

‘gamma’: An R Package for Dose Rate Estimation from In-Situ Gamma-Ray Spectrometry Measurements

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Abstract

In situ gamma spectrometry is a useful technique used by the Luminescence and ESR dating community to improve the representativity of dose rate measurements in the context of gamma dose rate heterogeneities around dated material. This paper presents ‘gamma’, a new R package and its graphical user interface ‘gammaShiny’, allowing a reliable and reproducible workflow for *in situ* gamma spectrometry data analysis in the context of luminescence and ESR dating.

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- The ‘window technique’, that consists in selecting different parts of the spectra to quantify the U and Th-series and K radioelements contents in the sediment, around the probe.
- The ‘threshold techniques’, that allow a direct determination of the gamma dose rate without individual determination of K, U and Th series radioelements. Murray et al. (1978) have shown that the gamma dose rate can be estimated using the proportionality existing between the number of counts measured above a certain energy and the gamma dose rate. Mercier & Falguères (2007) developed this approach for a NaI(Tl) probe. They conclude that the measurement time (and consequently the risk of changing temperature during the measurement) is significantly reduced in comparison with the ‘window technique’.

There are two methods based on the ‘threshold technique’: in counts and in energy. In both cases, Guérin & Mercier (2011) have shown that the environmental gamma dose rate determined in this way does not depend on water presence, nor on U-series disequilibrium. They have also shown few dependence on the gamma dose rate with the nature of the sediment.

The majority of *in situ* gamma-ray spectrometers produce energy shifted and spectrally distorted spectra. This could be due to the fact that detector crystals (usually LaBr or NaI) are often used in unstable temperature conditions (Casanovas et al., 2012). As a result, spectrum processing is required before conversion from a spectrum to gamma dose rate.

A typical workflow for energy shifting correction requires manual identification of reference peaks. This is usually

1. Introduction

In situ gamma spectrometry is a powerful tool used in luminescence dating to tackle gamma dose rate heterogeneity (Aitken, 1998; Klusůň, 2010). A gamma spectrometer probe records gamma rays emitted within a sphere of radius equal to 30–50 cm (Figure 1 in Guérin & Mercier, 2011) whereas a classic BeGe laboratory gamma spectrometer with planar or coaxial geometry only characterizes samples of a few dozen cubic centimeters, thus greatly improving the representativity of the measurement (Gilmore, 2008).

Different techniques are currently used in luminescence and ESR dating field to determine the gamma dose rate from *in situ* gamma spectrometry measurements:

