

Package ‘powerTCR’

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Type Package

Title Model-Based Comparative Analysis of the TCR Repertoire

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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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```

}
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 `symmetrix` 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 contained 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

```
# Simulate 3 sampled individuals
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 model to the data at the true thresholds
fits <- list("fit1" = fdiscgammagpd(s1, useq = 25),
            "fit2" = fdiscgammagpd(s2, useq = 26),
            "fit3" = fdiscgammagpd(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")
grid <- 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]]$mle['sigma'],
                                sigmaq = fits[[j]]$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 <code>fdiscgammagpd</code> . If this object is passed, all parameter fields will automatically populate with the maximum likelihood estimates for the parameters 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	Proportion 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

`ddiscgammagpd` gives the density, `pdiscgammagpd` gives the distribution function, `qdiscgammagpd` gives the quantile function, and `rdiscgammagpd` 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 <- rdiscgammagpd(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
```

```

pdiscgammagpd(24, shape = 5, rate = .25, u = 25,
               sigma = 15, xi = .5, phiu = .2, shift = 1)

# Plot simulated data versus theoretical quantiles
quantiles <- qdiscgammagpd((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
ddiscgammagpd(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 <- fdiscgammagpd(repertoires[[1]], useq = thresholds1, shift = min(repertoires[[1]]))
qdiscgammagpd(.6, fit1)

```

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

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 α is computed as

$$n * 1 / (\sum \log(x / Cmin)) + 1.$$

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

Usage

```
fdesponds(x)
```

Arguments

<code>x</code>	vector of counts.
----------------	-------------------

Value

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

Author(s)

<hbk5086@psu.edu>

References

Desponds, Jonathan, Thierry Mora, and Aleksandra M. Walczak. "Fluctuating fitness shapes the clone-size distribution of immune repertoires." *Proceedings of the National Academy of Sciences* 113.2 (2016): 274-279. APA

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>

Examples

```
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

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

Arguments

fits	A list of fits output from <code>fdiscgammagpd</code> .
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)

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See Also

[fdiscgammagpd](#)

Examples

```
data(repertoires)
fits <- lapply(repertoires,
  function(X) fdiscgammagpd(X, useq = unique(round(quantile(X, c(.75,.8,.85,.9))))))
names(fits) <- names(repertoires)

# You should in practice use a large number of resamples, say, 1000
boot <- get_bootstraps(fits, resamples = 10)

mles <- get_mle(boot[[1]])
xi_CI <- quantile(unlist(purrr::map(mles, 'xi')), c(.025, .5, .975))
xi_CI
```

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 <code>fdiscgammagpd</code> or <code>fdesponds</code> .
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

$$JSD(P, Q) = \sqrt{.5 * \int [P(t) \log P(t) / M(t)] + \int [Q(t) \log Q(t) / M(t)] dt}$$

where

$$M(t) = .5 * (P(t) + Q(t)).$$

Value

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

Author(s)

<hbk5086@psu.edu>

References

Desponds, Jonathan, Thierry Mora, and Aleksandra M. Walczak. "Fluctuating fitness shapes the clone-size distribution of immune repertoires." *Proceedings of the National Academy of Sciences* 113.2 (2016): 274-279. APA

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['pareto.alpha'],
  alphaq = fit2['pareto.alpha'])

dist
```

JS_dist

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

<code>fit1</code>	A fit from the specified <code>modelType</code> .
<code>fit2</code>	A fit from the specified <code>modelType</code> .
<code>grid</code>	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.
<code>modelType</code>	The type of model <code>fit1</code> and <code>fit2</code> are from. If they were generated using <code>fdiscgam-magpd</code> , the type of model is "Spliced". If they were generated using <code>fdesponds</code> , the type of model is "Desponds". Defaults to "Spliced".

Details

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

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

where

$$M_i = .5 * (P_i + Q_i).$$

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]], repertoire[[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 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.
phip	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

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

where

$$M_i = .5 * (P_i + Q_i).$$

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]], repertoire[[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

```
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

Nazarov, Vadim I., et al. "tcR: an R package for T cell receptor repertoire advanced data analysis." BMC bioinformatics 16.1 (2015): 175.

repertoires

Two toy examples of sample TCR repertoires.

Description

This data set gives to 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

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

Format

The format is:

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

Examples

```
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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