

# Package ‘BBEST’

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**Type** Package

**Title** Bayesian Estimation of Incoherent Neutron Scattering Backgrounds

**Description** We implemented a Bayesian-statistics approach for subtraction of incoherent scattering from neutron total-scattering data. In this approach, the estimated background signal associated with incoherent scattering maximizes the posterior probability, which combines the likelihood of this signal in reciprocal and real spaces with the prior that favors smooth lines.

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## R topics documented:

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|               |  |
|---------------|--|
| BBEST-package | <i>Bayesian Background Estimation.</i> |
|---------------|--|

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## Description

In this package we implemented a Bayesian-statistics approach for subtraction of incoherent scattering from neutron total-scattering data. In this approach, the estimated background signal associated with incoherent scattering maximizes the posterior probability, which combines the likelihood of this signal in reciprocal and real spaces with the prior that favors smooth lines.

To cite the BBEST package type: 'citation("BBEST")' (without the single quotes).

For a listing of all routines in the BBEST package type: 'library(help="BBEST")'

To start the Graphical User Interface type: 'runUI()'

To start a simple command-line guide type: 'guide()'

## Details

|          |            |
|----------|------------|
| Package: | BBEST      |
| Type:    | Package    |
| Version: | 0.1-0      |
| Date:    | 2014-08-11 |
| License: | GPL-3      |

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**References**

BBEST-package

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calc.Gr

*Calculate and plot the Pair Distribution Function*

---

**Description**

Calculates and plots the corrected Pair Distribution Function.

**Usage**

```
calc.Gr(fit.results, rho.0, plot=TRUE, r.min = 0, r.max = 5,
        dr = 0.01, Q.min = NA, Q.max = NA, nsd = 2, gr.compare=NA)
```

**Arguments**

|                  |   |
|------------------|---|
| fit.results      | the return value of <code>do.fit</code> .   |
| plot             | logical, whether to plot the PDF.   |
| rho.0            | numeric, the atomic number density of the material: the number of atoms per unit cell divided by a volume of the unit cell.   |
| r.min, r.max, dr | numerics. Function is plotted in the region <code>[r.min, r.max]</code> .   |
| Q.min, Q.max     | numerics. To calculate the sine-Fourier transform, the total scattering function $S(Q)$ is "terminated" at a certain $Q=Q_{max}$ point. The best $Q_{max}$ point to terminate $S(Q)$ (that corresponds to the value of $S(Q)-1$ closest to zero) is sought in the <code>[Q.min, Q.max]</code> region. |
| nsd              | numeric, the number of standard deviations to plot the uncertainty.   |
| gr.compare       | numeric vector. If not NA, specifies the function to add to the plot. Should correspond to the same grid ( <code>[r.min, r.max, dr]</code> ).   |

**Details**

The function uses `ggplot2` package for plotting. `ggplot2` package can be installed by typing `install.packages("ggplot2")`.

**Value**

A list with elements:

|       |   |
|-------|---|
| r     | numeric vector of grid points                                       |
| gr    | numeric vector, indicates the corrected Pair Distribution Function. |
| stdev | numeric vector, indicates estimated standard deviation.             |

**See Also**

[do.fit](#)

---

|        |                            |
|--------|----------------------------|
| do.fit | <i>Estimate background</i> |
|--------|----------------------------|

---

**Description**

do.fit estimates the bacground using the Bayesian approach and Differential Evolution algorithm.

**Usage**

```
do.fit(data, bounds.lower, bounds.upper, scale=c(1,1), knots.x=NA,
       knots.n=NA, analytical=FALSE, stdev=TRUE, control=list(), p.bkg=.5,
       save.to="")
```

**Arguments**

|                            |   |
|----------------------------|---|
| data                       | an object of type data. See <a href="#">set.data</a> for details.   |
| bounds.lower, bounds.upper | numerics specifying the lower and upper bounds for the fitted spline values.  |
| scale                      | numeric vector which, if applicable, determines the bounds for the fitted scale parameter. The default value of c(1,1) means a no-scale fit. See details.         |
| knots.x                    | numeric vector which, if not NA, specifies the knot positions.  |
| knots.n                    | numeric, the number of knots. If knots.x is NA then knots.n equidistant knots will be created.  |
| analytical                 | logical. If TRUE background is approximated by an analytical function $f(x) = P_1 \exp(-P_2 x) x^{P_3} + P_4 / [(x - P_5)^2 + P_6^2]$ .                           |
| stdev                      | logical, whether to calculate the uncertainty for the estimated background. Should be set to FALSE if analytical=TRUE.  |
| control                    | list, the return value of <a href="#">set.control</a> . Specifies various parameters of the Differential Evolution optimization algorithm implemented in DEoptim. |
| p.bkg                      | numeric, the probability that a single pixel contains "only" a background.  |
| save.to                    | character, a filename for saving the results.   |

