Supplement to: On the inference of positive and negative species interactions and their relation to abundance

Andrew J. Rominger

This supplement combines a narrative account of how to reproduce the results in the main text as well as additional analyses in support of the conclusions in the main text.

S1 Reproducibility

The results of this study can be fully reproduced by installing the package RarePlusComMinus (available on GitHub) written in \mathbb{R}^1 . Installation requires the package $devtools^2$:

```
dt <- require(devtools)
if(!dt) {
   install.packages('devtools')
   library(devtools)
}

thisPack <- require(RarePlusComMinus)
if(!thisPack) install_github('ajrominger/RarePlusComMinus')</pre>
```

Two additional custom packages are required, $socorro^3$ for plotting, and $pika^4$ for simulating and analyzing species abundance distributions (SAD):

```
socorroLoad <- require(socorro)
if(!socorroLoad) install_github('ajrominger/socorro')

pikaLoad <- require(pika)
if(!pikaLoad) install_github('ajrominger/pika')</pre>
```

All other required packages^{5–8} are installed with the installation of RarePlusComMinus. The RarePlus-ComMinus package includes documented⁹ and unit-tested¹⁰ functions to carry out all analyses. The help documentation explains these functions, for example

```
?plusMinus
?schoener
```

Now we can set-up our analysis.

```
library(RarePlusComMinus)
library(pika)
library(socorro)
library(parallel)
library(viridis)

# we can now set caching to be TRUE by default
knitr::opts_chunk$set(cache = TRUE)

# threading defaults
nthrd <- detectCores()
nthrd <- ifelse(round(nthrd * 0.8) >= nthrd - 1, nthrd - 1, round(nthrd * 0.8))
if(nthrd < 1) nthrd <- 1</pre>
```

```
# plotting defaults
parArgs <- list(mar = c(3, 3, 0, 0) + 0.5, mgp = c(1.5, 0.30, 0), tcl = -0.25)
cexDefault <- 1.4
lwdDefault <- 2
figW <- 3.75
figH <- 3.75
kmitr::opts_chunk$set(fig.width = figW, fig.height = figH, fig.align = 'center')</pre>
```

S2 Reproducing the results of Calatayud et al.

First we reproduce some of the key results of Calatayuda *et al.* $(CEA)^{11}$, namely how abundances relate to positive and negative association networks. To do this we first process the data from CEA which I include as data in the RarePlusComMinus package; more information about the data can be accessed through the R help document via ?abundMats.

```
# load data from paper
data('abundMats')

# clean it
obsdat <- lapply(abundMats, function(x) {
    x <- ceiling(x)
    x <- x[rowSums(x) > 0, colSums(x) > 0]

    return(x)
})
```

Now we use the plusMinus function to calculate positive and negative association networks and abundances from the observed data. Internally, this function produces B (default B = 999) randomly permuted matrices using the r2dtable algorithm¹² that fixes row and column marginals. It then compares the Schoener similarities from the original and permuted matrices. I use the custom function schoener (made to be more efficient) to compute these similarities, and this function is unit tested against spaa::niche.overlap.

The plusMinus function is based on, but not copied from, the function used by CEA in their analyses and made available by the authors at https://figshare.com/articles/Positive_associations_among_rare_species_and_their_persistence_in_ecological_assemblages/9906092. The new plusMinus function is streamlined to be faster and thus able to be applied to many more simulations. It is unit tested against the CEA's original function.

It should be noted that CEA retained 326 studies after filtering, whereas I retain 299. This is because I removed any dataset for which there were fewer than three links in either the positive or negative networks, whereas CEA removed only those datasets with fewer than two links¹¹.

