Package ‘powerTCR’

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**Type**  Package

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**Description**  This package provides a model for the clone size distribution of the TCR repertoire. Further, it permits comparative analysis of TCR repertoire libraries based on theoretical model fits.

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Accessors

Grab important output from a list of fits

Description

These are convenient accessors that will grab important output from a list of fits from fdiscgammagpd. They will grab the maximum likelihood estimates and/or the negative log likelihood for the maximum likelihood estimates.

Usage

```r
get_mle(fits)
get_nllh(fits)
get_diversity(fits)
```

Arguments

- `fits`: A list of fits output from fdiscgammagpd.

Value

A list of out either maximum likelihood estimates (`get_mle`) or negative log likelihoods (`get_nllh`) corresponding to the list of fits. For `get_diversity`, a data frame of diversity estimates (species richness, Shannon entropy, clonality, and proportion of highly stimulated clones) for the samples.

Author(s)

<hbk5086@psu.edu>

See Also

`fdiscgammagpd`
Examples

# Here is a good workflow using fdiscgammagpd:
# Choose quantiles for every sample repertoire in the same manner.
# Then fit the model in the same manner as well.

data("repertoires")

thresholds <- list()
fits <- list()
for(i in 1:2)
    thresholds[[i]] <- unique(round(quantile(repertoires[[i]], c(.8,.85,.9,.95))))
fits[[i]] <- fdiscgammagpd(repertoires[[i]], useq = thresholds[[i]],
shift = min(repertoires[[i]]))

names(fits) <- c("fit1", "fit2")

mles <- get_mle(fits)
nllhs <- get_nllh(fits)
diversity_ests <- get_diversity(fits)

mles
nllhs
diversity_ests

clusterPlot

Visualize hierarchical clustering of samples

Description

This function is just a simple wrapper for the hclust function. It takes a symmetrical matrix displaying pairwise distances between samples and outputs a plot of the hierarchical clustering using specified linkage. Note that the distances must be given as a matrix object, not a distance object.

Usage

clusterPlot(distances, method = c("complete", "ward.D", "ward.D2", "single",
"average", "mcquitty", "median", "centroid")

Arguments

distances A symmetric matrix containing the Jensen-Shannon distance between pairs of distributions.

method Linkage method, as in hclust

Value

A basic plot of the induced hierarchical clustering.
Note

The distances must be given as a matrix object, not a distance object. The distance between a distribution and itself is 0. This corresponds to a matrix diagonal of 0.

Author(s)
<hbk5086@psu.edu>

See Also
JS_spliced, JS_desponds

Examples

```r
# Simulate 3 sampled individuals
set.seed(123)
s1 <- rdiscgammapd(1000, shape = 3, rate = .15, u = 25, sigma = 15, xi = .5, shift = 1)
s2 <- rdiscgammapd(1000, shape = 3.1, rate = .14, u = 26, sigma = 15, xi = .6, shift = 1)
s3 <- rdiscgammapd(1000, shape = 10, rate = .3, u = 45, sigma = 20, xi = .7, shift = 1)

# Fit model to the data at the true thresholds
fits <- list("fit1" = fdiscgammapd(s1, useq = 25),
              "fit2" = fdiscgammapd(s2, useq = 26),
              "fit3" = fdiscgammapd(s3, useq = 45))

# Compute the pairwise JS distance between 3 fitted models
distances <- matrix(rep(0, 9), nrow = 3)
colnames(distances) <- rownames(distances) <- c("s1", "s2","s3")
ggrid <- min(c(s1,s2,s3)):10000
for(i in 1:2){
  for(j in (i+1):3){
    distances[i,j] <- JS_spliced(grid,
                                shiftp = min(fits[[i]]$x),
                                shiftq = min(fits[[j]]$x),
                                phip = fits[[i]]$mle['phi'],
                                phiq = fits[[j]]$mle['phi'],
                                shapep = fits[[i]]$mle['shape'],
                                shapeq = fits[[j]]$mle['shape'],
                                ratep = fits[[i]]$mle['rate'],
                                rateq = fits[[j]]$mle['rate'],
                                threshp = fits[[i]]$mle['thresh'],
                                threshq = fits[[j]]$mle['thresh'],
                                sigmap = fits[[i]]$mle['sigma'],
                                sigmam = fits[[j]]$mle['sigma'],
                                xip = fits[[i]]$mle['xi'],
                                xiq = fits[[j]]$mle['xi'])
  }
}

# Distances are symmetric
distances <- distances + t(distances)
```

