# A Quick Introduction to iNEXT.3D via Examples

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#### 2024-02-06

INEXT.3D (INterpolation and EXTrapolation for three dimensions of biodiversity) is a sequel to iNEXT (Hsieh et al., 2016). Here the three dimensions (3D) of diversity include taxonomic diversity (TD), phylogenetic diversity (PD) and functional diversity (FD). An online version "iNEXT.3D Online" (https://chao.shinyapps.io/iNEXT\_3D/) is also available for users without an R background.

A unified framework based on Hill numbers (for TD) and their generalizations (Hill-Chao numbers, for PD and FD) is adopted to quantify 3D. In this framework, TD quantifies the effective number of species, PD quantifies the effective total branch length, mean-PD (PD divided by tree depth) quantifies the effective number of lineages, and FD quantifies the effective number of virtual functional groups (or functional "species"). Thus, TD, mean-PD, and FD are all in the same units of species/lineage equivalents and can be meaningfully compared; see Chao et al. (2014) for the basic standardization theory for TD, and Chao et al. (2021) for a review of the unified theory for 3D.

For each of the three dimensions of biodiversity, inext.3D features two statistical analyses (non-asymptotic and asymptotic):

 A non-asymptotic approach based on interpolation and extrapolation for 3D diversity (i.e., Hill-Chao numbers)

INEXT. 3D computes the estimated 3D diversity for standardized samples with a common sample size or sample completeness. This approach aims to compare diversity estimates for equally-large (with a common sample size) or equally-complete (with a common sample coverage) samples; it is based on the seamless rarefaction and extrapolation (R/E) sampling curves of Hill-Chao numbers for q = 0, 1 and 2. For each dimension of biodiversity, inext.3D offers three types of R/E sampling curves:

- Sample-size-based (or size-based) R/E sampling curves: This type of sampling curve plots the diversity estimates with respect to sample size.
- Coverage-based R/E sampling curves: This type of sampling curve plots the diversity estimates with respect to sample coverage.
- Sample completeness curve: This curve depicts how sample coverage varies with sample size. The sample completeness curve provides a bridge between the size- and coverage-based R/E sampling curves.
- 2. An asymptotic approach to infer asymptotic 3D diversity (i.e., Hill-Chao numbers)

inext.3D computes the estimated asymptotic 3D diversity and also plots 3D diversity profiles (q-profiles) for q between 0 and 2, in comparison with the observed diversity. Typically, the asymptotic estimates for  $q \ge 1$  are reliable, but for q < 1 (especially for q = 0, species richness), the asymptotic estimates represent only lower bounds. inext.3D also features a time-profile (which depicts the observed and asymptotic estimate of PD or mean PD with respect to reference times), and a tau-profile (which depicts the observed and asymptotic estimate of FD with respect to threshold level tau).

## How to cite

If you publish your work based on results from inext.3D package, you should make references to the following methodology paper and the package:

- Chao, A., Henderson, P. A., Chiu, C.-H., Moyes, F., Hu, K-H., Dornelas, M and. Magurran, A. E. (2021).
   Measuring temporal change in alpha diversity: a framework integrating taxonomic, phylogenetic and functional diversity and the iNEXT.3D standardization. Methods in Ecology and Evolution, 12, 1926-1940.
- Chao, A. and Hu, K.-H. (2023). The iNEXT.3D package: interpolation and extrapolation for three dimensions of biodiversity. R package available from CRAN.

## SOFTWARE NEEDED TO RUN INEXT.3D IN R

• Required: R

• Suggested: RStudio IDE

# **HOW TO RUN INEXT.3D:**

The inext.3D package can be downloaded from CRAN or Anne Chao's iNEXT.3D github using the commands below. For a first-time installation, some additional packages must be installed and loaded; see package manual.

```
## or install the latest version from github
install.packages('devtools')
library(devtools)
install_github('AnneChao/iNEXT.3D')

## import packages
library(iNEXT.3D)
```

There are six main functions in this package:

Two functions for non-asymptotic analysis with graphical displays:

- **iNEXT3D** computes standardized 3D diversity estimates of order q = 0, 1 and 2 for rarefied and extrapolated samples at specified sample coverage values and sample sizes.
- ggiNEXT3D visualizes the output from the function inext3D.

Two functions for point estimation and basic data information

- estimate3D computes 3D diversity of order q = 0, 1 and 2 with a particular set of user-specified level of sample sizes or sample coverage values.
- DataInfo3D provides basic data information based on the observed data.

Two functions for asymptotic analysis with graphical displays:

- ObsAsy3D computes observed and asymptotic diversity of order q between 0 and 2 (in increments of 0.2) for 3D diversity; it also computes observed and asymptotic PD for specified reference times, and observed and asymptotic FD for specified threshold levels.
- ggObsAsy3D visualizes the output from the function ObsAsy3D.

#### **DATA INPUT FORMAT**

## Species abundance/incidence data format

Although species identities/names are not required to assess TD or compare TD across individual assemblages (as in the <code>inext</code> package), they are required for PD and FD. Thus, for <code>inext</code>. 3D package, information on species identity (or any unique identification code) and assemblage affiliation is required. Two types of species abundance/incidence data are supported:

- 1. Individual-based abundance data (datatype = "abundance"): When there are multiple assemblages, in addition to the assemblage/site names (as column names) and the species names (as row names), species abundance data (reference sample) can be input as a species (in rows) by assemblage (in columns) matrix/data.frame or a list of species abundance vectors. In the special case that there is only one assemblage, all data should be read in one column.
- 2. Sampling-unit-based incidence data: Incidence-raw data (datatype = "incidence\_raw"): for each assemblage, input data for a reference sample consist of a species-by-sampling-unit matrix, in addition to the sampling-unit names (as column names) and the species names (as row names). When there are N assemblages, input data consist of N lists of matrices, and each matrix is a species-by-sampling-unit matrix. Each element in the incidence raw matrix is 1 for a detection, and 0 for a non-detection. Input a matrix which combines data for all assemblages is allowed, but the argument nT in the function inext3D must be specified so that the number of sampling units in each assemblage is specified.

For example, the dataset <code>Brazil\_rainforest\_abun\_data</code> included in the <code>iNEXT.3D</code> package consists of species sample abundances of two assemblages/habitats: "Edge" and "Interior". Run the following code to view the first 15 rows of the abundance data.

```
data("Brazil_rainforest_abun_data")
Brazil_rainforest_abun_data
```

```
Edge Interior
Carpotroche_brasiliensis 11 21
Astronium_concinnum 110
Astronium_graveolens
Spondias_macrocarpa
                         36
                         12
2
7
                                   1
Spondias venulosa
Tapirira_guianensis
                                     1
Thyrsodium_spruceanum 11 11
Anaxagorea_silvatica 1 13
Annona_acutiflora 1 1
Annona_acutiflora
                                   2
Annona_cacans
                          0
                         3
Annona_dolabripetala
                                     3
Annona sp
Annona_sp

Duguetia_chrysocarpa 1

-1 1
                                     1
                                     1
                                     0
Ephedranthus sp2
                                     1
```

We use data (Fish\_incidence\_data) collected from two time periods, namely "2013-2015" and "2016-2018", as an example. Each time period is designated as an assemblage. The purpose was to compare 3D diversity of the two time periods. In each time period, species incidence/occurrence was recorded in 36 sampling units in each assemblage; each sampling unit represents a sampling date. Thus, there are 36 columns in each time period. Run the following code to view the first 6 rows and 6 columns for each matrix.

## Phylogenetic tree format for PD

labels are shown below.

To perform PD analysis, the phylogenetic tree (in Newick format) spanned by species observed in the pooled data is required. For the dataset <code>Fish\_incidence\_data</code>, the phylogenetic tree for all observed species (including species in both time periods) is stored in the file <code>fish\_phylo\_tree</code>; for the dataset <code>Brazil\_rainforest\_abun\_data</code>, the phylogenetic tree for all observed species (including species in both Edge and Interior habitats) is stored in the file <code>Brazil\_rainforest\_phylo\_tree</code>. A partial list of the tip labels and node

## Species pairwise distance matrix format for FD

To perform FD analysis, the species-pairwise distance matrix (Gower distance computed from species traits) for species observed in the pooled data is required in a matrix/data.frame format. For the dataset <code>Fish\_incidence\_data</code>, the distance matrix for all observed species (including species in both time periods) is stored in the file <code>fish\_dist\_matrix</code>; for the dataset <code>Brazil\_rainforest\_abun\_data</code>, the distance matrix for all species (including species in both Edge and Interior habitats) is stored in the file <code>Brazil\_rainforest\_dist\_matrix</code>. The distance matrix for the first 3 Brazil rainforest tree species is shown below.

```
data("Brazil_rainforest_distance_matrix")
Brazil_rainforest_distance_matrix
```

	Carpotroche_brasiliensis	Astronium_concinnum	Astronium_graveolens
Carpotroche_brasiliensis	0.000	0.522	0.522
Astronium_concinnum	0.522	0.000	0.000
Astronium_graveolens	0.522	0.000	0.000

# MAIN FUNCTION INEXT3D(): RAREFACTION/EXTRAPOLATION

```
iNEXT3D(data, diversity = 'TD', q = c(0,1,2), datatype = "abundance",
    size = NULL, endpoint = NULL, knots = 40, nboot = 50, conf = 0.95, nT = NULL,
    PDtree = NULL, PDreftime = NULL, PDtype = 'meanPD',
    FDdistM, FDtype = 'AUC', FDtau = NULL, FDcut_number = 50)
```

The arguments of this function are briefly described below, and will be explained in more details by illustrative examples in later text. This main function computes standardized 3D diversity estimates of order q = 0, 1 and 2, the sample coverage estimates, and related statistics for K (if knots = K in the specified argument) evenly-spaced knots (sample sizes) between size 1 and the endpoint, where the endpoint is described below. Each knot represents a particular sample size for which 3D diversity estimates will be calculated. By default, endpoint = 0 double the reference sample size for abundance data or double the total sampling units for incidence data. For example, if endpoint = 10, knot = 4 is specified, diversity estimates will be computed for a sequence of samples with sizes (1, 4, 7, 10).

Argument	Description
data	<ul> <li>a. For datatype = "abundance", data can be input as a vector of species abundances (for a single assemblage), matrix/data.frame (species by assemblages), or a list of species abundance vectors.</li> <li>b. For datatype = "incidence_raw", data can be input as a list of matrices/data.frames (species by sampling units); data can also be input as a single matrix/data.frame by merging all sampling units across assemblages based on species identity; in this case, the number of sampling units (nT, see below) must be specified.</li> </ul>
diversity	selection of diversity type: $\t^T D' = Taxonomic diversity$ , $\t^T D' = Phylogenetic diversity$ , and $\t^T D' = Functional diversity$ .
q	a numerical vector specifying the diversity orders. Default is $\circ$ (0, 1, 2).
datatype	data type of input data: individual-based abundance data (datatype = "abundance"), or species by sampling-units incidence/occurrence matrix (datatype = "incidence_raw") with all entries being 0 (non-detection) or 1 (detection).
size	an integer vector of sample sizes (number of individuals or sampling units) for which diversity estimates will be computed. If <code>NULL</code> , then diversity estimates will be computed for those sample sizes determined by the specified/default <code>endpoint</code> and <code>knots</code> .
endpoint	an integer specifying the sample size that is the <code>endpoint</code> for rarefaction/extrapolation. If NULL, then <code>endpoint</code> = double the reference sample size.
knots	an integer specifying the number of equally-spaced knots (say K, default is 40) between size 1 and the endpoint; each knot represents a particular sample size for which diversity estimate will be calculated. If the endpoint is smaller than the reference sample size, then iNEXT3D() computes only the rarefaction estimates for approximately K evenly spaced knots. If the endpoint is larger than the reference sample size, then iNEXT3D() computes rarefaction estimates for approximately K/2 evenly spaced knots between sample size 1 and the reference sample size, and computes extrapolation estimates for approximately K/2 evenly spaced knots between the reference sample size and the endpoint.
nboot	a positive integer specifying the number of bootstrap replications when assessing sampling uncertainty and constructing confidence intervals. Enter 0 to skip the bootstrap procedures. Default is 50.
conf	a positive number < 1 specifying the level of confidence interval. Default is 0.95.
nT	(required only when <code>datatype = "incidence_raw"</code> and input data in a single matrix/data.frame) a vector of nonnegative integers specifying the number of sampling units in each assemblage. If assemblage names are not specified(i.e., <code>names(nT) = NULL</code> ), then assemblages are automatically named as "assemblage1", "assemblage2", etc.
PDtree	(required argument for ${\tt diversity} = {\tt ``PD''}$ ), a phylogenetic tree in Newick format for all observed species in the pooled assemblage.
PDreftime	(argument only for <code>diversity = "PD"</code> ), a vector of numerical values specifying reference times for PD. Default is <code>NULL</code> (i.e., the age of the root of PDtree).
PDtype	(argument only for diversity = "PD"), select PD type: PDtype = "PD" (effective total branch length) or PDtype = "meanPD" (effective number of equally divergent lineages).  Default is "meanPD", where meanPD = PD/tree depth.
FDdistM	(required argument for diversity = "FD"), a species pairwise distance matrix for all species in the pooled assemblage.
	(argument only for diversity = "FD"), select FD type: FDtype = "tau_values" for FD

FDtype	under specified threshold values, or FDtype = "AUC" (area under the curve of tau-profile) for an overall FD which integrates all threshold values between zero and one. Default is "AUC".
FDtau	(argument only for diversity = "FD" and FDtype = "tau_values"), a numerical vector between 0 and 1 specifying tau values (threshold levels). If NULL (default), then threshold is set to be the mean distance between any two individuals randomly selected from the pooled assemblage (i.e., quadratic entropy).
FDcut_number	(argument only for diversity = "FD" and FDtype = "AUC"), a numeric number to cut [0, 1] interval into equal-spaced sub-intervals to obtain the AUC value by integrating the tau-profile. Equivalently, the number of tau values that will be considered to compute the integrated AUC value. Default is FDcut_number = 50. A larger value can be set to obtain more accurate AUC value.

