Package 'BayLum'

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Type Package

Title Chronological Bayesian Models Integrating Optically Stimulated
Luminescence and Radiocarbon Age Dating

Description Bayesian analysis of luminescence data and C-14 age estimates. Bayesian models are based on the following publications: Combes, B. & Philippe, A. (2017) <doi:10.1016/j.quageo.2017.02.003> and Combes et al (2015) <doi:10.1016/j.quageo.2017.02.003> and Combes et al (2015) <doi:10.1016/j.quageo.2017.02.003> and Combes et al (2015) <doi:10.1016/j.q cludes, amongst others, data import, export, application of age models and palaeodose model.

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utils,
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Imports methods,
hexbin (>= 1.28.3),
cli (>= 3.6.1),
KernSmooth (>= 2.23),
rjags (>= 4-13),
runjags (>= 2.2.1),
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yaml (>= 2.3.7)

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Contents

BayLum-package	*Chronological Bayesian Models Integrating Optically Stimulated Luminescence and C-14 Dating*

Description

A collection of various R functions for Bayesian analysis of luminescence data and C-14 age estimates. This includes, amongst others, data import, export, application of age and palaeodose models.

Details

This package is based on the functions: Generate_DataFile and Generate_DataFile_MG to import luminescence data. These functions create a list containing all informations to compute age of single-grain OSL measurements for the first function and multi-grain OSL measurements for the second.

The functions: Age_Computation and AgeS_Computation use Bayesian analysis for OSL age estimation for one or various samples according to difference models (e.g. different dose-response curves and different equivalent dose distributions around the palaeodose).

It is possible to consider various BIN/BINX-files per sample, to compute ages of samples in stratigraphic constraints and to integrate systematic errors.

It is possible to calibrate C-14 age with the function AgeC14_Computation. We can also estimate chronology containing 14C age and OSL samples with the function Age_OSLC14.

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References

Philippe, A., Guérin, G., Kreutzer, S., 2019. BayLum - An R package for Bayesian analysis of OSL ages: An introduction. Quaternary Geochronology 49, 16–24. doi:10.1016/j.quageo.2018.05.009

See Also

Useful links:

- https://CRAN.r-project.org/package=BayLum
- Report bugs at https://github.com/crp2a/BayLum/issues

AgeC14_Computation   *Bayesian analysis for C-14 age estimations of various samples*

Description

This function calibrates the C-14 age of samples to get an age (in ka). The user can choose one of the following radiocarbon calibration curve: Northern or Southern Hemisphere or marine atmospheric. It must be the same curve for all samples.

Usage

```
AgeC14_Computation(
  Data_C14Cal,
  Data_SigmaC14Cal,
  SampleNames,
  Nb_sample,
  PriorAge = rep(c(10, 50), Nb_sample),
  SavePdf = FALSE,
  OutputFileName = c("MCMCplot", "HPD_CalC-14Curve", "summary"),
  OutputFilePath = c(""),
  SaveEstimates = FALSE,
  OutputTableName = c("DATA"),
  OutputTablePath = c(""),
  StratiConstraints = c(),
  sepSC = c(","),
  Model = c("full"),
  CalibrationCurve = c("IntCal20"),
  Iter = 50000,
  t = 5,
  n.chains = 3,
  quiet = FALSE,
  roundingOfValue = 3
)
```

Arguments

Data_C14Cal	numeric (**required**): corresponding to C-14 age estimate.
Data_SigmaC14Cal	
	numeric (**required**): corresponding to the error of C-14 age estimates.
SampleNames	character (**required**): names of sample. The length of this vector is equal to Nb_sample.
Nb_sample	integer: number of samples.
PriorAge	numeric (with default): lower and upper bounds for age parameter of each sample in years (not in ka). Note that, length(PriorAge) == 2 * Nb_sample and PriorAge[2i-1,2i] corresponds to the lower and upper bounds of sample whose number ID is equal to i.
SavePdf	logical (with default): if TRUE save graphs 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 SavePd=TRUE, length(OutputFileName) = =3, see **PLOT OUTPUT** in **Value** section for more informations.

OutputFilePath   character (with default): path to the pdf file that will be generated by the function if SavePdf=TRUE. If it is not equal to "", it must be terminated by "/".

SaveEstimates   logical (with default): if TRUE save Bayes' estimates, credible interval at level 68% and 95% and the result of the Gelman and Rubin test of convergence, in a csv table named OutputFileName in folder OutputFilePath.

OutputTableName

   logical (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. If it is not equal to "", it must be terminated by "/".

StratiConstraints

   numeric matrix or character(with default): input object for the stratigraphic relation between samples. If there is stratigraphic relation between samples see the details section for instructions regarding how to correctly fill StratiConstraints; the user can refer to a matrix (numeric matrix) or to a csv file (character). If there is no stratigraphic relation default value is suitable.

sepSC   character (with default): if StratiConstraints is character, indicate column separator in StratiConstraints csv file.

Model   character (with default): if **"full"**, error on estimate calibration curve is taken account. If **"naive"** this error is not taken account in the age estimate.

CalibrationCurve

   character (with default): calibration curve chosen. Allowed inputs are

   - **"Intcal13"** or **"Intcal13"** for Northern Hemisphere atmospheric radiocarbon calibration curve,
   - **"Marine13"** or **"Marine13"** for Marine radiocarbon calibration curve,
   - **"SHCal13"** or **"SHCal20"** for Southern Hemisphere atmospheric radiocarbon calibration curve
   - **a csv file, with tree columns, the first column is dedicated to** "Cal.BP"**, the second to** "XC-14.age"**, the third to** "Error"**. The decimal of this file must be a dot, and the separator must be a comma.**

Iter   integer (with default): number of iterations for the MCMC computation (for more information see rjags::jags.model).

t   integer (with default): 1 every t iterations of the MCMC is considered for sampling the posterior distribution (for more information see rjags::jags.model.

n.chains   integer (with default): number of independent chains for the model (for more information see rjags::jags.model.

quiet   logical (with default): enables/disables rjags messages

roundingOfValue

   integer (with default): Integer indicating the number of decimal places to be used, default set to 3.

Details

How to fill StratiConstraints**?**

If there is stratigraphic relations between samples, *C-14 age in* `Data_C14Cal` *must be ordered by order of increasing ages*.

The user can fill the `StratiConstraints` matrix as follow.

1. **Size of the matrix**: row number of `StratiConstraints` matrix is equal to `Nb_sample+1`, and column number is equal to `Nb_sample`.

2. **First line of the matrix**: for all `i` in `{1,...,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.

3. **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+1,1:Nb_sample}` is a upper triangular matrix.

The user can also use SCMatrix or SC_Ordered (if all samples are ordered) functions to construct the `StratiConstraints` matrix.

The user can also refer to a .csv file that contains the relation between samples as defined above. The user must take care about the separator used in the csv file using the argument `sepSC`.

** More precision on `Model` **

We propose two models "full" or "naive". If `Model = 'full'` that means measurement error and error on calibration curve are taken account in the Bayesian model; if `Model = "naive"` that means only error on measurement are taken account in the mode.

More precisely, the model considered here, as the one developed by Christen, JA (1994), assume multiplicative effect of errors to address the problem of outliers. In addition, to not penalise variables that are not outliers and damage theirs estimation, we introduce a structure of mixture, that means only variable that are considered as outlier have in addition a multiplicative error.

Value

NUMERICAL OUTPUT

1. **A list containing the following objects:**
   - **Sampling**: that corresponds to a sample of the posterior distributions of the age parameters;
   - **Outlier**: stating the names of samples that are considered as outliers;
   - **Model**: stating which model was chosen (″full″ or ″naive″);
   - **CalibrationCurve**: stating which radiocarbon calibration curve was chosen;
   - **PriorAge**: stating the priors used for the age parameter;
   - **StratiConstraints**: stating the stratigraphic relations between samples considered in the model.

2. **The Gelman and Rubin test of convergency**: print the result of the Gelman and Rubin test of convergence for the age estimate for each sample. A result close to one is expected.
   In addition, the user must visually assess the convergence of the trajectories by looking at the graph generated by the function (see **PLOT OUTPUT** for more informations).
   If both convergences (Gelman and Rubin test and plot checking) are satisfactory, the user can consider the estimates as valid. Otherwise, the user may try increasing the number of MCMC iterations (`Iter`) or being more precise if it is possible on the `PriorAge` parameter to reach convergence.

3. **Credible intervals and Bayes estimates**: prints the Bayes' estimates, the credible intervals at 95% and 68% for the age parameters for each sample.

PLOT OUTPUT

1. **MCMC trajectories**: A graph with the MCMC trajectories and posterior distributions of the age parameter is displayed.
   On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distribution of the parameter.

2. **Summary of sample age estimates**: plot credible intervals and Bayes' estimate of each sample age on one graph.

To give the results in a publication, we recommend to give the Bayes' estimate of the parameters as well as the credible interval at 95% or 68%.

How to cite

Christophe, C., Philippe, A., Guérin, G., Kreutzer, S., 2024. AgeC14_Computation(): Bayesian analysis for C-14 age estimations of various samples. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

Please note that the initial values for all MCMC are currently all the same for all chains since we rely on the automatic initial value generation of JAGS. This is not optimal and will be changed in future. However, it does not affect the quality of the age estimates if the chains have converged.

Author(s)

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References

Christen, JA (1994). Summarizing a set of radiocarbon determinations: a robust approach. Applied Statistics, 489-503.

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B, Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Hogg AG, Hua Q, Blackwell PG, Niu M, Buck CE, Guilderson TP, Heaton TJ, Palmer JG, Reimer PJ, Reimer RW, Turney CSM, Zimmerman SRH. 2013. SHCal13 Southern Hemisphere calibration, 0-50000 years cal. BP Radiocarbon 55(4):1889-1903

See Also

rjags, plot_MCMC, SCMatrix, plot_Ages

Examples

```
## Load data
data(DATA_C14,envir = environment())
C14Cal <- DATA_C14$C14[,1]
SigmaC14Cal <- DATA_C14$C14[,2]
Names <- DATA_C14$Names
nb_sample <- length(Names)

## Age computation of samples without stratigraphic relations
Age <- AgeC14_Computation(
 Data_C14Cal = C14Cal,
 Data_SigmaC14Cal = SigmaC14Cal,
 SampleNames = Names,
 Nb_sample = nb_sample,
 PriorAge = rep(c(20,60),nb_sample),
 Iter = 500,
 quiet = TRUE,
 roundingOfValue = 3)
```

AgeS   *Output of* `AgeS_Computation` *function for the samples: "GDB5" and "GDB3"*

Description

Output of `AgeS_Computation` function for the samples: "GDB5" and "GDB3", there is no stratigraphic relation neither systematic errors.

Usage

```
data("AgeS")
```

Format

A list containing

Sampling MCMC.list that corresponds to a sample of the posterior distributions of the ages (in ka), palaeodoses (in Gy) and equivalent dose dispersions (in Gy) parameters of samples "GDB5" and "GDB3";

Model_GrowthCurve stating which dose response fitting option was chosen to run the function

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 (in ka);

StratiConstraints stating the matrix of stratigraphic relations between samples considered in the model;

CovarianceMatrix stating the covariance matrix of error used in the model, highlighting not common errors between samples in our cases (diagonal matrix).

References

Tribolo, C., Asrat, A., Bahain, J. J., Chapon, C., Douville, E., Fragnol, C., Hernandez, M., Hovers, E., Leplongeon, A., Martin, L, Pleurdeau, D, Pearson, O , Puaud, S, Assefa, Z. (2017). Across the Gap: Geochronological and Sedimentological Analyses from the Late Pleistocene-Holocene Sequence of Goda Buticha, Southeastern Ethiopia. PloS one, 12(1), e0169418.

Examples

```
data(AgeS)
str(AgeS)
```

AgeS_Computation   *Bayesian analysis for OSL age estimation of various samples*

Description

This function computes the age (in ka) of at least two samples according to the model developed in Combès and Philippe (2017), based on outputs of Generate_DataFile or Generate_DataFile_MG or both of them using combine_DataFiles.
Samples, for which data is available in several BIN files, can be analysed.
Single-grain or Multi-grain OSL measurements can be analysed simultaneously.

Usage

```
AgeS_Computation(
  DATA,
  SampleNames = DATA$SampleNames,
  Nb_sample = DATA$Nb_sample,
  PriorAge = rep(c(0.01, 100), Nb_sample),
  BinPerSample = rep(1, Nb_sample),
  SavePdf = FALSE,
  OutputFileName = c("MCMCplot", "summary"),
  OutputFilePath = c(""),
  SaveEstimates = FALSE,
  OutputTableName = c("DATA"),
  OutputTablePath = c(""),
  THETA = c(),
  sepTHETA = c(","),
  StratiConstraints = c(),
  sepSC = c(","),
  LIN_fit = TRUE,
  Origin_fit = FALSE,
  distribution = c("cauchy"),
  model = NULL,
  Iter = 10000,
  burnin = 4000,
  adapt = 1000,
  t = 5,
  n.chains = 3,
  jags_method = "rjags",
  autorun = FALSE,
```

```
    quiet = FALSE,
    roundingOfValue = 3,
    ...
)
```

Arguments

DATA
(**required**) Two inputs are possible: (1): DATA list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function Generate_DataFile, Generate_DataFile_MG or combine_DataFiles. DATA contains informations for more than one sample. If there is stratigraphic relations between samples, informations in DATA must be ordered by order of increasing ages. See the details section to for more informations. (2): An object of class BayLum.list which is provided by the output of AgeS_Computation. When input of class BayLum.list is identified, no new JAGS model is created. Instead, the JAGS model specified by the AgeS_Computation output is extended. Useful for when convergence was not originally achieved and a complete restart is not desirable.

