

Package ‘HDANOVA’

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Type Package

Title High-Dimensional Analysis of Variance

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Description

Functions and datasets to support Smilde, Marini, Westerhuis and Liland (2025, ISBN: 978-1-394-21121-0)

``Analysis of Variance for High-Dimensional Data - Applications in Life, Food and Chemical Sciences".

This implements and imports a collection of methods for HD-ANOVA data analysis with common interfaces, result- and plotting functions, multiple real data sets and four vignettes covering a range different applications.

Depends R (>= 3.5.0)

Imports car, lme4, MASS, mixlm (>= 1.4.3), pls, pracma, progress, RSpectra

Suggests knitr, vegan

License GPL (>= 2)

URL <https://khliland.github.io/HDANOVA/>,
<https://github.com/khliland/HDANOVA/>

BugReports <https://github.com/khliland/HDANOVA/issues/>

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apca	<i>ANOVA Principal Component Analysis - APCA</i>
------	--

Description

APCA function for fitting ANOVA Principal Component Analysis models.

Usage

```
apca(  
  formula,  
  data,  
  add_error = TRUE,  
  contrasts = "contr.sum",  
  permute = FALSE,  
  perm.type = c("approximate", "exact"),
```

```
    ...  
)
```

Arguments

formula	Model formula accepting a single response (block) and predictors.
data	The data set to analyse.
add_error	Add error to LS means (default = TRUE).
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").
...	Additional parameters for the hdanova function.

Value

An object of class `apca`, inheriting from the general `asca` class. Further arguments and plots can be found in the [asca](#) documentation.

References

Harrington, P.d.B., Vieira, N.E., Espinoza, J., Nien, J.K., Romero, R., and Yergey, A.L. (2005) Analysis of variance–principal component analysis: A soft tool for proteomic discovery. *Analytica chimica acta*, 544 (1-2), 118–127.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
data(candies)
ap <- apca(assessment ~ candy, data=candies)
scoreplot(ap)

# Numeric effects
candies$num <- eff <- 1:165
mod <- apca(assessment ~ candy + assessor + num, data=candies)
summary(mod)
scoreplot(mod, factor=3, gr.col=rgb(eff/max(eff), 1-eff/max(eff),0), pch.scores="x")
```

Description

This is a quite general and flexible implementation of APLS.

Usage

```
apls(
  formula,
  data,
  add_error = TRUE,
  contrasts = "contr.sum",
  permute = FALSE,
  perm.type = c("approximate", "exact"),
  ...
)
```

Arguments

formula	Model formula accepting a single response (block) and predictors. See Details for more information.
data	The data set to analyse.
add_error	Add error to LS means (default = TRUE).
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").
...	Additional arguments to hdanova .

Details

APLS is a method which decomposes a multivariate response according to one or more design variables. ANOVA is used to split variation into contributions from factors, and PLS is performed on the corresponding least squares estimates, i.e., $Y = X_1 B_1 + X_2 B_2 + \dots + E = T_1 P_1' + T_2 P_2' + \dots + E$. For balanced designs, the PLS components are equivalent to PCA components, i.e., APLS and APCA are equivalent. This version of APLS encompasses variants of LiMM-PLS, generalized APLS and covariates APLS.

The formula interface is extended with the function `r()` to indicate random effects and `comb()` to indicate effects that should be combined. See Examples for use cases.

Value

An `apls` object containing loadings, scores, explained variances, etc. The object has associated plotting ([asca_plots](#)) and result ([asca_results](#)) functions.

References

- Smilde, A., Jansen, J., Hoefsloot, H., Lamers, R., Van Der Greef, J., and Timmerman, M. (2005). ANOVA-Simultaneous Component Analysis (ASCA): A new tool for analyzing designed metabolomics data. *Bioinformatics*, 21(13), 3043–3048.
- Liland, K.H., Smilde, A., Marini, F., and Næs, T. (2018). Confidence ellipsoids for ASCA models based on multivariate regression theory. *Journal of Chemometrics*, 32(e2990), 1–13.
- Martin, M. and Govaerts, B. (2020). LiMM-PCA: Combining ASCA+ and linear mixed models to analyse high-dimensional designed data. *Journal of Chemometrics*, 34(6), e3232.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Load candies data
data(candies)

# Basic APLS model with two factors
mod <- apls(assessment ~ candy + assessor, data=candies)
print(mod)

# APLS model with interaction
mod <- apls(assessment ~ candy * assessor, data=candies)
print(mod)

# Result plotting for first factor
loadingplot(mod, scatter=TRUE, labels="names")
scoreplot(mod)
# No backprojection
scoreplot(mod, projections=FALSE)
# Spider plot
scoreplot(mod, spider=TRUE)

# APLS model with compressed response using 5 principal components
mod.pca <- apls(assessment ~ candy + assessor, data=candies, pca.in=5)

# Mixed Model APLS, random assessor
mod.mix <- apls(assessment ~ candy + r(assessor), data=candies)
scoreplot(mod.mix)

# Mixed Model APLS, REML estimation
mod.mix <- apls(assessment ~ candy + r(assessor), data=candies, REML=TRUE)
```

```

scoreplot(mod.mix)

# Load Caldana data
data(caldana)

# Combining effects in APLS
mod.comb <- apls(compounds ~ time + comb(light + time:light), data=caldana)
summary(mod.comb)
timeplot(mod.comb, factor="light", time="time", comb=2)

# Permutation testing
mod.perm <- apls(assessment ~ candy * assessor, data=candies, permute=TRUE)
summary(mod.perm)

