ComStruc – a FORTRAN program for comparing ecological communities
Version 1.1

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1. Introduction

ComStruc is a small program that computes basic patterns of community structure in ecological matrices like species x site or site x variable matrices. In ecological research this is sometimes necessary for analysing species co-occurrences, or for the computation of rarefied species numbers.

The recent standard program for analysing community structure and species co-occurrence patterns is EcoSim (Gotelli and Entsminger 2002). However, EcoSim lacks some important features and ComStruc is intended as a supplementary program. The actual version of ComStruc contains five modules: rarefaction, species overlap, community similarity, a variance test, and a fitting module for relative abundance distributions.

2. Data structure

ComStruc needs unformatted ASCII files (text files) as shown in the table beside. The first line must always be a comment lines that starts with an asterisk (*). The program asks whether species are in columns or in rows. The data sets need not to be sorted. Data have to be separated by one or more spaces. Matrix size is only limited by the available computer memory. However, analysing larger matrices may become very time consuming.

3. Program run

After the input of the data file name the programs checks the data structure and shows the number of rows and columns. ComStruc contains six basic modules:

- Rarefaction
- Species overlap
- Site overlap

* Data matrix

| 102 | 54 | 84.32 | 17.705 | 49 |
| 954 | 302 | 149.39 | 273.713 | 16 |
| 342 | 1 | 260.38 | 0.631 | 114 |
| 2 | 5 | 0.90 | 1.367 | 1 |
| 4 | 8 | 3.24 | 2.903 | 2 |
| 6 | 47 | 3.87 | 43.081 | 2 |
| 56 | 0 | 8.29 | 3.105 | 5 |
| 20 | 28 | 8.85 | 5.1 | 0 |
| 17 | 40 | 0 | 0 | 52 |
| 584 | 0 | 0 | 0 | 17 |
| 350 | 20 | 0 | 3.2 | 3 |
3. Rarefaction

Rarefaction attempts to calculate expected species richness at a standardized size. In order to do this it uses a random sample models based on the hypergeometric distribution (Heck et al. 1975) (sampling without replacement). Rarefied species numbers are computed from the following equations.

\[
E(Sm) = \sum_{i=1}^{S} \left( 1 - \frac{N - n_i}{m} \right)
\]

and

\[
Var(Sm) = \sum_{i=1}^{S} \left( \frac{N - n_i}{m} \right) \left( 1 - \frac{N - n_i}{m} \right) + \frac{2 \sum_{j=2}^{S} \sum_{i=1}^{j-1} \left( \frac{N - n_i}{m} \right) \left( \frac{N - n_j}{m} \right) \left( \frac{N - n_j - n_i}{m} \right)}{m}
\]

Sm is the expected species number in a sample of size m from a total community of S species and N individuals. \( n_i \) and \( n_j \) are the numbers of individuals of species i and j in the whole community (Heck et al. 1975, Olszewski 2004).

The Table below shows the rarefaction results of six subsamples (columns 1 to 6) from a data matrix of 170 species and 7881 individuals. If abundance data are given as densities ComStruc first normalizes the data set by dividing all density data through the density of the least abundant species in order to rescale to individual numbers. Instead of the variance the output file Output.txt gives the standard deviation of the expected species number at sample size m.

Additionally ComStruc computes the Simpson index of evenness for the site (ESite) and for the total matrix (ETotal), and the alpha diversity index for the sample (AlphaS), for the rarefacted sample (AlphaR), and for the total matrix (AlphaT). Evenness is computed from

\[
E = \frac{N}{N-1} - 1 - \sum_{i=1}^{S} \frac{1}{p_i^2}
\]

The variance of E is given by

\[
Var(E) = \frac{4(N-1) \sum_{i=1}^{S} p_i^4 + 2 \sum_{i=1}^{S} p_i^2 - 2(N-3) \left( \sum_{i=1}^{S} p_i^2 \right)^2}{N(N-1)}
\]

with \( p_i \) being the relative abundance of species i and N the total number of individuals. It should be emphasised that Var(E) is a sample theoretical variance that decreases fast with N (due to the division by \( N^2 \)). Real variances are often larger.

Alpha is given by

\[
S = \alpha \ln(1 + \frac{N}{\alpha})
\]

With S and N being the number of species and the number of individuals.

