Package 'weitrix'

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Title Tools for matrices with precision weights, test and explore weighted or sparse data

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Description Data type and tools for working with matrices having precision weights and missing data. This package provides a common representation and tools that can be used with many types of high-throughput data. The meaning of the weights is compatible with usage in the base R function ``lm'' and the package ``limma''. Calibrate weights to account for known predictors of precision. Find rows with excess variability. Perform differential testing and find rows with the largest confident differences. Find PCA-like components of variation even with many missing values, rotated so that individual components may be meaningfully interpreted. DelayedArray matrices and BiocParallel are supported.

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`as_weitrix` *Convert data to a weitrix*

Description

Ensure data is a weighted matrix or "weitrix". A weitrix is a SummarizedExperiment or subclass thereof with some metadata fields set. If it is ambiguous how to do this, produce an error.

Usage

```
as_weitrix(object, weights = NULL)
```

Arguments

object	Object to convert.
weights	Optional, weights matrix if not present in object.

Details

Input can be a matrix or DelayedArray.

Input can be anything the limma package recognizes, notably the limma EList class (for example as output by voom or vooma).

If weights are not present in "object" and not given with "weights", they default for 0 for NA values and 1 for everything else.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Examples

```
mat <- matrix(c(1,2,NA,3,NA,4), ncol=2)
weitrix <- as_weitrix(mat)

metadata(weitrix)
weitrix_x(weitrix)
weitrix_weights(weitrix)
```

---

bless_weitrix *Bless a SummarizedExperiment as a weitrix*

Description

Set metadata entries in a SummarizedExperiment object so that it can be used as a weitrix.

Usage

```
bless_weitrix(object, x_name, weights_name)
```

Arguments

object	A SummarizedExperiment object.
x_name	Name of the assay containing the observations.
weights_name	Name of the assay containing the weights.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Examples

```
mat <- matrix(c(1,2,NA,3,NA,4), ncol=2)
weights <- matrix(c(1,0.5,0,2,0,1), ncol=2)
se <- SummarizedExperiment(assays=list(foo=mat, bar=weights))

weitrix <- bless_weitrix(se, "foo", "bar")

metadata(weitrix)
weitrix_x(weitrix)
weitrix_weights(weitrix)
```

`components_seq_scree` *Proportion more variance explained by adding components one at a time*

Description

Based on the output of `components_seq`, work out how much further variance is explained by adding further components.

Usage

```
components_seq_scree(comp_seq, rand_comp = NULL)

components_seq_screeplot(comp_seq, rand_comp = NULL)
```

Arguments

`comp_seq`	A list of Components objects, as produced by `components_seq`.
`rand_comp`	Optional. A Components object with a single component. This should be based on a randomized version of the weitrix, for example as produced by `weitrix_components(weitrix_randomize(my_weitrix), p=1)`.

Details

If `rand_comp` is given, some possible threshold levels for including further components are also calculated.

The "Parallel analysis" threshold is chosen based on varianced explained by a single component in a randomized weitrix.

The "Optimistic" thresholds are chosen starting from the "Parallel Analysis" threshold. We view the Parallel Analysis threshold as indicating random variance is split amongst an effective number of samples, which will be somewhat smaller than the real number of samples. As each component is accepted, the pool of remaining variance is reduced by its contribution, and also the number of effective samples is reduced by one. The threshold is then the size of the remaining variance pool divided by the effective remaining number of samples. This is a somewhat ad-hoc method, but may indicate more components are justified than by criteria based on a flat threshold.

Value

components_seq_scree returns a data frame listing the variance explained by each further component.

components_seq_screeplot returns a ggplot2 plot object.

Examples

```
comp_seq <- weitrix_components_seq(simwei, 4, verbose=FALSE)

components_seq_scree(comp_seq)
components_seq_screeplot(comp_seq)
```

---

counts_proportions *Produce a weitrix of proportions within groups*

Description

Produce a weitrix of proportions between 0 and 1. The input is read counts at a collection of features in a collection of samples. The features need to be grouped, for example by gene. The proportions will add to 1 within each group.

