Package 'flintyR'

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flintyR-package

Flexible and Interpretable Non-parametric Tests of Exchangeability

Description

Given a multivariate dataset and some knowledge about the dependencies between its features, it is important to ensure the observations or individuals are exchangeable before fitting a model to the data in order to make inference from it, or assigning randomized treatments in order to estimate treatment effects. This package provides a flexible non-parametric test of exchangeability, allowing the user to specify the feature dependencies by hand. See Aw, Spence and Song (2021) for the accompanying paper.

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Fast Bitwise Hamming Distance Vector

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weightedChi2P Tail Probability for Chi Square Convolution

Random Variable

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blockGaussian Approximate p-value for Test of Exchangeability (Assuming Large N

and P with Block Dependencies)

Description

Computes the large (N, P) asymptotic p-value for dataset X, assuming its P features are independent within specified blocks.

Usage

blockGaussian(X, block_boundaries, block_labels, p)

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Arguments

X The binary or real matrix on which to perform test of exchangeability block_boundaries

Vector denoting the positions where a new block of non-independent features

starts.

block_labels Length P vector recording the block label of each feature.

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is the large N and large P asymptotics of the permutation test.

Dependencies: getBinVStat, getRealVStat, getBlockCov, getChi2Weights

Value

The asymptotic p-value

blockLargeP Approximate p-value for Test of Exchangeability (Assuming Large P with Block Dependencies)

Description

Computes the large P asymptotic p-value for dataset X, assuming its P features are independent within specified blocks.

Usage

blockLargeP(X, block_boundaries, block_labels, p = 2)

Arguments

X The binary or real matrix on which to perform test of exchangeability block_boundaries

Vector denoting the positions where a new block of non-independent features starts.

 $block_labels$ Length P vector recording the block label of each feature.

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is the large P asymptotics of the permutation test.

 $Dependencies:\ getBinVStat,\ getRealVStat,\ getChi2Weights,\ weightedChi2P,\ getBlockCov$

Value

The asymptotic p-value

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blockPermute	p-value Computation for Test of Exchangeability with Block Dependencies

Description

Generates a block permutation p-value. Uses a heuristic to decide whether to use distance caching or simple block permutations.

Usage

```
blockPermute(X, block_boundaries = NULL, block_labels = NULL, nruns, p = 2)
```

Arguments

Χ	The binary or real matrix on which to perform permutation resampling	
block_boundaries		
	Vector denoting the positions where a new block of non-independent features starts. Default is NULL.	
block_labels	Length ${\cal P}$ vector recording the block label of each feature. Default is NULL.	
nruns	The resampling number (use at least 1000)	
р	The power p of l_p^p , i.e., $ x _p^p = (x_1^p + x_n^p)$	

Details

Dependencies: buildForward, buildReverse, cachePermute, cacheBlockPermute1, cacheBlockPermute2, getHammingDistance, getLpDistance, naiveBlockPermute1, naiveBlockPermute2

Value

The block permutation p-value

buildForward	Map from Indices to Label Pairs	
--------------	---------------------------------	--

Description

Builds a map from indexes to pairs of labels. This is for caching distances, to avoid recomputing Hamming distances especially when dealing with high-dimensional (large P) matrices.

Usage

```
buildForward(N)
```

Arguments

N Sample size, i.e., nrow(X)

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Details

Dependencies: None

Value

 $N \times N$ matrix whose entries record the index corresponding to the pair of labels (indexed by the matrix dims)

buildReverse

Map from Label Pairs to Indices

Description

Builds a map from pairs of labels to indexes. This is for caching distances, to avoid recomputing Hamming distances especially when dealing with high-dimensional (large P) matrices.

Usage

buildReverse(N)

Arguments

N

Sample size, i.e., nrow(X)

Details

Dependencies: None

Value

 $N \times N$ matrix whose entries record the index corresponding to the pair of labels (indexed by the matrix dims)

cacheBlockPermute1

Resampling Many V Statistics (Version 1)

Description

Generates a block permutation distribution of V statistic. Precomputes distances and some indexing arrays to quickly generate samples from the block permutation distribution of the V statistic of \mathbf{X} .

