nature ecology & evolution

SUPPLEMENTARY INFORMATION

https://doi.org/10.1038/s41559-017-0391-4

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Biodiversity–multifunctionality relationships depend on identity and number of measured functions

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Supplementary Material Section 1: List of all variables included in the analysis

A large number of ecosystem variables were included in the analysis to approximate as wide a range of different ecosystem functions as possible (Supplementary Table 1.1). Variables include measurements on the level of the abiotic environment, of plants and consumers. Information on consumers was separated into different functional groups when possible. Otherwise, different taxonomic groups were separated as these groups not only indicate secondary productivity but also mediate different ecosystem functions: herbivory, predation, parasitism, decomposition, scavenging, pollination, and seed predation.

Supplementary Table 1.1: List of the 82 ecosystem variables measured in the Jena Experiment included in the analysis. Variables are indicative of ecosystem functions. The abbreviation and names of the variables are given with a short description of exemplary ecosystem functions that are approximated by the respective variable, as well as the year in which the variable was measured, and whether an increase or decrease in the variable is considered to indicate increased functioning. If different months or depths are listed, an average of these measurements was used in the analysis.

Abbreviation	Variable	Approximated ecosystem function: process rates, functional roles, ecosystem properties	Year	Direction of increased functioning	Month	Depth layers	Included in 2004
BM_coarseroot	Biomass of coarse roots	Belowground primary productivity, anchorage of plants, soil erosion control	2004	1	7		yes
BM_dead_DW	Aboveground biomass of dead plant material	Plant senescence, accumulation of aboveground litter	2007	0	5, 8		yes
BM_fineroot	Biomass of fine roots	Belowground primary productivity (reactive fraction), water and nutrient uptake, soil erosion control	2004	1	7		yes
BM_microbes	Biomass of soil microbes	Belowground secondary productivity, potential decomposition, mineralisation, soil carbon dynamics, high microbial biomass as indicator for biologically active soils	2007	1	5		yes
BM_targ_DW	Aboveground biomass of sown (target) plant community	Aboveground primary productivity	2007	1	5, 8		yes
BM_weed_DW	Aboveground biomass of weeds	Inverse to community stability (biomass component)	2007	-1	5, 8		yes

C_targ	Percentage of carbon in biomass of sown (target) plant community	Aboveground primary productivity, carbon sequestration	2007	1	5, 8	yes
Cov_bare	Cover of bare ground	Inverse to community productivity and aboveground space filling, inverse to soil erosion control	2007	-1	6, 8	yes
Cov_dead	Cover of dead plant material	Plant death rate, accumulation of dead material	2007	0	6, 8	no
Cov_targ	Cover of sown (target) plant species	Component of aboveground space filling and plant productivity, soil protection	2007	1	6, 8	yes
Cov_weed	Cover of weeds	Inverse to community stability (structural component)	2007	-1	6, 8	yes
Cperc_fineroot	Carbon concentration in fine roots	Belowground primary productivity, carbon sequestration	2004	1	7	yes
Delta13C_targ	δ13C in biomass of sown (target) plant species	Carbon cycling; indication of source of carbon fluxes	2004	0	5	yes
Delta15N_targ	δ15N in biomass of sown (target) plant species	Nitrogen cycling; contribution of atmospheric dinitrogen fixation (lower $\delta^{15}N$)	2004	0	5, 8	yes
Diam_root	Mean diameter of roots	Resource uptake, root morphology: associated positively with root herbivory and pathogen attack and negatively with mycorrhiza colonisation, desiccation protection	2004	1	7, 9	yes
Growth_root	Growth of root length between September and July	Belowground primary productivity	2004	1	7	yes
Height_targ	Mean of sown (target) plant community plant height	Component of 3D space filling and productivity, importance for light interception	2007	1	5, 8	yes
Height_weeds	Mean of weed plant height	Inverse to community stability (structural component)	2002	-1	7	no

Herbiv	Mean of herbivory in percent	Herbivory, i.e. transfer of energy to higher trophic levels	2005	0	8	yes
LAI	LAI measured 5cm above the ground	Light interception, measure of aboveground space filling	2007	1	5, 8	yes
Mortality_hymenopt	Mortality of trap nesting Hymenoptera	Arthropod death rate, proxy for infection and parasitism	2005	-1		no
N_aphidina	Abundance of Aphidina	Aboveground secondary productivity, herbivory	2004	1	10	yes
N_chilop	Abundance of Chilopoda	Belowground secondary productivity, predation	2006	1	5, 11	yes
N_cicada	Abundance of Auchenorrhyncha	Aboveground secondary productivity, herbivory	2004	1	10	yes
N_Col_phatoph	Abundance of phytophagous beetles	Aboveground secondary productivity, herbivory	2006	1	5, 11	no
N_Col_pred	Abundance of predatory beetles	Aboveground secondary productivity, predation	2006	1	5, 11	no
N_coleopt	Total abundance of Coleoptera including all feeding guilds	Aboveground secondary productivity, herbivory, predation, decomposition, fungivory	2004	1	10	yes
N_collemb	Abundance of Collembola	Belowground secondary productivity, decomposition, predation	2006	1	5, 11	no
N_dermap	Abundance of Dermaptera	Aboveground secondary productivity, decomposition, herbivory, predation	2004	1	10	yes
N_diplop	Abundance of Diplopoda	Belowground secondary productivity, decomposition	2004	1	5, 10	yes
N_dipt	Abundance of Diptera	Aboveground secondary productivity, pollination, herbivory, predation, scavenging, decomposition	2006	1	5, 11	no

N_earthw_endo	Abundance of endogeic earthworms	Belowground secondary productivity, bioturbation, soil fertility, decomposition	2006	1	5, 11	yes
N_enchy	Abundance of Enchytraeidae	Belowground secondary productivity, decomposition	2004	1	10	yes
N_gamasida	Abundance of Gamasida	Aboveground secondary production, predation	2006	1	5, 11	no
N_gastro	Abundance of Gastropoda	Aboveground secondary productivity, herbivory, scavenging	2006	1	5, 11	yes
N_herb_suck	Abundance of sucking herbivores	Aboveground secondary productivity, herbivory	2006	1	5, 11	no
N_heteropt	Abundance of Heteroptera	Aboveground secondary productivity, herbivory, predation	2004	1	10	yes
N_holes_voles	Number of burrowing holes by voles	Secondary productivity, seed predation, predation, bioturbation	2005	1	6, 9	no
N_hymenopt	Abundance of Hymenoptera	Aboveground secondary productivity, pollination, predation, parasitism	2006	1	5, 11	no
N_isop	Abundance of Isopoda	Belowground secondary productivity, decomposition	2006	1	5, 11	yes
N_larv_phytoph	Abundance of phytophagous insect larvae	Belowground secondary productivity, root herbivory	2006	1	5	no
N_larv_pred	Abundance of predatory beetle larvae	Belowground secondary productivity, belowground predation	2006	1	5, 11	no
N_lumbricus	Abundance of *Lumbricus terrestris*	Belowground secondary productivity, bioturbation, leaf litter decomposition, soil fertility	2004	1	5, 10	yes
N_mites	Abundance of mites	Belowground secondary productivity, predation, decomposition, herbivory, fungivory, parasitism	2006	1	5, 11	no

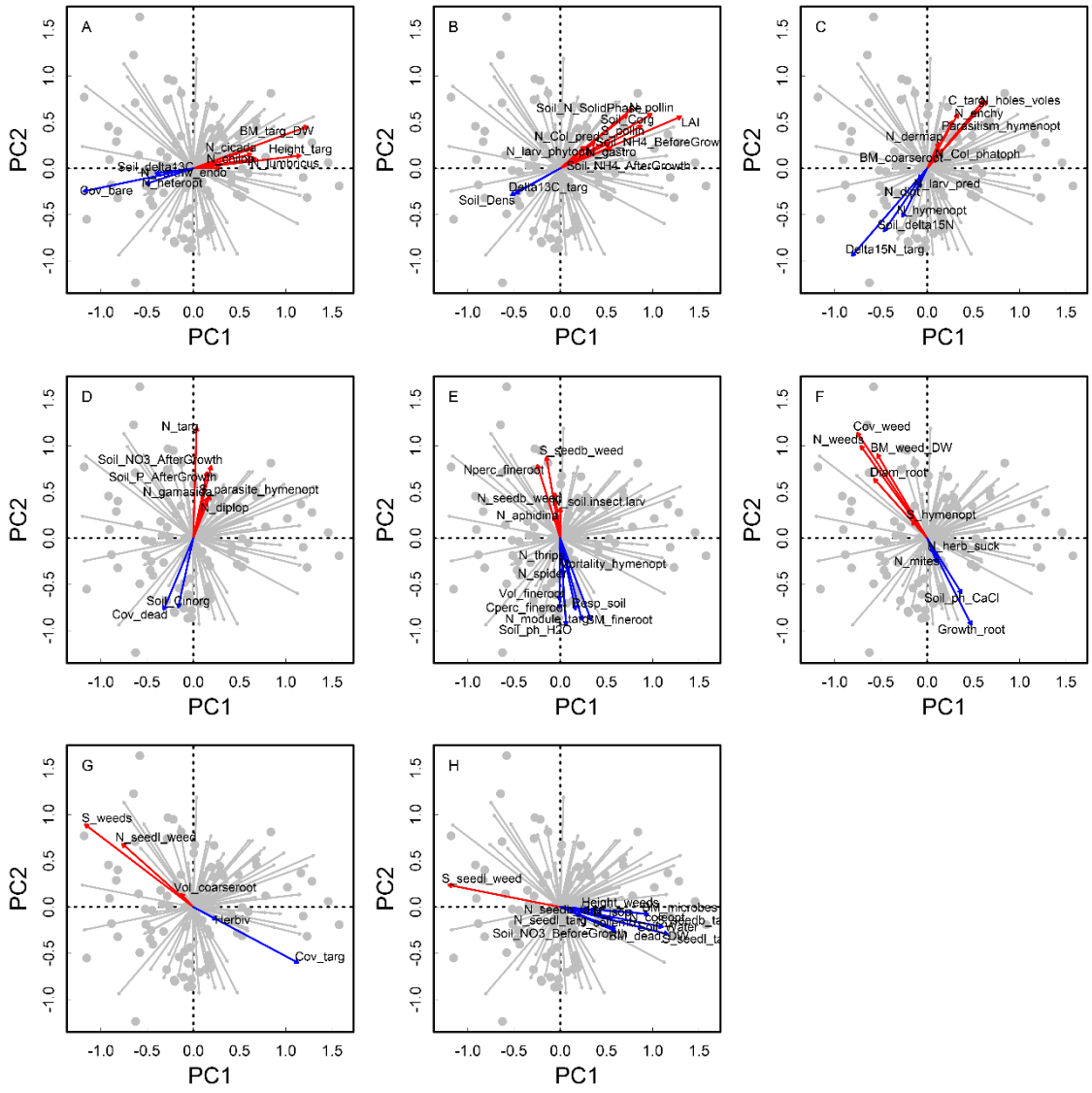
N_module_targ	Number of target plant modules per meter square	Aboveground space filling, indication of plant allocation strategies, aboveground primary productivity	2006	1	6	no
N_pollin	Flower visitor frequency	Pollination	2006	1	6, 8	no
N_seedb_targ	Number of viable seeds of target species in the seed bank per meter square	Plant community regeneration (abundance component)	2004	1	3	yes
N_seedb_weed	Number of viable seeds of weed species in the seed bank per meter square	Inverse to community stability (regeneration component)	2004	-1	3	yes
N_seedl_targ	Number of target plant seedlings per meter square	Plant community regeneration (abundance component)	2006	1	4, 7, 10	no
N_seedl_weed	Number of weed plant seedlings per meter square	Inverse to community stability (regeneration component)	2006	-1	4, 7, 10	no
N_soil.insect.larv	Abundance of insect larvae	Arthropod mediated functions	2004	1	10	yes
N_spider	Abundance of spiders	Aboveground secondary productivity, predation	2006	1	5, 11	yes
N_targ	Percent nitrogen in biomass of sown plant species	Plant nutrient uptake, growth strategies, nitrogen cycling	2007	1	5, 8	yes
N_thrips	Abundance of Thysanoptera	Aboveground secondary productivity, herbivory, pollination, fungivory, predation	2004	1	10	yes
N_weeds	Number of weeded individuals	Inverse to community stability (diversity component)	2004	-1	5, 8	yes
Nperc_fineroot	N concentration in fine roots	Plant nutrient uptake, growth strategies, plant water uptake	2004	1	7	yes
Parasitism_hymenopt	Parasitism rate of trap nesting Hymenoptera	Parasitism rate	2005	0		no
Resp_soil	Basal soil respiration	Microbial decomposition / mineralization, soil carbon	2007	1	5	yes

		dynamics, loss of organic soil carbon via respiration					
S_hymenopt	Species richness Hymenoptera	Stability of pollination and predation	2005	1			no
S_parasite_hymenopt	Species richness of parasites of Hymenoptera	Stability of parasitism	2005	1			no
S_pollin	Species richness of flower visitors per 6 minutes	Stability of pollination	2006	1	6, 8		no
S_seedb_targ	Species richness of seed bank of sown (target) plant species	Plant regeneration, stability of plant community composition	2004	1	3		yes
S_seedb_weed	Species richness of seed bank of weed plant species	Plant regeneration, inverse of stability of plant community composition	2004	-1	3		yes
S_seedl_targ	Species richness of seedlings of sown (target) plant species	Plant regeneration, stability of plant community composition	2006	1	4, 7, 10		no
S_seedl_weed	Species richness of seedlings of weed plant species	Plant regeneration, inverse of stability of plant community composition	2006	-1	4, 7, 10		no
S_weeds	Species richness of weeds	Inverse to stability of plant community (diversity component)	2004	-1	5, 8		yes
Soil_Cinorg	Concentration of inorganic carbon in solid phase soil samples	Component of soil formation, soil stability	2006	1	4	0, 5, 10, 15, 20, 25	yes
Soil_Corg	Concentration of organic carbon in solid phase soil samples	Component of soil formation, soil fertility, Carbon sequestration	2006	1	4	0, 5, 10, 15, 20, 25	yes
Soil_delta13C	$\delta^{13}C$ in soil samples	Carbon cycling, indication of organic plant derived carbon in the soil	2004	0	4	0, 5, 10, 15, 20, 25	yes
Soil_delta15N	$\delta^{15}N$ in soil samples	Nitrogen cycling, relative contribution of fixed atmospheric nitrogen (lower $\delta^{15}N$)	2004	0	4	0, 5, 10, 15, 20, 25	yes

