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## Supplementary information

**Tab. S1.** Difference equations and mathematical expression for the likelihood functions for models  $M_0$ ,  $M_1$ ,  $M_2$  and for the full model in monocultures.

Model	Difference equation	Likelihood function
<b>Full</b>	$B_i(t+1, p, T) = B_i(t, p, T) + \left( r_{mi} + \sigma_{ei} u_{ei}(T) + \frac{\sigma_{di} u_{di}(T, p)}{\sqrt{B_i(0, p, T)}} \right) \cdot B_i(t, p, T) \cdot \left( 1 - \frac{B_i(t, p, T)}{K_i} \right)$	$\prod_{i, T, p, s} \left( \frac{1}{\sigma_{oi} \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \cdot \left( \frac{\ln(B_i^{obs}(T, p, s)) - \ln(B_i(T, p))}{\sigma_{oi}} \right)^2 \right] \right) \cdot \prod_{i, T} \int_{-\infty}^{+\infty} \frac{1}{(\sqrt{2\pi})^{Np+1}} \frac{1}{\sigma_{ei} \sigma_{di}^{Np}} \sqrt{B_0}^{Np} \exp \left[ -\frac{1}{2} \cdot \left( \frac{t}{\sigma_{ei}} \right)^2 + \sum_p \left( \frac{\hat{r}_i(T, p) - r_{mi} - t \sqrt{B_0}}{\sigma_{di}} \right)^2 \right] dt$
<b>M<sub>2</sub></b>	$B_i(t+1, T) = B_i(t, T) + (r_{mi} + \sigma_{ei} u_{ei}(T)) \cdot B_i(t, T) \cdot \left( 1 - \frac{B_i(t, T)}{K_i} \right)$	$\prod_{i, T, p, s} \left( \frac{1}{\sigma_{oi} \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \cdot \left( \frac{\ln(B_i^{obs}(T, p, s)) - \ln(B_i(T))}{\sigma_{oi}} \right)^2 \right] \right) \cdot \prod_{i, T} \frac{1}{\sigma_{ei} \sqrt{2\pi}} \cdot \exp \left[ -\frac{1}{2} \cdot \left( \frac{\hat{r}_i(T) - r_{mi}}{\sigma_{ei}} \right)^2 \right]$
<b>M<sub>1</sub></b>	$B_i(t+1) = B_i(t) + r_{mi} \cdot B_i(t) \cdot \left( 1 - \frac{B_i(t)}{K_i} \right)$	$\prod_{i, T, p, s} \frac{1}{\sigma_{oi} \sqrt{2\pi}} \cdot \exp \left[ -\frac{1}{2} \cdot \left( \frac{\ln(B_i^{obs}(T, p, s)) - \ln(B_i(T))}{\sigma_{oi}} \right)^2 \right]$

<b>M<sub>0</sub></b>	$B_i(t+1) = B(t) + r_m \cdot B(t) \cdot \left(1 - \frac{B(t)}{K}\right)$	$\prod_{i,T,p,s} \frac{1}{\sigma_o \sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2} \cdot \left(\frac{\ln(B_i^{obs}(T,p,s)) - \ln(B(T))}{\sigma_o}\right)^2\right]$
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**Tab. S2.** Model selection based on monoculture data. The  $AIC_m$  is computed for each model  $m$  from the number of parameters estimated for the model  $k_m$  and the log-likelihood function  $L(\theta/B)$  provided in Table S1.

	<b>Full</b>	<b>M<sub>2</sub></b>	<b>M<sub>1</sub></b>	<b>M<sub>0</sub></b>
$L(\theta/B)$	2506.7	154.2	-4140.0	-4938.6
$k_m$	280	224	168	3
$AIC_m$	-4453.4	139.5	8616.1	9863.2