I use these calculations to make Supplementary Figure 1, which reproduce Figure 2 (B-C) from CEA.

```
# ----
# helper function for making fancy histograms
```

```
specialHist <- function(x, breaks, col, add = FALSE, ...) {</pre>
    h <- hist(x, breaks, plot = FALSE)
    if(!add) plot(range(h$breaks), range(h$counts), type = 'n', ...)
    rect(xleft = h$breaks[-length(h$breaks)], xright = h$breaks[-1],
         ybottom = 0, ytop = h$counts, col = col)
}
# helper function for labeling subfigures
figLetter <- function(1, lab, bg = 'transparent', cex = 1, ...) {</pre>
    legend('topleft', legend = lab, bg = bg, box.col = 'transparent',
           x.intersp = 0, y.intersp = 0.25, adj = c(0.5, 0.5), cex = cex, ...)
}
# function to remake Fig 2(b-c)
fig2bc <- function(x, breaksRho, breaksWM, addxlab = TRUE, figLabs = LETTERS[1:2],</pre>
                    insetxprop = 0.5, insetyprop = 0.5) {
    # ----
    # relative bounds for inset figures
    insetxMax <- 0.975</pre>
    insetxMin <- insetxMax - insetxprop</pre>
    insetyMax <- 0.975
    insetyMin <- insetyMax - insetyprop</pre>
    # set up plot
    plot.new()
    par(parArgs)
    par(cex = 1)
    # ----
    # split into two main plots and fill in
    fi <- split.screen(c(1, 2), erase = FALSE)</pre>
    # correlation differences
    screen(fi[1], new = FALSE)
    par(parArgs)
    if(addxlab) {
        par(mar = parArgs\$mar + c(0, 0, 0, -0.5))
        xlab <- 'Abundance-species degree differences\n(positive - negative)'</pre>
        par(mar = parArgs\$mar + c(-2.25, 0, 0, -0.5))
        xlab <- ''
    }
    specialHist(x$pos.rho.rho - x$neg.rho.rho, xlim = c(-2, 2),
```

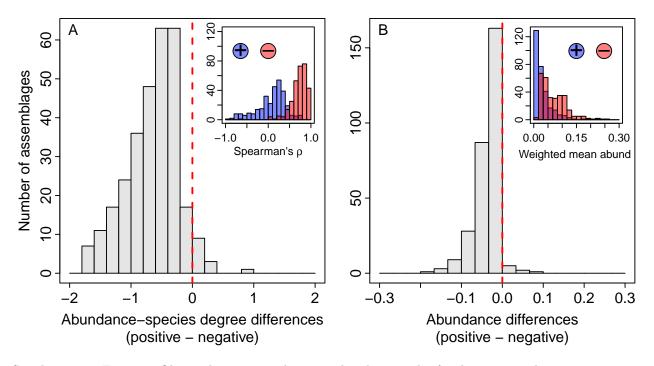
```
breaks = breaksRho, col = 'gray90',
            xlab = '', ylab = 'Number of assemblages')
mtext(xlab, side = 1, line = 2.5)
abline(v = 0, col = 'red', lty = 2, lwd = 2)
figLetter('topleft', figLabs[1])
# raw correlations
fj <- split.screen(matrix(c(insetxMin + 0.02, insetxMax + 0.02,
                             insetyMin, insetyMax), nrow = 1),
                    erase = FALSE)
screen(fj, new = FALSE)
par(parArgs)
par(cex = 0.75)
par(mgp = par('mgp') * par('cex'))
rhoYmax <- 90
rhoFmax <- max(hist(x$pos.rho.rho, breaks = breaksRho / 2, plot = FALSE)$counts,</pre>
               hist(x$neg.rho.rho, breaks = breaksRho / 2, plot = FALSE)$counts)