Soil_Dens	Bulk density soil	Soil compaction, soil fertility	2006	-1	4	0, 5, 10, 15, 20, 25	no
Soil_N_SolidPhase	Concentration of mineral nitrogen in solid phase soil samples	Soil fertility	2006	1	4	0, 5, 10, 15, 20, 25	yes
Soil_NH4_AfterGrowth	Ammonium concentration in the soil after the growing season	Nitrogen cycling, nutrients left after plant growth, potential for nitrogen leaching	2007	-1	10	0	yes
Soil_NH4_BeforeGrowth	Ammonium concentration in the soil before the growing season	Nitrogen cycling, nutrients available for plant growth	2007	1	3	0	yes
Soil_NO3_AfterGrowth	Nitrate concentration in the soil after growing season	Nitrogen cycling, nutrients left after plant growth, potential for nitrogen leaching	2007	-1	10	0	yes
Soil_NO3_BeforeGrowth	Nitrate concentration in the soil before growing season	Nitrogen cycling, nutrients available for plant growth	2007	1	3	0	yes
Soil_P_AfterGrowth	Phosphate concentration in the soil after growing season	Phosphorus cycling, nutrients left after plant growth, potential for phosphorus leaching	2002	-1	9	0, 15	no
Soil_ph_CaCl	Soil pH in CaCl	Nutrient relations, decomposition, cation exchange on organic soil particles	2002	0	9	0, 15	no
Soil_ph_H2O	Soil pH in H_2O	Nutrient relations, decomposition, cation exchange on organic soil particles	2002	0	9	0, 15	no
Soil_Water	Soil water content per mass	Water availability, growth, nutrient transport	2007	1	3, 10	0	yes
Vol_coarseroot	Volume of coarse root standing stock	Plant-nutrient relations (accessed soil volume), size of the rhizosphere	2004	1	9		yes
Vol_fineroot	Volume of fine root standing stock	Plant-nutrient relations (accessed soil volume), size of the rhizosphere (reactive fraction), water uptake	2004	1	9		yes

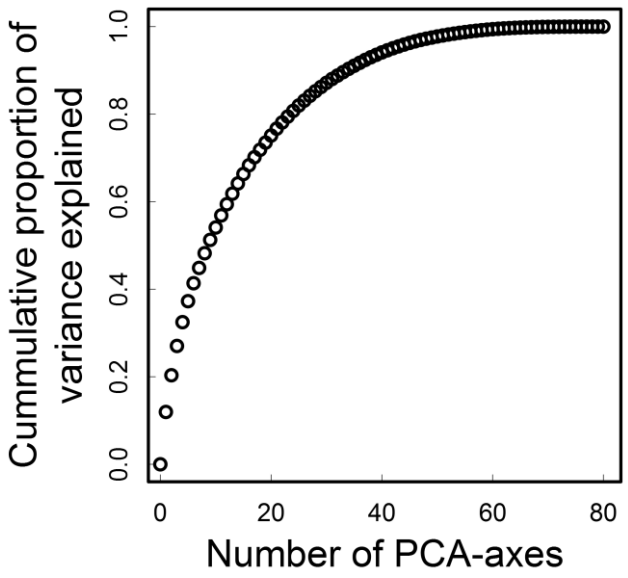
Supplementary Material Section 2: Correlations and trade-offs among functions

To calculate the multifunctionality index, a PCA was computed based on the 82 ecosystem variables indicative of ecosystem functions that were included in the analysis. The resulting PCA graph can be inspected for correlations and trade-offs between the ecosystem functions approximated by the variables. This is possible because angles between functions (depicted as arrows in the PCA-graph) represent the strength of correlations. Angles close to 0° represent strong positive correlations and angles close to 180° strong negative correlations. To visualise the correlations among the different functions, the functional space spanned by the PCA-axis 1 and 2 (360°) was divided into 16 segments; each of which was defined to be 22.5° wide. PCA-axis 1 was defined to be the first separation between segments. From there, segments were defined clockwise. Functions located in the same segment are positively correlated, functions located in opposing segments are negatively correlated as depicted in Supplementary Fig. 2.1. Note that these segments are only for visualisation. Angles close to 0° between two functions indicate strong positive correlations, while angles close to 180° indicate strong negative correlations. In a second approach, all 82 ecosystem variables and also the multifunctionality index were correlated pair-wise using the R-function chart.correlation from the package PerformanceAnalytics [12] (Supplementary Fig. 2.4).

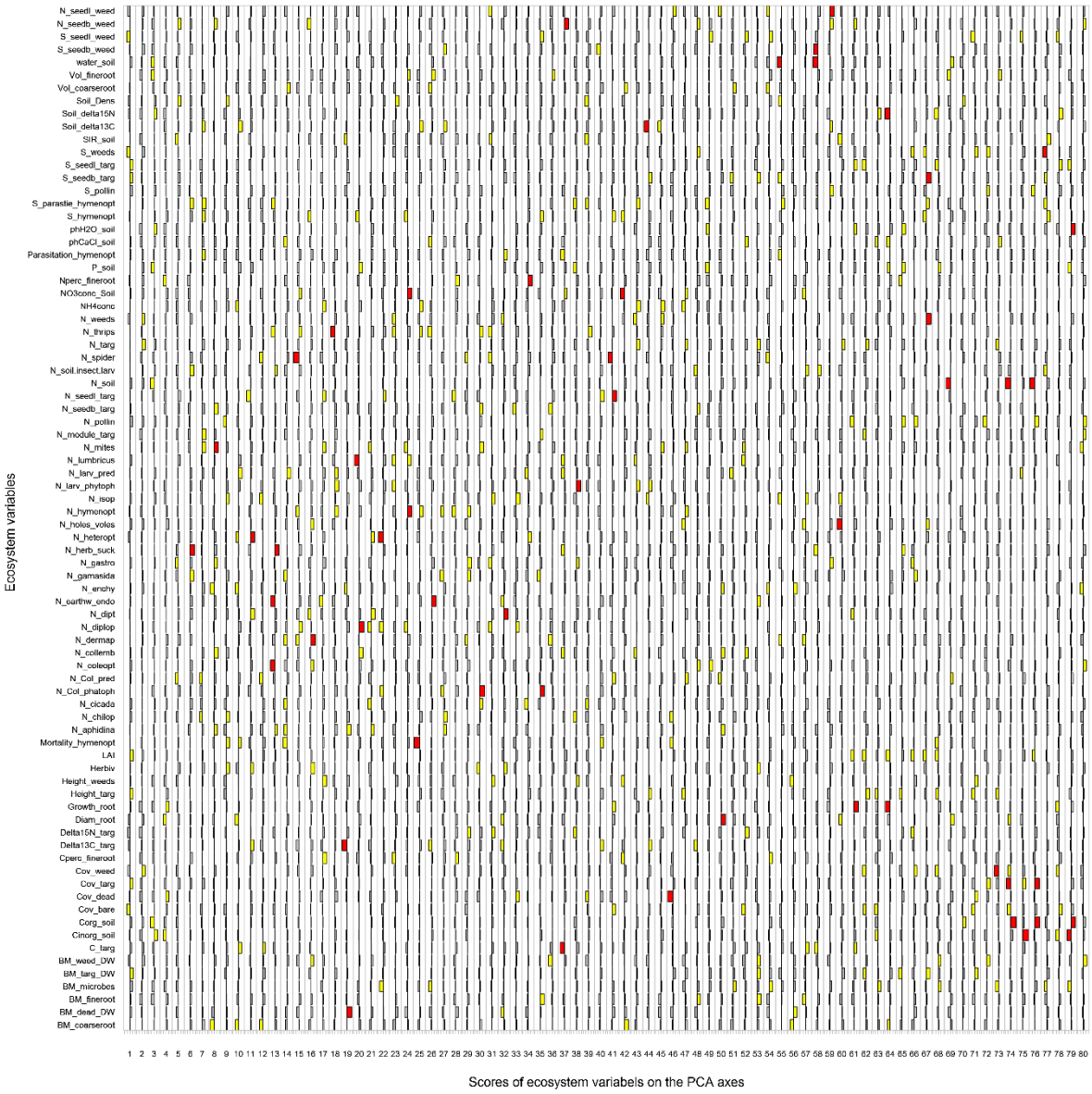


▲Supplementary Figure 2.1: Visualisation of the correlations among functions as indicated by the PCA. Angles among functions (depicted as arrows in the PCA-graph) represent the strength of correlations. Angles close to 0° represent strong positive correlations and angles close to 180° strong negative correlations. To visualise the correlations among the different functions, the functional space spanned by the PCA-axis 1 and 2 was divided into 16 segments. Functions in opposing segments show trade-offs and are coloured in blue and red and labelled with the short name of the function. For a definition of short names, see Supplementary Table 1.1.

The proportion of explained variance increased steadily with the number of PCA-axis included, without showing any clearly visible cut-offs (Supplementary Fig. 2.2). The large number of 24 PCA-axis was needed to explain at least 80% of the variance contained in the multifunctional space. The number of axes needed to reach a large cumulative percentage of variance explained can be interpreted as an indication of the amount of independent information in a dataset. In our case, a large number of needed axes indicated many independent ecosystem functions. This interpretation can be illustrated by a simple example. If all functions included in the dataset would be perfectly correlated (positively or negatively), then all variability in the data would be explained by one axis, and the first principle component axis would explain 100% of the variance. If in the other extreme case, all functions would be completely independent, i.e. having a covariance of zero, then each function would represent an independent principle component, and the number of PCA-axes needed to explain the variance in the data would be equal to the number of functions. Real datasets will produce intermediate results between these two extremes, depending on the interrelations among the included functions.



Supplementary Figure 2.2: Cumulative proportion of variance explained by an increasing number of PCA-axes. PCA-axis 1 explained 12% of the variance in trait-space, and all further PCA-axis explained less with axis 2 accounting for additional 8% of variance explained.

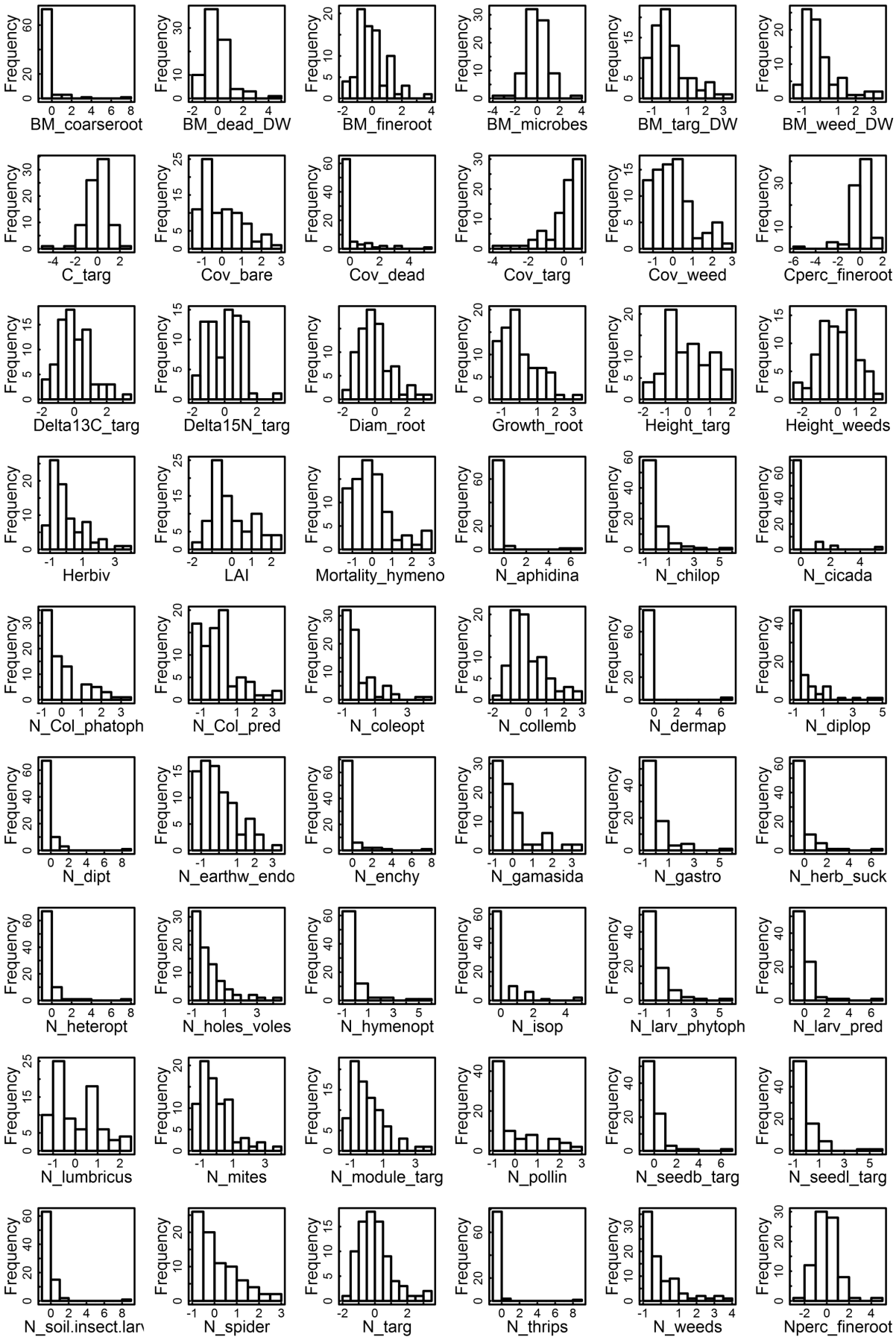


Supplementary Figure 2.3: Loadings of all 82 ecosystem variables on principle components of the ordination shown in Fig. 1a. Loadings ranged from -0.41 to 0.43. Loadings with absolute values in the range of 0.2 to 0.3 are shown in yellow, loadings exceeding 0.3 in absolute values are shown in red. No axis is clearly associated with a number of variables low enough to enable easy interpretation. Rather all axes represent a combination of many different ecosystem variables. A high-resolution version of the graphic is provided as a separate file in the supplementary material.