# Perform clustering. Note that s1 and s2 were generated using similar
# parameters, so we might expect them to be clustered together
## Not run: clusterPlot(distances, method = c("ward.D"))

discgammagpd

The discrete gamma-GPD spliced threshold distribution

Description

Density, distribution function, quantile function and random generation for the discrete gamma-
GPD spliced threshold distribution. The distribution has gamma bulk with shape equal to shape
and rate equal to rate. It is spliced at a threshold equal to u and has a GPD tail with sigma equal to
sigma and xi equal to xi. The proportion of data above the threshold phi is equal to phiu and the
data are shifted according to shift.

Usage

ddiscgammagpd(x, fit, shape, rate, u, sigma, xi, phiu = NULL, shift = 0, log = FALSE)
pdiscgammagpd(q, fit, shape, rate, u, sigma, xi, phiu = NULL, shift = 0)
qdiscgammagpd(p, fit, shape, rate, u, sigma, xi, phiu = NULL, shift = 0)
rdiscgammagpd(n, fit, shape, rate, u, sigma, xi, phiu = NULL, shift = 0)

Arguments

x, q
vector of quantiles.
p
vector of probabilities.
n
number of observations.
fit
A fit output from fdiscgammagpd. If this object is passed, all parameter fields
will automatically populate with the maximum likelihood estimates for the pa-
rameters in fit.
shape
shape parameter alpha of the truncated gamma distribution.
rate
rate parameter beta of the gamma distribution.
u
threshold.
sigma
scale parameter sigma of the GPD.
xi
shape parameter xi of the GPD
phiu
Propotion of data greater than or equal to threshold u.
shift
value the complete distribution is shifted by. Ideally, this is the smallest value of
the count data from one sample.
log
Logical; if TRUE, probabilities p are given as log(p).

Details

The shape, rate, u, sigma, and xi parameters must be specified by the user. If phiu is left unspecified,
it defaults to 1 minus the distribution function of a discrete gamma distribution (not a discrete
truncated gamma) evaluated at u=1.
Value

discgammapd gives the density, pdiscgammapd gives the distribution function, qdiscgammapd gives the quantile function, and rdiscgammapd generates random variables from the described distribution.

Author(s)

<hbk5086@psu.edu>

Examples

# Generate and sort a random sample for a log-log plot
d <- rdiscgammapd(100, shape = 5, rate = .25, u = 25,
sigma = 15, xi = .5, shift = 1)
d <- sort(d, decreasing = TRUE)
plot(log(d), log(1:100))

# When phiu is specified to .2, exactly 80% 
of the data are below the threshold u
pdiscgammapd(24, shape = 5, rate = .25, u = 25,
sigma = 15, xi = .5, phiu = .2, shift = 1)

# Plot simulated data versus theoretical quantiles
quantiles <- qdiscgammapd((100:1)/101, shape = 5, rate = .25, u = 25,
sigma = 15, xi = .5, shift = 1)
plot(log(d), log(quantiles))
abline(0,1) # The line x=y

# Density below shift value should be 0
discgammapd(0, shape = 5, rate = .25, u = 25, sigma = 15, xi = .5, shift = 1)

# This is an example of using the "fit" input instead of manually specifying all parameters
data("repertoires")
thresholds1 <- unique(round(quantile(repertoires[[1]], c(.75,.8,.85,.9,.95))))
fit1 <- fdiscgammapd(repertoires[[1]], useq = thresholds1, shift = min(repertoires[[1]]))
qudiscgammapd(.6, fit1)

fdesponds  Fit the type-I Pareto distribution as according to Desponds et al. (2016)

Description

This function fits a continuous type-I pareto distribution to a vector of count data. Given data x, a threshold Cmin, and letting n be the number of clones greater than u, the shape parameter alpha is computed as

\[ n \star 1/(\sum \log(x/Cmin)) + 1. \]

The method considers every possible threshold (that is, every element of the vector unique(x)). The threshold and alpha which minimize the Kolmogorov-Smirnov statistic are selected.
Usage

fdesponds(x)

Arguments

x vector of counts.