For each dimension of diversity (TD, PD, FD), the main function inext3D() returns the inext3D object, which can be further used to make plots using the function gginext3D() to be described below. The "inext3D" object includes three lists:

- 1. \$TDInfo (\$PDInfo,or \$FDInfo) for summarizing data information.
- \$TDiNextEst (\$PDiNextEst, or \$FDiNextEst) for showing diversity estimates along with related statistics for a series of rarefied and extrapolated samples; there are two data frames (\$size\_based and \$coverage based) conditioning on standardized sample size or sample coverage, respectively.
- \$TDASYEST (\$PDASYEST, or \$FDASYEST) for showing asymptotic diversity estimates along with related statistics.

# FUNCTION ggiNEXT3D(): GRAPHIC DISPLAYS

The function <code>ggiNEXT3D()</code>, which extends <code>ggplot2</code> with default arguments, is described as follows:

```
ggiNEXT3D(output, type = 1:3, facet.var = "Assemblage", color.var = "Order.q")
```

Here output is the iNEXT3D() object. Three types of curves are allowed for 3D diversity:

- 1. Sample-size-based R/E curve (type = 1): This curve plots diversity estimates with confidence intervals as a function of sample size.
- 2. Sample completeness curve (type = 2): This curve plots the sample coverage with respect to sample size.
- 3. Coverage-based R/E curve (type = 3): This curve plots the diversity estimates with confidence intervals as a function of sample coverage.

The argument facet.var = "Order.q", facet.var = "Assemblage", facet.var = "Both", or facet.var = "None" is used to create a separate plot for each value of the specified variable.

The <code>ggiNEXT3D()</code> function is a wrapper with the package <code>ggplot2</code> to create a rarefaction/extrapolation sampling curve in a single line of code. The figure object is of class <code>"ggplot"</code>, so it can be manipulated by using the <code>ggplot2</code> tools.

# TAXONOMIC DIVERSITY (TD): RAREFACTION/EXTRAPOLATION VIA EXAMPLES

#### **EXAMPLE 1: TD rarefaction/extrapolation for abundance data**

Edge 1794 319 0.939 0.974 110 48 38 28 13

Based on the dataset (Brazil\_rainforest\_abun\_data) included in the package, the following commands return all numerical results for TD. The first list of the output (\$TDInfo) returns basic data information including the name of the Assemblage, sample size (n), observed species richness (\$S.obs), sample coverage estimate of the reference sample with size n (SC(n)), sample coverage estimate of the extrapolated sample with size 2n (SC(2n)) as well as the first five species abundance frequency counts in the reference sample (f1-f5). The output is identical to that based on the function DataInfo3D() by specifying diversity = 'TD' and datatype = "abundance"; see later text). Thus, if only data information is required, the simpler function DataInfo3D() (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later.

```
2 Interior 2074 356 0.941 0.973 123 48 41 32 19
```

The second list of the output (\$TDINEXTEST) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "Edge" assemblage, corresponding to the target sample size m = 1, 95, 189, ..., 1699, 1794, 1795, 1899, ..., 3588), which locates the reference sample size at the mid-point of the selected knots. There are two data frames (\$size based and \$coverage based).

The first data frame ( $\$size\_based$ ) includes the name of the Assemblage, diversity order (order.q), the target sample size (m), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the size m is less than, equal to, or greater than the reference sample size), the diversity estimate of order q (qTD), the lower and upper confidence limits of diversity (qTD.LCL and qTD.UCL) conditioning on the sample size, and the corresponding sample coverage estimate (sc) along with the lower and upper confidence limits of sample coverage (sc.LCL and sc.UCL). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the  $\$size\_based$  output are displayed:

```
output_TD_abun$TDiNextEst$size_based
```

```
Assemblage Order.q m Method qTD qTD.LCL qTD.UCL SC SC.LCL SC.UCL

1 Edge 0 1 Rarefaction 1.000 1.000 1.000 0.012 0.010 0.013

2 Edge 0 95 Rarefaction 66.306 65.043 67.569 0.484 0.468 0.500

3 Edge 0 189 Rarefaction 106.743 104.052 109.434 0.638 0.622 0.653

4 Edge 0 284 Rarefaction 137.029 133.025 141.033 0.718 0.704 0.733

5 Edge 0 378 Rarefaction 161.010 155.820 166.200 0.768 0.755 0.782

6 Edge 0 472 Rarefaction 181.073 174.781 187.366 0.803 0.790 0.816
```

The second data frame ( $$coverage\_based$ ) includes the name of assemblage, the diversity order (order.q), the target sample coverage value (sc), the corresponding sample size (m), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the coverage sc is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (qTD), the lower and upper confidence limits of diversity (qTD.LCL and qTD.UCL) conditioning on the target sample coverage value. Here only the first six rows of the  $$coverage\_based$  output are displayed below: (Note for a fixed coverage value, the confidence interval in the  $$coverage\_based$  table is wider than the corresponding interval in the  $$size\_based$  table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication, leading to higher uncertainty on the resulting diversity estimate.)

```
output_TD_abun$TDiNextEst$coverage_based
```

```
Assemblage Order.q SC m Method qTD qTD.LCL qTD.UCL

1 Edge 0 0.012 1 Rarefaction 1.000 0.970 1.030

2 Edge 0 0.484 95 Rarefaction 66.306 61.976 70.636

3 Edge 0 0.638 189 Rarefaction 106.743 99.830 113.657

4 Edge 0 0.718 284 Rarefaction 137.029 127.987 146.072

5 Edge 0 0.768 378 Rarefaction 161.010 150.075 171.946

6 Edge 0 0.803 472 Rarefaction 181.073 168.376 193.771
```

The third list of the output (\$TDAsyEst) includes the name of the Assemblage, diversity label (qTD, species richness for q = 0, Shannon diversity for q = 1, and Simpson diversity for q = 2), the observed diversity ( $TD_obs$ ), asymptotic diversity estimate ( $TD_asy$ ) and its estimated bootstrap standard error (s.e.) as well as the confidence intervals for asymptotic diversity ( $qTD_LCL$  and  $qTD_UCL$ ). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function ObsAsy3D(). The output for \$TDAsyEst is shown below:

```
output_TD_abun$TDAsyEst
```

```
Assemblage qTD TD_obs TD_asy s.e. qTD.LCL qTD.UCL

1 Edge Species richness 319.000 444.971 28.910 388.309 501.634

2 Edge Shannon diversity 155.386 178.000 4.920 168.357 187.642

3 Edge Simpson diversity 82.023 85.905 3.753 78.550 93.261

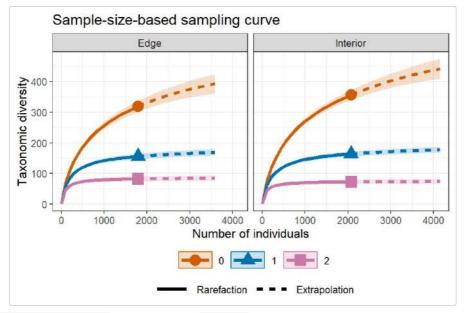
4 Interior Species richness 356.000 513.518 28.411 457.834 569.202

5 Interior Shannon diversity 163.514 186.983 6.553 174.139 199.827

6 Interior Simpson diversity 72.153 74.718 4.713 65.481 83.955
```

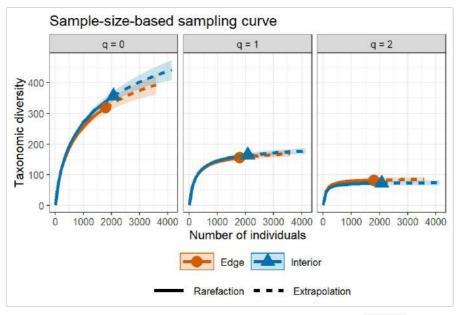
The ggiNEXT3D function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When facet.var = "Assemblage" is specified in the ggiNEXT3D function, it creates a separate plot for each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (type = 1) is given below:

```
# TD sample-size-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_TD_abun, type = 1, facet.var = "Assemblage")
```



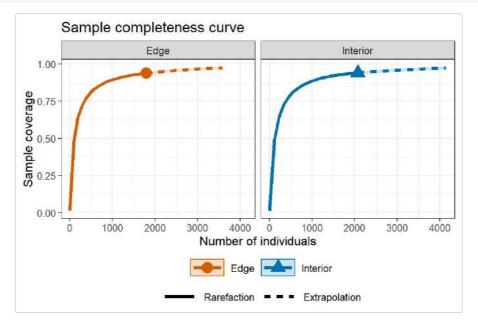
When facet.var = "Order.q" is specified in the ggiNEXT3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# TD sample-size-based R/E curves, separating by "Order.q"
ggiNEXT3D(output_TD_abun, type = 1, facet.var = "Order.q")
```



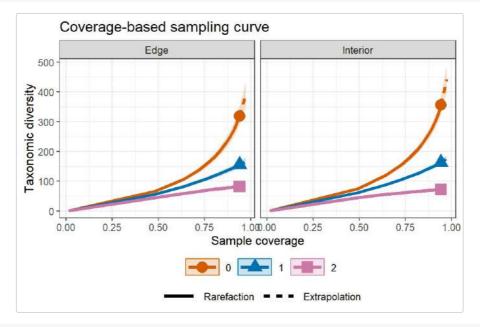
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors represent different assemblages.

```
# Sample completeness curves for abundance data, separating by "Assemblage"
ggiNEXT3D(output_TD_abun, type = 2, color.var = "Assemblage")
```

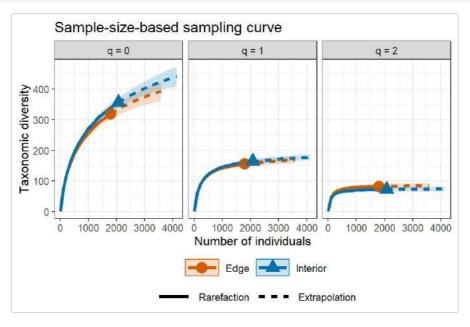


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# TD coverage-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_TD_abun, type = 3, facet.var = "Assemblage")
```



```
# TD coverage-based R/E curves, separating by "Order.q"
ggiNEXT3D(output_TD_abun, type = 3, facet.var = "Order.q")
```



## **EXAMPLE 2: TD rarefaction/extrapolation for incidence data**

Based on the dataset (Fish\_incidence\_data) included in the package, the following commands return all numerical results for TD. The first list of the output (\$TDInfo) returns basic data information including the name of the Assemblage, number of sampling units (T), total number of incidences (U), observed species richness (S.obs), sample coverage estimate of the reference sample with size T (SC(T)), sample coverage estimate of the extrapolated sample with size 2T (SC(2T)) as well as the first five species incidence frequency counts in the reference sample (Q1-Q5). The output is identical to that based on the function DataInfo3D() by specifying diversity = 'TD' and datatype = "incidence\_raw"; see later text). Thus, if only data information is required, the simpler function DataInfo3D() (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later.

