

dataprep

Lauren Olinger

9/30/2023

Loading Necessary Libraries

```
library(readr)
```

```
## Warning: package 'readr' was built under R version 4.1.2
```

```
library(plyr)
```

```
## Warning: package 'plyr' was built under R version 4.1.2
```

```
library(vegan)
```

```
## Warning: package 'vegan' was built under R version 4.1.2
```

```
## Loading required package: permute
```

```
## Warning: package 'permute' was built under R version 4.1.2
```

```
## Loading required package: lattice
```

```
## This is vegan 2.6-2
```

```
library(ggplot2)
```

```
library(pairwiseAdonis)
```

```
## Loading required package: cluster
```

```
library(dplyr)
```

```
## Warning: package 'dplyr' was built under R version 4.1.2
```

```
##
```

```
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:plyr':
```

```
##
```

```
##      arrange, count, desc, failwith, id, mutate, rename, summarise,
```

```
##      summarize
```

```
## The following objects are masked from 'package:stats':
```

```
##
```

```
##      filter, lag
```

```
## The following objects are masked from 'package:base':
```

```
##
```

```
##      intersect, setdiff, setequal, union
```

Data Import

We are importing three CSV files, each corresponding to a different genetic marker (16S, 18S, and CO1). Another dataset (origdeltadat) containing sample information is also imported.

```
s16s <- read_csv("input/16S ESV Taxonomy Sequence Table (no tissue).csv")

## Rows: 33820 Columns: 49
## -- Column specification -----
## Delimiter: ","
## chr (9): hash, sequence, kingdom, phylum, class, order, family, genus, species
## dbl (40): ST 1-18, ST 2-18, ST 3-18, ST 4-18, ST 5-18, SS 1-18, SS 2-18, SS ...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.

s18s <- read_csv("input/18S ESV Taxonomy Sequence Table (no tissue).csv")

## Rows: 18640 Columns: 51
## -- Column specification -----
## Delimiter: ","
## chr (9): hash, sequence, kingdom, phylum, class, order, family, genus, species
## dbl (42): ST 1-18, ST 2-18, ST 3-18, ST 4-18, ST 5-18, SS 1-18, SS 2-18, SS ...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.

sCOI <- read_csv("input/CO1 ESV Taxonomy Sequence Table (no tissue).csv")

## Rows: 3126 Columns: 49
## -- Column specification -----
## Delimiter: ","
## chr (9): hash, sequence, kingdom, phylum, class, order, family, genus, species
## dbl (40): ST 1-18, ST 2-18, ST 3-18, ST 4-18, ST 5-18, SS 1-18, SS 2-18, SS ...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.

origdeltadat <- read_csv("input/sampleinfodelta_4july.csv")

## Rows: 186 Columns: 28
## -- Column specification -----
## Delimiter: ","
## chr (19): category, sample type, species, spp code, samplespp, sample note, ...
## dbl (9): Index, Year, Sample Mass (mg), sample mass (mg) acidified, Carbon ...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

Data Manipulation

We add a new column named “marker” to each of the three genetic marker dataframes to identify the source of the data. The three datasets are then combined into one dataframe (seqdat_all). To achieve this, the columns of each dataset are reordered to match a common order, after which the datasets are concatenated.

```
#make new dataframe "seqdat_all" that combines the top three markers, also adding a column for "marker"
s16s <- cbind(marker = rep('16s', nrow(s16s)), s16s)
s18s <- cbind(marker = rep('18s', nrow(s18s)), s18s)
```

```

sCOI <- cbind(marker = rep("COI", nrow(sCOI)), sCOI)

#column list from the three csus (they dont match up across the markers so have to xref)
newcols <- unique(c(colnames(s16s), colnames(sCOI), colnames(s18s)))

#preallocate the dataframe & set colnames
seqdat_all <-
  data.frame(matrix(
    ncol = length(newcols),
    nrow = c(nrow(s16s) + nrow(s18s) + nrow(sCOI))
  ))
colnames(seqdat_all) <- newcols

#reordering colnames of seqdat, s16s, s18s, sCOI, so they match up
reorddat<- function(colname,dfname){
  dfname2 <- dfname[,1:which(colnames(dfname) == colname)]
  dfnametoReord <- dfname[,c((which(colnames(dfname) == colname)+1):ncol(dfname))]
  dfnametoReord <- dfnametoReord[,order(colnames(dfnametoReord))]
  dfname3 <- cbind(dfname2, dfnametoReord)
  return(dfname3)
}

seqdat_all <- reorddat("species",seqdat_all)
s16s <- reorddat("species",s16s)
s18s <- reorddat("species",s18s)
sCOI <- reorddat("species",sCOI)

#populate seqdat_all
seqdat_all[1:nrow(sCOI), which(colnames(seqdat_all) %in% colnames(sCOI))] <-
  sCOI
seqdat_all[(nrow(sCOI) + 1):(nrow(sCOI) + nrow(s16s)), which(colnames(seqdat_all) %in% colnames(s16s))] <-
  s16s
seqdat_all[(nrow(sCOI) + nrow(s16s) + 1):(nrow(seqdat_all)), which(colnames(seqdat_all) %in% colnames(s18s))] <-
  s18s

seqdat_all[which(is.na(seqdat_all),arr.ind = T)] <- 0
newcols <- colnames(seqdat_all)

