Pairs – a FORTRAN program for studying pair wise species associations in ecological matrices

Version 1.0

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1. Introduction

The study of species co-occurrences has a long tradition in ecology (Weiher and Keddy 1999). Particularly the long lasting and still ongoing discussion around community assembly rules (Diamond 1975, Diamond and Gilpin 1982, Gilpin and Diamond 1982, Connor and Simberloff 1979, 1983, 1984, Gotelli and McCabe, 2002, Ulrich 2004) has inspired the development of statistical tools to infer non random patterns in community assembly (Gotelli and Graves 1996, Gotelli 2000, 2001, Ulrich and Gotelli 2007a, b).

Community assembly is often studied in terms of nestedness (Patterson and Atmar 1986, Wright et al. 1998, Ulrich and Gotelli 2007a) and non-random patterns of species co-occurrences (Diamond 1975, Gotelli 2000, 2001, Ulrich and Gotelli 2007b) and the respective standard software is widely used: The *Nestedness Temperature Calculator* (Atmar and Patterson 1995), *EcoSim* (Gotelli and Entsminger 2002, and *Nestedness* (Ulrich 2006).

The present program *Pairs* extends these approaches and implements beside standard nestedness and co-occurrence metrics a new metric to study pairwise species associations: The software implements:

The discrepancy metric of Brualdi and Sanderson (1999),

the species combinations score (Pielou and Pielou 1968),

the C-score (Stone and Roberts 1990),

the checkerboard score (Gotelli 2000),

the Soerensen metric,

the togetherness score (Stone and Roberts 1992),

the species absences score (Stone and Roberts 1992),

the variance test (Schluter 1984),

a pairwise correlation test.

Pairs contains therefore similar metrics than the software *CoOccurrence* (Ulrich 2006) and is designed for the study of multiple matrices in null model analysis, the analysis of the statistical behaviour of certain metrics, and in studies of neutral models.

2. Metrics

Nestedness

A proper metric (Ulrich and Gotelli 2007a) to measure nestedness is the discrepancy *BR* (Brualdi and Sanderson 1999) that counts the number of discrepancies (absences or presence) that must be erased to produce a perfectly nested matrix. BR is standardized by dividing its values through the total number of occurrences in the matrix (the matrix fill) (Greve and Chown 2006).

Co-occurrence

The present program implements five matrix wide measures of co-occurrences:

1. The species combinations score (COMBO) screens the columns of the presence absence or abundance matrix for unique species combinations (Pilou and Pielou 1968). Hence, it counts the number of species that always co-occur.

2. The checkerboard score (Gotelli 2000) screens the matrix for checkerboards. These are 2*2 submatrices of the structure $\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$ or $\begin{matrix}0 & 1\\ 1 & 0\end{matrix}$. The score is a simple count of the numer of such submatrices.

3. The C-score (Stone and Roberts 1990) is the average number of checkerboards for two species i and j. The score is calculated from

$$CS = \frac{2\sum_{i=1}^{S(S-1)/2}(n_i - N_{ij})(n_j - N_{ij})}{S(S-1)}$$

where S is the number of species and n_i and n_j are the row totals (numbers of occurrences) of species i and j and N_{ij} is the number of co-occurrences of both species.

4. the togetherness score (Stone and Roberts 1992) is based on presences and absences and calculated from

$$t = \frac{2}{S(S-1)}\sum_{1}^{S(S-1)/2}\frac{4p_{ij}a_{ij}}{sites^2}$$

Where p_{ij} and a_{ij} are the numbers of pairs presences and absences, respectively.

5. The absences score equals the C-score but counts joint absences instead of joint presences. For comparing matrices of different size and shape the metrics have to be standardized. This is done by dividing the effect size through the expected value.

