# Package 'BayLum'

June 14, 2017

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| Description  |
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### **Description**

Chronological Bayesian Models Integrating Optically Stimulated Luminescence Dating

| AgeS_Computation | Bayesian analysis for the OSL age estimation of various samples |
|------------------|---|
| AgeS_Computation | Bayesian analysis for the OSL age estimation of various samples |

# **Description**

This function computes the age of at leat two samples according to the model developed in Combes and Philippe (2017), based on an output of the Generate\_DataFile function.

Samples, for which data is available in several BIN files, can be analysed.

### Usage

```
AgeS_Computation(DATA, Nb_sample, BinPerSample = rep(1, Nb_sample),
SampleNames, SavePdf = FALSE, OutputFileName = c("MCMCplot", "summary",
"2per2Laws"), OutputFilePath = c(""), SaveEstimates = FALSE,
OutputTableName = c("DATA"), OutputTablePath = c(""), THETA = c(),
sepTHETA = c(","), PriorAge = rep(c(0.01, 100), Nb_sample),
StratiConstraints = c(), sepSC = c(","), LIN_fit = TRUE,
Origin_fit = FALSE, distribution = c("cauchy"), Taille = 50000, t = 5,
Nb_chaines = 3)
```

### **Arguments**

| - 7 | 9              |  |
|-----|----------------|--|
|     | DATA           | list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function Generate_DataFile. DATA contains information for more than one sample.   |
|     | Nb_sample      | integer (required): number of samples, Nb_sampe>1.   |
|     | BinPerSample   | integer vector (with default): vector with the number of BIN files per sample. The length of this vector is equal to Nb_sample. BinPerSample[i] correponds to the number of BIN files for the sample whose number ID is equal to i. For more information to fill this vector, we refer to detatils in Generate_DataFile. |
|     | SampleNames    | character vector: names of sample. The length of this vector is equal to Nb_sample.  |
|     | SavePdf        | boolean (with default): if TRUE save graph in pdf file named OutputFileName in folder OutputFilePath.  |
|     | OutputFileName | character (with default): name of the pdf file that will be generated by the function if SavePdf=TRUE.   |
|     | OutputFilePath | character (with default): path to the pdf file that will be generated by the function if SavePdf=TRUE.   |
|     | SaveEstimates  | boolean (with default): if TRUE save Bayes estimates and confidence interval at level $68\%$ and $95\%$ , in a csv table named OutputFileName in folder OutputFilePath.  |

OutputTableName

character (with default): name of the table that will be generated by the function if SaveEstimates=TRUE.

OutputTablePath

character (with default): path to the table that will be generated by the function

if SaveEstimates=TRUE.

THETA numeric matrix or character (with default): input object for systematic and in-

dividual error. If systematic errors are considered, see the details section for instructions regarding how to correctly fill THETA. Otherwise, default value is

suitable, and only individual error is considered.

sepTHETA character (with default): if THETA is character, indicate column separator in

THETA .csv file.

PriorAge numeric vector (with default): lower and upper bounds for age parameter of

each sample. length(PriorAge)=2\*Nb\_sample and PriorAge[2i-1,2i] correponds to the lower and upper bounds of sample whose number ID is equal to

i.

StratiConstraints

numeric matrix or character(with default): input object for the statigraphic relation between samples. If there is stratigraphic relation between samples see the details section for instructions regarding how to correctly fill StratiConstraints.

Otherwise, default value is suitable.

sepSC character (with default): if StratiConstraints is character, indicate column

separator in StratiConstraints .csv file.

LIN\_fit logical (with default): if TRUE (default) allows a linear component, on top of

the (default) saturating exponential curve, for the fitting of dose response curves. Please see details for more informations on the proposed dose response curves.

Origin\_fit logical (with default): if TRUE, forces the dose response curves to pass through

the origin. Please see details for more informations on the proposed growth

curves.

distribution character (with default): type of distribution that defines how individual equiv-

alent dose values are distributed around the palaeodose. Allowed inputs are

"cauchy", "gaussian" and "lognormal".

Taille integer (with default): number of iterations for the MCMC computation (for

more information see jags.model).

t integer (with default): 1 every t iterations of the MCMC is considered for sam-

pling the posterior distribution (for more information see jags.model).

Nb\_chaines integer (with default): number of independent chains for the model (for more

information see jags.model).

# **Details**

#### \*\* How to fill StratiConstraints? \*\*

If there is stratigraphic relations between samples, information in DATA must be ordered by order of increasing ages. The user can fill the StratiConstraints matrix as follow.

First, concerning the **size of the matrix**, row number of StratiConstraints matrix is equal to Nb\_sample+1, and column number is equal to Nb\_sample.

Secondly, conserning the **first line of the matrix**, for all i in  $\{1, \ldots, Nb\_Sample\}$ , StratiConstraints[1,i]=1 that means the lower bound of the sample age given in PriorAge[2i-1] for the sample whose number ID is equal to i, is taken into account.