Usage

```
cacheBlockPermute1(X, block_labels, nruns, p = 2)
```

Arguments

X The binary or real matrix on which to perform permutation resampling

block_labels Length P vector recording the block label of each feature

nruns The resampling number (use at least 1000) $p \qquad \qquad \text{The power } p \text{ of } l_p^p \text{, i.e., } ||x||_p^p = (x_1^p + ... x_n^p)$

cacheBlockPermute2 7

Details

This version is with block labels specified.

Dependencies: buildForward, buildReverse, cachePermute, getHammingDistance, getLpDistance

Value

A vector of resampled values of the V statistic

cacheBlockPermute2

Resampling Many V Statistics (Version 2)

Description

Generates a block permutation distribution of V statistic. Precomputes distances and some indexing arrays to quickly generate samples from the block permutation distribution of the V statistic of \mathbf{X} .

Usage

```
cacheBlockPermute2(X, block_boundaries, nruns, p = 2)
```

Arguments

X The binary or real matrix on which to perform permutation resampling

 $block_boundaries$

Vector denoting the positions where a new block of non-independent features

starts

nruns The resampling number (use at least 1000)

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This version is with block boundaries specified.

 $Dependencies:\ buildForward,\ buildReverse,\ cache Permute,\ get Hamming Distance,\ get Lp Distance$

Value

A vector of resampled values of the V statistic

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cac	hePe	rmıد	ute

Permutation by Caching Distances

Description

What do you do when you have to compute pairwise distances many times, and those damn distances take a long time to compute? Answer: You cache the distances and permute the underlying sample labels!

Usage

```
cachePermute(dists, forward, reverse)
```

Arguments

dists $\binom{N}{2}$ by B matrix, with each column containing the distances (ex: Hamming, l_p^p)

for the block

forward $N \times N$ matrix mapping the pairs of sample labels to index of the $\binom{N}{2}$ -length

vector

reverse $\binom{N}{2} \times 2$ matrix mapping the index to pairs of sample labels

Details

This function permutes the distances (Hamming, l_p^p , etc.) within blocks. Permutations respect the fact that we are actually permuting the underlying labels. Arguments forward and reverse should be precomputed using buildForward and buildReverse.

Dependencies: buildForward, buildReverse

Value

A matrix with same dimensions as dists containing the block-permuted pairwise distances

distDataLargeP

Asymptotic p-value of Exchangeability Using Distance Data

Description

Generates an asymptotic p-value.

Usage

```
distDataLargeP(dist_list)
```

Arguments

dist_list

The list (length B) of pairwise distance data. Each element in list should be either a distance matrix or a table recording pairwise distances.

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Details

Generates a weighted convolution of chi-squares distribution of V statistic by storing the provided list of distance data as an $\binom{N}{2} \times B$ array, and then using large-P theory to generate the asymptotic null distribution against which the p-value of observed V statistic is computed.

Each element of dist_list should be a $N \times N$ distance matrix.

Dependencies: buildReverse, getChi2Weights, weightedChi2P

Value

The asymptotic p-value obtained from the weighted convolution of chi-squares distribution.

distDataPermute

p-value Computation for Test of Exchangeability Using Distance Data

Description

Generates a block permutation p-value.

Usage

```
distDataPermute(dist_list, nruns)
```

Arguments

dist_list The list (length B) of pairwise distance data. Each element in list should be

either a distance matrix or a table recording pairwise distances.

nruns The resampling number (use at least 1000)

Details

Generates a block permutation distribution of V statistic by storing the provided list of distance data as an $\binom{N}{2} \times B$ array, and then permuting the underlying indices of each individual to generate resampled $\binom{N}{2} \times B$ arrays. The observed V statistic is also computed from the distance data.

Each element of dist_list should be a $N \times N$ distance matrix.

Dependencies: buildForward, buildReverse, cachePermute

Value

The p-value obtained from comparing the empirical tail cdf of the observed V statistic computed from distance data.

