kernel (o), DK3 (□), DK4 (×) and DK5 (○).
Figure 4: Dependence of unfolding accuracy on spectrum statistics for the Gaussian (◦) and DK5 (+) case. The horizontal axis represents the total number of counts recorded.