Usage

```
counts_proportions(counts, grouping, verbose = TRUE, typecast = identity)
```

Arguments

counts	A matrix of read counts. Rows are peaks and columns are samples.
grouping	A data frame defining the grouping of features. Should have a column "group" naming the group and a column "name" naming the feature (corresponding to rownames(counts)).
verbose	If TRUE, output some debugging and progress information.
typecast	A function to convert a matrix to a matrix-like type. Applied at the chunk level, before all chunks are rbinded. Allows use of memory-efficient matrix representations.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Examples

```
grouping <- data.frame(
    group=c("A","A","A","B","B"),
    name=c("p1","p2","p3","p4","p5"))

counts <- rbind(
    p1=c(1,2,0),
    p2=c(0,1,0),
    p3=c(1,0,0),
    p4=c(0,0,1),
    p5=c(0,2,1))

wei <- counts_proportions(counts, grouping)

weitrix_x(wei)
weitrix_weights(wei)
rowData(wei)
```

`counts_shift` *Produce a weitrix of shift scores*

Description

Produce a weitrix of shift scores between -1 and 1. The input is read counts at a collection of peaks (or other features) in a collection of samples. The peaks can be grouped by gene, and are ordered within each gene.

Usage

```
counts_shift(counts, grouping, verbose = TRUE, typecast = identity)
```

Arguments

`counts`	A matrix of read counts. Rows are peaks and columns are samples.
`grouping`	A data frame defining the grouping of peaks into genes. Should have a column "group" naming the gene and a column "name" naming the peak (corresponding to `rownames(counts)`). Within each group, peak names should be ordered from 5' to 3' position.
`verbose`	If TRUE, output some debugging and progress information.
`typecast`	A function to convert a matrix to a matrix-like type. Applied at the chunk level, before all chunks are `rbind`ed. Allows use of memory-efficient matrix representations.

Details

For a particular gene, a shift score measures measures the tendency of reads to be upstrand (negative) or downstrand (positive) of the average over all samples. Shift scores range between -1 and 1.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Examples

```
grouping <- data.frame(
    group=c("A","A","A","B","B"),
    name=c("p1","p2","p3","p4","p5"))

counts <- rbind(
    p1=c(1,2,0),
    p2=c(0,1,0),
    p3=c(1,0,0),
    p4=c(0,0,1),
    p5=c(0,2,1))

wei <- counts_shift(counts, grouping)

weitrix_x(wei)
weitrix_weights(wei)
rowData(wei)
```

---

matrix_long *Convert a matrix to long form for ggplotting*

Description

A convenience function which melts the matrix and then joins row and column information.

Usage

```
matrix_long(
  matrix,
  row_info = NULL,
  col_info = NULL,
  varnames = c("name", "col")
)
```

Arguments

matrix	A matrix, or object that can be converted to a matrix.
row_info	Information about rows of the matrix. A data frame, or object that can be converted to a data frame.
col_info	Information about columns of the matrix. A data frame, or object that can be converted to a data frame.
varnames	Vector of two column names in the output, the first for the row and the second for the column.

Value

A data frame containing the matrix and associated information in long format.

Examples

```
matrix_long(weitrix_x(simwei), rowData(simwei), colData(simwei))
```

---

simwei *Simulated weitrix dataset.*

Description

This is a small simulated weitrix used in examples. There is one component of variation to be found, plus Gaussian noise with variance inversely proportional to the weights.

Usage

```
simwei
```

Format

A weitrix object.

---

weitrix_calibrate *Adjust weights row-wise based on given row dispersions*

Description

Based on estimated row dispersions, adjust weights in each row.

