Package 'ELISAtools'

March 8, 2019

Title ELISA Data Analysis with Batch Correction

Version 0.1.0

Description To run data analysis for enzyme-link immunosorbent assays (ELISAs). Either the five- or four-parameter logistic model will be fitted for data of single ELISA. Moreover, the batch effect correction/normalization will be carried out, when there are more than one batches of ELISAs. Feng (2018) <doi:10.1101/483800>.

Depends R (>= 3.4.0), R2HTML (>= 2.3.2), stringi (>= 1.1.7), minpack.lm (>= 1.2-1), methods

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ELISAtools-package ELISA data analysis with batch correction

Description

An R package to run ELISA data analysis with the ability to do batch correction/normalization

Details

Index

This package is developed to run analysis of ELISA data. First, the calibration data are used to fit either the five- or four-parameter logistic model. Then the fitted model is used to predict the concentrations of unknown samples. If the batches of calibration data exist, the correction/normalization could be done. The corrected calibration curve are then used for predication.

Please refer to the vignettes to see details.

Author(s)

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References

Feng, et al 2018 https://doi.org/10.1101/483800

annotate.plate

Description

to write annotations for an ELISA plate as an input to guide the functions to read OD values

Usage

```
annotate.plate(sample.id, sample.prefix, sample.suffix, num.sample,
num.std = 8, byRow.sample = TRUE, byRow.replicates = TRUE,
replicates.sample = 3, replicates.std = 3, rows, columns,
std.first = TRUE)
```

Arguments

| sample.id | character vector to specify the names/ids of the samples on the plate. Note, standard/calibration sample ids/names is fixed to be "s1","s2", etc, which are specified by the software and users don't need to privide. | |
|--------------------------|--|--|
| <pre>sample.prefix</pre> | characters will be added to the beginning of sample names | |
| <pre>sample.suffix</pre> | characters will be added to the end of sample names | |
| num.sample | numeric number of samples to write | |
| num.std | numeric number of standards | |
| byRow.sample | boolean indicate whether to write sample names horizontally by row (TURE) or vertically by column (FALSE) | |
| byRow.replicates | | |
| | boolean indicate whether to write sample replicates horizontally by row (TURE) or vertically by column (FALSE) | |
| replicates.sample | | |
| | numeric number of replicates for each sample | |
| replicates.std | numeric number of replicates for each standards | |
| rows | numeric vector to specify which rows to be included in the annotation | |
| columns | numeric vector to specify which columns to be included in the annotation | |
| std.first | boolean to indicate whether to write standards first or the samples first. | |

Details

Based on the input to quickly write the annotations for ELISA plate. The output is in a 96-well format and will be used to giude the reading of OD plates. This way only a nxm dataframe can be used. To write non-regular annotation, you have to do it mannually.

Value

a dataframe holding the annotations for the plate.

avoidZero

Description

Get rid of zeros in a numeric vector before taking the logarithm of them. We basically replace the "zeros" with a negligible small value in order to avoid NaN upon the log-transformation.

Usage

avoidZero(x, fac = 10)

Arguments

| х | numeric values as input |
|-----|--|
| fac | numeric a factor of scale in order to get a "small" value to replace zeros |

Value

a vector of value with zeros replaced.

combineData Combine elisa_batch data

Description

Combine the two lists of elisa_batch data.

Usage

combineData(eb1, eb2)

Arguments

| eb1 | list of elisa_batch data |
|-----|--------------------------|
| eb2 | list of elisa_batch data |

Details

When combining, we not only concatenate the two data sets, but also combine batches, meaning the two batches with same batch ID will be merged into one. We will not merge the runs. Therefore, same batch from different list will always have different runs. It is the user's responsibility to make sure the runs are different.

elisa_batch

Value

a list of elisa_batch data combining the two input lists (sorted);