Thirdly, concerning the **sample relations**, for all j in {2,...,Nb\_Sample+1} and all i in {j,...,Nb\_Sample},

StratiConstraints[j,i]=1 if sample age whose number ID is equal to j-1 is lower than sample age whose number ID is equal to i. Otherwise, StratiConstraints[j,i]=0.

Note that  $StratiConstraints_{2:Nb\_sample+A,1:Nb\_sample}$  is a upper triangular matrix.

The user can also use SCMatrix function to construct he StratiConstraints matrix.

The user can also refer to a .csv file that containts the relation between samples as defined above.

#### \*\* How to fill THETA concerning common and individual error? \*\*

If systematic errors are considered, the user can fill the THETA matrix as follow.

Note that row number of THETA is equal the column number. For all i in  $\{1, \ldots, Nb\_sample\}$ , THETA[i,i] containts individual error plus systematic error of the sample whose number ID is equal to i. For all i, j in  $\{1, \ldots, Nb\_sample\}$  and i different from j, THETA[i,j] containts common error between samples whose number ID are equal to i and j.

Note that THETA[i, j] is a symetric matrix.

The user can also refer to a .csv file that containts the errors as defined above.

#### \*\* Different growth curves \*\*

As for Age\_Computation, the user can choose from 4 dose response curves:

• Saturating exponential plus linear growth (AgeMultiBF\_EXPLIN):

```
for all x in IR+, f(x)=a(1-exp(-x/b))+cx+d; select
```

- LIN\_fit=TRUE
- Origin\_fit=FALSE
- Saturating exponential growth (AgeMultiBF\_EXP):

```
for all x in IR+, f(x)=a(1-exp(-x/b))+d; select
```

- LIN\_fit=FALSE
- Origin\_fit=FALSE
- Saturating exponential plus linear growth and fitting through the origin (AgeMultiBF\_EXPLINZO):

```
for all x in IR+, f(x)=a(1-exp(-x/b))+cx; select
```

- LIN\_fit=TRUE
- Origin\_fit=TRUE
- Saturating exponential growth and fitting through the origin (AgeMultiBF\_EXPZO):

```
for all x in IR+, f(x)=a(1-exp(-x/b)); select
```

- LIN\_fit=FALSE
- Origin\_fit=TRUE

#### Value

#### 1- NUMERICAL OUTPUT

#### A list containing the following objects:

- **Sampling** that corresponds to a sample of the posterior distributions of the Age, palaeodose and equivalent dose dispersion parameters.
- Model\_GrowthCurve, stating which dose response fitting option was chosen;
- **Distribution**, stating which distribution was chosen to model the dispersion of individual equivalent dose values around the palaeodose of the sample;
- PriorAge, stating the priors used for the age parameter.

#### The Gelman and Rudin test of convergency

Prints the result of the Gelman and Rudin test of convergency for the age, palaeodose and equivalent dose dispersion parameters for each sample. A result close to one is expected.

In addition, the user must visually assess the convergency of the trajectories by looking at the pdf file generated by the function (see 2- for more informations).

If both convergencies (Gelman and Rudin test and plot checking) are satisfactory, the user can consider the printed estimates as valid. Otherwise, the user may try increasing the number of MCMC interations (Taille) to reach convergency.

#### Credible intervals and Bayes estimates

Prints the Bayes esitmates, the credible intervals at level 95% and 68% for the age, palaeodose and equivalent dose dispersion parameters for each sample.

#### 2- PLOT OUTPUT

#### MCMC trajectories

A pdf file with the MCMC trajectories and posterior distributions of the age, palaeodose and equivalent dose dispersion parameters. There is one page per sample.

The first line of the figure correponds to the age parameter, the second to the palaeodose parameter and the third to the equivalent dose dispersion parameter. On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distribution of the parameter.

#### **Summary of sample ages**

Plot credible intervals and bayes estimate of each sample age on a same graph.

#### Stratigraphic constraints

If there are stratigraphic constraints, plot sampling of each sample two by two...

#### Author(s)

Claire Christophe, Guillaume Guerin

### References

Combes, Benoit and Philippe, Anne, 2017. Bayesian analysis of multiplicative Gaussian error for multiple ages estimation in optically stimulated luminescence dating. Quaternary Geochronology (in press)

Combes, B., Philippe, A., Lanos, P., Mercier, N., Tribolo, C., Guerin, G., Guibert, P., Lahaye, C., 2015. A Bayesian central equivalent dose model for optically stimulated luminescence dating. Quaternary Geochronology 28, 62-70. doi:10.1016/j.quageo.2015.04.001