Usage

```
weitrix_calibrate(weitrix, dispersions)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.
dispersions	A dispersion for each row.

Details

For large numbers of samples this can be based directly on weitrix_dispersions. For small numbers of samples, when using limma, it should be based on a trend-line fitted to known co-variates of the dispersions. This can be done using weitrix_calibrate_trend.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Examples

```
# Adjust weights so dispersion for each row is exactly 1. This is dubious
# for a small dataset, but would be fine for a dataset with many columns.
comp <- weitrix_components(simwei, p=1, verbose=FALSE)
disp <- weitrix_dispersions(simwei, comp)
cal <- weitrix_calibrate(simwei, disp)
weitrix_dispersions(cal, comp)
```

---

weitrix_calibrate_all *Adjust weights element-wise by fitting a trend to squared residuals*

Description

This is a very flexible method of calibrating weights. It should be especially useful if your existing weights account for technical variation, but there is also biological variation. In this case large weights will tend to be overly optimistic, and a non-linear transformation of weights is needed.

Usage

```
weitrix_calibrate_all(
  weitrix,
  design = ~1,
  trend_formula = NULL,
  mu_min = NA,
  mu_max = NA,
  keep_fit = FALSE
)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.
design	A formula in terms of colData(weitrix or a design matrix, which will be fitted to the weitrix on each row. Can also be a pre-existing Components object, in which case the existing fits (design$row) are used.
trend_formula	A formula specification for predicting squared residuals. See below. If absent, metadata(weitrix)$weitrix$calibrate_all_formula is used.
mu_min	When fitting the GLM, omit observations where the estimated mu is less than this value. When calculating weights from the fitted GLM, clip mu to be at least this value.
mu_max	When fitting the GLM, omit observations where the estimated mu is greater than this value. When calculating weights from the fitted GLM, clip mu to be at most this value.

keep_fit — Keep glm fit and the data used to create it. This can be large! If TRUE, these will be stored in `metadata(weitrix)$weitrix$all_fit` and `metadata(weitrix)$weitrix$all_data`.

Details

Residuals are found relative to a fitted model. A trend model is then fitted to the squared residuals using a gamma GLM with log link function. Weitrix weights are set based on the inverse of the fitted trend.

Residuals from a fitted model are generally smaller than residuals from the true model. A simple adjustment to the weights is made to account for this. Weights are reduced by a factor of (n-ncol(design)*nrow(weitrix))/n where n is the number of non-missing values in the weitrix.

`trend_formula` may reference any row or column variables, or `mu` for the predicted value, or `weight` for the existing weights, or special factors `row` and `col`. Keep in mind also that a log link function is used.

Unlike in `weitrix_calibrate_trend`, existing weights must be explicitly included in the formula if they are to be retained (see examples).

This function is currently not memory efficient, it should be fine for bulk experiments but may struggle for single cell. To reduce memory usage somewhat, when constructing the data frame on which to fit the glm, only columns referenced in `trend_formula` are included.

Example formulas:

`trend_formula=~1+offset(-log(weight))` Apply a global scaling, otherwise keeping weights the same.

`trend_formula=~log(weight)` Moderate weights by raising them to some power and applying some overall scaling factor. This will allow for biological variation.

`trend_formula=~poly(log(weight),2))` Apply a more complex quadratic curve-based moderation of weights.

`trend_formula=~col+offset(-log(weight))` Calibrate each sample's weights by a scaling factor. Note that due to the simplistic adjustment for using a fitted model rather than the true model, this may give misleading results when the design is unbalanced and there are few samples, i.e. when there are some samples with much higher leverage than others.

`trend_formula=~col*poly(log(weight),2)` Quadratic curve moderation of weights, applied to each sample individually.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

`metadata(weitrix)$weitrix` will contain the fitted trend model, and if requested the data frame used to fit the model.

Examples

```
simcal <- weitrix_calibrate_all(simwei, ~1, ~log(weight), keep_fit=TRUE)

metadata(simcal)$weitrix$all_fit
```

`weitrix_calibrate_trend` *Adjust weights row-wise by fitting a trend to estimated dispersions*

Description

Dispersions are estimated using `weitrix_dispersions`. A trend line is then fitted to the dispersions using a gamma GLM with log link function. Weitrix weights are calibrated based on this trend line.