```

asca

Analysis of Variance Simultaneous Component Analysis - ASCA

Description

This is a quite general and flexible implementation of ASCA.

Usage

```

asca(
  formula,
  data,
  contrasts = "contr.sum",
  permute = FALSE,
  perm.type = c("approximate", "exact"),
  ...
)

```

Arguments

formula	Model formula accepting a single response (block) and predictors. See Details for more information.
data	The data set to analyse.
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").
...	Additional arguments to hdanova .

Details

ASCA is a method which decomposes a multivariate response according to one or more design variables. ANOVA is used to split variation into contributions from factors, and PCA is performed on the corresponding least squares estimates, i.e., $Y = X_1 B_1 + X_2 B_2 + \dots + E = T_1 P_1' + T_2 P_2' + \dots + E$. This version of ASCA encompasses variants of LiMM-PCA, generalized ASCA and covariates ASCA. It includes confidence ellipsoids for the balanced crossed-effect ASCA.

The formula interface is extended with the function `r()` to indicate random effects and `comb()` to indicate effects that should be combined. See Examples for use cases.

Value

An `asca` object containing loadings, scores, explained variances, etc. The object has associated plotting ([asca_plots](#)) and result ([asca_results](#)) functions.

References

- Smilde, A., Jansen, J., Hoefsloot, H., Lamers, R., Van Der Greef, J., and Timmerman, M. (2005). ANOVA-Simultaneous Component Analysis (ASCA): A new tool for analyzing designed metabolomics data. *Bioinformatics*, 21(13), 3043–3048.
- Liland, K.H., Smilde, A., Marini, F., and Næs, T. (2018). Confidence ellipsoids for ASCA models based on multivariate regression theory. *Journal of Chemometrics*, 32(e2990), 1–13.
- Martin, M. and Govaerts, B. (2020). LiMM-PCA: Combining ASCA+ and linear mixed models to analyse high-dimensional designed data. *Journal of Chemometrics*, 34(6), e3232.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Load candies data
data(candies)

# Basic ASCA model with two factors
mod <- asca(assessment ~ candy + assessor, data=candies)
print(mod)

# ASCA model with interaction
mod <- asca(assessment ~ candy * assessor, data=candies)
print(mod)

# Result plotting for first factor
loadingplot(mod, scatter=TRUE, labels="names")
scoreplot(mod)
# No backprojection
scoreplot(mod, projections=FALSE)
# Spider plot
```

```

scoreplot(mod, spider=TRUE)

# ASCA model with compressed response using 5 principal components
mod.pca <- asca(assessment ~ candy + assessor, data=candies, pca.in=5)

# Mixed Model ASCA, random assessor
mod.mix <- asca(assessment ~ candy + r(assessor), data=candies)
scoreplot(mod.mix)

# Mixed Model ASCA, REML estimation
mod.mix <- asca(assessment ~ candy + r(assessor), data=candies, REML=TRUE)
scoreplot(mod.mix)

# Load Caldana data
data(caldana)

# Combining effects in ASCA
mod.comb <- asca(compounds ~ time + comb(light + time:light), data=caldana)
summary(mod.comb)
timeplot(mod.comb, factor="light", time="time", comb=2)

# Permutation testing
mod.perm <- asca(assessment ~ candy * assessor, data=candies, permute=TRUE)
summary(mod.perm)

```

asca_plots

ASCA Plot Methods

Description

Various plotting procedures for [asca](#) objects.

Usage

```

## S3 method for class 'asca'
loadingplot(object, factor = 1, comps = 1:2, ...)

## S3 method for class 'asca'
scoreplot(
  object,
  factor = 1,
  comps = 1:2,
  within_level = "all",
  pch.scores = 19,
  pch.projections = 1,
  gr.col = NULL,
  projections = TRUE,
  spider = FALSE,

```