\$TDInfo

```
Assemblage T U S.obs SC(T) SC(2T) Q1 Q2 Q3 Q4 Q5
1 2013-2015 36 532 50 0.980 0.993 11 6 4 1 3
2 2016-2018 36 522 53 0.976 0.989 13 5 5 2 3
```

The second list of the output (\$TDINEXTEST) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "2013-2015" time period, corresponding to the target number of sample units mT = 1, 2, 4, ..., 34, 36, 37, 38, ..., 72), which locates the reference sampling units at the mid-point of the selected knots. There are two data frames ( $\$size\_based$  and  $\$coverage\_based$ ).

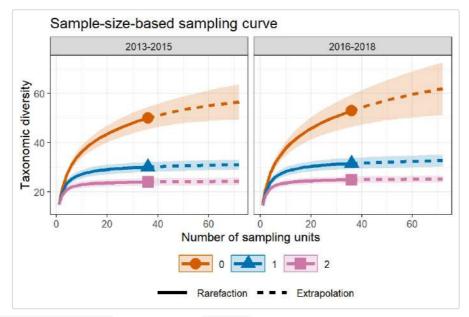
The first data frame ( $$size\_based$ ) includes the name of the Assemblage, diversity order (order.q), the target number of sampling units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the target number of sample units mT is less than, equal to, or greater than the number of sampling units in the reference sample), the diversity estimate of order q (qTD), the lower and upper confidence limits of diversity (qTD.LCL and qTD.UCL) conditioning on the sample size, and the corresponding sample coverage estimate (sc) along with the lower and upper confidence limits of sample coverage (sc.LCL and sc.UCL). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the \$size based output are displayed:

The second data frame ( $$coverage\_based$ ) includes the name of assemblage, the diversity order (order.q), the target sample coverage value (sc), the corresponding number of sampling units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the coverage sc is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (qTD), the lower and upper confidence limits of diversity (qTD.LCL and qTD.UCL) conditioning on the target sample coverage value. Here only the first six rows of the  $$coverage\_based$  output are displayed below: (Note for a fixed coverage value, the confidence interval in the  $$coverage\_based$  table is wider than the corresponding interval in the  $$size\_based$  table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication, leading to higher uncertainty on the resulting diversity estimate.)

The third list of the output (\$TDASyEst) includes the name of the Assemblage, diversity label (qTD, species richness for q = 0, Shannon diversity for q = 1, and Simpson diversity for q = 2), the observed diversity ( $TD_obs$ ), asymptotic diversity estimate ( $TD_asy$ ) and its estimated bootstrap standard error (s.e.) as well as the confidence intervals for asymptotic diversity ( $qTD_LCL$  and  $qTD_UCL$ ). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function ObsAsy3D(). The output is shown below:

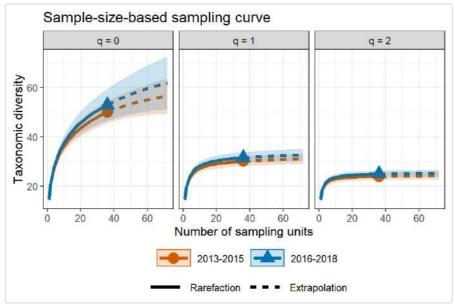
```
Assemblage qTD TD_obs TD_asy s.e. qTD.LCL qTD.UCL
1 2013-2015 Species richness 50.000 59.803 18.179 24.173 95.433
2 2013-2015 Shannon diversity 30.089 31.542 1.173 29.243 33.840
3 2013-2015 Simpson diversity 23.961 24.394 0.885 22.659 26.128
4 2016-2018 Species richness 53.000 69.431 9.946 49.937 88.924
5 2016-2018 Shannon diversity 31.534 33.393 1.388 30.674 36.113
6 2016-2018 Simpson diversity 24.889 25.409 0.848 23.746 27.072
```

The <code>ggiNEXT3D</code> function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When <code>facet.var = "Assemblage"</code> is specified in the <code>ggiNEXT3D</code> function, it creates a separate plot for each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (<code>type = 1</code>) for incidence data is given below:



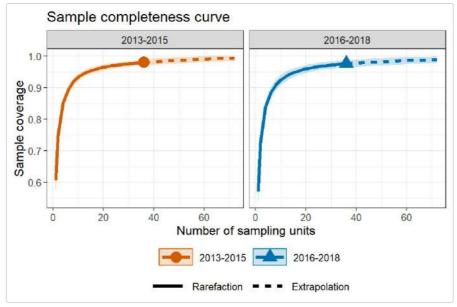
When facet.var = "order.q" is specified in the ggiNEXT3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# TD sample-size-based R/E curves for incidence data, separating by "Order.q"
ggiNEXT3D(output_TD_inci, type = 1, facet.var = "Order.q")
```



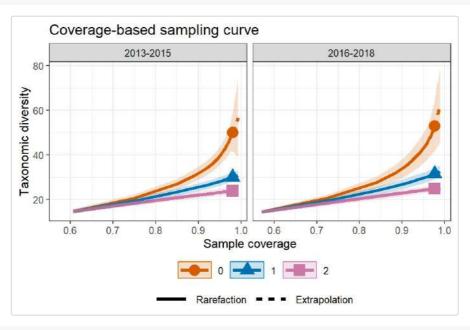
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors are used for different assemblages.

```
# Sample completeness curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_TD_inci, type = 2, color.var = "Assemblage")
```

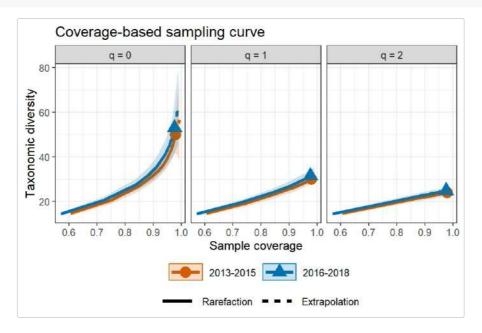


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# TD coverage-based R/E curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_TD_inci, type = 3, facet.var = "Assemblage")
```



# TD coverage-based R/E curves for incidence data, separating by "Order.q" ggiNEXT3D(output\_TD\_inci, type = 3, facet.var = "Order.q")



#### **EXAMPLE 3: PD rarefaction/extrapolation for abundance data**

Based on the dataset (Brazil\_rainforest\_abun\_data) and the phylogentic tree (Brazil\_rainforest\_phylo\_tree) included in the package, the following commands return all numerical results for PD. The first list of the output (\$PDInfo</code>) returns basic data information including the name of the Assemblage, sample size (n), observed species richness (\$S.obs\$), sample coverage estimate of the reference sample with size n (\$C(n)\$), sample coverage estimate of the extrapolated sample with size 2n (\$C(2n)\$), the observed total branch length in the phylogenetic tree spanned by all observed species (\$PD.obs\$), the number of singletons and doubletons in the node/branch abundance set (\$f1\*, \$f2\*\$), the total branch length of those singletons and doubletons in the node/branch abundance set (\$g1, \$g2\$), and the reference time (\$Reftime\$). The output is identical to that based on the function \$PataInfo3D()\$ by specifying diversity = 'PD' and \$datatype = "abundance"; see later text). Thus, if only data information is required, the simpler function \$PataInfo3D()\$ (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later.

The required argument for performing PD analysis is PDtree. For example, the phylogenetic tree for all observed species (including species in both Edge and Interior habitats) is stored in <code>Brazil\_rainforest\_phylo\_tree</code>. Then we enter the argument <code>PDtree = Brazil\_rainforest\_phylo\_tree</code>. Two optional arguments are: <code>PDtype</code> and <code>PDreftime</code>. There are two options for <code>PDtype</code>: "PD" (effective total branch length) or "meanPD" (effective number of equally divergent lineages, <code>meanPD = PD/tree</code> depth). Default is <code>PDtype = "meanPD"</code>. <code>PDreftime</code> is a numerical value specifying a reference time for computing phylogenetic diversity. By default (<code>PDreftime = NULL</code>), the reference time is set to the tree depth, i.e., age of the root of the phylogenetic tree. Run the following code to perform PD analysis.

The second list of the output (\$PDINextEst) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "Edge" assemblage, corresponding to the target sample size m = 1, 95, 189, ..., 1699, 1794, 1795, 1899, ..., 3588), which locates the reference sample size at the mid-point of the selected knots. There are two data frames (\$size\_based and \$coverage\_based).

The first data frame ( $size\_based$ ) includes the name of the Assemblage, diversity order (order.q), the target sample size (m), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the size m is less than, equal to, or greater than the reference sample size), the diversity estimate of order q (qpD), the lower and upper confidence limits of diversity (qpD.LCL and qpD.UCL) conditioning on the sample size, the corresponding sample coverage estimate (sc) along with the lower and upper confidence limits of sample coverage (sc.LCL and sc.UCL), the reference time (Reftime) and the type of PD (Type). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the \$size\_based output are displayed:

```
Assemblage Order.q m Method qPD qPD.LCL qPD.UCL SC SC.LCL SC.UCL Reftime Type

1 Edge 0 1 Rarefaction 1.000 0.984 1.016 0.012 0.011 0.013 400 meanPD

2 Edge 0 95 Rarefaction 18.547 17.956 19.137 0.484 0.469 0.499 400 meanPD

3 Edge 0 189 Rarefaction 26.723 25.867 27.579 0.638 0.624 0.652 400 meanPD

4 Edge 0 284 Rarefaction 32.305 31.275 33.336 0.718 0.706 0.731 400 meanPD

5 Edge 0 378 Rarefaction 36.498 35.336 37.661 0.768 0.757 0.780 400 meanPD

6 Edge 0 472 Rarefaction 39.882 38.610 41.153 0.803 0.792 0.814 400 meanPD
```

The second data frame ( $scoverage\_based$ ) includes the name of assemblage, the diversity order (order.q), the target sample coverage value (sc), the corresponding sample size (m), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the coverage sc is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (qpd), the lower and upper confidence limits of diversity (qpd).LCL and qpd).UCL) conditioning on the target sample coverage value, the reference times (Reftime) and the

type of PD (Type). Here only the first six rows of the \$coverage\_based output are displayed below: (Note for a fixed coverage value, the confidence interval in the \$coverage\_based table is wider than the corresponding interval in the \$size\_based table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication, leading to higher uncertainty on the resulting diversity estimate.)

```
output_PD_abun$PDiNextEst$coverage_based
```

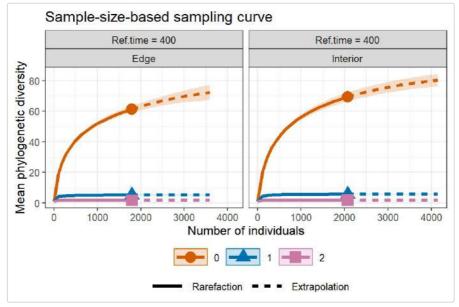
```
Assemblage Order.q
                   SC
                               Method
                                       qPD qPD.LCL qPD.UCL Reftime
                        1 Rarefaction 1.000 0.983 1.017
1
    Edge 0 0.012
               0 0.484 95 Rarefaction 18.547 17.553 19.541
2
      Edge
                                                            400 meanPD
                                                          400 meanPD
3
               0 0.638 189 Rarefaction 26.723 25.350 28.097
      Edge
4
               0 0.718 284 Rarefaction 32.305 30.674 33.936
                                                           400 meanPD
      Edge
      Edge
5
              0 0.768 378 Rarefaction 36.498 34.671 38.325
                                                            400 meanPD
                0 0.803 472 Rarefaction 39.882 37.898 41.866
                                                             400 meanPD
```

The third list of the output (\$PDASyEst\$) includes the name of the Assemblage, PD (or meanPD) for q = 0, 1, and 2 (qPD), the observed diversity ( $PD_obs$ ), asymptotic diversity estimates ( $PD_asy$ ), estimated asymptotic bootstrap standard error (s.e.) as well as the confidence intervals for asymptotic diversity with q = 0, 1, and 2 (qPD.LCL and qPD.UCL), the reference times (Reftime) and the type of PD (Type). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function ObsAsy3D(). The output is shown below:

```
qPD PD_obs PD_asy s.e. qPD.LCL qPD.UCL Reftime Type
    Edge q = 0 PD 61.290 80.027 5.580 69.091 90.964 400 meanPD
1
      Edge q = 1 PD 5.246 5.372 0.095 5.184
2
                                             5.559
                                                       400 meanPD
      Edge q = 2 PD 1.797 1.798 0.022
                                       1.754
  Interior q = 0 PD 69.318 86.375 4.457 77.640 95.110
4
                                                       400 meanPD
   Interior q = 1 PD 5.721 5.854 0.093 5.672
5
                                             6.036
                                                     400 meanPD
   Interior q = 2 PD 1.914 1.915 0.023 1.869 1.961 400 meanPD
```