6. The Soerensen score is calculated from

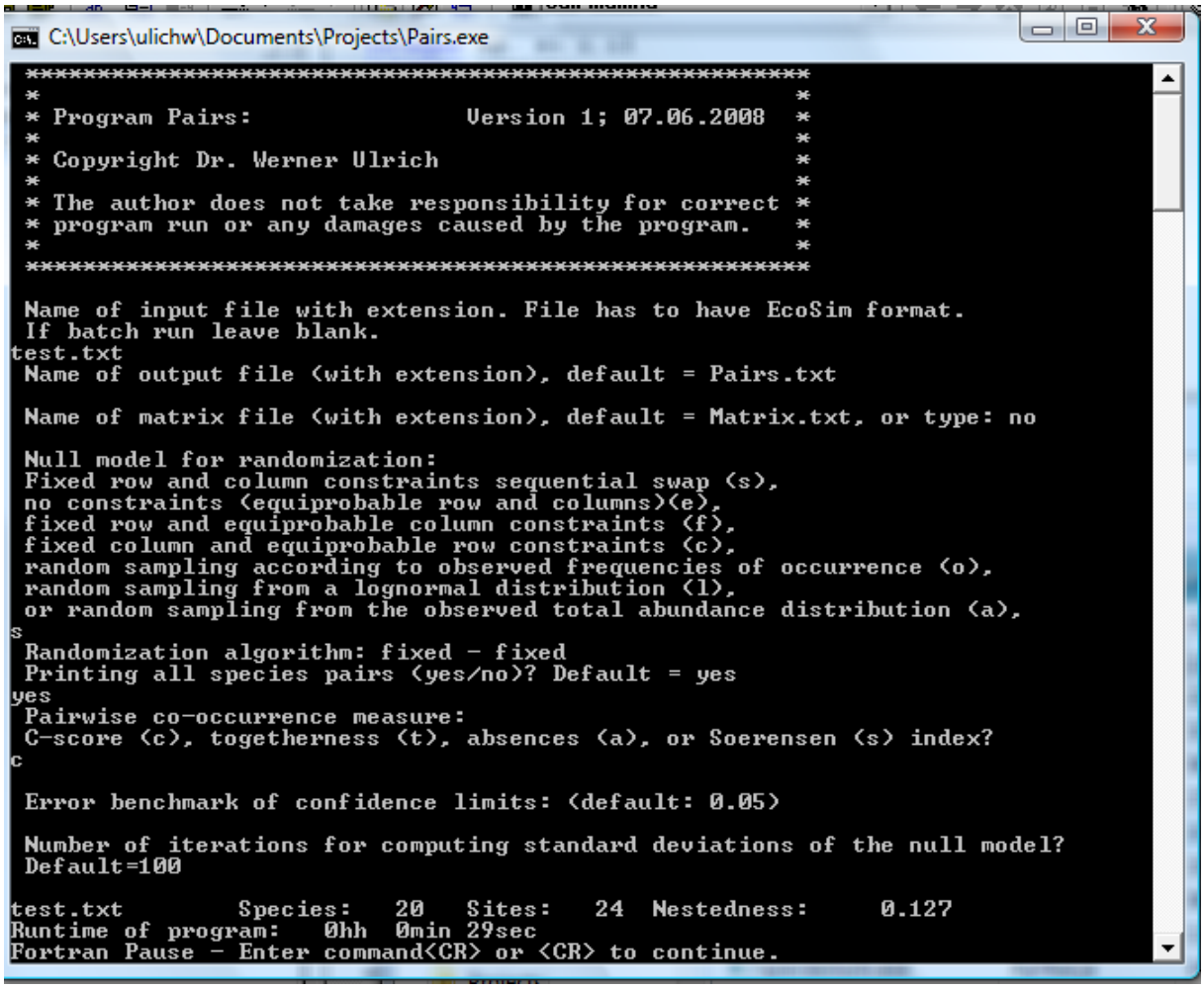
$$Soe = \frac{2}{S(S-1)}\sum_{1}^{S(S-1)/2}\frac{2n_{ij}}{n_i + n_j}$$

7. The variance test of Schluter (1984)

8. A matrix wide correlation coefficient calculated as the mean of the Spearman rank order correlations between all pair-wise site correlations. This option is only available for matrices that contain abundance data.