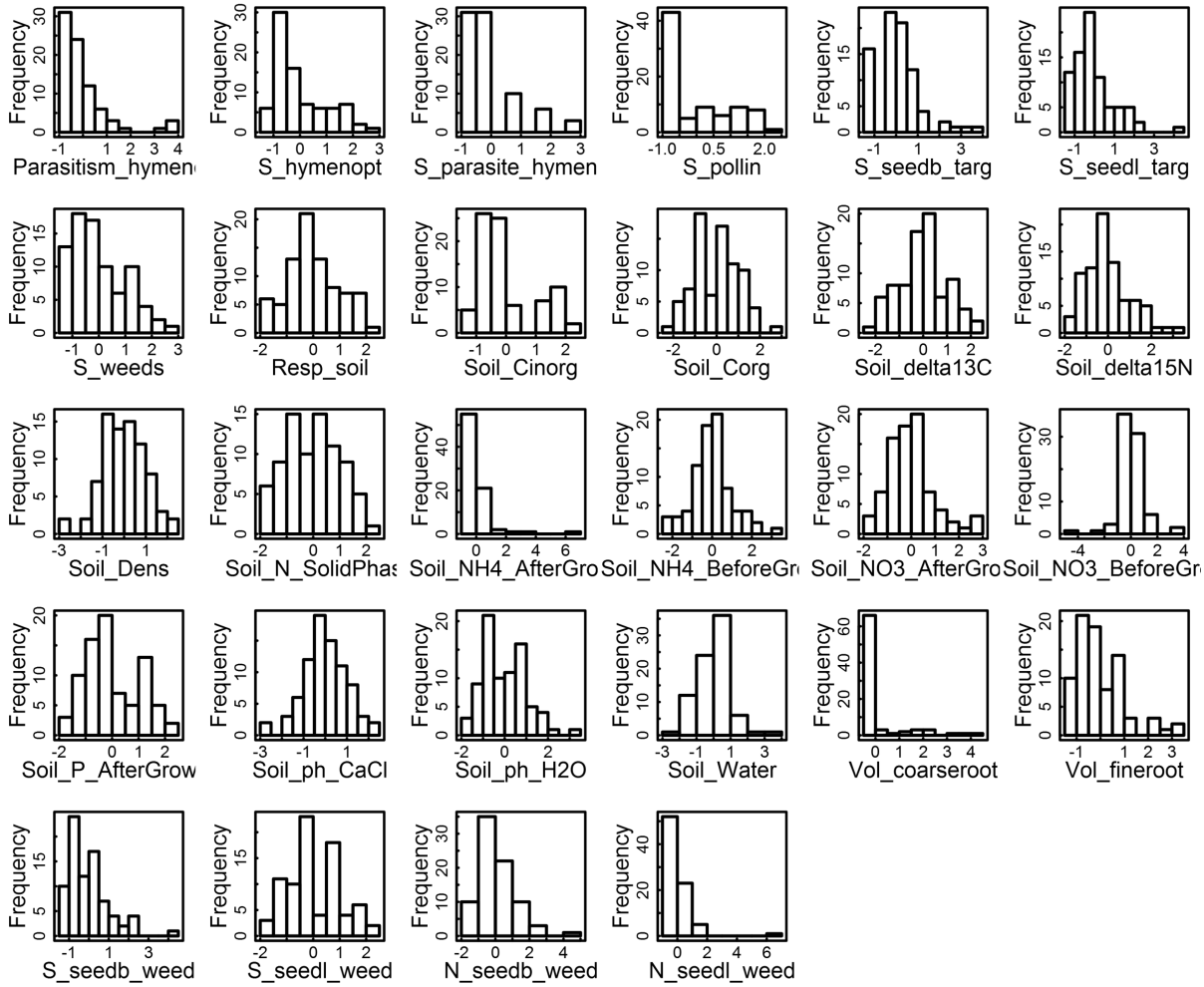
Supplementary Figure 2.4: Pairwise correlations between all 82 ecosystem variables included in the analysis to indicate ecosystem functions and the calculated index of multifunctionality. A high-resolution version of the graphic is provided as a separate file in the supplementary material.

Supplementary Material Section 3: Sensitivity analysis for non-normally distributed data on ecosystem functions

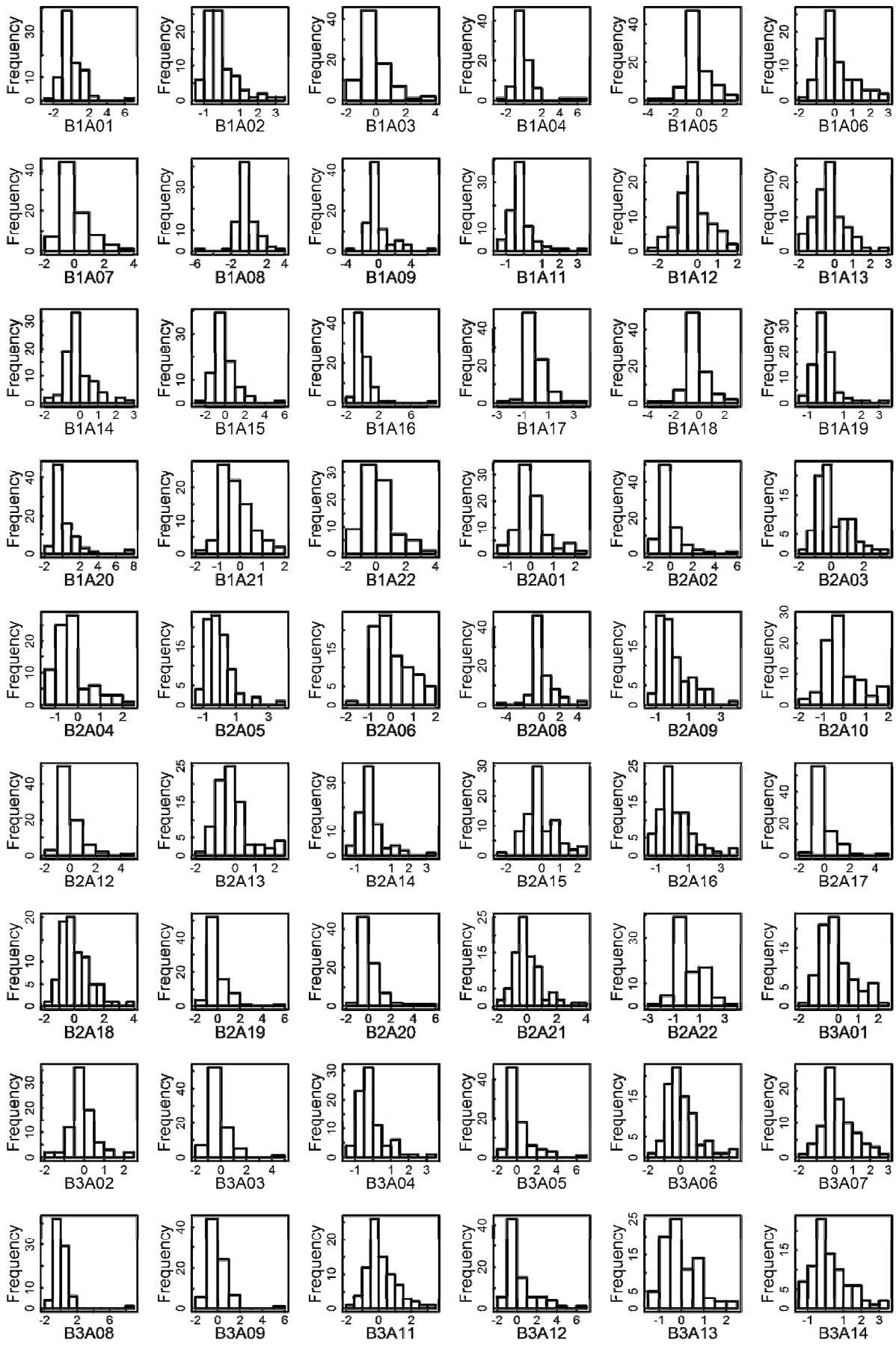
The variables indicating ecosystem functions in the different plots of the Jena Experiment were often not normally distributed across the different plots within a variable (Supplementary Fig. 3.1) or across the different variables within a plot (Supplementary Fig. 3.2). Such distributions indicate that the relationships between variables might be non-linear. Because the principal component analysis (PCA) used in our analysis assumes linear relationships, we conducted a sensitivity analysis testing for the influence of potential non-linear relationships on our results. To do so, we calculated a principle coordinate analysis (PCoA) based on Gower distances that are not assuming any shape of the relationship between variables. The multifunctional space covered by the experimental plots in the PCoA (Supplementary Fig. 3.3A) was very similar to the results of the PCA. This visual inspection was confirmed by a formal comparison of the results of the two approaches via a Procrustes rotation (Supplementary Fig. 3.3B) that showed only minimal differences in the configuration of the experimental plots in multifunctional space created by the two approaches. Similarly, the configurations resulting from an NMDS based on a Gower distance matrix of all plots showed large similarity with the configurations resulting from the PCA or the PCoA method (Supplementary Fig. 3.4) Consequently, potential non-linear relationships between ecosystem variables were of minor importance in our dataset and the PCA used in the analysis was robust against their occurrence.



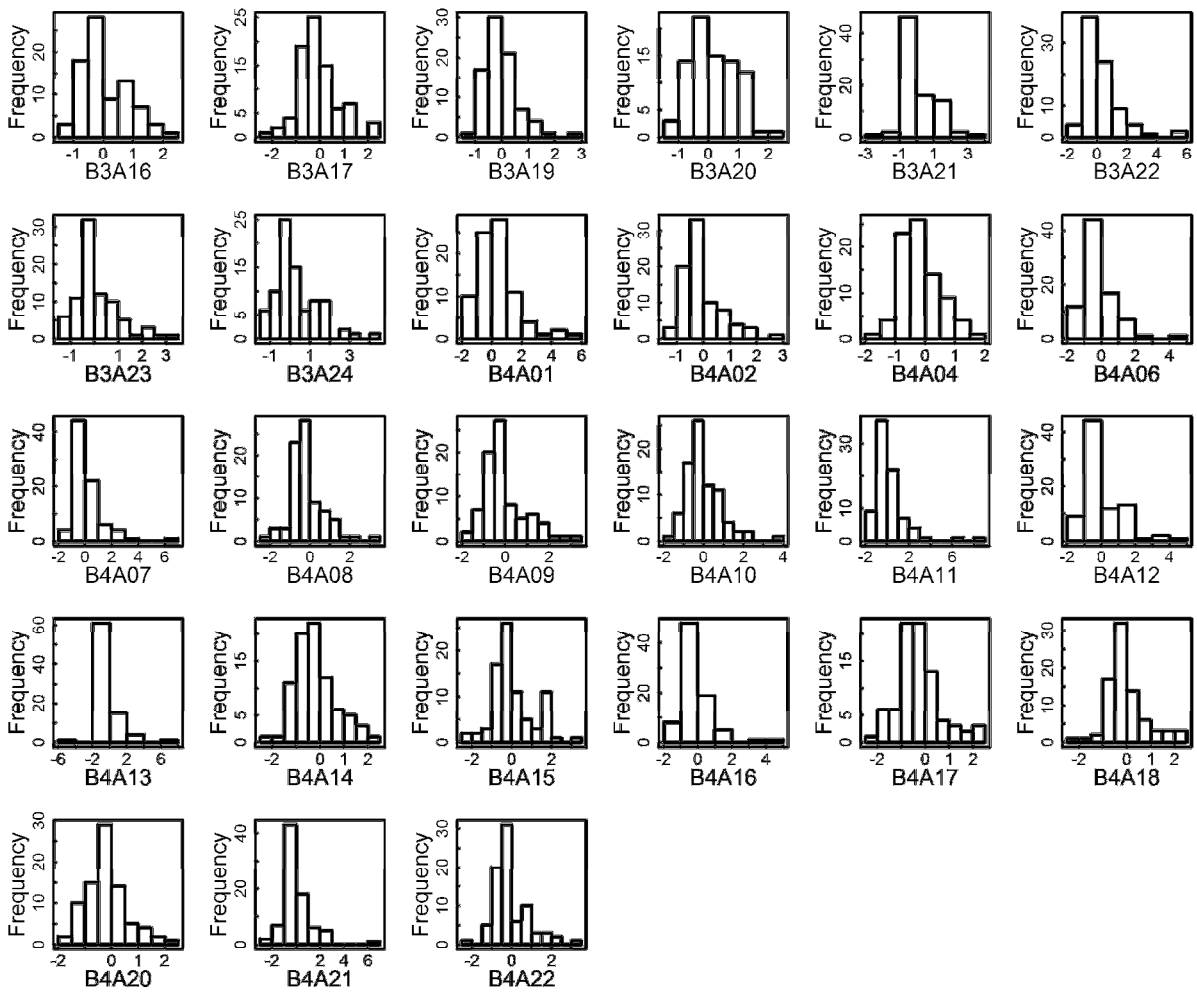
Supplementary Figure 3.1: Distribution of the column vectors of the ecosystem variable matrix on which the multivariate analysis was based. Histograms for the distribution of all 82 ecosystem variables over the 81 experimental plots of the Jena Experiment are given. All variables have been centred on their mean and standardised to units of standard deviations (z-transformed).