#### See Also

```
Generate_DataFile, rjags package, MCMC_plot, Age_Computation, SCMatrix
```

### **Examples**

```
## Load data
# data(DATA1,envir = environment())
# data(DATA2,envir = environment())
# DATA=Concat_DataFile(DATA2,DATA1)

## Age computation of samples GDB5 and GDB3,
## without common error and without stratigraphic constraints
# Age=AgeS_Computation(DATA,Nb_sample=2,SampleNames=c("GDB5","GDB3"),SavePdf=FALSE,Taille=1000)
```

```
## Age computation of samples GDB5 and GDB3,
## without common error, assuming GDB5 age younder than GDB3 age
# SC=matrix(data=c(1,1,0,1,0,0),ncol=Nb_sample,nrow = (Nb_sample+1),byrow = T)
# Age=AgeS_Computation(DATA,Nb_sample=2,SampleNames=c("GDB5","GDB3"),
# StratiConstraints=SC,Taille=10000)
```

Age\_Computation

Bayesian analysis for the OSL age estimation of one sample

#### **Description**

This function computes the age of a sample according to the model developed in Combes and Philippe (2017), based on an output of the Generate\_DataFile function.

A sample, for which data is avalilable in several BIN files, can be analysed.

#### Usage

```
Age_Computation(DATA, samplename, SavePdf = FALSE,
  OutputFileName = c("MCMCplot"), OutputFilePath = c(""),
  SaveEstimates = FALSE, OutputTableName = c("DATA"),
  OutputTablePath = c(""), BinPerSample = c(1), PriorAge = c(0.01, 100),
  LIN_fit = TRUE, Origin_fit = FALSE, distribution = c("cauchy"), I = 1,
  Taille = 50000, t = 5, Nb_chaines = 3)
```

#### **Arguments**

DATA list of objects: LT, sLT, ITimes, dLab, ddot\_env, regDose, J, K, Nb\_measurement,

provided by the function Generate\_DataFile. DATA can contain information

for more than one sample.

samplename character: name of the sample.

SavePdf boolean (with default): if TRUE save graph in pdf file named OutputFileName

in folder OutputFilePath.

OutputFileName character (with default): name of the pdf file that will be generated by the func-

tion if SavePdf=TRUE.

OutputFilePath character (with default): path to the pdf file that will be generated by the function

if SavePdf=TRUE.

SaveEstimates boolean (with default): if TRUE save Bayes estimates and confidence inter-

val at level 68% and 95%, in a csv table named OutputFileName in folder

OutputFilePath.

OutputTableName

character (with default): name of the table that will be generated by the function

if SaveEstimates=TRUE.

OutputTablePath

character (with default): path to the table that will be generated by the function

if SaveEstimates=TRUE.

BinPerSample integer vector (with default): vector with the number of BIN files per sample.

If in DATA there is more than one sample, the BinPerSample vector must be the same as that used to run the function Generate\_DataFile for generating the

DATA object.

| PriorAge     | numeric vector (with default): lower and upper bounds for the sample age parameter. length(PriorAge)=2.  |
|--------------|--|
| LIN_fit      | logical (with default): if TRUE (default) allows a linear component, on top of the (default) saturating exponential curve, for the fitting of dose response curves. Please see details for more informations on the proposed dose response curves. |
| Origin_fit   | logical (with default): if TRUE, forces the dose response curves to pass through the origin. Please see details for more informations on the proposed growth curves.   |
| distribution | character (with default): type of distribution that defines how individual equivalent dose values are distributed around the palaeodose. Allowed inputs are "cauchy", "gaussian" and "lognormal".  |
| I            | integer (with default): if DATA contains data from more than one sample, I indicates the ID number of the sample to be analysed.   |
| Taille       | integer (with default): number of iterations for the MCMC computation (for more information see jags.model).   |
| t            | integer (with default): 1 every t iterations of the MCMC is considered for sampling the posterior distribution (for more information see jags.model).  |
| Nb_chaines   | integer (with default): number of independent chains for the model (for more information see jags.model).  |

### **Details**

For more flexibility, the user can choose from 4 dose response curves:

• Saturating exponential plus linear growth (AgeMultiBF\_EXPLIN):

for all x in IR+, f(x)=a(1-exp(-x/b))+cx+d; select

- LIN\_fit=TRUE
- Origin\_fit=FALSE
- **Saturating exponential growth** (AgeMultiBF\_EXP):

for all x in IR+, f(x)=a(1-exp(-x/b))+d; select

- LIN\_fit=FALSE
- Origin\_fit=FALSE
- Saturating exponential plus linear growth and fitting through the origin (AgeMultiBF\_EXPLINZO):

for all x in IR+, f(x)=a(1-exp(-x/b))+cx; select

- LIN\_fit=TRUE
- Origin\_fit=TRUE
- **Saturating exponential growth and fitting through the origin** (AgeMultiBF\_EXPZ0):

for all x in IR+, f(x)=a(1-exp(-x/b)); select

- LIN\_fit=FALSE
- Origin\_fit=TRUE

#### Value

# 1- NUMERICAL OUTPUT

A list containing the following objects:

• **Sampling** that corresponds to a sample of the posterior distributions of the Age, palaeodose and equivalent dose dispersion parameters.