```

    ellipsoids,
    confidence,
    xlim,
    ylim,
    xlab,
    ylab,
    legendpos,
    ...
)

permutationplot(object, factor = 1, xlim, xlab = "SSQ", main, ...)

```

Arguments

object	asca object.
factor	integer/character for selecting a model factor. If factor <= 0 or "global", the PCA of the input is used (negativ factor to include factor level colouring with global PCA).
comps	integer vector of selected components.
...	additional arguments to underlying methods.
within_level	MSCA parameter for chosing plot level (default = "all").
pch.scores	integer plotting symbol.
pch.projections	integer plotting symbol.
gr.col	integer vector of colours for groups.
projections	Include backprojections in score plot (default = TRUE).
spider	Draw lines between group centers and backprojections (default = FALSE).
ellipsoids	character "confidence" or "data" ellipsoids for balanced fixed effect models.
confidence	numeric vector of ellipsoid confidences, default = c(0.4, 0.68, 0.95).
xlim	numeric x limits.
ylim	numeric y limits.
xlab	character x label.
ylab	character y label.
legendpos	character position of legend.
main	Plot title.

Details

Usage of the functions are shown using generics in the examples in [asca](#). Plot routines are available as `scoreplot.asca` and `loadingplot.asca`.

Value

The plotting routines have no return.

References

- Smilde, A., Jansen, J., Hoefsloot, H., Lamers, R., Van Der Greef, J., and Timmerman, M. (2005). ANOVA-Simultaneous Component Analysis (ASCA): A new tool for analyzing designed metabolomics data. *Bioinformatics*, 21(13), 3043–3048.
- Liland, K.H., Smilde, A., Marini, F., and Næs, T. (2018). Confidence ellipsoids for ASCA models based on multivariate regression theory. *Journal of Chemometrics*, 32(e2990), 1–13.
- Martin, M. and Govaerts, B. (2020). LiMM-PCA: Combining ASCA+ and linear mixed models to analyse high-dimensional designed data. *Journal of Chemometrics*, 34(6), e3232.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

asca_results

ASCA Result Methods

Description

Standard result computation and extraction functions for ASCA ([asca](#)).

Usage

```
## S3 method for class 'hdanova'
print(x, ...)

## S3 method for class 'hdanova'
summary(object, extended = TRUE, df = FALSE, ...)

## S3 method for class 'summary.hdanova'
print(x, digits = 2, ...)

## S3 method for class 'asca'
loadings(object, factor = 1, ...)

## S3 method for class 'asca'
scores(object, factor = 1, ...)

projections(object, ...)

## S3 method for class 'asca'
projections(object, factor = 1, ...)
```

Arguments

x	asca object.
...	additional arguments to underlying methods.
object	asca object.
extended	Extended output in summary (default = TRUE).
df	Show degrees of freedom in summary (default = FALSE).
digits	integer number of digits for printing.
factor	integer/character for selecting a model factor.

Details

Usage of the functions are shown using generics in the examples in [asca](#). Explained variances are available (block-wise and global) through `blockexpl` and `print.rosaexpl`. Object printing and summary are available through: `print.asca` and `summary.asca`. Scores and loadings have their own extensions of `scores()` and `loadings()` through `scores.asca` and `loadings.asca`. Special to ASCA is that scores are on a factor level basis, while back-projected samples have their own function in `projections.asca`.

Value

Returns depend on method used, e.g. `projections.asca` returns projected samples, `scores.asca` return scores, while `print` and `summary` methods return the object invisibly.

References

- Smilde, A., Jansen, J., Hoefsloot, H., Lamers, R., Van Der Greef, J., and Timmerman, M. (2005). ANOVA-Simultaneous Component Analysis (ASCA): A new tool for analyzing designed metabolomics data. *Bioinformatics*, 21(13), 3043–3048.
- Liland, K.H., Smilde, A., Marini, F., and Næs, T. (2018). Confidence ellipsoids for ASCA models based on multivariate regression theory. *Journal of Chemometrics*, 32(e2990), 1–13.
- Martin, M. and Govaerts, B. (2020). LiMM-PCA: Combining ASCA+ and linear mixed models to analyse high-dimensional designed data. *Journal of Chemometrics*, 34(6), e3232.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

biplot.asca

Biplot for ASCA models

Description

Biplot for ASCA models

Usage

```
## S3 method for class 'asca'
biplot(
  x,
  factor = 1,
  comps = 1:2,
  xlim = NULL,
  ylim = NULL,
  col = "darkgray",
  expand = 1,
  labels,
  legendpos,
  ...
)
```

Arguments

x	asca object.
factor	Factor number or name.
comps	integer vector of selected components.
xlim	numeric vector of length 2 for x-axis limits of the loadings.
ylim	numeric vector of length 2 for y-axis limits of the loadings.
col	vector of colours for score axes and loading axes and points/texts.
expand	numeric expansion for the scores, defaulting to 1.
labels	optional. If "names", row names are used as labels. If "numbers", row numbers are used as labels. (Can also be a vector of labels.)
legendpos	character position of legend.
...	Additional arguments to plot and scoreplot.

Value

No return, only a plot.

Examples