## Details

If information on the low- $r$  behavior of  $G(r)$  is provided, the global intensity scale and atomic displacement parameters can be fitted along with the positions of the knots, ([set.Gr](#)). To fit normalization parameter set bounds in `scale` for the desired values. To fit Atomic Displacement Parameters see [set.SB](#).

In most cases `p.bkg` should be set to its default value 0.5.

For further details see [BBEST-package](#).

## Value

A list with elements:

|                          |   |
|--------------------------|---|
| <code>x</code>           | numeric vector of grid points   |
| <code>curves</code>      | list, see below.  |
| <code>uncrt</code>       | list, see below.  |
| <code>knots</code>       | list with elements <code>x</code> and <code>y</code> that specify the positions of the knots and the corresponding fitted intensity values, respectively. |
| <code>pars</code>        | numeric vector. If the background is approximated using the analytical function, contains all the relevant parameters <code>P</code> .                    |
| <code>scale</code>       | fitted value of the <code>scale</code> parameter, if used.  |
| <code>ADP</code>         | fitted values of the atomic displacement parameters, if applicable.   |
| <code>fit.details</code> | list, see below.  |

Element `curves` is a list with sub-elements:

|                  |   |
|------------------|---|
| <code>y</code>   | numeric vector of the (normalized) function values. |
| <code>bkg</code> | numeric vector, the estimated background.           |
| <code>SB</code>  | numeric vector, the (fitted) coherent baseline.     |

Element `uncrt` is a list with sub-elements:

|                           |   |
|---------------------------|---|
| <code>stdev</code>        | numeric vector, indicates estimated standard deviations for the reconstructed signal.             |
| <code>stdev.r</code>      | numeric vector, indicates estimated standard deviations for a reconstructed signal in $r$ -space. |
| <code>hess</code>         | Hessian matrix for a $\psi(c)$ function.  |
| <code>cov.matrix</code>   | covariance matrix, i.e. the inverse of the Hessian.   |
| <code>cov.matrix.r</code> | covariance matrix in $r$ -space.  |

Element `fit.details` is a list with sub-elements:

|                      |   |
|----------------------|---|
| <code>lambda</code>  | numeric vector, the estimated mean magnitude of the signal. |
| <code>sigma</code>   | numeric vector, the estimated Gaussian noise.               |
| <code>knots.n</code> | the number of knots used in the fit.                        |
| <code>knots.x</code> | knot positions used in the fit.                             |

|                |  |
|----------------|--|
| control        | see the control argument.  |
| Gr             | list containing information on the low-r behaviour of G(r) . See <a href="#">set.Gr</a> for details. |
| n.atoms        | numeric vector, number of different atoms per unit cell.   |
| scatter.length | numeric vector, atomic scattering factors.   |

## References

- Ardia, D., Mullen, K., Peterson, B. & Ulrich, J. (2011): DEoptim. R Package Version 2.2-2. <http://CRAN.R-project.org/package=DEoptim>.
- Mullen, K.M., Ardia, D., Gil, D., Windover, D., Cline, J. (2011): DEoptim: An R Package for Global Optimization by Differential Evolution. *J. Stat. Softw.*, **40**(6), 1-26. <https://www.jstatsoft.org/article/view/v040i06>.