- Model\_GrowthCurve, stating which dose response fitting option was chosen;
- **Distribution**, stating which distribution was chosen to model the dispersion of individual equivalent dose values around the palaeodose of the sample;
- PriorAge, stating the priors used for the age parameter.

#### The Gelman and Rudin test of convergency

Prints the result of the Gelman and Rudin test of convergency for the age, palaeodose and equivalent dose dispersion parameters. A result close to one is expected.

In addition, the user must visually assess the convergency of the trajectories by looking at the pdf file generated by the function (see 2- for more informations).

If both convergencies (Gelman and Rudin test and plot checking) are satisfactory, the user can consider the printed estimates as valid. Otherwise, the user may try increasing the number of MCMC interations (Taille) to reach convergency.

#### Credible intervals and Bayes estimates

Prints the Bayes esitmates, the credible intervals at level 95% and 68% for the age, palaeodose and equivalent dose dispersion parameters of the sample.

#### 2- PLOT OUTPUT

A pdf file with the MCMC trajectories and posterior distributions of the age, palaeodose and equivalent dose dispersion parameters.

The first line of the figure correponds to the age parameter, the second to the palaeodose parameter and the third to the equivalent dose dispersion parameter. On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distribution of the parameter.

# Author(s)

Claire Christophe, Guillaume Guerin

#### References

Combes, Benoit and Philippe, Anne, 2017. Bayesian analysis of multiplicative Gaussian error for multiple ages estimation in optically stimulated luminescence dating. Quaternary Geochronology (in press)

Combes, B., Philippe, A., Lanos, P., Mercier, N., Tribolo, C., Guerin, G., Guibert, P., Lahaye, C., 2015. A Bayesian central equivalent dose model for optically stimulated luminescence dating. Quaternary Geochronology 28, 62-70. doi:10.1016/j.quageo.2015.04.001

#### See Also

```
Generate_DataFile, rjags package, MCMC_plot
```

#### **Examples**

```
## load data file generated by the function Generate_DataFile
# data(DATA1,envir = environment())
# Age=Age_Computation(DATA1,samplename="GDB3",SavePdf=FALSE,Taille=1000)
```

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Concat\_DataFile

Concatenates two outputs of the function Generate\_DataFile

### **Description**

This function allows concatenating two lists provided as output of the Generate\_DataFile function.

Only concatenation of 2 files is possible.

### Usage

```
Concat_DataFile(u1, u2)
```

### **Arguments**

```
    u1 list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement.
    u2 list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement.
```

#### Value

A List of objects: LT, sLT, ITimes, dLab, ddot\_env, regDose, J, K, Nb\_measurement.

#### Author(s)

Claire Christophe, Guillaume Guerin

#### See Also

```
Generate_DataFile
```

### **Examples**

```
# load data files
data(DATA1,envir = environment())
data(DATA2,envir = environment())
# concatenate two data files
DATA3=Concat_DataFile(DATA1,DATA2)
str(DATA3)
```

DATA1

DATA on sample named GDB3

# Description

list of objects: LT, sLT, ITimes, dLab, ddot\_env, regDose, J,K,Nb\_measurement obtained using Generate\_DataFile function from luminescence data.

```
data("DATA1")
```

DATA2

#### **Format**

A data frame with 0 observations on the following 2 variables.

LT (one list per sample); each list contains all L/T values for the corresponding sample;

sLT (one list per sample); each list contains all uncertainties on L/T values for the corresponding sample;

ITimes (one list per sample); each list contains irradiation time values for the corresponding sample;

dLab, a matrix containing in line i, the laboratory dose rate and its variance for sample i;

ddot\_env , a matrix containing in line i, the environmental dose rate and its variance (excluding the common error terms) for sample i;

regDose (one list per sample); each list contains all regenerated doses;

J , a vector giving, for each BIN file, the number of aliquots selected for the analysis;

K, a vector giving, for each BIN file, the number of regenerative doses in the SAR protocol;

Nb\_measurement , a vector giving, for each BIN file, the number of measurements;

#### **Details**

A FAIRE

#### Source

A FAIRE

#### References

A FAIRE

### **Examples**

data(DATA1)
str(DATA1)

DATA2

DATA on sample named GDB5

# **Description**

list of objects: LT, sLT, ITimes, dLab, ddot\_env, regDose, J,K,Nb\_measurement obtained using Generate\_DataFile function from luminescence data.

```
data("DATA2")
```

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#### **Format**

A data frame with 0 observations on the following 2 variables.