if(0.75 * rhoYmax < rhoFmax + 0.1 * rhoYmax) {
    rhoYmax <- 1.35 * rhoYmax</pre>
}
specialHist(x$pos.rho.rho, xlim = c(-1, 1), ylim = c(0, rhoYmax),
            breaks = breaksRho / 2, col = hsv(0.65, alpha = 0.5),
            xlab = expression("Spearman's"~rho),
            ylab = '')
specialHist(x$neg.rho.rho,
            breaks = breaksRho / 2, col = hsv(0, alpha = 0.5),
            add = TRUE)
usr <- par('usr')</pre>
points(usr[1] + c(0.2, 0.5) * diff(usr[1:2]), rep(usr[3] + 0.75 * diff(usr[3:4]), 2),
       cex = 3, bg = hsv(c(0.65, 0), alpha = 0.5), <math>pch = 21)
text(usr[1] + c(0.2, 0.5) * diff(usr[1:2]), rep(usr[3] + 0.75 * diff(usr[3:4]), 2),
     labels = c('+', '-'), cex = 2)
# mean differences
screen(fi[2])
par(parArgs)
if(addxlab) {
    par(mar = parArgs\$mar + c(0, -1, 0, +0.5))
    xlab <- 'Abundance differences\n(positive - negative)'</pre>
} else {
    par(mar = parArgs\$mar + c(-2.25, -1, 0, +0.5))
    xlab <- ''
specialHist(x$pos.wm - x$neg.wm, xlim = c(-0.3, 0.3),
            breaks = breaksWM, col = 'gray90',
```

```
xlab = '', ylab = '')
    mtext(xlab,
          side = 1, line = 2.5)
    abline(v = 0, col = 'red', lty = 2, lwd = 2)
    figLetter('topleft', figLabs[2])
    # raw means
    fk <- split.screen(matrix(c(insetxMin - 0.04, insetxMax - 0.04,
                                 insetyMin, insetyMax), nrow = 1),
                         erase = FALSE)
    screen(fk, new = FALSE)
    par(parArgs)
    par(cex = 0.75)
    par(mgp = par('mgp') * par('cex'))
    specialHist(x$pos.wm, xlim = c(0, 0.3),
                breaks = (breaksWM + 0.3) / 2, col = hsv(0.65, alpha = 0.5),
                xlab = 'Weighted mean abund.',
                ylab = '')
    specialHist(x$neg.wm,
                breaks = (breaksWM + 0.3) / 2, col = hsv(0, alpha = 0.5),
                add = TRUE)
    usr <- par('usr')</pre>
    points(usr[1] + (1 - c(0.5, 0.2)) * diff(usr[1:2]),
           rep(usr[3] + 0.75 * diff(usr[3:4]), 2),
           cex = 3, bg = hsv(c(0.65, 0), alpha = 0.5), <math>pch = 21)
    text(usr[1] + (1 - c(0.5, 0.2)) * diff(usr[1:2]),
           rep(usr[3] + 0.75 * diff(usr[3:4]), 2),
         labels = c('+', '-'), cex = 2)
    foo <- close.screen(c(fi, fj, fk))</pre>
    invisible(NULL)
fig2bc(commStats, breaksRho = seq(-2, 2, by = 1/5),
       breaksWM = seq(-0.3, 0.3, by = 0.1/3))
foo <- close.screen(all.screens = TRUE)</pre>
```