---

|              |   |
|--------------|---|
| do.fit.banks | <i>Estimate the background for individual banks</i> |
|--------------|---|

---

## Description

do.fit estimates the background for individual banks according to the Bayesian approach using the Differential Evolution algorithm

## Usage

```
do.fit.banks(data, bounds.lower, bounds.upper, knots.n.left,
             knots.n.right, x.boundary, analytical=FALSE, control,
             save.to="")
```

## Arguments

|   |   |
|---|---|
| data                                    | an object of type data. See <a href="#">set.data</a> for details.   |
| bounds.lower, bounds.upper              | numerics, lower and upper bounds for the fitted spline values.  |
| knots.n.left, knots.n.right, x.boundary | numerics that specify the number of knots. knots.n.left and knots.n.right knots are created on the left and on the right of x.boundary point, respectively.       |
| analytical                              | logical. If TRUE background is approximated by an analytical function $f(x) = P_1 \exp(-P_2 x) x^{P_3} + P_4 / [(x - P_5)^2 + P_6^2]$ .                           |
| control                                 | list, the return value of <a href="#">set.control</a> . Specifies various parameters of the Differential Evolution optimization algorithm implemented in DEoptim. |
| save.to                                 | character, a filename for saving the results.   |

**Details**

This function simplifies the procedure for estimating the background for several detector banks by a multiple call of `do.fit`. Other relevant parameters are set to: `stdev=FALSE`, `scale=NA`, `p.bkg=.5`.

For neutron scattering, the incoherent background exhibits a broad peak at low Q and decays gradually at higher Q. Hence, we suggest to use different numbers of knots for the low- and high-Q regions. See [BBEST-package](#) for details.

**Value**

A list of elements. Each element contains a return value of `do.fit` for the corresponding data bank.

**See Also**

[do.fit](#), [BBEST-package](#)

---

|                      |                                |
|----------------------|--------------------------------|
| <code>do.iter</code> | <i>Estimate the background</i> |
|----------------------|--------------------------------|

---

**Description**

`do.iter` performs adaptive Bayesian estimation of the background.

**Usage**

```
do.iter(fit.results, local = TRUE, eps = 1e-04,
        n.iter = 10000, save.to = "")
```

**Arguments**

|                          |  |
|--------------------------|--|
| <code>fit.results</code> | list. The return value of <code>do.fit</code> .  |
| <code>local</code>       | logical. If TRUE, gradient descent method is used to find background estimation. If FALSE, Differential Evolution is used. |
| <code>eps</code>         | numeric, the desired accuracy for spline values.   |
| <code>n.iter</code>      | numeric, number of iterations for a gradient descent method, see details.  |
| <code>save.to</code>     | character, the filename for saving the results.  |

**Details**

An adaptation of neutron scattering data for a Bayesian background separation procedure. The method is detailed elsewhere\*.

First, use the function `do.fit` to estimate the background *from* the low-r information in  $G(r)$ . `do.iter` procedure estimates the background *without* low-r information, calculates the difference between the two estimates, subtracts this difference from the scattering data and finds the new estimate of the background.

**Value**

An object `fit.results` with modified elements `fit.results$curves$bkg`, `fit.results$curves$y` and `fit.results$curves$corr`. See [do.fit](#) for details.

**References**

\*Gagin, A. and Levin, I. Hydrogen background estimation in neutron total scattering experiments. Submitted for publication.

---

|                        |                         |
|------------------------|-------------------------|
| <code>fix.merge</code> | <i>Merge .fix files</i> |
|------------------------|-------------------------|

---

**Description**

`fix.merge` merges several `.fix` files into a specified file in a form suitable for *PDFgetN*.

**Usage**

```
fix.merge(outfile, infile1, infile2, ...)
```

**Arguments**

`outfile` character, the filename for saving the data.  
`infile1, infile2, ...`  
files to merge.

**See Also**

[write.fix](#), [read.sqa](#), [do.fit.banks](#), [BBEST-package](#)

---

|                    |                    |
|--------------------|--------------------|
| <code>guide</code> | <i>BBEST guide</i> |
|--------------------|--------------------|

---

**Description**

`guide` is a function that guides through the Bayesian procedure for estimating the background

**Usage**

```
guide()
```

**Value**

A list with elements:

`fit.res` the return value of [do.fit](#).  
`data` an object of type `data`, see [set.data](#).  
`gr` the return value of [calc.Gr](#).



---

|               |                                     |
|---------------|-------------------------------------|
| mPlot.results | <i>Plot the background estimate</i> |
|---------------|-------------------------------------|

---

**Description**

Plots the estimated background and the corrected function.