LT (one list per sample); each list contains all L/T values for the corresponding sample;

sLT (one list per sample); each list contains all uncertainties on L/T values for the corresponding sample;

ITimes (one list per sample); each list contains irradiation time values for the corresponding sample;

dLab, a matrix containing in line i, the laboratory dose rate and its variance for sample i;

ddot\_env , a matrix containing in line i, the environmental dose rate and its variance (excluding the common error terms) for sample i;

regDose (one list per sample); each list contains all regenerated doses;

- J, a vector giving, for each BIN file, the number of aliquots selected for the analysis;
- K, a vector giving, for each BIN file, the number of regenerative doses in the SAR protocol;

Nb\_measurement, a vector giving, for each BIN file, the number of measurements;

#### **Details**

A FAIRE

#### **Source**

A FAIRE

#### References

A FAIRE

# **Examples**

data(DATA2)
str(DATA2)

Generate\_DataFile

Generates, from one (or several) BIN file(s), a list of luminescence data and information before statistical analysis

# Description

This function is used to generate, from the BIN file(s), a list of values of: OSL intensities and associated uncertainties, regenerative doses, etc., which will be the input of the Bayesian models. To be easy-to-use, this function requires a rigorous organisation - all needed files should be arranged in one folder - of informations concerning each BIN file. It is possible to process data for various samples simultaneously and to consider more than one BIN file per sample.

```
Generate_DataFile(Path, Names, Nb_sample, Nb_binfile = length(Names),
BinPerSample = rep(1, Nb_sample), sepDP = c(","), sepDE = c(","),
sepDS = c(","), sepR = c("="))
```

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#### **Arguments**

| Path           | character ( <b>required</b> ): the path to the project folder, containing one or more subfolders in which the BIN files are located.  |
|----------------|---|
| Names          | character vector ( <b>required</b> ): list of names of the sub-folders containing the BIN files - each subfolder must contain a BIN file and associated .csv files. See details for more informations on associated .csv files required in the subfolders. If there is more than one BIN file per sample, see the details section for instructions regarding how to correctly fill the Names vector.        |
| Nb_sample      | integer (required): number of samples.  |
| Nb_binfile     | integer (with default): number of BIN files. It must be equal to, or greater than Nb_sample.  |
| BinPerSample   | integer vector (with default): vector with the number of BIN files per sample. The length of this vector must be equal to Nb_sample and the sum of entries of this vector must be equal to Nb_binfile. If there is more than one BIN file per sample, see the details section for instructions regarding how to correctly fill BinPerSample vector. Otherwise, this vector must contain a list of 1 values. |
| sepDP          |   |
|                | character (with default): column separator in the DiscPose.csv files.   |
| sepDE          | character (with default): column separator in the DiscPose.csv files.  character (with default): column separator in the DoseEnv.csv files.   |
| sepDE<br>sepDS | •   |

#### **Details**

With Path and Names, this function goes to the subfolders containing the BIN files and associated information to compute the luminescence data.

#### \*\* What are the required files in each subfolder? \*\*

Each subfolder can be named, for example, as the sample name followed by a number; it must contain:

- bin.BIN, the bin file renamed as bin.BIN (note: the name of all files matters);
- **DiscPos.csv**, a two columns .csv file containing the list of disc and grain position number of the previously selected grains (typically this list will include the position of grains based on their sensitivity, recycling or other properties);
- **DoseEnv.csv**, a two columns file containing the observation of the natural (or environmental), dose rate, and its non-shared variance (i.e. after removing all shared errors). Note: the user shall provide the squared value of the error associated with the dose rate experienced by the sample grains in nature;
- **DoseSourve.csv**, a two columns file containing the observation of the laboratory dose rate, and its variance (squared error);
- rule.csv, a .csv file containing information on
  - beginSignal= the first channel for summing the natural or regenerative OSL signal (typically 1 or 6);
  - endSignal= the last channel for summing the natural or regenerative OSL signal (typically 5 or 10);
  - beginBackground= the first channel for background estimation of the natural or regenerative OSL signal (typically 76 or 81);
  - endBackground= the last channel for background estimation of the natural or regenerative OSL signal (typically 95 or 100);

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- beginTest,
- endTest,
- beginTestBackground,
- endTestBackground= same values as above, for the test dose response (typically the same values should be used);
- inflatePercent= uncertainty arising from the instrument reproducibility (typically 0.02, i.e. 2%);
- nbOfLastCycleToRemove= number of cycles at the end of the SAR protocol which should not be included in the dose response curve fitting (typically 1 if only a recycling test is performed, or 2 if both recycling and IR depletion are tested).