SampleNames
character vector: names of samples. The length of this vector is equal to Nb_sample.

Nb_sample
integer: number of samples, Nb_sample>1.

PriorAge
numeric vector (with default): lower and upper bounds for age parameter of each sample (in ka). Note that, length(PriorAge)=2*Nb_sample and PriorAge[2i-1,2i] corresponds to the lower and upper bounds of sample whose number ID is equal to i.

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] corresponds 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 details in Generate_DataFile or in Generate_DataFile_MG.

SavePdf
logical (with default): if TRUE save graphs 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; length(OutputFileName)=2, see **PLOT OUTPUT** in **Value** section for more informations.

OutputFilePath
character (with default): path to the pdf file that will be generated by the function if SavePdf=TRUE. If it is not equal to "", it must be terminated by "/".

SaveEstimates
logical (with default): if TRUE save Bayes' estimates, credible interval at level 68% and 95% and the result of the Gelman en Rubin test of convergence, 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. If it is not equal to "", it must be terminated by "/".

THETA
numeric matrix or character (with default): input object for systematic and individual error. If systematic errors are considered, see the details section for instructions regarding how to correctly fill THETA; the user can refer to a matrix (numeric matrix) or to a csv file (character). Otherwise, default value is suitable, and only individual errors are considered.

sepTHETA	character (with default): if THETA is character, indicate column separator in THETA CSV-file.
StratiConstraints	numeric matrix or character(with default): input object for the stratigraphic relation between samples. If there is stratigraphic relation between samples see the details section for instructions regarding how to correctly fill StratiConstraints; the user can refer to a matrix (numeric matrix) or to a csv file (character). If there is no stratigraphic relation 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. See details section 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. See details section 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″, ″lognormal_A″ and ″lognormal_M″, see details section for more informations.
model	character (*optional*): allows to provide a custom model to the function as text string. Please note that if this option is chosen the parameter distribution is ignored and no safety net is applied. If the function crashes it is up to the user.
Iter	integer (with default): the number of iterations to run which will be used to assess convergence and ages (see runjags::run.jags).
burnin	integer (with default): the number of iterations used to "home in" on the stationary posterior distribution. These are not used for assessing convergence (see runjags::run.jags).
adapt	integer (with default): the number of iterations used in the adaptive phase of the simulation (see runjags::run.jags).
t	integer (with default): 1 every t iterations of the MCMC is considered for sampling the posterior distribution. (for more information see runjags::run.jags).
n.chains	integer (with default): number of independent chains for the model (for more information see runjags::run.jags).
jags_method	character (with default): select which method to use in order to call JAGS. jags_methods ″rjags″ (the default) and ″rjparallel″ have been tested. (for more information about these possibilities and others, see runjags::run.jags)
autorun	logical (with default): choose to automate JAGS processing. JAGS model will be automatically extended until convergence is reached (for more information see runjags::autorun.jags).
quiet	logical (with default): enables/disables rjags messages
roundingOfValue	integer (with default): Integer indicating the number of decimal places to be used, default = 3.
...	further arguments that can be passed to control the Bayesian process. 1) When creating a new JAGS model, see details for supported arguments. 2) If extending a JAGS model see arguments of runjags::extend.JAGS.

Details

Supported ... arguments

ARGUMENT	INPUT	METHOD	DEFAULT	DESCRIPTION
max.time	character	rjparallel	Inf	maximum allowed processing time, e.g., 10m for 10 minutes (c
interactive	logical	rjparallel	FALSE	enable/disable interactive mode (cf. runjags::autorun.jags)
startburnin	integer	rjparallel	4000	number of burn-in iterations (cf. runjags::autorun.jags)
startsample	integer	rjparallel	10000	total number of samples to assess convergence (cf. runjags::au
inits	named list	rjparallel	NA	fine control over random seeds and random number generator

How to fill StratiConstraints

If there is stratigraphic relations between samples, *informations in DATA must be ordered by order of increasing ages*. To do this the user can either fill right Names in Generate_DataFile or in Generate_DataFile_MG (as it is indicated in Details section of these function), or ordered by order of increasing ages outputs of Generate_DataFile or Generate_DataFile_MG in combine_DataFiles

The user can fill the StratiConstraints matrix as follow.

1. **Size of the matrix**: row number of StratiConstraints matrix is equal to Nb_sample+1, and column number is equal to Nb_sample.

2. **First line of the matrix**: for all i in {1,...,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.

3. **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 or SC_Ordered (if all samples are ordered) functions to construct the StratiConstraints matrix.

The user can also refer to a csv file that contains the relation between samples as defined above. The user must take care about the separator used in the csv file using the argument sepSC.

How to fill THETA **covariance matrix concerning common and individual error?**

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

- row number of THETA is equal the column number, equal to Nb_sample.
- For all i in {1,...,Nb_sample}, THETA[i,i] contains individual error plus systematic error of the sample whose number ID is equal to i.
- For all i,j in {1,...,Nb_sample} and i different from j , THETA[i,j] contains 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 contains the errors as defined above.

Alternatively you can use the function create_ThetaMatrix.

Option on growth curves

As for `Age_Computation` and `Palaeodose_Computation`, the user can choose from 4 dose response curves:

- **Saturating exponential plus linear growth** (AgesMultiCS2_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** (AgesMultiCS2_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** (AgesMultiCS2_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** (AgesMultiCS2_EXPZO):
  for all x in IR+, f(x)=a(1-exp(-x/b)); select
  - `LIN_fit=FALSE`
  - `Origin_fit=TRUE`

Option on equivalent dose distribution around the palaeodose

The use can choose between :

- `cauchy`: a Cauchy distribution with location parameter equal to the palaeodose of the sample;
- `gaussian`: a Gaussian distribution with mean equal to the palaeodose of the sample;
- `lognormal_A`: a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample:
- `lognormal_M`: a log-normal distribution with **M**edian equal to the palaeodose of the sample.

Value

NUMERICAL OUTPUT

1. **A list of type** `BayLum.list` **containing the following objects:**
   - **Sampling**: that corresponds to a sample of the posterior distributions of the age (in ka), palaeodose (in Gy) and equivalent dose dispersion (in Gy) parameters for each sample;
   - **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 (in ka);
   - **StratiConstraints**: stating the stratigraphic relations between samples considered in the model;
   - **CovarianceMatrix**: stating the covariance matrix of error used in the model, highlighting common errors between samples or not.
   - **model**: returns the model that was used for the Bayesian modelling as a character
   - **JAGS model output**: returns the JAGS model with class "runjags".

2. **The Gelman and Rubin test of convergency**: prints the result of the Gelman and Rubin test of convergence 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 convergence of the trajectories by looking at the graph generated by the function (see **PLOT OUTPUT** for more informations).

   If both convergences (Gelman and Rubin test and plot checking) are satisfactory, the user can consider the estimates as valid. Otherwise, the user may try increasing the number of MCMC iterations (`Iter`) or being more precise on the `PriorAge` parameter (for example specify if it is a young sample `c(0.01,10)` an old sample `c(10,100)`), or changing the parameter `distribution` or the growth curve, to reach convergence.

3. **Credible intervals and Bayes estimates**: prints the Bayes estimates, the credible intervals at 95% and 68% for the age, palaeodose and equivalent dose dispersion parameters for each sample.

PLOT OUTPUT

1. **MCMC trajectories**: A graph with the MCMC trajectories and posterior distributions of the age, palaeodose and equivalent dose dispersion parameters is displayed, there is one page per sample.

   The first line of the figure corresponds 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.

2. **Summary of sample age estimates**: plot credible intervals and Bayes estimate of each sample age on a same graph.

To give the results in a publication, we recommend to give the Bayes' estimate of the parameters as well as the credible interval at 95% or 68%.

How to cite

Christophe, C., Philippe, A., Guérin, G., Kreutzer, S., 2024. AgeS_Computation(): Bayesian analysis for OSL age estimation of various samples. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

Please note that the initial values for all MCMC are currently all the same for all chains since we rely on the automatic initial value generation of JAGS. This is not optimal and will be changed in future. However, it does not affect the quality of the age estimates if the chains have converged.

Author(s)

Claire Christophe, Anne Philippe, Guillaume Guérin, Sebastian Kreutzer

References

Combes, Benoit and Philippe, Anne, 2017. Bayesian analysis of multiplicative Gaussian error for multiple ages estimation in optically stimulated luminescence dating. Quaternary Geochronology (39, 24-34)

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, Generate_DataFile_MG, rjags, plot_MCMC, SCMatrix, Age_Computation, Palaeo-dose_Computation, plot_Ages, create_ThetaMatrix, runjags

Examples

```
## Age computation of samples GDB5 and GDB3,
## load data
data(DATA2) # GD85
data(DATA1) # GD83

## produce DataFile
Data <- combine_DataFiles(DATA2, DATA1)

## without common error, assuming GDB5 age younger than GDB3 age
Nb_sample <- 2
SC <- matrix(
  data = c(1,1,0,1,0,0),
  ncol = 2,
  nrow = (Nb_sample+1),
  byrow = TRUE)

## Not run:
## run standard
Age <- AgeS_Computation(
  DATA = Data,
  Nb_sample = Nb_sample,
  SampleNames = c("GDB5","GDB3"),
  PriorAge = rep(c(1,100), 2),
  StratiConstraints = SC,
  Iter = 100,
  quiet = FALSE,
  jags_method = "rjags"
)

## extend model
Age_extended <- AgeS_Computation(
  DATA = Age,
  Nb_sample = Nb_sample,
  SampleNames = c("GDB5","GDB3"),
  PriorAge = rep(c(1,100), 2),
  StratiConstraints = SC,
  adapt = 0,
  burnin = 500,
  Iter = 1000,
  quiet = FALSE,
  jags_method = "rjags"
)

## autorun mode
Age <- AgeS_Computation(
  DATA = Data,
  Nb_sample = Nb_sample,
  SampleNames = c("GDB5","GDB3"),
  PriorAge = rep(c(1,100), 2),
  StratiConstraints = SC,
```

```
    Iter = 10000,
    quiet = FALSE,
    jags_method = "rjags",
    autorun = TRUE)

## parallel mode
Age <- AgeS_Computation(
  DATA = Data,
  Nb_sample = Nb_sample,
  SampleNames = c("GDB5","GDB3"),
  PriorAge = rep(c(1,100), 2),
  StratiConstraints = SC,
  Iter = 10000,
  quiet = FALSE,
  jags_method = "rjparallel")

## End(Not run)
```

Age_Computation   *Bayesian analysis for the OSL age estimation of one sample*

Description

This function computes the age (in ka) of a sample according to the model developed in Combes
and Philippe (2017), based on an output of Generate_DataFile or Generate_DataFile_MG.
A sample, for which data is available in several BIN files, can be analysed.

Usage

```
Age_Computation(
  DATA,
  SampleName = DATA$SampleNames[1],
  PriorAge = c(0.01, 100),
  BinPerSample = c(1),
  SavePdf = FALSE,
  OutputFileName = c("MCMCplot"),
  OutputFilePath = c(""),
  SaveEstimates = FALSE,
  OutputTableName = c("DATA"),
  OutputTablePath = c(""),
  LIN_fit = TRUE,
  Origin_fit = FALSE,
  distribution = c("cauchy"),
  I = 1,
  Iter = 50000,
  t = 5,
  n.chains = 3,
  quiet = FALSE,
  roundingOfValue = 3
)
```

Arguments

DATA	list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function Generate_DataFile or Generate_DataFile_MG. DATA can contain information for more than one sample.
SampleName	character: name of the sample.
PriorAge	numeric (with default): lower and upper bounds for the sample age parameter (in ka). Note that, length(PriorAge)=2.
BinPerSample	integer (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 or in Generate_DataFile_MG for generating the DATA object.
SavePdf	logical (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; length(OutputFileName = 2, see **PLOT OUTPUT** in **Value** section for more informations.
OutputFilePath	character (with default): path to the pdf file that will be generated by the function if SavePdf = TRUE. If it is not equal to "", it must be terminated by "/".
SaveEstimates	logical (with default): if TRUE save Bayes estimates and credible interval at level 68% and 95% and the result of the gelman en Rubin test of convergency, 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. If it is not equal to "", it must be terminated by "/".
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. See details section 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. See details section 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", "lognormal_A" and "lognormal_M", see details section for more informations.
I	integer (with default): if DATA contains data from more than one sample, I indicates the ID number of the sample to be analysed.
Iter	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).
n.chains	integer (with default): number of independent chains for the model (for more information see jags.model).
quiet	logical (with default): enables/disables rjags messages
roundingOfValue	integer (with default): Integer indicating the number of decimal places to be used, default = 3.

Details

Option on growth curves

As for AgeS_Computation and Palaeodose_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

Option on equivalent dose distribution around the palaeodose

The use can choose between :

- cauchy: a Cauchy distribution with location parameter equal to the palaeodose of the sample

- gaussian: a Gaussian distribution with mean equal to the palaeodose of the sample

- lognormal_A: a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample

- lognormal_M: a log-normal distribution with **M**edian equal to the palaeodose of the sample

Value

NUMERICAL OUTPUT

1. **A list containing the following objects**:
   - **Sampling** that corresponds to a sample of the posterior distributions of the age (in ka), palaeodose (in Gy) and equivalent dose dispersion (in Gy) 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 (in ka).

2. **The Gelman and Rubin test of convergency**: prints the result of the Gelman and Rubin 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 graph generated by the function (see **PLOT OUTPUT** for more informations).