Usage

```
weitrix_calibrate_trend(weitrix, design = ~1, trend_formula = NULL)
```

Arguments

`weitrix`	A weitrix object, or an object that can be converted to a weitrix with `as_weitrix`.
`design`	A formula in terms of `colData(weitrix)` or a design matrix, which will be fitted to the weitrix on each row. Can also be a pre-existing Components object, in which case the existing fits (`design$row`) are used.
`trend_formula`	A formula specification for predicting log dispersion from columns of row-Data(weitrix). If absent, metadata(weitrix)$weitrix$calibrate_trend_formula is used.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

Several columns are added to the `rowData`:

- deg_free Degrees of freedom for dispersion calculation.
- dispersion_before Dispersion before calibration.
- dispersion_trend Fitted dispersion trend.
- dispersion_after Dispersion for these new weights.

Examples

```
rowData(simwei)$total_weight <- rowSums(weitrix_weights(simwei))

# To estimate dispersions, use a simple model containing only an intercept
# term. Model log dispersion as a straight line relationship with log total
# weight and adjust weights to remove any trend.
cal <- weitrix_calibrate_trend(simwei,~1,trend_formula=~log(total_weight))

# This dataset has few rows, so calibration like this is dubious.
# Predictors in the fitted model are not significant.
summary( metadata(cal)$weitrix$trend_fit )

# Information about the calibration is added to rowData
```

```
rowData(cal)


# A Components object may also be used as the design argument.
comp <- weitrix_components(simwei, p=1, verbose=FALSE)
cal2 <- weitrix_calibrate_trend(simwei,comp,trend_formula=~log(total_weight))

rowData(cal2)
```

`weitrix_calplot` *Weight calibration plots, optionally versus a covariate*

Description

Various plots based on weighted squared residuals of each element in the weitrix. `weight*residual^2` is the Pearson residual for a gamma GLM plus one, as used by `weitrix_calibrate_all`.

Usage

```
weitrix_calplot(
  weitrix,
  design = ~1,
  covar,
  cat,
  funnel = FALSE,
  guides = TRUE
)
```

Arguments

`weitrix`	A weitrix object, or an object that can be converted to a weitrix with `as_weitrix`.
`design`	A formula in terms of `colData(weitrix` or a design matrix, which will be fitted to the weitrix on each row. Can also be a Components object.
`covar`	Optional. A covariate. Specify as you would with `ggplot2::aes`. Can be a matrix of the same size as `weitrix`.
`cat`	Optional. A categorical variable to break down the data by. Specify as you would with `ggplot2::aes`.
`funnel`	Flag. Produce a funnel plot? Note: `covar` can not be used for funnel plots.
`guides`	Show blue guide lines.

Details

This function is not memory efficient. It is suitable for typical bulk data, but generally not not for single-cell.

Defaults to a boxplot of sqrt(weight) weighted residuals. Blue guide bars are shown for the expected quartiles, these will ideally line up with the boxplot.

If `cat` is given, it will be used to break the elements down into categories.

If `covar` is given, sqrt(weight) weighted residuals are plotted versus the covariate, with red trend lines for the mean and for the mean +/- one standard deviation. If the weitrix is calibrated, the trend lines should be horizontal lines with y intercept close to -1, 0 and 1. Blue guide lines are shown for this ideal outcome.

Any of the variables available with `weitrix_calibrate_all` can be used for `covar` or `cat`.

Value

A ggplot2 plot.

