Supplementary material

An ensemble-forecasting model for airborne grass pollen at three climatically distinct sites

Supplementary tables

***Table S1**. Out-of-sample performance of all 61 candidate models evaluated during the initial screening phase using the Augsburg (Hirst) dataset. Models were trained on 2018–2023 data and evaluated on the independent 2024 test year. Reported metrics include root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2). Rankings are based on RMSE (ascending order). The final ensemble members were selected from the top-performing tier while ensuring methodological diversity.*

Model	Family	rmse 2024	mae 2024	r2 2024	Runtime (s)	bestTune	rank rmse	rank mae	rank r2
ctree2	Tree (single/rule)	7.41	2.12	0.32	7.41	maxdepth=4; mincriterion=0.255	1	2	6
ranger	Tree/Forest	7.41	2.14	0.33	7.41	predFixed=2; minNode=3	2	3	1
gbm	Boosting	7.45	2.08	0.31	7.45	n.trees=50; interaction.depth=5; shrinkage=0.1; n.minobsinnode=10	3	1	8
Rborist	Tree/Forest	7.46	2.15	0.32	7.46	mtry=2; coefReg=0.7525; coefImp=0.5	4	5	2
parRF	Tree/Forest	7.46	2.17	0.32	7.46	mtry=2	5	9	3
RRFglobal	Tree/Forest	7.48	2.16	0.32	7.48	mtry=2; coefReg=0.2575	6	6	4
rf	Tree/Forest	7.49	2.16	0.32	7.49	mtry=2	7	7	5
rpart1SE	Tree (single/rule)	7.50	2.29	0.28	7.50	parameter=none	8	22	13
rpart2	Tree (single/rule)	7.50	2.29	0.28	7.50	maxdepth=4	9	23	14
cforest	Tree (single/rule)	7.52	2.15	0.31	7.52	mtry=3	10	4	7
ctree	Tree (single/rule)	7.54	2.22	0.28	7.54	mincriterion=0.745	11	15	15
bam	Other	7.55	2.19	0.30	7.55	select=TRUE; method=1	12	11	9
gam	Other	7.55	2.19	0.30	7.55	select=TRUE; method=1	13	12	10
bstTree	Boosting	7.60	2.17	0.29	7.60	mstop=50; maxdepth=2; nu=0.1	14	8	12
RRF	Tree/Forest	7.62	2.17	0.29	7.62	mtry=2; splitrule=2; min.node.size=5	15	10	11
gaussprPoly	Kernel/SVM/GP	7.65	2.25	0.26	7.65	degree=3; scale=0.1	16	16	17
blackboost	Boosting	7.69	2.21	0.26	7.69	mstop=50; maxdepth=2	17	13	16
gamboost	Boosting	7.70	2.29	0.24	7.70	mstop=250; prune=no	18	21	21
bstSm	Boosting	7.71	2.28	0.25	7.71	mstop=250; nu=0.1	19	19	18
partDSA	Other	7.71	2.34	0.24	7.71	cut.off.growth=5; MPD=0.1	20	25	23
rpart	Tree (single/rule)	7.71	2.34	0.24	7.71	cp=0.00969763808658574	21	24	24
cubist	Tree (single/rule)	7.76	2.22	0.24	7.76	committees=1; neighbors=0	22	14	22
xgbLinear	Boosting	7.81	2.58	0.24	7.81	nrounds=50; lambda=0.1; alpha=0.1; eta=0.3	23	34	20

nnetar	Neural network/DL	7.83	2.27	0.22	7.83	hidden1=3; n.ensemble=1	24	18	25
gaussprRadial	Kernel/SVM/GP	7.85	2.25	0.25	7.85	sigma=0.72311537165214	25	17	19
gamLoess	Other	7.88	2.28	0.21	7.88	span=0.5; degree=1	26	20	26
gcvEarth	Other	8.10	2.35	0.17	8.10	degree=1	27	26	33
xgbTree	Boosting	8.10	2.71	0.20	8.10	nrounds=50; max_depth=1; eta=0.3; gamma=0; colsample_bytree=0.8; min_child_weight=1; subsample=0.5	28	35	28
ppr	Other	8.11	2.55	0.20	8.11	nterms=1	29	33	27
glmnet	Regularized regression	8.13	2.85	0.17	8.13	fraction=0.7625; lambda=0.1	30	41	37
earth	Other	8.14	2.38	0.17	8.14	nprune=6; degree=1	31	28	36
lars	Regularized regression	8.15	2.89	0.16	8.15	fraction=0.7625	32	42	38
lasso	Regularized regression	8.20	2.73	0.17	8.20	fraction=0.9	33	38	34
ridge	Regularized regression	8.24	2.72	0.18	8.24	lambda=0	34	36	30
lm	Linear/GLM	8.24	2.72	0.18	8.24	intercept=TRUE	35	37	31
rlm	Linear/GLM	8.29	2.36	0.16	8.29	intercept=TRUE; psi=1	36	27	39
M5Rules	Tree (single/rule)	8.33	2.48	0.12	8.33	pruned=1; smoothed=2	37	29	40
avNNet	Neural network/DL	8.77	2.49	0.17	8.77	size=7; decay=0.01; bag=FALSE	38	31	35
nnet	Neural network/DL	8.78	2.49	0.18	8.78	size=9; decay=0.01	39	30	32
pcaNNet	Neural network/DL	8.78	2.50	0.18	8.78	size=3; decay=0.01	40	32	29
mlpWeightDecay	Neural network/DL	9.08	2.91	0.00	9.08	size=1; decay=0.1	41	44	59
mlpML	Neural network/DL	9.08	2.91		9.08	layer1=1; layer2=0; layer3=0	42	43	
mlpWeightDecayML	Neural network/DL	9.22	2.82	0.05	9.22	layer1=1; layer2=0; layer3=0; decay=0.1	43	39	41
mlp	Neural network/DL	9.22	2.82		9.22	size=1	44	40	
glmboost	Boosting	45.21	4.69	0.01	45.21	mstop=50; prune=no	45	45	42
enet	Regularized regression	51.60	5.02	0.01	51.60	alpha=1; lambda=0.0117572649875026	46	46	43
BstLm	Boosting	52.25	5.06	0.01	52.25	mstop=200; nu=0.1	47	47	44
msaenet	Regularized regression	57.03	5.30	0.01	57.03	alphas=0.95; nsteps=2; scale=2	48	48	45
glmStepAIC	Linear/GLM	57.35	5.31	0.01	57.35	parameter=none	49	49	46
gaussprLinear	Kernel/SVM/GP	58.87	5.40	0.01	58.87	parameter=none	50	50	47
bayesglm	Linear/GLM	59.02	5.41	0.01	59.02	parameter=none	51	51	48
glm	Linear/GLM	59.02	5.41	0.01	59.02	parameter=none	52	52	49