### \*\* How to fill the Names vector? \*\*

Names is a vector of length Nb\_binfile. Names[i] is the name (e.g., Sample1-File1, or successive names separated by "/" signs, if BIN files are in subfolders, e.g. Sample1/File1) of the subfolder containing all informations on the BIN file of ID number i. The names in Names are ordered following two rules:

- The names in the Names vector must be ordered following the sample order (the names of subfolders containing BIN files for the same sample should follow each other in the Names vector, e.g. Sample1, Sample2-File1, Sample2-File2, etc.).
- If stratigraphic constraints apply to samples, and so a Bayesian model with stratigraphic
  constraints is implemented, then the names in the Names vector must be ordered by order of
  increasing ages.

For example, Names=c(noun1, noun2), in which case noun1 (respectively, noun2) corresponds to the subfolder name containing the BIN file of sample 1 (respectively of sample 2). In addition, if we know that sample 1 is younger than sample 2, then Names vector is correctly filled. If conversely, Names=c(noun2, noun1), the analysis performed by AgeS\_Computation would not be consistent.

#### \*\* How to fill the BinPerSample vector? \*\*

BinPerSample[i] correponds to the number of BIN files for the sample whose number ID is equal to i.

For example, let us consider a case with two samples (Sample1 and Sample2), with 2 BIN files for Sample1 and 1 for Sample2. In this case, Nb\_binfile=3 and Nb\_sample=2. The user may then set Names=c("Sample1-File1", "Sample1-File2", "Sample2-File1"), in which case "Sample1-1" is the name of the subfolder containing the first BIN file for Sample1, "Sample1-File2" the name of the subfolder for the second BIN file of Sample1; eventually, "Sample2-1" is the name of the subfolder containing the BIN file for the second sample. In this case, BinPerSample=c(2,1).

For the general BIN-file structure, the reader is referred to the following website: http://www.nutech.dtu.dk/ The function read\_BIN2R developed in Luminescence package is used to read the BIN files.

### Value

A list containing the following objects:

- LT (one list per sample); each list contains all L/T values for the corresponding sample;
- **sLT** (one list per sample); each list contains all uncertainties on L/T values for the corresponding sample;
- **ITimes** (one list per sample); each list contains irradiation time values for the corresponding sample;

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- dLab, a matrix containing in line i, the laboratory dose rate and its variance for sample i;
- **ddot\_env**, a matrix containing in line i, the environmental dose rate and its variance (excluding the common error terms) for sample i;
- regDose (one list per sample); each list contains all regenerated doses;
- J, a vector giving, for each BIN file, the number of aliquots selected for the analysis;
- **K**, a vector giving, for each BIN file, the number of regenerative doses in the SAR protocol;
- **Nb\_measurement**, a vector giving, for each BIN file, the number of measurements;

#### Author(s)

Claire Christophe, Guillaume Guerin

#### See Also

```
read_BIN2R, Concat_DataFile, LT_RegenDose
```

### **Examples**

```
## 1) Example for one sample with one Bin File
## give the name of the path to data folder
# Path=c("inst/extdata/")
## give the name of the folder datat
# Names=c("GDB3")
## give the number of sample
# Nb_sample=1
# DATA=Generate_DataFile(Path,Names,Nb_sample)
# str(DATA)
## 2) Example for 2 samples and one Bin file each
## give the name of the path to data folder
# Path=c("inst/extdata/")
## give the name of the folder datat
# Names=c("GDB5","GDB3")
## give the number of sample
# Nb_sample=2
# DATA=Generate_DataFile(Path,Names,Nb_sample)
# str(DATA)
```

LT\_RegenDose

Plots L/T as a function of regenerative dose

### **Description**

This function plots L/T values as a function of Regenerative Dose, for every selected aliquot.

```
LT_RegenDose(DATA, Path, Names, BinPerSample = rep(1), SampleNumber = 1,
    sepDP = c(","))
```

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### **Arguments**

| DATA         | list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function Generate_DataFile. DATA can contain information from more than one sample.                        |
|--------------|---|
| Path         | character: path to the project folder (the same as the one used in Generate_DataFile to provide DATA)   |
| Names        | character vector: list of names of the sub-folders containing the BIN files, which were used by Generate_DataFile to generate the DATA object.  |
| BinPerSample | integer vector (with default): vector with the number of BIN files per sample, which was used in Generate_DataFile to generate the DATA object.   |
| SampleNumber | integer(with default): ID number (in [1,Nb_sample]) of the sample selected for plotting L/T as a function of regenerative doses. Required if the DATA object contains information for more than one sample. |

# **Details**

sepDP

To fill Names and BinPerSample, we refer to the detail section from the Generate\_DataFile function.

character(with default): column separator in the DiscPose.csv file.

### Value

L/T plots; there are as many plots as selected aliquots in the DiscPos.csv file. There are 9 plots per page. There is not interpolation.

