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Appendix

A Competing architectures

In the section we detail the predictive performances (Fig. 7) and computational requirements (Fig. 8) of 7 different ANN architectures at the species occupancy problem. We show those for two validation procedures: (i) a 50/50 train test split and a (ii) 5-fold cross validation retaining 3 out of 15 clusters at each iteration, those are clusters of samples built with a kmeans approach on the scaled coordinates. This second approach is called a block cross-validation. It prevents information leakage from train to test datasets, caused e.g by pairs of samples that can be practically in the same local area but nonetheless distributed on both side of the split.

Additionally we present the performances for the full set of traits and environmental covariates, as well as for a reduced set. The reduced set consists of the traits and covariates highlighted by Figs. 4 and 6 for the butterflies and the moths respectively. In other words, we restrict the inputs to the traits and covariates underlying the 10% most important trait-environment interactions.

For reference we also show the performance of *Hmsc*, arguably the best existing approach to joint distribution modelling (?). Convergence was achieved in butterflies with the following hyper-parameters: 3 chains, thinning of 10, 1000 (chain) samples, 1000 transient samples. Because of the computational requirements of this method, no random effects were used, and only 10% of each data sets was used (before train/test splits). For moths however, we had to reduce to 300 chain samples so that it could be computed in less than a week.

In addition to *ensemble* and *multi-branch* architectures defended in this paper, 5 architectures are tested. We detail below their specificities, as well as the dimensions of their inputs (X) and outputs (Y):

- *sp-specific* [X: n samples \times m covariates \rightarrow Y: n samples \times q species] is the simplest MSDM form, it does not use traits but only environmental covariates, it is multi-output but does not build on trait mediation;
- *trait-mediated* [X: n samples \times (m covariates \cdot ($1 + p$ traits)) \rightarrow Y: n samples \times q species] is the time distributed construct we advocate to support trait-mediation and explain it;
- *ensemble* [X: n samples \times (m covariates \cdot ($1 + p$ traits)) \rightarrow Y: n samples \times q species] is the ensemble averaging of the two previous models;
- *multi-branch* [X: n samples \times (m covariates \cdot ($1 + p$ traits)) \rightarrow Y: n samples \times q species] is the sequential training of the *trait-mediated* and the *sp-specific* branches; conversely to the *ensemble* approach, *sp-specific* branch is conditional on the *trait-mediated* branch as the former is trained on the residual of the later;

- *multi-branch concat* [$X: n \text{ samples} \times (m \text{ covariates} \cdot p \text{ traits}) \rightarrow Y: n \text{ samples} \times q \text{ species}$] is the same as the previous one, except that it does not build on a Kronecker product of the traits and covariates but simply their concatenation; in the current form of SHAP, even if it builds on trait-mediation it cannot explain it (interaction values are not available for *deep explainers*);
- *long* [$X: (n \text{ samples} \cdot q \text{ species}) \times (m \text{ covariates} \cdot (1 + p \text{ traits})) \rightarrow Y: n \text{ samples} \times 1$] is a single output model which build on a long tabular form in which each sample is a site.year.species rather than a site.year; the input for a sample is a Kronecker product of all the covariates of the site with all the traits of the focal species;
- *long concat* [$X: (n \text{ samples} \cdot q \text{ species}) \times (m \text{ covariates} + p \text{ traits}) \rightarrow Y: n \text{ samples} \times 1$] is the same as *long* except it builds on a simple concatenation of traits and covariates rather than the Kronecker product.