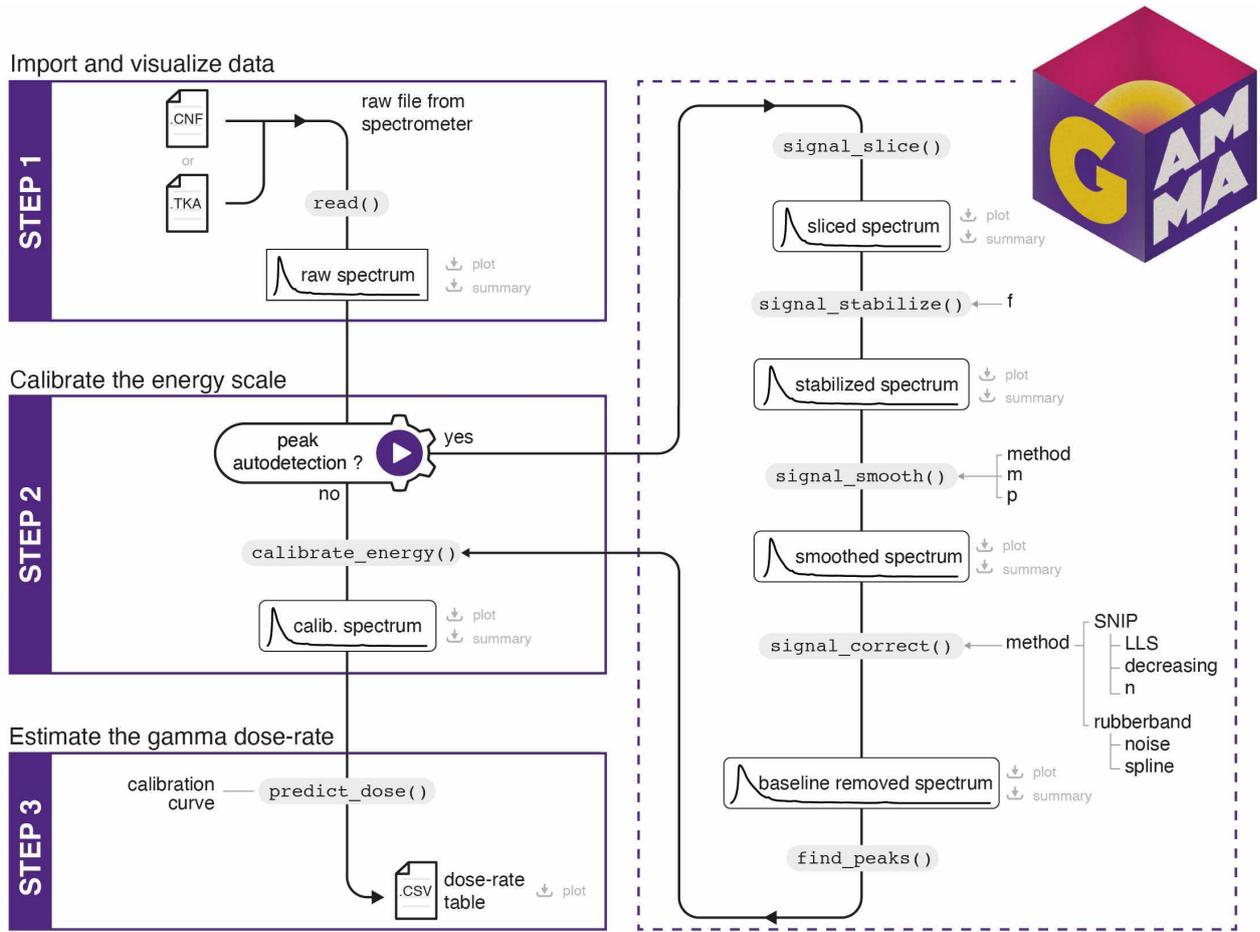


Figure 1. A typical workflow within the ‘gamma’ package.

performed using proprietary software such as Genie2000® (Canberra division of Mirion technologies, Windows OS only). Once reference peaks are identified, a new channel-energy curve is generated, taking into account the apparent shift between the observed and theoretical energies of these peaks. To this day, there is no turnkey solution for these steps and personal or laboratory-based solutions are implemented, e.g. Visual Basic Advance® macros within Microsoft Excel®.

There are two challenging issues to these existing approaches. The first one is the lack of transparency: details of spectrum processing are not presented in the publications and researcher’s internally developed solutions are not made available to the community, greatly limiting reproducibility and reliability of the measurements (see Kreutzer et al., 2017 for a broader discussion in the field of luminescence dating). Secondly, the use of proprietary software limits their access by the community, hindering their maintenance and evolution.

To address these different issues, we present an integrated solution to analyse *in situ* gamma spectrometry data, from raw spectrum processing to gamma dose-rate estimation: the R package ‘gamma’. The R programming language (R Core Team, 2020) has many advantages, starting

with its ease of learning and use. R is available on all computer platforms and its community offers efficient support. R is distributed under the GNU General Public License (therefore free of charge), ensuring transparency and modularity. Finally, several R packages dedicated to geochronology already exist (such as the ‘Luminescence’ package; Kreutzer et al., 2012).

2. The R package ‘gamma’

The ‘gamma’ package allows the user to import, inspect and correct the energy scale of one or multiple spectra. It provides methods for estimating the gamma dose rate by the use of built-in or custom calibration curves. A graphical user interface (GUI) is also provided through the dedicated R package ‘gammaShiny’, using the ‘shiny’ package (Chang et al., 2020).

2.1. Workflow overview

This section presents a typical workflow within the ‘gamma’ package (Figure 1). A walk-through guide is also provided in the package manual. The following examples can be reproduced in any integrated development environ-

ment (like RStudioTM Desktop; <http://rstudio.org>) or in the R terminal.

Once the ‘gamma’ package is loaded with `library(gamma)`, processing a spectrum is achieved in three steps: import, energy calibration and dose-rate estimation which are detailed hereafter.