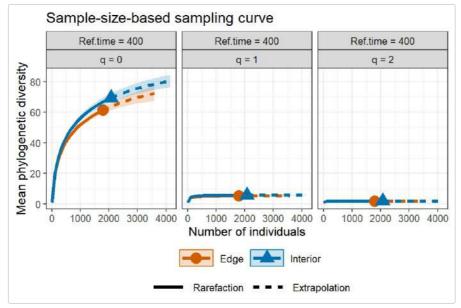
The <code>ggiNEXT3D</code> function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When <code>facet.var = "Assemblage"</code> is specified in the <code>ggiNEXT3D</code> function, it creates a separate plot for each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (<code>type = 1</code>) is given below:

```
# PD sample-size-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_PD_abun, type = 1, facet.var = "Assemblage")
```



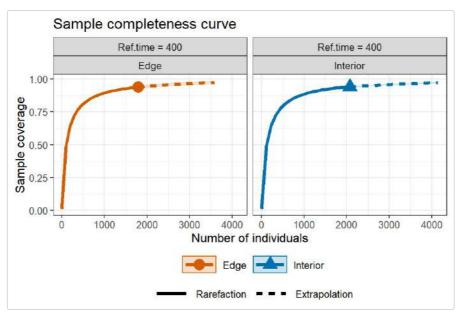
When facet.var = "Order.q" is specified in the ggiNEXT3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# PD sample-size-based R/E curves, separating by "Order.q"
ggiNEXT3D(output_PD_abun, type = 1, facet.var = "Order.q")
```



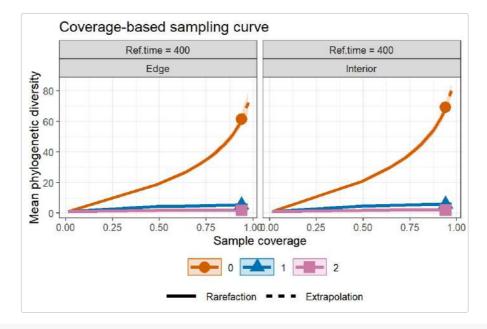
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors are used for different assemblages.

```
# Sample completeness curves for abundance data, separating by "Assemblage"
ggiNEXT3D(output_PD_abun, type = 2, color.var = "Assemblage")
```

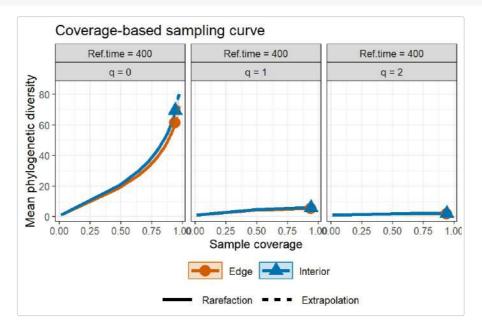


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# PD coverage-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_PD_abun, type = 3, facet.var = "Assemblage")
```



# PD coverage-based R/E curves, separating by "Order.q"
ggiNEXT3D(output\_PD\_abun, type = 3, facet.var = "Order.q")



# **EXAMPLE 4: PD rarefaction/extrapolation for incidence data**

Based on the dataset (Fish\_incidence\_data) included in the package and the phylogentic tree (Fish\_phylo\_tree), the following commands return all numerical results for PD. The first list of the output (\$PDInfo) returns basic data information including the name of the Assemblage, number of sampling units (T), total number of incidences (U), observed species richness (S.obs), sample coverage estimate of the reference sample with size T (SC(T)), sample coverage estimate of the extrapolated sample with size 2T (SC(2T)), the observed total branch length in the phylogenetic tree spanned by all observed species (PD.obs), the singletons/doubletons in the sample branch incidence (Q1\*,Q2\*), the total branch length of those singletons/doubletons in the sample branch incidence (R1,R2), and the reference time (Reftime). The output is identical to that based on the function DataInfo3D() by specifying diversity = 'PD' and datatype = "incidence\_raw"; see later text). Thus, if only data information is required, the simpler function DataInfo3D() (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later.

The required argument for performing PD analysis is PDtree. For example, the phylogenetic tree for all observed species (including species in both "2013-2015" and "2016-2018" time periods) is stored in Fish\_phylo\_tree. Then we enter the argument PDtree = Fish\_phylo\_tree. Two optional arguments are: PDtype and PDreftime. There are two options for PDtype: "PD" (effective total branch length) or "meanPD" (effective number of equally divergent lineages, meanPD = PD/tree depth). Default is PDtype = "meanPD". PDreftime is a numerical value specifying a reference time for computing phylogenetic diversity. By default (PDreftime = NULL), the reference time is set to the tree depth, i.e., age of the root of the phylogenetic tree. Run the following code to perform PD analysis.

```
data(Fish_incidence_data)
data(Fish_phylo_tree)
data <- Fish_incidence_data
tree <- Fish_phylo_tree</pre>
```

The second list of the output (proinextest) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "2013-2015" time period, corresponding to the target number of sample units mT = 1, 2, 4, ..., 34, 36, 37, 38, ..., 72), which locates the reference sampling units at the mid-point of the selected knots. There are two data frames ( $size_based$  and  $coverage_based$ ).

The first data frame ( $\$size\_based$ ) includes the name of the Assemblage, diversity order (order.q), the target number of sample units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the target number of sample units mT is less than, equal to, or greater than the number of sampling units in the reference sample), the diversity estimate of order q (qPD), the lower and upper confidence limits of diversity (qPD.LCL and qPD.UCL) conditioning on the sample size, the corresponding sample coverage estimate (sC) along with the lower and upper confidence limits of sample coverage (sc.LCL and sc.UCL), the reference time (Reftime) and the type of PD (Type). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the \$size based output are displayed:

```
output_PD_inci$PDiNextEst$size_based
```

The second data frame (\$coverage\_based) includes the name of assemblage, the diversity order (order.q), the target sample coverage value (sc), the corresponding number of sample units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the coverage sc is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (qPD), the lower and upper confidence limits of diversity (qPD.LCL and qPD.UCL) conditioning on the target sample coverage value, the reference time (Reftime) and the type of PD (Type). Here only the first six rows of the \$coverage\_based output are displayed below: (Note for a fixed coverage value, the confidence interval in the \$coverage\_based table is wider than the corresponding interval in the \$size\_based table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication, leading to higher uncertainty on the resulting diversity estimate.)

```
output_PD_inci$PDiNextEst$coverage_based
```

The third list of the output (\$PDASyEst) includes the name of the Assemblage, PD (or meanPD) for q = 0, 1, and 2 (qPD), the observed diversity ( $PD_obs$ ), asymptotic diversity estimate ( $PD_asy$ ) and its estimated bootstrap standard error (s.e.), the confidence intervals for asymptotic diversity (qPD\_LCL and qPD\_UCL), the reference time (Reftime) and the type of PD (Type). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function obsAsy3D(). The output is shown below:

```
output_PD_inci$PDAsyEst
```

```
Assemblage qPD PD_obs PD_asy s.e. qPD.LCL qPD.UCL Reftime Type

1 2013-2015 q = 0 PD 9.847 10.039 0.702 8.663 11.416 0.977 meanPD

2 2013-2015 q = 1 PD 7.635 7.729 0.157 7.421 8.037 0.977 meanPD

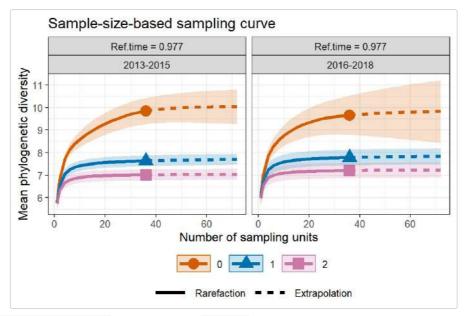
3 2013-2015 q = 2 PD 7.013 7.057 0.152 6.760 7.355 0.977 meanPD

4 2016-2018 q = 0 PD 9.659 9.854 0.796 8.295 11.413 0.977 meanPD
```

```
5 2016-2018 q = 1 PD 7.781 7.859 0.141 7.583 8.136 0.977 meanPD 6 2016-2018 q = 2 PD 7.202 7.244 0.116 7.016 7.471 0.977 meanPD
```

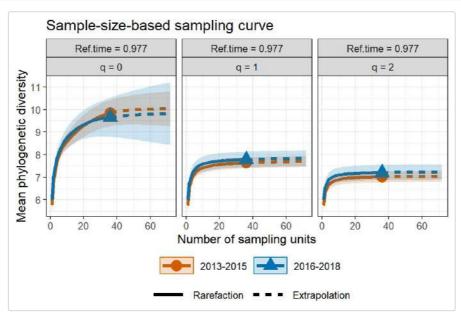
The gginext3D function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When facet.var = "Assemblage" is specified in the gginext3D function, it creates a separate plot for each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (type = 1) is given below:

```
# PD sample-size-based R/E curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_PD_inci, type = 1, facet.var = "Assemblage")
```



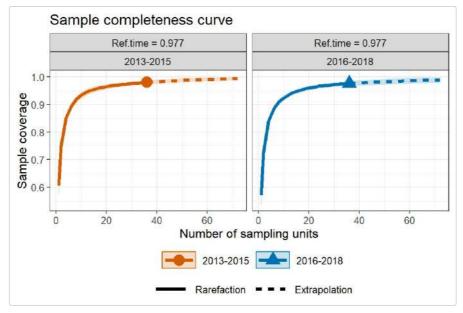
When facet.var = "Order.q" is specified in the ggiNEXT3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# PD sample-size-based R/E curves for incidence data, separating by "Order.q"
ggiNEXT3D(output_PD_inci, type = 1, facet.var = "Order.q")
```



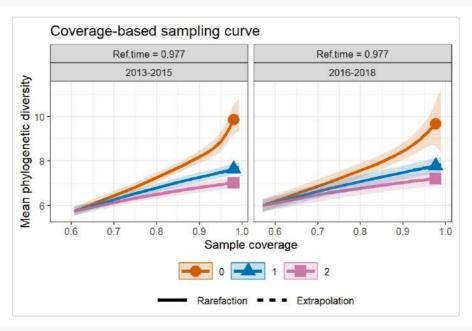
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors are used for different assemblages.

```
# Sample completeness curves for incidence data, separating by "Assemblage" ggiNEXT3D(output_PD_inci, type = 2, color.var = "Assemblage")
```

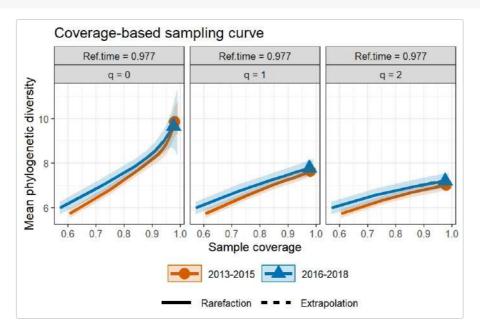


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# PD coverage-based R/E curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_PD_inci, type = 3, facet.var = "Assemblage")
```



# PD coverage-based R/E curves for incidence data, separating by "Order.q" ggiNEXT3D(output\_PD\_inci, type = 3, facet.var = "Order.q")



## **EXAMPLE 5: FD rarefaction/extrapolation for abundance data**

Based on the dataset (Brazil\_rainforest\_abun\_data) and the the distance matrix (Brazil\_rainforest\_distance\_matrix) included in the package, the following commands return all numerical results for FD. The first list of the output (\$FDInfo) returns basic data information including the name of the Assemblage, sample size (n), observed species richness (\$S.obs), sample coverage estimate of the reference sample with size n (SC(n)), sample coverage estimate of the extrapolated sample with size 2n(SC(2n)), and the minimum, mean, and maximum distance among all non-diagonal elements in the distance matrix(dmin, dmean, dmax). The output is identical to that based on the function DataInfo3D() by specifying diversity = 'FD' and datatype = "abundance"; see later text). Thus, if only data information is required, the simpler function DataInfo3D() (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later

The required argument for performing FD analysis is FDdistM. For example, the distance matrix for all species (including species in both Edge and Interior habitats) is stored in Brazil\_rainforest\_distance\_matrix. Then we enter the argument FDdistM = Brazil\_rainforest\_distance\_matrix Three optional arguments are (1) FDtype: FDtype = "AUC" means FD is computed from the area under the curve of a tau-profile by integrating all plausible threshold values between zero and one; FDtype = "tau\_values" means FD is computed under specific threshold values to be specified in the argument FD\_tau. (2) FD\_tau: a numerical value specifying the tau value (threshold level) that will be used to compute FD. If FDtype = "tau\_values" and FD\_tau = NULL, then the threshold level is set to be the mean distance between any two individuals randomly selected from the pooled data over all data (i.e., quadratic entropy).

```
$FDInfo
Assemblage n S.obs SC(n) SC(2n) dmin dmean dmax

1 Edge 1794 319 0.939 0.974 0 0.372 0.776

2 Interior 2074 356 0.941 0.973 0 0.329 0.776
```

The second list of the output (\$FDINEXTEST) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "Edge" assemblage, corresponding to the target sample size m = 1, 95, 189, ..., 1699, 1794, 1795, 1899, ..., 3588), which locates the reference sample size at the mid-point of the selected knots. There are two data frames (\$size\_based and \$coverage\_based).