**Usage**

```
mPlot.results(fit.results, label.x = "x", label.y = "y",
              xlim=NA, ylim=NA)
```

**Arguments**

`fit.results` the return value of `do.fit`.  
`label.x, label.y` characters, titles for x and y axes.  
`xlim, ylim` numeric vectors with two entries. If not NA, specify x- and y-axis limits.

**Details**

The function uses `ggplot2` and `gridExtra` packages for plotting. Packages can be installed by typing `install.packages("ggplot2")` and `install.packages("gridExtra")`.

**See Also**

[do.fit](#)

---

|                     |  |
|---------------------|--|
| mPlot.results.banks | <i>Plot the background estimate for individual banks</i> |
|---------------------|--|

---

**Description**

Plots the background estimate for individual detector banks.

**Usage**

```
mPlot.results.banks(fit.results, label.x = "x", label.y = "y",
                    xlim=NA, ylim=NA)
```

**Arguments**

`fit.results` the return value of `do.fit.banks`.  
`label.x, label.y` characters, titles for x and y axes.  
`xlim, ylim` numeric matrices of size  $(NB, 2)$ , where NB is the number of data banks. If not NA, specify x- and y-axis limits.

**See Also**

[do.fit.banks](#)

---

|           |  |
|-----------|--|
| mPlot.sqa | <i>Plot the total normalized scattering intensity function <math>S(Q)</math> for individual detector banks</i> |
|-----------|--|

---

**Description**

The function plots the total scattering functions  $S(Q)$  returned by PDFgetN in [read.sqa](#).

**Usage**

```
mPlot.sqa(data)
```

**Arguments**

data            list, the return value of [read.sqa](#).

**See Also**

[read.sqa](#)

---

|                    |   |
|--------------------|---|
| prepare.banks.data | <i>Prepare data for estimating the background</i> |
|--------------------|---|

---

**Description**

prepare.banks.data sets all the fit parameters, such as sigma, lambda and SB for a set of detector banks.

**Usage**

```
prepare.banks.data(data, n.banks=4, lambda_1, lambda_2, lambda_0,
                   x_1, x_2, n.atoms, scatter.length, ADP, n.regions)
```

**Arguments**

data            list of objects of type data. See [read.sqa](#) and [set.data](#) for details.

n.banks        numeric, number of banks.

lambda\_1, lambda\_2, lambda\_0, x\_1, x\_2  
               parameters to be passed to [set.lambda](#).

n.atoms, scatter.length, ADP  
               parameters to be passed to [set.SB](#).

n.regions      parameter to be passed to [set.sigma](#).

**Details**

This function simplifies setting the fit parameters for a set of detector banks by a multiple call of [set.sigma](#), [set.SB](#), and [set.lambda](#).

**Value**

A list of objects of type data suitable for [do.fit.banks](#).

**See Also**

[set.sigma](#), [set.SB](#), [set.lambda](#)

---

|           |                            |
|-----------|----------------------------|
| read.data | <i>Read data from file</i> |
|-----------|----------------------------|

---

**Description**

Reads data from a text file with columns "x", "y", and, optionally, "lambda", "sigma" and "SB".

**Usage**

```
read.data(file = stop("'file' must be specified"), ...)
```

**Arguments**

|      |   |
|------|---|
| file | character, the name of the file which the data are to be read from.   |
| ...  | further arguments to be passed to <code>read.table</code> (optional). |

**Details**

This function implements one of the ways to load experimental data. The file must consist of a header with column names and several columns below. First two columns in file must be x and y values. The others could specify lambda, sigma and SB.

**Value**

An object of type data. See [set.data](#) for details.

---

|          |                                   |
|----------|-----------------------------------|
| read.sqa | <i>Read data from a .sqa-file</i> |
|----------|-----------------------------------|

---

### Description

This function reads .sqa-files generated by *PDFgetN*, which contain corrected total-scattering functions bank by bank.

### Usage

```
read.sqa(file = stop("'file' must be specified"))
```

### Arguments

file                    character, the name of the file which the data are to be read from.

### Value

List those elements are objects of type data. See [set.data](#) for details.