See Also

elisa_batch-class loadData saveDB

Examples

```
#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")</pre>
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
#make a guess for the parameters, the other two parameters a and d
#will be estimated based on data.
model<-"5pl"
pars<-c(7.2,0.5, 0.015) #5pl inits
names(pars)<-c("xmid", "scal", "g")</pre>
#do fitting. model will be written into data set.
batches<-runFit(pars=pars, batches=batches, refBatch.ID=1, model=model )</pre>
#call to do predications based on the model.
batches<-predictAll(batches);</pre>
batches.old<-batches;</pre>
#now suppose want to join/combine the two batches, old and new
batches.com<-combineData(batches.old, batches);</pre>
```

elisa_batch

Constructor function to build an elisa_batch object

Description

S3 method as a constructor to build the S4 class object of elisa_batch elisa_batch-class

Usage

```
elisa_batch(batchID = NA_character_, desc = NA_character_,
runs = list(), model.fit = list(), model.name = NA_character_,
pars = c(-1), num.runs = 1, range.ODs = c(-1, -1),
normFactor = NaN)
```

Arguments

| batchID | character string to specify a batches |
|------------|--|
| desc | character string for the data/experiment information |
| runs | list of elisa_plates in this run. There could be one or many plates in a run. |
| model.fit | list intend to contain information for the fitting of nls.lm. But not using it now. |
| model.name | character string of either the 5pl (5-parameter) or 4pl (4-parameter) logistic function |
| pars | numeric the actually parameters for the fitting. for example for the 5pl model they are $c(a, d, xmid, scal, g)$. |
| num.runs | numeric the number of plates in this run. |
| range.ODs | numeric the min and max ODs |
| normFactor | numeric the batch effect normalization factor ("S"). |

Details

S3 method as a constructor to build the S4 class object of elisa_batch elisa_batch-class. Normally this is called to build a empty object with default values and then load the elisa_run data into it

Value

an elisa_batch object

See Also

nls.lm elisa_run-class elisa_plate-class elisa_batch-class

Examples

elisa_batch();

elisa_batch-class S4 class definition of an elisa_batch object

Description

elisa_batch-class define the S4 class of an elisa_batch object

elisa_batch-class

Arguments

| batchID | characters to specify the batch |
|------------|--|
| runs | list of elisa_run objects |
| num.runs | numeric the number of elisa_runs in this batch |
| pars | numeric the actually parameters for the fitting. for example for the 5pl they are c(a, d,xmid, scal, g). |
| model.fit | list intend to contain information for the fitting of nls.lm. But not using it now. |
| model.name | characters of either the 5pl (5-parameter) or 4pl (4-parameter) logistic function |
| range.ODs | numeric the min and max ODs |
| normFactor | numeric the batch normalization factor ("S"). |

Details

defining the S4 class of the elisa_batch. This holds the data for elisa batch. It contains one or many elisa_run objects.

Slots

batchID character desc character runs list num.runs numeric pars numeric model.fit list model.name character range.ODs numeic normFactor numeric

See Also

nls.lmelisa_plate-class elisa_run-class elisa_batch-class

Examples

elisa_batch();

```
elisa_plate
```

Description

S3 method as a constructor to build the S4 class object of the elisa_plate elisa_plate

Usage

```
elisa_plate(batchID = NA_character_, expID = NA_character_,
  desc = NA_character_, data.std = data.frame(),
  mdata.std = data.frame(), data.unknown = data.frame(),
  mdata.unknown = data.frame(), normFactor = NaN, range.ODs = c(-1,
  -1))
```

Arguments

| batchID | characters to specify the batch |
|---------------|---|
| expID | characters to specify experiment or plate ID |
| desc | characters for the data/experiment information |
| data.std | data.frame for standard curve data |
| mdata.std | data.frame containing the mean ODs and concentration of the calibration data |
| data.unknown | data.frame for data of samples with unknown concentration fitted with either four- or five-parameter logistic function. |
| mdata.unknown | data.frame containing the mean ODs and concentration by sample IDs. |
| normFactor | numeric the correction factor for batch effects. |
| range.ODs | numeric the min and max ODs in the plate. |
| | |

Details

S3 method as a constructor to build the S4 class object of elisa_plate elisa_plate. Normally this is called to build an empty object with default values and then load data into it by calling loadData loadData or load.ODs load.ODs