spls	Regularized regression	62.00	5.56	0.01	62.00	K=2; eta=0.7; kappa=0.5	53	53	50
plsRglm	Regularized regression	65.73	5.76	0.01	65.73	nt=2; alpha.pvals.expli=0.1	54	54	51
kernelpls	PLS/PCR	89.94	7.03	0.01	89.94	ncomp=2	55	55	52
pls	PLS/PCR	89.94	7.03	0.01	89.94	ncomp=2	56	56	54
simpls	PLS/PCR	89.94	7.03	0.01	89.94	ncomp=2	57	57	53
widekernelpls	PLS/PCR	89.94	7.03	0.01	89.94	ncomp=2	58	58	55
svmLinear3	Kernel/SVM/GP	441.54	25.43	0.00	441.54	cost=0.25; Loss=1	59	59	56
svmLinear2	Kernel/SVM/GP	3724.58	197.13	0.00	3724.58	cost=1	60	60	57
svmLinear	Kernel/SVM/GP	3724.58	197.13	0.00	3724.58	C=1	61	61	58

Table S2. *Grass pollen season parameters in Augsburg, Córdoba and Thessaloniki (2018–2024), including season start and end dates (95% cumulative method), peak date and peak daily concentration (Peak value), Seasonal Pollen Integral (SPIn), and season length (days).*

Station	year	Start date	End date	Peak date	Peak value	SPIn	Length days
Augsburg	2018	27/04/2018	26/07/2018	10/05/2018	53.3	713.6	91
Augsburg	2019	08/05/2019	03/09/2019	06/06/2019	46.4	469.6	119
Augsburg	2020	08/05/2020	25/08/2020	28/07/2020	143.2	2308.6	110
Augsburg	2021	15/05/2021	19/08/2021	12/06/2021	85.9	880.3	97
Augsburg	2022	12/05/2022	05/09/2022	26/05/2022	130.6	780.8	117
Augsburg	2023	10/05/2023	24/08/2023	02/06/2023	65.3	784.7	107
Augsburg	2024	01/05/2024	29/08/2024	05/06/2024	126	1030.7	121
Córdoba	2018	21/04/2018	11/09/2018	03/06/2018	275	5865	144
Córdoba	2019	02/03/2019	05/08/2019	11/05/2019	366	6237	157
Córdoba	2020	02/03/2020	05/10/2020	06/05/2020	267	4497.9	218
Córdoba	2021	17/03/2021	10/08/2021	18/05/2021	1335	14875	147
Córdoba	2022	22/02/2022	19/09/2022	21/05/2022	226	3312.1	210
Córdoba	2023	19/02/2023	02/10/2023	25/04/2023	112.8	2165.8	226
Córdoba	2024	15/03/2024	01/07/2024	12/05/2024	906.2	5006.1	109
Thessaloniki	2018	30/03/2018	15/10/2018	03/05/2018	13	267	200
Thessaloniki	2019	24/03/2019	27/10/2019	20/05/2019	18	286	218
Thessaloniki	2020	01/04/2020	23/10/2020	26/05/2020	17	284	206
Thessaloniki	2021	06/04/2021	05/10/2021	11/05/2021	27	370	183
Thessaloniki	2022	01/04/2022	17/10/2022	16/05/2022	21	628	200
Thessaloniki	2023	01/04/2023	09/10/2023	22/05/2023	44	1010	192
Thessaloniki	2024	10/04/2024	16/10/2024	18/05/2024	63	1031	190

Table S3. *Summary of seasonal and pre-season weather conditions in Augsburg, Córdoba and Thessaloniki during the grass pollen seasons (2018–2024). Variables include mean_tavg_season – mean daily average temperature (°C) during the pollen season, mean_tmax_season – mean daily maximum temperature (°C) during the pollen season, mean_rhum_season – mean daily relative humidity (%) during the pollen season, total_prcp_season – cumulative precipitation (mm) during the pollen season, rain_days_season – number of days with precipitation ≥1 mm during the pollen season, gdd_season – growing degree days (base 5 °C) accumulated during the pollen season, dryspell_max_season – maximum length of a consecutive dry spell (days with precipitation <1 mm) during the pollen season, mean_tavg_pre – mean daily average temperature (°C) during the 30 days preceding the pollen season, total_prcp_pre – cumulative precipitation (mm) during the 30 days preceding the pollen season and rain_days_pre – number of days with precipitation ≥1 mm during the 30 days preceding the pollen season.*