All of these steps can be performed through the GUI, which can be launched with `launch_app()` after loading the package with `library(gammaShiny)`. Note that we chose to develop a GUI to allow the use of ‘gamma’ for users who might not feel comfortable with the use of the command line. However, only the full publication of scripts along with the results guarantees the reproducibility of published studies.

2.1.1 Step 1: import and inspect a gamma spectrum

The ‘gamma’ package supports the most common type of spectrum files: Canberra CAM (.CNF) and Programmers Toolkit files (.TKA). This prevents spending time on data transformation and preserves file metadata. The `read()` function allows to import a CNF-file with the path of the file as a single argument. When the path leads to a directory instead of a single file, all spectra included in the directory are imported.

```
1 ## Get an example file
2 cnf <- system.file(
3   "extdata/LaBr.CNF",
4   package = "gamma"
5 )
6 ## Import data
7 spc <- read(cnf)
8 spc
```

Spectra are stored as instances of an S4 class. Many mutator methods and group generic functions are available for basic operations and data wrangling. The `plot(spc)` method allows to quickly graphically inspect the data.

2.1.2 Step 2: adjust the energy scale

The energy calibration of a spectrum is a challenging part and must be performed before dose rate estimation. The solution presented here requires the user to specify the position (channel) of at least three observed peaks and their corresponding theoretical energies (in keV). A second order polynomial model is fitted on these energy *versus* channel values, then used to predict the new energy scale of the spectrum.

The package allows the user to provide the channel-energy pairs to be used. However, the spectrum can be noisy so it is difficult to properly identify the peak channel. In this case, a better approach may be to pre-process the spectrum (variance-stabilization, smoothing and baseline correction) and perform a peak detection (Figure 2). Once the peak detection is satisfactory, the user can set the corresponding energy values (in keV) and use these lines to calibrate the energy scale of the spectrum. All signal processing methods are prefixed with `signal_`.

Cleaning Several channels can be dropped to retain only part of the spectrum with `signal_slice()`. If no specific value is provided, an attempt is made to define the number of channels to skip at the beginning of the spectrum. This drops all channels before the highest count maximum. This is intended to deal with the artefact produced by the rapid growth of random background noise towards low energies.

Stabilization The stabilization step aims at improving the identification of peaks with a low signal-to-noise ratio. This particularly targets higher energy peaks. To perform this step, a function is applied to all the intensity values of the spectrum with `signal_stabilize()`. The example below uses a square root transformation but any user defined function can be used.

Smoothing Counting artefacts can be removed by smoothing intensities with `signal_smooth()`. Several methods are implemented here such as (weighted) sliding-average and Savitzky-Golay filter (Savitzky & Golay, 1964; Gorry, 1990). The example below uses the Savitzky-Golay filter as this method usually provides better results, at the expense of a longer computing time.

Baseline correction Spectrum baseline can be estimated and removed with `signal_correct()` using specialized SNIP algorithm (Ryan et al., 1988; Morháč et al., 1997; Morháč & Matoušek, 2008).

Peak detection `find_peaks()` allows automatic peak position detection on a baseline-corrected spectrum. For a successful detection, a local maximum has to be the highest one in a given window and has to be higher than k times the noise (estimated as the Median Absolute Deviation) to be recognized as a peak.

Energy calibration The energy scale calibration needs the energy values of detected peaks to be set. `calibrate_energy()` then fits a second order polynomial model to predict the new spectrum energy scale.

```
1 library(magrittr)
2 ## Signal processing
3 tmp <- spc %>%
4   signal_slice() %>%
5   signal_stabilize(f = sqrt) %>%
6   signal_smooth(method = "savitzky", m = 21)
7   ↪ %>%
8   signal_correct(method = "SNIP")
9 ## Peak detection
10 pks <- peaks_find(tmp)
11 set_energy(pks) <- c(238, NA, NA, NA,
12                    1461, NA, NA, 2615)
13 ## Energy scale calibration
14 spc2 <- energy_calibrate(spc, pks)
```

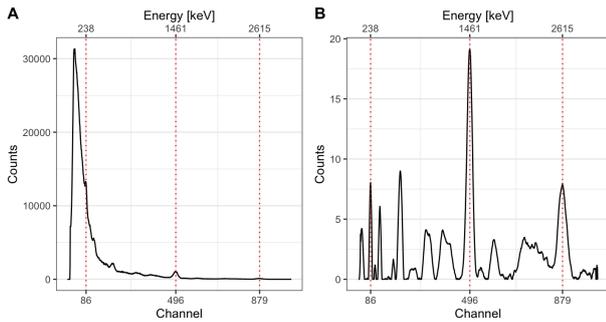


Figure 2. (A) Raw gamma ray spectrum from in situ measurement; (B) Processed spectrum used for peak finding along with the detected peaks.