Value

an elisa_plate object

See Also

nls.lmloadData elisa_plate load.ODs

Examples

elisa_plate();

elisa_plate-class S4 class definition of an elisa_plate object

Description

elisa_plate define the S4 class of an elisa_plate object

Arguments

| batchID | characters to specify the batch |
|---------------|---|
| expID | characters to specify experiment or plate ID |
| desc | characters for the data/experiment information |
| data.std | data.frame for standard curve data |
| data.unknown | data.frame containing data for samples with unknown concentration |
| normFactor | numeric the correction factor for batch effects ("S"). |
| mdata.unknown | data.frame containing the mean ODs and concentration by sample IDs. |
| mdata.std | data.frame containing the mean ODs and concentrations for standard data |

Details

defining the S4 class of the elisa_plate object. This is the data structure to hold the elisa_plate Data. It contains different slots for holding both standard and unknown data. It also defines the regression model and the correction parameter for the batch effects. Note: we assume each plate has its own standard curve.

Slots

batchID character expID character data.std data.frame data.unknown data.frame normFactor numeric desc character range.ODs numeric mdata.unknown data.frame mdata.std data.frame

See Also

nls.lm

Examples

elisa_plate();

elisa_run

Description

S3 method as a constructor to build the S4 class object of elisa_run elisa_run-class

Usage

```
elisa_run(batchID = NA_character_, desc = NA_character_,
plates = list(), num.plates = 1, date = NA_character_,
range.ODs = c(-1, -1))
```

Arguments

| batchID | characters to specify the batch |
|------------|--|
| desc | characters for data/experiment information |
| plates | list of elisa_plates in this run. could be one or many |
| num.plates | numeric the number of plates in this run. |
| date | charaters the date to run ELISA measurements |
| range.ODs | numeric the range of ODs for the measurements |

Details

S3 method as a constructor to build the S4 class object of elisa_run elisa_run-class. Normally this is called to build a empty object with default values and then load the elisa_run data into. #

Value

an elisa_run object

See Also

nls.lm elisa_run-class elisa_plate-class

Examples

elisa_run();

elisa_run-class

Description

elisa_run-class defines the S4 class of elisa_run

Arguments

| batchID | characters to specify the batch |
|------------|---|
| desc | characters for the data/experiment information |
| plates | list of elisa_plates |
| num.plates | numeric the number of plates in this run |
| date | characters for the date of running the ELISA measurements |

Details

defining the S4 class of the elisa_run object. This is list to hold the data for each elisa run. It contains one or many elisa plate objects.

Slots

batchID character plates list desc character num.plates numeric date character range.ODs numeric

See Also

nls.lm

Examples

elisa_run();

Description

read in the paramters and the independent variable value(s), and then return the 5pl function value(s). For the 4pl model, set g to be 1.

Usage

f5pl(pars, x)

Arguments

| pars | numeric the parameters of the 5pl (or 4pl). It has the following content: [a, d, |
|------|--|
| | xmid, scal, g]. |
| x | numeric the log-transformed x value(s). |

Details

The function has the following form $f(x)=a+(d-a)/((1+exp((xmid-x)/scal))^g)$

Value

the 5pl function value(s).

| inv. | f5pl |
|------|------|
|------|------|

The inverse of the 5-parameter logistic function

Description

The inverse function of the 5pl. Set the value of g to be 1, if the 4pl is of interest.

Usage

inv.f5pl(pars, y)

Arguments

| pars | the parameters of the function. It has the following content: [a, d, xmid, scale, |
|------|---|
| | g]. |
| У | the value to be reverse calculated. |

Value

the value of the reverse function

load.ODs

Description

Generic function to load OD data into an elisa_plate object

Usage

```
load.ODs(x, plate.header, plate.data, plate.blank, annotation, ....)
```

```
## S4 method for signature 'elisa_plate'
load.ODs(x, plate.header, plate.data, plate.blank,
    annotation)
```

Arguments

| Х | the elisa_plate object to load data into |
|--------------|---|
| plate.header | characters |
| plate.data | data.frame OD readings |
| plate.blank | data.frame OD blank readings |
| annotation | data.frame annotation to guide reading. |
| | other parameters that will help reading data. |

Details

It loads OD data into an elisa_plate object. The data usually read int from design file, annotation file, OD file and standard concentration data.

