

# **- Supplementary Data - Introducing an R package for luminescence dating analysis Ancient TL**

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## Contents

1	Example: Fitting loop	5
2	Fitting comparison	7
	References	12

**List of Figures**

1	Fitting comparison I . . . . .	8
2	Fitting comparison II . . . . .	9
3	Fitting comparison III . . . . .	10

**List of Tables**

1	Samples used for the fitting test . . . . .	10
2	Results fitting . . . . .	11

# 1 Example: Fitting loop

This **R** script uses the *Luminescence* package and selects all ramped signal data from a BIN-file. It is assumed that every 2nd curve is a background curve. A 3-component fit is tried for every curve after background subtraction. For every fit a plot is produced. The output is written in the previously defined output folder. The numerical values of the parameter output are written in a CSV-file. Additional values are appended.

```
1  ##fit loop for LM-OSL curve data
2
3  ##INSERT INPUT AND OUTPUT PATH HERE
4  input<-"~/Desktop/LM_CurveMeasurement.BIN"
5  output.path<-"~/Desktop/"
6  n.components<-3
7
8
9  ##load library
10 library(Luminescence)
11
12  ##=====##
13  ## READ AND PREPARE DATA
14  ##=====##
15
16  ##read BIN file
17  temp<-readBIN2R(input)
18
19  ##grep IDs for signal and background curves
20  values.ID<-temp@METADATA[temp@METADATA[, "LTYPE"]=="RBR", "ID"]
21  values.HIGH<-temp@METADATA[temp@METADATA[, "LTYPE"]=="RBR", "HIGH"]
22
23  ##set IDs for curves
24  values.signal.ID<-values.ID[seq(1, length(values.ID), 2)]
25  values.BG.ID<-values.ID[seq(2, length(values.ID), 2)]
26
27  #set stimulation time for curves
28  values.signal.HIGH<-values.HIGH[seq(1, length(values.HIGH), 2)]
29  values.BG.HIGH<-values.HIGH[seq(2, length(values.HIGH), 2)]
30
31  ##=====##
32  ## FIT LOOP
33  ##=====##
34
35  for(i in 1:(length(values.ID)/2)){
36
37      ##set individual data.frame for signal and BG
38
39      ##assuming that signal and bg have the same resolution and stimulation time
40      x<-seq(values.signal.HIGH[i]/length(unlist(temp@DATA[values.signal.ID[i]])),
41            values.signal.HIGH[i],
42            values.signal.HIGH[i]/length(unlist(temp@DATA[values.signal.ID[i]])))
43
44      ##set data.frame
45      values.signal<-data.frame(x=x, y=unlist(temp@DATA[values.signal.ID[i]]))
46      values.BG<-data.frame(x=x, y=unlist(temp@DATA[values.BG.ID[i]]))
47
48      ##=====##
49      ##START FITTING WITH JPEG OUTPUT
50      jpeg(file=paste(output.path, "FittedCurves_", i, ".jpg", sep=""), quality=100,
51           height=3000, width=3000, res=300)
52
53      fit_LMCurve(values.signal, values.BG,
54                  log_scale="x",
55                  n.components=n.components,
56                  fit.advanced=TRUE,
```

```
57         output.path=output.path,
58         main=paste("sample_",i,sep=""))
59     dev.off()
60     ##-----##
61
62 }#EOF
```

## 2 Fitting comparison

To provide a comparison of different approaches to fit models to luminescence curves the routine of the *Luminescence* package is compared with those of the programs Fitbin9 (Bailey, 2008) and Hybfit (Grzegorz Adamiec, principle described in Bluszcz and Adamiec (2006)) (Tab. 1). Without applying any background subtraction the curves almost coincide (indistinguishable curve shapes). The results as a sum curve for a 2-,3- and 4-component function are shown in Fig. 1. In addition, for 7-components the result for sample Rom16 is shown in Fig. 3 using **R** and the program Hybfit. In Fig. 2 the outcome seems to be affected by the way the background is subtracted (linear or polynomial fit) and therefore differences between the programs can be noticed. However, as far as the BG is fitted in the course of one of the slow components, the outcomes of the three programs appear to be very comparable. The detailed results ( $n$ - and  $b$ -values) are listed in Tab. 2. All fits were produced using the automatic start parameter estimation functions of the programs. Note: Not all possible combinations of components, samples and programs were applied.

