Package 'multiscan'

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Title R package for combining multiple scans

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Description Estimates gene expressions from several laser scans of the same microarray

License GPL (>= 2)

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multiscan   *Combining multiple laser scans of microarray data*

Description

Estimates gene expressions from multiple laser scans of microarrays using non-linear functional regression model with additive plus multiplicative errors.

Usage

```
multiscan(data, initial = NULL, na.rm = TRUE, verbose = FALSE, control = list())
```

Arguments

data   A numeric matrix or data frame containing the intensity data of a single microar-
                ray scanned at multiple (two or more) scanner settings. For dual channel arrays,
                multiscan should be run on each channel of data separately. The number of
                rows (n) is equal to the number of spots/probes on the array, and the number of
                columns (m) equals the number of scans. Columns will be arranged in order of
                scanner's sensitivity before fitting the model. Replicated probes on the array are
                treated as individual spots.

initial   A vector of length m+2 to be used as initial values for the scanning effects
                $(\beta_2, \cdots, \beta_m)$ and scale $(\sigma_1, \sigma_2, \nu)$ parameters. If it is NULL (default), the initial
                values are determined from the data.

na.rm   Logical. Should missing values be removed? Defaults to TRUE.

verbose   Logical. If TRUE, some intermediate results are printed as the iteration proceeds.

control   A list of control parameters. See 'Details'.

Details

The function implements the method of Khondoker *et. al.* (2006) for combining multiple laser
scans of microarrays. This function is computationally slow and memory-intensive. That is due
to the nested iteration loops of the numerical optimization of the likelihood function involving a
large number $(n + m + 2)$ of parameters. The optimization uses an alternating algorithm with the
Nelder-Mead simplex method (Nelder and Mead, 1965) in the inner loops. The function multiscan
directly uses the C function nmmin, the internal code used in the general-purpose optimization tool
[optim](), for implementing the Nelder-Mead simplex method. For large data sets with many tens of
thousands of probes, it is recommended to consider first fitting the model using a random subset
(e.g. 10,000 rows) of the data matrix, and then using the estimated scanning effects and scale
parameters obtained as initial values for fitting the model to the full data set.

The control is a list of arguments. The users can change/supply any of the following components:

trace Indicator (0 or 1) of tracing information of Nelder-Mead algorithm. If 1, tracing informa-
       tion on the progress of the optimization is produced. Because Nelder-Mead may be calllled
       thousands of times during the estimation process, setting trace = 1 will print too much infor-
       mation very rapidly, which may not be useful. Defaults to 0.

gmaxit The maximum number of global iterations. Defaults to 150.

maxit The maximum number of Nelder-Mead iterations. Defaults to 5000.

reltol Relative convergence tolerance of Nelder-Mead. The algorithm stops if it is unable to reduce the value by a factor of reltol * (abs(val) + reltol) at a step. Defaults to 1e-5.

globaltol Convergence tolerance of the outer (alternating) iteration. The estimation process converges if the gain in loglikelihood from one complete cycle of the outer iteration is less than globaltol. Defaults to 1e-10.

alpha, beta, gamma Scaling parameters for the Nelder-Mead method. alpha is the reflection factor (default 1.0), beta the contraction factor (0.5) and gamma the expansion factor (2.0).

Value

Returns an object of class multiscan with components

call	The call of the multiscan function.
beta	A vector of length m containing the maximum likelihood estimates of the scanning effects, the first component fixed at 1.
scale	A vector of length 3 containing the maximum likelihood estimates of the scale parameters $\sigma_1, \sigma_2,$ and ν.
mu	A vector of length n containing the estimated gene expressions.
data	A matrix of the input data with columns rearranged in order of scanner's sensitivity.
fitted	A matrix of the fitted model on the data.
sdres	A matrix of the standardised residuals.
outerit	Number of global iterations completed.
gconv, conv, convmu	

Integer convergence codes.