3. Species pairs

Pairs not only studies matrix wide patterns. It uses a Bayesian approach to detect non-random associations of pairs of species. The number of species pairs of a matrix is S(S-1/2. Hence even for medium sized matrices many 'significantly non-random' species pairs are expected at the 1% or 5% error level. For instance in a matrix of 50 species 61 significant pairs are expected just by chance at the 5% error benchmark. To reduce this high false detection error rate *Pairs* calculates first the expected empirical Bayes distribution of co-occurrence scores (C-score, togetherness score, Soerensen score and joint absences score) and compares this expectation with the observed distribution

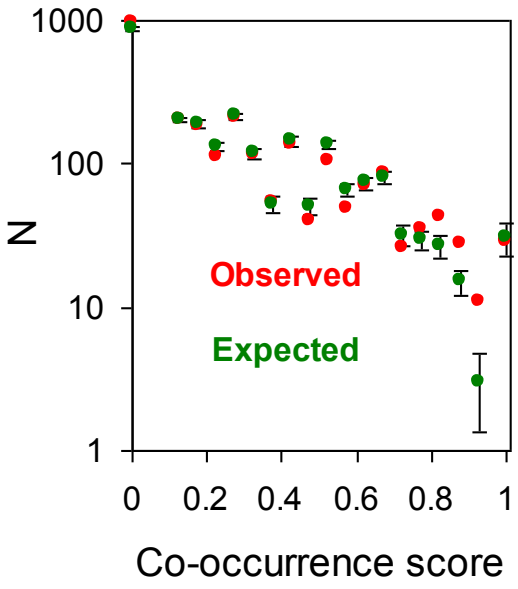


of scores. This is done from the predefined number of random matrices. To compares observation and expectation scores of all metrics are standardized in the range of 0 to 1 and classified into 22 groups: 0, 0-0.04999,0.05-0.09999,….,0.9-0.94999, 0.95-0.99999,1.

The scores are calculated as above but instead dividing through S(S-1) they are divided through $n_i n_j$ for each pair .

The Fig. above shows such a comparison. In many cases the observed number of scores will be well within the confidence limits of the null expectation irrespective of whether the pair wise scores are later identified as being significant or not. *Pairs* chooses only those scores for further analysis where the number of observed instances is either larger than the mean expectation (Bayes M criterion) or larger than the upper 5% or 1% confidence limit (Bayes CL criterion). In the Figure the number of observed scores having values between 0.8 and 0.95 are well above the null expectation and pairs having such scores are first candidates to look for on-random associations.

For each pairs a Z-transformed value (Obs-Exp)/StDev. is calculated. For each of the above defined score classes *Pairs* calculates the two odds ratios = (Obs-Exp)/Obs. The first uses the mean of the Bayes distribution, the second its upper confidence limit. This value equals 1- false detection error rate. For all classes with positive odds ratios it chooses those pairs with scores above the respective pair wise confidence limit of the null model and prints it Z-scores. A further selection step (the Bayes M criterion) involves the odd



ratios. Only those pairs with the highest Z-scores are chosen. The benchmark is the number of pairs in the score class multiplied with the ML odds ratio. The most conservative third criterion (Byes CL) uses the CL odds ratio.

In the next analysis step the program calculates all S(S-1)/2 species pair scores and compares these with the null expectation. As a default null expectations are calculated from 100 randomized matrices for each pair.

An example: In the Figure above in the score class 0.5-0.55 106 pairs were observed but 136 pairs expected. The pairs of this class are not further considered as candidates for non-random associations. In the class from 0.85-0.9 28 pairs were observed but only 15 expected with an upper confidence limit of 22. Hence the Bayes M odds ratio is (28-15)/28 = 0.46 and the respective Bayes CL odd ratio = 0.21. That means only the 46% (ME) or 21% (CL) of species pairs with the highest pair wise significant Z-scores are considered as candidates for non-random association.

4. Data structure

Pairs needs one main plain text data file of the following structure. The columns of the matrix are sites, the rows species. Hence the matrix above contains 12 species distributed over 6 sites. The data file has to be a simple ASCII file with data delimitated by one or more spaces. Accepted are either abundance or presences absence data of the integer (In) or real format (Fn.k) The first row contains site names, the first column species names. The file has therefore the same format that is needed for *EcoSim* (Gotelli and Entsminger 2002). The number of species is not limited, the maximum number of sites is about 150.