## Sum Curves without Background Subtraction

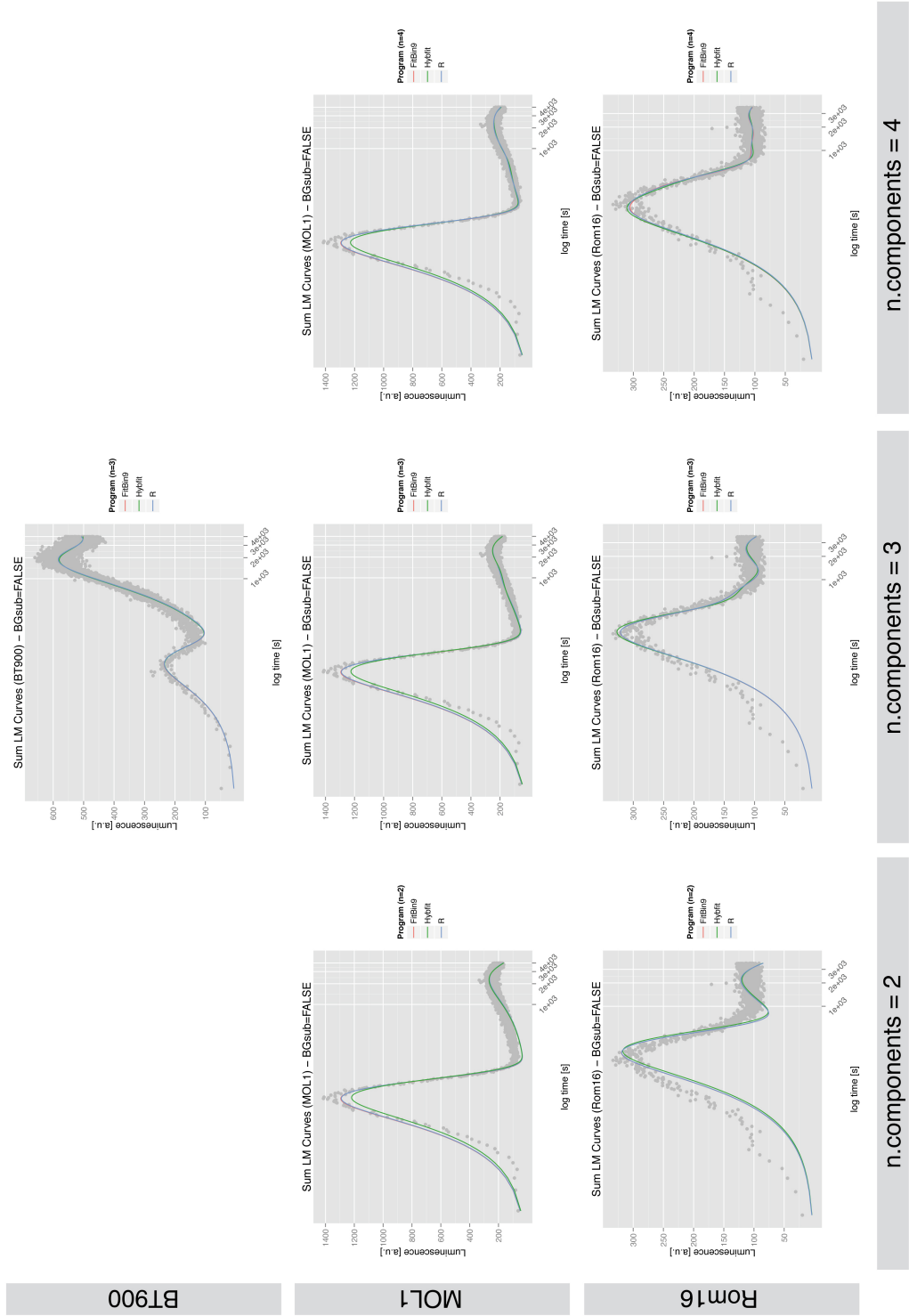


Figure 1: LM-OSL fitting results as sum curves using three different programs for three different samples without background subtraction.