```
# Load candies data
data(candies)

# Basic ASCA model with two factors and interaction
mod <- asca(assessment ~ candy * assessor, data=candies)

# Biplot
biplot(mod)

# Biplot with named loadings
biplot(mod, labels="names")
```

block.data.frame	<i>Block-wise indexable data.frame</i>
------------------	--

Description

This is a convenience function for making `data.frames` that are easily indexed on a block-wise basis.

Usage

```
block.data.frame(X, block_inds = NULL, to.matrix = TRUE)
```

Arguments

<code>X</code>	Either a single <code>data.frame</code> to index or a list of matrices/ <code>data.frames</code>
<code>block_inds</code>	Named list of indexes if <code>X</code> is a single <code>data.frame</code> , otherwise <code>NULL</code> .
<code>to.matrix</code>	logical indicating if input list elements should be converted to matrices.

Value

A `data.frame` which can be indexed block-wise.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Random data
M <- matrix(rnorm(200), nrow = 10)
# .. with dimnames
dimnames(M) <- list(LETTERS[1:10], as.character(1:20))

# A named list for indexing
inds <- list(B1 = 1:10, B2 = 11:20)

X <- block.data.frame(M, inds)
str(X)
```

caldana

Arabidopsis thaliana growth experiment

Description

A dataset containing 67 metabolites from plants grown under different light and temperature conditions. This subset of the data contains only the light effect and time effect for limited conditions, while the full data also contains gene expressions.

Usage

```
data(caldana)
```

Format

A data.frame having 140 rows and 3 variables:

light Light levels

time Time of measurement

compound Metabolic compounds

References

Caldana C, Degenkolbe T, Cuadros-Inostroza A, Klie S, Sulpice R, Leisse A, et al. High-density kinetic analysis of the metabolomic and transcriptomic response of Arabidopsis to eight environmental conditions. Plant J. 2011;67(5):869-884.

candies	<i>Sensory assessment of candies.</i>
---------	---------------------------------------

Description

A dataset containing 9 sensory attributes for 5 candies assessed by 11 trained assessors.

Usage

```
data(candies)
```

Format

A data.frame having 165 rows and 3 variables:

assessment Matrix of sensory attributes

assessor Factor of assessors

candy Factor of candies

References

Luciano G, Næs T. Interpreting sensory data by combining principal component analysis and analysis of variance. Food Qual Prefer. 2009;20(3):167-175.

dummycode	<i>Dummy-coding of a single vector</i>
-----------	--

Description

Flexible dummy-coding allowing for all R's built-in types of contrasts and optional dropping of a factor level to reduce rank deficiency probability.

Usage

```
dummycode(Y, contrast = "contr.sum", drop = TRUE)
```

Arguments

Y vector to dummy code.

contrast Contrast type, default = "contr.sum".

drop logical indicating if one level should be dropped (default = TRUE).

Value

matrix made by dummy-coding the input vector.

Examples

```
vec <- c("a","a","b","b","c","c")
dummycode(vec)
```

extended.model.frame *Extracting the Extended Model Frame from a Formula or Fit*

Description

This function attempts to apply [model.frame](#) and extend the result with columns of interactions.

Usage

```
extended.model.frame(formula, data, ..., sep = ".")
```

Arguments

formula	a model formula or terms object or an R object.
data	a data.frame, list or environment (see model.frame).
...	further arguments to pass to model.frame .
sep	separator in contraction of names for interactions (default = ".").

Value

A [data.frame](#) that includes everything a [model.frame](#) does plus interaction terms.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
dat <- data.frame(Y = c(1,2,3,4,5,6),
                 X = factor(LETTERS[c(1,1,2,2,3,3)]),
                 W = factor(letters[c(1,2,1,2,1,2)]))
extended.model.frame(Y ~ X*W, dat)
```

extract_estimates	<i>Extract estimates for a given factor combination</i>
-------------------	---

Description

Extracts and sums the LS estimates for a given factor combination from an object of class `hdanova`. If `add_residuals` is `TRUE`, the residuals are added to the LS estimates. If `subtract` is `TRUE`, the returned matrix is the data with chosen estimates subtracted.

Usage