Site	year	mean_tavg_season	mean_rhum_season	total_prcp_season	rain_days_season	dryspell_max_season	mean_tavg_pre	total_prcp_pre	rain_days_pre
Augsburg	2018	17.03	73.11	213.95	25	10	12.06	15.8	4
Augsburg	2019	17.20	73.53	350.95	36.5	11	9.03	38.6	6.5
Augsburg	2020	16.57	74	278.7	31.5	11	10.85	26.1	6
Augsburg	2021	16.21	76.75	430	52	10	7.91	104.05	11
Augsburg	2022	17.99	68.3	181.55	31	12	9.16	28.55	8.5
Augsburg	2023	17.51	68.49	303.55	33	17	9.5	90.4	14.5
Augsburg	2024	17.54	76.83	538.05	43	7	9.33	48.95	9.5
Córdoba	2018	23.0	51.38	37.9	6	84	12.78	68.1	9
Córdoba	2019	20.83	51.92	67.9	14	103	10.37	0	0
Córdoba	2020	22.58	54.48	216.8	27	40	12.85	2	1
Córdoba	2021	22.18	51.34	78.7	17	59	11.88	19.8	4
Córdoba	2022	22.55	52.43	215.5	24	100	10.51	0.6	0
Córdoba	2023	22.84	48.35	116.1	16	88	7.57	40.4	3
Córdoba	2024	20.12	60.56	133.2	12	41	11.43	65.2	8
Thessaloniki	2018	21.81	56.45	115	10	6	10.58	30.6	4
Thessaloniki	2019	21.07	62.21	166.2	19	7	9.82	11.5	1
Thessaloniki	2020	20.94	63.34	128	12	5	9.96	28.2	4
Thessaloniki	2021	21.89	61.79	23.9	8	5	9.15	14.5	4
Thessaloniki	2022	21.37	64.22	94.7	11	4	6.64	21.8	4
Thessaloniki	2023	21.44	66.17	113.8	17	5	10.48	28.4	5
Thessaloniki	2024	23.3	60.26	55.7	9	7	13.2	0.5	0

Table S4. *Predictive performance of the seven forecasting sub-models for Poaceae pollen concentrations in Augsburg, Córdoba and Thessaloniki. Reported metrics include root mean squared error (rmse), coefficient of determination (rsq), mean absolute error (mae), mean absolute scaled error (mase), and ensemble weight assigned to each model. Lower RMSE and MAE values indicate better performance. ARIMA orders were automatically selected by the auto_arima procedure (modeltime package, which internally uses forecast) and varied across sites (e.g., ARIMA (4,0,0), ARIMA (5,0,0)).*

.model_desc	rmse	rsq	mae	mase	weight	station
RLR	5.577398	0.658034	2.049181	0.629637	0.176373	Augsburg
XGB	5.785206	0.654554	2.077016	0.638189	0.170037	Augsburg
NNETAR(4,1,10)[7]	25.59741	0.088087	18.70144	5.746254	0.03843	Augsburg
RF	6.95358	0.479569	2.312269	0.710474	0.141467	Augsburg
SVR	6.762546	0.572885	2.340688	0.719206	0.145463	Augsburg
PROPHET-XGB-XGB	6.629591	0.564097	2.459774	0.755797	0.14838	Augsburg
ARIMA(4,0,0)	5.469584	0.670717	1.834504	0.563675	0.179849	Augsburg
RLR	46.79723	0.586994	11.47059	0.709541	0.156344	Córdoba
XGB	53.80967	0.457589	12.53358	0.775294	0.135969	Córdoba
NNETAR(4,1,10)[7]	42.04199	0.688243	17.12968	1.059597	0.174027	Córdoba
RF	60.83858	0.299584	16.35833	1.011884	0.12026	Córdoba
SVR	57.50956	0.374412	15.20939	0.940814	0.127222	Córdoba
PROPHET-XGB	56.13708	0.403727	17.63485	1.090846	0.130332	Córdoba
ARIMA(5,0,0)	46.94681	0.58283	10.69411	0.66151	0.155846	Córdoba
RLR	3.509575	0.807488	1.450196	0.609205	0.148391	Thessaloniki
XGB	4.037075	0.724077	1.739454	0.730718	0.129002	Thessaloniki
NNETAR(4,1,10)[7]	2.647926	0.908392	0.982657	0.412799	0.196678	Thessaloniki
RF	4.355045	0.687455	1.828224	0.768009	0.119583	Thessaloniki
SVR	4.295597	0.771745	1.780898	0.748128	0.121238	Thessaloniki
PROPHET-XGB	4.177082	0.707819	1.996226	0.838584	0.124678	Thessaloniki
ARIMA(5,0,0)	3.246188	0.804421	1.37344	0.576961	0.160431	Thessaloniki

Table S5. *Predictive performance of the ensemble-forecasting model for Poaceae pollen concentrations in Augsburg, Córdoba and Thessaloniki. Reported metrics include mean absolute error (mae), mean absolute scaled error (mase), root mean squared error (rmse), and coefficient of determination (rsq). Lower RMSE and MAE values indicate better performance.*

.model_desc	mae	mase	rmse	rsq	station
ENSEMBLE (WEIGHTED): 7 MODELS	2.316623	0.711812	5.744712	0.661968	Augsburg
ENSEMBLE (WEIGHTED): 7 MODELS	12.38011	0.765801	45.61296	0.617318	Córdoba
ENSEMBLE (WEIGHTED): 7 MODELS	1.369919	0.575482	3.336829	0.841793	Thessaloniki

Table S6. *Predictive performance of the ensemble and individual models for lag 1-3 predictions across Augsburg, Córdoba and Thessaloniki. Metrics reported include mean absolute error (mae), mean absolute scaled error (mase), root mean squared error (rmse), and coefficient of determination (rsq). Lower RMSE and MAE values indicate better performance.*