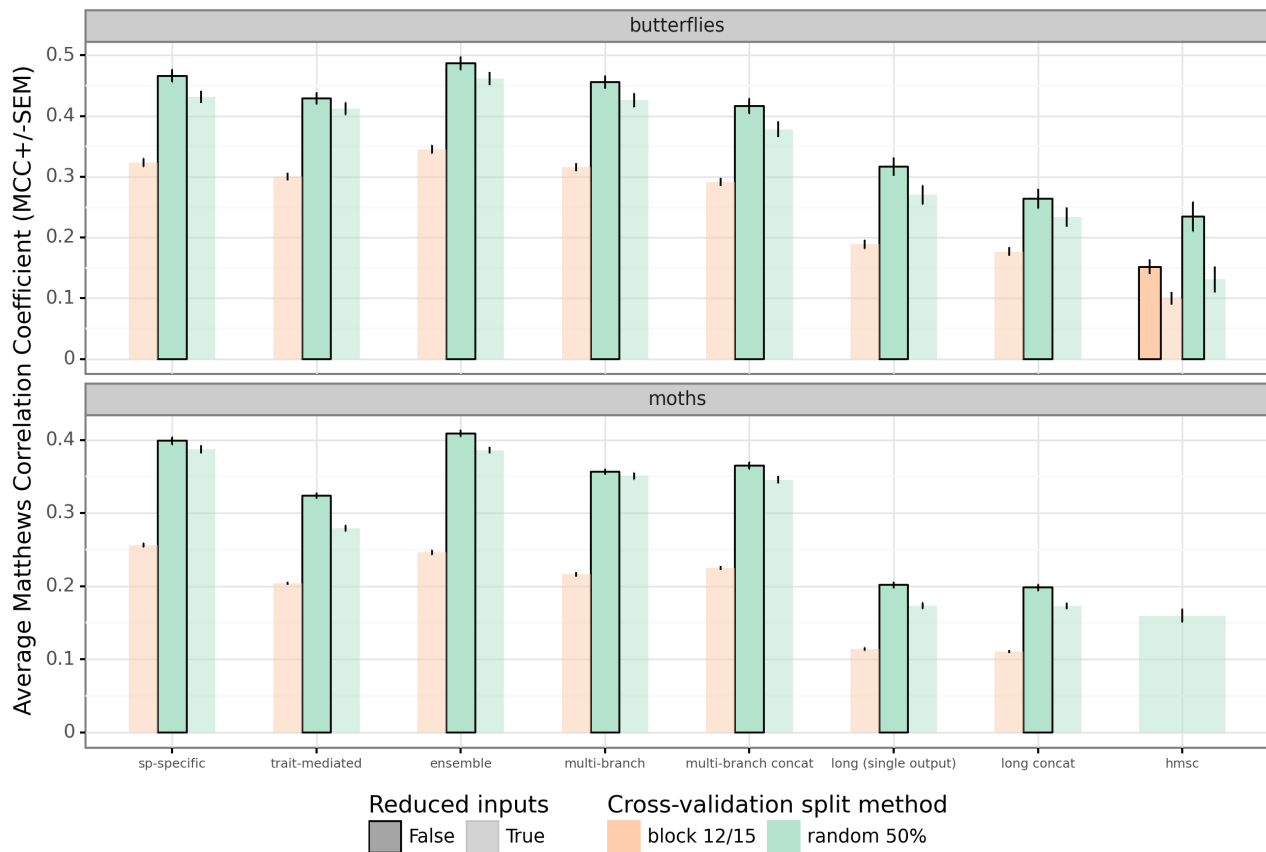


Figure 7: Predictive performance of 8 competing models depending on the validation procedure and whether or not the inputs (traits and covariates) have filtered first. The model *ensemble* and *multi-branch* are the two options defended in this paper as they allow for the explanation of trait mediation.

