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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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Contents

Accessors 2
clusterPlot 3

discgammagpd 5
fdesponds 6
fdiscgammagpd 7
get_bootstraps 9
get_distances 10
JS_desponds 11
JS_dist 13
JS_spliced 14
repertoires 16

Index **17**

`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

```
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 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 containined 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 fdiscgammagpd. 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`	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

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 — *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

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

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

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)

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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 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)

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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 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 havs 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

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

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

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 fdiscgammagpd, 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

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

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]], 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 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]], 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
```

`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))
```

Index

∗ **datasets**
repertoires, 16

Accessors, 2

clusterPlot, 3

ddiscgammagpd *(*discgammagpd*)*, 5
discgammagpd, 5

fdesponds, 6, *11*
fdiscgammagpd, *2*, 7, *10, 11*

get_bootstraps, 9
get_distances, 10
get_diversity *(*Accessors*)*, 2
get_mle *(*Accessors*)*, 2
get_nllh *(*Accessors*)*, 2

hclust, *3*

JS_desponds, *4*, 11, *14*
JS_dist, *10–12*, 13, *15*
JS_spliced, *4*, *12*, 14, *14, 15*

optim, *8*

pdiscgammagpd *(*discgammagpd*)*, 5

qdiscgammagpd *(*discgammagpd*)*, 5

rdiscgammagpd *(*discgammagpd*)*, 5
repertoires, 16