.model_desc	mae	mase	rmse	rsq	model_type	station	lag
RLR	2.049181	0.629637	5.577398	0.658034	Single	Augsburg	1
XGB	2.077016	0.638189	5.785206	0.654554	Single	Augsburg	1
NNETAR(4,1,10)[7]	24.20067	7.435962	33.0643	0.056683	Single	Augsburg	1
RF	2.315214	0.711379	6.94786	0.482532	Single	Augsburg	1
SVR	2.340852	0.719256	6.762776	0.572883	Single	Augsburg	1
PROPHET-XGB	2.459774	0.755797	6.629591	0.564097	Single	Augsburg	1
ARIMA(4,0,0)	1.834504	0.563675	5.469584	0.670717	Single	Augsburg	1
Ensemble (Weighted)	2.374905	0.72972	5.753772	0.661846	Ensemble	Augsburg	1
RLR	11.47059	0.709541	46.79723	0.586994	Single	Córdoba	1
XGB	12.53358	0.775294	53.80967	0.457589	Single	Córdoba	1
NNETAR(4,1,10)[7]	12.18941	0.754005	33.07108	0.793454	Single	Córdoba	1
RF	16.31217	1.009028	60.73258	0.301957	Single	Córdoba	1
SVR	15.21782	0.941335	57.50324	0.374562	Single	Córdoba	1
PROPHET-XGB	17.63485	1.090846	56.13708	0.403727	Single	Córdoba	1
ARIMA(5,0,0)	10.69411	0.66151	46.94681	0.58283	Single	Córdoba	1
Ensemble (Weighted)	11.4841	0.710377	44.4614	0.639253	Ensemble	Córdoba	1
RLR	1.450196	0.609205	3.509575	0.807488	Single	Thessaloniki	1
XGB	1.739454	0.730718	4.037075	0.724077	Single	Thessaloniki	1
NNETAR(4,1,10)[7]	1.022648	0.429599	2.628506	0.908647	Single	Thessaloniki	1
RF	1.830698	0.769048	4.356544	0.685388	Single	Thessaloniki	1
SVR	1.780761	0.748071	4.295274	0.771588	Single	Thessaloniki	1
PROPHET-XGB	1.996226	0.838584	4.177082	0.707819	Single	Thessaloniki	1
ARIMA(5,0,0)	1.37344	0.576961	3.246188	0.804421	Single	Thessaloniki	1
Ensemble (Weighted)	1.374515	0.577413	3.332897	0.841615	Ensemble	Thessaloniki	1
RLR	3.151479	0.968332	8.753321	0.197705	Single	Augsburg	2
XGB	3.115081	0.957148	8.843949	0.183977	Single	Augsburg	2
NNETAR(4,1,10)[7]	18.1485	5.576356	26.063	0.009108	Single	Augsburg	2
RF	2.804223	0.861633	8.189521	0.263295	Single	Augsburg	2
SVR	2.740726	0.842123	8.292774	0.281401	Single	Augsburg	2
PROPHET-XGB	3.001317	0.922193	8.664083	0.194687	Single	Augsburg	2
ARIMA(2,0,1)(1,0,1)[7]	3.168376	0.973524	8.841075	0.198771	Single	Augsburg	2
Ensemble (Weighted)	3.393984	1.042845	8.303789	0.243645	Ensemble	Augsburg	2
RLR	19.63875	1.214802	75.97492	0.115191	Single	Córdoba	2
XGB	17.49953	1.082475	66.94449	0.164454	Single	Córdoba	2
NNETAR(4,1,10)[7]	119.7102	7.404963	64.0292	1.23E-07	Single	Córdoba	2
RF	19.02224	1.176666	69.03896	0.114619	Single	Córdoba	2
SVR	19.06912	1.179566	72.22521	0.072982	Single	Córdoba	2
PROPHET-XGB	22.29096	1.378861	77.52718	0.050469	Single	Córdoba	2
ARIMA(0,0,5)	18.8204	1.164181	74.58881	0.09632	Single	Córdoba	2
Ensemble (Weighted)	22.52649	1.39343	70.61818	0.107966	Ensemble	Córdoba	2
RLR	2.132062	0.895647	4.934755	0.582669	Single	Thessaloniki	2
XGB	2.424989	1.018701	5.472492	0.471351	Single	Thessaloniki	2
NNETAR(4,1,10)[7]	2.282958	0.959036	5.10446	0.525161	Single	Thessaloniki	2

RF	2.138555	0.898374	4.945935	0.567196	Single	Thessaloniki	2
SVR	2.301462	0.966809	5.630717	0.527361	Single	Thessaloniki	2
PROPHET-XGB	2.353258	0.988568	4.886135	0.585256	Single	Thessaloniki	2
ARIMA(3,0,0)(1,0,1)[7]	2.119441	0.890345	4.812979	0.572459	Single	Thessaloniki	2
Ensemble (Weighted)	2.110082	0.886414	4.920391	0.583781	Ensemble	Thessaloniki	2
RLR	3.24639	0.997495	8.651018	0.190141	Single	Augsburg	3
XGB	3.343049	1.027194	9.061883	0.178051	Single	Augsburg	3
NNETAR(4,1,10)[7]	31.39845	9.647571	39.72345	0.064102	Single	Augsburg	3
RF	2.915102	0.895702	8.361802	0.234656	Single	Augsburg	3
SVR	2.741317	0.842304	8.510234	0.271892	Single	Augsburg	3
PROPHET-XGB	3.23846	0.995058	8.717836	0.194303	Single	Augsburg	3
ARIMA(3,0,0)(1,0,1)[7]	3.472683	1.067026	8.998358	0.127278	Single	Augsburg	3
Ensemble (Weighted)	3.661396	1.12501	8.40599	0.231101	Ensemble	Augsburg	3
RLR	21.96294	1.35857	79.06971	0.057377	Single	Córdoba	3
XGB	19.16292	1.185368	74.23754	0.049337	Single	Córdoba	3
NNETAR(4,1,10)[7]	23.88668	1.477568	67.93658	0.153305	Single	Córdoba	3
RF	20.26905	1.253791	73.79637	0.058255	Single	Córdoba	3
SVR	18.42533	1.139743	72.66833	0.051166	Single	Córdoba	3
PROPHET-XGB	22.81353	1.411186	72.40625	0.082007	Single	Córdoba	3
ARIMA(3,0,2)	21.37614	1.322272	81.40161	0.024237	Single	Córdoba	3
Ensemble (Weighted)	19.80579	1.225134	72.79833	0.071486	Ensemble	Córdoba	3
RLR	2.184666	0.917745	5.072809	0.563055	Single	Thessaloniki	3
XGB	2.442131	1.025902	5.348451	0.482333	Single	Thessaloniki	3
NNETAR(4,1,10)[7]	5.456584	2.292228	7.654705	0.137405	Single	Thessaloniki	3
RF	2.158865	0.906906	4.924468	0.572026	Single	Thessaloniki	3
SVR	2.364577	0.993323	5.816655	0.533723	Single	Thessaloniki	3
PROPHET-XGB	2.26665	0.952185	4.935291	0.571525	Single	Thessaloniki	3
ARIMA(2,0,2)	2.289895	0.96195	5.115452	0.51809	Single	Thessaloniki	3
Ensemble (Weighted)	2.32367	0.976138	4.991617	0.573237	Ensemble	Thessaloniki	3

