

Package ‘groupwalk’

October 13, 2022

Title Implement the Group Walk Algorithm

Version 0.1.2

Description A procedure that uses target-decoy competition (or knockoffs) to reject multiple hypotheses in the presence of group structure. The procedure controls the false discovery rate (FDR) at a user-specified threshold.

URL <https://www.biorxiv.org/content/10.1101/2022.01.30.478144v1>,
<https://github.com/freejstone/groupwalk>

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Suggests testthat (>= 3.0.0)

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NeedsCompilation no

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R topics documented:

group_walk	2
Index	4

group_walk

Implements group-walk algorithm

Description

This function returns a list of q-values corresponding to hypotheses that have been partitioned into groups. For FDR control, users should report the target-hypotheses with q-values less than or equal to their choice of threshold, alpha. For further details about how group-walk works, see: <https://www.biorxiv.org/content/10.1101/2022.01.30.478144v1>

Usage

```
group_walk(
  winning_scores,
  labels,
  all_group_ids,
  K = 40,
  return_frontier = FALSE,
  correction = 1
)
```

Arguments

winning_scores	A numerical vector of winning scores generated from the target-decoy competitions for each hypothesis.
labels	A vector of winning labels indicating whether it was a target (= 1) or a decoy (!= 1) for each hypothesis.
all_group_ids	A vector of group IDs associated to each hypothesis (can be recorded as integers, factors, characters).
K	A window size parameter (integer).
return_frontier	A boolean indicating whether the function should return the complete sequence of frontiers.
correction	A correction factor used to in the numerator of the estimated false discovery rate (FDR) (Use 1 for FDR control).

Value

A sequence of q-values for each hypothesis. If return_frontier = T, additionally the sequence of frontiers will be returned.

Examples

```
create_uncalibrated_hypotheses <- function(m_vec, pi_0_vec, mus, sds) {
  total <- sum(m_vec)
  g_total <- length(m_vec)
```

```

data <- matrix(0, ncol = 4, nrow = total)
for (g in 1:length(m_vec)){
  m <- m_vec[g]
  pi_0 <- pi_0_vec[g]
  mu <- mus[g]
  sd <- sds[g]
  if (g == 1) {
    start <- 0
  } else {
    start <- sum(m_vec[1:(g - 1)])
  }
  targets_nonnull <- rnorm(floor(m*pi_0), mean = mu, sd = sd)
  targets_null <- rnorm(m - floor(m*pi_0), mean = 0, sd = 1)
  decoys <- rnorm(m, mean = 0, sd = 1)
  targets <- c(targets_nonnull, targets_null)
  W <- pmax(targets, decoys)
  data[(start + 1):(start + m), 1] <- W
  data[(start + 1):(start + m), 2] <- g
  decoy_inds <- which(decoys > targets)
  inc_native_inds <- (which(targets_null > decoys[(floor(m*pi_0) + 1):m])) + floor(m*pi_0)
  X <- rep(0, m)
  X[decoy_inds] <- -1
  X[inc_native_inds] <- 1
  Y <- X
  X[X == 0] <- 1
  data[(start + 1):(start + m), 3] <- Y
  data[(start + 1):(start + m), 4] <- X
}
return(data)
}

data <- create_uncalibrated_hypotheses(m_vec = rep(1000, 3),
  pi_0_vec = rep(0.6, 3), mus = c(2.5, 3, 3.5), sds = rep(1, 3))

winning_scores <- data[, 1]
all_group_ids <- data[, 2]
labels <- data[, 4]
q_vals <- group_walk(winning_scores, labels, all_group_ids)

```

Index

`group_walk`, 2