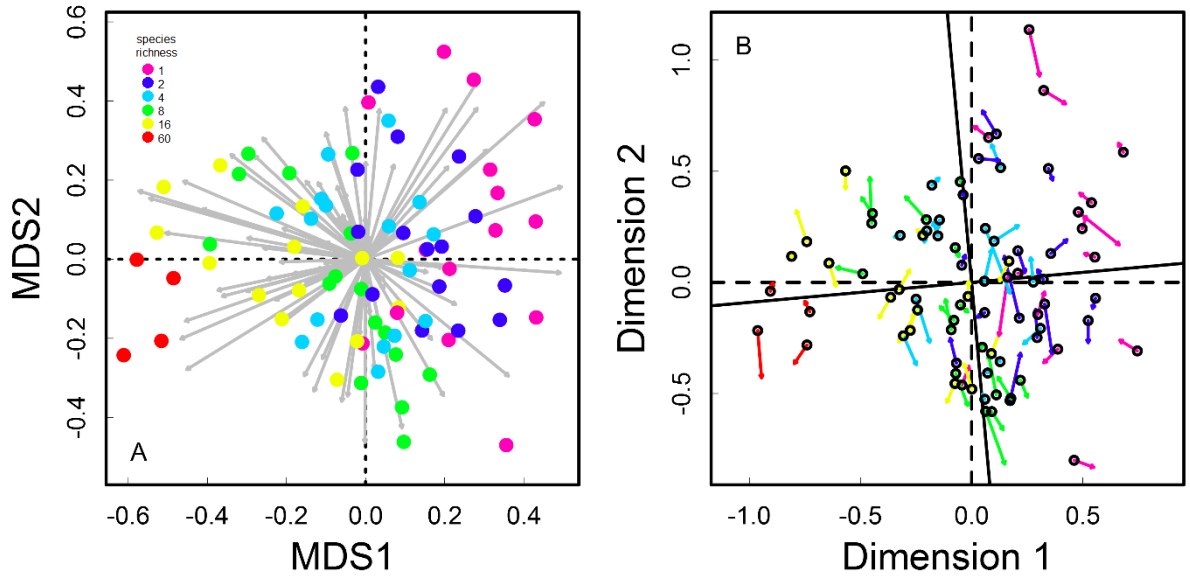
Supplementary Figure 3.1 continued



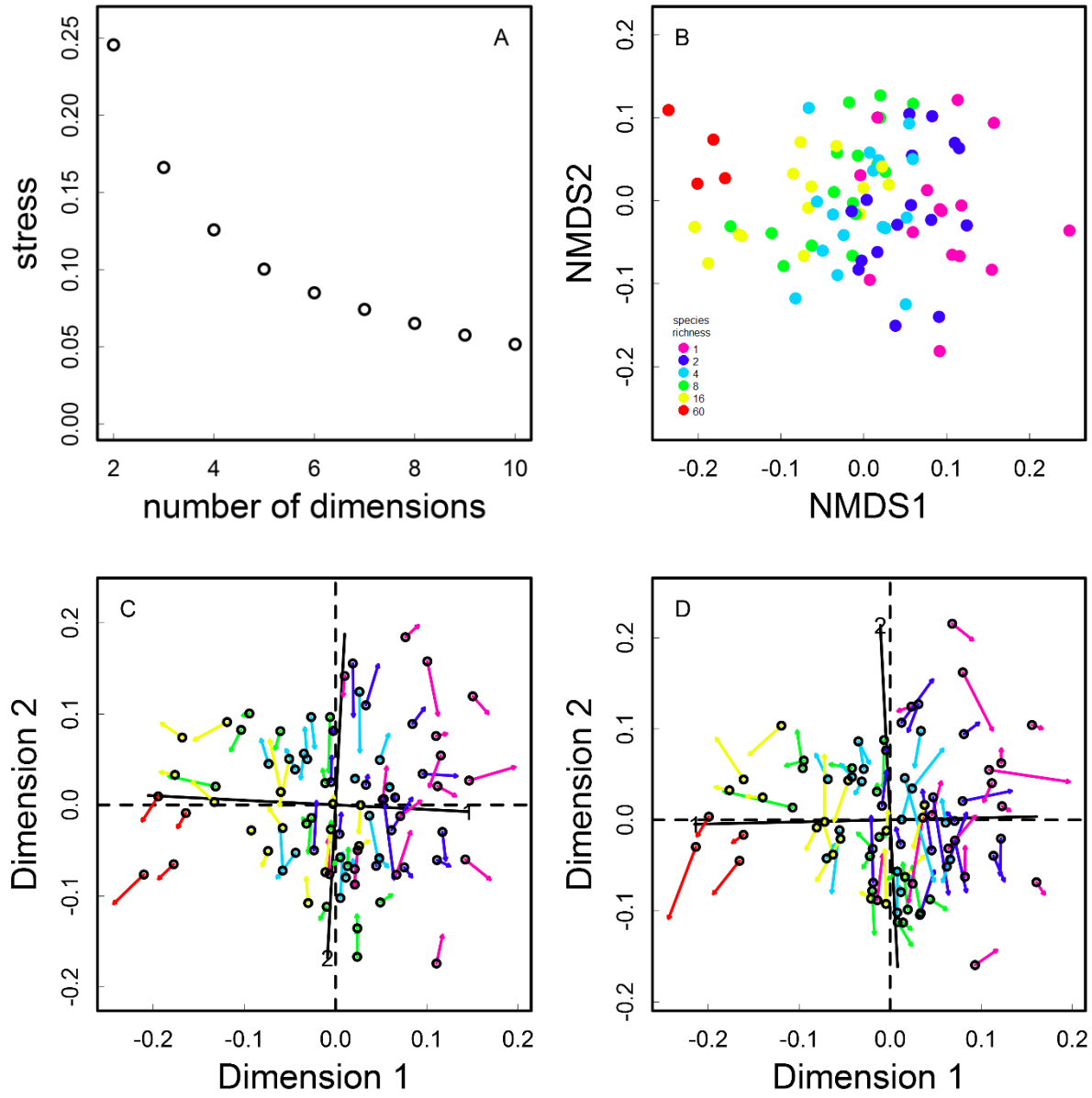
Supplementary Figure 3.2: Distribution of the row vectors of the ecosystem variable matrix on which the multivariate analysis was based. Histograms for the distribution of ecosystem variables measured on each of the 81 experimental plots of the Jena Experiment over all 82 ecosystem variables included in the analysis are given. All variables have been centred on their mean and standardised to units of standard deviations (z-transformed).



Supplementary Figure 3.2 continued



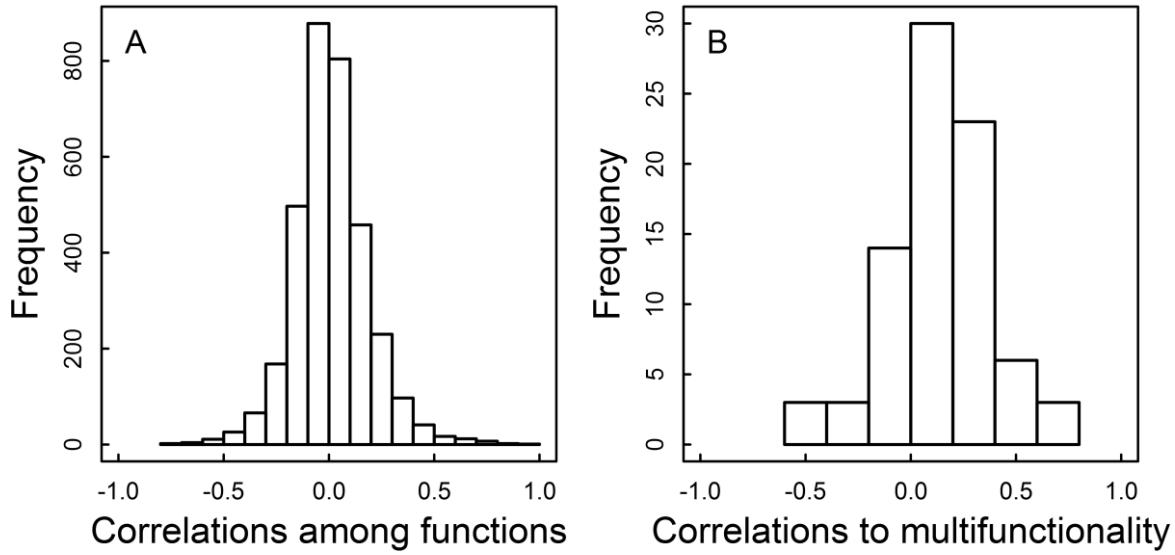
Supplementary Figure 3.3: (A) Results from a principle coordinates analysis based on Gower-distances, and (B) a comparison of the resulting multifunctional space to the results of the PCA shown in Fig. 1a. Panel A shows the position of each plot (coloured dots) in a multifunctional space spanned by the first two PCoA-axes derived from analysing different ecosystem variables measured in the Jena Experiment to indicate ecosystem functions. The red dots (60-species mixtures) form a distinct cluster at the left-hand side of the graph and are not in the centre of the plot. Each of the functions is shown by a grey arrow. Panel B shows the results of a Procrustes rotation comparing the PCoA results from Graph A to the PCA results shown in Fig. 1a. Dashed lines are the coordination system of the PCoA and the solid lines the coordination system of the PCA that has been turned around the origin to maximise overlap. Coloured arrows indicate how much the position of individual plots in multifunctional space change from the PCA (start of arrows and black circles) to the PCoA (end of arrows). Colours indicate the diversity level of plots, as indicated in the legend of Panel A.



Supplementary Figure 3.4: Results from a nonmetric multidimensional scaling (NMDS) based on Gower-distances. (A) A scree plot of stress of the NMDS against an increasing number of dimensions used in the NMDS configuration. (B) The NMDS result showing the first two dimensions of the configuration. (C) A comparison of the resulting multifunctional space of the NMDS to the results of the PCoA shown in Supplementary Fig. 3.3A. (D) A comparison of the resulting multifunctional space of the NMDS to the results of the PCA shown in Fig. 1a. Panel A shows that at least 5 dimensions are needed for the NMDS to adequately describe the multifunctional space. Panel B shows the position of each plot (coloured dots) in a multifunctional space spanned by the first two dimensions in the NMDS derived from analysing different ecosystem variables measured in the Jena Experiment to indicate ecosystem functions. The red dots (60-species mixtures) form a distinct cluster at the left-hand side of the graph and are not in the centre of the plot. Panel C and D shows the results of a Procrustes rotation comparing the NMDS results to the PCoA results (Supplementary Fig. 3.3A) and to the PCA results shown in Fig. 1a. Dashed lines are the coordination system of the NMDS and the solid lines the coordination system of the other analyses that have been turned around the origin to maximise overlap. Coloured arrows indicate how much the position of individual plots in multifunctional space change from the PCA or PC0A (start of arrows and black circles) to the NMDS (end of arrows). Colours indicate the diversity level of plots, as indicated in the legend of Panel B.

Supplementary Material Section 4: Correlations between functions and the index of multifunctionality

To quantified the correlations among all individual ecosystem functions, a correlation matrix including all pairwise combinations of the ecosystem variables included in the analysis to indicate ecosystem functions was calculated using the R-function cor. Restricting this matrix to the values below the 1:1 diagonal, correlation coefficients were extracted and were summed as a histogram. Similarly, correlations of all individual ecosystem functions and the index of multifunctionality were calculated. Resulting r and p values were tabulated (Supplementary Table 4.1). Scatter plots of the relationships can be found in the last row of Supplementary Fig. 2.4. A summary of the correlations among the individual functions and of individual functions with multifunctionality is shown in Supplementary Fig. 2.2.



Supplementary Figure 4.1. Pairwise correlations among all functions and between individual functions and multifunctionality. (A) The distribution of pairwise correlations observed between the ecosystem functions included in the analysis. A full matrix of pairwise correlations is shown in Supplementary Figure 2.4. (B) The distribution of pairwise correlations between the individual functions and the index of multifunctionality are shown in Fig. 2B. A full analysis of all pairwise correlations between all functions and multifunctionality is presented in Supplementary Table 4.1.

Supplementary Table 4.1: Individual correlations between the ecosystem variables indicating ecosystem functions and the index of multifunctionality and between the ecosystem variables and plant species richness. Given are r- and p-values of the correlations ordered by their significance of the correlation with multifunctionality. Significant correlations with multifunctionality are highlighted in bold and colour; blue indicates positive and red negative relationships.