Supplementary figures

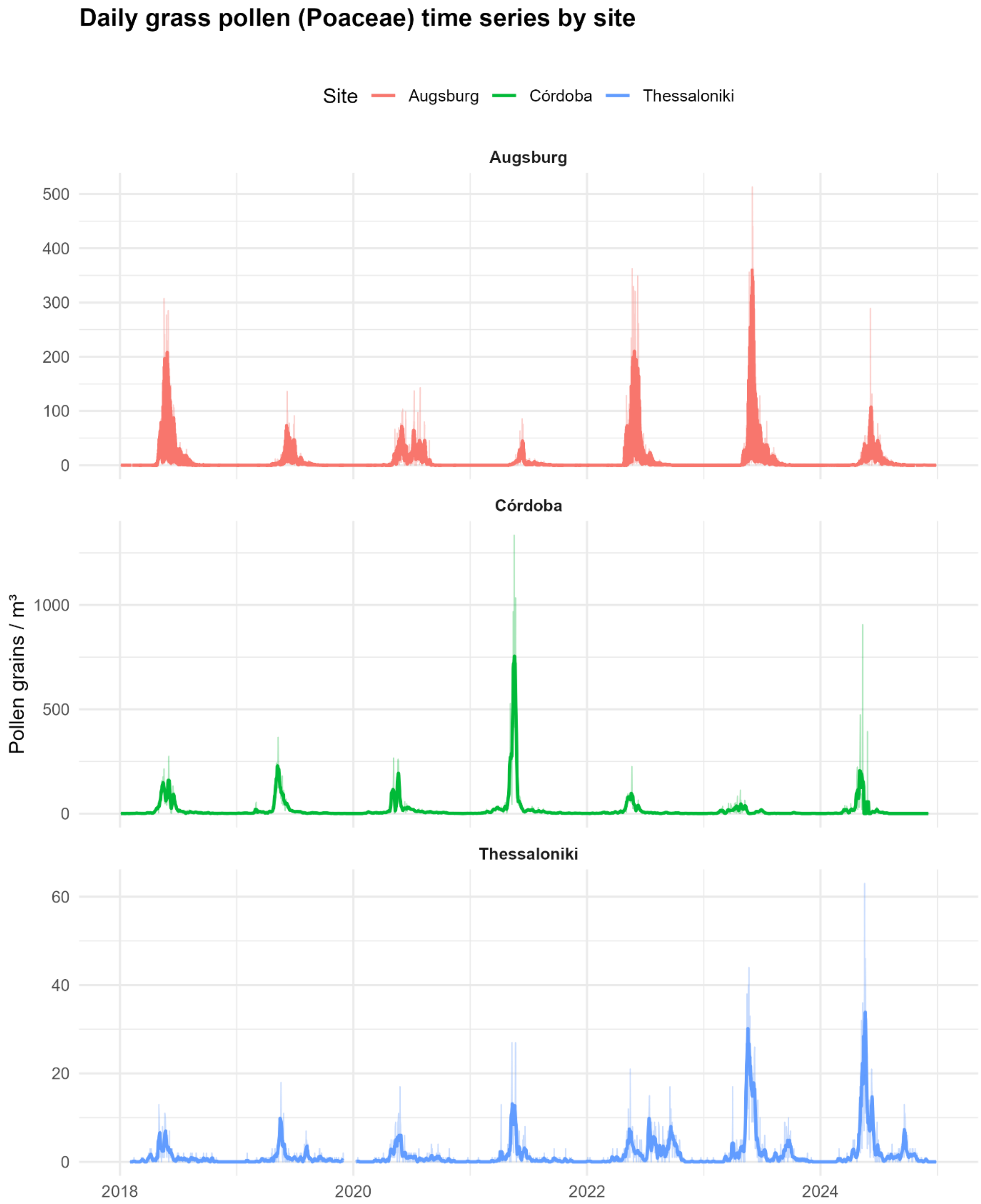

***Figure S1**. Daily grass pollen (Poaceae) concentrations in Augsburg (top panel), Córdoba (central panel) and Thessaloniki (bottom panel) from 2018–2024. Faint lines represent daily values, and bold lines indicate 7-day rolling means.*