Methods (by class)

• elisa_plate: to load ODs to an elisa_plate object

| loadData Read data according to the design file |
|---|
|---|

Description

Read the design file and then load the data according to the information in the design file.

Usage

loadData(design.file)

Arguments

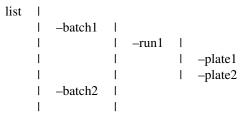
design.file characters to specify the path and the file name of the design file.

Details

The design file contains all the information necessary to read data. It has the following format

| ExpID | FileName | Batch | Num_Plate | Date | AnnotationFile | Std_Conc | Dir_Annotation | Dir_StdConc |
|-------|-----------|--------|-----------|-----------|----------------|-------------|----------------|-------------|
| Exp1 | file1.txt | Batch1 | 1 | 9/18/2009 | annote.txt | stdConc.txt | | |
| Exp2 | file2.txt | Batch2 | 2 | 9/18/2009 | annote.txt | stdConc.txt | | |

The return data is a list of batches (elisa_batch-class), which are made of one or many elisa runs(elisa_run-class). The run could contain one or many elisa plates (elisa_plate-class) with data or annotation of each plate.



Value

a list of batches holding different runs of elisa, which could contain one or many elisa_plates with data and annotations for each plate.

See Also

elisa_batch-class elisa_plate-class elisa_run-class

Examples

```
file.dir<-system.file("extdata", package="ELISAtools")
loadData(file.path(file.dir,"design.txt"));</pre>
```

loadDB

Read the saved elisa_batch data

Description

Load the serialized elisa_batch data from disk.

loadDB

Usage

loadDB(db)

Arguments

db

characters to specify the path and file name the elisa data file.

Details

Here we deserialize elisa_batch data by wrapping the readRds() function call. The serialized elisa_batch data are assumed to have been correctly analyzed. We will print a summary for what has been read.

Value

a list of batches holding different runs of elisa, which could contain one or many elisa_plates with data and annotations for each plate.

See Also

elisa_batch-class loadData saveDB

Examples

```
#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")</pre>
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
#make a guess for the parameters, the other two parameters a and d
#will be estimated based on data.
model<-"5pl"
pars<-c(7.2,0.5, 0.015) #5pl inits
names(pars)<-c("xmid", "scal", "g")</pre>
#do fitting. model will be written into data set.
batches<-runFit(pars=pars, batches=batches, refBatch.ID=1, model=model )</pre>
#now call to do predications based on the model.
batches<-predictAll(batches);</pre>
#now saving the data.
saveDB(batches, file.path(tempdir(),"elisa_tool1.rds"));
```

loadDB(file.path(tempdir(),"elisa_tool1.rds"));

plotAlignData

Description

Plot the batch data together for visualization.

Usage

plotAlignData(batches, graph.file = NULL)

Arguments

| batches | list of batch data objects either raw or analyzed data. |
|------------|---|
| graph.file | characters as the output graph file name. If specified, a SVG (*.svg) graph will be saved to the disk. Otherwise, the graph will be send to the stdout. |

Details

If the data has been analysed, a fitted line will be drawn too. If there are more than one batches, each batch will be plotted with different color and different symmbols. Different batches will also be shifted/adjusted based on their "S" factor, and one single fitted line (based on the "reference" batch) will be plotted.

Value

characters which specify the graph file name, if graph.file is specified. NULL otherwise.

Examples

```
#load the library
library(ELISAtools)
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")</pre>
```

```
#load the data
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
```

```
#plot the raw batch data together
plotAlignData(batches);
```

plotBatchData

Description

Plot the individual batch data for visualization.

Usage

```
plotBatchData(batch, graph.file = NULL)
```

Arguments

| batch | batch data objects with either raw or analyzed data. |
|------------|---|
| graph.file | characters as the output graph file name. If specified, a SVG (*.svg) graph will be saved to the disk. Otherwise, the graph will be send to the stdout. |

Details

If the data has been analysed, a fitted line will be drawn too.

Value

characters which is the graph file name, if graph.file is specified. NULL otherwise.