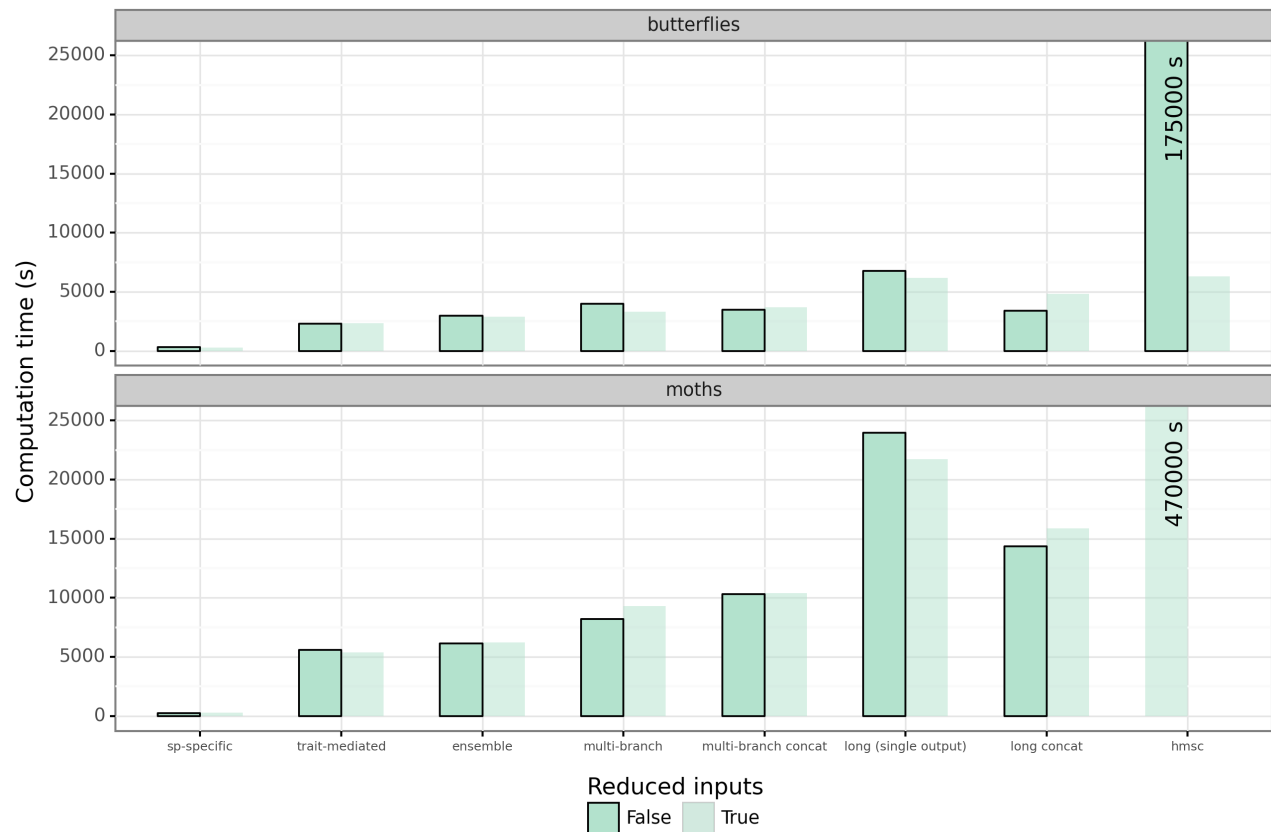


Figure 8: Computation times for the training of the 8 competing models depending on whether or not the inputs (traits and covariates) have filtered first. The ANNs model use 50% of the data sets, while the Hmsc model only uses 10%.