2.1.3 Step 3: gamma dose-rate estimation

To estimate the gamma dose rate, one of the calibration curves distributed with this package can be used (Figure 3). These built-in curves are in use in several luminescence dating laboratories and can be used to replicate published results. As these curves are instrument specific, the user may have to build its own curve. The ‘gamma’ package provides a set of functions to build custom calibration curves.

```

1 ## Load the calibration curve
2 data("BDX_LaBr_1", package = "gamma")
3 ## Estimate the gamma dose rate
4 doses <- dose_predict(BDX_LaBr_1, spc2)
5 doses

```

The construction of a calibration curve with `dose_fit()` requires a set of reference spectra for which the gamma dose rate is known (see Miallier et al., 2009 for the reference values in use at the CRP2A laboratory) and a background noise measurement. First, each reference spectrum is integrated over a given interval, then normalized to active time and corrected for background noise. The dose rate is finally modelled by the integrated signal value used as a linear predictor (York et al., 2004). `dose_predict()` returns the predicted dose rate value with both the count and energy threshold approaches.

3. Discussion

The ‘gamma’ package provides a convenient and reproducible toolkit for *in situ* gamma spectrometry data analysis. Along with the dedicated ‘gammaShiny’ package (GUI), it offers a useful set of functions for spectra processing, calibration curve building and dose rate estimation.

The ‘gamma’ package allows batch processing of spectra. To ensure the reliability of the produced results, manual verification is strongly recommended since automatic detection may sometime produce unreliable results, especially when the processed spectra display poor signal-to-noise ratios. In the future, improvement of the automatic peak detection process is to be expected (Guilhem Paradol, pers. comm.).

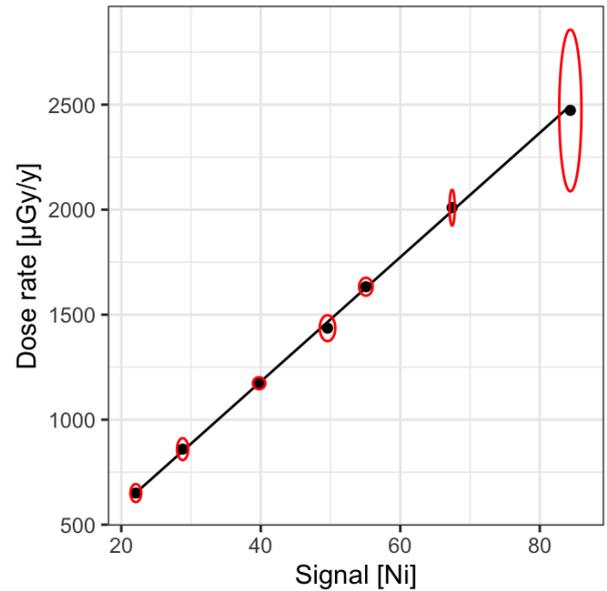


Figure 3. Built-in LaBr calibration curve in used at the CRP2A laboratory (Bordeaux).

4. Conclusions

The ‘gamma’ package is distributed over the Comprehensive R Archive Network (CRAN; <http://cran.r-project.org>). It is provided under the General Public Licence (GNU GPL3) conditions: the code is open and anyone can review it. Source code and installation instructions are available on GitHub at <https://github.com/crp2a/gamma> and <https://github.com/crp2a/gammaShiny>. Users are invited to contribute, share feedback, request new features or report bugs via the GitHub platform. As for the ‘Luminescence’ package (Kreutzer et al., 2012; Fuchs et al., 2015), future improvements to the ‘gamma’ package and associated GUI are intended to be community driven.

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Reviewer

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