   If both convergencies (Gelman and Rubin 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 (`Iter`), or being more precise on the `PriorAge` parameter (for example specify if it is a young sample `c(0.01,10)` an old sample `c(10,100)`), or changing the parameter `distribution` or the growth curve, to reach convergency.to reach convergency.

3. **Credible intervals and Bayes estimates**: prints the Bayes esitmates, the credible intervals at 95% and 68% for the age, palaeodose and equivalent dose dispersion parameters of the sample.

PLOT OUTPUT

A graph with the MCMC trajectories and posterior distributions of the age, palaeodose and equivalent dose dispersion parameters is displayed.

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.

To give the results in a publication, we recommend to give the Bayes estimate of the parameter as well as the credible interval at 95% or 68%.

How to cite

Christophe, C., Kreutzer, S., Philippe, A., Guérin, G., 2024. Age_Computation(): Bayesian analysis for the OSL age estimation of one sample. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

Please note that the initial values for all MCMC are currently all the same for all chains since we rely on the automatic initial value generation of JAGS. This is not optimal and will be changed in future. However, it does not affect the quality of the age estimates if the chains have converged.

Author(s)

Claire Christophe, Sebastian Kreutzer, Anne Philippe, Guillaume Guérin

References

Combes, Benoit and Philippe, Anne, 2017. Bayesian analysis of multiplicative Gaussian error for multiple ages estimation in optically stimulated luminescence dating. Quaternary Geochronology (39, 24-34)

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, Generate_DataFile_MG, rjags, plot_MCMC, AgeS_Computation, Palaeodose_Computation

Examples

```
## load data file generated by the function Generate_DataFile
data(DATA1,envir = environment())
priorage <- c(10,60) # GDB3 is an old sample
Age <- Age_Computation(
 DATA = DATA1,
 SampleName = "GDB3",
 PriorAge = priorage,
 Iter = 100,
 quiet = TRUE)
```

Age_OSLC14	*Bayesian analysis for age estimation of OSL measurements and C-14 ages of various samples*

Description

This function computes an age of OSL data consisting of at least two samples and calibrate C-14 ages of samples to get an age (in ka).

Ages of OSL data are computed according to the model given in Combes and Philippe (2017). Single-grain or Multi-grain OSL measurements can be analysed simultaneously (with output of Generate_DataFile or Generate_DataFile_MG or both of them using combine_DataFiles). Samples, for which data is available in several BIN files, can be analysed.

For C-14 data, the user can choose one of the following radiocarbon calibration curve: Northern or Southern Hemisphere or marine atmospheric.

Usage

```
Age_OSLC14(
  DATA,
  Data_C14Cal,
  Data_SigmaC14Cal,
  Nb_sample = DATA$Nb_sample,
  SampleNames = DATA$SampleNames,
  SampleNature,
  PriorAge = rep(c(10, 60), Nb_sample),
  SavePdf = FALSE,
  OutputFileName = c("MCMCplot", "HPD_Cal14CCurve", "summary"),
  OutputFilePath = c(""),
  SaveEstimates = FALSE,
  OutputTableName = c("DATA"),
  OutputTablePath = c(""),
  StratiConstraints = c(),
  sepSC = c(","),
  BinPerSample = rep(1, sum(SampleNature[1, ])),
  THETA = c(),
  sepTHETA = c(","),
  LIN_fit = TRUE,
  Origin_fit = FALSE,
  distribution = c("cauchy"),
```

```
    Model_C14 = c("full"),
    CalibrationCurve = c("IntCal20"),
    Iter = 10000,
    burnin = 4000,
    adapt = 1000,
    t = 5,
    n.chains = 3,
    jags_method = "rjags",
    autorun = FALSE,
    quiet = FALSE,
    roundingOfValue = 3,
    ...
)
```

Arguments

DATA   Two types of inputs are supported. (1): a list of objects: LT, sLT, ITimes,
                    dLab, ddot_env, regDose, J, K, Nb_measurement, provided by the function
                    Generate_DataFile, Generate_DataFile_MG or combine_DataFiles. DATA con-
                    tains information for more than one sample. If there is stratigraphic relations
                    between samples, informations in DATA must be ordered by order of increasing
                    ages. See the details section to for more informations. (2): an object of class
                    BayLum.list which is provided by the output of Age_OSLC14. When input
                    of class BayLum.list is identified, no new JAGS model is created. Instead, the
                    JAGS model specified within the BayLum.list is extended. Useful for when
                    convergence was not originally achieved and a complete restart is not desirable.

Data_C14Cal   numeric vector: corresponding to C-14 age estimate (in years, conversion in ka
                    is automatically done in the function). If there is stratigraphic relations between
                    samples, Data_C14Cal must be ordered by order of increasing ages.

Data_SigmaC14Cal
                    numeric: corresponding to the error of C-14 age estimates.

Nb_sample   numeric: number of samples (OSL data and C-14 age), (Nb_sample>3, at least
                    to sample of OSL data and one sample of C-14 age).

SampleNames   character: sample names for both OSL data and C14 data. The length of this vec-
                    tor is equal to Nb_sample. If there is stratigraphic relation, this vector must be
                    ordered by increasing order (to mix OSL samples and C-14 ages if it is needed).

SampleNature   matrix: states the nature of the sample. Row number of SampleNature matrix
                    is equal to 2 and column number is equal to Nb_sample. First line of the matrix:
                    SampleNature[1,i] states if sample whose number ID is equal to i, is an OSL
                    sample 1 or not 0. Second line of the matrix: SampleNature[2,i] states if
                    sample whose number ID is equal to i, is an C-14 sample 1 or not '0.

PriorAge   numeric (with default): lower and upper bounds for age parameter of each sam-
                    ple **(in ka)**. Note that, length(PriorAge) = 2*Nb_sample sand PriorAge[2i-1,2i]
                    corresponds to the lower and upper bounds of sample whose number ID is equal
                    to i.

SavePdf   logical (with default): if TRUE save graphs 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, length(OutputFileName)=3, see **PLOT OUTPUT** in
                    Value section for more informations.

OutputFilePath   character (with default): path to the pdf file that will be generated by the function
                 if SavePdf=TRUE. If it is not equal to "", it must be terminated by "/".

SaveEstimates   logical (with default): if TRUE save Bayes' estimates, credible interval at level
                 68% and 95% and the result of the Gelman en Rubin test of convergence, 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. If it is not equal to "", it must be terminated by "/".

StratiConstraints
                 matrix or character (with default): input object for the stratigraphic relation be-
                 tween samples. If there is stratigraphic relation between samples see the details
                 section for instructions regarding how to correctly fill StratiConstraints, the
                 user can refer to a matrix or to a CSV-file character. Otherwise, default value is
                 suitable.

sepSC   character (with default): if StratiConstraints is character, indicate column
                 separator in StratiConstraints CSV-file.

BinPerSample   numeric (with default): vector with the number of BIN-files per OSL sample.
                 The length of this vector is equal to the number of OSL samples. BinPerSample[i]
                 corresponds 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 details in Gener-
                 ate_DataFile or in Generate_DataFile_MG.

THETA   numeric matrix or character (with default): input object for systematic and indi-
                 vidual error for OSL samples. If systematic errors are considered, see the details
                 section for instructions regarding how to correctly fill THETA; the user can refer
                 to a matrix (numeric matrix) or to a csv file (character). 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.

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, for
                 OSL samples. See details for more informations on the proposed dose response
                 curves.

Origin_fit   plogical (with default): if TRUE, forces the dose response curves to pass through
                 the origin. See details for more informations on the proposed growth curves, for
                 OSL samples.

distribution   character (with default): type of distribution that defines how individual equiv-
                 alent dose values are distributed around the palaeodose, for OSL samples. Al-
                 lowed inputs are "cauchy", "gaussian", "lognormal_A" and "lognormal_M",
                 see details for more informations.

Model_C14   character (with default): if "full", error on estimate calibration curve is taken
                 account, for C-14 samples. If "naive" this error is not taken account in the age
                 estimate.

CalibrationCurve
                 character (with default): calibration curve chosen, for C-14 samples. Allowed
                 inputs are

                    • **"Intcal13"** or **"Intcal13"** for Northern Hemisphere atmospheric radiocar-
                      bon calibration curve,

- **"Marine13"** or **"Marine13"** for Marine radiocarbon calibration curve,
- **"SHCal13"** or **"SHCal20"** for Southern Hemisphere atmospheric radio-carbon calibration curve
- **a csv file, with tree columns, the first column is dedicated to "Cal.BP", the second to "XC-14.age", the third to "Error". The decimal of this file must be a dot, and the separator must be a comma.**

Iter	[integer](with default): the number of iterations to run and who will be used to assess convergence and ages (see [runjags::run.jags]).
burnin	[integer](with default): the number of iterations used to "home in" on the stationary posterior distribution. These are not used for assessing convergence (see [runjags::run.jags]).
adapt	[integer](with default): the number of iterations used in the adaptive phase of the simulation (see [runjags::run.jags]).
t	[numeric](with default): 1 every t iterations of the MCMC is considered for sampling the posterior distribution (for more information see [rjags::jags.model].
n.chains	[numeric](with default): number of independent chains for the model (for more information see [rjags::jags.model]).
jags_method	[character](with default): select which method to use in order to call JAGS, supported are "rjags" (the default), rjparallel, simple, interruptible, parallel, and snow (for more information about each of these possibilities, see [runjags::run.jags])
autorun	[logical](with default): choose to automate JAGS processing. JAGS model will be automatically extended until convergence is reached (for more information see [runjags::autorun.jags]).
quiet	[logical](with default): enables/disables [rjags] messages
roundingOfValue	
	[integer](with default): Integer indicating the number of decimal places to be used, default = 3.
...	further arguments that can be passed to control the Bayesian process, see details for supported arguments

Details

Note that there are three types of arguments in the previous list. There are arguments for information concerning only OSL samples: DATA, BinPerSample, THETA, sepTHETA, LIN_fit, Origin_fit, distribution.

There are arguments for information concerning only C14 samples: Data_C14Cal, Data_SigmaC14Cal, Model_C14, CalibrationCurve.

There are arguments for information concerning all the samples: Nb_sample, SampleNames, SampleNature, PriorAge, SavePdf, OutputFileName, OutputFilePath, SaveEstimates, OutputTableName, OutputTablePath, StratiConstraints, sepSC.

Supported ... arguments

ARGUMENT	INPUT	METHOD	DEFAULT	DESCRIPTION
max.time	[character]	rjparallel	Inf	maximum allowed processing time, e.g., 10m for 10 minutes (c
interactive	[logical]	rjparallel	FALSE	enable/disable interactive mode (cf. [runjags::autorun.jags])
startburnin	[integer]	rjparallel	4000	number of burn-in iterations (cf. [runjags::autorun.jags])

| startsample | integer | rjparallel | 10000 | total number of samples to assess convergence (cf. runjags::au |
| inits | named list | rjparallel | NA | fine control over random seeds and random number generator |

How to fill 'StratiConstraints?

If there are stratigraphic relations between samples, **14C estimate age in** Data_C14Cal **must be ordered by order of increasing ages, as informations in** DATA. Names in SampleNames must be ordered and corresponds to the order in Data_C14Cal and in DATA, also if it is needed to mix names of OSL samples and 14C samples.

The user can fill the StratiConstraints matrix as follow.

1. **Size of the matrix**: row number of StratiConstraints matrix is equal to Nb_sample+1, and column number is equal to Nb_sample.

2. **First line of the matrix**: for all i in {1,...,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.

3. **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+1,1:Nb_sample} is a upper triangular matrix.

The user can also use SCMatrix or SC_Ordered (if all samples are ordered) function to construct the StratiConstraints matrix.

The user can also refer to a csv file that contains the relation between samples as defined above. The user must be careful about which separator is used in the csv file using the argument sepSC.

How to fill THETA **covariance matrix concerning common and individual error?**

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

- row number of THETA is equal the column number, equal to Nb_sample.

- For all i in {1,...,Nb_sample}, THETA[i,i] contains individual error plus systematic error of the sample whose number ID is equal to i.

- For all i,j in {1,...,Nb_sample} and i different from j , THETA[i,j] contains common error between samples whose number ID are equal to i and j.

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

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

Option on growth curves

As for Age_Computation and Palaeodose_Computation, the user can choose from 4 dose response curves:

- **Saturating exponential plus linear growth** (AgesMultiCS2_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** (AgesMultiCS2_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** (AgesMultiCS2_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** (AgesMultiCS2_EXPZO):

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

  - LIN_fit=FALSE
  - Origin_fit=TRUE

Option on equivalent dose distribution around the palaeodose

The use can choose between :

- cauchy: a Cauchy distribution with location parameter equal to the palaeodose of the sample
- gaussian: a Gaussian distribution with mean equal to the palaeodose of the sample
- lognormal_A: a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample
- lognormal_M: a log-normal distribution with **M**edian equal to the palaeodose of the sample

More precision on Model

We propose two models "full" or "naive". If Model='full' that means measurement error and error on calibration curve are taken account in the Bayesian model; if Model="naive" that means only error on measurement are taken account in the mode.

More precisely, the model considered here, as the one developed by Christen, JA (1994), assume multiplicative effect of errors to address the problem of outliers. In addition, to not penalise variables that are not outliers and damage theirs estimation, we introduce a structure of mixture, that means only variable that are considered as outlier have in addition a multiplicative error.