S	1	2	3	4	5	6
1	1.00	1.00	1.00	1.00	1.00	1.00
2	1.00	1.00	1.00	0.00	1.00	0.00
3	1.00	0.00	1.00	1.00	1.00	0.00
4	1.00	1.00	1.00	1.00	0.00	0.00
5	1.00	1.00	1.00	1.00	0.00	0.00
6	1.00	1.00	1.00	1.00	0.00	0.00
7	1.00	1.00	1.00	0.00	0.00	0.00
8	1.00	1.00	1.00	0.00	1.00	0.00
9	1.00	1.00	0.00	1.00	0.00	0.00
10	1.00	1.00	0.00	0.00	0.00	0.00
11	1.00	1.00	0.00	0.00	0.00	1.00
12	1.00	1.00	0.00	0.00	0.00	0.00

- The batch file format

Test1.txt
Test2.txt
Test3.txt
Test4.txt
Test5.txt

5. Program run

First, the program asks for the files names. The default output file names are *Pairs.txt, SignPairs.txt,* and *Matrix.txt*. You get the default values after returning *enter*. If you don't give the name of the data file and return *enter* the program expects a batch run and a file name with the data files.

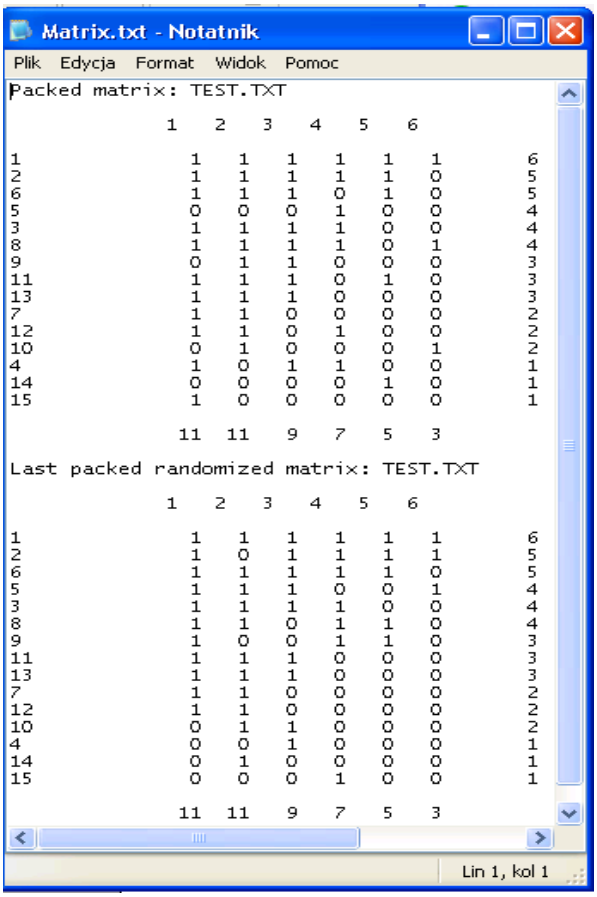
Next, the program asks for the model for randomization. You have seven possibilities: A null model with fixed row and column constraints (input: s) using the independent swap algorithm (Gotelli 2000, 2001),

no constraints (equiprobable row and columns, input: e), or fixed row (input: f) or fixed column (input: c) constraints only. For details of the null models used see Gotelli (2000, 2001) and Ulrich and Gotelli (2007a, b). The independent swap model uses ten times the matrix size (10*rows*columns) single swaps to generate a randomized matrix.

The fifth null model (o) assigns species with a probability according to the number of site occurrences. This model is therefore identical to the Random 1 model of Patterson and Atmar (1986) and Wright et al. (1998). The sixth null model is a sampling model, where the sites are filled with species using a random sampling of individuals from a common species pool that is structured according to a lognormal species abundance distribution. In this case the program asks for the shape generating parameter *a* of the lognormal model. This has the typical form $[S=S_0Exp(-a(R-R_0)^2]$ and is computed using a normally distributed random number on a log scale. Preston's canonical lognormal has the parameter value a = 0.2 (May 1975). In the case of the lognormal null model column (site) species numbers are fixed to the observed values (fixed column constraint).

