Signal component analysis of IR-RF decay curves of K-feldspars – Part 2

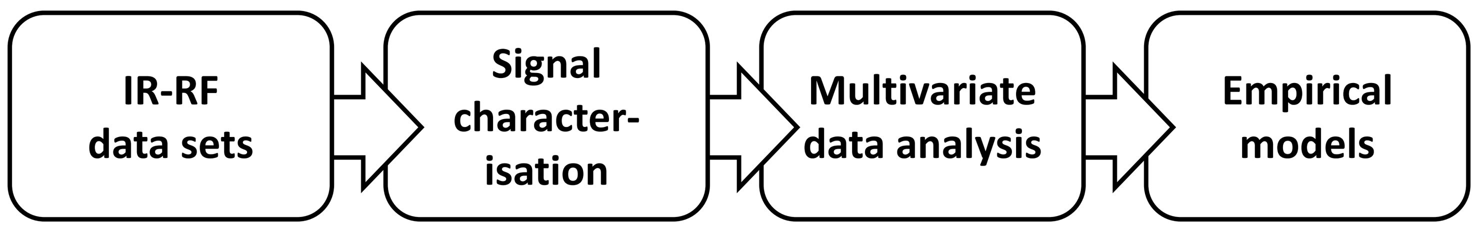
Dirk Mittelstraß
Independent Researcher, Dresden, Germany
dirk.mittelstrass@luminescence.de

Part 1
luminescence.de/RF/PosterLED2023_RF_components.pdf

Scope

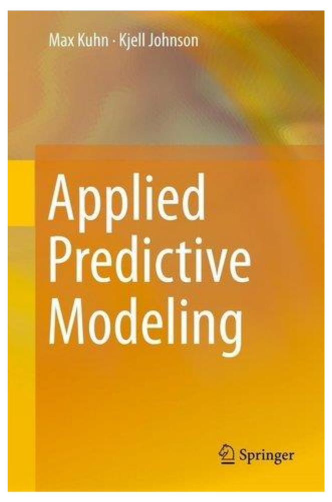
In geomorphology, not only the age of sedimentary deposits but also their origin and mineral properties are of interest. Obtaining this information can be more difficult and time-consuming than just determining the luminescence age. Here IR-RF can be an useful marker. Preliminary tests have shown that IR-RF measurements after sample bleaching have characteristic curve parameters depending on the origin of the sample [1]. These 'fingerprints' are measured at the bleached sample, are easy to calibrate and seem to be independent from the luminescence age and fading.

Multivariate data analysis might give us the tools to create empirical models about the origin and properties of feldspar sediments from the IR-RF fingerprints. This poster shows a short feasibility study for this approach.



What is multivariate data analysis?

Multivariate data analysis (MDA) is a collection of mathematical methods to find correlations in complex large data sets. These correlations are used to create empirical classification and prediction models. MDA is primarily used in pharmacy and chemometrics and is one main ancestor of modern AIs like ChatGPT. An excellent introduction for using MDA in **R** is the book Applied Predictive Modelling [2].



Signal curve fitting

The signal characterisation was done using the **R** package **OSLdecomposition** [3], see luminescence.de for more information.

This **R** package was originally developed for the separation of Fast, Medium and Slow components in CW-OSL measurements of quartz [4]. Here, we adapt the same algorithms for characterising IR-RF decay curves. Similar to CW-OSL of quartz, we assume that each K-feldspar IR-RF signal curve can be described by the sum of several exponential decay curves:

$$I_{RF}(d) = \sum_{k=1}^{K} \frac{n_k}{D_k} e^{-\frac{d}{D_k}}$$

I_{RF}	IR-RF signal
d	Accumulated dose during measurement, given by measurement time t and laboratory dose rate $\dot{D}_{lab}$, thus $d = t\dot{D}_{lab}$
K	Number of signal components
k	Signal component index
n_k	Signal component intensity, equals area below component curve
D_k	Half-decay dose of the signal component, related to the half-life τ by $D_k = \tau\dot{D}_{lab}$

The decay constants D_k are optimized iteratively by a genetic algorithm [5] while the component intensities n_k are calculated analytically [4]. The number of exponential terms K increases iteratively until a statistical test indicates that the fitting quality does not improve by additional components. Alternatively, the user can set a target number of components.

Acknowledgments

The data sets for this study were provided by multiple work groups. Many thanks to Margret Fuchs for providing B19-LU, Mariana Sontag-Gonzáles and Markus Fuchs for providing Gi361 and Gi326, Christoph Schmidt for providing BT1657 and Tobias Lauer for providing L-Eva-2275 and 2277.

References

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Luminescence data analysis as a service

https://luminescence.de/author.html

The algorithms and analyses presented here are an unfunded hobbyist project. However, Dirk can be booked to perform advanced analyses of OSL, IRSL and IR-RF data sets.

He has also a cooperation with the **LUNA lab** in Freiberg, Germany. The LUNA lab is a joint project of HZDR, TU Freiberg and Freiberg Instruments and is led by Dr. Margret Fuchs. The lab provides commercial services for **sample preparation**, luminescence dating and drill core mapping.