### References

Peterson, P.F., Gutmann, M., Proffen, TH. & Billinge, S.J.L. (2000): PDFgetN: A User-Friendly Program to Extract the Total Scattering Structure Function and the Pair Distribution Function from Neutron Powder Diffraction Data. *J. Appl. Cryst.*, **33**, 1192. [http://www.pa.msu.edu/cmp/billinge-group/programs/pdfgetn/pdfgetn\\_jac.pdf](http://www.pa.msu.edu/cmp/billinge-group/programs/pdfgetn/pdfgetn_jac.pdf).

Proffen, TH., Peterson, P.F., Gutmann, M. & Billinge, S.J.L. (2009): PDFgetN Users Guide Version 1.6.6. <http://pdfgetn.sourceforge.net/>.

### See Also

[mPlot.sqa](#)

---

|          |                                   |
|----------|-----------------------------------|
| read.sqb | <i>Read data from a .sqb-file</i> |
|----------|-----------------------------------|

---

### Description

This function reads .sqb-files generated by *PDFgetN*, which contain the corrected and blended total-scattering function  $S(Q)$ .

### Usage

```
read.sqb(file = stop("'file' must be specified"))
```

**Arguments**

file                    character, the name of the file which the data are to be read from.

**Value**

An object of type data. See [set.data](#) for details.

**References**

Peterson, P.F., Gutmann, M., Proffen, TH. & Billinge, S.J.L. (2000): PDFgetN: A User-Friendly Program to Extract the Total Scattering Structure Function and the Pair Distribution Function from Neutron Powder Diffraction Data. *J. Appl. Cryst.*, **33**, 1192. [http://www.pa.msu.edu/cmp/billinge-group/programs/pdfgetn/pdfgetn\\_jac.pdf](http://www.pa.msu.edu/cmp/billinge-group/programs/pdfgetn/pdfgetn_jac.pdf).

Proffen, TH., Peterson, P.F., Gutmann, M. & Billinge, S.J.L. (2009): PDFgetN Users Guide Version 1.6.6. <http://pdfgetn.sourceforge.net/>.

---

runUI

*Start the GUI*

---

**Description**

Starts the application and opens up the default web browser to view it.

**Usage**

```
runUI()
```

**Details**

Runs a **Shiny** application. This function normally does not return; interrupt boldR to stop the application (usually by pressing Ctrl+C or Esc).

---

set.control

*Set controls for the Differential Evolution Algorithm*

---

**Description**

Specifies various parameters of the Differential Evolution optimization algorithm implemented in DEoptim.

**Usage**

```
set.control(CR=.85, F=.7, NP=300, itermax=2000, parallelType=1)
```

**Arguments**

|              |  |
|--------------|--|
| CR           | numeric, crossover probability from interval [0,1].  |
| F            | numeric, differential weighting factor from interval [0,2].  |
| NP           | numeric, number of population members  |
| itermax      | numeric, the number of iterations  |
| parallelType | numeric, defines the type of parallelization to employ. 0 for a single-core run. If parallelType=1 the program will use all the available cores, via the parallel package. |

**Details**

For the most tasks, it is best to set NP to at least 10-15 times the length of the parameter vector.

**Value**

a list of elements suitable for `do.fit` and `do.fit.banks`.

**References**

Mullen, K.M., Ardia, D., Gil, D., Windover, D., Cline, J. (2011): DEoptim: An R Package for Global Optimization by Differential Evolution. *J. Stat. Softw.*, **40**(6), 1-26. <https://www.jstatsoft.org/article/view/v040i06>.

---

set.data

*Set data*

---

**Description**

The function sets key parameters necessary for the fit, such as sigma, lambda and SB

**Usage**

```
set.data(x, y, sigma=NA, lambda=NA, SB=NA)
```

**Arguments**

|        |   |
|--------|---|
| x      | numeric vector, specifies grid points.                                |
| y      | numeric vector, specifies function values.                            |
| sigma  | numeric vector, if not NA, specifies estimated noise.                 |
| lambda | numeric vector, if not NA, specifies estimated mean signal magnitude. |
| SB     | numeric vector, if not NA, specifies estimated coherent baseline.     |

## Details

One way (not the simplest) to prepare experimental data for the fit. This function returns a list of the above parameters – an object of type `data`. Objects of that type are used as arguments for some functions implemented in the package. In most cases only the elements `x` and `y` are required in the object `data`. However, all 5 elements (and one optional, see `set.Gr`) must be specified to execute the fit, i.e. prior to the `do.fit` call.