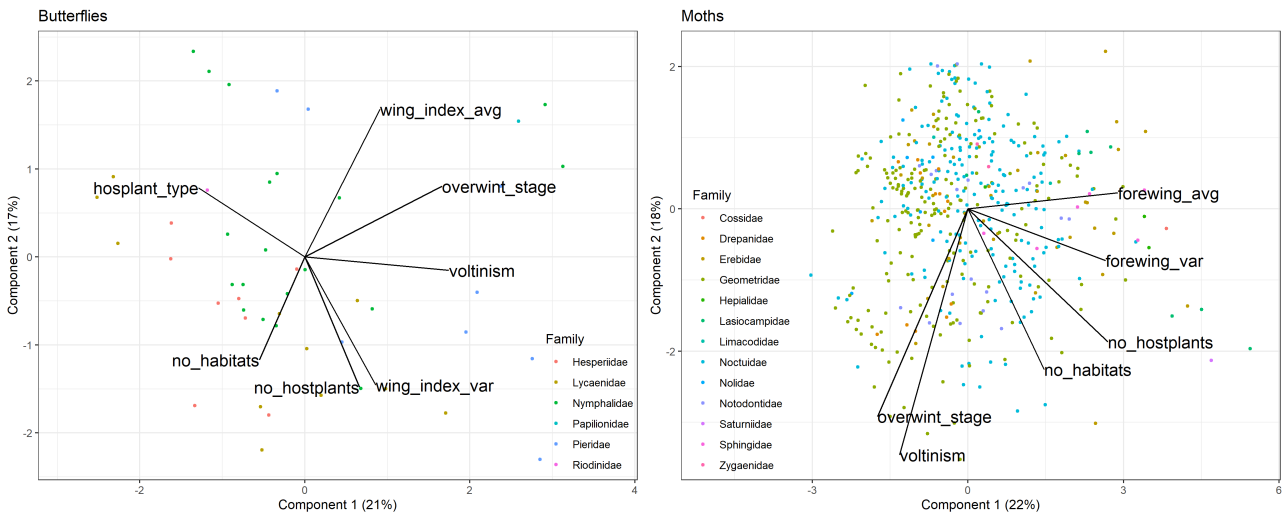


Figure 9: Biplots from the principal component analysis of the traits of the two communities. The coloured dots represent the species, while the segments show the traits' contributions to the two principal components.