Value

NUMERICAL OUTPUT

1. **A list containing the following objects:**
   - **Sampling**: that corresponds to a sample of the posterior distributions of the age parameters (in ka for both C14 samples and OSL samples);
   - **PriorAge**: stating the priors used for the age parameter;
   - **StratiConstraints**: stating the stratigraphic relations between samples considered in the model;
   - **Model_OSL_GrowthCurve**: stating which dose response fitting option was chosen;
   - **Model_OSL_Distribution**: stating which distribution was chosen to model the dispersion of individual equivalent dose values around the palaeodose of the sample;
   - **Model_C14**: stating which model was chosen (″full″ or ″naive″);

- **CalibrationCurve**: stating which radiocarbon calibration curve was chosen;
- **Outlier**: stating the names of samples that must be outliers.

2. **The Gelman and Rubin test of convergency**: prints the result of the Gelman and Rubin test of convergence for the age estimate for each sample. A result close to one is expected.

   In addition, the user must visually assess the convergence of the trajectories by looking at the graph generated by the function (see **PLOT OUTPUT** for more informations).

   If both convergences (Gelman and Rubin test and plot checking) are satisfactory, the user can consider the estimates as valid. Otherwise, the user may try increasing the number of MCMC iterations (`Iter`) or be more precise on the `PriorAge` parameter to reach convergence.

3. **Credible intervals and Bayes estimates**: prints the Bayes' estimates, the credible intervals at 95% and 68% for the age parameters for each sample.

4. **JAGS model output**: returns the JAGS model with class "runjags".

PLOT OUTPUT

1. **MCMC trajectories**: A graph with the MCMC trajectories and posterior distributions of the age parameter is displayed.

   On each line, the plot on the left represents the MCMC trajectories, and the one on the right the posterior distribution of the parameter.

2. **Age estimate and HPD at 95% of 14C samples on calibration curve**: plot age estimate and HPD on calibration plot.

3. **Summary of sample age estimates**: plot credible intervals and Bayes estimate of each sample age on a same graph.

How to cite

Christophe, C., Philippe, A., Kreutzer, S., Baumgarten, F.H., 2024. Age_OSLC14(): Bayesian analysis for age estimation of OSL measurements and C-14 ages of various samples. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

Please note that the initial values for all MCMC are currently all the same for all chains since we rely on the automatic initial value generation of JAGS. This is not optimal and will be changed in future. However, it does not affect the quality of the age estimates if the chains have converged.

Author(s)

Claire Christophe, Anne Philippe, Guillaume Guerin, Sebastian Kreutzer, Frederik Harly Baumgarten

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B, Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Hogg AG, Hua Q, Blackwell PG, Niu M, Buck CE, Guilderson TP, Heaton TJ, Palmer JG, Reimer PJ, Reimer RW, Turney CSM, Zimmerman SRH. 2013. SHCal13 Southern Hemisphere calibration, 0-50000 years cal BP. Radiocarbon 55(4):1889-1903

See Also

runjags, plot_MCMC, SCMatrix, plot_Ages

Examples

```
## Load data
# OSL data
data(DATA1,envir = environment())
data(DATA2,envir = environment())
Data <- combine_DataFiles(DATA2,DATA1)

# 14C data
C14Cal <- DATA_C14$C14[1,1]
SigmaC14Cal <- DATA_C14$C14[1,2]
Names <- DATA_C14$Names[1]

# Prior Age
prior <- rep(c(1,60),3)
samplenature <- matrix(
 data = c(1,0,1,0,1,0),
 ncol = 3,
 nrow = 2,
 byrow = TRUE)

SC <- matrix(
 data = c(1,1,1,0,1,1,0,0,1,0,0,0),
 ncol = 3,
 nrow =4 ,
 byrow = TRUE)

## Age computation of samples
## Not run:
Age <- Age_OSLC14(
 DATA = Data,
 Data_C14Cal = C14Cal,
 Data_SigmaC14Cal = SigmaC14Cal,
 SampleNames = c("GDB5",Names,"GDB3"),
 Nb_sample = 3,
 SampleNature = samplenature,
 PriorAge = prior,
 StratiConstraints = SC,
 Iter = 20,
 burnin = 20,
 adapt = 20,
 n.chains = 2)

## End(Not run)
```

---

combine_DataFiles   *Combine objects*

Description

Combine objects generated by Generate_DataFile and Generate_DataFile_MG

Usage

```
combine_DataFiles(...)

Concat_DataFile(...)
```

Arguments

...   list objects generated by Generate_DataFile or Generate_DataFile_MG

Details

The function allows to combine data already generated by Generate_DataFile or Generate_DataFile_MG. The number of input objects is not limited and the function works similar to the standard base R function `c()`, but preserves the particular structure of the objects imported and generated by 'Bay-Lum'. The elements are combined by list element names.

Combining such data is rather useful in two scenarios:

- The data have been already imported and treated and then stored in RData-files. Using the function `combine_DataFiles()` will significantly speed up the processing time,
- simultaneous analysis of single and multi-grain OSL measurements.

Value

A nested list combining the input objects.

Function version

0.1.1

How to cite

Kreutzer, S., Christophe, C., 2024. combine_DataFiles(): Combine objects. Function version 0.1.1. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France), adapting the idea from the function 'Concat_DataFile()' by Claire Christophe.

See Also

Generate_DataFile, Generate_DataFile_MG

Examples

```
# load data files
data(DATA1,envir = environment())
data(DATA2,envir = environment())

#combine objects
DATA3 <- combine_DataFiles(DATA1, DATA2)
str(DATA3)
```

create_DataFile *Prepare input data for subsequent BayLum Analysis*

Description

The function pre-processes input data from BIN/BINX file, XSYG files or [RLum.Analysis](#) objects for `'BayLum'`. The parameters for the modelling are controlled by a to be supplied YAML configuration file (please read package vignette).

Usage

```
create_DataFile(config_file, verbose = TRUE)
```

Arguments

config_file [character](#) (**required**): path to YAML configuration file; alternatively the config_file can be a [list](#) similar to the R representation of the imported YAML file. This enables on-the fly modifications

verbose [logical](#) (*with default*): enable/disable terminal feedback

Details

The function uses a single configuration file based on the YAML format and operates in two modes:

(1) The YAML file contains the path to the files and the function attempts to import them. In such a case, all files must be thoroughly prepared (e.g., strictly follow the SAR protocol etc.).

(2) Alternatively, the YAML file contains no file paths but the data were imported and processed before `create_DataFile()` was called (recommended). Then the function is searching for objects with the sample name in the global environment. Example: `samp1 <- Luminescence::read_BIN2R(...)` with `samp1` the sample name as specified in the YAML file.

For more details, please see the package vignette.

Value

Returns a [list](#) that can be processed by the modelling functions of 'BayLum'

- **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;
- **SampleNames**, a character vector with the sample names;
- **Nb_sample**, the number of samples in the dataset

Function version

0.1.0

How to cite

Kreutzer, S., Christophe, C., 2024. create_DataFile(): Prepare input data for subsequent BayLum Analysis. Function version 0.1.0. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl University of Heidelberg (Germany), in parts based on code by Claire Christophe

See Also

write_YAMLConfigFile, yaml::read_yaml, Luminescence::read_BIN2R, Luminescence::read_XSYG2R, Luminescence::subset_SingleGrainData

Examples

```
##set path to YAML file
yaml_file <- system.file("extdata/example.yml", package = "BayLum")

samp1_file <- system.file("extdata/samp1/bin.bin", package = "BayLum")
samp2_file <- system.file("extdata/samp2/bin.bin", package = "BayLum")

## import BIN files
samp1 <- Luminescence::read_BIN2R(samp1_file, verbose = FALSE) |>
 subset(POSITION == 2 & GRAIN == 32)
samp2 <- Luminescence::read_BIN2R(samp2_file, verbose = FALSE) |>
 subset(POSITION == 2 & GRAIN == 32)

## create file
create_DataFile(yaml_file)
```

---

create_FolderTemplates

Create Folder Templates

Description

Create file and folder structure templates on the user hard drive as expected by Generate_DataFile and Generate_DataFile_MG. Files and data in the folders must then be overwritten manually with user data. The function intends to minimise the errors going along with the creation of these folder structures. The function uses the example data of BayLum to create the templates.

Usage

```
create_FolderTemplates(
  path,
  mode = "SG",
  n_folders = 1,
  names = paste("Sample_", 1:n_folders),
  verbose = TRUE
)
```

Arguments

path	character (**required**): path to the folder where the templates should be created
mode	character (*with default*): depending on the dataset you can create templates or single grain (SG) or multi-grain (MG) data
n_folders	numeric (*with default*): number of template folders to be created
names	character (*optional*): allows give own names to the subfolders.
verbose	logical (*with default*): enables/disables verbose mode

Value

If the templates were created successfully on the hard drive, the function returns nothing.

Function version

0.1.0

How to cite

Kreutzer, S., 2024. create_FolderTemplates(): Create Folder Templates. Function version 0.1.0. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Geography & Earth Sciences, Aberystwyth University (United Kingdom)

See Also

Generate_DataFile, Generate_DataFile_MG

Examples

```
create_FolderTemplates(tempdir())
```

---

create_ThetaMatrix   *Create Theta Matrix*

Description

Create the Θ matrix with the shared uncertainties that can used as input in, e.g., AgeS_Computation and Age_OSLC14 which is used for the covariance matrix Σ (Combès & Philippe, 2017)

Usage

```
create_ThetaMatrix(input, output_file = NULL, sigma_s, ...)
```

Arguments

input	character or data.frame (*optional*): input data frame or file connection to import a CSV-file with the needed information. If nothing is provided the function returns an input template. The argument output_file can be used to write this input template to the file system
output_file	character (optional): file path for the output CSV-file, the field separator is hard set to ",". Please use utils::write.table for more flexibility.
sigma_s	numeric (**required**): named character with values for systematic uncertainties. Those values are lab-specific. Can be set to NULL to remove systematic uncertainties. The order of the *named* vector is not important, but the naming! **Note**: some of the uncertainties have a unit, please check details.
...	further arguments that can be passed to utils::read.table (for the CSV-file import)

Details

The function intends to ease the creation of the $Theta$ matrix, which cannot be created straight forward, e.g., base R functions such as stats::cov. The relationship between the covariance matrix $Sigma$ and $Theta$ is given with

$$\Sigma_i j = A_i * A_j * \Theta_i j$$

For details see Combès & Philippe, 2017 and Guérin et al. (2021).

Input modes

The function supports two different operation modes:

1. input is left empty: the function returns a data.frame template that can be used as input (the option output_file works as well)

2. input is fed with a data.frame or a character (file path), the Θ matrix is returned

Input format

The function expects either a CSV-file or a data.frame as input. To create template you can run the function leaving the argument input empty (see example). Please note the format of the input table (data.frame) needs to kept as specified in the template.

The following table lists the meaning of the columns:

COLUMN	DESCRIPTION	UNIT

SAMPLE_ID	sample name	-
DR_BETA_K	standard error beta-dose rate K	Gy/ka
DR_BETA_U	standard error beta-dose rate U	Gy/ka
DR_BETA_Th	standard error beta-dose rate Th	Gy/ka
DR_GAMMA_K	standard error gamma-dose rate K	Gy/ka
DR_GAMMA_U	standard error gamma-dose rate U	Gy/ka
DR_GAMMA_Th	standard error gamma-dose rate Th	Gy/ka
DR_GAMMA_TOTAL	standard error total gamma-dose rate	Gy/ka
DR_TOTAL	total dose rate	Gy/ka
DR_TOTAL_X	standard error total dose rate	Gy/ka

Note: All columns can be set to 0 or NA *but no column must be left empty! If a value > 0 is provided for* DR_GAMMA_TOTAL *this value is taken and values in, e.g.,* DR_GAMMA_K *are discarded (set to 0)!*

Systematic uncertainties

The following table provides information on the named argument that can be provided via the argument sigma_s. Missing values are not allowed, all values must be set.

ARGUMENT	DESCRIPTION	UNIT
s_betaK	relative uncertainty K concentration	-
s_betaU	relative uncertainty U concentration	-
s_betaTh	relative uncertainty Th concentration	-
s_gammaK	relative uncertainty K concentration	-
s_gammaU	relative uncertainty U concentration	-
s_gammaTh	relative uncertainty Th concentration	-
s_gammaDR	relative uncertainty gamma-dose rate	-
s_CAL	relative uncertainty beta-source calibration	-
s_intDR	absolute uncertainty internal dose rate	Gy/ka

Value

A symmetric $Theta$ matrix or if input is missing, a data.frame with an input template

Function version

0.1.0

How to cite

Kreutzer, S., Guérin, G., 2024. create_ThetaMatrix(): Create Theta Matrix. Function version 0.1.0. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS-Université Bordeaux Montaigne (France), based on an 'MS Excel' sheet by Guillaume Guérin, IRAMAT-CRP2A, UMR 5060, CNRS-Université Bordeaux Montaigne (France)

References

Combès, B., Philippe, A., 2017. Bayesian analysis of individual and systematic multiplicative errors for estimating ages with stratigraphic constraints in optically stimulated luminescence dating. Quaternary Geochronology 39, 24–34. doi:10.1016/j.quageo.2017.02.003

Guérin, G., Lahaye, C., Heydari, M., Autzen, M., Buylaert, J.-P., Guibert, P., Jain, M., Kreutzer, S., Lebrun, B., Murray, A.S., Thomsen, K.J., Urbanova, P., Philippe, A., 2021. Towards an improvement of optically stimulated luminescence (OSL) age uncertainties: modelling OSL ages with systematic errors, stratigraphic constraints and radiocarbon ages using the R package BayLum. Geochronology 3, 229—245. doi:10.5194/gchron32292021

See Also

AgeS_Computation, Age_OSLC14, utils::read.table, utils::write.table

Examples

```
##(1) return template data.frame (no file output)
create_ThetaMatrix()

## Not run:
##(2) return template as data.frame + file
file_path <- tempfile(fileext = ".csv")
create_ThetaMatrix(output_file = file_path )

##NOT RUNNING EXAMPLE for sigma_s
calc_ThetaMatrix(...,
sigma_s =  c(
 s_betaK = 0.010,
 s_betaU = 0.007,
 s_betaTh = 0.006,
 s_gammaK = 0.010,
 s_gammaU = 0.007,
 s_gammaTh = 0.006,
 s_gammaDR = 0.05,
 s_CAL = 0.020,
 s_intDR = 0.030))


## End(Not run)
```

DATA1   *DATA of sample named GDB3*

Description

list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J,K,Nb_measurement obtained using Generate_DataFile function with single-grain OSL measurementsl of the sample GDB3.

