Processing of Airborne Gamma-Ray Spectra: Extracting Photopeaks

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SUMMARY

Receiving information from airborne gamma-ray spectra is based on the ability to estimate the photopeak areas in the regular spectra of natural and other sources. In the airborne gamma-ray spectrometry, extracting the photopeaks of radionuclides from regular one-second spectra is a complicated problem. In the region of higher energies, e.g., above 1.6 MeV, the difficulties are associated with low count rates, while in the region of lower energies, difficulties are due to a significant background level and its statistical noise. In this article a new procedure is proposed to process the measured spectra up to extracting evident photopeaks. The procedure consists of decreasing noises in energy channels along the flight lines, transforming spectra to equal resolution spectra, removing baselines from each spectrum, sharpening details, and transforming spectra back to original channel scale. The resulting spectra are better suited for examining and using the photopeaks. No assumptions regarding the number, positions and magnitudes of photopeaks are needed. Non-negativity of photopeak areas is ensured by the procedure. The proposed technique is likely to contribute to studies of environmental issues, soil characterization and other near surface geophysical methods.

Key words: Airborne Spectrometry, Photopeak, Baseline, Spectrum Denoising, Equal Resolution

INTRODUCTION

In Airborne Gamma-Ray (AGR) spectra, the photopeaks are the primary and only information about the geological and geophysical state of soil and subsurface rocks. The availability of photopeaks and possibility to measure them allow for solving a number of geological, geophysical and geochemical problems, from estimating the concentrations of radioactive elements on vast areas (Grasty and Minty, 1995; AIRBORNE, 1991) to achieving detailed polytypic solutions of inverse problems (Druker, 2012). However, regular AGR spectra are too complicated and noisy to enable easy extraction of the photopeaks. Therefore, averaging and/or smoothing methods should be applied to extracting reasonable photopeaks from regular spectra. One such method is used by standard processing (Grasty and Minty, 1995; AIRBORNE, 1991), where the averaging is the summation of all the counts in the energy windows. This method is notably effective to decrease the influence of noises. However, these data are used in accurate formulas designed for the data with quite low noises. Such low-noise regular data usually do not exist, and Airborne Gamma-Ray Spectrometry (AGRS) data processing applies various averaging and/or smoothing methods over time and area. The averaging in many cases is of arbitrary choice, including suspicious non-local variants. Even with these simplifications the result might be not so good, e.g., it is possible to have spacious areas of negative values – and not only above the water. Generally, strong averaging and/or smoothing procedures may result in enormous losses of spatial resolution and low-quality output data.

There are two primary problems to be solved by standard processing: removal of Compton influence in energy windows and considering the mutual influence of natural radioactive elements in the energy windows. Standard processing solves the problems with a set of special calibrations and it has a convenient advantage in ignoring the unused parts of spectra. However, it has to be noted that the calibrations should be somewhat accurate, and also certain extrapolations and averaging are used (e.g., for cosmic radiation). Typically, real mutual influences between the energy windows are not significant, and they can be taken into account (approximately) after processing - if this step is deemed worthwhile. Moreover, it is quite difficult to add new energy windows into processing and certain man-made radioactive elements cannot be detected with the standard procedure.

Alternatively, one can use directly computed photopeak areas instead, although this approach needs to have right notion regarding the background of photopeaks. Commonly a background is a segment between the end values of an energy window. Unfortunately, the end values are random values and have rather large scatter, depending on the window ends and on the manner used to obtain the end values. Such random values may change abruptly from spectrum to spectrum or from channel to channel (when slightly moving the windows). Therefore, directly calculated photopeak areas should be (well) averaged.

In this study, a procedure to acquire more reliable and accurate results is proposed. General elements of the technique are smoothing the spectra along lines and along the energy axis, building the (Compton) baseline to obtain spectra of photopeaks only.

Note that all the numbers, values, examples and figures below are related to input airborne spectra with 512 channels of a 6.0 keV width each, with the usable measured data being between approximately 0.3 MeV and 3.0 MeV, i.e., in channels from approximately 40 to 510.
PROCESSING THE SPECTRA

A. Smoothing along the lines

As is well-known, the count rate in the spectrometer channels agrees with Poisson distribution (Billings et al., 2003; Markova and Velichko, 2011; Minty, 2003; Tsoulfanidis, 1995). Poisson distribution variables have equal mean $M$ and variance $V$:

$$M = V. \quad (1)$$

The number of pulses in energy channels along the flight lines is a Poisson process, at least on short distances comparable to a footprint size where $M$ is almost constant. Competent smoothing of Poisson data is a separate problem because of the strong relation (1) between “signal” $M$ and “noise” $V$. For large values of mean value, e.g. $M > 20$, the problem can be replaced by regular smoothing of the data with an additive Gaussian noise. However, in AGRS it is not the case because in AGR spectra at higher energies, many of $M$ values are noticeably lesser, e.g. $M < 5$, and often $M < 1$.