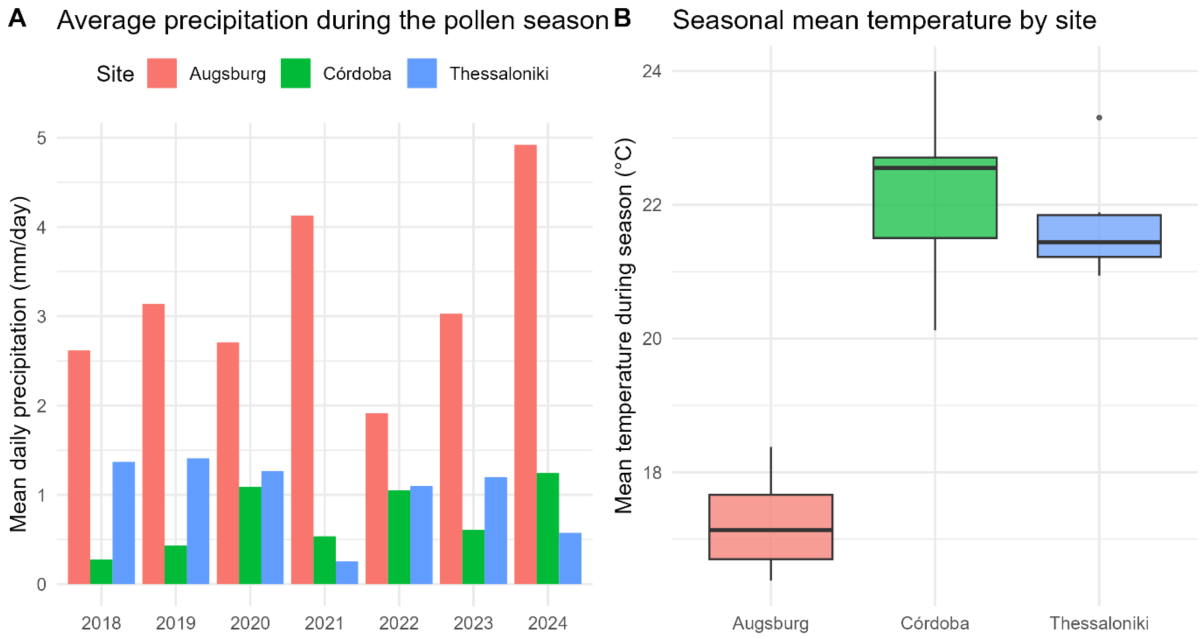

Figure S2. *Meteorological conditions during the pollen season (2018–2024) in Augsburg, Córdoba and Thessaloniki. (A) Mean daily precipitation, and (B) Mean daily air temperature.*

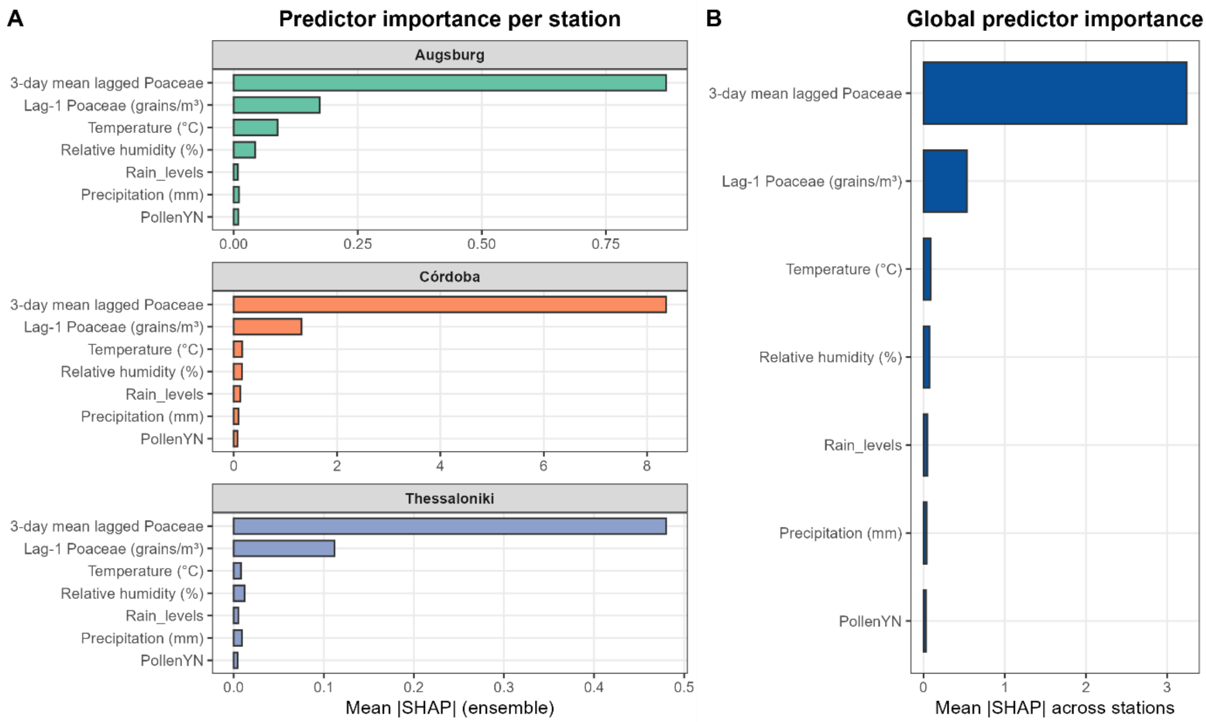

Figure S3*. SHAP (SHapley Additive exPlanations) feature importance for predicting daily Poaceae pollen concentrations using the ensemble forecast in (A) Station-specific mean absolute SHAP values across Augsburg, Córdoba, and Thessaloniki, showing how the relative contribution of each factor varies by climate and local pollen dynamics. (B) Global importance aggregated across the three stations. Bars represent the mean absolute SHAP value of each predictor, quantifying its average contribution to model output. Larger bar lengths indicate higher predictive importance.*