Examples

```
weitrix_calplot(simwei, ~1)
weitrix_calplot(simwei, ~1, covar=mu)
weitrix_calplot(simwei, ~1, cat=col)

# weitrix_calplot should generally be used after calibration
cal <- weitrix_calibrate_all(simwei, ~1, ~col+log(weight))
weitrix_calplot(cal, ~1, cat=col)

# You can use a matrix of the same size as the weitrix as a covariate.
# It will often be useful to assess vs the original weighting.
weitrix_calplot(cal, ~1, covar=weitrix_weights(simwei))
```

---

weitrix_components *Principal components of a weitrix*

Description

Finds principal components of a weitrix. If varimax rotation is enabled, these are then rotated to enhance interpretability.

Usage

```
weitrix_components(
  weitrix,
  p = 0,
  design = ~1,
  n_restarts = 3,
```

```
  max_iter = 1000,
  tol = 1e-05,
  use_varimax = TRUE,
  initial = NULL,
  verbose = TRUE
)

weitrix_components_seq(
  weitrix,
  p,
  design = ~1,
  n_restarts = 3,
  max_iter = 1000,
  tol = 1e-05,
  use_varimax = TRUE,
  verbose = TRUE
)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.
p	Number of components to find.
design	A formula referring to colData(weitrix) or a matrix, giving predictors of a linear model for the experimental design. By default only an intercept term is used, i.e. rows are centered before finding components. A more complex formula might be used to account for batch effects. ~0 can be used if rows are already centered.
n_restarts	Number of restarts of the iteration to use.
max_iter	Maximum iterations.
tol	Stop iterating if R-squared increased by less than this amount in an iteration.
use_varimax	Use varimax rotation to enhance interpretability of components.
initial	Optional, an initial guess for column components (scores). Can have fewer columns than p, in which remaining components are initialized randomly. Can have more columns than p, in which case a randomly chosen subspace is used in each restart.
verbose	Show messages about the progress of the iterations.

Details

Note that this is a slow numerical method to solve a gnarly problem, for the case where weights are not uniform. The case of uniform weights or weights that can be written as an outer product of row and column weights is somewhat faster, however there are much faster algorithms for this available elsewhere.

An iterative method is used, starting from a random initial set of components. It is possible for this to get stuck at a local minimum. To ameliorate this, the iteration is initially run n_restarts times and the best result used. This is then iterated further. Examine all_R2s in the output to see if this

is happening – if the values are not all nearly identital, the iteration is sometimes getting stuck at local minima. Increase `n_restarts` to increase the odds of finding the global minimum.

Value

A "Components" object with the following elements accessible using `$`.

- row Row matrix, aka loadings. Rows are rows in the weitrix, and columns contain the experimental design (usually just an intercept term), and components.
- col Column matrix, aka scores. Rows are columns in the weitrix, and columns contain fitted coefficients for the experimental design, and components.
- R2 Weighted R squared statistic. The proportion of total variance explained by the components.
- all_R2s R2 statistics from all restarts. This can be used to check how consistently the iteration finds optimal components.
- ind_designColumn indices associated with experimental design.
- ind_componentsColumn indices associated with components.

For a result `comp`, the original measurements are approximated by `comp$row %*% t(comp$col)`.

`weitrix_components_seq` returns a list of Components objects, with increasing numbers of components from 1 up to p.

Functions

- `weitrix_components()`: Find a matrix decomposition with the specified number of components.
- `weitrix_components_seq()`: Produce a sequence of weitrix decompositions with 1 to p components.

Examples

```
# Variables in rows, observations in columns, as per Bioconductor convention
dat <- t(iris[,1:4])

# Find two components
comp <- weitrix_components(dat, p=2, max_iter=5, n_restart=1)

# Examine row and col matrices
pairs(comp$row, panel=function(x,y) text(x,y,rownames(comp$row)))
pairs(comp$col)
```

`weitrix_confects` *Top confident effects based on one or more contrasts of a linear model for each row*

Description

This function provides topconfects-style testing of a linear model contrast, as well as a multi-contrast extension of this method for F-tests with effect sizes.

Usage