Usage

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

Format

A list containing:

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;

References

For more informations on this sample we refer to the following publication:

Tribolo, C., Asrat, A., Bahain, J. J., Chapon, C., Douville, E., Fragnol, C., Hernandez, M., Hovers, E., Leplongeon, A., Martin, L, Pleurdeau, D, Pearson, O , Puaud, S, Assefa, Z. (2017). Across the Gap: Geochronological and Sedimentological Analyses from the Late Pleistocene-Holocene Sequence of Goda Buticha, Southeastern Ethiopia. PloS one, 12(1), e0169418.

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 with single-grain OSL measurementsl of the sample GDB5.

Usage

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

Format

A data frame containing:

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;

References

For more informations on this sample we refer to the following publication:

Tribolo, C., Asrat, A., Bahain, J. J., Chapon, C., Douville, E., Fragnol, C., Hernandez, M., Hovers, E., Leplongeon, A., Martin, L, Pleurdeau, D, Pearson, O , Puaud, S, Assefa, Z. (2017). Across the Gap: Geochronological and Sedimentological Analyses from the Late Pleistocene-Holocene Sequence of Goda Buticha, Southeastern Ethiopia. PloS one, 12(1), e0169418.

Examples

```
data(DATA2)
str(DATA2)
```

DATA3   *DATA of sample named FER1*

Description

list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J,K,Nb_measurement obtained using Generate_DataFile function with multi-grain OSL measurementsl of the sample FER1.

Usage

```
data("DATA3")
```

Format

A list containing:

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;

References

For more informations on this sample we refer to the following publication:

Guerin, G., Frouin, M., Talamo, S., Aldeias, V., Bruxelles, L., Chiotti, L., Goldberg, P., Hublin, J.J., Jain, M., Lahaye, C., Madelaine, S., Maureille, B., McPherron, S., Mercier, N., Murray, A., Sandgathe, D., Steele, T., Thomsen, K., Turq, A. (2015). A multi-method luminescence dating of the Palaeolithic sequence of La Ferrassie based on new excavations adjacent to the La Ferrassie 1 and 2 skeletons. Journal of Archaeological Science, 58, 147-166.

Examples

```
data(DATA3)
str(DATA3)
```

DATA_C14 *C14 cal age estiamte and its error*

Description

C14 cal age estiamtes and theirs error of samples S-EVA-26510, S-EVA-26506, S-EVA-26507, S-EVA-26508.

Usage

```
data("DATA_C14")
```

Format

A list containing:

Names: character vector of the sample names;

C14: numeric matrix, in the first column the 14C Cal age of the samples, and in the second column theirs errors.

References

For more informations on this sample we refer to the following publication:

Guerin, G., Frouin, M., Talamo, S., Aldeias, V., Bruxelles, L., Chiotti, L., Goldberg, P., Hublin, J.J., Jain, M., Lahaye, C., Madelaine, S., Maureille, B., McPherron, S., Mercier, N., Murray, A., Sandgathe, D., Steele, T., Thomsen, K., Turq, A. (2015). A multi-method luminescence dating of the Palaeolithic sequence of La Ferrassie based on new excavations adjacent to the La Ferrassie 1 and 2 skeletons. Journal of Archaeological Science, 58, 147-166.

Examples

```
data(DATA_C14)
(DATA_C14)
```

Generate_DataFile-deprecated

Generates, from one (or several) BIN-file(s) of Single-grain OSL measurements, a list of luminescence data and information before statistical analysis (DEPRECATED)

Description

This function is used to generate, from the BIN file(s), a list of values of: **Single-grain** 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.

Usage

```
Generate_DataFile(
  Path,
  FolderNames,
  Nb_sample,
  Nb_binfile = length(FolderNames),
  BinPerSample = rep(1, Nb_sample),
  sepDP = c(","),
  sepDE = c(","),
  sepDS = c(","),
  sepR = c("="),
  verbose = TRUE,
  ...
)
```

Arguments

Path	[character](#) (**required**): the path to the project folder, containing one or more sub folders in which the BIN files are located. If it is not equal to "", it must be terminated by "/".
FolderNames	[character](#) (**required**): list of names of the sub-folders containing the BIN files
	• each sub folder must contain a BIN file and associated csv files. See details for more informations on associated csv files required in the sub folders. If there is more than one BIN file per sample, see the details section for instructions regarding how to correctly fill the FolderNames 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 DoseEnv.csv files.
sepDS	[character](with default): column separator in the 'DoseLab.csv" files.
sepR	[character](with default): column separator in the Rule.csv files.
verbose	[logical](with default): enable/disable verbose mode
...	further arguments that can be passed to [Luminescence::read_BIN2R].

Details

With Path and FolderNames, this function goes to the sub folders containing the BIN files and associated information to compute the luminescence data.

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

Each sub folder 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), both in Gy. 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) both in Gy;
- **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);
  - 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 FolderNames **vector? ****

FolderNames is a vector of length Nb_binfile. FolderNames[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 FolderNames are ordered following two rules:

- The names in the FolderNames 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 FolderNames 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 FolderNames vector must be ordered by order of increasing ages.
  For example, FolderNames=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 FolderNames vector is correctly filled.
  If conversely, FolderNames=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 FolderNames=c("Sample1-File1", "Sample1-File2", "Sample2-File1"), in which case "Sample1-File1" 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-File1" 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 developped 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;

- **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.

** How to save this list **

You can save this list in a .RData object. To do this, you can use the fonction save. Then, to load this list you can use the function load (see example section fore more details).

How to cite

Christophe, C., Kreutzer, S., Philippe, A., 2024. Generate_DataFile-deprecated(): Generates, from one (or several) BIN-file(s) of Single-grain OSL measurements, a list of luminescence data and information before statistical analysis (DEPRECATED). In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Claire Christophe, Sebastian Kreutzer, Anne Philippe, Guillaume Guerin

See Also

read_BIN2R, combine_DataFiles, Generate_DataFile_MG, LT_RegenDose Age_Computation, AgeS_Computation, Palaeodose_Computation

Examples

```
## Not run:
## Example for one sample with one Bin File
path<- system.file("extdata/samp1", "", package="BayLum")
folder=""
nbsample=1  # give the number of sample
Data <- Generate_DataFile(
 Path = path,
 FolderNames = folder,
 Nb_sample = nbsample,
 verbose = FALSE)
str(Data)

## to save information in RData object in folder containing bin file
# save(Data,file=c(paste(path,folder,'Data.RData',sep="")))
## to load information containing Data.RData object
# load(file=c(paste(path,folder,"Data.RData",sep="")))

## End(Not run)
```

Generate_DataFile_MG-deprecated

Generates, from one (or several) BIN file(s) of Multi-grain OSL measurements a list of luminescence data and information before statistical analysis (DEPRECATED)

Description

This function is used to generate, from the BIN file(s), a list of values of:

Multi-grain 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.

Usage

```
Generate_DataFile_MG(
  Path,
  FolderNames,
  Nb_sample,
  Nb_binfile = length(FolderNames),
  BinPerSample = rep(1, Nb_sample),
  sepD = c(","),
  sepDE = c(","),
  sepDS = c(","),
  sepR = c("="),
  verbose = TRUE,
  force_run1_at_a_time = FALSE,
  ...
)
```

Arguments

Path	[character](#) (**required**): the path to the project folder, containing one or more sub folders in which the BIN files are located. If it is not equal to `""`, it must end with `"/"`.
FolderNames	[character](#) (**required**) vector: list of names of the sub-folders containing the BIN files
	• each sub folder must contain a BIN file and associated csv files. See details for more informations on associated csv files required in the sub folders. If there is more than one BIN file per sample, see the details section for instructions regarding how to correctly fill the FolderNames 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.
sepD	[character](#) (with default): column separator in the `DiscPose.csv` files.
sepDE	[character](#) (with default): column separator in the `DoseEnv.csv` files.
sepDS	[character](#) (with default): column separator in the `DoseLab.csv` files.
sepR	[character](#) (with default): column separator in the `Rule.csv` files.
verbose	[logical](#) (with default): enable/disable verbose mode

force_run1_at_a_time

> logical (*with default*): if set to TRUE, the order of the records is pushed to follow the one "Run 1 at a time" order (this is, all sequence steps were performed on one aliquot before moving to the next aliquot), regardless of their original sequence. The default is FALSE because 'BayLum' assumes that the sample was measured with the "Run 1 at a time" option (only Risø readers, lexsyg readers do not have another option). In other words, the argument allows you to automatically correct your input data to follow the order 'BayLum' expects. Why isn't the default value TRUE?. Because this re-ordering must fail if a measurement position was used more than once for different samples! This typically happens when different BIN/BINX files are merged.

...   further arguments that can be passed to Luminescence::read_BIN2R.

Details

With Path and FolderNames, this function goes to the sub folders 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);
- **Disc.csv**, a one columns csv file containing the list of disc 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), both in Gy. 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), both in Gy;
- **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);
  - 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 FolderNames vector? **

FolderNames is a vector of length Nb_binfile. FolderNames[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 FolderNames are ordered following two rules:

- The names in the FolderNames 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 FolderNames 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 FolderNames vector must be ordered by order of increasing ages.
  For example, FolderNames=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 FolderNames vector is correctly filled.
  If conversely, FolderNames=c(noun2,noun1), the analysis performed by AgeS_Computation would not be consistent.

** How to fill the BinPerSample vector? **

BinPerSample[i] corresponds 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 FolderNames=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 Luminescence::read_BIN2R 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;

- **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;

** How to save this list **

You can save this list in a .RData object. To do this, you can use the function save. Then, to load this list you can use the function load (see example section fore more details).

How to cite

Christophe, C., Kreutzer, S., Philippe, A., Guérin, G., 2024. Generate_DataFile_MG-deprecated(): Generates, from one (or several) BIN file(s) of Multi-grain OSL measurements a list of luminescence data and information before statistical analysis (DEPRECATED). In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

The function imports only BIN/BINX-file records which have been previously selected.

Author(s)

Claire Christophe, Sebastian Kreutzer, Anne Philippe, Guillaume Guérin

See Also

read_BIN2R, combine_DataFiles, LT_RegenDose Age_Computation, AgeS_Computation, Palaeodose_Computation

Examples

```
## Not run:
path <- system.file("extdata/FER1", "", package="BayLum")
folder <- ""
# give the number of sample
nbsample <- 1
DATA <- Generate_DataFile_MG(
 Path = path,
 FolderNames = folder,
 Nb_sample = nbsample)
str(DATA)

# to save information in RData object in folder containing bin file
#save(DATA,file=c(paste(path,folder,'DATA.RData',sep="")))
# to load information containing DATA.RData object
#load(file=c(paste(path,folder,"DATA.RData",sep="")))

## End(Not run)
```

IntCal13   *Atmospheric North data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in AtmosphericNorth_CalC14 allows a calibration for mid-latitude Northern Hemisphere atmospher reservoir.

Usage

```
data("IntCal13")
```

Format

A data frame with 3 variables.

CAL.BP a numeric vector correpondig to calendar years befor present

X14C.age a numeric vector correponding to 14C age

Error a numeric vector correponding to error arround 14C age measurement

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B, Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Examples

```
data(IntCal13)
## maybe str(IntCal13) ; head(IntCal13) ...
```

IntCal20   *Atmospheric North data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in AtmosphericNorth_CalC14 allows a calibration for mid-latitude Northern Hemisphere atmospher reservoir.

Usage

```
data("IntCal20")
```

Format

A data frame with 3 variables.

`CAL.BP` a numeric vector correpondig to calendar years befor present

`X14C.age` a numeric vector correponding to 14C age

`Error` a numeric vector correponding to error arround 14C age measurement

References

Reimer, P., Austin, W., Bard, E., Bayliss, A., Blackwell, P., Bronk Ramsey, C., . . . Talamo, S. (2020). The IntCal20 Northern Hemisphere Radiocarbon Age Calibration Curve (0–55 cal kBP). Radiocarbon, 62(4), 725-757. doi:10.1017/RDC.2020.41

Examples

```
data(IntCal20)
## maybe str(IntCal20) ; head(IntCal20) ...
```

LT_RegenDose-deprecated

Plots Lx/Tx as a function of the regenerative dose (DEPRECATED)

Description

This function plots `Lx/Tx` values as a function of regenerative dose, for every selected aliquot and for each sample.