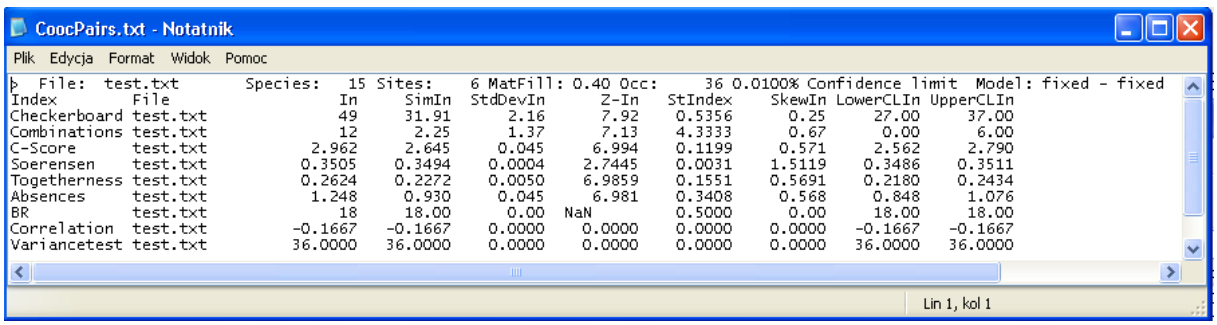
The seventh null model resamples rows according to the observed species abundance distribution calculated from row totals of abundance. This last null model, of course, needs abundance data as input.

Next the program asks for the number of randomizations to compute the null model means and standard deviations, as well as upper and lower confidence limits. In most cases 100 such randomizations will be enough.



6. The output files

Pairs produces four output files. The first file (*CoocPairs.txt*) contains basic information about the matrix and the measurements. First it gives species and site numbers, matrix fill, the total number of occurrences, the confidence limit benchmark, and the null model algorithm. Then observed metric values, simulated values, the respective standard deviations, Z-scores, standardized values, skews of the null model distribution, and upper and lower confidence limits of



this distribution are provided.

The second file *Matrix.txt* contains the packed original data matrix and the last randomized packed matrix. The examples above show both files.

The third output file *Pairs.txt* contains the observed and the empirical Bayes distribution, its mean, standard deviation, skewness and the lower and upper confidence limits. The two last columns contain the odds ratios of the respective score with regard to the Bayes M and the Bayes CL criterion. The odds ratio is the proportion of pairs above expectation = (Obs-Exp)/ Obs.

Next the program gives all species pairs. The last six columns contain Z-transformed scores [= (obs.-exp.)/ StDev] and associated probability levels. In the Z-score case it gives the Z-scores for those species with observed scores greater or smaller than the upper or lower confidence limit for that pair and the associated probability level. In the MeanScore and CLScore case it selects further according to the above defined Bayes M and Bayes CL criteria.

The last two columns contain false error rate corrected Z-scores and probability levels according to the method of Benjamini and Yekutieli (2001).This refinement modifies the test wise H_0 probability benchmark a from the ordered sequence (largest to smallest) of H_0 of the species pairs r probabilities p_k to

$$p_k^* = \alpha \frac{k}{r} \frac{1}{\sum_{i=1}^{r} \frac{1}{i}} \qquad (1)$$

where the k = 1 to r probability values p_k are ordered from largest to smallest, and p^*_k is the adjusted probability benchmark. The second last column contains the associated Z-score.

The last output file *SignPairs.txt* contains the significant species pairs. It contains also counts of species pairs and significant species (lower and upper 95% confidence limits) pairs for each score class and for the total matrix.

The file contains also expected numbers of significant values (simple CL criterion) obtained from 100 random matrices.