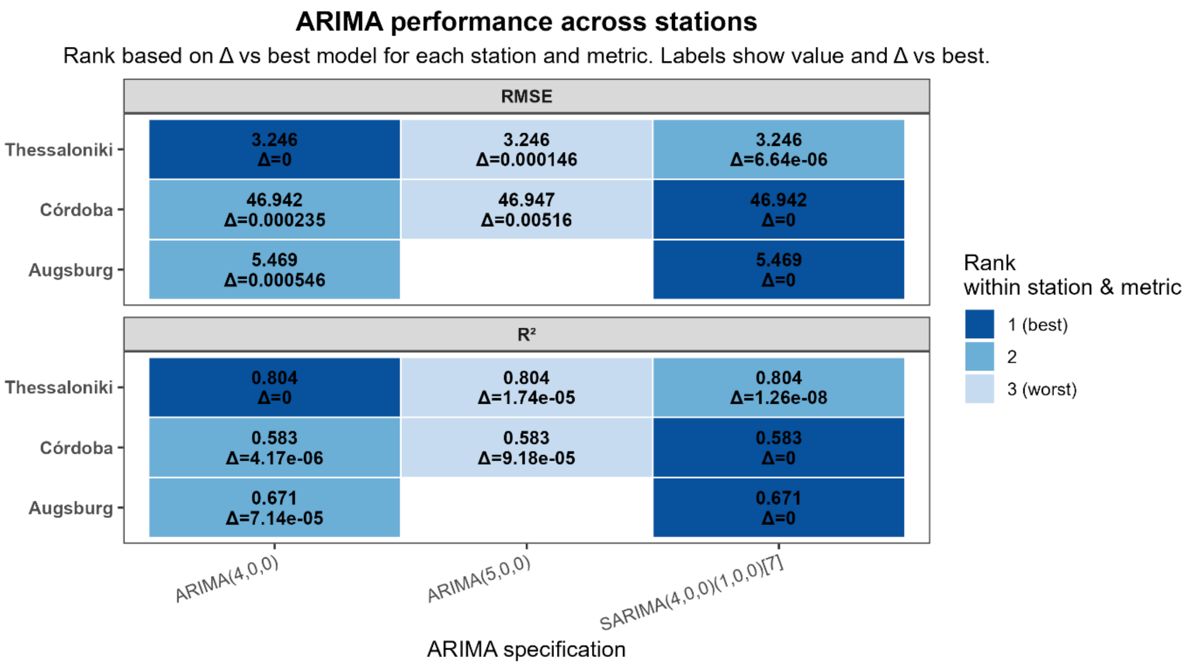

Figure S4*. Sensitivity of ARIMA specifications to station and metric. Rank-based heatmap comparing three time-series structures—ARIMA(4,0,0), ARIMA(5,0,0), and SARIMA(4,0,0)(1,0,0)[7]—for Augsburg, Córdoba and Thessaloniki. Panels show RMSE (top) and R² (bottom). Within each station and metric combination, darker tiles indicate better rank (1 = best, 3 = worst). Numerical labels give the absolute metric value and its difference (Δ) relative to the best-performing ARIMA specification at that station.*

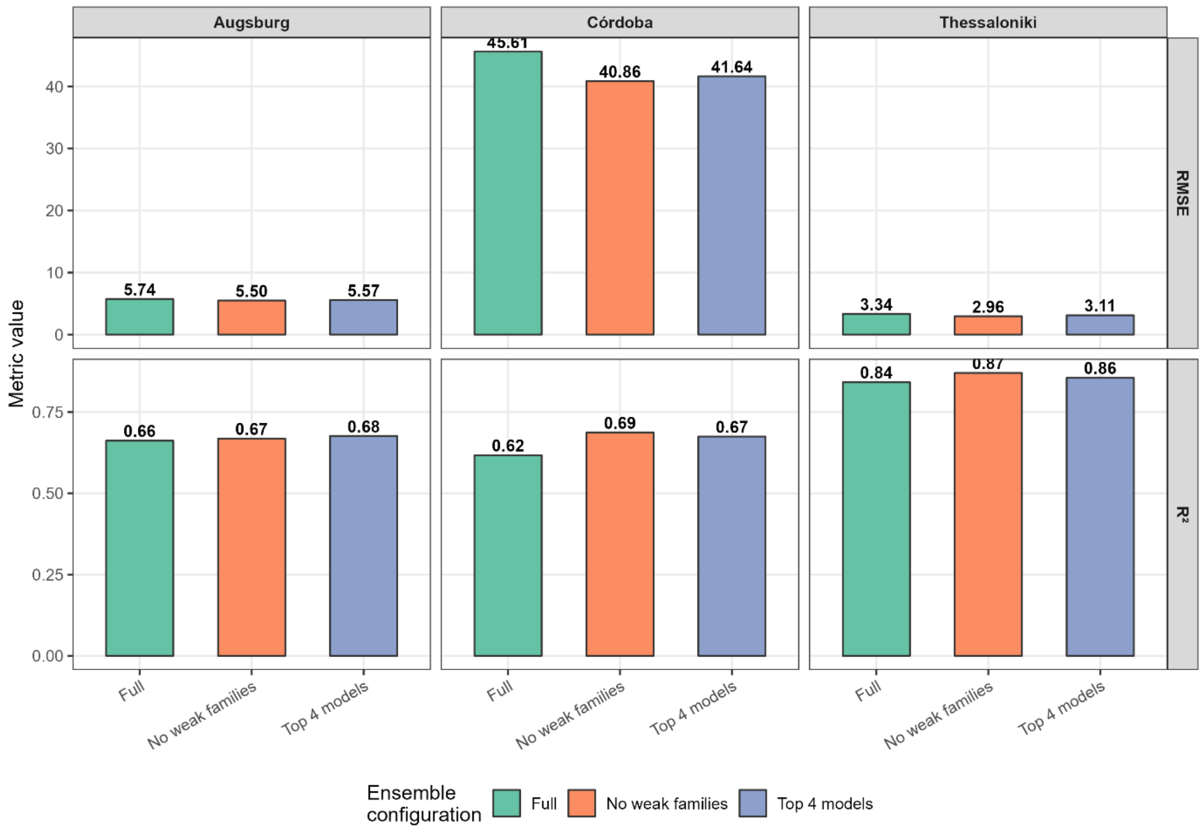

Figure S5*. Performance of three ensemble configurations, Full 7-model ensemble, 4-model ensemble without weak families, and Top-4 highest-performing models, evaluated at the three study stations (Augsburg, Córdoba, and Thessaloniki). Bars show RMSE (top row) and R² (bottom row) for each ensemble variant.*