Value

min.KS The value of the KS statistic for the fitted Pareto distribution.
Cmin The inferred threshold.
powerlaw.exponent The powerlaw exponent. This is equal to pareto.alpha + 1
pareto.alpha The inferred shape parameter alpha of the fitted Pareto distribution.

Author(s)

<hbk5086@psu.edu>

References


Examples

# Fit the model to sample data
data("repertoires")

fit1 <- fdesponds(repertoires[[1]])
fit2 <- fdesponds(repertoires[[2]])

fit1
fit2

fdiscgammagpd  Fit the discrete gamma-GPD spliced threshold model

Description

This function takes count data and fits the gamma-GPD spliced threshold model to it. The model consists of a discrete truncated gamma as the bulk distribution, up to the threshold, and a discrete GPD at and above the threshold. The 'shift' is ideally the minimum count in the sample.
Usage

`fdiscgammagpd(x, useq, shift = NULL, pvector=NULL, std.err = TRUE, method = "Nelder-Mead", ...)`

Arguments

- **x**: A vector of count data.
- **useq**: A vector of possible thresholds to search over. These should be discrete numbers.
- **shift**: The amount the distribution is shifted. It is recommended to use the minimum number in the count data when modeling the clone size distribution of the TCR repertoire.
- **pvector**: A vector of 5 elements corresponding to the initial parameter estimates. These 5 initial values are for the gamma shape and rate, the threshold, and the GPD sigma and xi. If they are not prespecified, the function computes pvector automatically.
- **std.err**: Logical. Should the standard errors on the estimates be computed from the Hessian matrix?
- **method**: Character string listing optimization method fed to optim. Defaults to Nelder-Mead.
- **...**: Other arguments passed to the function.

Value

- **x**: Numerical vector of the original data input.
- **shift**: Numeric specifying the original shift input.
- **init**: Numerical vector of the initial values of the parameter estimates. This is the same as pvector.
- **useq**: Numerical vector containing the thresholds the grid search was performed over.
- **nllhuseq**: Numerical vector of negative log likelihoods computed at each threshold in useq.
- **optim**: Output from optim for the bulk and tail distributions.
- **nllh**: The negative log likelihood corresponding to the maximum likelihood fitted distribution.
- **mle**: A numerical vector containing the estimates for phi, shape, rate, threshold, sigma, and xi.
- **fisherInformation**: The Fisher information matrix computed from the Hessian output from optim.

Author(s)

<hbk5086@psu.edu>
**get_bootstraps**

**Examples**

```r
data("repertoires")
thresholds1 <- unique(round(quantile(repertoires[[1]], c(.75,.8,.85,.9,.95))))
thresholds2 <- unique(round(quantile(repertoires[[2]], c(.75,.8,.85,.9,.95))))

fit1 <- fdiscgammagpd(repertoires[[1]], useq = thresholds1,
shift = min(repertoires[[1]]))
fit2 <- fdiscgammagpd(repertoires[[2]], useq = thresholds1,
shift = min(repertoires[[2]]))

fit1
fit2
```

---

**get_bootstraps**  
Get bootstrapped fits for a list of fitted models

**Description**

In order to get confidence bands on parameter estimates, a parametric bootstrap is recommended. This bootstrapping procedure takes bootstraps above and below the threshold separately, retaining the correct proportion of data that are above or below the threshold.

**Usage**

```r
get_bootstraps(fits, resamples = 1000, cores = 1, gridStyle = "copy")
```

**Arguments**

- **fits**  
  A list of fits output from fdiscgammagpd.

- **resamples**  
  Number of bootstrap replicates to execute for each model fit. Defaults to 1000.

- **cores**  
  Number of cores to use, if running in parallel. Defaults to 1.