Examples

```
#load the library
library(ELISAtools)
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")
#load the data</pre>
```

```
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
```

```
#plot the raw batch 1 data
plotBatchData(batches[[1]]);
```

predictAll

Description

Based on the 5pl or 4pl regression, predict the concentration of of unknown samples. Assume the regression has been accomplished.

Usage

predictAll(batches)

Arguments

batches list of elisa_batch objects containing both the raw data and the fitted regression model.

Details

The input data structure contains both the data (ODs) and the fitted regression model. The estimation of unknonw concentration based on the ODs and the standard curve of each plate. The batch effects are corrected/normalized and the corrected concentrations also are also written into the batch data structure, if there are more than one batches in the data.

Value

The same list of elisa_batch with estimated sample concentrations based on ODs and the fitted regression model. The estimated concentrations normalized/corrected between different batches are also calculated and recorded.

References

Feng 2018 https://doi.org/10.1101/483800

See Also

elisa_batch elisa_run elisa_plate

prepareInitsLM Prepare initial values for fitting shifts

Description

Generate the initial values for fitting shifts with a model of the 5-parameter logistic function.

Usage

```
prepareInitsLM(batches, ref.batch = 1)
```

Arguments

| batches | list of elisa_batch data |
|-----------|---|
| ref.batch | numeric the index of the reference batch. It is 1 by default. |

Details

This is a more complicated way to prepare the initials for shifting.

Value

a data list contain the following elements,

- inits, the initial values for the standard curves of all the plates
- ref.ibatch, the index of the reference batch
 - This one is specified by the input ref.batch.
- ref.irun,the index of the reference run
- ref.index,the index of the reference line in the order of the inits vector

prepareRegInput Prepare the input for regressoin

Description

Prepare the input data to feed in the fitting.

Usage

prepareRegInput(batches)

Arguments

batches list of the ELISA data arranged in batches. Each element of list contains a batch (list) data, and each batch contains one or many the elisa_run objects elisa_plate

Value

list of data that will feed in to do regression.

See Also

elisa_plate elisa_batchelisa_run

rangeOD Get the OD ranges (min/max)

Description

Going through the list of batches to get the OD range (min and max)

Usage

rangeOD(batches)

Arguments

batches list of batches data

read.annotation Read the annotation of single ELISA plate

Description

Parse the annotations for one single ELISA plate from a section of a file and output the annotations for standard and unknown separately.

Usage

read.annotation(annotation, std.conc)

Arguments

| annotation | characters to specify the path and name of the annotation file |
|------------|---|
| std.conc | data.frame containing standard concentration data. Only first two columns are |
| | used with first one to be the standard IDs and second the concentrations. |

read.annotations

Details

The annotation file may contain annotations for more than one plate. Each plate is marked by "Plate: plate 1..." and "~End". This function is fed in with the content for each section and we do actually parsing in here. Store the annotations into data frame. It also parse the standard concentration and include this information in the data frame. For each section, we expect the following format

1 2 3 4 ... С s1 sample1 sample1 s1 ... D s2 s2 sample2 sample ... ••• ••• •••

In addition, the row name and column names indicate the plate row and column indices. As input, the stardard and unknown are returned separately in two tables.

Value

a list of data.frames holding the annotations for the plate.

Examples

```
#get example annotation file path from the system folder
fileName<-system.file("extdata", "annote_single.txt", package="ELISAtools")
#prepare the standard concentration file.
std.conc<-data.frame(id=c("s1","s2","s3","s4","s5","s6"), conc=c(1:6))
#read the data as a data frame.
ann<-read.table(fileName, header=TRUE, sep="\t", stringsAsFactors=FALSE)</pre>
```

#call to do the reading.

read.annotations Read the annotations of plates

Description

Parse annotations for multiple ELISA plates from files, one annotation file and one standard concentration file, and output the annotations for standard and unknown separately.