## Sum Curves with Background Subtraction

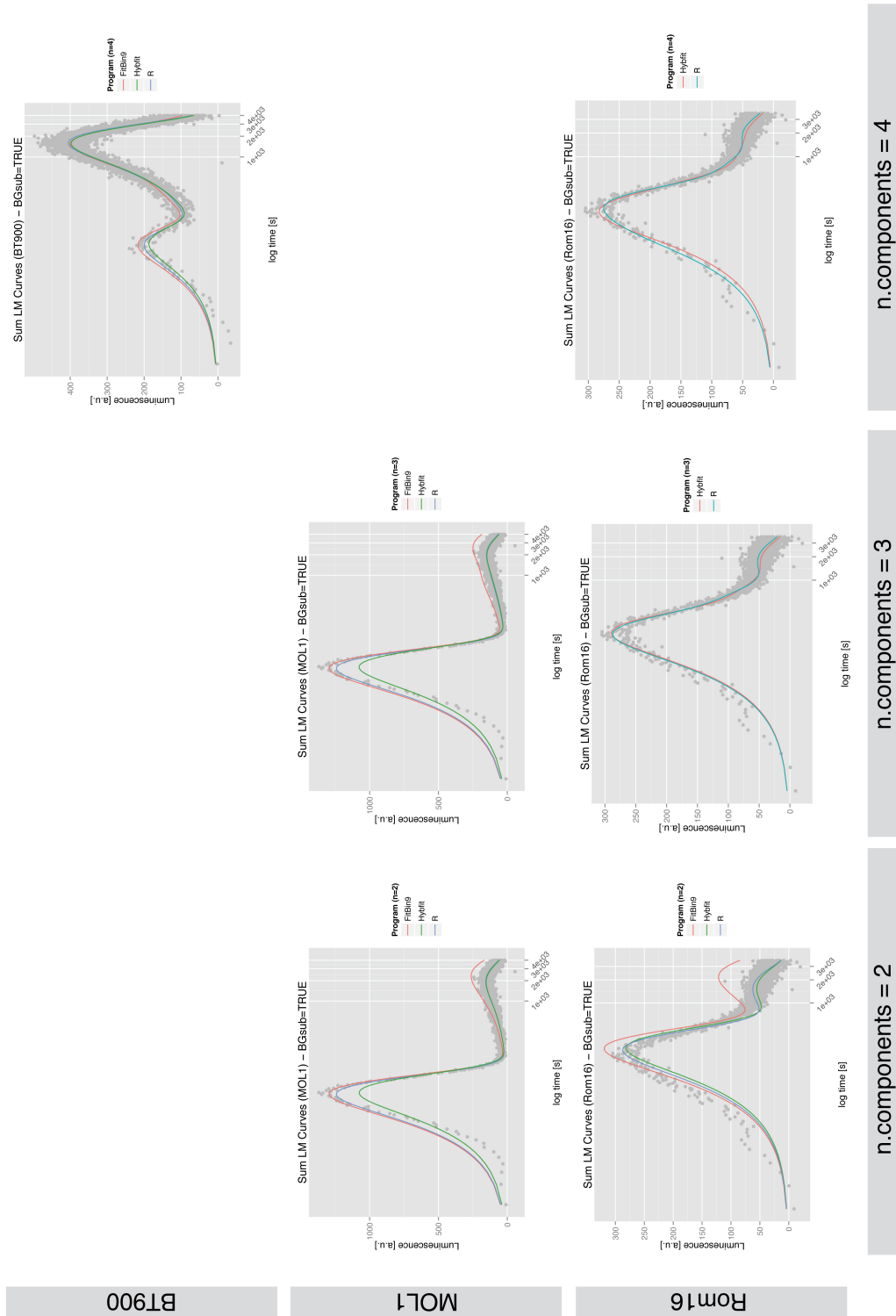


Figure 2: LM-OSL fitting results as sum curves using three different programs for three different samples with background subtraction. Not for all combinations a fit was applied.