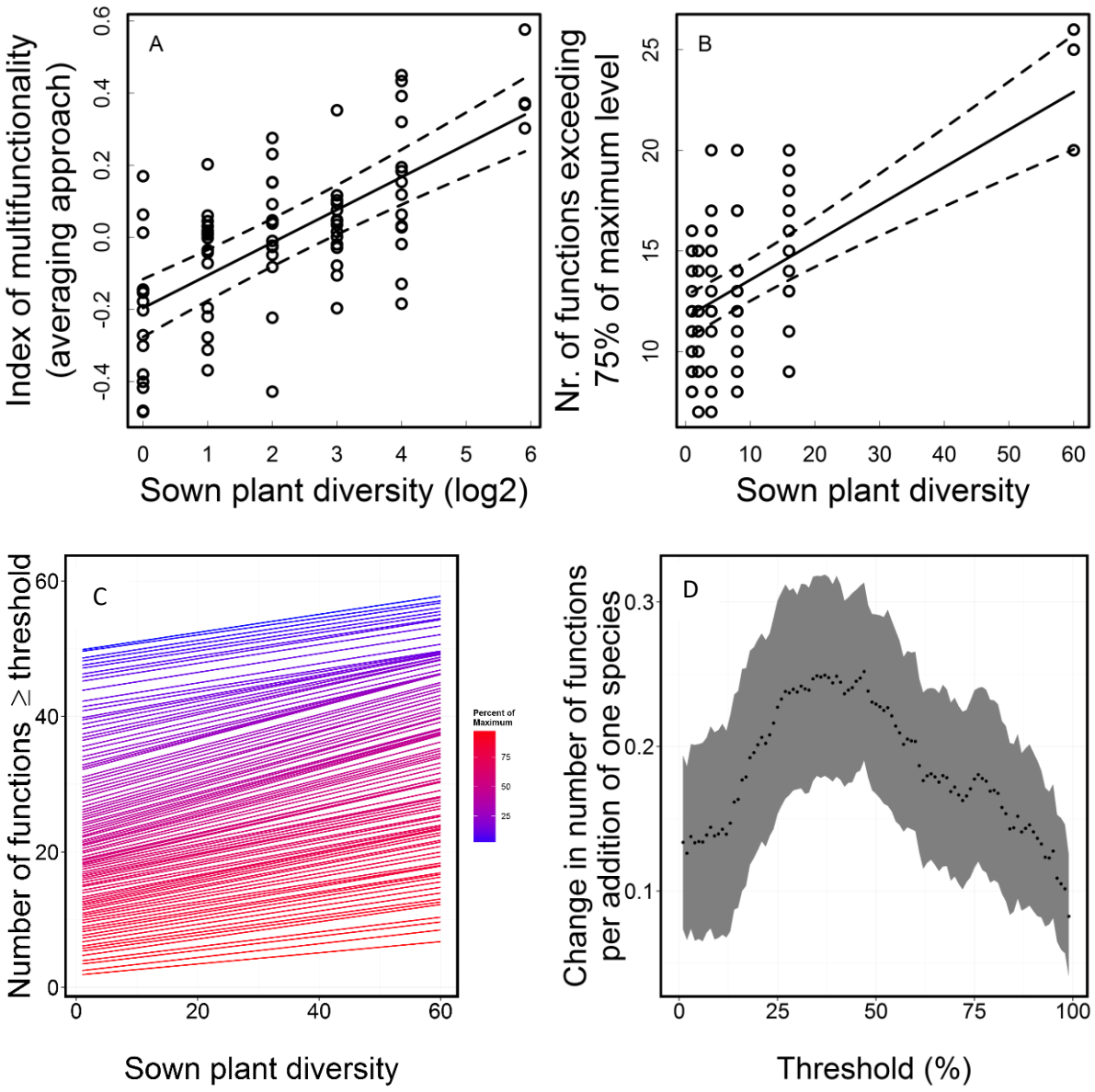
	Multifunctionality		Plant species richness	
Variable	r	P	R	p
Soil_Corg	0.69	**<0.001**	0.13	0.247
Soil_N_SolidPhase	0.63	**<0.001**	0.16	0.144
BM_microbes	0.61	**<0.001**	0.30	0.007
LAI	0.54	**<0.001**	0.59	<0.001
Cov_bare	-0.52	**<0.001**	-0.44	<0.001
N_coleopt	0.51	**<0.001**	0.25	0.027
Soil_Dens	-0.50	**<0.001**	-0.07	0.543
Soil_Water	0.47	**<0.001**	0.23	0.039
N_gamasida	0.44	**<0.001**	0.01	0.925
Soil_P_AfterGrowth	0.43	**<0.001**	-0.16	0.163
Delta15N_targ	-0.41	**<0.001**	-0.31	0.005
C_targ	0.41	**<0.001**	0.07	0.515
Soil_NH4_BeforeGrowth	0.38	**<0.001**	0.19	0.085
BM_targ_DW	0.37	**0.001**	0.52	<0.001
Parasitism_hymenopt	0.37	**0.001**	-0.08	0.481
N_collemb	0.36	**0.001**	0.16	0.150
Height_weeds	0.34	**0.002**	0.03	0.781
N_chilop	0.33	**0.003**	0.53	<0.001
Cov_targ	0.32	**0.003**	0.40	<0.001
N_enchy	0.31	**0.005**	0.01	0.960
Height_targ	0.31	**0.005**	0.54	<0.001
N_earthw_endo	0.30	**0.007**	0.09	0.402
S_seedb_weed	0.30	**0.007**	-0.12	0.274
N_targ	0.30	**0.007**	-0.10	0.395
S_parasite_hymenopt	0.29	**0.008**	-0.09	0.426
N_larv_phytoph	0.28	**0.010**	0.02	0.835
Cov_dead	-0.28	**0.011**	-0.18	0.100
Soil_delta15N	-0.28	**0.011**	-0.19	0.092
N_gastro	0.27	**0.016**	0.16	0.145
S_seedl_weed	-0.25	**0.022**	-0.52	<0.001
Herbiv	0.25	**0.027**	0.15	0.195
S_seedl_targ	0.24	**0.029**	0.77	<0.001
Vol_coarseroot	0.24	**0.030**	-0.06	0.594
N_pollin	0.23	**0.037**	0.44	<0.001
S_seedb_targ	0.23	**0.042**	0.83	<0.001
BM_dead_DW	0.22	**0.049**	0.30	0.006
N_Col_pred	0.22	0.052	0.18	0.107
N_cicada	0.22	0.054	0.31	0.005
Soil_Cinorg	-0.19	0.084	0.00	0.981

Soil_NO3_AfterGrowth	0.19	0.091	0.05	0.673
N_seedb_targ	0.19	0.094	0.01	0.922
N_Col_phatoph	0.17	0.122	-0.02	0.855
Nperc_fineroot	0.17	0.125	-0.21	0.056
S_weeds	-0.17	0.134	-0.49	<0.001
S_pollin	0.16	0.160	0.49	<0.001
Soil_ph_CaCl	0.16	0.166	0.17	0.123
N_isop	0.15	0.175	0.35	0.001
Diam_root	0.15	0.181	-0.22	0.048
N_holes_voles	0.14	0.214	0.26	0.019
N_thrips	0.13	0.239	-0.07	0.560
N_hymenopt	-0.11	0.322	-0.03	0.797
Cperc_fineroot	0.11	0.339	0.08	0.492
Soil_ph_H2O	-0.11	0.341	0.07	0.523
N_weeds	0.10	0.354	-0.34	0.002
BM_weed_DW	0.10	0.396	-0.32	0.004
N_mites	0.09	0.424	-0.08	0.457
Soil_NH4_AfterGrowth	0.08	0.464	0.20	0.075
N_larv_pred	-0.08	0.466	-0.04	0.744
N_lumbricus	0.07	0.521	0.29	0.008
N_diplop	0.07	0.526	0.11	0.341
Resp_soil	-0.07	0.527	0.01	0.941
N_seedb_weed	0.07	0.536	-0.10	0.379
N_seedl_targ	0.07	0.544	0.01	0.926
Delta13C_targ	-0.07	0.553	-0.24	0.029
N_heteropt	-0.07	0.553	-0.12	0.291
N_seedl_weed	0.06	0.569	-0.32	0.003
Soil_delta13C	-0.06	0.576	-0.20	0.069
Vol_fineroot	0.06	0.581	-0.01	0.957
Mortality_hymenopt	-0.06	0.589	0.01	0.958
S_hymenopt	-0.06	0.603	-0.09	0.429
BM_coarseroot	0.04	0.720	0.00	0.981
N_dermap	0.04	0.727	0.02	0.884
Soil_NO3_BeforeGrowth	0.04	0.734	0.20	0.074
Growth_root	-0.04	0.755	0.23	0.043
N_soil.insect.larv	-0.03	0.786	-0.04	0.691
N_aphidina	0.03	0.787	-0.06	0.582
N_dipt	0.03	0.790	0.00	0.970
Cov_weed	0.02	0.838	-0.35	0.001
BM_fineroot	0.02	0.869	0.18	0.113
N_module_targ	0.02	0.875	-0.15	0.170
N_herb_suck	-0.01	0.911	0.09	0.403
N_spider	0.01	0.912	0.06	0.579

Supplementary Material Section 5: Different approaches to multifunctionality

Based on the review by Byrnes, et al. [8], we calculated multifunctionality with all reviewed approaches provided in the package multifunc [9]. Our data were unsuitable for an additional multiplicative approach presented by Bowker, et al. [13] for three reasons: (1) All ecosystem variables included some plots for which zeros were measured, resulting in a multiplicative multifunctionality index of zero for all plots. (2) Some ecosystem variables would have to be inverted because lower values are indicators of better functioning. This would require multiplication with -1 causing the whole index to become negative. (3) Some ecosystem variables change their sign along the diversity gradient from positive to negative or negative to positive. These variables cannot be transformed because adding a constant to shift the whole variable to positive or negative values would distort the results for the multiplicative index. Results from all different approaches that could be applied to our data support the conclusion that multifunctionality increases with sown plant diversity for the investigated 82 ecosystem variables measured in the Jena Experiment (Fig. 1B).

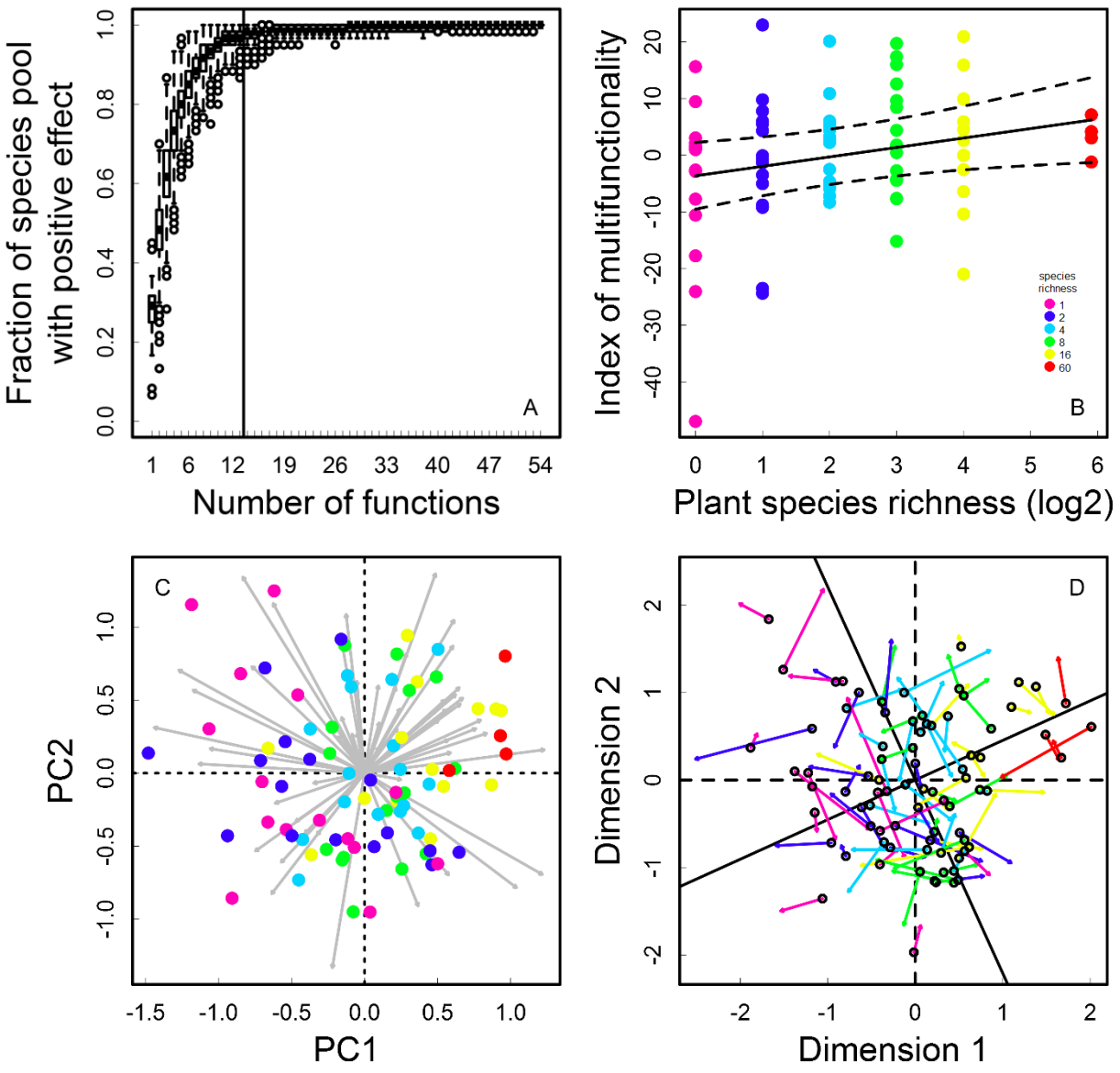
Similar results to the multivariate index of multifunctionality were obtained with the averaging, the threshold and the multiple-threshold approaches calculating multifunctionality [8]. With increasing plant species richness, multifunctionality increased independently of the approach chosen (Supplementary Fig. 5.1). In the averaging approach [6], all functions were averaged per plot, and this measure of multifunctionality was regressed against plant species richness. In the threshold approach, the number of functions that exceeds 75% of the maximum level of functioning was calculated for each plot. Following the recommendation by Byrnes et al. [8], the maximum level of functioning was calculated as the average of the five plots with the highest values measured for the respective function. While in the averaging approach, multifunctionality saturated with increasing plant species richness (Supplementary Fig. 5.1A), multifunctionality and species richness were linearly related in the threshold approach (Supplementary Fig. 5.1B). This qualitative difference can result from the fact that in the averaging approach, functions with large absolute differences along the diversity gradient tend to dominate the results, thus reducing the effective number of functions on which the calculation of multifunctionality is based. In contrast, in the threshold approach, each function contributes equally. Therefore, the results from the threshold approach are less likely to saturate along a gradient of plant diversity. Finally, in the multiple-threshold approach, the same calculations were performed as in the threshold approach but with all threshold values from 1 to 99% [8] (Supplementary Fig. 5.1C-D). This analysis revealed that multifunctionality increased with plant species richness over the whole range of tested thresholds. Thus, in contrast to previous studies [8,14], there was no threshold above or below which there was no significant effect of biodiversity on multifunctionality anymore. The strongest effects of plant species richness on multifunctionality were observed at medium high threshold values between 25% and 50% (Supplementary Fig. 5.1D).



Supplementary Figure 5.1: Results from alternative approaches to calculating multifunctionality. (A) Results from the averaging approach ($F_{1,76}$=76.0; p=5 * 10^{-13}). (B) Results from the threshold approach ($F_{1,76}$=49.2; p=8 * 10^{-10}). Each dot represents one of the 81 plots of the Jena Experiment. (C and D) Results from the multiple-thresholds approach; (C) The number of functions exceeding the defined critical threshold plotted against sown plant diversity. Different colours indicate the critical threshold of the level of functioning that needs to be reached in a plot for this plot being considered functioning with respect to this function. Cold colours indicate low thresholds, while warm colours indicate high thresholds. (D) The slope between the number of functions exceeding the threshold and sown plant diversity plotted against the values of the critical threshold on the x-axis. The shaded area identifies confidence bands around the slopes that are plotted as black symbols.

Supplementary Material Section 6: A sensitivity analysis for the effect of including data on ecosystem functions measured in different years.