Usage

```
read.annotations(annotation, std.conc, dir.annotation, dir.stdConc,
    num.plate = 1)
```

Arguments

| annotation | characters to specify the path and name of the annotation file |
|----------------|--|
| std.conc | characters to specify the standard concentration file. |
| dir.annotation | characters specifying the file to the annotatoin file. |
| dir.stdConc | characters specifying the path to the annotatoin file. |
| num.plate | numeric indicating the number of plates in the annotation files. |

Details

The annotation file may contain annotations for more than one plate. Each plate is marked by "Plate: plate 1..." and "~End". This function parses each section in both annotation file and standard concentration file. Then passes the section on to do the parsing. For each section, we expect the following format

| | 1 | 2 | 3 | 4 | |
|-----|----|----|---------|---------|-----|
| С | s1 | s1 | sample1 | sample1 | |
| D | s2 | s2 | sample2 | sample | |
| ••• | | | | | ••• |

Value

a list of annotations for elisa plates.

Examples

```
#get example annotation file path from the system folder
ann<-system.file("extdata", "annote.txt", package="ELISAtools")
std.conc<-system.file("extdata", "stdConc.txt", package="ELISAtools")</pre>
```

#read them in and there are 2 plates.
read.annotations(annotation=ann, std.conc=std.conc, num.plate=2)

read.plate

Read the single ELISA OD plate

Description

Read the individual ELISA plate to parse the ODs.

Usage

read.plate(ODs, annotation, batchID, expID)

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read.plates

Arguments

| ODs | characters containing data of ODs for one plate |
|------------|--|
| annotation | list of data containing annotations of the plate |
| batchID | characters specifying the batchID read from the design file |
| expID | characters specifying the expID or plateID read from the design file |

Details

The input is a text file imported from the sdf file. We only read the first section with both the OD and blank file. The OD data are read in according to the annotation file.

Value

an object of elisa_plate holding data and annotations for a single plate.

| read.plates | Read the ELISA OD files | |
|-------------|-------------------------|--|
|-------------|-------------------------|--|

Description

Read the ELISA OD file to parse the ODs.

Usage

Arguments

| fileName | characters containing file name of OD data |
|-------------|---|
| annotations | list of data containing annotations of the plates |
| num.plate | numeric number of OD plates in the OD file. |
| batchID | characters specify the batchID read from the design file |
| expID | characters specify the expID or plateID read from the design file |
| date | characters the date running the ELISA exps. |

Details

The input is a text file imported from the sdf file. The file may contain multiple plates of OD. We will parse each file section and then read them according to the annotation to load the data. We assume for each file the data are for the same batch and experiment. If otherwise, please split the file into different ones.

Value

an object of elisa_run holding data and annotations for one or multiple plates.

Examples

```
#get example annotation file path from the system folder
ann<-system.file("extdata", "annote.txt", package="ELISAtools")
std.conc<-system.file("extdata", "stdConc.txt", package="ELISAtools")
#read them in and there are 2 plates.
annotations<-read.annotations(annotation=ann, std.conc=std.conc, num.plate=2)
#now start reading the OD plate file
fileName <-system.file("extdata", "Assay_3_and_4.txt", package="ELISAtools")
plates<-read.plates(fileName, annotations=annotations, num.plate=2, batchID="b1", expID="e1")</pre>
```

reportHtml

Report ELISA data in HTML format.

Description

Writting the ELISA analysis results by batch in HTML format.

Usage

```
reportHtml(batches, file.name = "report", file.dir = ".", desc = "")
```

Arguments

| batches | list of elisa batch data objects. The data can be raw or after analyzed and batch- corrected. |
|-----------|--|
| file.name | character string denoting the report file. The file will be written in HTML for- mat. |
| file.dir | character string denoting the directory to save the report. |
| desc | character string describing the project and experiment. Will be written into the report. |

Value

the function returns NULL. But it will save the html report to the disk. Therefore, it is IMPORTANT to specify a directory you have write permission to run this function.