IR-RF data sets

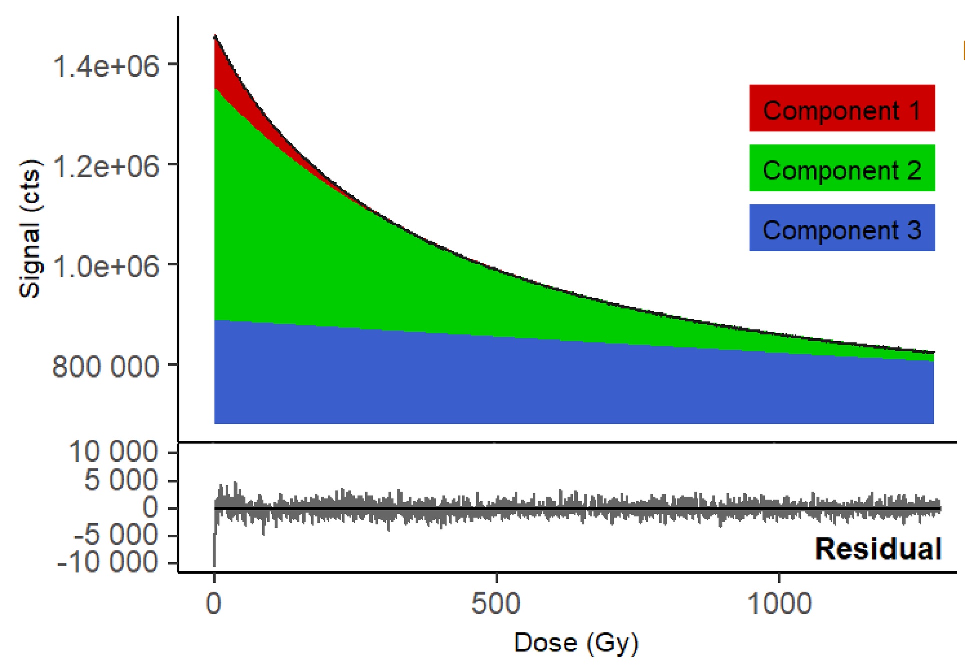
K-feldspar measurements from different locations and luminescence dating campaigns were compared. All were measured with *lexsyg Research* devices [6] using the default RF_{70} protocol [7]. For this study, only the IR-RF measurements after bleaching (RF_{reg}) were used.

Sample	Origin	Sedimentation	Age	Grain size	Measurement device	Ref.
B19-LU	Batagay mega-slump, Siberia	Syngenetic permafrost deposits from multiple cold stages	100 ka – 500 ka	63–100 µm	Lexsyg Research Leipzig	[8]
BT1657	Persani mountains, Romania	Baked paleosol below lava flow	~ 1 Ma	90–200 µm	Lexsyg Research Bayreuth	
Gi361	Cuddalore, India	Recently formed coastal dune	Modern	150–200 µm	Lexsyg Research Giessen	[9]
Gi326	Bayreuth, Germany	Triassic sandstone	Very old	90–200 µm	Lexsyg Research Giessen	
L-Eva-2275 & 2277	Fordwich, UK	Fluvial sands from stone age excavation site	~ 500 ka	90–250 µm	Lexsyg Research Leipzig	[10]

Table 1: Overview over K-feldspar sediment samples used for this study.

Signal characterisation

Preliminary tests showed that IR-RF measurements of K-feldspars can sufficiently described by four signal components up to a dose of at least 4000 Gy. Up to a dose of about 1500 Gy, only three components are necessary. Here, all measurements were reduced to 1250 Gy to be in line with the shortest measurements (L-Eva-2275). All fittings were performed with K = 3 components, using `fit_RFcurve()` of the upcoming version 1.1 of `OSLdecomposition`.



	Half-decay dose (Gy)	Area below curve (cts)
Component 1	103.2	2.19e+07 ± 7.95e+04
Component 2	408.2	3.70e+08 ± 1.98e+05
Component 3	1.305e+04	2.25e+10 ± 1.42e+06

Figure 1: IR-RF signal components of aliquot 56 of sample L-Eva-2275, measured on a lexsyg research device [6] using the RF_{70} protocol [7], thus IR-RF was measured at 70°C with a 850/40 filter. The sample was solar simulator bleached before this measurement.

Multivariate data analysis

The half-decay doses and component intensities were normalized and linearized to reduce imbalances in the value weighting. A **Principal Component Analysis** (PCA) was performed. Principal Components (PCs) are vectors along the highest variance in the value space. The PCs form a transformed coordinate system in which similarities and dissimilarities between the samples are worked out much better.