```
extract_estimates(object, factors, subtract = FALSE, add_residuals = FALSE)
```

Arguments

<code>object</code>	asca object.
<code>factors</code>	vector of factor names or numbers.
<code>subtract</code>	logical subtract the estimates from the data (default = <code>FALSE</code>).
<code>add_residuals</code>	logical add residuals to the estimates (default = <code>FALSE</code>).

Value

A matrix of the extracted estimates.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors and interaction
mod <- hdanova(assessment ~ candy * assessor, data=candies)

# Extract estimates for the interaction
inter <- extract_estimates(mod, c("candy:assessor"))

# Visualize the interaction effect
image(t(inter), main="Interaction effect", xlab="Attribute", ylab="Sample")
```

hdanova

*High-Dimensional Analysis of Variance***Description**

This function provides a high-dimensional analysis of variance (HDANOVA) method which can be used alone or as part of a larger analysis, e.g., ASCA, APCA, LiMM-PCA, MSCA or PC-ANOVA. It can be called directly or through the convenience functions [asca](#), [apca](#), [limmpca](#), [msca](#) and [pcanova](#).

Usage

```
hdanova(
  formula,
  data,
  subset,
  weights,
  na.action,
  family,
  unrestricted = FALSE,
  add_error = FALSE,
  aug_error = "denominator",
  use_ED = FALSE,
  pca.in = FALSE,
  contrasts = "contr.sum",
  coding,
  equal_baseline = FALSE,
  SStype = "II",
  REML = NULL,
  scale = FALSE
)
```

Arguments

formula	Model formula accepting a single response (block) and predictors. See Details for more information.
data	The data set to analyse.
subset	Expression for subsetting the data before modelling.
weights	Optional object weights.
na.action	How to handle NAs (no action implemented).
family	Error distributions and link function for Generalized Linear Models.
unrestricted	Use unrestricted ANOVA decomposition (default = FALSE).
add_error	Add error to LS means, e.g., for APCA.
aug_error	Augment score matrices in backprojection. Default = "denominator" (of F test), "residual" (force error term), numeric value (alpha-value in LiMM-PCA).

use_ED	Use "effective dimensions" for score rescaling in LiMM-PCA.
pca.in	Compress response before ASCA (number of components).
contrasts	Effect coding: "contr.sum" (default = sum-coding), "contr.weighted" (not for lme4 models), "contr.reference", "contr.treatment".
coding	Defunct. Use 'contrasts' instead.
equal_baseline	Experimental: Set to TRUE to let interactions, where a main effect is missing, e.g., a nested model, be handled with the same baseline as a cross effect model. If TRUE the corresponding interactions will be put in quotation marks and included in the <code>model.frame</code> .
SStype	Type of sum-of-squares: "I" = sequential, "II" (default) = last term, obeying marginality, "III" = last term, not obeying marginality.
REML	Parameter to <code>mixlm</code> : NULL (default) = sum-of-squares, TRUE = REML, FALSE = ML.
scale	Scaling of the response matrix. Defaults to FALSE (no scaling). For alternatives, see Details.

Details

Scaling of the response matrix can be done by setting the `scale` parameter. If `scale=TRUE`, each column is scaled by its standard deviation (autoscaling). A numeric value can be provided to scale the columns by specific quantities. If `scale` is a character string, the first element is interpreted as a factor name and the second element is interpreted as a factor level, whose samples the standard deviations are calculated from (reference group scaling).

Value

An `hdanova` object containing loadings, scores, explained variances, etc. The object has associated plotting ([asca_plots](#)) and result ([asca_results](#)) functions.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors
mod <- hdanova(assessment ~ candy + assessor, data=candies)
summary(mod)
```

limmpca

Linear Mixed Model PCA

Description

This function mimics parts of the LiMM-PCA framework, combining ASCA+ and linear mixed models to analyse high-dimensional designed data. The default is to use REML estimation and scaling of the backprojected errors. See examples for alternatives.

Usage