The object of that type can also be created via `read.data`, `read.sqa` and `read.sqb`. Parameters "sigma", "lambda" and "SB" can be determined automatically, see `set data` keyword.

The general recipe for setting an object `data` is the following. If vectors `x` and `y` are stored in the text file, use `read.data`. If they are stored in a `.sqb`-file, call `read.sqb`. If they are stored in the memory, use `set.data`. Then use functions `set.sigma`, `set.lambda`, and `set.SB` to specify the remaining parameters.

## Value

A list with elements

|                     |  |
|---------------------|--|
| <code>x</code>      | numeric vector, specifies gridpoints.                      |
| <code>y</code>      | numeric vector, specifies function values.                 |
| <code>sigma</code>  | numeric vector, specifies estimated noise.                 |
| <code>lambda</code> | numeric vector, specifies estimated mean signal magnitude. |
| <code>SB</code>     | numeric vector, specifies estimated coherent baseline.     |

---

`set.Gr`

*Add information on the low-r behaviour of  $G(r)$*

---

## Description

Function to incorporate information on the low-r behaviour of  $G(r)$  into the Bayesian model.

## Usage

```
set.Gr(data, r1=seq(0, 1, 0.005), r2=NA, rho.0,
       type1="gaussianNoise", type2=NA, sigma.f=NA, l=NA)
```

## Arguments

|                           |   |
|---------------------------|---|
| <code>data</code>         | an object of type <code>data</code> . See <code>set.data</code> for details.  |
| <code>r1, r2</code>       | numeric vectors, specify grids on which the $G(r)$ behaviour is controlled.   |
| <code>rho.0</code>        | numeric, atomic number density of the material: a number of atoms per unit cell divided by a volume of the unit cell. |
| <code>type1, type2</code> | characters, specify the way to control the behavior of $G(r)$ . See details.  |
| <code>sigma.f, l</code>   | numerics or numeric vectors, specify parameters for a squared-exponential covariance function.                        |

**Details**

type1 can be either "gaussianNoise" or "correlatedNoise".  $G(r)$  is restricted to the  $-4\pi\rho_0r_1$  line plus independent Gaussian noise or correlated Gaussian noise, respectively.

type2 can be either "secondDeriv" or "gaussianProcess" to impose smoothness conditions over the interval  $r_2$ . If type2 is "secondDeriv", a minimum of the second derivative is sought. If type2 is "gaussianProcess", the smoothness is controlled via the Gaussian process using parameters sigma.f and l.

According to our experience, the most efficient way is to impose type1="gaussianNoise" and type2=NA conditions.

**Value**

An object of type data.

---

|            |                                  |
|------------|----------------------------------|
| set.lambda | <i>Set mean signal magnitude</i> |
|------------|----------------------------------|

---

**Description**

set.lambda sets the mean height of the peaks over region x.

**Usage**

```
set.lambda(data, lambda=NA, lambda_1=NA, lambda_2=NA,
           lambda_0=NA, x_1=NA, x_2=NA)
```

**Arguments**

data            an object of type data. See [set.data](#) for details.

lambda         numeric vector. If not NA, specifies (approximate) the mean magnitude of the signal. This estimate does not need to be accurate. lambda can be estimated as a smooth function that crosses centres of the signal peaks.

lambda\_1, lambda\_2, lambda\_0, x\_1, x\_2  
                numerics. If lambda is NA help to estimate lambda. See details.

**Details**

lambda is calculated as a linear piecewise function which is equal to lambda\_0 outside the  $[x_1, x_2]$  region. Inside this region, lambda is approximated by a line connecting points  $(x_1; \lambda_1)$  and  $(x_2; \lambda_2)$ .

**Value**

An object of type data. Element

lambda         numeric vector containing an approximate mean magnitude of the signal.

is replaced with its new value.



---

|        |                                  |
|--------|----------------------------------|
| set.SB | <i>Set the coherent baseline</i> |
|--------|----------------------------------|

---

### Description

set.SB sets the baseline, describing coherent neutron scattering caused by uncorrelated atomic motion or any other baseline that needs to be preserved in the recovered signal.