- **gridStyle**  
  Defines how the sequence of thresholds is selected in the bootstrap fits. If the default "copy", each bootstrapped fit will be computed using the same grid of thresholds from the original fit. Otherwise, an integer can be supplied. If an integer is supplied, the bootstraps will be fit using a grid of thresholds defined by the originally estimated threshold plus or minus the supplied integer.

**Value**

If only one fit is passed, `get_bootstraps` returns a list of length resamples, where each element is a bootstrapped fit output from fdiscgammagpd. If a list of fits is passed, then the output is a list of lists. Each element of that list is a list of length resamples, where each element is a bootstrapped fit output from fdiscgammagpd.

**Author(s)**

<hbk5086@psu.edu>
get_distances

Compute matrix of pairwise Jensen-Shannon Distances

Description
For a list of model fits (either the spliced model or the Desponds et al. model), compute the matrix of Jensen-Shannon distances. This can then be used for clustering or multi-dimensional scaling.

Usage
get_distances(fits, grid, modelType = "Spliced")

Arguments

- **fits**: A list of fits output from either fdiscgammagpd or fdesponds.
- **grid**: Vector of integers over which to compute the JS distance. The minimum of the grid is ideally the minimum count of all samples being compared. The maximum is ideally something very large (e.g. 100,000) in order to all or nearly all of the model density. The grid should include every integer in its range. See `JS_dist`.
- **modelType**: Either "Spliced" or "Desponds", depending on what sort of fits you are supplying. Defaults to "Spliced".

Value
A symmetric matrix of pairwise Jensen-Shannon distances, with 0 on the diagonal.

Author(s)
<hbk5086@psu.edu>
See Also

JS_dist, fdiscgammagpd, fdesponds

Examples

# Simulate 3 datasets
set.seed(123)
s1 <- rdiscgammagpd(1000, shape = 3, rate = .15, u = 25, sigma = 15,
                     xi = .5, shift = 1)
s2 <- rdiscgammagpd(1000, shape = 3.1, rate = .14, u = 26, sigma = 15,
                     xi = .6, shift = 1)
s3 <- rdiscgammagpd(1000, shape = 10, rate = .3, u = 45, sigma = 20,
                     xi = .7, shift = 1)

# Fit the spliced model to each
# Here, we use true thresholds for fast computation for this example
# In practice, you need to select a whole sequence of potential thresholds
sim_fits <- list("s1" = fdiscgammagpd(s1, useq = 25),
                 "s2" = fdiscgammagpd(s2, useq = 26),
                 "s3" = fdiscgammagpd(s3, useq = 45))

# Compute the pairwise JS distance between 3 fitted models
grid <- min(c(s1,s2,s3)):10000
distances <- get_distances(sim_fits, grid, modelType="Spliced")
distances

JS_desponds

Compute the Jensen-Shannon distance between two fitted distributions using the Desponds model

Description

After the Desponds et al. (2016) model has been fit to your samples, the pairwise JS distance can be computed between them. This function takes the fitted model parameters from 2 distributions and computes the JS distance between them. When all pairwise distances have been computed, they can be used to do hierarchical clustering. This function assumes you denote one distribution as P and one as Q.

Usage

JS_desponds(grid, Cminp, Cminq, alphap, alphaq)

Arguments

grid Vector of integers over which to compute the JS distance. The minimum of the grid is ideally the minimum count of all samples being compared. The maximum is ideally something very large (e.g. 100,000) in order to all or nearly all of the model density. The grid should include every integer in its range. See Examples.
Cminp       The estimated threshold for distribution P.
Cminq       The estimated threshold for distribution Q.
alphap      The estimated parameter alpha for distribution P.
alphaq      The estimated parameter alpha for distribution Q.

Details

For 2 discrete distributions P and Q, the Jensen-Shannon distance between them is
\[ JSD(P, Q) = \sqrt{\alpha} \int \left( P(t) \log P(t) / M(t) \right) + \int \left( Q(t) \log Q(t) / M(t) \right) dt \]

where
\[ M(t) = 0.5 \times (P(t) + Q(t)) \].

Value

The function directly returns the Jensen-Shannon distance between two fitted distributions P and Q.

