

Package ‘bandsfdp’

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Title Compute Upper Prediction Bounds on the FDP in Competition-Based Setups

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Suggests fdpbandsdata

Description Implements functions that calculate upper prediction bounds on the false discovery proportion (FDP) in the list of discoveries returned by competition-based setups, implementing Ebadi et al. (2022) <[doi:10.48550/arXiv.2302.11837](https://doi.org/10.48550/arXiv.2302.11837)>. Such setups include target-decoy competition (TDC) in computational mass spectrometry and the knockoff construction in linear regression (note this package typically uses the terminology of TDC). Included is the standardized (TDC-SB) and uniform (TDC-UB) bound on TDC's FDP, and the simultaneous standardized and uniform bands. Requires pre-computed Monte Carlo statistics available at <<https://github.com/uni-Arya/fdpbandsdata>>. This data can be downloaded by running the command 'devtools::install_github("`uni-Arya/fdpbandsdata")' in R and restarting R after installation. The size of this data is roughly 81Mb.

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Encoding UTF-8

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URL <https://github.com/uni-Arya/bandsfdp>

BugReports <https://github.com/uni-Arya/bandsfdp/issues>

NeedsCompilation no

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gen_bound	<i>Generalized band</i>
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Description

This function computes an upper prediction bound on the FDP among target wins in any set R of hypotheses of TDC. See details for more information.

Usage

```
gen_bound(
  labels,
  indices,
  gamma,
  type,
  d_max = NULL,
  max_fdp = 0.5,
  c = 0.5,
  lambda = 0.5
)
```

```
genband(
  labels,
  indices,
  gamma,
  type,
  d_max = NULL,
  max_fdp = 0.5,
  c = 0.5,
  lambda = 0.5
)
```

Arguments

labels	A vector of (ordered) labels. See details below.
indices	A vector specifying the indices of hypotheses for which an upper prediction bound on the FDP is computed.
gamma	The confidence parameter of the band. Typical values include $\gamma = 0.05$ or $\gamma = 0.01$.

type	A character string specifying which band to use. Must be one of "stband" or "uniband".
d_max	An optional positive integer specifying the maximum number of decoy wins considered in calculating the bands.
max_fdp	A number specifying the maximum FDP considered by the user in calculating the bands. Used to compute d_max if d_max is set to NULL.
c	Determines the ranks of the target score that are considered winning. Defaults to $c = 0.5$ for (single-decoy) TDC.
lambda	Determines the ranks of the target score that are considered losing. Defaults to $\lambda = 0.5$ for (single-decoy) TDC.

Details

In (single-decoy) TDC, each hypothesis is associated to a winning score and a label (1 for a target win, -1 for a decoy win). This function assumes that the hypotheses are ordered in decreasing order of winning scores (with ties broken at random). The argument labels, therefore, must be ordered according to this rule.

This function also supports the extension of TDC that uses multiple decoys. In that setup, the target score is competed with multiple decoy scores and the rank of the target score after competition is used to determine whether the hypothesis is a target win (label = 1), decoy win (-1) or uncounted (0). The top c proportion of ranks are considered winning, the bottom $1-\lambda$ losing, and all the rest uncounted.

The threshold of TDC is given by the formula (assuming hypotheses are ordered):

$$\max\{k : \frac{D_k + 1}{T_k \vee 1} \cdot \frac{c}{1 - \lambda} \leq \alpha\}$$

where T_k is the number of target wins among the top k hypotheses, and D_k is the number of decoy wins similarly.

The argument gamma sets a confidence level of $1-\gamma$. Both the uniform and standardized bands require pre-computed Monte Carlo statistics, so only certain values of gamma are available to use. Commonly used confidence levels, like 0.95 and 0.99, are available. We refer the reader to the README of this package for more details.

The argument d_max controls the rate at which the returned bounds increase: a larger d_max results in a more conservative bound. If, however, $D_k + 1$ exceeds d_max for some index k , each target win thereafter is considered a false discovery when computing the bound. Thus it is important that d_max, chosen a priori, is large enough. Given it is sufficiently large, the precise value of d_max does not have a significant effect on the resulting bounds (see <https://arxiv.org/abs/2302.11837> for more details).