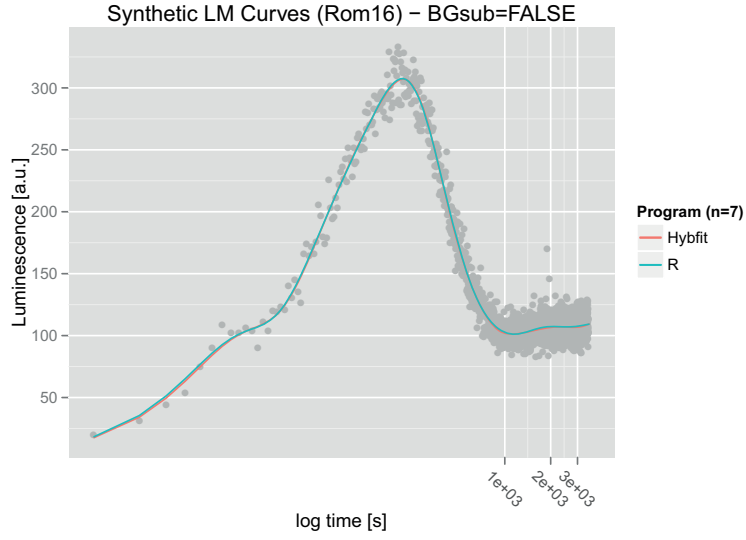


Figure 3: LM-OSL fitting result comparing R and the program Hybfit for sample Rom16 using a 7-component function.

Table 1: Samples used for the fitting test

sample id	description	grain size	laboratory	reference
BT900	beach deposit Norway (quartz)	90 - 250 $\mu\text{m}$	Bayreuth	Fuchs et al. (2011)
MOL1	Mol sand Belgium (quartz)	90 - 200 $\mu\text{m}$	Bayreuth	Gullentops and Vandenberghe (1995)
Rom16	archaeological artefact Romania (chalcedony)	100 - 200 $\mu\text{m}$	Cologne	Schmidt et al. (prep)