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distDataPValue	A Non-parametric Test for Exchangeability and Homogeneity (Dis-
	tance List Version)

Description

Computes the p-value of a multivariate dataset, which informs the user if the sample is exchangeable at a given significance level, while simultaneously accounting for feature dependencies. See Aw, Spence and Song (2021) for details.

Usage

```
distDataPValue(dist_list, largeP = FALSE, nruns = 1000)
```

Arguments

dist_list The list of distances

largeP Boolean indicating whether to use large *P* asymptotics. Default is FALSE.

nruns Resampling number for exact test. Default is 1000.

Details

This version takes in a list of distance matrices recording pairwise distances between individuals across B independent features.

Dependencies: distDataLargeP and distDataPermute from auxiliary.R

Value

The p-value to be used to test the null hypothesis of exchangeability

```
# Example
suppressWarnings(require(doParallel))
registerDoParallel()

N <- 100
num_rows <- choose(N,2)
B <- 20
dist_list <- list()
for (b in 1:B) {
    # generate fake data
    fake_samples <- replicate(10, rbinom(N,1,0.5))

# compute pairwise distance
    fake_dist <- as.matrix(dist(fake_samples, method = "manhattan"))

# add to list
    dist_list[[b]] <- fake_dist
}

distDataPValue(dist_list)</pre>
```

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```
# should be larger than 0.05
```

getBinVStat

V Statistic for Binary Matrices

Description

Computes V statistic for a binary matrix X, as defined in Aw, Spence and Song (2021+).

Usage

```
getBinVStat(X)
```

Arguments

Χ

The $N \times P$ binary matrix

Details

Dependencies: getHammingDistance

Value

 $V(\mathbf{X})$, the variance of the pairwise Hamming distance between samples

Examples

```
X <- matrix(nrow = 5, ncol = 10, rbinom(50, 1, 0.5))
getBinVStat(X)</pre>
```

getBlockCov

Covariance Computations Between Pairs of Distances (Block Dependencies Case)

Description

Computes covariance matrix entries and associated alpha, beta and gamma quantities defined in Aw, Spence and Song (2021), for partitionable features that are grouped into blocks. Uses precomputation to compute the unique entries of the asymptotic covariance matrix of the pairwise Hamming distances in $O(N^2)$ time.

Usage

```
getBlockCov(X, block_boundaries, block_labels, p = 2)
```

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Arguments

X The binary or real matrix

block_boundaries

Vector denoting the positions where a new block of non-independent features

starts.

block_labels Length P vector recording the block label of each feature.

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is used in the large P asymptotics of the permutation test.

Dependencies: buildReverse, getHammingDistance, getLpDistance

Value

The three distinct entries of covariance matrix, (α, β, γ)

getChi2Weights

Get Chi Square Weights

Description

Computes weights for the asymptotic random variable from the α, β and γ computed of data array ${\bf X}.$

Usage

```
getChi2Weights(alpha, beta, gamma, N)
```

Arguments

alpha covariance matrix entry computed from getCov beta covariance matrix entry computed from getCov gamma covariance matrix entry computed from getCov

N The sample size, i.e., nrow(X) where X is the original dataset

Details

This is used in the large P asymptotics of the permutation test.

Dependencies: None

Value

The weights (w_1, w_2)

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getCov

Covariance Computations Between Pairs of Distances (Independent Case)

Description

Computes covariance matrix entries and associated alpha, beta and gamma quantities defined in Aw, Spence and Song (2021), assuming the P features of the dataset \mathbf{X} are independent.

Usage

```
getCov(X, p = 2)
```

Arguments

X The binary or real matrix

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is used in the large P asymptotics of the permutation test.

Dependencies: buildReverse, getLpDistance

Value

The three distinct entries of covariance matrix, (α, β, γ)

getHammingDistance

A Hamming Distance Vector Calculator

Description

Computes all pairwise Hamming distances for a binary matrix X.

Usage