```
limmpca(
  formula,
  data,
  pca.in = 5,
  aug_error = 0.05,
  use_ED = FALSE,
  REML = TRUE,
  contrasts = "contr.sum",
  permute = FALSE,
  perm.type = c("approximate", "exact"),
  SStype = "III",
  ...
)
```

Arguments

formula	Model formula accepting a single response (block) and predictors. See Details for more information.
data	The data set to analyse.
pca.in	Compress response before ASCA (number of components), default = 5.
aug_error	Error term of model ("denominator", "residual", numeric alpha-value). The latter implies the first with a scaling factor.
use_ED	Use Effective Dimensions instead of degrees of freedom when scaling.
REML	Use restricted maximum likelihood estimation. Alternatives: TRUE (default), FALSE (ML), NULL (least squares).
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").
SStype	Type of sum-of-squares: "I" = sequential, "II" = last term, obeying marginality, "III" (default) = last term, not obeying marginality.
...	Additional arguments to hdanova .

Details

The Sum of Squares for the model is dependent on the SStype of the model. For SStype = "I" and SStype = "II" the SSQ is based on LLR (possibly inflating large contributions), while it is directly estimated from the model for SStype = "III". SStype = "III" is the default for LiMM-PCA and should be combined with sum coding. Sum of Squares for the random effects are based on the variance components.

Value

An object of class `limmpca`, inheriting from the general `asca` class.

References

- Martin, M. and Govaerts, B. (2020). LiMM-PCA: Combining ASCA+ and linear mixed models to analyse high-dimensional designed data. *Journal of Chemometrics*, 34(6), e3232.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Load candies data
data(candies)

# Default LiMM-PCA model with two factors and interaction, 5 PCA components
mod <- limmpca(assessment ~ candy*r(assessor), data=candies)
summary(mod)
scoreplot(mod, factor = "candy")

# LiMM-PCA with least squares estimation and 8 PCA components
modLS <- limmpca(assessment ~ candy*r(assessor), data=candies, REML=NULL, pca.in=8)
summary(modLS)
scoreplot(modLS, factor = "candy")

# Load Caldana data
data(caldana)

# Combining effects in LiMM-PCA (assuming light is a random factor)
mod.comb <- limmpca(compounds ~ time + comb(r(light) + r(time:light)), data=caldana, pca.in=8)
summary(mod.comb)
```

model.frame.asca

Model Frame and Model Matrix for ASCA-like Models

Description

Extraction functions to retrieve the `model.frame` and `model.matrix` of an `asca` object.

Usage

```
## S3 method for class 'asca'
model.frame(formula, ...)

## S3 method for class 'asca'
model.matrix(object, ...)
```

Arguments

formula	The asca object.
...	Not implemented
object	The asca object.

Value

A data.frame or matrix object.

Examples

```
# Load candies data
data(candies)

# Basic ASCA model with two factors
mod <- asca(assessment ~ candy + assessor, data=candies)

# Extract model frame and model matrix
mf <- model.frame(mod)
head(mf)
mm <- model.matrix(mod)
par.old <- par(mar=c(3,3,3,1), mgp=c(1,0.7,0))
image(t(mm[seq(165,1,-1),]), main="Model Matrix", xlab="dummy values", ylab="samples",
      axes=FALSE)
par(par.old)
```

msca

Multilevel Simultaneous Component Analysis - MSCA

Description

This MSCA implementation assumes a single factor to be used as between-individuals factor.

Usage

```
msca(
  formula,
  data,
  contrasts = "contr.sum",
  permute = FALSE,
  perm.type = c("approximate", "exact"),
  ...
)
```

Arguments

formula	Model formula accepting a single response (block) and predictors. See Details for more information.
data	The data set to analyse.
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").
...	Additional arguments to hdanova .

Value

An `asca` object containing loadings, scores, explained variances, etc. The object has associated plotting ([asca_plots](#)) and result ([asca_results](#)) functions.

References

- Smilde, A., Jansen, J., Hoefsloot, H., Lamers, R., Van Der Greef, J., and Timmerman, M. (2005). ANOVA-Simultaneous Component Analysis (ASCA): A new tool for analyzing designed metabolomics data. *Bioinformatics*, 21(13), 3043–3048.
- Liland, K.H., Smilde, A., Marini, F., and Næs, T. (2018). Confidence ellipsoids for ASCA models based on multivariate regression theory. *Journal of Chemometrics*, 32(e2990), 1–13.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Load candies data
data(candies)

# Basic MSCA model with a single factor
mod <- msca(assessment ~ candy, data=candies)
print(mod)
summary(mod)

# Result plotting for first factor
loadingplot(mod, scatter=TRUE, labels="names")
scoreplot(mod)

# Within scores
scoreplot(mod, factor="within")

# Within scores per factor level
```

```

par.old <- par(mfrow=c(3,2), mar=c(4,4,2,1), mgp=c(2,0.7,0))
for(i in 1:length(mod$scores.within))
  scoreplot(mod, factor="within", within_level=i,
            main=paste0("Level: ", names(mod$scores.within)[i]),
            panel.first=abline(v=0,h=0,col="gray",lty=2))
par(par.old)

# Permutation testing
mod.perm <- asca(assessment ~ candy * assessor, data=candies, permute=TRUE)
summary(mod.perm)

```

pcanova	<i>Principal Components Analysis of Variance Simultaneous Component Analysis - PC-ANOVA</i>
---------	---

Description

This is a quite general and flexible implementation of PC-ANOVA.

Usage