### Usage

```
set.SB(data, SB=NA, n.atoms=NA, scatter.length=NA, ADP=NA,
       fit=FALSE, oneADP=TRUE, ADP.lim = c(0, 0.05))
```

### Arguments

|                              |  |
|------------------------------|--|
| data                         | an object of type data. See <a href="#">set.data</a> for details.  |
| SB                           | numeric vector which, if not NA, determines the baseline. See <a href="#">BBEST-package</a> for details.   |
| n.atoms, scatter.length, ADP | numerics. Specify the number of atoms of each atomtype in the unit cell, atomic scattering factors and atomic displacement parameters (ADP), respectively. |
| fit                          | logical, whether to fit ADP.   |
| oneADP                       | logical. If TRUE a single parameter is used for all the APDs.  |
| ADP.lim                      | numeric vector that specifies the lower and upper bounds for the fitted ADP.   |

### Details

Baseline SB has to be specified. If no baseline is needed fill SB with zeroes. If n.atoms, scatter.length and ADP parameters are specified, the baseline is calculated according to

$$SB(x) = 1 - \frac{\sum_i N_i f_i^2 e^{-ADP_i x^2}}{N \langle f^2 \rangle} \left(1 - \frac{\langle f \rangle^2 - \langle f^2 \rangle}{\langle f \rangle^2}\right).$$

If ADP parameters are to be fitted, indicate n.atoms, scatter.length and set parameter fit to TRUE. Set oneADP to the desired value.

### Value

An object of type data. Element

SB                    numeric vector containing the baseline.

is replaced with its new value. Element

fitADP                a list of values.

might be added to describe the fit details.

---

|           |   |
|-----------|---|
| set.sigma | <i>Set the experimental uncertainty</i> |
|-----------|---|

---

### Description

This function either sets the pointwise experimental uncertainty or estimates it using `wmts` library.

### Usage

```
set.sigma(data, sigma=NA, x.bkg.only=NA, n.regions=10, thresh.scale=1)
```

### Arguments

|                           |   |
|---------------------------|---|
| <code>data</code>         | an object of type <code>data</code> . See <a href="#">set.data</a> for details.   |
| <code>sigma</code>        | numeric vector which, if not <code>NA</code> , determines the pointwise experimental uncertainty.   |
| <code>x.bkg.only</code>   | if parameter <code>sigma</code> is <code>NA</code> , determines the peak-free region used to estimate the noise.  |
| <code>n.regions</code>    | if both parameters <code>sigma</code> and <code>x.bkg.only</code> are <code>NA</code> , the grid is split into <code>n.regions</code> equal regions. The noise is then estimated for each of these regions. See details |
| <code>thresh.scale</code> | numeric vector or scalar which is used to amplify or attenuate the threshold values for a wavelet shrinkage.  |

### Details

We assume the experimental uncertainty to have a Gaussian distribution with `x`-dependent amplitude. Splitting the grid into `n.regions` segments and estimating Gaussian standard deviations over each of these segments allows us to approximate the true distribution.

The function uses `wavShrink` package that performs a decimated discrete wavelet transform for signal smoothing. The use of `thresh.scale` argument signifies a departure from a model driven estimate of the thresholds and can be used to tweak the levels to obtain a smoother or rougher result.

### Value

An object of type `data`. Elements

|                       |  |
|-----------------------|--|
| <code>sigma</code>    | numeric vector containing the estimated noise level.   |
| <code>smoothed</code> | if both parameters <code>sigma</code> and <code>x.bkg.only</code> are <code>NA</code> contains a smoothed estimate of the regression function. |

are replaced with their new values.

### References

Percival, D. B. and Walden, A. T. (2000): *Wavelet Methods for Time Series Analysis*, Cambridge University Press.

Percival, D. B. (2013): `wmts`: Wavelet Methods for Time Series Analysis Version 2.0-0. <http://CRAN.R-project.org/package=wmts>.

**Examples**

```
# Setting x and y
x <- seq(.7, 30, 0.01)
y <- sin(x)
# Adding x-dependent noise
y <- y + rnorm(sd=0.05+x/240, n=length(x))

# estimating noise
dat <- list(x=x, y=y)
dat <- set.sigma(dat, n.regions=1)
# use
# dat <- set.sigma(dat, n.regions=5)
# to see the difference

# Plotting results: noisy function and a
# smoothed estimate +/- 2 standard deviations
plot(x, y, t="l")
lines(dat$x, dat$smoothed, col=3, lwd=2)
lines(dat$x, dat$smoothed+2*dat$sigma, col=2)
lines(dat$x, dat$smoothed-2*dat$sigma, col=2)
abline(v=seq(min(x), max(x),length=5), col=4)
```

---

sqa.split

*Split .sqa file into individual files for each databank*

---

**Description**

sqa.split splits *PDFgetN* .sqa-file into individual files for each databank.