There is a correct modern approach to properly smooth AGRS data with various values of $M$ in channels: transform a Poisson signal into a signal with Gaussian noise, smooth it with a well-known filter, and subsequently transform it back to the original domain. A number of such Anscombe transforms (Anscombe, 1948) is available to replace a Poisson process by a process with an additive Gaussian noise:

$$\text{Poisson (}M\text{)} \rightarrow \text{Signal (}M\text{)} + \text{Noise (0)}, \quad (2)$$

where Noise (0) is close to the standard Gaussian noise from distribution $N(0,1)$ with the mean and the variance approximately equal to 0 and 1, respectively. The Anscombe transform (2) is good for moderate signal levels, say, $M > 4$; even the better transform (Freeman and Tukey, 1950) is good only for $M > 1$. Most of commonly known linear filters are good for suppressing Gaussian noises. As for back transform, only Anscombe transform has it in quite accurate form (Makitalo, 2011). The problem is that such transformation of data is somewhat ambiguous. The data representation in the form on the right hand side of transformation (2) usually implies an independent source of noise, i.e., the output signal is noisy even with zero input signal. By contrast, the Poisson process on the left hand side of (2) does not imply an independent source of noise. Therefore, even if the transform (2) can be easily done with simple formula, the back transform cannot be done with the inversion of the formula – the back transform should be valid statistically, just because in that case the noise is suppressed. According to these facts and simulating with Monte Carlo method, there are three ranges of $M$ values, (a) low, where the back transform for (2) is unknown (and the quality of output also), (b) moderate, where the approach is pertinent (but leads to output quite similar to simple smoothing), (c) large, where the approach is redundant, because of similarity of Poisson and Gaussian processes. As a result, for AGRS this approach is unsuitable – at least because of unavoidable jumps between the described ranges.

Thus, the smoothing of energy channel data along the lines needs suitable filters. Such filters should be local and short to avoid notable shift of field items along the lines. In particular, an effective width of the filter should be comparable to a footprint size, that is, the filter width might depend on the energy. A correct filter does not distort the phase of signal too much. For example, Blackman and similar bell-shaped filters are correct, while rectangular filters are not, because, generally, they can result in introducing false anomalies or in making the real ones to disappear. A good choice is Savitzky-Golay filters (Press et al., 2007), which keep several first moments of the process, although these filters may produce (rather rare) negative values. Given this, good filter lengths are 5 to 9 points, which usually correspond to the distance of small changes along the line. An example of the smoothing with the Savitzky-Golay filter of length 9 and degree 2 is given in Figure 1.

![Figure 1. Smoothing the spectrum channels along the flight line (horizontal axis), for an energy channel near 1.1 MeV (a), and an energy channel near 2.6 MeV (b). Spectra count rates are in cps. The thin lines show the input data, and the thick lines show the smoothed data.](image)

After smoothing the output variance of data is much less than the input one and the output spectra are more suitable for extracting the local parts with photopeaks. See an example in Figure 2.
B. Estimation of spectra baselines

The next step is to build the baselines of spectra, which are essentially approximations of the Compton continuum. Then the photopeak spectrum is the result of subtracting a baseline from a spectrum. Generally, this problem is notably complicated, even for spectra with large Signal-to-Noise-Ratio (SNR) that looks like cumulative AGR spectra. For the spectra with large SNR the problem is mostly in clarifying a more precise baseline, rather than in finding it (Morhac, 2009; Ramos and Ruisanchez, 2005; Schulze et al., 2005). There are a number of approaches to the problem of finding baselines. First, there are attempts to approximate the entire spectrum with polynomials; this approach may lead to unstable math operations. Second, there is iterative smoothing, and the number of iterations may be unpleasantly amazing. Third is a wavelet transform to remove higher frequency noises; to date, how to segregate signals from noises in very noisy gamma-ray spectra has not been straightforward. There are also other more sophisticated methods that yield unclear results. Actually, the primary difficulty is to define a baseline. Usually, it is explicitly or implicitly adopted that baseline is very smooth compared to the original spectrum or their difference.