Author(s)

<hbk5086@psu.edu>

References


See Also

JS_spliced, JS_dist

Examples

data("repertoires")

# Fit the discrete gamma-gpd spliced model at some selected threshold on 2 samples
fit1 <- fdesponds(repertoires[[1]])
fit2 <- fdesponds(repertoires[[2]])

# Create a grid of every integer from the minimum threshold to a large value
# When comparing many distributions in advance of clustering,
# the same grid should be used across every comparison
# The chosen "large value" here is only 1,000, for the sake of quick computation.
# Ideally, the large value will be at least 100,000
grid <- min(c(fit1[['Cmin']], fit2[['Cmin']])):1000

# Compute the Jensen-Shannon distance between fit1 and fit2
dist <- JS_desponds(grid,
                   Cminp = fit1[['Cmin']],
                   Cminq = fit2[['Cmin']],
                   alphap = fit1[['alpha']],
                   alphaq = fit2[['alpha']])
Compute the Jensen-Shannon distance between two model fits

Description
This function is a convenient wrapper for JS_spliced and JS_desponds. After models have been fit to your samples, the pairwise JS distance can be computed between them. This function takes two model fits and outputs the JS distance between them. The model fits must be of the same type. That is, they are both fits from the spliced threshold model, or they are both fits from the Desponds et al. model. When all pairwise distances have been computed, they can be used to do hierarchical clustering.

Usage

JS_dist(fit1, fit2, grid, modelType = "Spliced")

Arguments

fit1 A fit from the specified modelType.
fit2 A fit from the specified modelType.
grid Vector of integers over which to compute the JS distance. The minimum of the grid is ideally the minimum count of all samples being compared. The maximum is ideally something very large (e.g. 100,000) in order to all or nearly all of the model density. The grid should include every integer in its range. See Examples.
modelType The type of model fit1 and fit2 are from. If they were generated using fdiscgam-magpd, the type of model is "Spliced". If they were generated using fdesponds, the type of model is "Desponds". Defaults to "Spliced".

Details
For 2 discrete distributions P and Q, the Jensen-Shannon distance between them is

\[ JSD(P, Q) = \sqrt{75 \times \left[ \sum (P_i \log P_i / M_i) \right] + \sum (Q_i \log Q_i / M_i)} \]

where

\[ M_i = .5 \times (P_i + Q_i). \]

Value
The function directly returns the Jensen-Shannon distance between two fitted distributions.

Author(s)
<hbk5086@psu.edu>
See Also

JS_spliced, JS_desponds

Examples

data("repertoires")

# Fit the discrete gamma-GPD spliced model at some selected threshold on 2 samples
fit1 <- fdiscgammagpd(repertoires[[1]],
  useq = quantile(repertoires[[1]], .8),
  shift = min(repertoires[[1]]))
fit2 <- fdiscgammagpd(repertoires[[2]],
  useq = quantile(repertoires[[2]], .8),
  shift = min(repertoires[[2]]))

# Create a grid of every integer from the minimum count to a large value
# The chosen "large value" here is only 1,000, for the sake of quick computation.
# Ideally, the large value will be at least 100,000
grid <- min(c(repertoires[[1]], repertoires[[2]])):1000

# Compute the Jensen-Shannon distance between fit1 and fit2
dist <- JS_dist(fit1, fit2, grid, "Spliced")
dist

JS_spliced

Compute the Jensen-Shannon distance between two fitted discrete
gamma-GPD spliced threshold distributions

Description

After models have been fit to your samples, the pairwise JS distance can be computed between them. This function takes the fitted model parameters from 2 distributions and computes the JS distance between them. When all pairwise distances have been computed, they can be used to do hierarchical clustering. This function assumes you denote one distribution as P and one as Q.