**Usage**

```
sqa.split(file = stop("'file' must be specified"))
```

**Arguments**

file                    character, name of the source file.

**See Also**

[read.sqa](#), [do.fit.banks](#), [BBEST-package](#)

---

|             |   |
|-------------|---|
| test.signal | <i>A random function with a smooth background</i> |
|-------------|---|

---

### Description

test.signal creates a random function that consists of peaks, a smooth background, and a Gaussian noise.

### Usage

```
test.signal(x, lambda, sigma, x.delta, knots.n, peaks.widthRange, peaks.n)
```

### Arguments

|                  |   |
|------------------|---|
| x                | numeric vector, the x-points where data should be generated.                              |
| lambda           | numeric, the mean signal magnitude.   |
| sigma            | numeric, the noise level.   |
| x.delta          | numeric, the minimum spacing allowed between spline knots. Defines background smoothness. |
| knots.n          | numeric, a number of spline knots to generate.  |
| peaks.widthRange | numeric vector, specifies range in peak widths.   |
| peaks.n          | numeric, the number of peaks to generate.   |

### Details

The background is calculated as a sum of fundamental splines on the randomly generated knots. The function is a sum of the background, random peaks, and Gaussian noise.

### Value

An object of type data (see [set.data](#)) with the following elements added:

|       |   |
|-------|---|
| knots | list with elements x and y that specify the knot positions and knot values, respectively. |
| bkg   | numeric vector containing the generated background.                                       |

### Examples

```
# 1. Create test function
f <- test.signal(x=seq(0,30,0.01), lambda=5,
  sigma=0.1, x.delta=1.0, knots.n=5,
  peaks.widthRange=c(0.1, 0.3), peaks.n=7)

# 2. Plot results
plot(f$x, f$y, t="l", xlab="x", ylab="f")
```

```

lines(f$x, f$bkg, col=2)
lines(f$x, f$y - f$bkg, col="gray")
legend(20, .9*max(f$y), c("test function", "background",
      "peaks+noise"), lty=1, col=c(1,2,"gray"))

```

---

trim.data

*Truncate data*


---

## Description

The function truncates the data (deletes low- and high-x information).

## Usage

```
trim.data(data, x.min, x.max)
```

## Arguments

`data` an object of type data. See [set.data](#) for details.  
`x.min, x.max` numeric values determining the region to keep.

## Details

Frequently, the experimental data need to be truncated to remove unwanted ranges.

## Value

an object of type data with all functions cropped to the region [`x.min`, `x.max`]

## Examples

```

# prepare data
x <- seq(0, 50, 0.01)
y <- .8*exp(-x)*x^4
dat <- list(x=x, y=y)
# truncate
dat <- trim.data(dat, 1, 25)
# plot results
plot(x,y,t="1",lwd=4, col=4)
lines(dat$x, dat$y, lwd=4, col=2)
legend(15,3,c("initial", "truncated"), lty=1, col=c(4,2))

```

`write.fit.results`      *Save results of the fit*

---

**Description**

`write.fit.results` writes the returned value of `do.fit` to a specified text file.

**Usage**

```
write.fit.results(fit.results, file = stop("'file' must be specified"))
```

**Arguments**

`fit.results`      list, the return value of `do.fit`.  
`file`              character, the filename for saving the data.

**See Also**

[do.fit](#), [BBEST-package](#)

---

`write.fix`              *Save a correction file for individual detector banks*

---

**Description**

`write.fix` writes corrections obtained using `do.fit.banks` to a specified file in a form suitable for *PDFgetN*.

**Usage**

```
write.fix(fit.results, file = stop("'file' must be specified"))
```

**Arguments**

`fit.results`      list, the return value of `do.fit.banks`.  
`file`              character, the filename for saving the data.

**See Also**

[read.sqa](#), [do.fit.banks](#), [BBEST-package](#)

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