A more promising approach seems to be using the formulations that are similar to those in solution of ill-posed problems (Eilers, 2003; Eilers and Boelens, 2005):

\[
\sum_i w_i (b_i - f_i)^2 + \lambda \Omega(b) \to \min ,
\]

where
- \( b \) – vector of baseline values,
- \( f \) – vector of spectrum values,
- \( W \) – vector of weight,
- \( \lambda \) – regularization parameter,
- \( \Omega \) – a functional to define a desired form of the baseline; for smooth baselines it usually depends on second differences (as stabilizers in ill-posed problems are).

In this formulation the problem seems to be more complicated than the original one: in addition to the baseline vector \( b \), which has the length of the spectrum \( f \), one also has to find \( W \), a vector of weights, and parameter \( \lambda \). Moreover, it is quite possible that the uniqueness of a solution is not ascertained. Therefore, the next approach is applied. One first sets a fixed (large) value of \( \lambda \) based on experiments and later iteratively sets the weights equal to two values, for example, 0.9 for the quiet, background parts of spectra and 0.1 for the peak areas. This method may work well on a series of spectra with explicit peaks and good SNR, but it is not the case for AGRS spectra due to their large changeability and low SNR.

Regardless of drawbacks, the idea of iterative weighting is a fruitful one if applied without a stabilizer. Let \( \lambda = 0 \) in (3) to make the problem less complicated. The smoothness of a solution should be provided by the algorithm. To make a smooth baseline, an effective width of a smoothing linear filter \( F \) should be several times more than FWHM (Full Width at Half Magnitude) of sought photopeaks. For example, by experience, the effective width of a Blackman filter should be 2 to 4 times greater than the FWHM of peaks.

C. Algorithm for building a baseline of spectrum

Let \( S_m \) be measured or smoothed (as in subsection A above) spectrum.

a) Initialization
1. Set all the initial weights of vector \( W \) to be equal: \( w_i = 1 \).
2. Set iteration number \( I = 0 \).
3. Set weight modifier \( u = 0.9 \).

b) Iterations
1. Smooth the spectrum \( S_m \) with weights \( W \) by filter \( F \) to obtain the spectrum \( S_c \).
2. Change the weights according to the rule:
   a. if \( S_c[k] < S_m[k] \), then \( w_k = w_k / u \).
   b. if \( S_c[k] > S_m[k] \), then \( w_k = w_k * u \).
3. Increase iteration number: $I = I + 1$.
4. Repeat the iterations until: (a) functional (3) decreases slowly and/or (b) weights $W$ become stable within some tolerance and/or (c) the numbers of iterations run up to maximum, and/or (d) some other criteria are met.
5. Now $S_c$ is baseline spectrum (as approximation of Compton continuum) and the difference $S_p = S_m - S_c$ is the sought photopeaks spectrum.

Thus, every spectrum value has two weights – the weight of the value related to the spectrum and its baseline and the weight of the position in current filter window.

A drawback of the approach is that FWHM noticeably depends on the energy (on channel number), which means that at least the filter $F$ should be changed according to the energy. There are several ways to overcome this drawback. First, it is possible (and not highly expensive) to use several filters for various energy channels up to using an individual filter for every spectrum channel. A simple special case of this possibility is to make an operation twice: once with parameters for low energies and once with parameters for high energies, as well as subsequently obtaining the result by interpolation. Yet there is another, more convenient and definite, way, which is to transform a regular spectrum to another spectrum with a constant value of FWHM, that is, to the spectrum with the resolution which is independent of the channel number. In some respects, at least in statistics, this variant is better.

D. Reducing the spectrum to constant resolution

Recall that the resolution of NaI(Tl) spectrometers is strongly related to the energy of gamma rays. This resolution depends mainly on the sensor size and the energy range (Knoll, 2000; Tsoulfanidis, 1995). Numerically (in the airborne energy range) such relations are close to the general rule:

$$ E^K R(E) = \text{const}, \quad (4) $$

where $\alpha \approx 0.5$ is an appropriate value for large (airborne) gamma-ray spectrometers, both theoretically and by experiments (Gilmore, 2008; Knoll, 2000; Kogan et al., 1969; Petersen, 1996; Tsoulfanidis, 1995). For typical small spectrometers the values of $\alpha$ usually are about 0.4 or less (Heath, 1997; Meng and Ramsden, 2000). As for AGRS, relation (4) is more conveniently expressed in the form:

$$ E R^2 p (E) = \text{const}, \quad (5) $$

where $p = 1$, is the value to improve the approximation (5) if desirable. The relation (5) shows how to transform the channels of an input spectrum:

$$ k = c n^{2p}, \quad (6) $$

where $k$ - channel number of input (measured) spectrum,
$n$ - channel number of output (transformed) spectrum,
$c$ - coefficient to choose.