```
weitrix_confects(
  weitrix,
  design,
  coef = NULL,
  contrasts = NULL,
  effect = c("auto", "contrast", "sd", "cohen_f"),
  dispersion_est = c("ebayes_limma", "row", "none"),
  fdr = 0.05,
  step = NULL,
  full = FALSE
)
```

Arguments

`weitrix`	A weitrix object, or an object that can be converted to a weitrix with `as_weitrix`.
`design`	A formula in terms of `colData(weitrix` or a design matrix, which will be fitted to the weitrix on each row. Can also be a pre-existing Components object, in which case the existing fits (`design$row`) are used.
`coef`	Give either coef or contrasts but not both. If coef is given, it is converted into a set of contrasts that simply test each given coefficient. Coefficients can be specified by number of name.
`contrasts`	Give either coef or contrasts but not both. One or more contrasts of interest, i.e. specifications of linear combination of coefficients. Each contrast should be placed in a columns. The number of rows should match the number of coefficients.
`effect`	Effect to estimate and provide confidence bounds on. See description.
`dispersion_est`	Method of estimating per-row dispersion. See description.
`fdr`	False Discovery Rate to control for.
`step`	Granularity of effect sizes to test.
`full`	If TRUE, output some further columns related to the calculations.

Details

Based on the `effect` argument, the estimated effect may be:

- `"auto"` Choose `"contrast"` or `"sd"` as appropriate.
- `"contrast"` The estimated contrast. This should produce results identical to a limma-topconfects analysis.
- `"sd"` Standard deviation explained (i.e. square root of the variance explained) by the part of the model captured by the contrasts provided.
- `"cohen_f"` Cohen's f, i.e. the signal to noise ratio. Ranking is similar to traditional ranking of results by p-value.

Based on the `dispersion_est` argument, the estimated residual dispersion is estimated as:

- `"none"` Weitrix is assumed to be fully calibrated already. Dispersion is assumed to be 1. If the assumption is correct, this is most powerful, as there is no uncertainty to the dispersion.
- `"row"` Dispersion is estimated based on the residuals for each row. With a limited number of columns, this estimate is uncertain (low residual degrees of freedom), so may lack power.
- `"ebayes_limma"` Default, recommended. Perform Empricial Bayes squeezing of dispersions, using `limma::squeezeVar`. This also reduces the uncertainty about the dispersion (mainfesting as extra "prior" degrees of freedom), increasing the power of the test.

In results from this function, whenever we talk about the mean, standard deviation explained, or typical observation error, this should be understood to be weighted. Standard deviation explained is in the same units as the observations, but its estimation is weighted by the weights, so in a row with some high weight observations and other low weight observations, estimated standard deviation explained will mostly be driven by the high weight observations.

Value

A topconfects result. The `$table` data frame contains columns:

- effect Estimated effect (as requested using the `effect` parameter).
- confect An inner confidence bound on effect.
- fdr_zero FDR-adjusted p-value for the null hypothesis that effect is zero.
- row_mean Weighted row mean.
- typical_obs_err Typical residual standard deviation (square root of variance) associated with observations in this row. Note that each observation has its own associated variance, based on its weight and the row dispersion estimate used. This column is calculated from the weighted average variance of observations.

Examples

```
# Simplest possible test
# Which rows have an average different from zero?
weitrix_confects(simwei, ~1, coef="(Intercept)")

# See vignettes for more substantial examples
```

weitrix_dispersions *Calculate row dispersions*

Description

Calculate the dispersion of each row. For each observation, this value divided by the weight gives the observation's variance.

Usage

```
weitrix_dispersions(weitrix, design = ~1)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.
design	A formula in terms of colData(weitrix or a design matrix, which will be fitted to the weitrix on each row. Can also be a pre-existing Components object, in which case the existing fits (design$row) are used.

Value

A numeric vector.