**Tab.S3.** Names and functional groups of the species used in the Jena biodiversity experiment and their code.

<b>Species name</b>	<b>Functional group</b>	<b>Abbreviation</b>
Achillea millefolium	Tall herb	Ach.mil
Ajuga reptans	Small herb	Aju.rep
Alopecurus pratensis	Grass	Alo.pra
Anthoxanthum odoratum	Grass	Ant.odo
Anthriscus sylvestris	Tall herb	Ant.syl
Arrhenatherum elatius	Grass	Arr.ela
Avenula pubescens	Grass	Ave.pub
Bellis perennis	Small herb	Bel.per
Bromus erectus	Grass	Bro.ere
Bromus hordeaceus	Grass	Bro.hor
Campanula patula	Tall herb	Cam.pat
Carum carvi	Tall herb	Car.car
Cardamine pratensis	Tall herb	Car.pra
Centaurea jacea	Tall herb	Cen.jac
Cirsium oleraceum	Tall herb	Cir.ole
Crepis biennis	Tall herb	Cre.bie
Cynosurus cristatus	Grass	Cyn.cri
Dactylis glomerata	Grass	Dac.glo
Daucus carota	Tall herb	Dau.car
Festuca pratensis	Grass	Fes.pra
Festuca rubra	Grass	Fes.rub
Galium mollugo	Tall herb	Gal.mol
Geranium pratense	Tall herb	Ger.pra
Glechoma hederacea	Small herb	Gle.hed
Heracleum sphondylium	Tall herb	Her.sph
Holcus lanatus	Grass	Hol.lan
Knautia arvensis	Tall herb	Kna.arv
Lathyrus pratensis	Legume	Lat.pra
Leontodon autumnalis	Small herb	Leo.aut
Leontodon hispidus	Small herb	Leo.his
Leucanthemum vulgare	Tall herb	Leu.vul
Lotus corniculatus	Legume	Lot.cor
Luzula campestris	Grass	Luz.cam

Medicago lupulina	Legume	Med.lup
Medicago × varia	Legume	Med.var
Onobrychis viciifolia	Legume	Ono.vic
Pastinaca sativa	Tall herb	Pas.sat
Phleum pratense	Grass	Phl.pra
Pimpinella major	Tall herb	Pim.maj
Plantago lanceolata	Small herb	Pla.lan
Plantago media	Small herb	Pla.med
Poa pratensis	Grass	Poa.pra
Poa trivialis	Grass	Poa.tri
Primula veris	Small herb	Pri.ver
Prunella vulgaris	Small herb	Pru.vul
Ranunculus acris	Tall herb	Ran.acr
Ranunculus repens	Small herb	Ran.rep
Rumex acetosa	Tall herb	Rum.ace
Sanguisorba officinalis	Tall herb	San.off
Taraxacum officinale	Small herb	Tar.off
Tragopogon pratensis	Tall herb	Tra.pra
Trifolium campestre	Legume	Tri.cam
Trifolium dubium	Legume	Tri.dub
Trisetum flavescens	Grass	Tri.fla
Trifolium fragiferum	Legume	Tri.fra
Trifolium hybridum	Legume	Tri.hyb
Trifolium pratense	Legume	Tri.pra
Trifolium repens	Legume	Tri.rep
Veronica chamaedrys	Small herb	Ver.cha
Vicia cracca	Legume	Vic.cra

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**Tab.S4.** P-values obtained with the Kolmogorov-Smirnov normality test for the environmental variables  $u_{ei}$ , the demographic variables  $u_{di}$ , and the observation variables  $u_{oi}$  estimated from replicated monocultures with our inference method as well as p-values associated with stochastic model predictions regarding average community biomass  $\bar{B}$  and standard deviation of the community biomass  $\sigma_B$ . Values highlighted in red correspond to failures regarding model validation.

Species	$u_{ei}$	$u_{di}$	$u_{oi}$	$\bar{B}$	$\sigma_B$
Ach.mil	0.226	0.161	0.988	0.21	0.07
Aju.rep	0.471	0.773	0.342	1	0.86
Alo.pra	0.982	0.784	0.991	0.4	0.58
Ant.odo	0.889	0.317	0.078	0.51	0.73
Ant.syl	0.977	0.62	0.569	0.47	0.62
Arr.ela	0.947	0.549	0.944	0.44	0.42
Ave.pub	0.998	0.337	0.232	0.37	0.54
Bel.per	0.621	0.366	0.224	0.84	0.64
Bro.ere	0.86	0.779	0.799	0.42	0.27
Bro.hor	0.968	0.774	0.075	0.8	0.86
Cam.pat	0.745	0.339	0.995	0.7	0.46
Car.car	0.312	0.81	0.958	0.36	0.12
Car.pra	NA	NA	NA	0	0
Cen.jac	0.348	0.325	0.99	0.18	0.22
Cir.ole	0.768	0.441	1	0.33	0.27
Cre.bie	0.897	0.162	0.17	0.38	0.61
Cyn.cri	0.533	0.463	0.342	0.68	0.55
Dac.glo	0.905	0.49	0.798	0.43	0.32
Dau.car	0.983	0.632	0.659	0.41	0.57
Fes.pra	0.873	0.654	0.199	0.37	0.44
Fes.rub	0.949	0.741	0.354	0.25	0.51
Gal.mol	0.929	0.797	0.868	0.43	0.36
Ger.pra	0.002	0.964	0.486	0.8	0.81
Gle.hed	0.857	0.316	0.154	0.45	0.68
Her.sph	0.803	0.66	0.297	0.56	0.74
Hol.lan	0.889	0.674	0.711	0.33	0.37
Kna.arv	0.994	0.291	0.928	0.34	0.3
Lat.pra	0.398	0.488	0.772	0.28	0.5
Leo.aut	0.946	0.371	0.054	0.25	0.5