# get the info part from seqdat_all so can tack on to subsetted pieces later
seqdat_info <- seqdat_all[,1:which(colnames(seqdat_all) == "species")]

#crossref sample names with the years/ groups/categories from origdeltadat,
#note: deltadat_all includes delta values- this is where could come back and pull those from if want
deltadat_all <-
  origdeltadat[which(origdeltadat$ednacode %in% newcols[grepl("-", newcols)]), ]

#remove stuff
rm(s16s, s18s, sCOI, newcols, origdeltadat)

```

Taxonomic Level Summarization

The data is summarized at different taxonomic levels such as kingdom, phylum, class, order, family, genus, and species. The data is further aggregated at the kingdom-phylum (kp), kingdom-phylum-class-order (kpco),

and species-level resolution.

```
#functions needed to summarize (may not use max)
aggFunctionSum <- function(dataframe, toAverage, toGroup) {
  aggregate(dataframe[, toAverage], dataframe[, toGroup], sum)
}

#sample names for later agg function
seqcolnames <- colnames(seqdat_all)[c((which(colnames(seqdat_all) == "species")+1):ncol(seqdat_all))]

seqdat_all$kingdom[which(seqdat_all$kingdom=="0")]<- "K"
seqdat_all$phylum[which(seqdat_all$phylum=="0")]<- "P"
seqdat_all$class[which(seqdat_all$class=="0")]<- "C"
seqdat_all$order[which(seqdat_all$order=="0")]<- "O"
seqdat_all$family[which(seqdat_all$family=="0")]<- "F"
seqdat_all$genus[which(seqdat_all$genus=="0")]<- "G"
seqdat_all$species[which(seqdat_all$species=="0")]<- "S"

#seqdat_kpcofgs = kingdom/phylum/class/order/fam/genus/species
seqdat_kpcofgs <- cbind(
  kingdom = seqdat_all$kingdom,
  phylum = seqdat_all$phylum,
  class = seqdat_all$class,
  order = seqdat_all$order,
  family = seqdat_all$family,
  genus = seqdat_all$genus,
  species = seqdat_all$species,
  seqdat_all[,c((which(colnames(seqdat_all) == "species")+1):ncol(seqdat_all))]
)

#kp - for nice overview tables
seqdat_kp <- aggFunctionSum(seqdat_kpcofgs, seqcolnames, c("kingdom", "phylum"))

#kpco - for matching to multivariate
seqdat_kpco <- aggFunctionSum(seqdat_kpcofgs, seqcolnames, c("kingdom", "phylum", "class", "order"))

#seqdat_kpcofgs - for species-level resolution, where species are identified
seqdat_kpcofgs <- aggFunctionSum(seqdat_kpcofgs, seqcolnames, c("kingdom", "phylum", "class", "order", "family", "genus", "species"))
```

Sample Type Matrix Creation

A matrix containing different sample types and categories, with sample counts (ns), is created.

```
#make list of all groups care about
group_df <- ddply(
  deltatad_all, ~category*`sample type`*samplespp*Year, summarise,
  n = length(ednacode))
```

Functions

We define a set of helper functions for subsetting, calculating frequency, and plotting.

```
# basic subsetting and xrefing to deltatad_all to keep samplenames consistent
subset_seq <- function(type, year, seqvar) {
  sampleinfordeltatemp <-
```

```

      deltadat_all[which(deltadat_all$samplespp == type &
                        deltadat_all$Year == year),]
sND18 <-
  seqvar[, which(colnames(seqvar) %in% sampleinfodeltatemp$ednacode)]
return(sND18)
}

# calculate frequency of occurrence = number of samples ESV for a given taxa was found in, divided by t
calcFoo <- function(type, year, seqvar){
  sampleinfodeltatemp <-
    deltadat_all[which(deltadat_all$samplespp == type &
                      deltadat_all$Year == year),]
  sND18 <- seqvar[, which(colnames(seqvar) %in% sampleinfodeltatemp$ednacode)]
  # sND18 <- rowSums(sND18 != 0)/ncol(sND18)
  sND18 <- rowSums(sND18 != 0)
  return(sND18)
}

# ellipsess in nmfs
veganCovEllipse <- function (cov, center = c(0, 0), scale = 1, npoints = 100)
{
  theta <- (0:npoints) * 2 * pi/npoints
  Circle <- cbind(cos(theta), sin(theta))
  t(center + scale * t(Circle %*% chol(cov)))
}

```

Saving Data and Cleanup

Finally, the current R environment is saved for future use and all temporary objects are removed to free up memory.

```

save.image("preppeddata.RData")
graphics.off()
gc()

##          used  (Mb) gc trigger  (Mb) limit (Mb) max used  (Mb)
## Ncells 2232170 119.3   4432914 236.8      NA  3174138 169.6
## Vcells 9621187  73.5   23596091 180.1    65536 23596045 180.1

rm(list=ls())

```