The first data frame (\$size\_based) includes the name of the Assemblage, diversity order (Order.q), the target sample size (m), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the size m is less than, equal to, or greater than the reference sample size), the diversity estimate of order q (qFD), the lower and upper confidence limits of diversity (qFD.LCL and qFD.UCL) conditioning on the sample size, and the corresponding sample coverage estimate (SC) along with the lower and upper confidence limits of sample coverage (SC.LCL and SC.UCL). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the \$size\_based output are displayed:

```
Assemblage Order.q m Method qFD qFD.LCL qFD.UCL SC SC.LCL SC.UCL

1 Edge 0 1 Rarefaction 1.000 1.000 0.012 0.010 0.013

2 Edge 0 95 Rarefaction 10.900 10.442 11.358 0.484 0.466 0.502

3 Edge 0 189 Rarefaction 12.993 12.117 13.868 0.638 0.619 0.657

4 Edge 0 284 Rarefaction 14.129 12.888 15.371 0.718 0.702 0.735

5 Edge 0 378 Rarefaction 14.860 13.304 16.416 0.768 0.755 0.782

6 Edge 0 472 Rarefaction 15.383 13.549 17.216 0.803 0.792 0.814
```

The second data frame (<code>Scoverage\_based</code>) includes the name of assemblage, the diversity order (<code>Order.q</code>), the target sample coverage value (<code>SC</code>), the corresponding sample size (<code>m</code>), the <code>Method</code> (<code>Rarefaction</code>, <code>Observed</code>, or <code>Extrapolation</code>, depending on whether the coverage <code>SC</code> is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (<code>QFD</code>), and the lower and upper confidence limits of diversity (<code>QFD.LCL</code> and <code>QFD.UCL</code>) conditioning on the target sample coverage value. Here only the first six rows of the <code>\$coverage\_based</code> output are displayed below: (Note for a fixed coverage value, the confidence interval in the <code>\$coverage\_based</code> table is wider than the corresponding interval in the <code>\$size\_based</code> table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication,

```
output_FD_abun$FDiNextEst$coverage_based
```

```
Assemblage Order.q SC m
                               Method
                                       qFD qFD.LCL qFD.UCL
1
       Edge 0 0.012 1 Rarefaction 1.000 1.000 1.000
2
                0 0.484 95 Rarefaction 10.900 10.472 11.328
3
                0 0.638 189 Rarefaction 12.993
                                             12.328 13.657
4
       Edge
                0 0.718 284 Rarefaction 14.129 13.209 15.049
5
               0 0.768 378 Rarefaction 14.860 13.696 16.025
       Edge
               0 0.803 472 Rarefaction 15.383 13.991 16.775
```

The third list of the output ( ${\tt SFDASyEst}$ ) includes the name of the Assemblage, FD for q = 0, 1, and 2 ( ${\tt QFD}$ ), the observed diversity ( ${\tt FD\_obs}$ ), asymptotic diversity estimate ( ${\tt FD\_asy}$ ) and its estimated bootstrap standard error ( ${\tt s.e.}$ ) as well as the confidence intervals for asymptotic diversity ( ${\tt QFD.LCL}$  and  ${\tt QFD.UCL}$ ). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function  ${\tt ObsAsy3D}$ (). The output is shown below:

```
output_FD_abun$FDAsyEst
```

```
Assemblage qFD FD_obs FD_asy s.e. qFD.LCL qFD.UCL

1 Edge q = 0 FD(AUC) 17.851 19.008 4.997 9.214 28.801

2 Edge q = 1 FD(AUC) 11.781 12.037 0.521 11.016 13.057

3 Edge q = 2 FD(AUC) 9.139 9.228 0.397 8.451 10.006

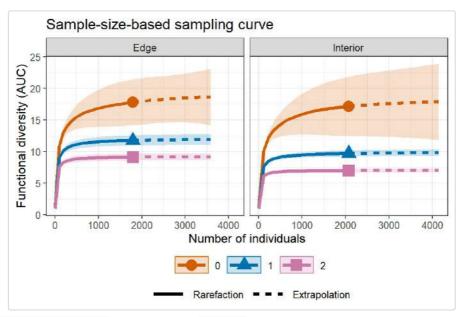
4 Interior q = 0 FD(AUC) 17.168 18.208 8.415 1.716 34.700

5 Interior q = 1 FD(AUC) 9.716 9.922 0.276 9.381 10.463

6 Interior q = 2 FD(AUC) 7.007 7.055 0.148 6.766 7.345
```

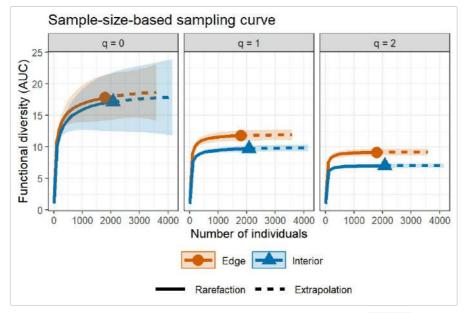
The <code>ggiNext3D</code> function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When <code>facet.var = "Assemblage"</code> is specified in the <code>ggiNext3D</code> function, it creates a separate plot for each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (<code>type = 1</code>) is given below:

```
# FD sample-size-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_FD_abun, type = 1, facet.var = "Assemblage")
```



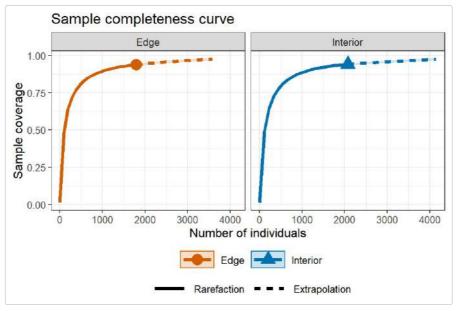
When facet.var = "Order.q" is specified in the ggiNEXT3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# FD sample-size-based R/E curves, separating by "Order.q"
ggiNEXT3D(output_FD_abun, type = 1, facet.var = "Order.q")
```



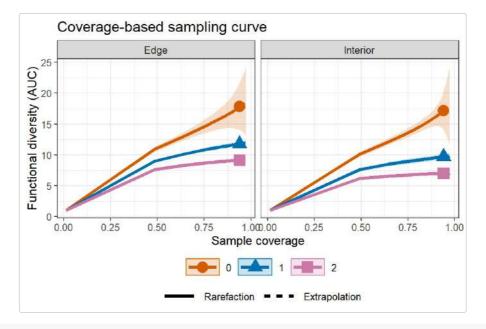
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors are used for different assemblages.

```
# Sample completeness curves for abundance data, separating by "Assemblage"
ggiNEXT3D(output_FD_abun, type = 2, color.var = "Assemblage")
```

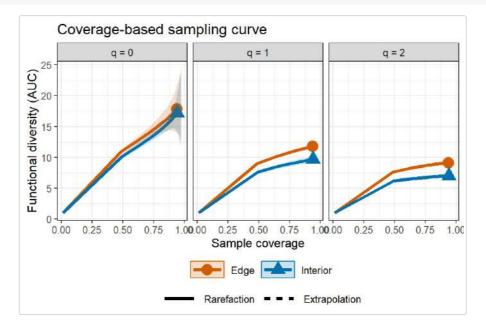


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# FD coverage-based R/E curves, separating by "Assemblage"
ggiNEXT3D(output_FD_abun, type = 3, facet.var = "Assemblage")
```



```
# FD coverage-based R/E curves, separating by "Order.q"
ggiNEXT3D(output_FD_abun, type = 3, facet.var = "Order.q")
```



# **EXAMPLE 6: FD rarefaction/extrapolation for incidence data**

Based on the dataset (Fish\_incidence\_data) and the the distance matrix (Fish\_distance\_matrix) included in the package, the following commands return all numerical results for FD. The first list of the output (\$FDInfo) returns basic data information including the name of the Assemblage, number of sampling units (T), total number of incidences (U), observed species richness (S.obs), sample coverage estimate of the reference sample with size T (SC(T)), sample coverage estimate of the reference sample with size 2T (SC(T)), and the minimum, mean, and maximum distance among all non-diagonal elements in the distance matrix(dmin, dmean, dmax). The output is identical to that based on the function DataInfo3D() by specifying diversity = 'FD' and datatype = "incidence\_raw"; see later text). Thus, if only data information is required, the simpler function DataInfo3D() (see later text) can be used to obtain the same output. More information about the observed diversity (for any order q between 0 and 2) can be obtained by function ObsAsy3D(), which will be introduced later.

The required argument for performing FD analysis is FDdistM. For example, the distance matrix for all species (including species in both "2013-2015" and "2016-2018" time periods) is stored in Fish\_distance\_matrix. Then we enter the argument FDdistM = Fish\_distance\_matrix Three optional arguments are (1) FDtype: FDtype = "AUC" means FD is computed from the area under the curve of a tau-profile by integrating all plausible threshold values between zero and one; FDtype = "tau\_values" means FD is computed under specific threshold values to be specified in the argument FD\_tau. (2) FD\_tau: a numerical value specifying the tau value (threshold level) that will be used to compute FD. If FDtype = "tau\_values" and FD\_tau = NULL, then the threshold level is set to be the mean distance between any two individuals randomly selected from the pooled data over all data (i.e., quadratic entropy).

```
data(Fish_incidence_data)
data(Fish_distance_matrix)
data <- Fish_incidence_data
distM <- Fish_distance_matrix
output_FD_inci <- iNEXT3D(data, diversity = 'FD', datatype = "incidence_raw", nboot = 20,</pre>
```

```
FDdistM = distM, FDtype = 'AUC')
output_FD_inci$FDInfo
```

```
$FDInfo

Assemblage T U S.obs SC(T) SC(2T) dmin dmean dmax

1 2013-2015 36 532 50 0.980 0.993 0.006 0.240 0.733

2 2016-2018 36 522 53 0.976 0.989 0.006 0.237 0.733
```

The second list of the output (\$FDINextEst) includes size- and coverage-based standardized diversity estimates and related statistics computed for 40 knots by default (for example in the "2013-2015" time period, corresponding to the target number of sample units mT = 1, 2, 4, ..., 34, 36, 37, 38, ..., 72), which locates the reference sampling units at the mid-point of the selected knots. There are two data frames ( $\$size\_based$  and  $\$coverage\_based$ ).

The first data frame ( $size_based$ ) includes the name of the Assemblage, diversity order (order.q), the target number of sample units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the target number of sample units mT is less than, equal to, or greater than the number of sampling units in the reference sample), the diversity estimate of order q (qFD), the lower and upper confidence limits of diversity (qFD.LCL and qFD.UCL) conditioning on the sample size, and the corresponding sample coverage estimate (sc) along with the lower and upper confidence limits of sample coverage (sc.LCL and sc.UCL). These sample coverage estimates with confidence intervals are used for plotting the sample completeness curve. If the argument nboot is greater than zero, then a bootstrap method is applied to obtain the confidence intervals for the diversity and sample coverage estimates. Otherwise, all confidence intervals will not be computed. Here only the first six rows of the  $size_based$  output are displayed:

The second data frame ( $$coverage\_based$ ) includes the name of assemblage, the diversity order (order.q), the target sample coverage value (sc), the corresponding number of sample units (mT), the Method (Rarefaction, Observed, or Extrapolation, depending on whether the coverage sc is less than, equal to, or greater than the reference sample coverage), the diversity estimate of order q (qFD), and the lower and upper confidence limits of diversity (qFD.LCL and qFD.UCL) conditioning on the target sample coverage value. Here only the first six rows of the  $$coverage\_based$  output are displayed below: (Note for a fixed coverage value, the confidence interval in the  $$coverage\_based$  table is wider than the corresponding interval in the  $$size\_based$  table. This is because, for a given coverage value, the sample size needed to attain a fixed coverage value varies with bootstrap replication, leading to higher uncertainty on the resulting diversity estimate.)