For the sake of simplicity, the only value of $p=1$ is used below. Thus, the inverse transform is:

$$ n = \sqrt{k/c}, \quad (7) $$

First, we consider the changes of the channel width:

$$ \frac{dk}{dn} = 2cn = 2\sqrt{ck}. \quad (8) $$

It is the equation to choose the $c$ coefficient. Let $m$ be the channel of the input spectrum with the same width before and after transformation, i.e. $\frac{dk}{dn}(m) = 1$. Hence,

$$ c = 1/4m. \quad (9) $$

It is convenient to take the value of $m$ somewhere in the middle of the spectra, for example, $m = 243$, which corresponds to the Potassium photopeak at 1.46 MeV. Transformation of spectra in both directions, (6) and (7), can be made by linear interpolation, which largely retains all of the details of spectra, and linear interpolation is sufficient for typical AGR spectra. Table 1 gives an idea regarding channel numbers and the resolutions before and after transformation.
Table 1. Some AGRS standard energy values, their input and output channels, input resolutions, and input and output FWHM. All the values are rounded.

<table>
<thead>
<tr>
<th>Energy (Element)</th>
<th>Input Channel</th>
<th>Output Channel</th>
<th>Input Resolution</th>
<th>Input FWHM</th>
<th>Output FWHM</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.62 (Th)</td>
<td>435</td>
<td>650</td>
<td>5 %</td>
<td>22</td>
<td>16</td>
</tr>
<tr>
<td>1.46 (K)</td>
<td>243</td>
<td>486</td>
<td>7 %</td>
<td>17</td>
<td>17</td>
</tr>
<tr>
<td>0.66 (Cs)</td>
<td>110</td>
<td>327</td>
<td>10 %</td>
<td>11</td>
<td>16</td>
</tr>
<tr>
<td>0.35 (Rn)</td>
<td>58</td>
<td>237</td>
<td>14 %</td>
<td>8</td>
<td>17</td>
</tr>
</tbody>
</table>

As Table 1 shows, the resolution in channel \( m \) is retained, and the resolution of output spectra almost does not depend on the energy. Therefore, the definition of resolution as ratio FWHM/E is not applicable to the output spectrum.

Note that channels at high energies become wider, e.g., the Thorium (2.62 MeV) photopeak has 16 channels of FWHM on output instead of 22 on input, which results in better output statistics. On the other end, the channels at low energies become narrower, e.g., the Caesium (0.66 MeV) photopeak has 16 output channels of FWHM instead of 11 on input, which means a noticeable decrease in magnitudes, almost without worsening the statistics. However, it should be noted that linear interpolation at very low energies produces certain evident saw-tooth artefacts, which may be obvious at \( dh > 2 \delta k \) and to the left, i.e., at energies below 0.36 MeV.

Thus, the transformation (7) of spectra channels improves the statistics of low counts at high energies and decreases the dynamic range of the spectra. The full working length of spectra, if a fixed channel is chosen according the relation (9), is approximately the same: channels \([40, 512]\) are transformed to channels \([197, 705]\), that is, 473 input channels are converted to 509 on output. An example of transformation to the spectrum of equal resolution is shown in Figure 3.

Figure 3. Transformation of a regular input spectrum to an output constant-resolution spectrum: (a) input spectrum smoothed as in Subsection A in channels \([44, 511]\), and (b) output spectrum of constant resolution in channels \([206, 704]\).

After the transformation (7), the spectrum is better suited for building a baseline according to the algorithm C above by applying the same rules to every channel of a spectrum. The baseline algorithm C does not ensure positive values for the difference between the spectrum and its baseline. The transformed photopeaks spectra, which resulted from subtraction, should have negative values. However, in the algorithm C, it is easy to provide the limitation on the negative areas, in comparison to positive areas. For example, the photopeak spectrum in Figure 4a has at most 7 % for a ratio of negative to positive areas for each position of the filter window. To make non-negative photopeak spectra, it is sufficient to set zeros instead of negative values; other approximations are also acceptable for such small negative-to-positive ratios.