It should be noted that my inset plot of mean weighted abundances (Supplementary Fig. 1 B) differs from CEA Figure 2C in that their y-axis ranges from 0 to 220, while mine ranges from 0 to 120. I suspected the original authors mislabeled their axis, because the scale as presented would suggest over 600 assemblages, while the number should be 326. Re-scaling their axis to range from 0 to 120 brings the rough estimate from their figure more in line with the reported number of assemblages.

S3 Exploring patterns of species abundance across space

Now we explore the shape of the spatial species abundance distributions (SSADs) in the real data provided by CEA¹¹. The main function we use is nbFit from the *RarePlusComMinus* package which calculates summary statistics about the negative binomial and Poisson fits to SSAD data.



Supplementary Figure 1: Observed association between abundance and infered positive and negative interactions, reproducing Figure 2(B-C) from CEA. This figure is also found in the main text and discussed further there.

In Supplementary Figure 2 I show that the data are well fit by the negative binomial via a likelihood-based goodness of fit $test^{13,14}$. This test scales the observed likelihood by the sampling distribution of likelihoods given the hypothesis that the negative binomial is the correct distribution. This test statistic, when squared, follows a χ -squared distribution with 1 degree of freedom¹⁴, allowing us to make a parametric cutoff of when the data are not well represented by a negative binomial. No assemblage analyzed rejected the negative binomial distribution. In Supplementary Figure 2 I also explore the relationship of the clustering parameter k with species relative abundance. The purpose of this later analysis is to be able to simulate random but realistic data.

```
# limit to only those communities that yielded meaningful networks
summStats <- mclapply(obsdat[rownames(commStats[!is.na(commStats$pos.n), ])],</pre>
                       mc.cores = nthrd, FUN = function(x) {
    nbInfo <- nbFit(x)</pre>
    cbind(nsite = nrow(x), nspp = ncol(x), J = sum(x), nbInfo)
})
summStats <- data.frame(study = rep(rownames(commStats[!is.na(commStats$pos.n), ]),</pre>
                                      sapply(summStats, nrow)),
                         do.call(rbind, summStats))
# data for linear model of k, excluding sites that didn't produce a good network
dat4k <- with(summStats[summStats$study %in%</pre>
                             rownames(commStats[!is.na(commStats$pos.n), ]) &
                             is.finite(summStats$size), ],
              data.frame(logk = log(size),
                          loga = log(abund / J),
                          logS = log(nspp))
)
```

```
kMod <- lm(logk ~ loga, data = dat4k)</pre>
kfun <- function(nspp, abund) {</pre>
    J <- sum(abund)
    exp(predict(kMod, newdata = data.frame(loga = log(abund / J))) +
            rnorm(nspp, sd = summary(kMod)$sigma))
layout(matrix(1:2, nrow = 1))
par(parArgs)
plot(summStats$abund, summStats$z, log = 'xy',
     ylim = range(summStats$z, qchisq(0.999, 1)),
     xaxt = 'n', yaxt = 'n',
     xlab = 'Abundance', ylab = expression('Goodness of fit '~z^2))
logAxis(1:2, expLab = TRUE)
abline(h = qchisq(0.95, 1), col = 'red', lwd = 2)
figLetter('topleft', 'A', bg = 'white')
box()
plot(summStats$abund / summStats$J, summStats$size, log = 'xy', xaxt = 'n', yaxt = 'n',
     xlab = 'Relative abundance', ylab = expression(k))
curve(kMod$coefficients[1] * x^kMod$coefficients[2], col = hsv(0.56, 0.6, 0.8),
      lwd = 2, add = TRUE)
logAxis(1:2, expLab = TRUE)
figLetter('topleft', 'B')
```

S4 Exploring the species abundance distribution

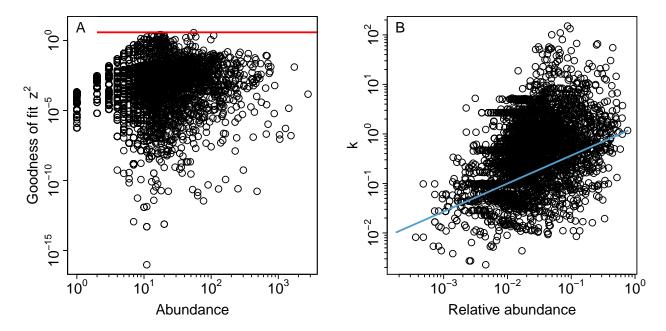
We also need to know the shapes of the species abundance distributions (SAD) of each assemblage to simulate realistic data. I do this using the function fitSAD from the custom *pika* package. I preform model selection on three standard SAD forms: the log-series, Poisson log-normal, and zero-truncated negative binomial, and record the best fit model and its parameter(s) for each assemblage.

```
mods <- c('fish', 'plnorm', 'tnegb')
sadStats <- mclapply(obsdat, mc.cores = nthrd, FUN = function(x) {
    nsite <- nrow(x)
    x <- colSums(x)
    s <- fitSAD(x, mods)

    i <- which.min(sapply(s, AIC))
    o <- s[[i]]$MLE
    if(i == 1) o <- c(o, NA)

    o <- c(i, o, sum(x), length(x), nsite)
    names(o) <- NULL

    return(o)
})
sadStats <- as.data.frame(do.call(rbind, sadStats))</pre>
```