We recommend setting d_max = NULL so that it is computed automatically using max_fdp. This argument ensures that $D_k + 1$ never exceeds d_max when the (non-interpolated) FDP bound on the top k hypotheses is less than max_fdp.

Value

An upper prediction bound on the FDP among target wins in the set of hypotheses whose indices are given as input.

References

Ebadi et al. (2022), Bounding the FDP in competition-based control of the FDR <https://arxiv.org/abs/2302.11837>.

Examples

```
if (requireNamespace("fdpbandsdata", quietly = TRUE)) {
  set.seed(123)
  labels <- c(
    rep(1, 250),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.9, 0.1)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.5, 0.5)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.1, 0.9))
  )
  indices <- c(1:100, 300:400, 600:650)
  gamma <- 0.05
  gen_bound(labels, indices, gamma, "stband")
}
```

sim_bound

Simultaneous Band

Description

This function computes upper prediction bounds on the target wins among the top k hypotheses of TDC, for each $k = 1, \dots, n$ where n is the total number of hypotheses.

Usage

```
sim_bound(
  labels,
  gamma,
  type,
  d_max = NULL,
  max_fdp = 0.5,
  c = 0.5,
  lambda = 0.5
)

simband(
  labels,
  gamma,
  type,
  d_max = NULL,
  max_fdp = 0.5,
  c = 0.5,
  lambda = 0.5
)
```

Arguments

labels	A vector of (ordered) labels. See details below.
gamma	The confidence parameter of the band. Typical values include $\gamma = 0.05$ or $\gamma = 0.01$.
type	A character string specifying which band to use. Must be one of "stband" or "uniband".
d_max	An optional positive integer specifying the maximum number of decoy wins considered in calculating the bands.
max_fdp	A number specifying the maximum FDP considered by the user in calculating the bands. Used to compute d_max if d_max is set to NULL.
c	Determines the ranks of the target score that are considered winning. Defaults to $c = 0.5$ for (single-decoy) TDC.
lambda	Determines the ranks of the target score that are considered losing. Defaults to $\lambda = 0.5$ for (single-decoy) TDC.

Details

In (single-decoy) TDC, each hypothesis is associated to a winning score and a label (1 for a target win, -1 for a decoy win). This function assumes that the hypotheses are ordered in decreasing order of winning scores (with ties broken at random). The argument labels, therefore, must be ordered according to this rule.

This function also supports the extension of TDC that uses multiple decoys. In that setup, the target score is competed with multiple decoy scores and the rank of the target score after competition is used to determine whether the hypothesis is a target win (label = 1), decoy win (-1) or uncounted (0). The top c proportion of ranks are considered winning, the bottom $1-\lambda$ losing, and all the rest uncounted.

The threshold of TDC is given by the formula (assuming hypotheses are ordered):

$$\max\{k : \frac{D_k + 1}{T_k \vee 1} \cdot \frac{c}{1 - \lambda} \leq \alpha\}$$

where T_k is the number of target wins among the top k hypotheses, and D_k is the number of decoy wins similarly.

The argument gamma sets a confidence level of $1-\gamma$. Both the uniform and standardized bands require pre-computed Monte Carlo statistics, so only certain values of gamma are available to use. Commonly used confidence levels, like 0.95 and 0.99, are available. We refer the reader to the README of this package for more details.

The argument d_max controls the rate at which the returned bounds increase: a larger d_max results in a more conservative bound. If, however, $D_k + 1$ exceeds d_max for some index k , each target win thereafter is considered a false discovery when computing the bound. Thus it is important that d_max, chosen a priori, is large enough. Given it is sufficiently large, the precise value of d_max does not have a significant effect on the resulting bounds (see <https://arxiv.org/abs/2302.11837> for more details).

We recommend setting d_max = NULL so that it is computed automatically using max_fdp. This argument ensures that $D_k + 1$ never exceeds d_max when the (non-interpolated) FDP bound on the top k hypotheses is less than max_fdp.