E. Sharpening the photopeaks

The transformed photopeak spectra are applicable for sharpening. To keep the solutions positive, the multiplicative methods are better suited. There are many such methods and their modifications (Meng and Ramsden, 2000). One of the well-studied, Gold’s ratio method (Jansson, 1984), will be considered below. The method is designed to solve the convolution equation

\[
f = A * u,
\]

where \( f \) – measured data; here the vector of (non-negative) photopeak areas,
\( u \) – primary data to find; here the vector of primary photopeaks,
\( A \) – the matrix of transformation.
Gold’s ratio method consists of the iterations:

\[ u_{i+1} = \frac{Bf}{BA = u}, \text{ where } B = \mathbf{I} \text{ or } B = \mathbf{A}^T; \quad u_0 = f; \quad i = 0, 1, 2, \ldots, \]  

(11) or (12)

If \( B = \mathbf{I} \), the solution (11) after several iterations takes a delta-like form; this solution is better for special problems like searching for man-made radionuclides. If \( B = \mathbf{A}^T \), the solution (12) after several iterations takes a clearer defined form. Both solutions depend on the system matrix \( \mathbf{A} \) in (10) that is essentially on the given resolution. After the sharpening, the spectrum should be scaled back to a regular energy scale to find the photopeaks and compute their areas.

There are practical differences between solutions (11) and (12). The solution (11) after several iterations assumes a delta-like form and continues to change with iterations. The solution (12) after several iterations becomes more distinct and later changes rather slowly with iterations. Generally, for typical AGRS problems the solution (12) is better, while for special problems the solution (11) may be more suitable. Both solutions do depend on the system matrix (10) that is essentially on a given resolution. It should be noted that in the sharpening process of the photopeak spectra it is not necessary to use the most accurate value of the resolution. On the contrary, in many cases using the worse resolution is preferable. In Figure 4, two versions of sharpening are shown. In Figure 4a, the input photopeak spectrum is shown. In Figure 4b, sharpening by (11) is shown, and it is a delta-like solution. In Figure 4c, sharpening by (12) is shown, and it is a conjugate solution. Both sharpened solutions in Figure 4 are built with twice worse (i.e., bigger value of) resolution than the true one; it should be noted that it is sharpening, not the real solution of (10).

![Figure 4. The photopeak spectra (a) before sharpening, (b) after delta-like sharpening by (11), and (c) after conjugate sharpening by (12).](image)

If the spectrum to process is smooth, e.g. cumulative, the photopeak spectrum, as shown in Figure 4a, after transformation to input channels, is suitable for calculating the resolution for any photopeaks, not only for Potassium. Using several values of the resolution, the parameter \( p \) in (8) can be improved.

**F. Peaks and their areas**

The next step of extracting photopeaks is to return from the sharpened spectrum scale to a regular energy scale. This step is shown in Figure 5. In Figure 5a the main result of the procedure is shown – the photopeak spectrum in the usual energy scale; there are several distinct photopeaks: 2.6 MeV (channel 430), 2.2 (360), 1.8 (300), 1.5 (240), 1.1 (190), 0.9 (150), 0.6 (100), 0.5 (80). Besides, there is no photopeak at 0.66 (110). An input spectrum in Figure 5b is also shown (logarithmic scale) to compare with the output spectrum.
Now it is much easier to analyse the photopeaks – create the list of their channels (energies), areas, noise levels, etc.

**DISCUSSION**

A full procedure to extract photopeaks from AGR spectra for a flight line is as follows:

A. Smooth spectra channel-by-channel along the line (subsection A).
B. For each spectrum:
   B.1. Transform it to constant resolution (subsection D).
   B.2. Remove the Compton background (subsection C).
   B.3. Sharpen the photopeak spectrum (subsection E).
   B.4. Transform it to input channels (subsection D).
   B.5. Calculate areas of photopeaks; create list of photopeaks.

Depending on such factors as the spectra quality and geophysical problem to solve, certain position in the full procedure might be skipped, e.g., for good low-noisy spectra, step A might be redundant. Additionally, to estimate the detector resolution, step B.3 for sharpening must be omitted. In certain cases, creating lists of photopeaks may be highly useful for searching non-standard sources of gamma radiation.

**CONCLUSIONS**

A new approach is proposed for transforming the input regular one-second AGR spectra to the photopeak spectra with essentially removed baselines. The primary stages of the procedure are the following: (a) suppressing the noise in the input spectra; (b) conversion of the spectra to a constant resolution spectra; (c) building baselines to approximate the Compton continuum; (d) sharpening the photopeaks; (e) returning to the input energy scale to create a list of photopeaks and/or calculate the areas of photopeaks. Mutual influences of radionuclides on each other in the photopeak vicinity can be accounted for afterwards. It is quite possible to use the cumulative photopeaks spectra (without sharpening) for estimations of resolutions at various energies throughout the spectra. The implementation of the technique is simple and rather straightforward.

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