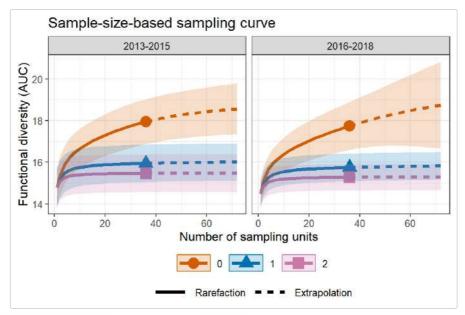
The third list of the output (\$FDASyEst) includes the name of the Assemblage, FD for q = 0, 1, and 2 (qFD), the observed diversity ( $FD\_obs$ ), asymptotic diversity estimate ( $FD\_asy$ ) and its estimated bootstrap standard error (s.e.), and the confidence intervals for asymptotic diversity (qFD.LCL and qFD.UCL). These statistics are computed only for q = 0, 1 and 2. More detailed information about asymptotic and observed diversity estimates for any order q between 0 and 2 can be obtained from function ObsAsy3D(). The output is shown below:

```
Assemblage qFD FD_obs FD_asy s.e. qFD.LCL qFD.UCL
1 2013-2015 q = 0 FD(AUC) 17.904 18.906 1.386 16.188 21.623
2 2013-2015 q = 1 FD(AUC) 15.944 16.043 0.469 15.124 16.961
3 2013-2015 q = 2 FD(AUC) 15.463 15.490 0.455 14.598 16.383
4 2016-2018 q = 0 FD(AUC) 17.739 19.770 4.931 10.106 29.434
5 2016-2018 q = 1 FD(AUC) 15.749 15.867 0.607 14.678 17.056
6 2016-2018 q = 2 FD(AUC) 15.275 15.305 0.532 14.262 16.348
```

The ggiNEXT3D function can be used to make graphical displays for rarefaction and extrapolation sampling curves. When facet.var = "Assemblage" is specified in the ggiNEXT3D function, it creates a separate plot for

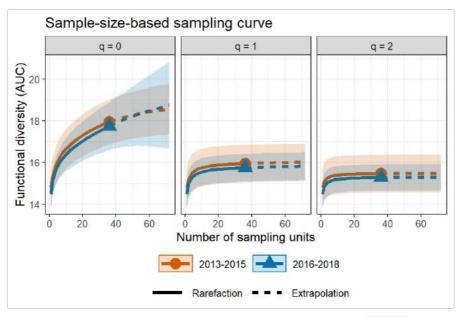
each assemblage; within each assemblage, different color curves represent diversity of different orders. An example for showing sample-size-based rarefaction/extrapolation curves (type = 1) is given below:

```
# FD sample-size-based R/E curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_FD_inci, type = 1, facet.var = "Assemblage")
```



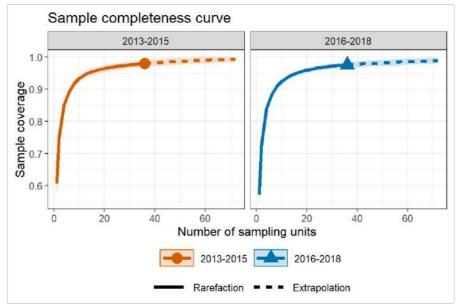
When facet.var = "order.q" is specified in the gginext3D function, it creates a separate plot for each diversity order; within each plot, different color curves represent different assemblages. An example is shown below:

```
# FD sample-size-based R/E curves for incidence data, separating by "Order.q"
ggiNEXT3D(output_FD_inci, type = 1, facet.var = "Order.q")
```



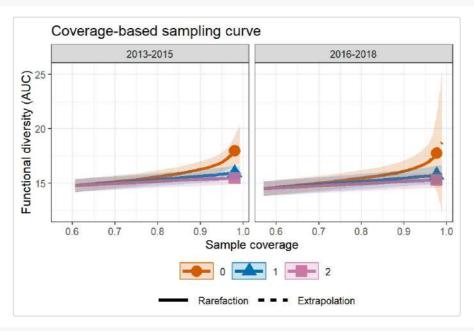
The following commands return the sample completeness (sample coverage) curve (type = 2) in which different colors are used for different assemblages.

```
# Sample completeness curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_FD_inci, type = 2, color.var = "Assemblage")
```

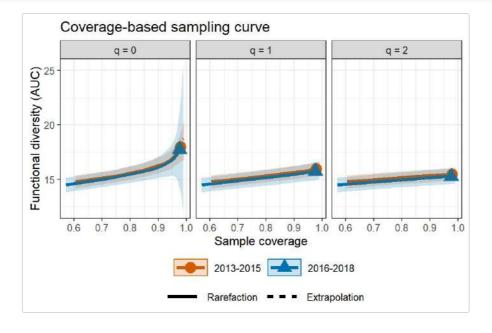


The following commands return the coverage-based rarefaction/extrapolation sampling curves in which different color curves represent three diversity orders within each assemblage (facet.var = "Assemblage"), or represent two assemblages within each diversity order (facet.var = "Order.q"), respectively.

```
# FD coverage-based R/E curves for incidence data, separating by "Assemblage"
ggiNEXT3D(output_FD_inci, type = 3, facet.var = "Assemblage")
```



# FD coverage-based R/E curves for incidence data, separating by "Order.q" ggiNEXT3D(output\_FD\_inci, type = 3, facet.var = "Order.q")



# **FUNCTION DataInfo3D(): DATA INFORMATION**

The function <code>DataInfo3D()</code> provides basic data information for the reference sample in each individual assemblage. The function <code>DataInfo3D()</code> with default arguments is shown below:

All arguments in the above function are the same as those for the main function inext3D. Running the DataInfo3D() function returns basic data information including sample size, observed species richness, two sample coverage estimates (SC(n) and SC(2n)) as well as other relevant information in each of the three dimensions of diversity. We use Brazil\_rainforest\_abun\_data and Fish\_incidence\_data to demo the function for each dimension of diversity.

# TAXONOMIC DIVERSITY (TD): Basic data information for abundance data

#### Output description:

- Assemblage = assemblage name.
- n = number of observed individuals in the reference sample (sample size).
- S.obs = number of observed species in the reference sample.
- sc(n) = sample coverage estimate of the reference sample with size n.
- sc (2n) = sample coverage estimate of the reference sample with size 2n.
- f1-f5 = the first five species abundance frequency counts in the reference sample.

# TAXONOMIC DIVERSITY (TD): Basic data information for incidence data

```
data(Fish_incidence_data)
DataInfo3D(Fish_incidence_data, diversity = 'TD', datatype = "incidence_raw")

Assemblage T U S.obs SC(T) SC(2T) Q1 Q2 Q3 Q4 Q5
1 2013-2015 36 532 50 0.980 0.993 11 6 4 1 3
2 2016-2018 36 522 53 0.976 0.989 13 5 5 2 3
```

## Output description:

- Assemblage = assemblage name.
- $\circ$  T = number of sampling units in the reference sample (sample size for incidence data).
- $\overline{u}$  = total number of incidences in the reference sample.
- $\circ~_{{\tt S.obs}}$  = number of observed species in the reference sample.
- sc(T) = sample coverage estimate of the reference sample with size T.
- $\circ$  SC (2T) = sample coverage estimate of the reference sample with size 2T.
- Q1-Q5 = the first five species incidence frequency counts in the reference sample.

## PHYLOGENETIC DIVERSITY (PD): Basic data information for abundance data

#### Output description:

- Assemblage, n, S.obs, SC(n) and SC(2n): definitions are the same as in the TD abundance output and thus
  are omitted.
- PD. obs = the observed total branch length in the phylogenetic tree spanned by all observed species.
- f1\*,f2\* = the number of singletons and doubletons in the node/branch abundance set.
- q1,q2 = the total branch length of those singletons/doubletons in the node/branch abundance set.
- Reftime = reference time for phylogenetic diversity (the age of the root of phylogenetic tree).

## PHYLOGENETIC DIVERSITY (PD): Basic data information for incidence data

#### Output description:

- Assemblage, T, U, S.obs, SC(T) and SC(2T): definitions are the same as in the TD incidence output and
  thus are omitted.
- PD.obs = the observed total branch length in the phylogenetic tree spanned by all observed species.
- Q1\*,Q2\* = the singletons/doubletons in the sample branch incidence.
- R1,R2 = the total branch length of those singletons/doubletons in the sample branch incidence.
- Reftime = reference time.

## FUNCTIONAL DIVERSITY (FD): Basic data information for abundance data

## Output description:

- Assemblage, n, S.obs, SC(n) and SC(2n): definitions are the same as in TD abundance output and thus are
  omitted.
- dmin = the minimum distance among all non-diagonal elements in the distance matrix.
- dmean = the mean distance between any two individuals randomly selected from each assemblage.
- dmax = the maximum distance among all elements in the distance matrix.

## FUNCTIONAL DIVERSITY (FD): Basic data information for incidence data

### Output description:

• Assemblage, T, U, S.obs, SC(T) and SC(2T): definitions are the same as in the TD incidence output and

thus are omitted.

3 2013-2015

4 2013-2015

5 2013-2015

6 2013-2015

2016-2018

2016-2018

- dmin = the minimum distance among all non-diagonal elements in the distance matrix.
- dmean = the mean distance between any two individuals randomly selected from each assemblage.
- dmax = the maximum distance among all elements in the distance matrix.

# FUNCTION estimate3D(): POINT ESTIMATION

estimate 3D is used to compute 3D diversity (TD, PD, FD) estimates with q = 0, 1, 2 under any specified levels of sample size (when base = "size") and sample coverage values (when base = "coverage") for abundance data (datatype = "incidence\_raw"). When base = "size", level can be specified with a particular vector of sample sizes (greater than 0); if level = NULL, this function computes the diversity estimates for the minimum sample size among all samples extrapolated to the double reference sizes. When base = "coverage", level can be specified with a particular vector of sample coverage values (between 0 and 1); if level = NULL, this function computes the diversity estimates for the minimum sample coverage among all samples extrapolated to the double reference sizes. All arguments in the function are the same as those for the main function inext3D.

```
estimate3D(data, diversity = "TD", q = c(0, 1, 2), datatype = "abundance",
   base = "coverage", level = NULL, nboot = 50, conf = 0.95,
   nT = NULL, PDtree, PDreftime = NULL, PDtype = "meanPD",
   FDdistM, FDtype = "AUC", FDtau = NULL, FDcut_number = 50)
```

# **TAXONOMIC DIVERSITY (TD): point estimation**

## Example 7a: TD for abundance data with two target coverage values (93% and 97%)

The following commands return the TD estimates with two specified levels of sample coverage (93% and 97%) based on the <code>Brazil\_rainforest\_abun\_data</code>.

```
data(Brazil rainforest abun data)
 \texttt{output\_est\_TD\_abun} < -\texttt{estimate3D}(\texttt{Brazil\_rainforest\_abun\_data}, \ \texttt{diversity} = \texttt{'TD'}, \ \texttt{q} = \texttt{c}(0,1,2), 
                                 datatype = "abundance", base = "coverage", level = c(0.93,
        0.97))
output_est_TD_abun
    Assemblage Order.q SC m Method qTD s.e. qTD.LCL qTD.UCL Edge 0 0.93 1547.562 Rarefaction 302.879 12.456 278.465 327.293
  Assemblage Order.q SC
                    0 0.97 3261.971 Extrapolation 383.307 18.571 346.909 419.705
       Edge
                   1 0.93 1547.562 Rarefaction 152.374 4.504 143.547 161.202
3
       Edge
                  1 0.97 3261.971 Extrapolation 166.837 4.992 157.052 176.622
       Edge
                  2 0.93 1547.562 Rarefaction 81.437 3.760 74.069 88.806
6 Eug
7 Interior
                  2 0.97 3261.971 Extrapolation 83.726 3.953 75.978 91.474
                   0 0.93 1699.021 Rarefaction 331.917 12.276 307.858 355.977
   Interior
Interior
                    0 0.97 3883.447 Extrapolation 433.807 18.549 397.452 470.162
                   1 0.93 1699.021 Rarefaction 159.330 4.855 149.814 168.847
10 Interior
                  1 0.97 3883.447 Extrapolation 175.739 5.128 165.689 185.790
11 Interior
                  2 0.93 1699.021 Rarefaction 71.611 3.922 63.924 79.297
                   2 0.97 3883.447 Extrapolation 73.326 4.068 65.353 81.299
```

# Example 7b: TD for incidence data with two target coverage values (97.5% and 99%)

The following commands return the TD estimates with two specified levels of sample coverage (97.5% and 99%) for the Fish\_incidence\_data.