Value

A vector of upper prediction bounds on the FDP of target wins among the top k hypotheses for each $k = 1, \dots, n$ where n is the total number of hypotheses.

References

Ebadi et al. (2022), Bounding the FDP in competition-based control of the FDR <https://arxiv.org/abs/2302.11837>.

Examples

```
if (requireNamespace("fdpbandsdata", quietly = TRUE)) {
  set.seed(123)
  labels <- c(
    rep(1, 250),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.9, 0.1)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.5, 0.5)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.1, 0.9))
  )
  gamma <- 0.05
  head(sim_bound(labels, gamma, "stband"))
}
```

tdc_sb

Standardized Band

Description

This function computes an upper prediction bound, derived from the standardized band, on the FDP in TDC's list of discoveries.

Usage

```
tdc_sb(
  thresholds,
  labels,
  alpha,
  gamma,
  c = 0.5,
  lambda = 0.5,
  n = length(labels),
  interpolate = TRUE
)

stband(
  thresholds,
  labels,
```

```

    alpha,
    gamma,
    c = 0.5,
    lambda = 0.5,
    n = length(labels),
    interpolate = TRUE
)

```

Arguments

thresholds	The rejection threshold of TDC. If given as a vector, an upper prediction bound is returned for each element.
labels	A vector of (ordered) labels. See details below.
alpha	The FDR threshold.
gamma	The confidence parameter of the bound. Typical values include $\gamma = 0.05$ or $\gamma = 0.01$.
c	Determines the ranks of the target score that are considered winning. Defaults to $c = 0.5$ for (single-decoy) TDC.
lambda	Determines the ranks of the target score that are considered losing. Defaults to $\lambda = 0.5$ for (single-decoy) TDC.
n	The number of hypotheses. Defaults to the length of labels.
interpolate	A boolean indicating whether the bands should be interpolated. Offers a slight boost in performance at the cost of computing power. Defaults to TRUE.

Details

In (single-decoy) TDC, each hypothesis is associated to a winning score and a label (1 for a target win, -1 for a decoy win). This function assumes that the hypotheses are ordered in decreasing order of winning scores (with ties broken at random). The argument labels, therefore, must be ordered according to this rule.

This function also supports the extension of TDC that uses multiple decoys. In that setup, the target score is competed with multiple decoy scores and the rank of the target score after competition is used to determine whether the hypothesis is a target win (label = 1), decoy win (-1) or uncounted (0). The top c proportion of ranks are considered winning, the bottom $1-\lambda$ losing, and all the rest uncounted.

The threshold of TDC is given by the formula:

$$\max\{k : \frac{D_k + 1}{T_k \vee 1} \cdot \frac{c}{1 - \lambda} \leq \alpha\}$$

where T_k is the number of target wins among the top k hypotheses, and D_k is the number of decoy wins similarly.

The argument gamma sets a confidence level of $1-\gamma$. Since the standardized band requires pre-computed Monte Carlo quantiles, only certain values of gamma are available to use. Commonly used confidence levels, like 0.95 and 0.99, are available. We refer the reader to the README of this package for more details.

The argument `alpha`, used to compute the threshold of TDC, is also used in this function. It serves to compute an appropriate `d_max` for a non-trivial bound. In particular, if the user inputs a vector of thresholds, a bound is returned for each element of thresholds using the same `d_max`. For more details, see: <https://arxiv.org/abs/2302.11837>.

We recommend the use of `interpolate = TRUE` (default), as it generally results in a tighter bound. This comes at the cost of performance: the bound for each threshold is computed in $O(n)$ time with interpolation and $O(1)$ without.

Value

An upper prediction bound on the FDP in TDC's list of discoveries. If `thresholds` is a vector, returns an upper prediction bound for each element of thresholds.

References

Ebadi et al. (2022), Bounding the FDP in competition-based control of the FDR <https://arxiv.org/abs/2302.11837>.