<table>
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<tr>
<th>Column</th>
<th>S obs.</th>
<th>Individuals</th>
<th>S expected</th>
<th>Std. Dev.</th>
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<th>StdSite</th>
<th>ETot</th>
<th>StDTot</th>
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<th>AlphaR</th>
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<td>0.002</td>
<td>14.56</td>
<td>23.68</td>
<td>30.60</td>
</tr>
</tbody>
</table>
ComStruc

4. Species overlap and site overlap

Instead of computation a metric for species co-occurrence patterns as does Eco Sim (Gotelli and Entsminger 2002) ComStruc calculates expected numbers of common species between all pairs of sites assuming a random sample out of a larger species pool. The program asks for the pool size. The probability of having k species in common if two samples from a pool of n species contain m and l species (m \leq l) is given by

$$p_k = \frac{k}{\binom{n}{k} \binom{m-k}{l-k}} \frac{\binom{n-k}{m}}{\binom{l}{l}}$$

with E(p_k) = ml/n and

$$\sigma_{pk}^2 = \sum_{i=0}^{m} \binom{n-l}{i} \binom{l}{m-i} \binom{m-i-ml}{n}$$

(Connor and Simberloff 1978, Ulrich 1999).

ComStruc computes the whole distribution for k = 0 to k = m and from this distribution the expected mean and standard deviation. Additionally it computes the Sørensen index of species overlap from

$$J = \frac{2k}{m + l}$$

The site overlap module does the same as the species overlap but compares sites using all species pairs. It is therefore a pairwise test of species co-occurrences.

5. Proportional similarity

For all pairs of sites the Colwell - Futuyma index of proportional similarity \( c_{j,k} \) is computed from (Colwell and Futuyma 1971)

$$c_{j,k} = 1 - 0.5 \sum_{i=1}^{S} \left| p_{i,j} - p_{i,k} \right|$$

with \( p_{i,j} \) and \( p_{i,k} \) being the relative abundances of species i in the sites j and k. These values are compared with randomized sites where the observed densities are randomly assigned to species. Simulated mean index values and the respective standard deviation are generated from 1000 replicates. In the example output above observed index values were always larger than the simulated ones. However, the simulated distribution is skewed. ComStruc computes the skewness from

$$\gamma = \frac{n}{(n-1)(n-2)} \sum_{j=1}^{s} \left( \frac{n_j - \overline{x}}{s} \right)^3$$

Additionally it gives the upper and lower 2.5% percentiles.
6. Variance test

Schluter (1984) popularized a test for identifying matrix wide patterns of species association or segregation. He used the quotient of row and column variances $V = R / C$. In a perfect random matrix this quotient should be 1 and for n sites the product n C should have a CHI$^2$ distribution with n degrees of freedom. Look at the following table. A standard species x sites input file is first transformed into relative abundances of species. Then the program computes the column variances and the row (species) sums. Next the variances of sums is divided through the sum of variances ($V = R / C$).

To compute expected $V$-values and associated standard deviations the program resuffles the matrix 1000 times either according to the sequential swap algorithm (Gotelli 2000) or according to the sums-of-squares reduction algorithm (Miklos and Podani 2004). In the first case the program needs absolute counts. This procedure is replicated 1000 times to get expected values and standard deviations.

The output looks as follows. ComStruc gives the number of sites and species, the observed $V$-ration, the simulated and its standard deviation and the Z-transforms (standardized) effect and the upper and lower 2.5 percentiles. A positive z-value points to species aggregation, a negative to segregation. Additionally, the program prints the last randomized matrix.

You should note, that the present test differs from the original version of Schluter. Schluter’s test is extremely sensitive to site differences like area or suitability. To account for this the program first transforms to relative abundances. Then however column sum are 1 and have a variance of zero. Therefore ComStruc turns the test around and computes column (site) variances and row (species) sums. By this the test rather is a measure of matrix wide differences of rank order distributions. However, these are made by differences in species abundances. Hence, the test is still a test for species co-occurrence patterns.