Our analysis is a stringent test of the relationship between multifunctionality and biodiversity because all data are collected under controlled conditions on a single field site. However, we included data of ecosystem functions measured in multiple years, so that variability among years (e.g., climatic variation, the age of the experiment) might have contributed to the documented effects on multifunctionality. That is because including a larger number of contexts (defined as years, habitats, experiments) when investigating the relationship between biodiversity and multifunctionality, increases the strength of this relationship [3]. To investigate if the detected effect of biodiversity on multifunctionality in our study depended on the inclusion of different contexts, we conducted a sensitivity analysis that restricted the data on ecosystem functions used to variables from 2004 only; which is the year with most data available. This resulted in a dataset with 54 ecosystem variables for which the number of species contributing to functioning and the multivariate index of multifunctionality was calculated in the same way as in the main analysis. As in the main analysis, all species contributed to at least one function when a sufficiently large number of functions was considered. The critical number of functions was 13 functions and therefore slightly higher than in the main analysis (Supplementary Fig. 6.1A). Thus, the sensitivity analysis confirms the result of the main analysis that very low redundancy among species is observed in our experimental grasslands. The multivariate index of multifunctionality calculated with data from 2004 increased significantly with plant diversity in the sensitivity analysis (Supplementary Fig. 6.1B; $F_{1,76}=4.73$; $p=0.033$). When inspecting the underlying PCA (Supplementary Fig. 6.1C), the diversity gradient is visible along the first PCA-axis as in the main analysis (Fig. 2A). As in the main analysis, the score of the experimental plots along PCA-axis 1 was highly significantly correlated to plant species richness ($r=0.63$, $t_{79}=7.14$, $p=4*10^{-10}$). However, the correlation was weaker than in the main analysis, and the experimental plots of different diversity levels formed a less distinct gradient along the first PCA-axis compared to the main analysis. The multifunctional configurations of experimental plots in the PCAs of the main and the sensitivity analysis were formally compared in a Procrustes rotation that shows large differences in the position of many plots in the multivariate space (Supplementary Fig. 6.1D). These differences and the resulting slight reduction in the effect of biodiversity on multifunctionality can be caused by at three effects. First, by restricting the analysis to data from a single year, thus reducing the number of contexts sensu Isbell, et al. [3]; second, by reducing the number of functions considered; and third by changes in the identity of functions included in the calculation of multifunctionality (Fig. 2). However, the results of the sensitivity analysis emphasise that the inclusion of different contexts is not a prerequisite for effects of diversity on multifunctionality and that both main conclusions of this analysis (all species contribute to ecosystem functioning and multifunctionality increases with plant species richness) are also valid when analysing data from only a single year.

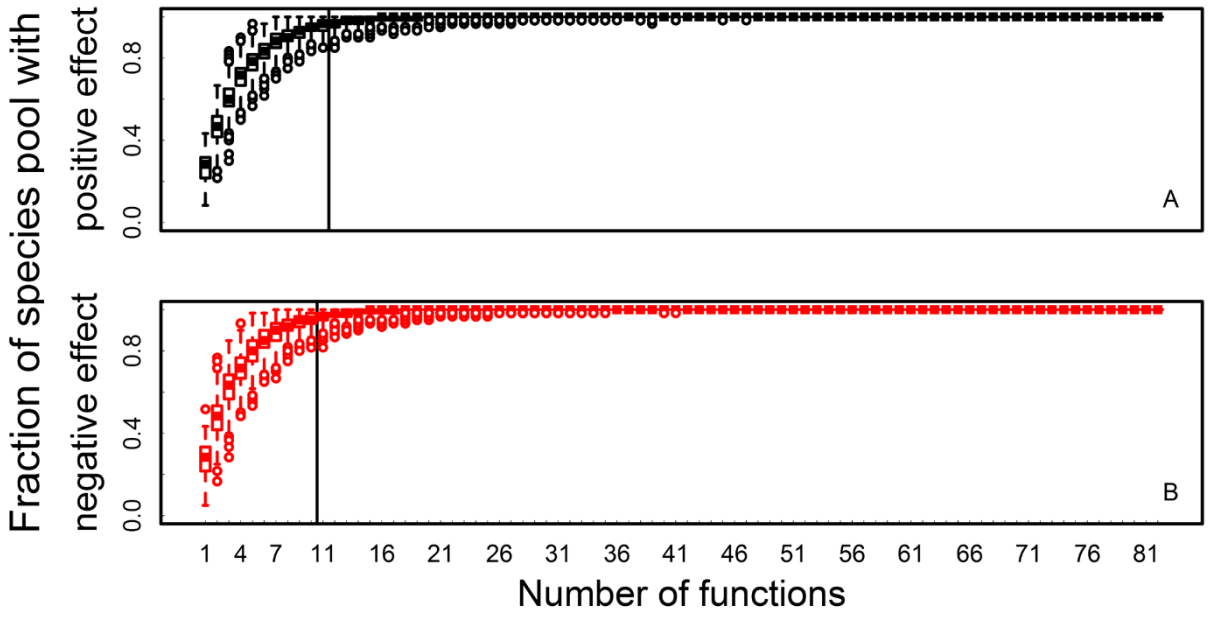


Supplementary Figure 6.1: Results from a sensitivity analysis that restricted the measurements of ecosystem functions included in the analysis to the 54 variables indicated in Supplementary Table 1 that were available from 2004, which was the one single year for which most data was available. (A) The proportion of the plant species pool with significant positive contributions to functioning when an increasing number of ecosystem functions was considered simultaneously. The plant species pool contained 60 species. When more than 13 functions were considered, the proportion of species contribution to functioning was statistically not distinguishable from 1. (B) The index of multifunctionality plotted against the plant species richness in the experimental plots. The solid lines visualise a significant increase in multifunctionality with plant species richness; broken lines show the upper and lower 95%-confidence interval for the linear relationship as estimated from a linear model. (C) The graph shows the position of each plot (coloured dots) in a multifunctional space spanned by the first two axes derived from of principal component analysis (PCA) based on 54 different ecosystem variables measured in 2004 in the Jena Experiment. The colour of the dots represents the diversity level of the experimental plot, as detailed in panel B. Plant diversity sown in the plots spans a gradient along the first principal component axis. Each of the functions is shown as a grey arrow. (D) Comparison of the results of a PCA calculated in the main analysis for 82 ecosystem variables that included measurements from different years and the PCA calculated on 54 ecosystem variables measured in 2004. The comparison was performed via a Procrustes rotation. Dashed lines are the

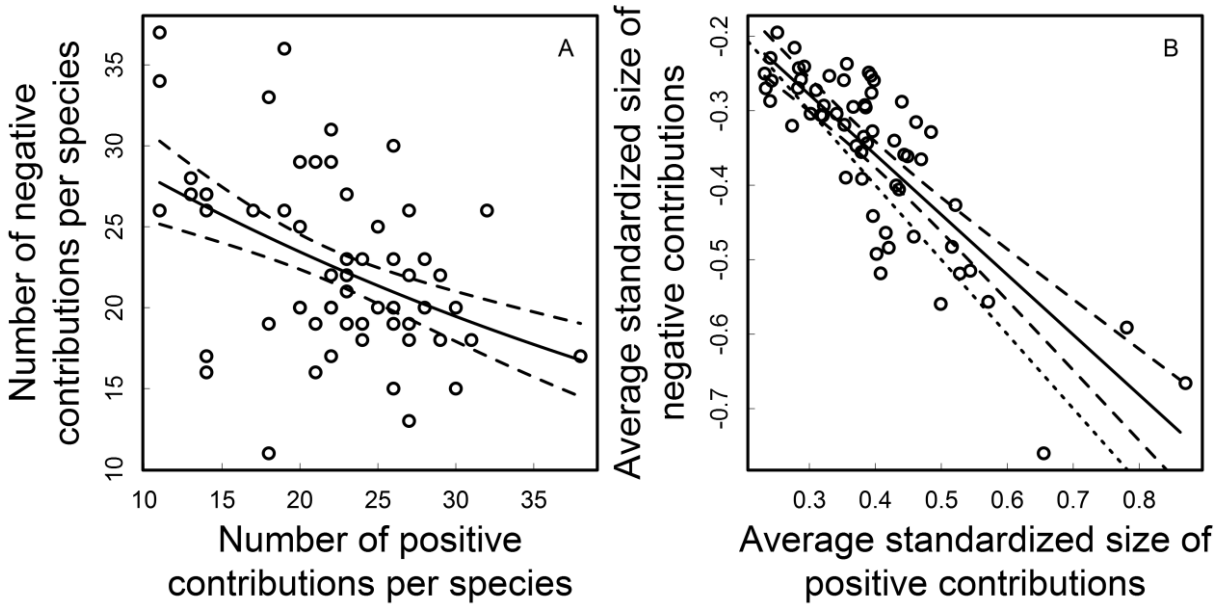
coordination system of the PCA shown in Supplementary Fig. 6.1C based on 54 variables and the solid lines the coordination system of the PCA based on 82 ecosystem variables. Axes have been turned around the origin to maximise overlap. Coloured arrows indicate how much the position of individual plots in multifunctional space change from the PCA based on 82 variables (start of arrows and black circles) to the PCA based on 54 variables measured in 2004 (end of arrows). Colours indicate the diversity level of plots, as indicated in the legend of panel B.

Supplementary Material Section 7: Positive and negative contributions of plant species to functioning

Following the turnover approach as original described by Hector and Bagchi [10] and being recently reviewed by Byrnes, et al. [8], we calculated the contribution of the presence and the absence of the individual plant species to the value of ecosystem functions observed in the different plots of the Jena Experiment. Using the R-functions provided in the package multifunc [9], we calculated the proportions of the species pool needed to sustain combinations of increasing numbers of ecosystem functions. Not all possible combinations of functions could be tested in this analysis because of a large number of functions included in our analysis. Therefore, for each number of functions (x-axis in Fig. 3), we calculated the average proportion for 2000 random combinations of ecosystem variables approximating ecosystem functions. The proportion of significant species effects was calculated both for the positive (Supplementary Fig. 7.1A) and negative (Supplementary Fig. 7.1B) contributions of the species. In a second step, the number of functions to which each species contributes positively and negatively and the respective effect sizes were calculated and correlated with each other (using the package multifunc [9]; Supplementary Fig. 7.2)



Supplementary Figure 7.1: Fraction of the species pool that significantly contributes to the level of functioning in a positive way (A) and in a negative way (B). Both curves approach a proportion of 100% that they reach when at least 11 different ecosystem functions are considered simultaneously.

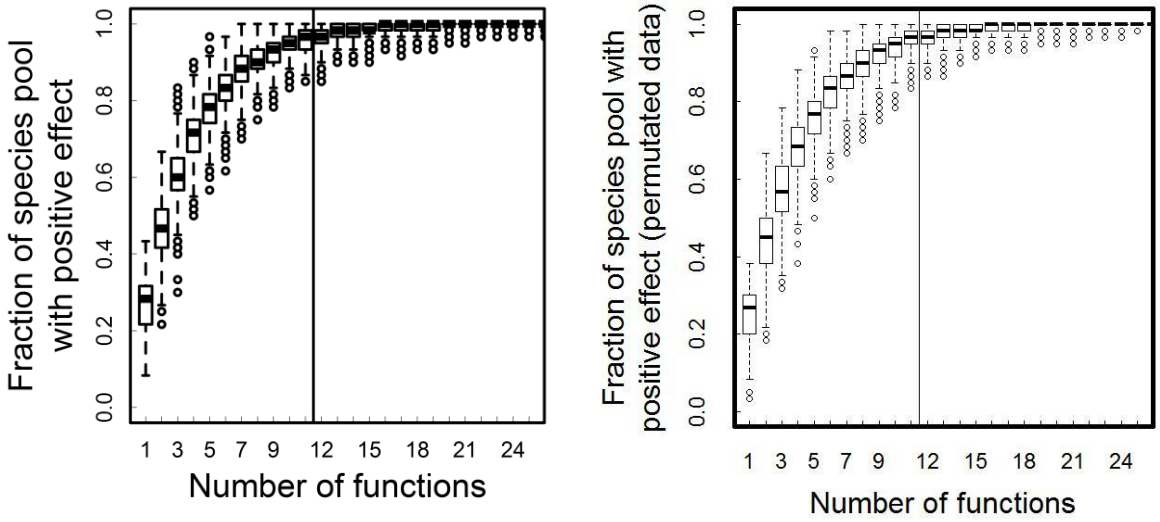


Supplementary Figure 7.2: The number of positive and negative contributions per species showed a significant negative correlation (A). When the average effect sizes per species for positive and negative correlations were plotted, effects correlate "positively" in size, but not in sign (B). That is species with large positive contributions also tended to show large negative contributions. The regression line (solid line with dashed lines indicating confidence intervals) was significantly shallower than the 1:1 line (dotted line), demonstrating that positive contributions of individual species to ecosystem functioning outweigh their negative contributions.

Supplementary Material Section 8: Effects of differently stringent selection criteria on the proportion of species with detectable effects on ecosystem functioning

The turnover approach published first by Hector and Bagchi [10] and reintroduced in a review on methods to calculate multifunctionality [8,9] has been used as the standard procedure to calculate the proportion of a species pool contributing to ecosystem functioning [3,10]. We have also used this method and conclude that all species of the pool of 60 plant species in the Jena Experiment contribute to at least one function out of the portfolio of 82 functions included in the analysis.

During the review of the manuscript one reviewer criticised the approach: “In the turnover analysis, you perform a linear model predicting the values of one of the 82 "functions" as a function of the presence/absence of each species. So, 82 models are performed. In doing so, you find that all species are an important term in at least one of the models. The more models you perform, the more likely that you will "discover" a pattern that is due to chance alone. […] Even if there was no true effect of species presence-absence on any "function", wouldn't you expect the number of detections of an effect to increase based on the number of models performed?” To test for a potential inflation in the number of detected effects we performed a permutation analysis. For this analysis, the presence/absence information for the different plant species was randomly redistributed over the plots, thus breaking up any existing relationships between the species composition of a plot and the values measured for the different functions. The resulting permutated data was analysed with the turnover approach in the same way as the original data. That is, for each ecosystem function, informative species effects were extracted from a full model with the presence-absence data of all 60 plant species as explanatory variables, using a stepwise AIC-approach. For 2000 randomly drawn subsets of functions at each number of ecosystem functions, numbering from 2 to 81, the proportion of species (out of the total of 60) that had informative, positive effects on at least one of the functions in the subset was calculated. Results from the measured and the permutated data were practically indistinguishable (Supplementary Fig. 8.1). This raised the question if the turnover approach is reliable to extract individual species contributions to ecosystem functioning in an experimental design as the one of the Jena Experiment. To investigate this question further, a data set with known species identity effects was simulated.