Leo.his	0.699	0.379	0.887	0.32	0.19
Leu.vul	0.64	0.144	1	0.39	0.35
Lot.cor	0.622	0.723	0.931	0.35	0.65
Luz.cam	0.028	0.175	0.541	1	0.56
Med.lup	0.53	0.746	0.487	0.67	0.62
Med.var	0.97	0.8	0.978	0.33	0.54
Ono.vic	0.988	0.836	0.998	0.83	0.79
Pas.sat	0.994	0.26	0.297	0.44	0.41
Phl.pra	0.957	0.551	0.31	0.58	0.78
Pim.maj	0.536	0.529	0.992	0.26	0.15
Pla.lan	0.37	0.289	0.043	0.68	0.71
Pla.med	0.943	0.062	0.886	0.32	0.46
Poa.pra	0.926	0.452	0.068	0.54	0.72
Poa.tri	0.565	0.565	0.1	0.59	0.7
Pri.ver	0.546	0.803	0.499	0.71	0.78
Pru.vul	0.343	0.458	0.143	0.34	0.35
Ran.acr	0.939	0.606	0.993	0.28	0.25
Ran.rep	0.997	0.281	0.151	0.48	0.57
Rum.ace	0.549	0.549	0.346	0.47	0.65
San.off	0.163	0.579	1	0.68	0.42
Tar.off	0.995	0.179	0.08	0.3	0.66
Tra.pra	0.807	0.24	0.277	0.5	0.51
Tri.cam	0.822	0.209	0.759	0.95	0.5
Tri.dub	0.295	0.159	0.434	0.83	0.58
Tri.fla	0.823	0.25	0.881	0.38	0.45
Tri.fra	0.903	0.009	0.515	0.94	0.78
Tri.hyb	0.624	0.67	0.031	0.55	0.75
Tri.pra	0.069	0.655	0.683	0.63	0.83
Tri.rep	0.848	0.402	0.094	0.63	0.82
Ver.cha	0.823	0.717	0.583	0.34	0.56
Vic.cra	0.378	0.85	0.486	0.67	0.62

**Tab.S5.** Correlation between model parameters when all the species are considered and when they are sorted according to their functional group.

		$\sigma_e$	$\sigma_d$	$\sigma_o$
$r_m$	All	-0.54***	-0.42***	-0.57***
	Grass	-0.79***	-0.54**	-0.63***
	Small herb	-0.18	-0.37	-0.70***
	Tall herb	-0.64***	-0.45*	-0.77***
	Legumes	-0.76***	-0.41	-0.25
$\sigma_e$	All		0.03	0.37***
	Grass		0.51*	0.57**
	Small herb		-0.27	0.23
	Tall herb		0.15	0.49**
	Legumes		0.06	0.43
$\sigma_d$	All			0.53***
	Grass			0.72***
	Small herb			0.53*
	Tall herb			0.65***
	Legumes			0.3

\*\*\*  $p < 0.025$ ; \*\*  $0.025 < p < 0.05$ ; \*  $0.05 < p < 0.1$



**Tab.S6.** Assessment of model predictive ability in species mixtures when the asynchrony between species in their response to environmental variations was not accounted for.  $R^2$  between observed and predicted values, proportion of mixtures  $N_{\text{dev}}$  significantly deviating from model predictions and overall deviation significance  $p$  from predictions for the studied summary statistics. Results are reported both for all the empirical mixtures, and for each diversity level separately.

		All	2 species	4 species	8 species	16 species
$\bar{B}$	$R^2$	0.66	0.89	0.66	0.76	0.88
	$N_{\text{dev}}$	0.15	1/16	2/11	1/10	2/3
	$p$	0.01	0.25	0.33	0.34	0.30
$\sigma_B$	$R^2$	0.59	0.64	0.71	0.67	0.45
	$N_{\text{dev}}$	0.08	1/16	1/11	0/10	1/3
	$p$	0.20	0.29	0.23	0.32	0.31
$\lambda$	$R^2$	0.77	0.48	0.02	0.00	0.09
	$N_{\text{dev}}$	0.31	5/16	3/11	4/10	0/3
	$p$	0.00	0.07	0.03	0.00	0.16