Supplementary Figure 2: Observed spatial species abundance distributions (SSAD) as characterized by (A) the goodness of fit of the negative binomial distribution and (B) the relationship between a given species' relative abundance and its clustering parameter k. The horizontal red line in (A) indicates the critical value above which we would reject the negative binomial; no points are above this line. The blue regression line in (B) shows the best fit log-log linear model.

```
names(sadStats) <- c('mod', 'par1', 'par2', 'J', 'nspp', 'nsite')</pre>
sadStats$mod <- mods[sadStats$mod]</pre>
# limit to only those sites that produced good networks
sadStats <- sadStats[rownames(sadStats) %in%</pre>
                          rownames(commStats[!is.na(commStats$pos.n), ]), ]
# helper function to make a rank abundance dist for a hypothetical community of
# `S` species given model `m` and parameters `p`
hypRAD <- function(m, p, S) {
    x \leftarrow sad(model = m, par = p[!is.na(p)])
    r <- sad2Rank(x, S)
    return(r / sum(r))
}
S <- 100
allRAD <- mclapply(1:nrow(sadStats), mc.cores = nthrd, FUN = function(i) {
    hypRAD(sadStats$mod[i], as.numeric(sadStats[i, c('par1', 'par2')]), S)
})
allRAD <- do.call(rbind, allRAD)
radEnv <- lapply(unique(sadStats$mod), function(m) {</pre>
    apply(allRAD[sadStats$mod == m, ], 2, quantile, probs = c(0.025, 0.975))
```

})

To demonstrate the marked unevenness of the SADs, in Supplementary Figure 3 we look at the outline of the shapes of all the rank abundance distributions for a hypothetical community of 100 species.

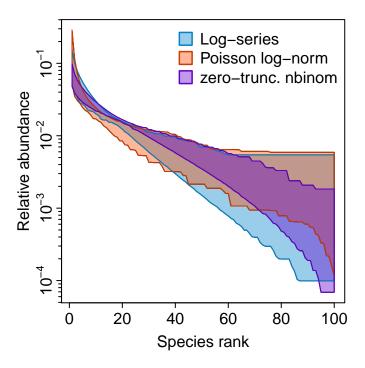
```
# ----
# helper function to make overlapping polygons more clear
specialPoly <- function(x, y, col) {</pre>
   polygon(x, y, col = colAlpha(col, 0.4), border = NA)
   polygon(x, y, border = col)
}
# ----
# plotting
par(parArgs)
plot(1, xlim = c(1, S), ylim = range(unlist(radEnv)), log = 'y', yaxt = 'n', type = 'n',
     xlab = 'Species rank', ylab = 'Relative abundance')
logAxis(2, expLab = TRUE)
polygon(c(1:S, S:1), c(radEnv[[1]][1, ], rev(radEnv[[1]][2, ])),
        col = hsv(0.56, 1, 0.8, 0.4))
polygon(c(1:S, S:1), c(radEnv[[2]][1, ], rev(radEnv[[2]][2, ])),
        col = hsv(0.05, 1, 1, 0.4))
polygon(c(1:S, S:1), c(radEnv[[3]][1, ], rev(radEnv[[3]][2, ])),
        col = hsv(0.75, 1, 0.8, 0.4))
polygon(c(1:S, S:1), c(radEnv[[1]][1, ], rev(radEnv[[1]][2, ])),
        border = hsv(0.56, 1, 0.8))
polygon(c(1:S, S:1), c(radEnv[[2]][1, ], rev(radEnv[[2]][2, ])),
        border = hsv(0.05, 1, 0.8))
polygon(c(1:S, S:1), c(radEnv[[3]][1, ], rev(radEnv[[3]][2, ])),
        border = hsv(0.75, 1, 0.8))
legend('topright',
       legend = c('Log-series', 'Poisson log-norm', 'zero-trunc. nbinom'),
       pch = 22, pt.cex = 2, pt.lwd = 1.5,
       col = hsv(c(0.56, 0.05, 0.75), 1, 0.8),
       pt.bg = hsv(c(0.56, 0.05, 0.75), 1, c(0.8, 1, 0.8), 0.4),
       bty = 'n')
```

S5 Simulating random data and artifactual interactions

Now we can simulate abundance data matching the overall shapes of the observed SADs and SSADs but with absolutely no real correlation or interaction between species.

```
# number of simulations to run
nsim <- round(1.25 * sum(!is.na(commStats$pos.wm)))</pre>
```

I simulate 374 random assemblages, slightly more than the 299 observed assemblages because some simulated assemblages will be rejected based on the data standards used. In Figure 1 of the main text I plot these simulated results alongside the results from the real data.