Supplementary Figure 8.1: Comparison of results from the turnover approach from the measured (left) and permutated (right) data on 82 functions from the Jena Experiment. Only values up to 25 functions are shown.

Creating and analysing a simulated dataset

Six different properties of the data were thought to influence the results of the turnover approach. These were (1) the number of plots in the dataset, (2) the number of species in the species pool, (3) the number of functions investigated, and (4) the proportion of the species pool that has an effect on functioning, (5) the number of species (or proportion of the pool of species with effects) that has an effect on an individual function, and (6) the signal to noise ratio in the data. Also, (7) the critical value that needs to be reached for an effect to be considered significant.

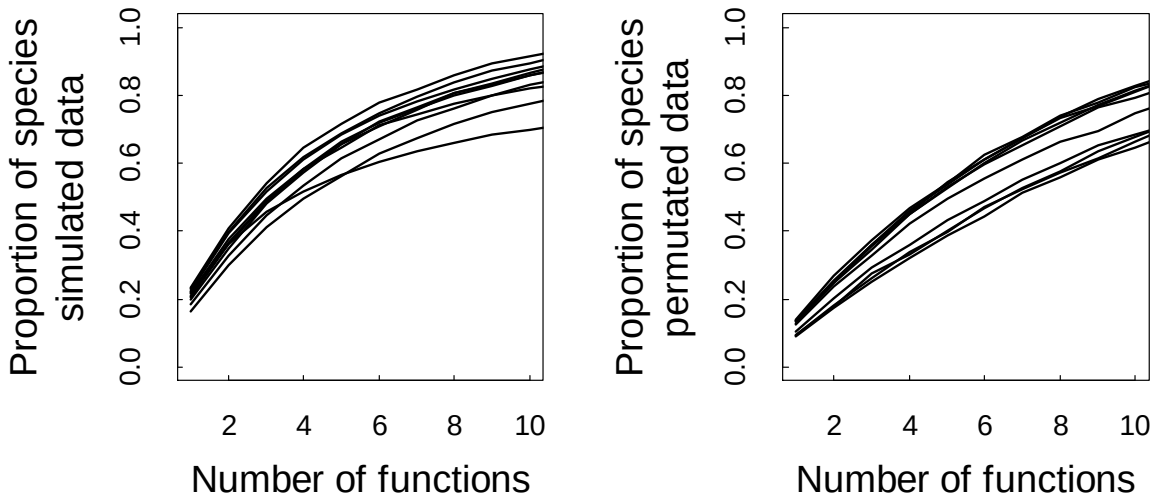
The data to test the effect of these properties was simulated (see R-code below) by assigning a quarter of the number of plots to each diversity levels of 1, 2, 4, and 8 species. In the next step, the species composition was assigned by randomly drawing for each plot the number of required species identities from the species pool. For each species, a column with the presence (1) and absence (0) data were stored. Finally, the values reached by each function in a given plot were simulated. To do so, first, the species were defined that have a potential effect (affecting species pool) by drawing the required number of species identities (proportion of the species pool with effects multiplied with the number of species). Second, the proportion of species with an effect on a single function was translated into an actual number of species by multiplying this proportion by the size of the affecting species pool. Next, a random subset of the affecting species pool of this size was drawn. For these species, their presence and absence values were summed per plot, and a small random number was added. The size of this number was controlled by the signal to noise ratio chosen. This procedure was repeated until the desired number of independent functions was reached.

The simulated data was permutated like the measured data described above, and both the original simulated data and the permutated simulated data were analysed with the turnover approach as exemplified above. To be able to draw the result from simulations of data with varying properties in the same graph not a boxplot over the resulting proportions of species per number of functions are presented but for each number of functions the average over the proportions is calculated, and these averages are connected with a line. Results from the original simulated data are always drawn on the left, results from the permutated data on the right panel in the graphs. For all simulation where not indicated otherwise the following default values were used: 40 plots and 20 simulated functions with a species pool of size 10; of these species 50% had an effect on functioning (5 species); individual functions were influenced by 20% of the affecting species pool (1 species per function); the critical ΔAIC value called k was set to 2, and the scaling factor for the noise to signal ratio was also set to 2.

Insights from the simulated data

Variability in repeated runs of the simulations

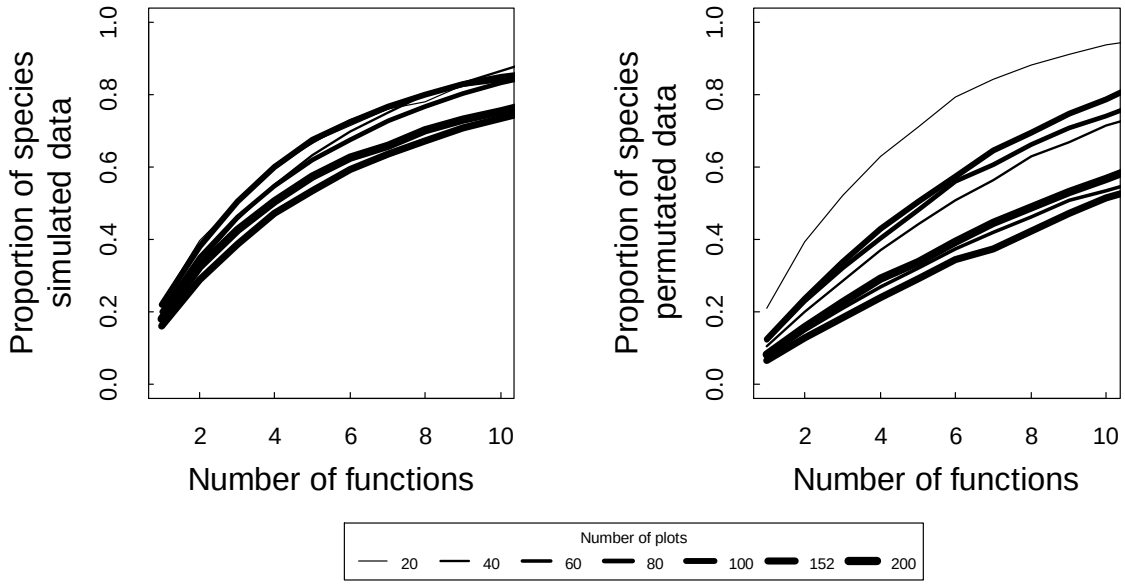
Repeating these simulations ten times gives an impression of the variability introduced in the simulations by drawing random species having effects on the functions. While the proportion of species that affect an individual function (0.2) is well estimated by the values obtained for a single function (Supplementary Fig. 8.2), The proportion of species identified to affect the 10 simulated functions jointly is much larger (0.7 – 1.0) than the proportion for which effects have been simulated (0.5). The permutated data shows only slightly reduced proportions of species with effects on functioning (Supplementary Fig. 8.2).



Supplementary Figure 8.2: Results of 10 independent runs of the simulation procedure with the standard setting as described in the text. Each line represents one run.

Number of plots

Increasing the number of plots did not change the shape of the curve for the simulated data or randomised data (Supplementary Fig. 8.3). Again the proportion of the species pool identified to affect functioning is too high. However, slopes for simulations with larger numbers of plots shifted the curves downwards in the direction of the real simulated values. Also, permutating the data shifted the curves downwards and did so stronger for simulations with more plots.

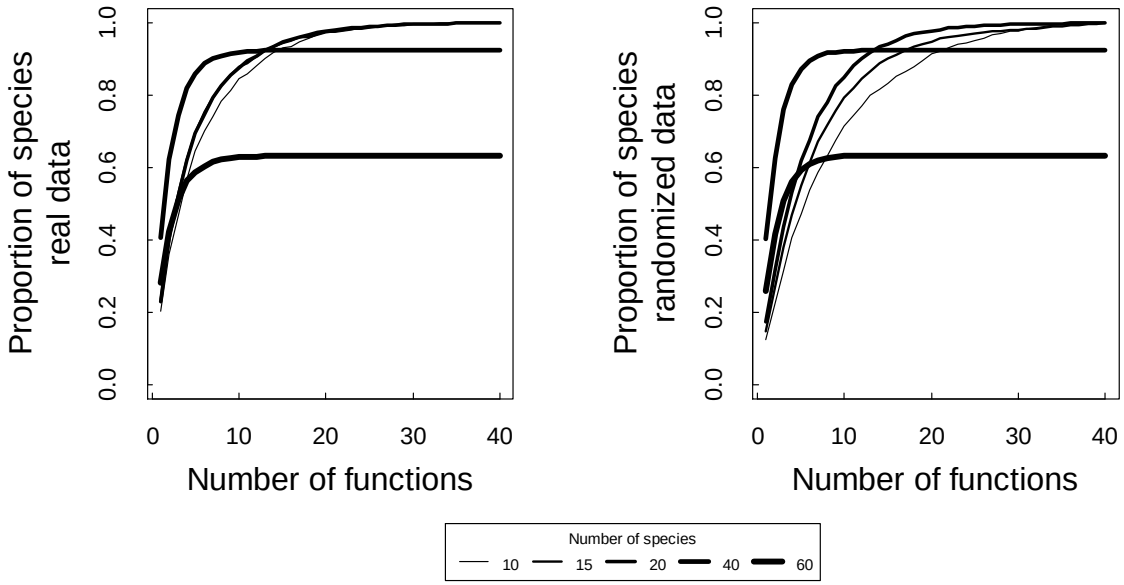


Supplementary Figure 8.3: Effects of an increasing number of plots. Other parameters of the simulation were set to standard values as described above.

Number of species

The number of species in the simulated dataset, i.e. the size of the species pool, did not change the shape the curves as long as the number of species was lower than the number of functions considered.

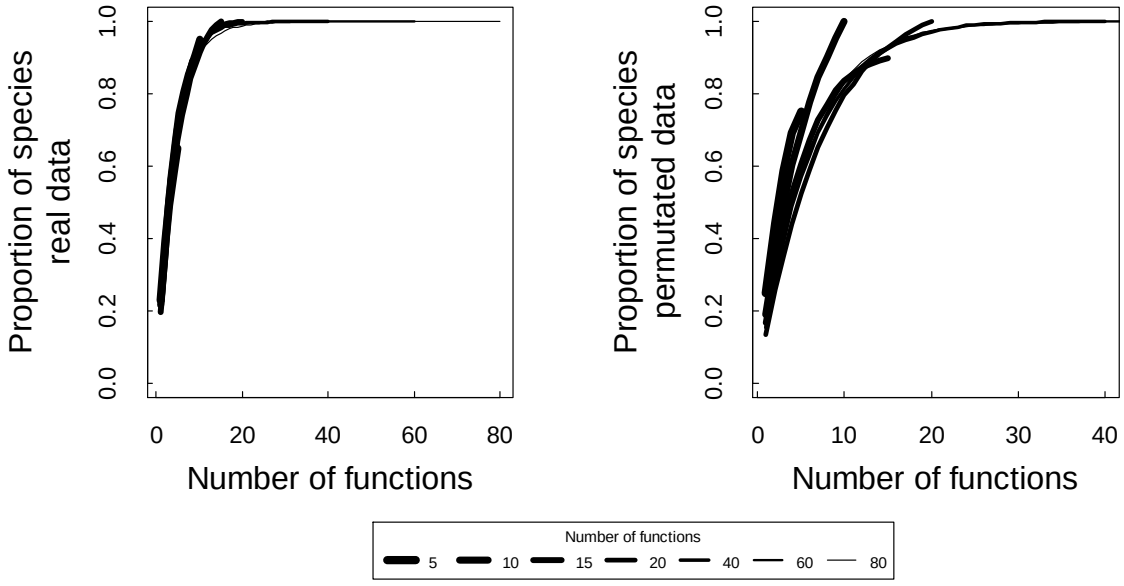
Note that with low numbers of species the proportion of the species pool showing an effect reaches 100% despite only half of the species having effects in the simulated data. When the number of species reached (40 species) or exceeded (60 species) the number of simulated functions (40) the curves reached a saturation that was lower than 100% but still higher than the 50% of the species for which effects had been created in the simulated data. Permuting the data did change the shape of the curves only little (Supplementary Fig. 8.4).



Supplementary Figure 8.4: Effects of an increasing number of species. Other parameters of the simulation were set to standard values as described above except the number of functions considered which was set to 40 instead of 10 for this analysis.

Number of functions

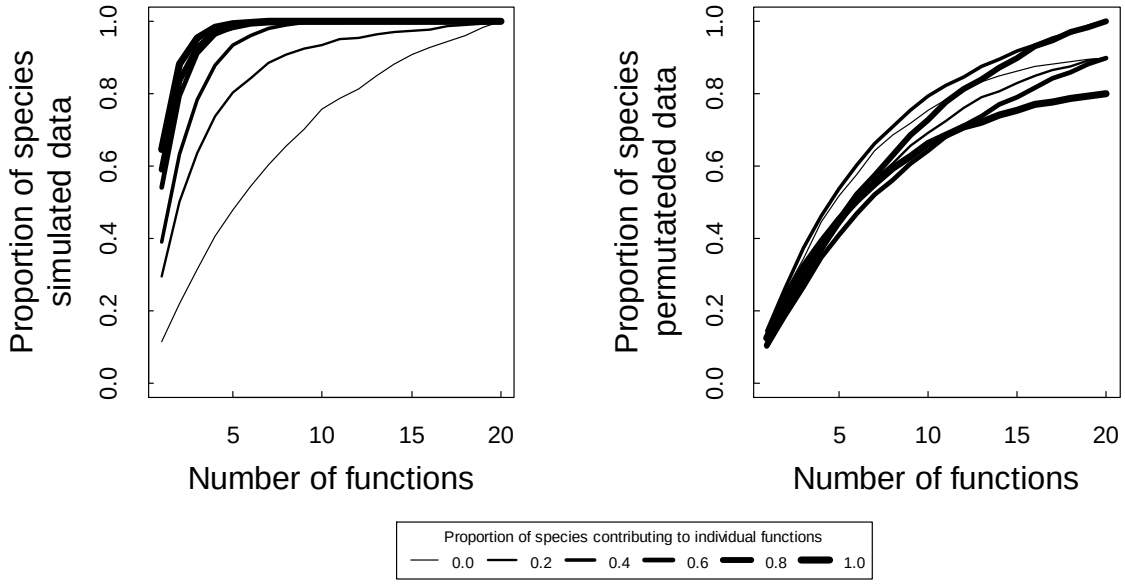
Increasing the number of functions simulated for the analysis did not change the shape of the curves. With fewer functions, an ever shorter section of the curve is produced (Supplementary Fig. 8.5). Note that with enough functions considered the proportion of the species pool showing an effect reaches 100% despite only half of the species having effects in the simulated data.