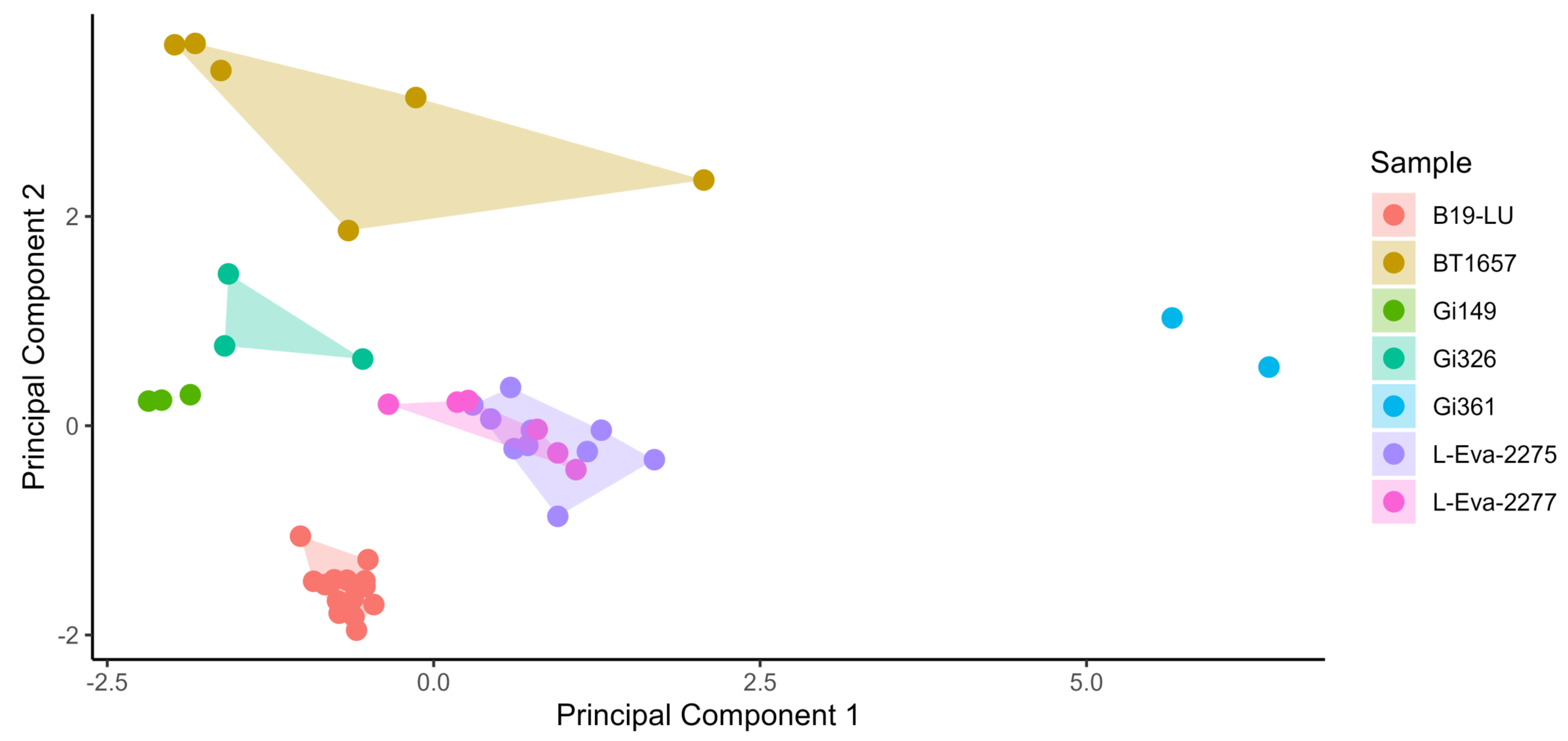


Figure 2: Score plot of of the two principal components with the highest contribution to the sample variance.

The PCA analysis was performed using the `prcomp()` function of the `stats` package. It returns five PCs of which PC1 and PC2 have the highest contribution to the sample variance with 48 % and 38 %. The input variable weights on the Principal Components (i.e. loadings) can be investigated to those input variables that have the greatest influence on sample variability:

$$\text{PC1 score} = 0.51\,\hat{D}_1 + 0.40\,\hat{D}_2 + 0.49\,\hat{D}_3 + 0.10\,\hat{n}_1 + 0.45\,\hat{n}_2 - 0.37\,\hat{n}_3$$

$$\text{PC2 score} = 0.29\,\hat{D}_1 + 0.45\,\hat{D}_2 + 0.11\,\hat{D}_3 - 0.58\,\hat{n}_1 - 0.31\,\hat{n}_2 + 0.51\,\hat{n}_3$$

$\hat{D}_k$ and $\hat{n}_k$ are transformed representations of D_k and n_k

Conclusion: The half-decay doses of all three components play a vital role for distinguishing between samples. The ratio of signal component 1 and 2 intensities (which dominate the curvature) against signal component 3 intensity (which dominates the signal background) seem also to be important.

Empirical models

More advanced MDA methods, like Partial Least Square Regression (PLSR) can build classification models and attribute predictors based well characterized data libraries and enable exciting new scientific applications.