Examples

```
# Using a model just containing an intercept
weitrix_dispersions(simwei, ~1)

# Allowing for one component of variation, the dispersions are lower
comp <- weitrix_components(simwei, p=1, verbose=FALSE)
weitrix_dispersions(simwei, comp)
```

weitrix_elist *Convert a weitrix object to a limma EList object*

Description

The resulting object can be used as input to limma::lmFit for a limma analysis.

Usage

```
weitrix_elist(weitrix)
```

Arguments

weitrix	A weitrix object.

Value

A limma EList object.

Examples

```
library(limma)

elist <- weitrix_elist(simwei)
design <- model.matrix(~true_score, data=colData(simwei))
fit <- lmFit(elist, design)
# ...perform further limma analysis steps as desired...
```

`weitrix_hill` *Calculate Hill numbers (effective number of observations) for rows or columns*

Description

Effective numbers of observations. `order=0` produces count of non-zero weights. `order=1` produces exp(entropy). `order=2` produces the inverse Simpson index.

Usage

```
weitrix_hill(weitrix, what = c("row", "col"), order = 2)
```

Arguments

`weitrix`	A weitrix object.
`what`	Calculate for rows ("row") (default) or columns ("col")?
`order`	Order of the Hill numbers.

Value

A numeric vector of effective numbers of observations.

Examples

```
weitrix_weights(simwei)

weitrix_hill(simwei, what="row", order=0)
weitrix_hill(simwei, what="row", order=1)
weitrix_hill(simwei, what="row", order=2)

weitrix_hill(simwei, what="col", order=0)
weitrix_hill(simwei, what="col", order=1)
weitrix_hill(simwei, what="col", order=2)
```

weitrix_randomize *Generate a random normally distributed version of a weitrix*

Description

Values are generated with variance equal to 1/weight. This can be used to see what R-squared would be achieved with purely random data, and therefore an appropriate number of components to use. This is known as Parallel Analysis.

Usage

```
weitrix_randomize(weitrix)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.

Value

A SummarizedExperiment object with metadata fields marking it as a weitrix.

See Also

components_seq_screeplot

Examples

```
weitrix_randomize(simwei)
```

weitrix_sd_confects *Find rows with confidently excessive variability in a calibrated weitrix*

Description

Find rows with confident excess standard deviation beyond what is expected based on the weights of a calibrated weitrix. This may be used, for example, to find potential marker genes.

Usage

```
weitrix_sd_confects(
  weitrix,
  design = ~1,
  fdr = 0.05,
  step = 0.001,
  assume_normal = TRUE
)
```

Arguments

weitrix	A weitrix object, or an object that can be converted to a weitrix with as_weitrix.
design	A formula in terms of colData(weitrix or a design matrix, which will be fitted to the weitrix on each row. Can also be a pre-existing Components object, in which case the existing fits (design$row) are used.
fdr	False Discovery Rate to control for.
step	Granularity of effect sizes to test.
assume_normal	Assume weighted residuals are normally distributed? Assumption of normality is quite a strong assemption here. If TRUE, tests are based on the weighted squared residuals following a chi-squared distribution. If FALSE, tests are based on assuming the dispersion follows an asymptotically normal distribution, with variance estimated from the weighted squared residuals. If FALSE, a reasonably large number of columns is required. Defaults to TRUE.

Details

Important note: With the default setting of assume_normal=TRUE, the "confect" values produced by this method are only valid if the weighted residuals are close to normally distributed. If you have a reasonably large number of columns (eg single cell data), you can and should relax this assumption by specifying assume_normal=FALSE.

This is a conversion of the "dispersion" statistic for each row into units that are more readily interpretable, accompanied by confidence bounds with a multiple testing correction.

We are looking for further perturbation of observed values beyond what is accounted for by a linear model and, further, beyond what is expected based on the observation weights (assumed to be calibrated and so interpreted as 1/variance). We are seeking to estimate the standard deviation of this further perturbation.

The weitrix must have been calibrated for results to make sense.

Top confident effect sizes are found using the topconfects method, based on the model that the observed weighted sum of squared residuals being non-central chi-square distributed.

Note that all calculations are based on weighted residuals, with a rescaling to place results on the original scale. When a row has highly variable weights, this is an approximation that is only sensible if the weights are unrelated to the values themselves.

Value

A topconfects result. The $table data frame contains columns:

- effect Estimated excess standard deviation, in the same units as the observations themselves. 0 if the dispersion is less than 1.
- confect A lower confidence bound on effect.
- row_mean Weighted mean of observations in this row.
- typical_obs_err Typical accuracy of each observation.
- dispersion Dispersion. Weighted sum of squared residuals divided by residual degrees of freedom.

- n_present Number of observations with non-zero weight.
- df Degrees of freedom. n minus the number of coefficients in the model.
- fdr_zero FDR-adjusted p-value for the null hypothesis that effect is zero.

Note that `dispersion = effect^2/typical_obs_err^2 + 1` for non-zero effect values.

Examples