Examples

```
if (requireNamespace("fdpbandsdata", quietly = TRUE)) {
  set.seed(123)
  thresholds <- c(250, 500, 750, 1000)
  labels <- c(
    rep(1, 250),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.9, 0.1)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.5, 0.5)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.1, 0.9))
  )
  alpha <- 0.05
  gamma <- 0.05
  tdc_sb(thresholds, labels, alpha, gamma)
}
```

 tdc_ub | *Uniform Band* |

Description

This function computes an upper prediction bound, derived from the uniform band, on the FDP in TDC's list of discoveries.

Usage

```
tdc_ub(
  thresholds,
  labels,
```

```

    alpha,
    gamma,
    c = 0.5,
    lambda = 0.5,
    n = length(labels),
    interpolate = TRUE
)

uniband(
  thresholds,
  labels,
  alpha,
  gamma,
  c = 0.5,
  lambda = 0.5,
  n = length(labels),
  interpolate = TRUE
)

```

Arguments

thresholds	The rejection threshold of TDC. If given as a vector, an upper prediction bound is returned for each element.
labels	A vector of (ordered) labels. See details below.
alpha	The FDR threshold.
gamma	The confidence parameter of the bound. Typical values include $\gamma = 0.05$ or $\gamma = 0.01$.
c	Determines the ranks of the target score that are considered winning. Defaults to $c = 0.5$ for (single-decoy) TDC.
lambda	Determines the ranks of the target score that are considered losing. Defaults to $\lambda = 0.5$ for (single-decoy) TDC.
n	The number of hypotheses. Defaults to the length of labels.
interpolate	A boolean indicating whether the bands should be interpolated. Offers a slight boost in performance at the cost of computing power. Defaults to TRUE.

Details

In (single-decoy) TDC, each hypothesis is associated to a winning score and a label (1 for a target win, -1 for a decoy win). This function assumes that the hypotheses are ordered in decreasing order of winning scores (with ties broken at random). The argument labels, therefore, must be ordered according to this rule.

This function also supports the extension of TDC that uses multiple decoys. In that setup, the target score is competed with multiple decoy scores and the rank of the target score after competition is used to determine whether the hypothesis is a target win (label = 1), decoy win (-1) or uncounted (0). The top c proportion of ranks are considered winning, the bottom $1-\lambda$ losing, and all the rest uncounted.

The threshold of TDC is given by the formula:

$$\max\{k : \frac{D_k + 1}{T_k \vee 1} \cdot \frac{c}{1 - \lambda} \leq \alpha\}$$

where T_k is the number of target wins among the top k hypotheses, and D_k is the number of decoy wins similarly.

The argument `gamma` sets a confidence level of $1 - \text{gamma}$. Since the uniform band requires pre-computed Monte Carlo statistics, only certain values of `gamma` are available to use. Commonly used confidence levels, like 0.95 and 0.99, are available. We refer the reader to the README of this package for more details.

The argument `alpha`, used to compute the threshold of TDC, is also used in this function. It serves to compute an appropriate `d_max` for a non-trivial bound. In particular, if the user inputs a vector of thresholds, a bound is returned for each element of thresholds using the same `d_max`. For more details, see: <https://arxiv.org/abs/2302.11837>.

We recommend the use of `interpolate = TRUE` (default), as it generally results in a tighter bound. This comes at the cost of performance: the bound for each threshold is computed in $O(n)$ time with interpolation and $O(1)$ without.

Value

An upper prediction bound on the FDP in TDC's list of discoveries. If `thresholds` is a vector, returns an upper prediction bound for each element of `thresholds`.

References

Ebadi et al. (2022), Bounding the FDP in competition-based control of the FDR <https://arxiv.org/abs/2302.11837>.

Examples

```
if (requireNamespace("fdpbandsdata", quietly = TRUE)) {
  set.seed(123)
  thresholds <- c(250, 500, 750, 1000)
  labels <- c(
    rep(1, 250),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.9, 0.1)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.5, 0.5)),
    sample(c(1, -1), size = 250, replace = TRUE, prob = c(0.1, 0.9))
  )
  alpha <- 0.05
  gamma <- 0.05
  tdc_ub(thresholds, labels, alpha, gamma)
}
```

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