7. Model fitting

7.1. The fitting algorithms

The model fitting module is a simplified version of the RAD fitting package that fits a wide range of rank abundance models to given data sets. ComStruc fits five models that represent basic shapes of rank abundance distributions.
**Generalized random assortment**

(Tokeshi 1990, Ulrich 2001):

\[ D_i = D_{\text{uni}(1)} ran^z \]

*ran* denotes always a random variable. In the original model is \( z = 1 \). The value of \( z \) may range between \( 0.00001 \leq z \leq 1 \). An input of \( z = 0 \) is equivalent with the original version of the model.

**Generalized Sugihara fraction**

(Generalized sequential breakage)

(Sugihara 1980, Ulrich 2001)

The program computes the model either via a fixed breakage value \( z \) (0.5 \( \leq z < 1 \))(X=0) or from a normally distributed breakage value with a mean of \( z \) (Sugihara 1980, Tokeshi 1996). In the latter case \( X \) is the input for the distribution variance. A triangular breakage probability is approximated by a variance input of \( X = 0.085 \). A simple linear random distribution of \( z \)-values is generated after a \( z \) and \( X \) input of 0. \( z = 0.66 \) and \( X = 0 \) is nearly identical with a canonical lognormal. The original Sugihara fraction has \( z = 0.75 \) and \( X = 0.085 \).

**Power fraction**

(Tokeshi 1996)

The single parameter \( z \) can take all values between \(-\infty \) and \(+\infty \). For \( z = 0 \) the model is equivalent to a random fraction, \( z = 1 \) results in a MacArthur fraction.

**Stochastic Zipf-Mandelbrot**

(Mouillot et al. 2000, Bell 2000, Ulrich 2001)

See Tab. 1. Both model parameters \( z \) and \( X \) have to be larger than 0.

**Stochastic normal and lognormal**

Either a simple normal distribution is computed (from a normal distributed random variable \( ran \); input option: \( X = 0 \)) or an exponential normal (from \( \ln(ran) \), input option: \( X = 1 \)), or a lognormal (from \( \exp(ran) \); input option: \( X = 2 \)).

In the latter case the single shape generating parameter \( z \) (the variance) is roughly \( 1/(2a) \) (\( a \) being the lognormal parameter).

The fit relies on least square fits where the Euclidean distances between predicted and observed data points are minimized. The main fitting variable \( r \) can then be defined as:

\[ r = \sum_{i=1}^{S} (d_i)^2 \]

with \( d_i \) being the Euclidean distance between theoretical and empirical ln-transformed densities and \( S \) the number of species. In the case of the stochastic models \( r \) is computed using mean densities of \( n \) replicates of the model. The fitting process runs with different values of the shape generating parameters \( z \) and \( X \) (by stepwise enclosure) until \( r \) reaches a minimum.

This test value is sensitive to the maximum density difference \( D \) of the species - defined as the quotient of most and least abundant species - of the data set (Fig. 6) (here data set always refers to an assemblages to be fitted). In the stochastic models low density species effect the value of \( r \) overproportional, mainly due to the higher variance. This makes it difficult to compare fits by different models.

Additionally, due to the summation process the test statistic \( r \) will depend on the total number of species \( S \) when comparing fits from assemblages of different species numbers. At first sight, the quotient \( r / S \) should be constant. However, the higher the number of species is the lower is the total variance of stochastic models after a finite number of iterations. Therefore, \( r \) will be relatively lower at high species numbers. To use \( r \) as a test statistic for comparing the fits of stochastic models at least a correction factor for
density is necessary. If one wants to compare $r$ at different species numbers a second correction factor has to be added. The correction factors and their behaviour are described in detail in the RAD manual and in Ulrich (2001)

A second main fitting statistic uses the number of species per binary density class (octave). As in the case of $r_{test}$ oct$_{test}$ computes squared differences, but in this case those of species numbers per octave of model and data set.

Again this measure depends on the maximum density difference and the total species number. ComStruc computes other statistics to assess the goodness of fit. These are described below in Chapter 6.3.

7.2. The input parameters

ComStruc fits the columns of the whole data matrix step by step

The module assumes that the columns represent local densities and are samples from a larger species pool. By default this is the number of rows (species) in the data matrix.

Iteration gives the number of iterations of the model fit. For most models convergence is quite fast and 20 iterations will result in a stable fit. The maximum number of iterations must not exceed the sum of species number and number of replicates of the model.