```
pcanova(formula, data, ncomp = 0.9, contrasts = "contr.sum", ...)
```

Arguments

formula	Model formula accepting a single response (block) and predictor names separated by + signs.
data	The data set to analyse.
ncomp	The number of components to retain, proportion of variation or default = minimum cross-validation error.
contrasts	Effect coding: "sum" (default = sum-coding), "weighted", "reference", "treatment".
...	Additional parameters for the hdanova function.

Details

PC-ANOVA works in the opposite order of ASCA. First the response matrix is decomposed using ANOVA. Then the components are analysed using ANOVA with respect to a design or grouping in the data. The latter can be ordinary fixed effects modelling or mixed models.

Value

A pcanova object containing loadings, scores, explained variances, etc. The object has associated plotting ([pcanova_plots](#)) and result ([pcanova_results](#)) functions.

References

Luciano G, Næs T. Interpreting sensory data by combining principal component analysis and analysis of variance. Food Qual Prefer. 2009;20(3):167-175.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
# Load candies data
data(candies)

# Basic PC-ANOVA model with two factors, cross-validated opt. of #components
mod <- pcanova(assessment ~ candy + assessor, data = candies)
print(mod)

# PC-ANOVA model with interaction, minimum 90% explained variance
mod <- pcanova(assessment ~ candy * assessor, data = candies, ncomp = 0.9)
print(mod)
summary(mod)

# Tukey group letters for 'candy' per component
lapply(mod$models, function(x)
  mixlm::cld(mixlm::simple.glht(x,
                              effect = "candy"))))

# Result plotting
loadingplot(mod, scatter=TRUE, labels="names")
scoreplot(mod)

# Mixed Model PC-ANOVA, random assessor
mod.mix <- pcanova(assessment ~ candy + r(assessor), data=candies, ncomp = 0.9)
scoreplot(mod.mix)
# Fixed effects
summary(mod.mix)
```

Description

Various plotting procedures for [pcanova](#) objects.

Usage

```
## S3 method for class 'pcanova'
scoreplot(object, factor = 1, comps = 1:2, col = "factor", ...)
```

Arguments

object	pcanova object.
factor	integer/character for selecting a model factor.
comps	integer vector of selected components.
col	character for selecting a factor to use for colouring (default = first factor) or ordinary colour specifications.
...	additional arguments to underlying methods.

Details

Usage of the functions are shown using generics in the examples in [pcanova](#). Plot routines are available as `scoreplot.pcanova` and `loadingplot.pcanova`.

Value

The plotting routines have no return.

References

Luciano G, Næs T. Interpreting sensory data by combining principal component analysis and analysis of variance. *Food Qual Prefer.* 2009;20(3):167-175.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

pcanova_results

PC-ANOVA Result Methods

Description

Standard result computation and extraction functions for ASCA ([pcanova](#)).

Usage

```
## S3 method for class 'pcanova'
summary(object, ...)

## S3 method for class 'summary.pcanova'
print(x, digits = 2, ...)

## S3 method for class 'pcanova'
print(x, ...)

## S3 method for class 'pcanova'
summary(object, ...)
```

Arguments

object	pcanova object.
...	additional arguments to underlying methods.
x	pcanova object.
digits	integer number of digits for printing.

Details

Usage of the functions are shown using generics in the examples in [pcanova](#). Explained variances are available (block-wise and global) through `blockexpl` and `print.rosaexpl`. Object printing and summary are available through: `print.pcanova` and `summary.pcanova`. Scores and loadings have their own extensions of `scores()` and `loadings()` through `scores.pcanova` and `loadings.pcanova`. Special to ASCA is that scores are on a factor level basis, while back-projected samples have their own function in `projections.pcanova`.

Value

Returns depend on method used, e.g. `projections.pcanova` returns projected samples, `scores.pcanova` return scores, while `print` and `summary` methods return the object invisibly.

References

Luciano G, Næs T. Interpreting sensory data by combining principal component analysis and analysis of variance. *Food Qual Prefer.* 2009;20(3):167-175.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

permanova

Permutation Based MANOVA - PERMANOVA

Description

Wrapper for the [adonis2](#) function to allow ordinary formula input.

Usage

```
permanova(formula, data, ...)
```

Arguments

formula	Model formula accepting a single response matrix and predictors. See details in adonis2 .
data	The data set to analyse.
...	Additional arguments to adonis2 .

Value

An ANOVA table with permutation-based p-values.

Examples

```
data(caldana)
(pr <- permanova(compounds ~ light * time, caldana))
```

permutation

Permutation for HDANOVA

Description

Permutation testing for HDANOVA. This function performs permutation testing for the effects in the HDANOVA model and adds them to the hdanova object.

Usage

```
permutation(object, permute = 1000, perm.type = c("approximate", "exact"))
```

Arguments

object	A hdanova object.
permute	Number of permutations to perform (default = 1000).
perm.type	Type of permutation to perform, either "approximate" or "exact" (default = "approximate").