# Author(s)

Claire Christophe, Guillaume Guerin

#### See Also

```
Generate_DataFile
```

#### **Examples**

```
## load data file generated by the function Generate_DataFile
# data(DATA1,envir = environment())
# LT_RegenDose(DATA1,Path=c('inst/extdata/'),Names=c("GDB3"))
```

MCMCsample

MCMC sample from the posterior distribution of the dataset GDB5

# Description

MCMC samples from the posterior distribution of "A" for age, "D" for palaeodose and "sD" for dispersion of equivalent doses around "D", of the data set GDB5.

```
data("MCMCsample")
```

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#### **Format**

It is a matric with 6000 row and tree column.

- A The first column of the matrice are sampled from the posterior distribution of the paramete A
- D The first column of the matrice are sampled from the posterior distribution of the paramete D
- sD The first column of the matrice are sampled from the posterior distribution of the paramete sD

#### **Details**

A FAIRE

#### **Source**

A FAIRE

#### References

A FAIRE

### **Examples**

```
data(MCMCsample)
## maybe str(MCMCsample); plot(MCMCsample[,1],type="l") ...
```

MCMC\_plot

MCMC trajectories and posterior distributions plot

### **Description**

This function uses the ouput of coda.samples to plot the trajectories of MCMC and densities of the posterior distributions of the age - if it is calculated, palaeodose and equivalent dose dispersion parameters of the sample. This function is used in the function Age\_Computation.

### Usage

```
MCMC_plot(sample, size, SampleNames, Nb_sample = 1, Nb_chaines = 3,
value = c(0, Nb_sample, 2 * Nb_sample), nom = c("A", "D", "sD"))
```

### **Arguments**

sample MCMC.list: this is generated by jags.model in Age\_Computation.

size integer: length of each chain.

SampleNames character vector: names of the samples, used in the figure titles.

Nb\_sample integer (with default): number of analysed samples.

Nb\_chaines integer (with default): number of independent chains for the model (for more

informations, see jags.model).

value integer vector (with default): position idex used to select age (if available),

palaeodose and equivalent dose dispersion parameters for the first sample.

nom character vector (with default): names of the selected parameters with value A

for age (if available), D for palaeodose and sD for equivalent dose dispersion.

#### Value

A pdf file with the MCMC trajectories and posterior distributions for each parameter defined in nom. There is one page per sample, which is divided by length(nom) vertically and by 2 horizontally. The first line of the figure correponds to the first parameter defined in nom, and so on. On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distributions of the parameter.

#### Author(s)

Claire Christophe, Guillaume Guerin

#### See Also

Age\_Computation, coda.samples and rjags packages.

# **Examples**

```
data(MCMCsample,envir = environment())
MCMC_plot(MCMCsample,2000,SampleNames="GDB3",Nb_sample=1,Nb_chaines=3)
```

PalaeodoseComputation Bayesian analysis for the palaeodose estimation of various samples

# Description

This function computes the palaeodose of one or various samples according to the model developed in Combes et al (2015), based on an output of the Generate\_DataFile function. Samples, for which data is available in several BIN files, can be analysed.

#### Usage

```
PalaeodoseComputation(DATA, Nb_sample, BinPerSample = rep(1, Nb_sample), SampleNames, SavePdf = FALSE, OutputFileName = c("MCMCplot", "summary"), OutputFilePath = c(""), SaveEstimates = FALSE, OutputTableName = c("DATA"), OutputTablePath = c(""), LIN_fit = TRUE, Origin_fit = FALSE, distribution = c("cauchy"), Taille = 50000, t = 5, Nb_chaines = 3)
```

#### **Arguments**

| DATA         | list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function Generate_DataFile. DATA contains information for more than one sample.   |
|--------------|--|
| Nb_sample    | integer ( <b>required</b> ): number of samples, Nb_sampe>1.  |
| BinPerSample | integer vector (with default): vector with the number of BIN files per sample. The length of this vector is equal to Nb_sample. BinPerSample[i] correponds to the number of BIN files for the sample whose number ID is equal to i. For more information to fill this vector, we refer to detatils in Generate_DataFile. |
| SampleNames  | character vector; names of sample. The length of this vector is equal to Nb. sample.   |

| SavePdf         | boolean (with default): if TRUE save graph in pdf file named ${\tt OutputFileName}$ in folder ${\tt OutputFilePath}.$  |
|-----------------|--|
| OutputFileName  | character (with default): name of the pdf files that will be generated by the function.  |
| OutputFilePath  | character (with default): path to the pdf files that will be generated by the function. $ \\$  |
| SaveEstimates   | boolean (with default): if TRUE save Bayes estimates and confidence interval at level 68 in a csv table named OutputFileName in folder OutputFilePath.   |
| OutputTableName |  |
|                 | character (with default): name of the table that will be generated by the function if $SaveEstimates=TRUE$ .   |
| OutputTablePath | l  |
|                 | character (with default): path to the table that will be generated by the function if $SaveEstimates=TRUE$ .   |
| LIN_fit         | logical (with default): if TRUE (default) allows a linear component, on top of the (default) saturating exponential curve, for the fitting of dose response curves. Please see details for more informations on the proposed dose response curves. |
| Origin_fit      | logical (with default): if TRUE, forces the dose response curves to pass through the origin. Please see details for more informations on the proposed growth curves.   |
| distribution    | character (with default): type of distribution that defines how individual equivalent dose values are distributed around the palaeodose. Allowed inputs are "cauchy", "gaussian" and "lognormal".  |
| Taille          | integer (with default): number of iterations for the MCMC computation (for more information see ${\tt jags.model}$ ).  |
| t               | integer (with default): 1 every t iterations of the MCMC is considered for sampling the posterior distribution (for more information see $jags.model$ ).   |
| Nb_chaines      | integer (with default): number of independent chains for the model (for more information see ${\tt jags.model}$ ).   |
|                 |  |