1 0.975 29.169 Rarefaction 29.773 1.197 27.427 32.118

1 0.990 58.667 Extrapolation 30.751 1.214 28.372 33.130

2 0.975 29.169 Rarefaction 23.861 0.825 22.245 25.478

2 0.990 58.667 Extrapolation 24.126 0.840 22.479 25.773

0 0.990 76.971 Extrapolation 62.688 14.646

0 0.975 34.825 Rarefaction 52.574 6.997 38.860 66.288

```
9 2016-2018 1 0.975 34.825 Rarefaction 31.479 1.223 29.082 33.875

10 2016-2018 1 0.990 76.971 Extrapolation 32.721 1.186 30.397 35.046

11 2016-2018 2 0.975 34.825 Rarefaction 24.872 0.755 23.392 26.352

12 2016-2018 2 0.990 76.971 Extrapolation 25.163 0.743 23.708 26.618
```

# PHYLOGENETIC DIVERSITY (PD): point estimation

# Example 8a: PD for abundance data with two target sample sizes (1500 and 3500)

The following commands return the PD estimates with two specified levels of sample sizes (1500 and 3500) for the Brazil rainforest abun data.

```
Assemblage Order.q
                            Method SC qPD s.e. qPD.LCL qPD.UCL Reftime Type
   Edge 0 1500 Rarefaction 0.928 58.370 1.007 56.396 60.344 400 meanPD
                0 3500 Extrapolation 0.973 71.893 2.233 67.516 76.270 400 meanPD
                1 1500 Rarefaction 0.928 5.224 0.103 5.021 5.426 400 meanPD
                1 3500 Extrapolation 0.973 5.320 0.105 5.115 5.526 400 meanPD
      Edge
4
      Edge
                 2 1500 Rarefaction 0.928 1.797 0.024 1.749
                                                              1.844
                                                                       400 meanPD
                                                       1.749
                 2 3500 Extrapolation 0.973 1.797 0.024
                                                              1.845
                                                                       400 meanPD
   Interior
                0 1500 Rarefaction 0.922 63.555 0.917 61.758 65.353 400 meanPD
8 Interior
                0 3500 Extrapolation 0.965 78.004 1.749 74.576 81.431 400 meanPD
                1 1500 Rarefaction 0.922 5.675 0.113 5.454 5.896 400 meanPD
10 Interior
                1 3500 Extrapolation 0.965 5.784 0.114 5.560 6.008 400 meanPD
                2 1500 Rarefaction 0.922 1.913 0.032 1.851 1.976 400 meanPD 2 3500 Extrapolation 0.965 1.914 0.032 1.852 1.977 400 meanPD
11 Interior
```

# Example 8b: PD for incidence data with two target coverage values (97.5% and 99%)

The following commands return the PD estimates with two specified levels of sample coverage (97.5% and 99%) for the Fish\_incidence\_data.

```
Assemblage Order.q
                                      Method qPD s.e. qPD.LCL qPD.UCL Reftime Type
1 2013-2015 0 0.975 29.169 Rarefaction 9.672 0.381 8.926 10.419 0.9770115 meanPD
2 2013-2015
                 0 0.990 58.667 Extrapolation 10.018 0.616 8.810 11.226 0.9770115 meanPD
   2013-2015
                 1 0.975 29.169 Rarefaction 7.612 0.149 7.320 1 0.990 58.667 Extrapolation 7.680 0.147 7.393
                                                                    7.905 0.9770115 meanPD
   2013-2015
                                                                    7.967 0.9770115 meanPD
                  2 0.975 29.169 Rarefaction 7.003 0.147 6.715 7.290 0.9770115 meanPD
   2013-2015
                 2 0.990 58.667 Extrapolation 7.030 0.146 6.745 7.315 0.9770115 meanPD
6 2013-2015
                 0 0.975 34.825 Rarefaction 9.646 0.464 8.737 10.556 0.9770115 meanPD
7 2016-2018
8 2016-2018
                 0 0.990 76.971 Extrapolation 9.831 0.896 8.075 11.587 0.9770115 meanPD
   2016-2018
                  1 0.975 34.825 Rarefaction 7.779 0.130 7.524 8.033 0.9770115 meanPD
10 2016-2018
11 2016-2018
12 2016-2018
                                                            7.561
                   1 0.990 76.971 Extrapolation 7.835 0.140
                                                                    8.109 0.9770115 meanPD
                   2 0.975 34.825 Rarefaction 7.201 0.121
                                                            6.963
                                                                    7.439 0.9770115 meanPD
                 2 0.990 76.971 Extrapolation 7.224 0.124 6.982 7.466 0.9770115 meanPD
```

# **FUNCTIONAL DIVERSITY (FD): point estimation**

# Example 9a: FD for abundance data with two target coverage values (93% and 97%)

The following commands return the FD estimates with two specified levels of sample coverage (93% and 97%) for the Brazil rainforest abun\_data.

```
data(Brazil_rainforest_abun_data)
```

```
Assemblage Order.q SC m
                                               qFD s.e. qFD.LCL qFD.UCL
                                       Method
   Edge 0 0.93 1547.562 Rarefaction 17.590 2.069 13.534 21.645
Edge 0 0.97 3261.971 Extrapolation 18.578 2.740 13.207 23.949
2
3
       Edge
                 1 0.93 1547.562 Rarefaction 11.732 0.311 11.123 12.341
      Edge
                1 0.97 3261.971 Extrapolation 11.920 0.313 11.307 12.534
5
      Edge
                2 0.93 1547.562 Rarefaction 9.120 0.261 8.609 9.632
       Edge
                2 0.97 3261.971 Extrapolation 9.183 0.264 8.665 9.701
6
   Interior
                  0 0.93 1699.021 Rarefaction 16.890 1.820 13.324 20.457
   Interior
8
                 0 0.97 3883.447 Extrapolation 17.839 4.980
                                                           8.079 27.599
                 1 0.93 1699.021 Rarefaction 9.668 0.258 9.161 10.175
   Interior
9
                1 0.97 3883.447 Extrapolation 9.834 0.275 9.294 10.374
10 Interior
11 Interior
                2 0.93 1699.021 Rarefaction 6.994 0.160 6.680 7.308
                2 0.97 3883.447 Extrapolation 7.033 0.162 6.716 7.350
12 Interior
```

# Example 9b: FD for incidence data with two target number of sampling units (30 and 70)

The following commands return the FD estimates with two specified levels of sample sizes (30 and 70) for the Fish\_incidence\_data.

```
Assemblage Order.q mT Method
                                          qFD s.e. qFD.LCL qFD.UCL
                                    SC
1 2013-2015 0 30 Rarefaction 0.976 17.748 0.519 16.730 18.766
2 2013-2015
                0 70 Extrapolation 0.993 18.550 0.696 17.186 19.914
3 2013-2015
                1 30 Rarefaction 0.976 15.929 0.314 15.314 16.545
4 2013-2015
                1 70 Extrapolation 0.993 16.006 0.315 15.388 16.624
  2013-2015
2013-2015
2016-2018
                2 30 Rarefaction 0.976 15.459 0.277 14.915 16.003
5
                 2 70 Extrapolation 0.993 15.477 0.278 14.932
                0 30 Rarefaction 0.972 17.503 0.562 16.401 18.606
8 2016-2018
                0 70 Extrapolation 0.988 18.705 1.207 16.340 21.070
9 2016-2018
                1 30 Rarefaction 0.972 15.729 0.371 15.001 16.457
                1 70 Extrapolation 0.988 15.816 0.364 15.103 16.530
10 2016-2018
11 2016-2018
               2 30 Rarefaction 0.972 15.268 0.386 14.512 16.025
12 2016-2018
                 2 70 Extrapolation 0.988 15.290 0.386 14.533 16.046
```

# FUNCTION ObsAsy3D: ASYMPTOTIC AND OBSERVED DIVERSITY PROFILES

All arguments in the above function are the same as those for the main function inext3D (except that the default of q here is seq(0, 2, 0.2)). The function ObsAsy3D() computes observed and asymptotic diversity of order q between 0 and 2 (in increments of 0.2) for 3D diversity; these 3D values with different order q can be used to depict a q-profile in the ggObsAsy3D function.

It also computes observed and asymptotic PD for various reference times by specifying the argument PDreftime; these PD values with different reference times can be used to depict a time-profile in the ggobsAsy3D function.

It also computes observed and asymptotic FD for various threshold tau levels by specifying the argument FDtau; these FD values with different threshold levels can be used to depict a tau-profile in the ggobsAsy3D function.

For each dimension, by default, both the observed and asymptotic diversity estimates will be computed.

# FUNCTION ggObsAsy3D(): GRAPHIC DISPLAYS OF DIVERSITY PROFILES

```
ggObsAsy3D(output, profile = "q")
```

ggobsAsy3D is a ggplot2 extension for an obsAsy3D object to plot 3D q-profile (which depicts the observed diversity and asymptotic diversity estimate with respect to order q) for q between 0 and 2 (in increments of 0.2).

It also plots time-profile (which depicts the observed and asymptotic estimate of PD or mean PD with respect to reference times when <code>diversity = "PD"</code> specified in the ObsAsy3D function), and tau-profile (which depicts the observed and asymptotic estimate of FD with respect to threshold level tau when <code>diversity = "FD"</code> and <code>FDtype = "tau\_values"</code> specified in the <code>ObsAsy3D</code> function) based on the output from the function <code>ObsAsy3D</code>.

In the plot of profiles, only confidence intervals of the asymptotic diversity will be shown when both the observed and asymptotic diversity estimates are computed.

# **TAXONOMIC DIVERSITY (TD): q-profiles**

## Example 10a: TD q-profiles for abundance data

9

10

Edge

The following commands returns the observed and asymptotic taxonomic diversity ('TD') for the <code>Brazil\_rainforest\_abun\_data</code>, along with its confidence interval for diversity order q between 0 to 2. Here only the first ten rows of the output are shown.

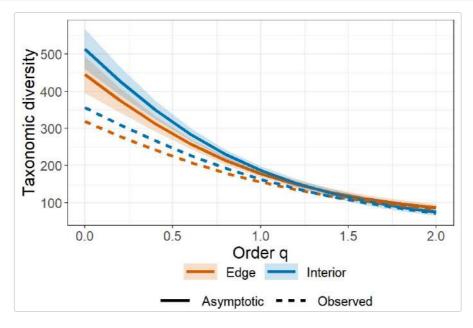
```
data(Brazil_rainforest_abun_data)
output ObsAsy_TD_abun <- ObsAsy3D(Brazil_rainforest_abun_data, diversity = 'TD',</pre>
                                     datatype = "abundance")
output ObsAsy TD abun
   Assemblage Order.q qTD s.e. qTD.LCL qTD.UCL
      Edge 0.0 444.971 25.175 395.629 494.314 Asymptotic
2
        Edge 0.2 375.270 16.678 342.582 407.958 Asymptotic
        Edge 0.4 312.452 10.496 291.880 333.024 Asymptotic
3
       Edge 0.6 258.379 6.878 244.900 271.859 Asymptotic Edge 0.8 213.730 5.445 203.057 224.403 Asymptotic Edge 1.0 178.000 5.138 167.930 188.069 Asymptotic
5
6
        Edge 1.2 149.914 5.123 139.874 159.955 Asymptotic
8
       Edge 1.4 127.945 5.135 117.879 138.010 Asymptotic
```

The following commands plot the corresponding q-profiles, along with its confidence interval for q between 0 to 2.