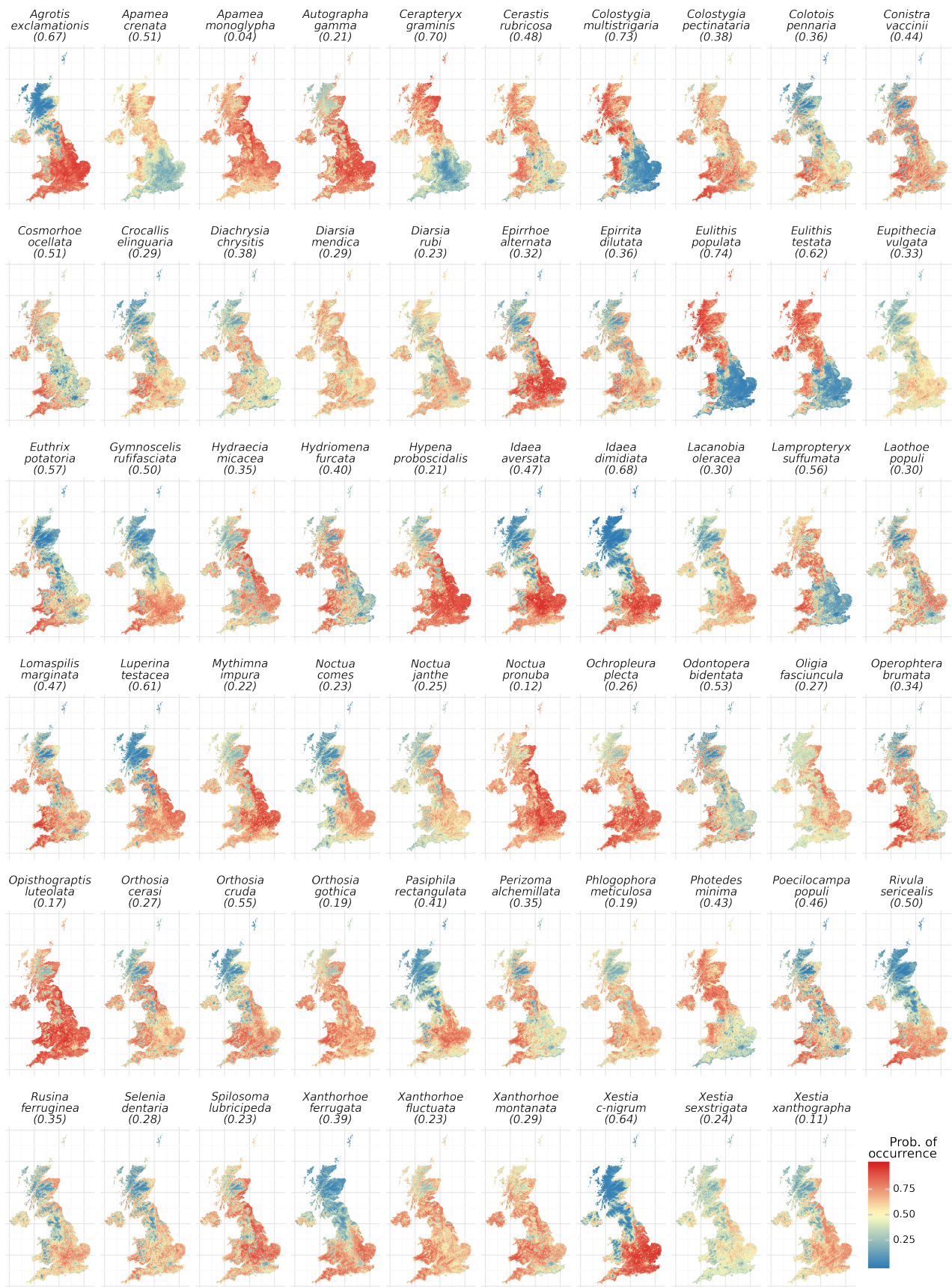


Figure 10: Predicted probability of occurrence of the 59 most common species of moths for the year 2020.

B Traits principal component analysis

C Moth predictions

D Moth species-specific response

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E Environmental covariates

Table 1: Environmental covariates used in the models. See [BIOCLIM19](#) for further details.

Name	Full name
temp_avg	Annual mean temperature
temp_diu_ran	Mean diurnal range
isotherm	Isothermality ($\text{temp_ran_dy}/\text{temp_yr_ran}$)
temp_season	Temp. seasonality (sd temp)
temp_max	Temp. of the warmest month
temp_min	Temp. of the coldest month
temp_yr_ran	Temp. annual range ($\text{temp_max}-\text{temp_min}$)
temp_wet_qtr	Temp. of the wettest quarter
temp_dry_qtr	Temp. of the driest quarter
temp_warm_qtr	Temp. of the warmest quarter
temp_cold_qtr	Temp. of the coldest quarter
rain_sum	Annual precipitation
rain_max	Prec. of the wettest month
rain_min	Prec. of the driest month
rain_season	Prec. seasonality
rain_wet_qtr	Prec. of the wettest quarter
rain_dry_qtr	Prec. of the driest quarter
rain_warm_qtr	Prec. of the warmest quarter
rain_cold_qtr	Prec. of the coldest quarter
no_frost_days	Number of frost days
wind_avg	Average wind speed
past_temp	temp of the previous year
past_rain	rain of the previous year
shdi_lc	Shannon diversity index of the land-covers
heterogeneity	contiguity of identical land-cover pixels
%broadleaf	Proportion of broadleaf woodlands
%conifer	Prop. of coniferous woodlands
%arable	Prop. of arable land
%imprv_grsl	Prop. of improved grassland
%seminat_grsl	Prop. of seminatural grassland
%mountain	Prop. of mountain and bog terrain
%coast	Prop. of coastal terrain
%urban	Prop. of urban terrain
dist_to_sea	Distance to the sea
elevation	Average altitude
slope	Average slope
aspect	Orientation of the slope
river_dens	Density of the river network