Supplementary Figure 3: Graphical summary of the shapes of the best-fit species abundance distribution models. Polygons represent the 95% conidence envelope of the rank abundance plots for each of the three SAD models considered.

Now we want to figure out if the correspondence between real and simulated results is specifically because of the shape of the SSAD (i.e. negative binomial) or if a spatially unclustered SSAD would also yield this close of a match. We do this by modeling the SSAD with a Poisson distribution.

Lastly we might be interested in whether we can produce a spurious association between abundance and interaction type without any reference to the observed data. For this experiment I imagine one arbitrary SAD and combine it with one of two arbitrary SSADs (either negative binomial or Poisson) and see if qualitatively similar results are found.

```
oneK <- 0.1
b <- 0.01
nsiteSimp <- 20
nsppSimp <- 50
nsimSimp <- nsim
```

In this case I use a log-series SAD with $\beta = 0.01$, a negative binomial with k = 0.1, and consider an assemblage with on average 20 sites and 50 species.

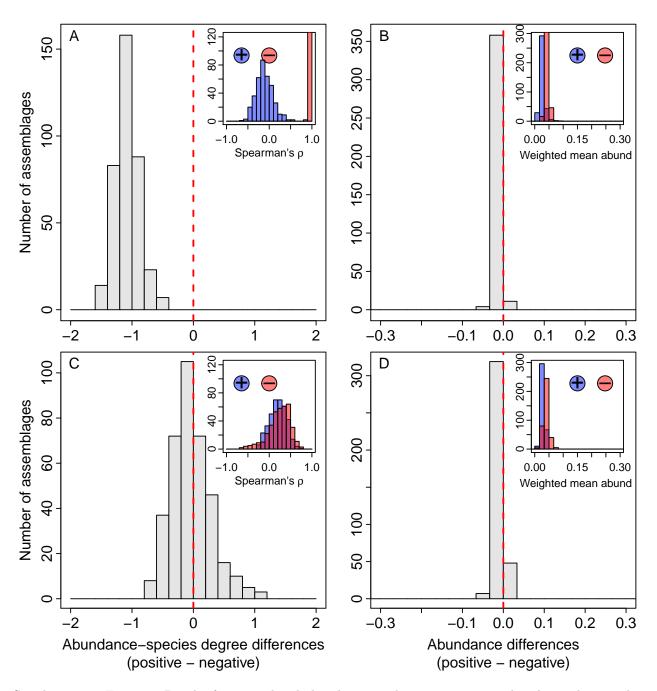
In Supplementary Figure 4 we see that indeed, when we use a realistic SAD and pair it with a negative binomial SSAD, we reconstruct a spurious association between rare species and positive interactions versus common species and negative interactions. When this same SAD shape is paired with a Poisson SSAD, we see this spurious association is substantially reduced.

To understand why these spurious results occur we must understand what the fixed-fixed null model 12,15 does to the underlying SSAD. We know that the fixed-fixed algorithm preserves, by definition, the SAD and the total abundances across sites, but within any given species, the allocation of its abundances has a potentially large combinatorial space. To understand what happens to SSADs when permuted, I simulate 100 assemblages, each with nspp species and nsite sites and compare the shape of the permuted SSAD with the true SSAD. I characterize SSAD shape by the number of sites occupied by a species and the maximum likelihood estimate of the negative binomial clustering parameter k. The results of this simulation are discussed in the main text.

Finally we very simply want to understand at a mathematical level why a spatially clustered versus spatially even SSAD would lead to these results. To explore this we consider a very simple example of two species and their Sch similarity.

```
N <- 5
Nrare <- 5
Ncomm <- 50
nsite <- 5

rarePair <- cbind(c(1, rep(0, nsite - 1)), c(Nrare, rep(0, nsite - 1)))
commPair <- cbind(c(Ncomm, rep(0, nsite - 1)), c(0, Ncomm, rep(0, nsite - 2)))</pre>
```