Usage

```
LT_RegenDose(
  DATA,
  Path,
  FolderNames,
  SampleNames = FolderNames,
  Nb_sample,
  BinPerSample = rep(1, Nb_sample),
  SG = rep(TRUE, Nb_sample),
  sepDP = c(","),
  nrow = 3L,
  ncol = nrow
)
```

Arguments

DATA	[list](#) (**required**): list of objects LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, #' provided by [Generate_DataFile](#) or [Generate_DataFile_MG](#) or [combine_DataFiles](#).DATA can contain information from more than one sample.
Path	[character](#) (**required**): path to the project folder (the same as the one used in [Generate_DataFile](#) or [Generate_DataFile_MG](#) to provide DATA)

FolderNames	character (**required**): vector of names of the sub-folders containing the BIN-files, which were used by Generate_DataFile or Generate_DataFile_MG to generate the DATA object.
SampleNames	character (with default): Names of samples. To use if there is more than one bin file per sample.
Nb_sample	integer (**required**): 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.
BinPerSample	integer (with default): integer vector (with default): vector with the number of BIN files per sample, which was used in Generate_DataFile or Generate_DataFile_MG to generate the DATA object.
SG	logical (with default): vector to set the type of measurement for each sample length(SG)=Nb_sample.If the sample of number ID equal to i, SG[i]=TRUE if it is a Single-grain OSL measurements, SG[i]=FALSE if it is a Multi-grain OSL measurements.
sepDP	character (with default): column separator in the DiscPos.csv file or in Disc.csv file. It must be the same separator for all samples, for single-grain OSL measurements or multi-grain OSL measurements.
nrow	integer (with default): controls the arrangement of the plots, here the number of rows. Can be set to NULL.
ncol	integer (with default): controls the arrangement of the plots, here the number of columns. Can be set to NULL.

Details

To fill FolderNames and BinPerSample, we refer to the **Detail** section from the Generate_DataFile or Generate_DataFile_MG function. As well for a precise description of input DATA.

Value

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

How to cite

Christophe, C., Kreutzer, S., Philippe, A., Guérin, G., 2024. LT_RegenDose-deprecated(): Plots Lx/Tx as a function of the regenerative dose (DEPRECATED). In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Claire Christophe, Sebastian Kreutzer, Anne Philippe, Guillaume Guérin

See Also

Generate_DataFile, Generate_DataFile_MG

Examples

```
## Not run:
## load data file generated by the function Generate_DataFile
data(DATA3,envir = environment())
path<- system.file("extdata/FER1", "", package="BayLum")
folder=""
samplename <- "FER1"
LT_RegenDose(
 DATA = DATA3,
 Path = path,
 FolderNames = folder,
 SampleNames = samplename,
 Nb_sample = 1,
 SG = FALSE)

## End(Not run)
```

Marine13   *Marine data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in marine_CalC14 allows a calibration for hypothetical "global" marine reservoir.

Usage

```
data("Marine13")
```

Format

A data frame with 3 variables.

CAL.BP a numeric vector correpondig to calendar years befor present

X14C.age a numeric vector correponding to 14C age

Error a numeric vector correponding to error arround 14C age measurement

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B, Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Examples

```
data(Marine13)
## maybe str(Marine13) ; head(Marine13) ...
```

Marine20   *Marine data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in marine_CalC14 allows a calibration for hypothetical "global" marine reservoir.

Usage

```
data("Marine20")
```

Format

A data frame with 3 variables.

CAL.BP a numeric vector correpondig to calendar years befor present

X14C.age a numeric vector correponding to 14C age

Error a numeric vector correponding to error arround 14C age measurement

References

Heaton, T., Köhler, P., Butzin, M., Bard, E., Reimer, R., Austin, W., . . . Skinner, L. (2020). Marine20—The Marine Radiocarbon Age Calibration Curve (0–55,000 cal BP). Radiocarbon, 62(4), 779-820. doi:10.1017/RDC.2020.68

Examples

```
data(Marine20)
## maybe str(Marine20) ; head(Marine20) ...
```

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.

Usage

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

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

References

Tribolo, C., Asrat, A., Bahain, J. J., Chapon, C., Douville, E., Fragnol, C., Hernandez, M., Hovers, E., Leplongeon, A., Martin, L, Pleurdeau, D, Pearson, O , Puaud, S, Assefa, Z. (2017). Across the Gap: Geochronological and Sedimentological Analyses from the Late Pleistocene-Holocene Sequence of Goda Buticha, Southeastern Ethiopia. PloS one, 12(1), e0169418.

Examples

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

ModelC14 *Likelihood of C14 samples for JAGS models use in* `Age_OSLC14`

Description

A list of models for C14 data to define likelyhood in JAGS models.

Usage

```
data("ModelC14")
```

Format

This list contains:

`full` a model considering error on calibration curve.

`naive` a model not considering error on calibration curve.

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B,Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Hogg AG, Hua Q, Blackwell PG, Niu M, Buck CE, Guilderson TP, Heaton TJ, Palmer JG, Reimer PJ, Reimer RW, Turney CSM, Zimmerman SRH. 2013. SHCal13 Southern Hemisphere calibration, 0-50000 years cal BP. Radiocarbon 55(4):1889-1903

Examples

```
data(Model_AgeC14)
writeLines(Model_AgeC14$full)
```

ModelOSL   *Likelihood of OSL samples for JAGS models use in* Age_OSLC14

Description

A list of models for OSL data to define likelyhood in JAGS models.

Usage

```
data("ModelOSL")
```

Format

This list contains:

AgesMultiCS2_EXPLIN a list of 4 models that all consider a saturating exponential plus linear
  growth. These 4 models have different distribution to describe equivalent dose values around
  the palaeodose.

AgesMultiCS2_EXP a list of 4 models that all consider a saturating exponential growth. These 4
  models have different distribution to describe equivalent dose values around the palaeodose.

AgesMultiCS2_EXPZO a list of 4 models that all consider a saturating exponential plus linear
  growth and fitting through the origin. These 4 models have different distribution to describe
  equivalent dose values around the palaeodose.

AgesMultiCS2_EXPLINZO a list of 4 models that all consider a saturating exponential growth and
  fitting through the origin. These 4 models have different distribution to describe equivalent
  dose values around the palaeodose.

Details

The different distibutions to describe equivalent dose values around the palaeodose are:

cauchy a Cauchy distribution with postition parameter equal to the palaeodose of the sample

gaussian a Gaussian distribution with mean equal to the palaeodose of the sample

lognormal_A a log-normal distribution with mean or **A**verage equal to the palaeodose of the sam-
  ple

lognormal_M a log-normal distribution with **M**edian equal to the palaeodose of the sample

For more information we refer to the function AgeS_Computation, section Details.

References

Plummer, M. (2003). JAGS: A program for analysis of Bayesian graphical models using Gibbs
sampling. In Proceedings of the 3rd international workshop on distributed statistical computing,
volume 124, page 125. Technische Universit at Wien, Austria.

Plummer, M. (2015). JAGS Version 4.0. 0 user manual.

Examples

```
data(ModelOSL)
## The JAGS model of the likelyhood for a saturating exponential plus linear growth
## (a function of the type \code{f(x)=a(1-exp(-x/b))+cx+d})
## and a gaussian distribution of equivalent doses around the palaeodose:
writeLines(ModelOSL$AgesMultiOSL_EXPLIN$gaussian)
```

ModelPrior   *Prior for JAGS models use in* Age_OSLC14

Description

A list to define prior in JAGS models, taking account OSL data and C14 data in stratigraphic constraint. The difficulty is in the fact that each cases is different. The youngest sample can be a C14 as well as a OSL sample. To resolve this problem we consider diferent cases thanks to this list.

Usage

```
data("ModelPrior")
```

Format

This list contains:

Sample1_C14 model considering that the youngest sample is a C14 sample

Sample1_OSL model considering that the youngest sample is a OSL sample

C14_OSL model considering that the second sample is a C14 sample

OSL_C14 model considering that the second sample is a OSL sample

C14 model considering that the last sample is a C14 sample

OSL model considering that the last sample is a OSL sample

References

Plummer, M. (2003). JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In Proceedings of the 3rd international workshop on distributed statistical computing, volume 124, page 125. Technische Universit at Wien, Austria.

Plummer, M. (2015). JAGS Version 4.0. 0 user manual.

Examples

```
data(ModelPrior)
## ModelPrior[[OSL]]
writeLines(ModelPrior$OSL)
```

Model_Age   *JAGS models use in* Age_Computation

Description

A list of JAGS models use to a Bayesian analysis of OSL age of one sample. There are models for various growth curves and various distrubution to describe equivalent dose distribution around the palaeodose.

Usage

```
data("Model_Age")
```

Format

This list contains:

AgeMultiBF_EXPLIN a list of 4 models that all consider a saturating exponential plus linear growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgeMultiBF_EXP a list of 4 models that all consider a saturating exponential growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgeMultiBF_EXPZO a list of 4 models that all consider a saturating exponential plus linear growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgeMultiBF_EXPLINZO a list of 4 models that all consider a saturating exponential growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

Details

The different distibutions to describe equivalent dose values around the palaeodose are:

cauchy a Cauchy distribution with postition parameter equal to the palaeodose of the sample

gaussian a Gaussian distribution with mean equal to the palaeodose of the sample

lognormal_A a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample

lognormal_M a log-normal distribution with **M**edian equal to the palaeodose of the sample

For more information we refer to the function Age_Computation, section Details.

References

Plummer, M. (2003). JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In Proceedings of the 3rd international workshop on distributed statistical computing, volume 124, page 125. Technische Universit at Wien, Austria.

Plummer, M. (2015). JAGS Version 4.0. 0 user manual.

See Also

rjags

Examples

```
data(Model_Age)
## Terminal print
## The JAGS model for a saturating exponential plus linear growth
## (a function of the type \code{f(x)=a(1-exp(-x/b))+cx+d})
## and a gaussian distribution of equivalent doses around the palaeodose:
writeLines(Model_Age$AgeMultiBF_EXPLIN$cauchy)
```

Model_AgeC14 *JAGS models use in* AgeC14_Computation

Description

A list of JAGS models use to a Bayesian analysis of C14 calibration age of various sample. Stratigraphic relations can be taken in count to calibrate C14 ages. This ages take into account that some data can be an outlier.

Usage

```
data("Model_AgeC14")
```

Format

This list contains:

full a model considering error on calibration curve.

naive a model not considering error on calibration curve.

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B,Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Hogg AG, Hua Q, Blackwell PG, Niu M, Buck CE, Guilderson TP, Heaton TJ, Palmer JG, Reimer PJ, Reimer RW, Turney CSM, Zimmerman SRH. 2013. SHCal13 Southern Hemisphere calibration, 0-50000 years cal BP. Radiocarbon 55(4):1889-1903

See Also

rjags

Examples

```
data(Model_AgeC14)
writeLines(Model_AgeC14$full)
```

Model_AgeS   *JAGS models use in* AgeS_Computation

Description

A list of JAGS models use to a Bayesian analysis of OSL age of various samples. There are models for various growth curves and various distrubution to describe equivalent dose distribution around the palaeodose.

Usage

```
data("Model_AgeS")
```

Format

This list contains:

AgesMultiCS2_EXPLIN a list of 4 models that all consider a saturating exponential plus linear growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgesMultiCS2_EXP a list of 4 models that all consider a saturating exponential growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgesMultiCS2_EXPZO a list of 4 models that all consider a saturating exponential plus linear growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

AgesMultiCS2_EXPLINZO a list of 4 models that all consider a saturating exponential growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

Details

The different distibutions to describe equivalent dose values around the palaeodose are:

cauchy a Cauchy distribution with postition parameter equal to the palaeodose of the sample

gaussian a Gaussian distribution with mean equal to the palaeodose of the sample

lognormal_A a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample

lognormal_M a log-normal distribution with **M**edian equal to the palaeodose of the sample

For more information we refer to the function AgeS_Computation, section Details.

References

Plummer, M. (2003). JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In Proceedings of the 3rd international workshop on distributed statistical computing, volume 124, page 125. Technische Universit at Wien, Austria.

Plummer, M. (2015). JAGS Version 4.0. 0 user manual.

See Also

rjags

Examples

```
data(Model_AgeS)
## The JAGS model for a saturating exponential plus linear growth
## (a function of the type \code{f(x)=a(1-exp(-x/b))+cx+d})
## and a gaussian distribution of equivalent doses around the palaeodose:
writeLines(Model_AgeS$AgesMultiCS2_EXP$gaussian)
```

Model_Palaeodose   *JAGS models use in* Palaeodose_Computation

---

Description

A list of JAGS models use to a Bayesian analysis of OSL palaeodose of one or various samples. There are models for various growth curves and various distrubution to describe equivalent dose distribution around the palaeodose.

Usage

```
data("Model_Palaeodose")
```

Format

This list contains:

PalaeodosesMultiBF_EXPLIN a list of 4 models that all consider a saturating exponential plus linear growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

PalaeodosesMultiBF_EXP a list of 4 models that all consider a saturating exponential growth. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

PalaeodosesMultiBF_EXPZO a list of 4 models that all consider a saturating exponential plus linear growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

PalaeodosesMultiBF_EXPLINZO a list of 4 models that all consider a saturating exponential growth and fitting through the origin. These 4 models have different distribution to describe equivalent dose values around the palaeodose.

Details

The different distibutions to describe equivalent dose values around the palaeodose are:

cauchy a Cauchy distribution with postition parameter equal to the palaeodose of the sample

gaussian a Gaussian distribution with mean equal to the palaeodose of the sample

lognormal_A a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample

lognormal_M a log-normal distribution with **M**edian equal to the palaeodose of the sample

For more information we refer to the function Palaeodose_Computation, section Details.

References

Plummer, M. (2003). JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In Proceedings of the 3rd international workshop on distributed statistical computing, volume 124, page 125. Technische Universit at Wien, Austria.

Plummer, M. (2015). JAGS Version 4.0. 0 user manual.