```
# weitrix_sd_confects should only be used with a calibrated weitrix
calwei <- weitrix_calibrate_all(simwei, ~1, ~1)

weitrix_sd_confects(calwei, ~1)
```

`weitrix_weights` *Get or set a weitrix object's "weights" matrix*

Description

Gets or sets the appropriate assay in the SummarizedExperiment object.

Usage

```
weitrix_weights(weitrix)

weitrix_weights(x) <- value
```

Arguments

`weitrix`	A weitrix object.
`x`	The weitrix to modify.
`value`	The new matrix.

Value

A matrix-like object such as a matrix or a DelayedArray.

Examples

```
weitrix_weights(simwei)
```

weitrix_x *Get or set a weitrix object's "x" matrix*

Description

Gets or sets the appropriate assay in the SummarizedExperiment object.

Usage

```
weitrix_x(weitrix)

weitrix_x(x) <- value
```

Arguments

weitrix	A weitrix object.
x	The weitrix to modify.
value	The new matrix.

Value

A matrix-like object such as a matrix or a DelayedArray.

Examples

```
weitrix_x(simwei)

simwei2 <- simwei
weitrix_x(simwei2) <- weitrix_x(simwei2) * 2
```

well_knotted_spline *Natural cubic spline with good choice of knots*

Description

For use in model formulas, natural cubic spline as in `splines::ns` but with knot positions chosen using k-means rather than quantiles. Automatically uses less knots if there are insufficient distinct values.

Usage

```
well_knotted_spline(x, n_knots, verbose = TRUE)
```

Arguments

x	The predictor variable. A numeric vector.
n_knots	Number of knots to use.
verbose	If TRUE, produce a message about the knots chosen.

Details

Wong (1982, 1984) showed the asymptotic density of k-means in 1 dimension is proportional to the cube root of the density of x. Compared to using quantiles (the default for ns), choosing knots using k-means produces a better spread of knot locations if the distribution of values is very uneven.

k-means is computed in an optimal, deterministic way using Ckmeans.1d.dp.

Value

A matrix of predictors, similar to ns.

This function supports "safe prediction" (see makepredictcall). Original knot locations will be used for prediction with predict.

References

Wong, M. (1982). Asymptotic properties of univariate sample k-means clusters. Working paper #1341-82, Sloan School of Management, MIT. https://dspace.mit.edu/handle/1721.1/46876

Wong, M. (1984). Asymptotic properties of univariate sample k-means clusters. *Journal of Classification*, 1(1), 255–270. https://doi.org/10.1007/BF01890126

See Also

ns, makepredictcall

Examples

```
lm(mpg ~ well_knotted_spline(wt,3), data=mtcars)

# When insufficient unique values exist, less knots are used
lm(mpg ~ well_knotted_spline(gear,3), data=mtcars)

library(ggplot2)
ggplot(diamonds, aes(carat, price)) +
   geom_point() +
   geom_smooth(method="lm", formula=y~well_knotted_spline(x,10))
```

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