See Also

elisa_batch elisa_run elisa_plate

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runFit

Examples

```
#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
##
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
```

```
#----IMPORTANT-----
#please make sure you have the write permission to save the html report
reportHtml(batches,file.dir=tempdir());
```

```
runFit
```

Fit 5- or 4-parameter logistic function

Description

Fit 5- or 4-parameter logistic function to estimate the parameters by pooling the standard curves from all batches

Usage

```
runFit(pars, a, d, batches, refBatch.ID = 1, model = c("5pl", "4pl"))
```

Arguments

| pars | numeric vector initial values to estimate the paramters |
|-------------|---|
| а | numeric the initial value for a (the lower limit of the function) |
| d | numeric the initial value for d (the upper limit of the function) |
| batches | list of the batch data used to fit the model |
| refBatch.ID | numeric or string indicating the reference batch, by default is set to be the first one. |
| model | characters to indicate either 5-parameter logistic function (5pl, default one) or 4-parameter logistic (4pl) to be used in the fitting. |

Details

In this fitting, we first "guess" the initial values and then estimate the parameters based on 5- or 4-parameter function by shifting every single standard curves towards the reference line. We are reasoning that the intra-batch and inter-batch factors affect the curve similarly by shifting the curve left or right without changing its shapes. So we combine them together to to fit one single reference

curve. To model the inter-batch effects, we take the average of the shifts of curves withine each batch, and use it to correct/normalize between different batches.

To summerize, each individual curve has its own shifts, which contains the information about intraand inter-batch effects. each batch has one batch level shifts (S Factor), which is an average of shifts of curves within its batch and contains information about inter-batch effects. When we try to normalize between batches, we will apply the batch level shift to all the curves within the same batch.

Value

the batch data with the fitted model

References

Feng, et al 2018 https://doi.org/10.1101/483800

Examples

```
#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
#get file folder
```

```
dir_file<-system.file("extdata", package="ELISAtools")</pre>
```

batches<-loadData(file.path(dir_file,"design.txt"))</pre>

```
#make a guess for the parameters, the other two parameters a and d
#will be estimated based on data.
model<-"5pl"
pars<-c(7.2,0.5, 0.015) #5pl inits
names(pars)<-c("xmid", "scal", "g")</pre>
```

```
#do fitting. model will be written into data set.
batches<-runFit(pars=pars, batches=batches, refBatch.ID=1, model=model )</pre>
```

saveDataText Save elisa_batch analysis results

Description

Save the data analysis results to disk in text format.

Usage

saveDataText(batches, file.name)

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saveDB

Arguments

| batches | list of elisa batch data to be serialized. |
|-----------|---|
| file.name | character specifying name of the output file. |

Details

The results are written to disk in the text format (tab-delimited) and is easy to be used for other analysis.

Examples

```
#'#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")</pre>
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
#make a guess for the parameters, the other two parameters a and d
#will be estimated based on data.
model<-"5pl"
pars<-c(7.2,0.5, 0.015) #5pl inits
names(pars)<-c("xmid", "scal", "g")</pre>
#do fitting. model will be written into data set.
batches<-runFit(pars=pars, batches=batches, refBatch.ID=1, model=model )</pre>
#now call to do predications based on the model.
batches<-predictAll(batches);</pre>
#now saving the data in text.
saveDataText(batches, file.path(tempdir(),"elisa_data.txt"));
```

saveDB

Save the elisa_batch data

Description

Serialize elisa_batch data to disk.

Usage

saveDB(batches, db)

saveDB

Arguments

| batches | list of elisa batch data to be serialized. |
|---------|--|
| db | character the file name specifying name of the db. |

Details

We serialize elisa_batch data by wrapping the saveRds() function call. The serialized elisa_batch data are assumed to have been correctly analyzed. We will print a summary for what has been saved.

See Also

elisa_batch-class loadData saveDB

Examples

```
#R code to run 5-parameter logistic regression on ELISA data
#load the library
library(ELISAtools)
```

```
#get file folder
dir_file<-system.file("extdata", package="ELISAtools")</pre>
```

```
batches<-loadData(file.path(dir_file,"design.txt"))</pre>
```

```
#make a guess for the parameters, the other two parameters a and d
#will be estimated based on data.
model<-"5pl"
pars<-c(7.2,0.5, 0.015) #5pl inits
names(pars)<-c("xmid", "scal", "g")</pre>
```

```
#do fitting. model will be written into data set.
batches<-runFit(pars=pars, batches=batches, refBatch.ID=1, model=model )</pre>
```

```
#now call to do predications based on the model.
batches<-predictAll(batches);</pre>
```

```
#now saving the data.
saveDB(batches, file.path(tempdir(),"elisa_tool1.rds"));
```

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