See Also

rjags

Examples

```
data(Model_Palaeodose)
writeLines(Model_Palaeodose$PalaeodosesMultiBF_EXPLIN$gaussian)
```

Palaeodose_Computation

Bayesian analysis for the palaeodose estimation of various samples

---

Description

This function computes the palaeodose (in Gy) of one or various samples according to the model developed in Combes et al (2015), based on an output of Generate_DataFile or Generate_DataFile_MG or both of them using combine_DataFiles.
Samples, for which data is avalilable in several BIN files, can be analysed.
Single-grain or Multi-grain OSL measurements can be analysed simultaneouly.

Usage

```
Palaeodose_Computation(
  DATA,
  SampleNames,
  Nb_sample,
  BinPerSample = rep(1, Nb_sample),
  SavePdf = FALSE,
  OutputFileName = c("MCMCplot"),
  OutputFilePath = c(""),
  SaveEstimates = FALSE,
  OutputTableName = c("DATA"),
  OutputTablePath = c(""),
  LIN_fit = TRUE,
  Origin_fit = FALSE,
  distribution = c("cauchy"),
  Iter = 50000,
  t = 5,
  n.chains = 3
)
```

Arguments

DATA	list of objects: LT, sLT, ITimes, dLab, ddot_env, regDose, J, K, Nb_measurement, provided by [Generate_DataFile] or [Generate_DataFile_MG]. DATA contains information for more than one sample.
SampleNames	character vector: names of sample. The length of this vector is equal to Nb_sample.
Nb_sample	integer: number of samples.
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] or [Generate_DataFile_MG].
SavePdf	boolean (with default): if TRUE save graph in pdf file named OutputFileName in folder 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 credible 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	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"**, **"lognormal_A"** and **"lognormal_M"**.
Iter	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]).
n.chains	integer (with default): number of independent chains for the model (for more information see [jags.model]).

Details

** Option on growth curves **

As for [Age_Computation] and [AgeS_Computation], the user can choose from 4 dose response curves:

- **Saturating exponential plus linear growth** (PalaeodosesMultiBF_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** (`PalaeodosesMultiBF_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** (`PalaeodosesMultiBF_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** (`PalaeodosesMultiBF_EXPZO`):

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

    – `LIN_fit=FALSE`

    – `Origin_fit=TRUE`

** Option on equivalent dose distribution around the palaeodose **

The use can choose between :

- `cauchy`: a Cauchy distribution with location parameter equal to the palaeodose of the sample

- `gaussian`: a Gaussian distribution with mean equal to the palaeodose of the sample

- `lognormal_A`: a log-normal distribution with mean or **A**verage equal to the palaeodose of the sample

- `lognormal_M`: a log-normal distribution with **M**edian equal to the palaeodose of the sample

Value

    NUMERICAL OUTPUT

1. **A list containing the following objects:**
   - **Sampling** that corresponds to a sample of the posterior distributions of palaeodose and equivalent dose dispersion parameters (both in Gy).
   - **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.

2. **The Gelman and Rubin test of convergency**: prints the result of the Gelman and Rubin 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 **PLOT OUTPUT** for more informations).
   If both convergencies (Gelman and Rubin 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 (`Iter`) to reach convergency.

3. **Credible intervals and Bayes estimates**: prints the Bayes esitmates, the credible intervals at 95 the palaeodose and equivalent dose dispersion parameters for each sample.

    PLOT OUTPUT

1. **MCMC trajectories** A graph with the MCMC trajectories and posterior distributions of the palaeodose and equivalent dose dispersion parameters is displayed, 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.

2. **Summary of palaeodose estimates**: plot credible intervals and Bayes estimate of each sample palaeodose on a same graph.

To give result in a publication, we recommend to give the Bayes estimate of the parameters as well as the credible interval at 95

How to cite

Christophe, C., Kreutzer, S., Philippe, A., Guérin, G., 2024. Palaeodose_Computation(): Bayesian analysis for the palaeodose estimation of various samples. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Note

Please note that the initial values for all MCMC are currently all the same for all chains since we rely on the automatic initial value generation of JAGS. This is not optimal and will be changed in future. However, it does not affect the quality of the age estimates if the chains have converged.

Author(s)

Claire Christophe, Sebastian Kreutzer, Anne Philippe, Guillaume Guérin

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, Generate_DataFile_MG, combine_DataFiles, rjags, plot_MCMC, Age_Computation, AgeS_Computation

Examples

```
## Load data
data(DATA1,envir = environment())
## Palaeodose computation of samples GDB3
P=Palaeodose_Computation(DATA=DATA1,Nb_sample=1,SampleNames=c("GDB5"),Iter=100)
```

---

plot_Ages   *Create Age Plot*

Description

Create Age Plot

Usage

```
plot_Ages(
  object,
  sample_names = NULL,
  sample_order = NULL,
  plot_mode = "ages",
  ...
)
```

Arguments

object	list or data.frame (**required**): Output as created by functions like AgeC14_Computation, which is a list of class BayLum.list. Alternatively the function supports a data.frame as input, however, in such a case the data.frame must resemble the ages data.frame created by the computation functions otherwise the input will be silently ignored.
sample_names	character (optional): alternative sample names used for the plotting. If the length of the provided character vector is shorter than the real number of samples, the names are recycled.
sample_order	numeric (optional): argument to rearrange the sample order, e.g., sample_order = c(4:1) plots the last sample first.
plot_mode	character (*with default*): allows to switch from displaying ages as points with lines ("ages") for the credible intervals to densities ("density")
...	further arguments to control the plot output, standard arguments are: cex, xlim, main, xlab, col further (non-standard) arguments are: grid (TRUE/FALSE), legend (TRUE/FALSE), legend.text (character input needed), legend.pos graphics::legend, legend.cex. Additional arguments: d_scale (scales density plots), show_ages (add ages to density plots)

Details

This function creates an age plot showing the mean ages along with the credible intervals. The function provides various arguments to modify the plot output, however, for an ultimate control the function returns the data.frame extracted from the input object for own plots.

Value

The function returns a plot and the data.frame used to display the data

Function version

0.1.5

How to cite

Kreutzer, S., Christophe, C., 2024. plot_Ages(): Create Age Plot. Function version 0.1.5. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl-University of Heidelberg (Germany), based on code written by Claire Christophe

See Also

AgeC14_Computation, AgeS_Computation

Examples

```
## load data
data(DATA_C14,envir = environment())
C14Cal <- DATA_C14$C14[,1]
SigmaC14Cal <- DATA_C14$C14[,2]
Names <- DATA_C14$Names
nb_sample <- length(Names)

## Age computation
Age <- AgeC14_Computation(
   Data_C14Cal = C14Cal,
   Data_SigmaC14Cal = SigmaC14Cal,
   SampleNames = Names,
   Nb_sample = nb_sample,
   PriorAge = rep(c(20,60),nb_sample),
   Iter = 500,
   quiet = TRUE)

## plot output
plot_Ages(Age)

## plot output
plot_Ages(Age, plot_mode = "density")
```

---

plot_MCMC   *Plot MCMC trajectories and posterior distributions*

Description

This function uses the output of rjags::jags.model to visualise the traces of the MCMC and the corresponding densities. In particular it displays the posterior distributions of the age, if it is calculated, palaeodose and the equivalent dose dispersion parameters of the sample. The function output is very similar to plot output produced with the 'coda' package, but tailored to meet the needs in the context of the 'BayLum' package.

Usage

```
plot_MCMC(
  object,
  sample_names = NULL,
  variables = c("A", "D", "sD"),
  axes_labels = c(A = "Age (ka)", D = "D (Gy)", sD = "sD (Gy)"),
  n.chains = NULL,
  n.iter = 1000,
  smooth = FALSE,
  rug = TRUE,
  plot_single = FALSE,
  ...
)
```

Arguments

object	coda::mcmc.list or coda::mcmc (**required**): Output generated by rjags::jags.model, e.g., in Age_Computation. Alternatively, limited support is provided for BayLum.list object input
sample_names	character (optional): Names of the used samples. This argument overrides the optional argument mtext.
variables	character (with default): Variables in your coda::mcmc object to be plotted.
axes_labels	character (with default): Axes labels used for the trace and density plots. The labels should be provided as named character vector with the parameter names as the names used to assign the axes labelling. The labelling for the x-axis (trace plots) and y-axis (density plot) cannot be modified.
n.chains	numeric (optional): Set the number of chains to visualise, if nothing is provided the number of chains is determined from the input object
n.iter	integer (with default): Set the number of iterations to be visualised in the trace plots, regardless of the size of the input dataset as long as the real number of iterations is > n.iter. Please note that large numbers impact the plot performance.
smooth	logical (with default): Enable/disables smooth of trace plots using stats::smooth
rug	logical (with default): Enable/disables rug under density plots
plot_single	logical (with default): Enables/disables the single plot mode of the function, i.e. if set to TRUE every plot is returned in a single plot and own par settings can be applied.
...	further arguments that can be passed to modify the plot output. Supported arguments are lwd, lty, col, type, cex,mtext, cf. mtext for mtext and plot.default for the other arguments.

Details

The function is used in the function Age_Computation, AgeS_Computation and Palaeodose_Computation, but can be used also as standalone plot function.

Value

Two plots: Traces of the MCMC chains and the corresponding density plots. This plots are similar to coda::traceplot and coda::densplot.

Function version

0.1.5

How to cite

Kreutzer, S., Christophe, C., 2024. plot_MCMC(): Plot MCMC trajectories and posterior distributions. Function version 0.1.5. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl University of Heidelberg (Germany). This function is a re-written version of the function 'MCMC_plot()' by Claire Christophe

See Also

Age_Computation, AgeS_Computation, Palaeodose_Computation, rjags::coda.samples and rjags packages.

Examples

```
data(MCMCsample,envir = environment())
object <- coda::as.mcmc(MCMCsample)
plot_MCMC(object)
```

---

plot_RegDosePoints   *Plot Regeneration Dose Points*

Description

Simple plot functionality to visualise L_x/T_x values against the dose extracted from data created by create_DataFile

Usage

```
plot_RegDosePoints(object, nrow = 3L, ncol = nrow, ...)
```

Arguments

object	list (**required**): input object created by create_DataFile
nrow	integer (*with default*): number of rows used for the plot panel
ncol	integer (*with default*): number of columns in the plot panel
...	further plot arguments passed down to modify the plot output. Supported arguments are xlab, ylab, type, pch, col, cex

Value

The function returns a plot

How to cite

Kreutzer, S., 2024. plot_RegDosePoints(): Plot Regeneration Dose Points. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Heidelberg University (Germany)

See Also

[create_DataFile](#)

Examples

```
data(DATA3,envir = environment())
plot_RegDosePoints(DATA3)
```

---

plot_Scatterplots   *Display Scatter Plot Matrix of the Bayesian Age Results*

Description

Create a hexbin plot matrix ([hexbin::hexplom](#)) of age results returned by the Bayesian age calculation.

Usage

```
plot_Scatterplots(
  object,
  variables = c("A"),
  sample_names = NULL,
  sample_selection = NULL,
  n.chains = NULL,
  plot_type = "hexbin",
  plot_mode = "matrix",
  ...
)

ScatterSamples(...)
```

Arguments

object   [coda::mcmc.list](#) or a [data.frame](#) (**required**): mcmc list objects generated by
                   [rjags::jags.model](#) in [AgeS_Computation](#), [AgeC14_Computation](#) or [Age_OSLC14](#).
                   If a [data.frame](#) is provided, only the first two columns are taken and NA values
                   are automatically removed. The function can also handle BayLum.list objects
                   directly for certain functions

variables	[character](*with default*): variable to be selected for the scatter plot, e.g., "A". Please note that you can only select one variable at the time
sample_names	[character](*optional*): sample names shown in the plot matrix
sample_selection	[numeric](*with default*): vector of samples to be plotted in the scatter matrix, e.g., c(1,2) will plot the first two samples, c(1,3) will plot samples 1 and 3 and c(1:3) will plot the first three samples
n.chains	[integer](*with default*): allows to limit the number of chains shown, by default the results of all chains are plotted.
plot_type	[character](*with default*): switch between different plot types, "hexbin" (the default), based on the function [hexbin::hexplom](#) and smoothScatter (the alternative) based on a highly customised plot function using the function [graphics::smoothScatter](#)
plot_mode	[character](*with default*): switch between a matrix plot mode and a single plot mode. The plot mode single only works for plot_type = smoothScatter and creates a single plot panel for each sample. Please note that this cannot be further combined with other par settings.
...	further arguments to control the plot output, standard plot arguments supported are main, xlab, ylab, xlim, ylim, cex. For additional arguments supporting a fine tuning of the plot, see details.

Details

Additional supported plot arguments

The following table lists additional arguments supported by the function in order to fine tune the graphical output. Such arguments, can just be added in the function call. Example, for disabling the [graphics::rug](#) in the plot mode smoothScatter you can type plot_Scatterplots(..., rug = FALSE) Please note that not all arguments are supported by all plot types.

ARGUMENT	SUPPORTED BY PLOT TYPE	DESCRIPTION
colramp	hexbin and smoothScatter	Option to define an own colour ramp, by defining an own func
pscales	hexbin and smoothScatter	Controls the number of ticks shown on the plot axes, please no
bw_smoothScatter	smoothScatter	Controls the bandwidth of the smooth scatter, cf. [graphics::sm](#)
rug	smoothScatter	enables/disables rugs
nlevels	smoothScatter	controls the number of isolines shown (cf. [graphics::contour](#))
nrpoints	smoothScatter	defines the number of nrpoints to be plotted [graphics::smooth](#)
col_contour	smoothScatter	defines the colour of the contour lines
col_nrpoints	smoothScatter	sets colour of the nrpoints in the scatter plot

Value

A scatter plot based on [hexbin::hexplom](#)

Function version

0.3.2

How to cite

Kreutzer, S., Christophe, C., Philippe, A., Guérin, G., 2024. plot_Scatterplots(): Display Scatter Plot Matrix of the Bayesian Age Results. Function version 0.3.2. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl University of Heidelberg (Germany) , based on the function 'ScatterSamples()' by Claire Christophe, Anne Philippe, Guillaume Guérin

See Also

Age_Computation, AgeS_Computation, AgeC14_Computation, and rjags packages.