ComStruc asks after the number of replicates (the sample size) of the data set has to be given. This is necessary for computing confidence limits (see below). In most cases IterAss will have a value of 1.

$Z_{min}$ and $z_{max}$ give the range of the main shape generating parameter z. The Table beside shows the default settings of the programs but other values inside these ranges are allowed (although these will sometimes result in errors communications of the program). For a good and faster model fit it will often be better to define more narrow ranges. X will not be changed during program run. In cases were X is important several runs with different X values have to be performed until a sufficiently good fit is reached.

Next the x% confidence limit probability has to be defined. ComStruc computes for each species the density range inside this limit and compares the respective data set density with this limit (see below). Allowed input values are (0.3, 0.7, 0.9, 0.95, and 0.99). They refer to confidence limit factors of (0.352, 0.6, 1.17, 1.645, 1.96, and 2.576). For other values ComStruc takes the default probability value of 0.95.

Instead of this a fixed confidence limit factors can be given (Input ConfLim = 0 and Deviat.F = value). Typi-

<table>
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<th>Col</th>
<th>Species</th>
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<th>Runs</th>
<th>RepM Model</th>
<th>Const z</th>
<th>Const X</th>
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</tr>
</tbody>
</table>

* p-value KolmogSmir p-value 50%Slope 50%Interc 15%Spe 15%Pro 15%SpeZM 15%ProZM

0.26589593573752254 0.1626251464939695 0.31874529338318373
0.1204238921001927 0.1113471251699064 0.2182403695805722
0.0716120745022479 0.0826177871905457 0.1619308660450881
0.0606936416184971 0.0591861397324860 0.1160048361334446
0.0566400770712909 0.0440035226049578 0.0862469059843184
0.0494540783558125 0.0375356241874162 0.0735698284392061
0.0321130378938479 0.033152398484509 0.0652978713738392
0.0240847784200385 0.0217853198476602 0.060255598821531
0.0217853198476602 0.0217853198476602 0.042692271725176
0.00525442517662 0.0217853198476602 0.042692271725176
0.0000000000000000 0.0000000000000000 0.0000000000000000

Testvariable Testvar Octaves FR<conf Rel.Sum R<conf Chi2confid p-value KolmogSmir p-value 50%Slope 50%Interc 15%Spe 15%Pro 15%SpeZM 15%ProZM

0.26589593573752254 0.1626251464939695 0.31874529338318373
0.1204238921001927 0.1113471251699064 0.2182403695805722
0.0716120745022479 0.0826177871905457 0.1619308660450881
0.0606936416184971 0.0591861397324860 0.1160048361334446
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0.0000000000000000 0.0000000000000000 0.0000000000000000

Next the x% confidence limit probability has to be defined. ComStruc computes for each species the density range inside this limit and compares the respective data set density with this limit (see below).

Allowed input values are (0.3, 0.7, 0.9, 0.95, and 0.99). They refer to confidence limit factors of (0.352, 0.6, 1.17, 1.645, 1.96, and 2.576).

Instead of this a fixed confidence limit factors can be given (Input ConfLim = 0 and Deviat.F = value). Typi-
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cal values should be between 0.5 and 3.

At last, correction factors may be defined. This refers to the density and species number dependence of $r$ and $oc$. With $CorrectF = dens$, only the density dependence is corrected. This is appropriate when comparing different communities with the same species numbers. To compare communities with different species numbers but similar density ranges the input $spec$ is indicated. To correct for species number and density $CorrectF$ must be ‘both’.

7.3. The Output

ComStruc produces the output file ‘Assemblage.txt’, of which the next table shows an example.

The first two file lines repeat the input values and give the value of $z$ for which the given model best fits the data set. Col refers to the column of a data matrix. If you have only one column Col will have the value 1.