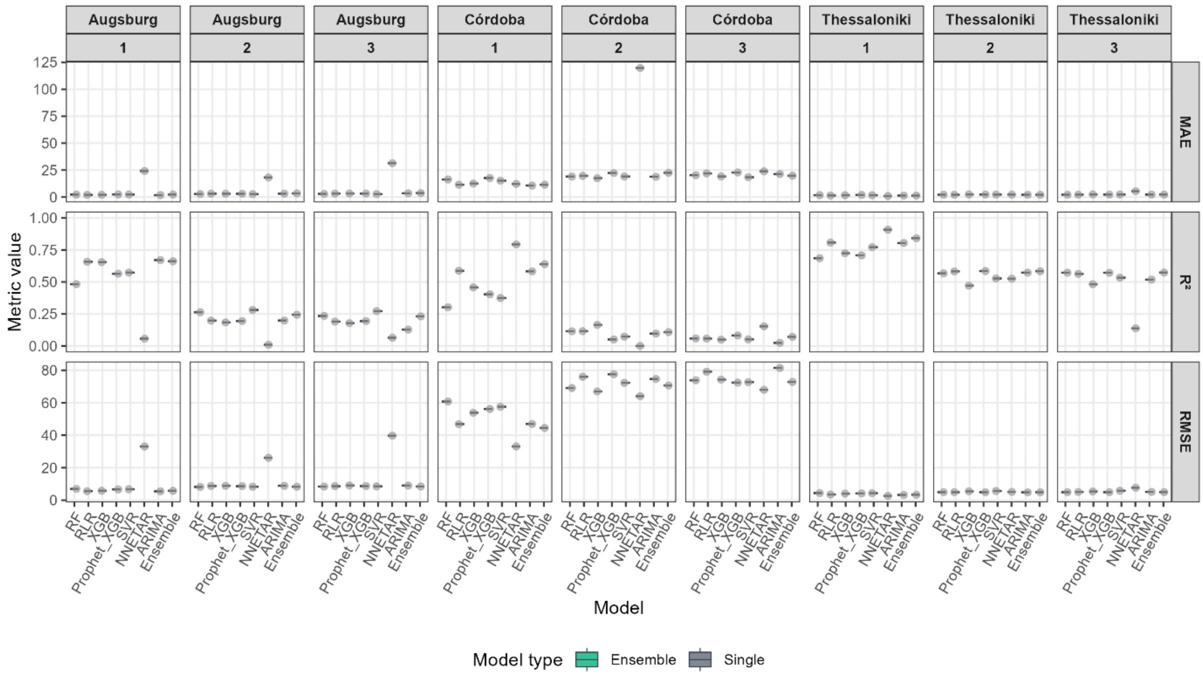

Figure S6. *Comparison of ensemble versus single-model performance across stations and lag structures. Panels show mean values (± standard deviation) of MAE, R2 and RMSE for lags of 1–3 days, faceted by station (Augsburg, Córdoba, Thessaloniki). Error bars indicate variability across years.*

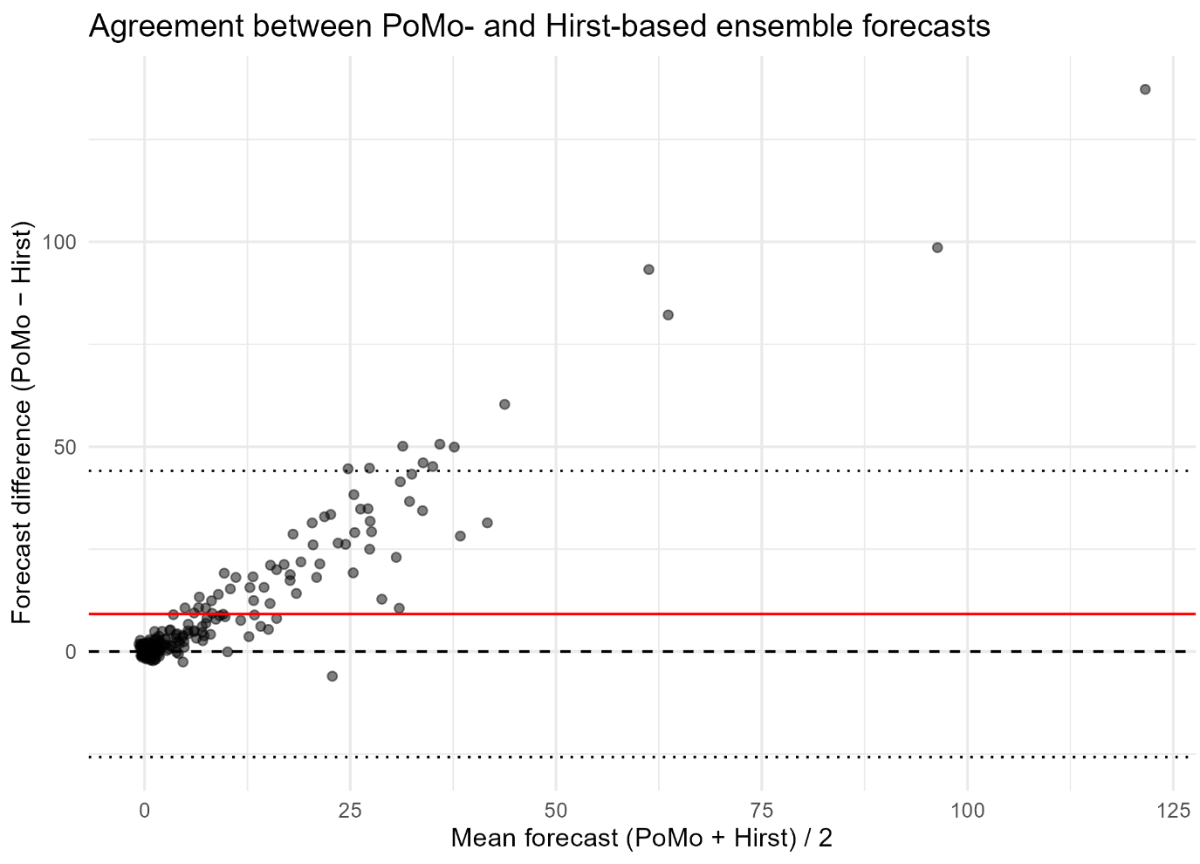

Figure S7. *Bland–Altman comparison of PoMo-based (BAA500 - Helmut Hund GmbH, Wetzlar, Germany) and Hirst-based (Hirst, 1952; Burkard Co. Ltd, UK) ensemble forecasts. The plot shows the difference between PoMo and Hirst predictions as a function of their mean value. The red line denotes the mean bias (PoMo − Hirst = 9.16 grains/m³), while dotted lines indicate the 95% limits of agreement (±1.96 SD). Points represent daily forecasts used in both models. Positive values indicate higher predicted concentrations from PoMo-driven ensembles.*