Examples

```
data(AgeS,envir = environment())

##hexbin
plot_Scatterplots(
   object = AgeS$Sampling,
   sample_names = c("GDB5", "GDB3"),
   sample_selection = c(1,2)
 )

##scatter smooth (matrix)
plot_Scatterplots(
   object = AgeS$Sampling,
   sample_names = c("GDB5", "GDB3"),
   sample_selection = c(1,2),
   plot_type = "smoothScatter")


##scatter smooth (single)
plot_Scatterplots(
   object = AgeS$Sampling,
   sample_names = c("GDB5", "GDB3"),
   sample_selection = c(1,2),
   plot_type = "smoothScatter",
   plot_mode = "single")
```

SCMatrix   *Construct the Stratigraphic Constrain Matrix Interactively*

Description

This function helps to define the stratigraphic relation between samples using questions. The output of this function can be used in the function AgeS_Computation.

Usage

```
SCMatrix(DATA = NULL, Nb_sample, SampleNames)
```

Arguments

DATA	BayLum.list (*with default*): Object of class BayLum.list, if provided the other parameters are not any longer mandatory.
Nb_sample	integer (**required**): the sample number, if DATA is provided, the input is not required
SampleNames	character (**required**): sample names, if DATA is provided, the input is not required

Details

The function will ask if sample i is younger than sample j to construct the stratigraphic constrain matrix.

Value

Returns a matrix that summarise the ordered relation between samples. This matrix can be integrate in AgeS_Computation function. We refer to detail on AgeS_Computation for more information concerning this matrix.

How to cite

Christophe, C., Philippe, A., Guérin, G., Kreutzer, S., 2024. SCMatrix(): Construct the Stratigraphic Constrain Matrix Interactively. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Claire Christophe, Anne Philippe, Guillaume Guérin, Sebastian Kreutzer

See Also

AgeS_Computation

Examples

```
## Not run:
SCMatrix(
 Nb_sample = 2,
 SampleNames = c("sample1","sample2"))

## End(Not run)
```

SC_Ordered   *Create Stratigraphically Ordered Sample Matrix*

Description

Construct the stratigraphic matrix used in the functions AgeS_Computation and AgeC14_Computation for samples that are all ordered by increasing age.

Usage

```
SC_Ordered(Nb_sample)
```

Arguments

Nb_sample   integer (**required**): the number of samples; alternatively an object of class
                 BayLum.list can be provided as input (such as produced by create_DataFile)

Value

Stratigraphic matrix where each sample are ordered by increasing order. This matrix can be integrated in the function AgeS_Computation. Please see AgeS_Computation for more information on this matrix.

How to cite

Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., 2024. SC_Ordered(): Create Stratigraphically Ordered Sample Matrix. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Claire Christophe, Anne Philippe, Sebastian Kreutzer, Guillaume Guérin

See Also

AgeS_Computation, SCMatrix

Examples

```
SC <- SC_Ordered(Nb_sample = 3)
```

SHCal13   *Atmospheric South data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in AtmosphericSouth_CalC14 allows a calibration for mid-latitude Southern Hemisphere atmospher reservoir.

Usage

```
data("SHCal13")
```

Format

A data frame with 3 variables.

CAL.BP a numeric vector correpondig to calendar years (in ky) befor present

X14C.age a numeric vector correponding to 14C age

Error a numeric vector correponding to error arround 14C age measurement

References

Reimer PJ, Bard E, Bayliss A, Beck JW, Blackwell PC, Bronl Ramsey C, Buck CE, Cheng H, Edwards RL, Friedrich M, Grootes PM, Guilderson TP, Haflidason H, Hajdas I, Hatte C, Heaton TJ, Hoffmann DL, Hogg AG, Hughen KA, Kaiser KF, Kromer B, Manning SW, Niu M, Reimer RW, Richards DA, Scott EM, Southon JR, Staff RA, Turney CSM, van der Plicht J. 2013. IntCal13 ans Marine13 radiocarbon age calibration curves 0-50000 years cal BP. Radiocarbon 55(4)=1869-1887.

Examples

```
data(SHCal13)
## maybe str(SHCal13) ; head(SHCal13) ...
```

SHCal20   *Atmospheric South data for calibration of 14C age*

Description

As 14C years is not equal to calendar years because atmospheric 14C concentration varies through time. Hence, data in AtmosphericSouth_CalC14 allows a calibration for mid-latitude Southern Hemisphere atmospher reservoir.

Usage

```
data("SHCal20")
```

Format

A data frame with 3 variables.

`CAL.BP` a numeric vector correpondig to calendar years (in ky) befor present

`X14C.age` a numeric vector correponding to 14C age

`Error` a numeric vector correponding to error arround 14C age measurement

References

Hogg, A., Heaton, T., Hua, Q., Palmer, J., Turney, C., Southon, J., . . . Wacker, L. (2020). SHCal20 Southern Hemisphere Calibration, 0–55,000 Years cal BP. Radiocarbon, 62(4), 759-778. doi:10.1017/RDC.2020.59

Examples

```
data(SHCal20)
## maybe str(SHCal20) ; head(SHCal20) ...
```

---

write_BayLumFiles *Write BayLum .csv-files*

Description

This function allows the user to write all .csv files expected by Generate_DataFile and Generate_DataFile_MG. Unlike create_FolderTemplates, this function makes it possible to write .csv files with all information directly from R. No further modification of .csv files are required. The purpose of this function is (i) to reduce tedious manual editing of .csv-files and the errors that result (ii) to introduce an easy way to review information inside .csv-files (by revisiting code rather than opening individual .csv-files) and (iii) to streamline folder and file creation when preparing data to run BayLum's modelling functions. Note: the user will still need to move the appropriate .bin-files into all the sample folders.

Usage

```
write_BayLumFiles(
  folder,
  SampleNames = "Sample_1",
  BinPerSample = rep(1, length(SampleNames)),
  SubSampleNames = NULL,
  DiscPos = NULL,
  DRenv = 1,
  DRenv.error = 0.04,
  DRsource = 0.1,
  DRsource.error = 0.002,
  signal.integral.min = 6,
  signal.integral.max = 10,
  background.integral.min = 346,
  background.integral.max = 395,
  inflatePercent = 0.025,
  nbOfLastCycleToRemove = 2
)
```

Arguments

folder	character (*required**): The name of the main folder in which all subsequent BayLum files and folders will be located. This could be a path to an already existing folder, or the path/name of a folder to be created.
SampleNames	character (*required*): Vector of sample names.
BinPerSample	numeric (*with default*): Vector of numbers indicating the number of .bin-files per sample.
SubSampleNames	character (*optional*): Vector of names to give each subfolder within a sample when the number of .bin-files in a sample counts more than one. If omitted or NULL, the subfolders are named by the subfolder count number.
DiscPos	numeric (*with default*): List of data frames with each data frame having one or two columns to identify aliquots/grains to be included in the analysis. The first column corresponds to the position number, and the second column corresponds to the grain number. If the data frame has only one column, a Disc.csv will be written. If the data.frame has two columns, a DiscPos.csv will be written. The length of the list should be the number of .bin-files included.
DRenv	numeric (*with default*): Vector where DRenv[i] corresponds to environmental dose rate for .bin-file[i]. Length should be one or the number of .bin-files included in the analysis.
DRenv.error	numeric (*with default*): Vector where DRenv.error[i] corresponds to environmental dose rate error for .bin-file[i]. Length should be one or the number of .bin-files included in the analysis.
DRsource	numeric (*with default*): Vector where DRsource[i] corresponds to source dose rate for .bin-file[i]. Length should be one or the number of .bin-files included in the analysis.
DRsource.error	numeric (*with default*): Vector where DRsource.error[i] corresponds to source dose rate error for .bin-file[i]. Length should be one or the number of .bin-files included in the analysis.
signal.integral.min	numeric (*with default*): Vector where signal.integral.min[i] corresponds to the channel number where the OSL signal should be summed from forbin-file[i] Length should be one or the number of .bin-files included in the analysis.
signal.integral.max	numeric (*with default*): Vector where signal.integral.max[i] corresponds to the channel number where the OSL signal should be summed from to for bin-file[i] Length should be one or the number of .bin-files included in the analysis.
background.integral.min	numeric (*with default*): Vector where background.integral.min[i] corresponds to the channel number where the OSL background signal should be summed from forbin-file[i] Length should be one or the number of .bin-files included in the analysis.
background.integral.max	numeric (*with default*): Vector where background.integral.max[i] corresponds to the channel number where the OSL background signal should be summed to for .bin-file[i]. Length should be one or the number of .bin-files included in the analysis.
inflatePercent	numeric (*with default*): Vector where inflatePercent[i] corresponds to uncertainty due to instrumental reproducibility tobin-file[i] Length should be one or the number of .bin-files included in the analysis.

nbOfLastCycleToRemove

> numeric (*with default*): Vector where nbOfLastCycleToRemove[i] corresponds to the number of regeneration points to remove in analysis for bin-file[i] Length should be one or the number of .bin-files included in the analysis.

Value

The function returns nothing, but writes the folder structure.

Function version

0.1.0

How to cite

Baumgarten, F.H., 2024. write_BayLumFiles(): Write BayLum .csv-files. Function version 0.1.0. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Frederik Baumgarten, RadPhys, DTU Physics, Technical University of Denmark (Denmark)

See Also

Generate_DataFile, Generate_DataFile_MG

Examples

```
# example samples
SampleNames <- c("OSL-1-MG","OSL-2-SG")

# number of .bin-files for each sample
BinPerSample <- c(1,3)

# List of data.frames of accepted aliquot/grain to be included
# in the analysis for each .bin-file.
DiscPos <- list(
data.frame("position" = 1:48),
data.frame("position" = c(1,1,1,1), "grain" = c(4,67,92,99)),
data.frame("position" = c(2,2,2,2), "grain" = c(7,13,41,72)),
data.frame("position" = c(3,3,3,3), "grain" = c(7,52,67,88)))

# example 1: write to disk (all together)
write_BayLumFiles(
folder = paste(tempdir(),"new_BayLum_folder",sep = "/"),
SampleNames = SampleNames,
BinPerSample = BinPerSample,
DiscPos = DiscPos,
DRenv = c(1.75, 1.52, 1.52, 1.52),
DRenv.error = c(0.04, 0.03, 0.03, 0.03),
DRsource = c(0.2075, 0.1501, 0.1501, 0.1501),
DRsource.error = c(0.0010, 0.0008, 0.0008, 0.0008))

# example 2: write to disk (by sample)
```

```
write_BayLumFiles(
folder = paste(tempdir(),"new_BayLum_folder",sep = "/"),
SampleNames = "OSL-1-MG",
BinPerSample = 1,
DiscPos = DiscPos[[1]],
DRenv = 1.75,
DRenv.error = 0.04,
DRsource = 0.2075,
DRsource.error = 0.0010)

write_BayLumFiles(
folder = paste(tempdir(),"new_BayLum_folder",sep = "/"),
SampleNames = "OSL-2-SG",
BinPerSample = 3,
DiscPos = DiscPos[2:4],
DRenv = 1.75,
DRenv.error = 0.04,
DRsource = 0.2075,
DRsource.error = 0.0010)
```

---

write_YAMLConfigFile *Write Auto Generated YAML BayLum Configuration File to the Disc*

Description

This little function helps to auto-generate a the BayLum YAML configuration file or a list that can be passed to create_DataFile. The YAML file itself can be modified in any text editor. The allowed parameters are extracted from the reference YAML file

Usage

```
write_YAMLConfigFile(output_file = NULL, ...)
```

Arguments

output_file   character (*with default*): valid file path of the output file

...   parameters to be preset in the YAML file (run write_YAMLConfigFile() to
                see allowed parameters) The parameter sample is special, because it can be
                provided as a character vector of any length. The number of elements in the
                vector (sample names) are then used to multiply the records in the configuration
                file.

Value

The function has two output modes:

- (1) output_file = <file_path>: Writes a YAML into the specified path and returns this
  path.

- (2) output_file = NULL: Returns a list of allowed function parameters that can be passed to
  the function **and** it returns a list that can be used a passed on to create_DataFile.

Function version

0.1.0

How to cite

Kreutzer, S., 2024. write_YAMLConfigFile(): Write Auto Generated YAML BayLum Configuration File to the Disc. Function version 0.1.0. In: Christophe, C., Philippe, A., Kreutzer, S., Guérin, G., Baumgarten, F.H., Frerebeau, N., 2024. BayLum: Chronological Bayesian Models Integrating Optically Stimulated. R package version 0.3.2. https://CRAN.r-project.org/package=BayLum

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl University of Heidelberg (Germany)

See Also

create_DataFile, yaml::read_yaml, Luminescence::read_BIN2R, Luminescence::read_XSYG2R

Examples

```
## generate list
write_YAMLConfigFile(
sample = c("samp1", "samp2"),
settings.rules.endTest = 10)

## generate file (here written in tempdir)
write_YAMLConfigFile(
 output_file = tempfile("configuration.yml"),
 sample = c("samp1", "samp2"),
 settings.rules.endTest = 10)
```

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