Supplementary Figure 4: Results from simulated abundances and interaction networks when only a single SAD shape and a single SSAD shape are used (as described in the text). Panel (A) shows correlations between abundance and centrality in positive or negative associations networks; panel (B) shows frequencies of different abundances in the two types of interaction networks.

```
commPairMax <- matrix(rep(Ncomm / nsite, nsite * 2), ncol = 2)</pre>
```

First we consider two rare species, one with abundance 1, and the other with abundance 5. If we consider a dataset with 5 total sites, then the configuration that maximizes the Schoener similarity between these two species is

 $\begin{bmatrix} 1 & 5 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

We can calculate how likely this configuration is under a negative binomial versus a Poisson SSAD like this

```
k <- 0.1
nbRareP <- prod(dnbinom(rarePair[, 2], k, mu = Nrare / nsite))
poRareP <- prod(dpois(rarePair[, 2], Nrare / nsite))</pre>
```

We see that the negative binomial SSAD is more likely to maximize the Schoener similarity compared to the Poisson, and thus compared to the null model rare species will appear to be aggregated with each other.

Conversely for the common species, in our simple example represented by two species both with abundance 50, we want to compare the probabilities of minimizing the Schoener similarity between them as derived from the negative binomial versus the Poisson SSAD. This occurs in any configuration such as this one where their total abundances fail to overlap

 $\begin{bmatrix} 50 & 0 \\ 0 & 50 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

We can calculate the probabilities of any such configuration like this

```
nbCommP <- prod(dnbinom(commPair[, 1], k, mu = Ncomm / nsite)) * (nsite - 1) *
    prod(dnbinom(commPair[, 2], k, mu = Ncomm / nsite))

poCommP <- prod(dpois(commPair[, 1], Ncomm / nsite)) * (nsite - 1) *
    prod(dpois(commPair[, 2], Ncomm / nsite))</pre>
```

We can further compare this to a scenario that would maximize the Schoener similarity between common species:

```
\begin{bmatrix} 10 & 10 \\ 10 & 10 \\ 10 & 10 \\ 10 & 10 \\ 10 & 10 \end{bmatrix}
```

We calculate the probability of this configuration like

```
nbCommPMax <- prod(dnbinom(as.vector(commPairMax), k, mu = Ncomm / nsite))
poCommPMax <- prod(dpois(as.vector(commPairMax), Ncomm / nsite))</pre>
```

The conclusions of these probability calculations are discussed in the main text.

References

- 1. R Core Team. R: A language and environment for statistical computing. (R Foundation for Statistical Computing, 2018).
- 2. Wickham, H., Hester, J. & Chang, W. devtools: Tools to make developing R Packages easier. (2018).
- 3. Rominger, A. J. socorro: Helper functions for R. (2016).
- 4. Rominger, A. J. pika: Tools for macroecology. (2016).
- 5. Oksanen, J. et al. vegan: Community ecology package. (2019).
- 6. Garnier, S. viridis: Default color maps from 'matplotlib'. (2018).
- 7. Csardi, G. & Nepusz, T. The igraph software package for complex network research. *InterJournal, Complex Systems* **1695**, 1–9 (2006).
- 8. Zhang, J. spaa: Species association analysis. (2016).
- 9. Wickham, H., Danenberg, P. & Eugster, M. roxygen2: In-line documentation for R. (2018).
- 10. Wickham, H. testthat: Get started with testing. The R Journal 3, 5–10 (2011).
- 11. Calatayud, J. et al. Positive associations among rare species and their persistence in ecological assemblages. Nat Ecol Evol (2019).
- 12. Patefield, W. M. Algorithm as 159: An efficient method of generating random $r \times c$ tables with given row and column totals. Journal of the Royal Statistical Society. Series C (Applied Statistics) 30, 91–97 (1981).
- 13. Etienne, R. S. A neutral sampling formula for multiple samples and an 'exact'test of neutrality. *Ecology letters* **10**, 608–618 (2007).
- 14. Rominger, A. J. & Merow, C. *meteR*: An R package for testing the maximum entropy theory of ecology. *Methods in Ecology and Evolution* **8**, 241–247.
- 15. Ulrich, W. & Gotelli, N. J. Null model analysis of species associations using abundance data. *Ecology* **91**, 3384–3397 (2010).