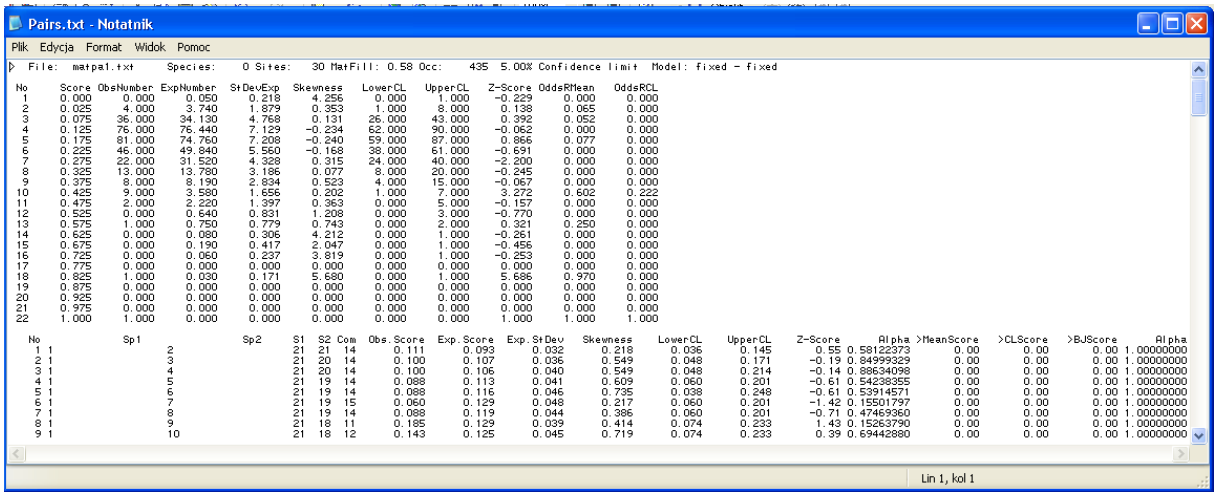
7. Citing *Pairs*

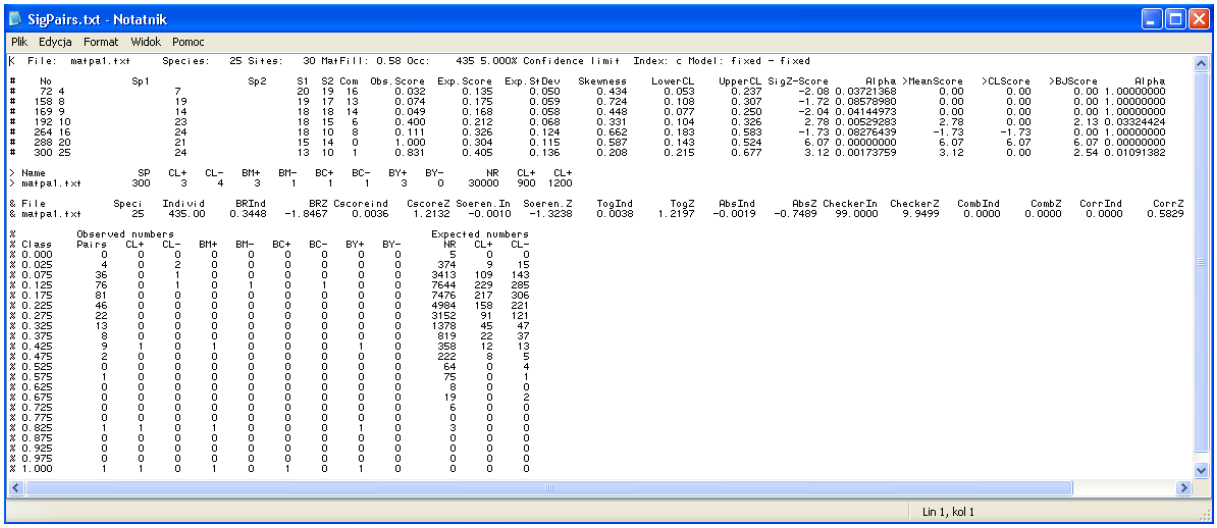
Pairs is freeware but nevertheless if you use *Pairs* in scientific work you should cite *Pairs* as follows:

Ulrich W. 2008. Pairs – a FORTRAN program for studying pair-wise species associations in ecological matrices. www.uni.torun.pl/~ulrichw

8. System requirements

Pairs is written in FORTRAN 95 and runs under Windows 9.x, XP, and Vista. The present version is





limited to 5000 sites, otherwise computation abilities are only limited by the computer's memory.

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