# **Details**

As for Age\_Computation and AgeS\_Computation, the user can choose from 4 dose response curves:

• Saturating exponential plus linear growth (AgeMultiBF\_EXPLIN):

for all x in IR+, f(x)=a(1-exp(-x/b))+cx+d; select

- LIN\_fit=TRUE
- Origin\_fit=FALSE
- **Saturating exponential growth** (AgeMultiBF\_EXP):

for all x in IR+, f(x)=a(1-exp(-x/b))+d; select

- LIN\_fit=FALSE
- Origin\_fit=FALSE
- $\bullet \ \ \textbf{Saturating exponential plus linear growth and fitting through the origin} \ (\texttt{AgeMultiBF\_EXPLINZO}):$

for all x in IR+, f(x)=a(1-exp(-x/b))+cx; select

- LIN\_fit=TRUE
- Origin\_fit=TRUE

• Saturating exponential growth and fitting through the origin (AgeMultiBF\_EXPZO):

for all x in IR+, f(x)=a(1-exp(-x/b)); select

- LIN\_fit=FALSE
- Origin\_fit=TRUE

#### Value

#### 1- NUMERICAL OUTPUT

# A list containing the following objects:

- **Sampling** that corresponds to a sample of the posterior distributions of palaeodose and equivalent dose dispersion parameters.
- Model\_GrowthCurve, stating which dose response fitting option was chosen;
- **Distribution**, stating which distribution was chosen to model the dispersion of individual equivalent dose values around the palaeodose of the sample;
- PriorAge, stating the priors used for the age parameter.

#### The Gelman and Rudin test of convergency

Prints the result of the Gelman and Rudin test of convergency for palaeodose and equivalent dose dispersion parameters for each sample. A result close to one is expected.

In addition, the user must visually assess the convergency of the trajectories by looking at the pdf file generated by the function (see 2- for more informations).

If both convergencies (Gelman and Rudin test and plot checking) are satisfactory, the user can consider the printed estimates as valid. Otherwise, the user may try increasing the number of MCMC interations (Taille) to reach convergency.

#### Credible intervals and Bayes estimates

Prints the Bayes esitmates, the credible intervals at level 95% and 68% for the palaeodose and equivalent dose dispersion parameters for each sample.

#### 2- PLOT OUTPUT

# MCMC trajectories

A pdf file with the MCMC trajectories and posterior distributions of the palaeodose and equivalent dose dispersion parameters. There is one page per sample.

The first line of the figure correponds to the palaeodose parameter and the second to the equivalent dose dispersion parameter. On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distribution of the parameter.

#### Author(s)

Claire Christophe, Guillaume Guerin

# References

Combes, B., Philippe, A., Lanos, P., Mercier, N., Tribolo, C., Guerin, G., Guibert, P., Lahaye, C., 2015. A Bayesian central equivalent dose model for optically stimulated luminescence dating. Quaternary Geochronology 28, 62-70. doi:10.1016/j.quageo.2015.04.001

# See Also

Generate\_DataFile, rjags package, MCMC\_plot, Age\_Computation, SCMatrix

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### **Examples**

```
## Load data
# data(DATA1,envir = environment())
## Palaeodose computation of samples GDB3
# P=PalaeodoseComputation(DATA1,Nb_sample=1,SampleNames=c("GDB5"),Taille=1000)
```

SCMatrix

Definition of the stratigraphic constraint matrix

# Description

This function helps to define the stratigraphic relation between samples, with questions. The output of this function can be used in function AgeS\_Computation.

#### Usage

```
SCMatrix(Nb_sample, Names)
```

# Arguments

Nb\_sample interger: the sample number.

Names charcater vector: sample names.

#### Value

A Matrix that summarise the ordered relation between samples. This matrix can be intergrate in AgeS\_Computation function. We refer to detail on AgeS\_Computation for more information concerning this matrix.

# Author(s)

Claire Christophe, Guillaume Guerin

#### See Also

```
AgeS_Computation
```

### **Examples**

```
## Assume that "sample1" is younger than "sample2"
# SCMatrix(2,c("sample1","sample2"))
# 1
```

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