```
getHammingDistance(X)
```

Arguments

Χ

The $N \times P$ binary matrix

Details

Dependencies: hamming_bitwise from fast_dist_calc.cpp

Value

A length ${N \choose 2}$ vector of pairwise Hamming distances

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Examples

```
X <- matrix(nrow = 5, ncol = 10, rbinom(50, 1, 0.5))
getHammingDistance(X)</pre>
```

getLpDistance

 $A l_p^p Distance Vector Calculator$

Description

Computes all pairwise l_p^p distances for a real matrix \mathbf{X} , for a specified choice of Minkowski norm exponent p.

Usage

```
getLpDistance(X, p)
```

Arguments

```
X The N \times P real matrix
```

```
The power p of l_p^p, i.e., ||x||_p^p = (x_1^p + ... x_n^p)
```

Details

Dependencies: lp_distance from fast_dist_calc.cpp

Value

```
A length \binom{N}{2} vector of pairwise l_p^p distances
```

Examples

```
X <- matrix(nrow = 5, ncol = 10, rnorm(50))
getLpDistance(X, p = 2)</pre>
```

 ${\tt getPValue}$

A Non-parametric Test for Exchangeability and Homogeneity

Description

Computes the p-value of a multivariate dataset X, which informs the user if the sample is exchangeable at a given significance level, while simultaneously accounting for feature dependencies. See Aw, Spence and Song (2021) for details.

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Usage

```
getPValue(
   X,
   block_boundaries = NULL,
   block_labels = NULL,
   largeP = FALSE,
   largeN = FALSE,
   nruns = 5000,
   p = 2
)
```

Arguments

X The binary or real matrix on which to perform test of exchangeability block_boundaries

Vector denoting the positions where a new block of non-independent features

starts. Default is NULL.

block_labels Length P vector recording the block label of each feature. Default is NULL. largeP Boolean indicating whether to use large P asymptotics. Default is FALSE. largeN Boolean indicating whether to use large N asymptotics. Default is FALSE.

nruns Resampling number for exact test. Default is 5000.

The power p of l_n^p , i.e., $||x||_n^p = (x_1^p + ... x_n^p)$. Default is 2.

Details

Automatically detects if dataset is binary, and runs the Hamming distance version of test if so. Otherwise, computes the squared Euclidean distance between samples and evaluates whether the variance of Euclidean distances, V, is atypically large under the null hypothesis of exchangeability. Note the user may tweak the choice of power p if they prefer an l_p^p distance other than Euclidean.

Under the hood, the variance statistic, V, is computed efficiently. Moreover, the user can specify their choice of block permutations, large P asymptotics, or large P and large N asymptotics. The latter two return reasonably accurate p-values for moderately large dimensionalities.

User recommendations: When the number of independent blocks B or number of independent features P is at least 50, it is safe to use large P asymptotics. If P or B is small, however, stick with permutations.

Dependencies: All functions in auxiliary.R

Value

The p-value to be used to test the null hypothesis of exchangeability

```
# Example 1 (get p-value of small matrix with independent features using exact test)
suppressWarnings(require(doParallel))
registerDoParallel()