Value

An updated hdanova object with permutation results.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors
mod <- hdanova(assessment ~ candy + assessor, data=candies)
mod <- permutation(mod)
summary(mod)
```

pls

Partial Least Squares (PLS) for HDANOVA

Description

This function performs Partial Least Squares (PLS) on a hdanova.

Usage

```
pls(object, ...)

## Default S3 method:
pls(object, ...)
```

Arguments

object	A hdanova object.
...	Additional arguments (not used).

Details

For residuals, PCA is performed instead of PLS as there is no natural response.

Value

An updated hdanova object with PLS results.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors
mod <- hdanova(assessment ~ candy + assessor, data=candies)
mod <- pls(mod)
scoreplot(mod)
```

prc

Principal Response Curves

Description

Wrapper for the [prc](#) function to allow for formula input.

Usage

```
prc(formula, data, ...)
```

Arguments

formula	Model formula accepting a single response (block) and predictors. If no predictor is called 'time', time is assumed to be the second predictor.
data	The data set to analyse.
...	Additional arguments to prc .

Value

An object of class prc.

See Also

Main methods: [asca](#), [apca](#), [limmpca](#), [msca](#), [pcanova](#), [prc](#) and [permanova](#). Workhorse function underpinning most methods: [hdanova](#). Extraction of results and plotting: [asca_results](#), [asca_plots](#), [pcanova_results](#) and [pcanova_plots](#)

Examples

```
data(caldana)
(pr <- prc(compounds ~ light * time, caldana))
summary(pr)
```

sca

Simultaneous Component Analysis

Description

This function performs Simultaneous Component Analysis (SCA) on a hdanova object.

Usage

```
sca(object)
```

Arguments

object A hdanova object.

Value

An updated hdanova object with SCA results.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors
mod <- hdanova(assessment ~ candy + assessor, data=candies)
mod <- sca(mod)
scoreplot(mod)
```

signflip

Flip signs of a component/factor combination in a SCA/PCA object

Description

This function flips the sign of a selected component in a selected factor of an asca object. This affects both scores, loadings and projected data.

Usage

```
signflip(object, factor, comp)
```

Arguments

object asca object.
factor integer/character for selecting a model factor.
comp integer for selected component.

Value

An asca object with the sign of the selected component flipped.

Examples

```
# Load candies data
data(candies)

# Basic HDANOVA model with two factors
mod <- hdanova(assessment ~ candy + assessor, data=candies)
mod <- sca(mod)
old.par <- par(mfrow=c(1,2), mar=c(4,4,1,1))
scoreplot(mod, factor="candy")
loadingplot(mod, factor="candy")
par(old.par)

# Flip the sign of the first component of the candy factor
mod <- signflip(mod, factor="candy", comp=1)
old.par <- par(mfrow=c(1,2), mar=c(4,4,1,1))
scoreplot(mod, factor="candy")
loadingplot(mod, factor="candy")
par(old.par)
```

timeplot

Timeplot for Combined Effects

Description

Timeplot for Combined Effects

Usage

```
timeplot(
  object,
  factor,
  time,
  comb,
  comp = 1,
  ylim,
  x_time = FALSE,
  xlab = time,
  ylab = paste0("Score ", comp),
  lwd = 2,
  ...
)
```

Arguments

object	asca object.
factor	integer/character main factor.
time	integer/character time factor.
comb	integer/character combined effect factor.
comp	integer component number.
ylim	numeric y limits.
x_time	logical use time levels as non-equispaced x axis (default = FALSE).
xlab	character x label.
ylab	character y label.
lwd	numeric line width.
...	additional arguments to plot.

Value

Nothing

Examples

```
data("caldana")
mod.comb <- asca(compounds ~ time + comb(light + time:light), data=caldana)

# Default time axis
timeplot(mod.comb, factor="light", time="time", comb=2)

# Non-equispaced time axis (using time levels)
timeplot(mod.comb, factor="light", time="time", comb=2, x_time=TRUE)

# Second component
timeplot(mod.comb, factor="light", time="time", comb=2, comp=2, x_time=TRUE)
```

update_without_factor *Update a Model without Factor*

Description

Perform a model update while removing a chosen factor. Hierarchical corresponds to type "II" sum-of-squares, i.e., obeying marginality, while non-hierarchical corresponds to type "III" sum-of-squares.

Usage

```
update_without_factor(model, fac, hierarchical = TRUE)
```

Arguments

<code>model</code>	model object to update.
<code>fac</code>	character factor to remove.
<code>hierarchical</code>	logical obey hierarchy when removing factor (default = TRUE).

Value

An updated model object is returned. If the supplied model is of type `lmerMod` and no random effects are left, the model is automatically converted to a linear model before updating.

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