Edge 1.6 110.672 5.139 100.599 120.745 Asymptotic

1.8 96.948 5.137 86.880 107.016 Asymptotic

```
# q-profile curves
ggObsAsy3D(output_ObsAsy_TD_abun)
```



### Example 10b: TD q-profiles for incidence data

Fish\_incidence\_data, along with its confidence interval for diversity order q between 0 to 2. Here only the first ten rows of the output are shown.

```
Assemblage Order.q qTD s.e. qTD.LCL qTD.UCL Method

1 2013-2015 0.0 59.803 9.908 40.384 79.223 Asymptotic

2 2013-2015 0.2 50.828 5.806 39.449 62.207 Asymptotic

3 2013-2015 0.4 43.790 3.281 37.359 50.221 Asymptotic

4 2013-2015 0.6 38.458 1.911 34.713 42.204 Asymptotic

5 2013-2015 0.8 34.490 1.248 32.044 36.936 Asymptotic

6 2013-2015 1.0 31.542 0.947 29.685 33.398 Asymptotic

7 2013-2015 1.2 29.328 0.803 27.754 30.902 Asymptotic

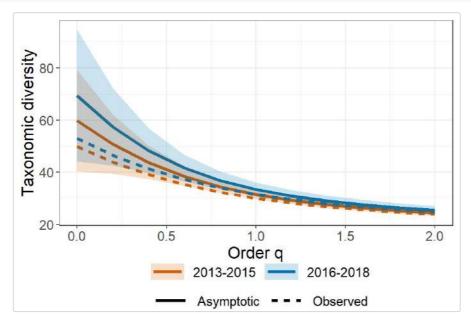
8 2013-2015 1.4 27.635 0.724 26.217 29.053 Asymptotic

9 2013-2015 1.6 26.312 0.673 24.992 27.632 Asymptotic

10 2013-2015 1.8 25.255 0.639 24.002 26.509 Asymptotic
```

The following commands plot the corresponding q-profiles, along with its confidence interval for q between 0 to 2.

```
# q-profile curves
ggObsAsy3D(output_ObsAsy_TD_inci)
```



# PHYLOGENETIC DIVERSITY (PD): time-profiles and q-profiles

## Example 11a: PD time-profiles for abundance data

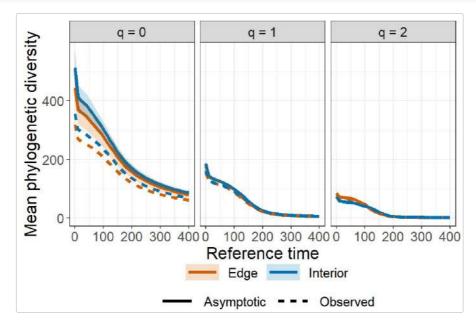
The following commands return the observed and asymptotic phylogenetic diversity ('PD') estimates for the  $Brazil\_rainforest\_abun\_data$ , along with its confidence interval for diversity order q = 0, 1, 2 under reference times from 0.01 to 400 (tree height). Here only the first ten rows of the output are shown.

```
Method Reftime Type
  Assemblage Order.q
                      qPD s.e. qPD.LCL qPD.UCL
     Edge 0 444.971 29.001 388.130 501.812 Asymptotic 0.100 meanPD
                  1 178.000 5.074 168.055 187.944 Asymptotic 0.100 meanPD
        Edge
2
                 2 85.905 4.149 77.773 94.038 Asymptotic 0.100 meanPD
       Edge
3
   Interior
                 0 513.518 29.215 456.256 570.779 Asymptotic 0.100 meanPD
5
                 1 186.983 5.190 176.812 197.154 Asymptotic 0.100 meanPD
   Interior 2 74.718 4.210 66.466 82.969 Asymptotic 0.100 meanPD Edge 0 371.100 25.520 321.082 421.117 Asymptotic 10.354 meanPD
6
   Edge 1 141.418 3.841 133.891 148.946 Asymptotic 10.354 meanPD
```

```
9 Edge 2 72.848 3.260 66.458 79.238 Asymptotic 10.354 meanPD 10 Interior 0 413.568 22.401 369.663 457.472 Asymptotic 10.354 meanPD
```

The argument profile = "time" in the ggobsAsy3D function creates a separate plot for each diversity order q = 0, 1, and 2 with x-axis being "Reference time". Different assemblages will be represented by different color lines.

```
# time-profile curves
ggObsAsy3D(output_ObsAsy_PD_abun, profile = "time")
```



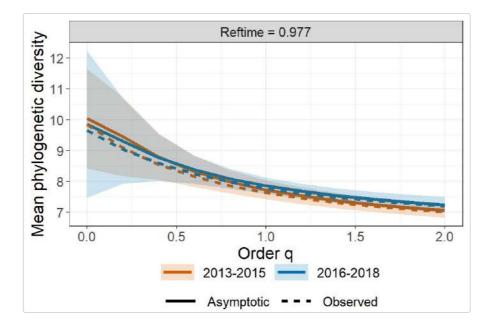
# Example 11b: PD q-profiles for incidence data

The following commands return the observed and asymptotic taxonomic diversity ('PD') estimates for the <code>Fish\_incidence\_data</code>, along with its confidence interval for diversity order q between 0 to 2. Here only the first ten rows of the output are shown.

```
Assemblage Order.q qPD s.e. qPD.LCL qPD.UCL Method Reftime Type
1 2013-2015 0.0 10.039 0.823 8.426 11.653 Asymptotic 0.977 meanPD
2 2013-2015 0.2 9.462 0.656 8.177 10.748 Asymptotic 0.977 meanPD
3 2013-2015 0.4 8.802 0.387 8.043 9.561 Asymptotic 0.977 meanPD
4 2013-2015 0.6 8.329 0.257 7.825 8.833 Asymptotic 0.977 meanPD
5 2013-2015 0.8 7.985 0.192 7.608 8.362 Asymptotic 0.977 meanPD
6 2013-2015 1.0 7.729 0.158 7.419 8.039 Asymptotic 0.977 meanPD
7 2013-2015 1.2 7.533 0.139 7.260 7.805 Asymptotic 0.977 meanPD
8 2013-2015 1.4 7.378 0.128 7.126 7.629 Asymptotic 0.977 meanPD
9 2013-2015 1.6 7.252 0.122 7.012 7.492 Asymptotic 0.977 meanPD
10 2013-2015 1.8 7.147 0.119 6.913 7.381 Asymptotic 0.977 meanPD
```

The following commands plot the corresponding q-profiles, along with its confidence interval for q between 0 to 2, for the default reference time = 0.977 (the tree depth).

```
# q-profile curves
ggObsAsy3D(output_ObsAsy_PD_inci, profile = "q")
```



# FUNCTIONAL DIVERSITY (FD): tau-profiles and q-profiles

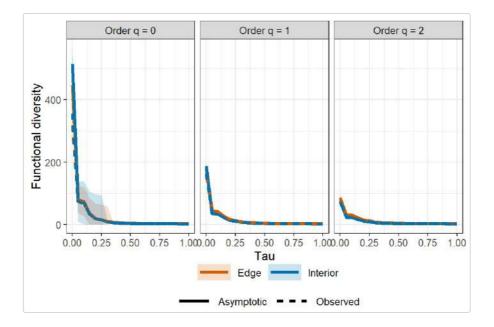
# Example 12a: FD tau-profiles for abundance data

The following commands returns observed and asymptotic functional diversity ('FD') for  ${\tt Brazil\_rainforest\_abun\_data}$ , along with its confidence interval at diversity order q = 0, 1, 2 under tau values from 0 to 1. Here only the first ten rows of the output are shown.

```
Assemblage Order.q qFD s.e. qFD.LCL qFD.UCL
                                                     Method Tau
       Edge 0 444.971 22.481 400.909 489.034 Asymptotic 0.00
                  1 178.000 5.377 167.461 188.538 Asymptotic 0.00
2
        Edge
       Edge
                2 85.905 4.471 77.143 94.668 Asymptotic 0.00
3
                 0 79.904 22.161 36.468 123.340 Asymptotic 0.05
       Edge
5
       Edge
                 1 45.187 1.216 42.804 47.569 Asymptotic 0.05
                  2 32.092 0.799 30.526 33.658 Asymptotic 0.05
       Edge
6
                  0 73.276 23.497 27.223 119.328 Asymptotic 0.10
1 42.200 1.137 39.972 44.427 Asymptotic 0.10
       Edge
8
        Edge
                2 30.182 0.683 28.843 31.521 Asymptotic 0.10
       Edge
9
                0 35.372 24.511 0.000 83.413 Asymptotic 0.15
10
       Edge
```

The following commands plot the corresponding tau-profiles, along with its confidence interval for diversity order q = 0, 1, 2.

```
# tau-profile curves
ggObsAsy3D(output_ObsAsy_FD_abun_tau, profile = "tau")
```



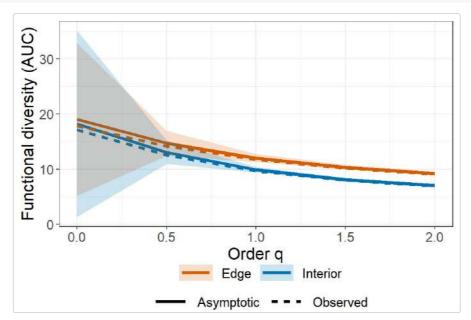
# Example 12b: FD q-profiles for abundance data

The following commands returns the observed and asymptotic taxonomic diversity ('FD') for the <code>Brazil\_rainforest\_abun\_data</code>, along with its confidence interval for diversity order q between 0 to 2 with <code>FDtype = 'AUC'</code>. Here only the first ten rows of the output are shown.

```
Assemblage Order.q $\operatorname{\mathsf{qFD}}$ s.e. \operatorname{\mathsf{qFD}}.\operatorname{\mathsf{LCL}} \operatorname{\mathsf{qFD}}.\operatorname{\mathsf{UCL}}
                                                              Method
      Edge 0.0 19.008 7.049 5.191 32.824 Asymptotic
Edge 0.5 14.698 1.144 12.456 16.941 Asymptotic
2
                    1.0 12.037 0.362 11.328 12.746 Asymptotic
        Edge
3
        Edge 1.5 10.345 0.233 9.889 10.802 Asymptotic
        Edge 2.0 9.228 0.189 8.857 9.600 Asymptotic
6
   Interior 0.0 18.208 8.615 1.322 35.094 Asymptotic
     Interior
                    0.5 13.071 1.076 10.963 15.179 Asymptotic
8
                    1.0 9.922 0.249 9.434 10.410 Asymptotic
     Interior 1.5 8.103 0.167 7.776 8.430 Asymptotic
9
10 Interior 2.0 7.055 0.143 6.776 7.335 Asymptotic
```

The following commands plot the corresponding q-profiles, along with its confidence interval for q between 0 to 2.

```
# q-profile curves
ggObsAsy3D(output_ObsAsy_FD_abun, profile = "q")
```



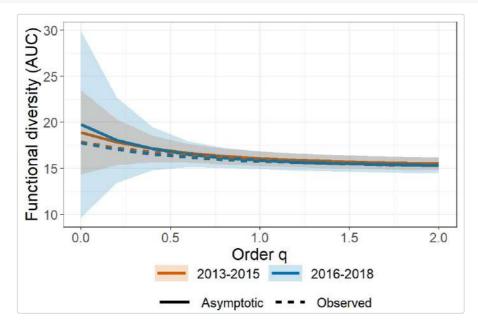
## Example 12c: FD q-profiles for incidence data

The following commands returns observed and asymptotic functional diversity ('FD') for Fish\_incidence\_data, along with its confidence interval at diversity order q from 0 to 2. Here only the first ten rows of the output are shown.

```
Assemblage Order.q qFD s.e. qFD.LCL qFD.UCL
 1
  2013-2015
           0.2 17.826 1.264 15.348 20.303 Asymptotic
2
3
  2013-2015
           0.4 17.115 0.736 15.673 18.557 Asymptotic
  2013-2015
           0.6 16.624 0.518 15.609 17.639 Asymptotic
4
  5
  2013-2015 1.0 16.043 0.401 15.257 16.828 Asymptotic
  2013-2015 1.2 15.868 0.383 15.117 16.618 Asymptotic
8
  2013-2015 1.4 15.736 0.372 15.007 16.466 Asymptotic
  9
           1.8 15.555 0.360 14.849 16.262 Asymptotic
10 2013-2015
```

The following commands plot the corresponding q-profiles, along with its confidence interval for q between 0 to 2.

```
# q-profile curves
ggObsAsy3D(output_ObsAsy_FD_inci, profile = "q")
```



#### License

The iNEXT.3D package is licensed under the GPLv3. To help refine iNEXT.3D, your comments or feedback would be welcome (please send them to Anne Chao or report an issue on the iNEXT.3D github iNEXT.3D github.

#### References

- Chao, A., Henderson, P. A., Chiu, C.-H., Moyes, F., Hu, K.-H., Dornelas, M. and Magurran, A. E. (2021).
   Measuring temporal change in alpha diversity: a framework integrating taxonomic, phylogenetic and functional diversity and the iNEXT.3D standardization. Methods in Ecology and Evolution, 12, 1926-1940.
- Hsieh, T. C., Ma, K-H, and Chao, A. (2016). iNEXT: An R package for rarefaction and extrapolation of species diversity (Hill numbers). Methods in Ecology and Evolution, 7, 1451-1456.

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