The next two output lines first contain $r_{test}$ and $oc_{test}$. Then, the frequency of species ranging inside the $x\%$ confidence limits are given. Tokeshi (1990) introduced this method for fitting relative abundance distributions (see for a modification also Bersier and Sugihara 1997). In principle this method is very simple. It compares the relative abundance of species of the data set with the mean density of the $i$-th species of the fitting model using the $x\%$ confidence limit:

$$Con_i(x\%) = \mu_i \pm \frac{r(x\%)\sigma_i}{\sqrt{n}}$$

Again, $n$ is the number of replicates of the model. If more than say 1 or 5\% of species range outside this limit, the model does not fit the data set. We see, however, immediately the problem with this approach. First of all, the method does not take systematic deviations into account. Although all species may range inside the 5\% confidence limit, their relative abundances may all be too low or too high. Secondly, the quality of data sets might be very different. In one case 100 specimens had been sampled, in another 100000. We have therefore also to include confidence

Figure 4: A power fraction model generates a S-shaped frequency distribution. We can compute a regression line through the middle ranking 50\% of species. They have the output values $50\%$Slop and $50\%$Int together with their standard deviations (SISIDev and IntStDe). 15\%Spe and 15\%SpZM count the number of species of the upper and lower 15\% percentile that are above and below (15\%Spe) or only above (15\%SpZM) the regression line. 15\%Pro and 15\%PrZM give the probability that this will be the case just by chance. Note that $slope$ is a diversity statistics similar to the alpha-index.
limits for the data set abundances. ComStruc does this by modifying the above equation to incorporate the (estimated) sample accuracy of the data set $n_{\text{data}}$. This is the assumed number of replicates of the data set that has to be estimated from the sample size (see Ulrich 2001b for a detailed discussion of this point).

$$C_{\text{con}}(x\%) = \mu \pm \frac{r(x\% \sigma)}{\sqrt{n} \sqrt{n_{\text{data}}}}$$

It then computes the frequency of species ranging inside this confidence limit ($FR < \text{conf}$). Additionally, a measure for the magnitude of deviation is given as the sum of deviations of those species ranging outside the $x\%$ confidence limit.

$$R_{\text{sum,}i>\text{conf}} = \sum x_{\text{Model}} \frac{C_{\text{con}}(x\%)}{n_{\text{data}}}$$

In a next step ComStruc computes the probability (via a CHI$^2$-test) whether the ordering of deviations of those species ranging outside the $x\%$ confidence limit deviates from the null hypothesis of a random distribution around the model mean ($\text{Chi}^2_{\text{confid}}$ and $p$-value). In the example below the probability that the deviators are distributed non-randomly is less than 50%.

Lastly, a Kolmogorov-Smirnov test gives the probability that the ordering of relative abundances of all data set species in relation to the model species deviates from the expectation of a random ordering. KolmogSmir gives the number of occurrences where the density differences of data set and model species of consecutive species have the same sign. $p$-value then gives the probability of rejecting the null hypothesis of a random distribution around the mean. In our case 5 times consecutive species deviated in different ways from the model.

The probability for such a pattern is less than 1% and we have to conclude, that our model does not fit the data set although an optical inspection of the fit looks not as bad. The 95% confidence limit method also indicates no good fit.

The next six output values of the program (50%Slope, 50%Interc, 15%Spe, 15%Pro, 15%SpeZM, 15%ProZM) give slopes and intercepts (together with their standard deviations) of exponential regression lines through the middle ranking 50% of the species of the data set. At last, species numbers (of the upper and lower 15% percentile) of species ranging above and below this regression line are counted. ComStruc gives also the probability that these species numbers deviate from the null hypothesis of a random pattern around the regression line. The program estimates therefore deviations from linearity.

For real data sets with a high variability in density the Kolmogorov-Smirnov test will often give poor results because of high numbers of species with identical or similar numbers of individuals. In these cases $r_{\text{test}}$ and $oc_{\text{test}}$ are better suited to compare fits by different models. However, in these cases no probability levels are available.

ComStruc then prints the relative abundances of the original data set and the model fitted as well as the species numbers per abundance octave of both assemblages.

Lastly, ComStruc gives the progress of the fitting procedure and shows $r_{\text{test}}$, $oc_{\text{test}}$ and $z$ at each step.

8. Citing ComStruc

ComStruc is freeware but nevertheless if you use ComStruc in scientific work you should cite ComStruc as follows:

Ulrich W. 2005 - ComStruc – a FORTRAN program for comparing ecological communities - www.uni.torun.pl/~ulrichw

9. Acknowledgements

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10. References