X1 <- matrix(nrow = 5, ncol = 10, rbinom(50, 1, 0.5)) # binary matrix, small
getPValue(X1) # perform exact test with 5000 permutations
# should be larger than 0.05</pre>
```

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```
# Example 2 (get p-value of high-dim matrix with independent features using asymptotic test)
X2 <- matrix(nrow = 10, ncol = 1000, rnorm(1e4)) # real matrix, large enough
getPValue(X2, p = 2, largeP = TRUE) # very fast
# should be larger than 0.05
# getPValue(X2, p = 2) # slower, do not run (Output: 0.5764)
# Example 3 (get p-value of high-dim matrix with partitionable features using exact test)
suppressWarnings(require(doParallel))
registerDoParallel()
X3 \leftarrow matrix(nrow = 10, ncol = 1000, rbinom(1e4, 1, 0.5))
getPValue(X3, block_labels = rep(c(1,2,3,4,5), 200))
# Warning message: # there are features that have zero variation (i.e., all 0s or 1s)
# In getPValue(X3, block_labels = rep(c(1, 2, 3, 4, 5), 200)):
# There exist columns with all ones or all zeros for binary X.
# Example 4 (get p-value of high-dim matrix with partitionable features using asymptotic test)
## This elaborate example generates binarized versions of time series data.
# Helper function to binarize a marker
# by converting z-scores to \{0,1\} based on
# standard normal quantiles
binarizeMarker <- function(x, freq, ploidy) {</pre>
 if (ploidy == 1) {
   return((x > qnorm(1-freq)) + 0)
 } else if (ploidy == 2) {
   if (x \le qnorm((1-freq)^2)) {
     return(0)
   } else if (x \le qnorm(1-freq^2)) {
    return(1)
   } else return(2)
 } else {
   cat("Specify valid ploidy number, 1 or 2")
 }
}
getAutoRegArray <- function(B, N, maf_1 = 0.38, maf_u = 0.5, rho = 0.5, ploid = 1) {
# get minor allele frequencies by sampling from uniform
mafs <- runif(B, min = maf_1, max = maf_u)</pre>
# get AR array
ar_array <- t(replicate(N, arima.sim(n = B, list(ar=rho))))</pre>
# theoretical column variance
column_var <- 1/(1-rho^2)</pre>
# rescale so that variance per marker is 1
ar_array <- ar_array / sqrt(column_var)</pre>
# rescale each column of AR array
for (b in 1:B) {
  ar_array[,b] <- sapply(ar_array[,b],</pre>
                          binarizeMarker,
                          freq = mafs[b],
                          ploidy = ploid)
return(ar_array)
```

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getRealVStat

V Statistic for Real Matrices

Description

Computes V statistic for a real matrix \mathbf{X} , where $V(\mathbf{X})$ = scaled variance of l_p^p distances between the row samples of \mathbf{X} .

Usage

```
getRealVStat(X, p)
```

Arguments

```
X The N \times P real matrix  \text{ The power } p \text{ of } l_p^p \text{, i.e., } ||x||_p^p = (x_1^p + ... x_n^p) \mathbf{s}
```

Details

Dependencies: getLpDistance

Value

 $V(\mathbf{X})$, the variance of the pairwise l_p^p distance between samples

```
X <- matrix(nrow = 5, ncol = 10, rnorm(50))
getRealVStat(X, p = 2)</pre>
```

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hamming_bitwise

Fast Bitwise Hamming Distance Vector Computation

Description

Takes in a binary matrix X, whose transpose t(X) has N rows, and computes a vector recording all N choose 2 pairwise Hamming distances of t(X), ordered lexicographically.

Usage

```
hamming_bitwise(X)
```

Arguments

Χ

binary matrix (IntegerMatrix class)

Value

vector of Hamming distances (Numeric Vector class)

Examples

```
# t(X) = [[1,0], [0,1], [1,1]] \longrightarrow output = [2,1,1]
```

 $ind {\it Gaussian}$

Approximate p-value for Test of Exchangeability (Assuming Large N and P)

Description

Computes the large (N,P) asymptotic p-value for dataset \mathbf{X} , assuming its P features are independent

Usage

```
indGaussian(X, p = 2)
```

Arguments

X The binary or real matrix on which to perform test of exchangeability

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is the large ${\cal N}$ and large ${\cal P}$ asymptotics of the permutation test.

Dependencies: getBinVStat, getRealVStat, getCov, getChi2Weights

Value

The asymptotic p-value

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indLargeP

Approximate p-value for Test of Exchangeability (Assuming Large P)

Description

Computes the large P asymptotic p-value for dataset X, assuming its P features are independent.

Usage

```
indLargeP(X, p = 2)
```

Arguments

X The binary or real matrix on which to perform test of exchangeability

p The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ...x_n^p)$

Details

This is the large P asymptotics of the permutation test.

Dependencies: getBinVStat, getRealVStat, getChi2Weights, weightedChi2P, getCov

Value

The asymptotic p-value

lp_distance

Fast l_p^p Distance Vector Computation

Description

Takes in a double matrix X, whose transpose t(X) has N rows, and computes a vector recording all $\binom{N}{2}$ pairwise l_p^p distances of t(X), ordered lexicographically.