▲**Supplementary Figure 8.5:** Effects of an increasing number of functions. Other parameters of the simulation were set to standard values as described above.

Proportion of the species contributing to individual functions

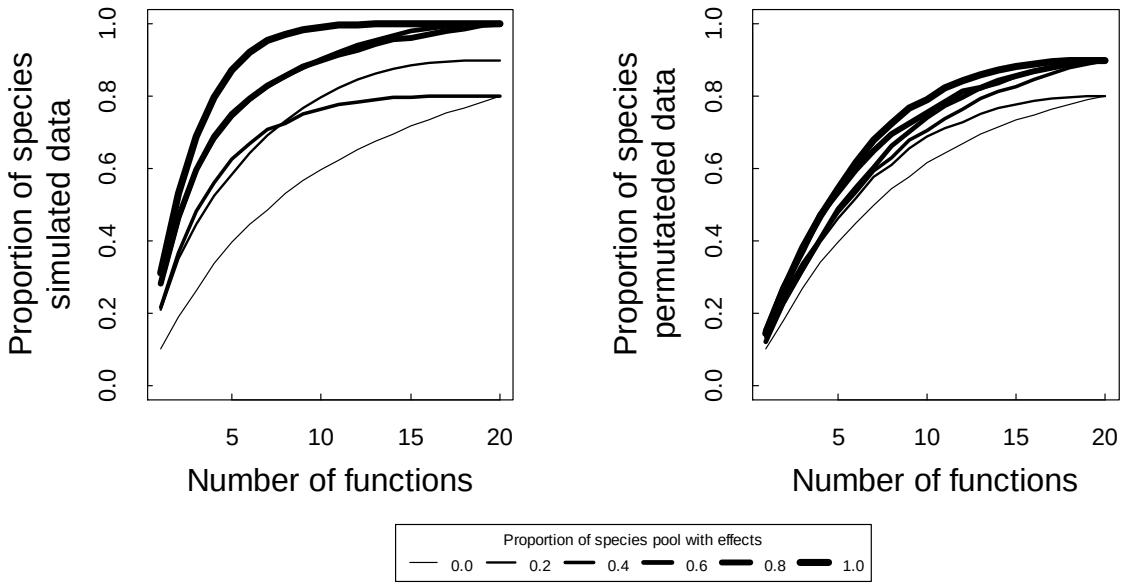
It can be seen that in the case where the functional values have been simulated to be completely independent of the presence of any species (thinnest line in the panel on the left in Supplementary Fig. 8.6), the proportion of species identified to contribute to functioning increases somewhat linearly with an increasing number of functions considered. With an increasing proportion of species contributing to an individual function (thicker lines in the panel on the left Supplementary Fig. 8.6) the lines became more and more curved and reached a proportion of 1 at lower numbers of functions. Importantly, these simulations show that it was not the height of the asymptote reached by the proportion of species but the shape of the curve that changed when the number of species contributing to an individual function was changed. The permutated data was always very similar to the case where functions are simulated as purely random numbers (thinnest line on the left). However, the asymptote reached was too high both for the simulated and the permutated data.



Supplementary Figure 8.6: Effects of an increasing proportion of species with effects. Simulated was data in which all species contribute to functioning. Other parameters of the simulation were set to standard values as described above.

Proportion of species pool affecting at least one function

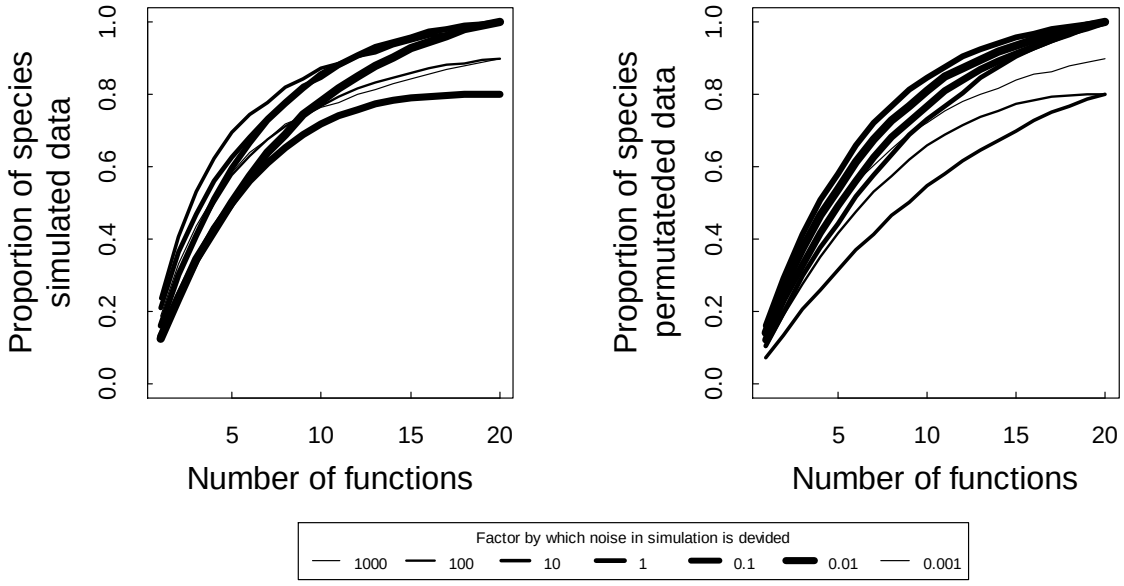
For simulated data with a lower proportion of the species pool contributing to functioning the asymptote reached by the curve was, as expected, lower. However, for both the simulated data and the permutated data the proportion of species contributing to functioning was higher than the simulated true value (Supplementary Fig. 8.7).



Supplementary Figure 8.7: Effects of an increasing proportion of species with effects. Other parameters of the simulation were set to standard values as described above.

Error to signal ration

Increasing the noise to signal ratio did not change the shape of the relationships (Supplementary Fig. 8.8).



Supplementary Figure 8.8: Effects of an increasing noise to signal ratio (smaller values of the factor are larger noise) Other parameters of the simulation were set to standard values as described above.

Summary of analysis of simulated data

The simulations show that the proportion of species affecting functioning increases just by chance because type 1 errors accumulate with an increasing number of models tested even when there are no true effects. Generally, the proportion of species with effects was estimated too high using the

turnover-approach as published in the literature [8,10] and used in analyses before. One way of reducing this bias is by applying stricter criteria for an effect of a species on a function to be considered informative.

Effects of changing the critical AIC value to identify a species effect as informative

The potential inflation of false positives in the analysis of species contributions to ecosystem functioning could be reduced by applying stricter criteria for a species to be considered having an effect on an ecosystem function. The classical turnover approach is based on a stepwise model selection approach in which candidate models are compared regarding their Akaike information criterion (AIC-value). A difference larger than two AIC-points between a model with and without the presence of an individual species as an explanatory variable is taken to indicate that this species has an informative effect on the respective function [8,10]. However, for model selection based on AIC scores a wide range of critical differences in AIC scores has been suggested reviewed in [11]. Also, it can be shown that any critical difference in AIC scores can be converted to an equivalent α-level in a p-value based model selection approach. The relationship between difference in AIC scores and p-values can be expressed as

$$P = \Pr(\chi_k^2 > \Delta AIC + 2k)$$

and

$$\Delta AIC = F_{\chi_k^2}^{-1}(1-p) - 2k$$

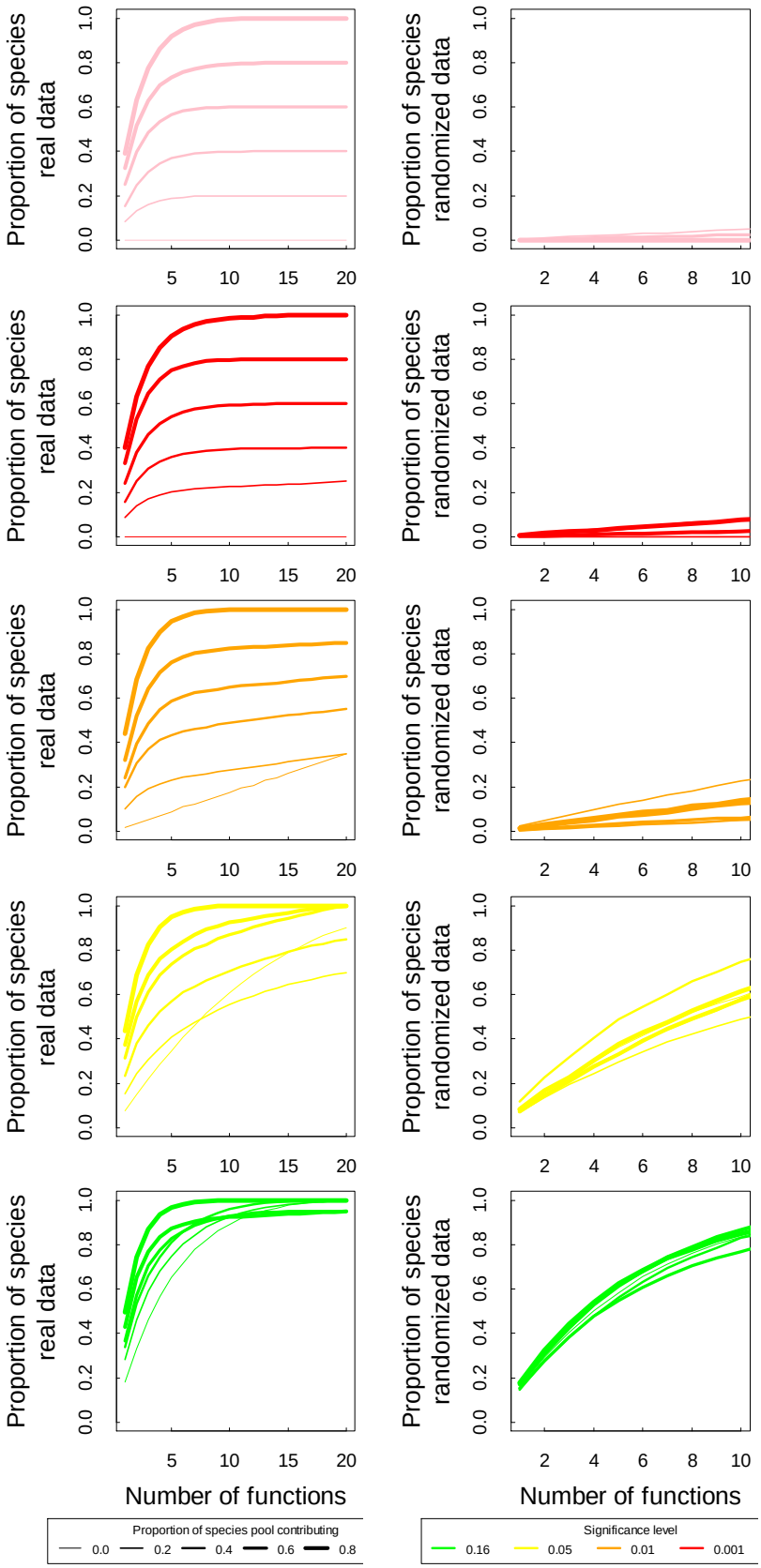
Where χ_k^2 is a chi-square random variable with *k* degrees of freedom, and

$$F_{\chi_k^2}^{-1}(1-p)$$

Is the (1-*p*) quantile of the χ_k^2distribution [11]. Consequently, a ΔAIC value of 2 is quivalent to a critical p-value of 0.16. By increasing the ΔAIC value needed to consider an effect of a species to be informative this p-value can be lowered. We have adapted the functions used to calculate the turnover approach provided in the multifunc package[9] to apply the step-AIC functions used to compute the informaive effects with a freely choosable critical ΔAIC value called k. Applying this functions we have repeated the analysis of simulated data with a variing proportion of the species pool affecting at least one function using a range of ΔAIC values (2, 3.8, 6.6, 7.9, 18.8, and 15.1) wich are equivalent to p-values of (0.16, 0.05, 0.01, 0.005, 0.001, and 0.0001 respectively.

The asymptote reached by the curve, indicating the proportion of the species pool that contributes to functioning, was depended on the specified critical difference in AIC scores. With the classically used difference of 2 AIC points to define significant contributions of a species (green curves in Supplementary Fig. 8.9), the number of significant effects is highly overestimated. When the significance level is raised to a difference in AIC points that is equivalent to a significance level of 0.01 (orange curves in Supplementary Fig. 8.9) the correct asymptotes as defined in the simulated data are reached. With this critical value (or even higher critical values), permutating the data causes the proportions of species with significant contributions be close to zero, which is also the expected behaviour expected. Thus, raising the critical difference in AIC scores to 6.6 (the equivalent to a significance level of 0.01) resolves the issue of a large number of models and parameters beeing estimated in the turnover approach as criticism raised by the reviewer. Especially, when comparing the results of the turnover approach to the results of a sensitivity analysis where the data has been permutated, and a stricter critical AIC value is used as normally done, the contributions of individual species to ecosystem functioning can be shown conclusively. However, it is important to note that this approach is extremely conservative because while lowering the type 1 error rate (that is rejecting the null-hypothesis while it is true) the type 2 error rate (failing to reject the null hypothesis despite it

being false) is strongly increased. Therefore, results of obtained with a turnover approach with stricter critical AIC-values cannot be directly compared to results of analyses using the standard AIC-value of 2.



▲**Supplementary Figure 8.9:** Effects of increasing proportion of the species pool with functional effects on the proportion of species with significant positive effects on an increasing number of functions as depending on the significance level.

The R code used to do the simulation and produce all graphs in this section is given as a separate file in the supplementary material.

Supplementary references

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