Table 2: Results fitting

#	program	sample	BG <sup>1</sup>	n <sup>2</sup>	n1	b1	n2	b2	n3	b3	n4	b4	n5	b5	n6	b6	n7	b7
1	FitBin9	BT900	F	3	1.88E+04	1.28E+00	8.76E+05	1.91E-03	8.19E+06	6.55E-05	NV	NV	NV	NV	NV	NV	NV	NV
2	Hybfit	BT900	F	3	1.86E+04	1.28E+00	7.70E+05	2.09E-03	4.52E+06	1.40E-04	NV	NV	NV	NV	NV	NV	NV	NV
3	R	BT900	F	3	1.88E+04	1.27E+00	8.78E+05	1.90E-03	8.30E+06	6.44E-05	NV	NV	NV	NV	NV	NV	NV	NV
4	FitBin9	BT900	T	4	1.44E+04	1.72E+00	1.05E+04	1.09E-01	9.54E+05	1.75E-03	1.49E+09	3.09E-08	NV	NV	NV	NV	NV	NV
5	R	BT900	T	4	1.27E+04	1.78E+00	4.26E+03	2.59E-01	5.54E+03	4.43E-02	1.06E+06	1.58E-03	NV	NV	NV	NV	NV	NV
6	FitBin9	MOL1	F	2	9.05E+04	2.19E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
7	FitBin9	MOL1	T	2	9.05E+04	2.19E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
8	R	MOL1	F	2	9.07E+04	2.17E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
9	R	MOL1	T	2	8.63E+04	2.23E+00	4.94E+05	1.08E-03	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
10	FitBin9	MOL1	F	3	8.95E+04	2.23E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
11	FitBin9	MOL1	T	3	8.95E+04	2.23E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
12	R	MOL1	F	3	8.97E+04	2.20E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
13	R	MOL1	T	3	8.60E+04	2.24E+00	1.55E+04	1.46E-02	4.92E+05	1.02E-03	NV	NV	NV	NV	NV	NV	NV	NV
14	FitBin9	MOL1	F	4	8.87E+04	2.25E+00	1.99E+04	4.37E-02	9.48E+04	3.62E-03	1.06E+06	5.24E-04	NV	NV	NV	NV	NV	NV
15	Hybfit	MOL1	F	4	8.52E+04	2.18E+00	1.54E+04	6.40E-02	7.78E+04	4.76E-03	1.05E+06	5.56E-04	NV	NV	NV	NV	NV	NV
16	R	MOL1	F	4	8.89E+04	2.23E+00	2.02E+04	4.23E-02	9.66E+04	3.54E-03	1.06E+06	5.21E-04	NV	NV	NV	NV	NV	NV
17	FitBin9	Rom16	F	2	1.18E+05	6.14E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
18	FitBin9	Rom16	T	2	1.18E+05	6.14E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
19	Hybfit	Rom16	F	2	1.23E+05	5.60E-02	4.36E+05	7.38E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
20	Hybfit	Rom16	T	2	8.06E+04	1.00E-01	7.20E+04	1.48E-02	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
21	R	Rom16	F	2	1.19E+05	6.12E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
22	R	Rom16	T	2	1.04E+05	6.61E-02	1.54E+05	1.59E-03	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
23	FitBin9	Rom16	F	3	7.25E+04	1.08E-01	7.66E+04	1.74E-02	4.74E+05	5.69E-04	NV	NV	NV	NV	NV	NV	NV	NV
24	Hybfit	Rom16	F	3	8.06E+04	1.00E-01	7.20E+04	1.48E-02	4.76E+05	5.49E-04	NV	NV	NV	NV	NV	NV	NV	NV
25	R	Rom16	F	3	7.29E+04	1.07E-01	7.64E+04	1.72E-02	4.74E+05	5.68E-04	NV	NV	NV	NV	NV	NV	NV	NV
26	R	Rom16	T	3	5.89E+04	1.15E-01	6.55E+04	2.48E-02	1.49E+05	1.21E-03	NV	NV	NV	NV	NV	NV	NV	NV
27	FitBin9	Rom16	F	4	1.92E+04	2.84E-01	8.78E+04	5.78E-02	6.25E+04	7.26E-03	5.18E+05	4.43E-04	NV	NV	NV	NV	NV	NV
28	Hybfit	Rom16	F	4	2.83E+04	2.27E-01	8.59E+04	4.82E-02	6.26E+04	5.69E-03	5.37E+05	4.01E-04	NV	NV	NV	NV	NV	NV
29	R	Rom16	F	4	2.25E+04	2.49E-01	8.70E+04	5.42E-02	6.25E+04	6.67E-03	5.25E+05	4.29E-04	NV	NV	NV	NV	NV	NV
30	R	Rom16	T	4	5.07E+03	6.48E-01	7.16E+04	8.66E-02	5.25E+04	1.79E-02	1.48E+05	1.13E-03	NV	NV	NV	NV	NV	NV
31	R	Rom16	F	5	3.74E+03	1.68E+00	5.50E+04	1.17E-01	6.74E+04	3.11E-02	7.22E+04	3.61E-03	6.14E+05	3.02E-04	NV	NV	NV	NV
32	R	Rom16	T	5	2.89E+03	1.15E+00	5.47E+04	1.09E-01	5.82E+04	3.04E-02	5.07E+04	3.48E-03	1.33E+05	6.55E-04	NV	NV	NV	NV
33	R	Rom16	F	6	9.60E+02	2.06E+01	4.55E+03	9.04E-01	5.96E+04	1.06E-01	6.33E+04	2.83E-02	7.54E+04	3.32E-03	6.38E+05	2.80E-04	NV	NV
34	R	Rom16	T	6	5.20E+02	1.96E+01	3.34E+03	7.82E-01	5.67E+04	1.04E-01	5.62E+04	2.90E-02	5.35E+04	3.27E-03	1.32E+05	6.18E-04	NV	NV
35	Hybfit	Rom16	F	7	9.35E+02	2.02E+01	4.20E+03	9.59E-01	5.23E+04	1.14E-01	5.80E+04	3.62E-02	2.82E+04	1.02E-02	1.24E+05	1.77E-03	1.77E+06	6.37E-05
36	R	Rom16	F	7	9.13E+02	2.18E+01	3.60E+03	1.12E+00	3.39E+04	1.40E-01	5.17E+04	5.82E-02	4.39E+04	1.96E-02	8.80E+04	2.62E-03	7.44E+05	2.10E-04
37	R	Rom16	T	7	5.01E+02	2.02E+01	2.74E+03	9.15E-01	4.28E+04	1.20E-01	4.45E+04	4.71E-02	3.10E+04	1.85E-02	7.63E+04	2.31E-03	1.39E+05	3.29E-04

Note

<sup>1</sup> background subtraction T (TRUE) or F (FALSE)<sup>2</sup> number of components used for fitting $n$  is the number of initial trapped electrons $b$  is the detrapping probability

NV = No Value

## References

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