Usage

JS_spliced(grid, shiftp, shiftq, phip, phiq, shapep, shapeq,
  ratep, rateq, threshp, threshq, sigmap, sigmaq, xip, xiq)

Arguments

grid Vector of integers over which to compute the JS distance. The minimum of the grid is ideally the minimum count of all samples being compared. The maximum is ideally something very large (e.g. 100,000) in order to see all or nearly all of the model density. The grid should include every integer in its range. See Examples.

shiftp The shift for distribution P.
shiftq The shift for distribution Q.
The estimated phi for distribution P.

phiq
The estimated phi for distribution Q.

shapep
The estimated gamma shape parameter for distribution P.

shapeq
The estimated gamma shape parameter for distribution Q.

ratep
The estimated gamma rate parameter for distribution P.

rateq
The estimated gamma rate parameter for distribution Q.

threshp
The estimated threshold for distribution P.

threshq
The estimated threshold for distribution Q.

sigmap
The estimated parameter sigma for distribution P.

sigmaq
The estimated parameter sigma for distribution Q.

xip
The estimated parameter xi for distribution P.

xiq
The estimated parameter xi for distribution Q.

Details

For 2 discrete distributions P and Q, the Jensen-Shannon distance between them is

\[ JSD(P, Q) = \sqrt{.5 \times \left[ \sum (P_i \log P_i / M_i) + \sum (Q_i \log Q_i / M_i) \right] } \]

where

\[ M_i = .5 \times (P_i + Q_i) \].

Value

The function directly returns the Jensen-Shannon distance between two fitted distributions P and Q.

Author(s)

<hbk5086@psu.edu>

See Also

JS_spliced JS_dist

Examples

data("repertoires")

# Fit the discrete gamma-gpd spliced model at some selected threshold on 2 samples
fit1 <- fdiscgammagpd(repertoires[[1]],
  useq = quantile(repertoires[[1]], .8),
  shift = min(repertoires[[1]]))
fit2 <- fdiscgammagpd(repertoires[[2]],
  useq = quantile(repertoires[[2]], .8),
  shift = min(repertoires[[2]]))

# Create a grid of every integer from the minimum count to a large value
# The chosen "large value" here is only 1,000, for the sake of quick computation.
# Ideally, the large value will be at least 100,000
grid <- min(c(repertoires[[1]], repertoires[[2]])):1000

# Compute the Jensen-Shannon distance between fit1 and fit2
dist <- JS_spliced(grid,
    shiftp = min(repertoires[[1]]),
    shiftq = min(repertoires[[2]]),
    phip = fit1$mle['phi'],
    phiq = fit2$mle['phi'],
    shapep = fit1$mle['shape'],
    shapeq = fit2$mle['shape'],
    ratep = fit1$mle['rate'],
    rateq = fit2$mle['rate'],
    threshp = fit1$mle['thresh'],
    threshq = fit2$mle['thresh'],
    sigmap = fit1$mle['sigma'],
    sigmaq = fit2$mle['sigma'],
    xip = fit1$mle['xi'],
    xiq = fit2$mle['xi']
)

dist

---

### parseFile

**Load in and parse TCR data files for use by powerTCR**

**Description**

This function leverages repLoad functions from the immunarch package. They are wrappers that output data in the format taken by powerTCR.

**Usage**

```r
parseFile(path, inframe = TRUE)
```

**Arguments**

- **path**
  - Path to input file with TCR repertoire sample data.
- **inframe**
  - Logical. Should counts only from in-frame sequences be returned? Defaults to TRUE.

**Details**

See the immunarch package on GitHub: https://github.com/immunomind/immunarch

**Value**

parseFile returns a vector of counts corresponding to the sample repertoire.

**References**

repertoires

Two toy examples of sample TCR repertoires.

Description
This data set gives two toy examples of TCR repertoires. Sample "samp1" contains 1,000 clones with a total of 26,288 sequenced T cells. Sample "samp2" contains 800 clones with a total of 24,267 sequenced T cells. These samples have been sorted from largest to smallest clone size.

Usage

```r
data("repertoires")
```

Format

The format is:

```
List of 2 $ samp1: num [1:1000] 1445 451 309 ... $ samp2: num [1:800] 2781 450 447 ...```

Examples

```r
data(repertoires)
n1 <- length(repertoires$samp1)
n2 <- length(repertoires$samp2)

# Generates plot on log-log scale
par(mfrow = c(2,1))
plot(log(repertoires$samp1), log(1:n1))
plot(log(repertoires$samp2), log(1:n2))
```
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