gconv Indicator of global convergence. 0 indicates successful convergence, 1 indicates premature termination.

conv Convergence codes for the Nelder-Mead simplex method in the last global iteration while updating scanning effects and scale parameters. 0 for successful convergence, 1 indicates that the iteration limit maxit had been reached, 10 indicates degeneracy of the Nelder-Mead simplex method.

convmu Convergence codes for the Nelder-Mead simplex method in the last global iteration while updating the gene expression parameters. This is an integer vector of length n where each component takes the value 0, 1, or 10 depending on whether the Nelder-Mead simplex method successfully converged, reached iteration limit maxit or produced degeneracy respectively while updating the corresponding gene expression parameter.

outerit	Number of global iterations completed.
loglf	Value of the loglikelihood function at convergence (gconv=0). NA if not converged (gconv=1).

References

Khondoker, M. R., Glasbey, C. A. and Worton, B. J. (2006). Statistical estimation of gene expression using multiple laser scans of microarrays. *Bioinformatics* **22**, 215–219.

Nelder, J. A. and Mead, R. (1965). A simplex method for function minimization. *The Computer Journal* **7** 308–313.

See Also

A web interface, created by David Nutter of Biomathematics & Statistics Scotland (BioSS), based on the original Fortran code written by Khondoker *et al.* (2006) is available at http://www.bioss.ac.uk/ktshowcase/create.cgi. Although it uses the same algorithm, results from the web interface may not be exactly identical to that of multiscan as it uses a different (non-free IMSL routine) implementation of Nelder-Mead simplex.

Examples

```
## load the multiscan library
library(multiscan)

## load the murine data set included in multiscan package
data(murine)
murine[1:10, ] ## see first few rows of data

## fit the model on murine data with default options
fit <- multiscan(murine)
fit

## plot the fitted model
plot(fit)

## get the estimated gene expressions
gene.exprs <- fit$mu

## see more details as iteration progresses

fit1 <- multiscan(murine, verbose = TRUE)
fit1
```

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murine   *A subset of murine macrophage gene expression data from Khondoker et al.(2006).*

Description

This data set contains a subset of 1000 rows of murine macrophage array1 data (Khondoker *et al.*, 2006). The data set has 4 columns corresponding to 4 laser scans of one channel of a microarray scanned at four different scanner settings. This data set is used in an example to illustrate the use of multiscan package.

Usage

```
data(murine)
```

Format

A 1000 by 4 data frame.

References

Khondoker, M. R., Glasbey, C. A. and Worton, B. J. (2006). Statistical estimation of gene expression using multiple laser scans of microarrays. *Bioinformatics* **22**, 215–219.

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plot.multiscan   *Plot fitted model and standardised residuals for a multiscan object*

Description

This function provides plots for fitted model and standardised residual for [multiscan](#) fitted objects.

Usage

```
## S3 method for class 'multiscan'
plot(x, residual=FALSE,...)
```

Arguments

x	a `multiscan` fitted object.
residual	Logical. Should residuals be plotted instead of the fitted model?. Defaults to `FALSE`.
...	Further arguments passed to the `plot` function.

Details

Fitted model on the input data, after rescaling by the corresponding scanning effects, is plotted against the estimated gene expressions. Standardised residuals for each scan of data are plotted against the rank of estimated gene expressions.

Value

Returns either one plot of the fitted model (`residual=FALSE`) on the input data or `m` plots of the residuals (`residual=TRUE`) corresponding to each scan of data.

References

Khondoker, M. R., Glasbey, C. A. and Worton, B. J. (2006). Statistical estimation of gene expression using multiple laser scans of microarrays. *Bioinformatics* **22**, 215–219.

See Also

multiscan

Examples

```
data(murine)

fit<-multiscan(murine)

## plot the fitted model

plot(fit)

## plot the residuals

op<-par(mfrow=c(2,2))
plot(fit, residual=TRUE)
par(op)
```

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