Usage

```
lp_distance(X, p)
```

Arguments

X double matrix (arma::mat class)

p numeric Minkowski power (double class)

Value

```
vector of l_p^p distances (arma::vec class)
```

```
# X = [[0.5,0.5],[0,1],[0.3,0.7]] --> lPVec = [x,y,z] # with x = (0.5^p + 0.5^p)
```

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naiveBlockPermute1

Resampling V Statistic (Version 1)

Description

Generates a new array X' under the permutation null and then returns the V statistic computed for X'.

Usage

```
naiveBlockPermute1(X, block_labels, p = 2)
```

Arguments

Details

This is Version 1, which takes in the block labels. It is suitable in the most general setting, where the features are grouped by labels. Given original \mathbf{X} and a list denoting labels of each feature, independently permutes the rows within each block of \mathbf{X} and returns resulting V. If block labels are not specified, then features are assumed independent, which is to say that block_labels is set to 1:ncol(\mathbf{X}).

Dependencies: getBinVStat, getRealVStat

Value

 $V(\mathbf{X}')$, where \mathbf{X}' is a resampled by permutation of entries blockwise

```
X \leftarrow matrix(nrow = 5, ncol = 10, rnorm(50)) \# real matrix example naiveBlockPermute1(X, block_labels = c(1,1,2,2,3,3,4,4,5,5), p = 2) # use Euclidean distance <math>X \leftarrow matrix(nrow = 5, ncol = 10, rbinom(50, 1, 0.5)) \# binary matrix example naiveBlockPermute1(X, block_labels = c(1,1,2,2,3,3,4,4,5,5))
```

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naiveBlockPermute2

Resampling V Statistic (Version 2)

Description

Generates a new array X' under the permutation null and then returns the V statistic computed for X'.

Usage

```
naiveBlockPermute2(X, block_boundaries, p = 2)
```

Arguments

X The $N \times P$ binary or real matrix

block_boundaries

A vector of length at most P, whose entries indicate positions at which to demarcate blocks

The power p of l_p^p , i.e., $||x||_p^p = (x_1^p + ... x_n^p)$

Details

This is Version 2, which takes in the block boundaries. It is suitable for use when the features are already arranged such that the block memberships are determined by index delimiters. Given original \mathbf{X} and a list denoting labels of each feature, independently permutes the rows within each block of \mathbf{X} and returns resulting V. If block labels are not specified, then features are assumed independent, which is to say that block_labels is set to 1:ncol(\mathbf{X}).

Dependencies: getBinVStat, getRealVStat

Value

 $V(\mathbf{X}')$, where \mathbf{X}' is a resampled by permutation of entries blockwise

```
X \leftarrow matrix(nrow = 5, ncol = 10, rnorm(50)) # real matrix example naiveBlockPermute2(X, block_boundaries = c(4,7,9), p = 2) # use Euclidean distance X \leftarrow matrix(nrow = 5, ncol = 10, rbinom(50, 1, 0.5)) # binary matrix example naiveBlockPermute2(X, block_boundaries = c(4,7,9))
```

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weightedChi2P

Tail Probability for Chi Square Convolution Random Variable

Description

Computes P(X > val) where $X = w_1Y + w_2Z$, where Y is chi square distributed with d_1 degrees of freedom, Z is chi square distributed with d_2 degrees of freedom, and w_1 and w_2 are weights with w_2 assumed positive. The probability is computed using numerical integration of the densities of the two chi square distributions. (Method: trapezoidal rule)

Usage

```
weightedChi2P(val, w1, w2, d1, d2)
```

Arguments

val	observed statistic
w1	weight of first chi square rv
w2	weight of second chi square rv, assumed positive
d1	degrees of freedom of first chi square rv
d2	degrees of freedom of second chi square rv

Details

This is used in the large P asymptotics of the permutation test.

Dependencies: None

Value

```
1 - CDF = P(X > val)
```

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