

Ecography

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**Supplementary material**

## Appendix 1

### List of reference used to extract species richness information

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## Appendix 2

### Collinearity assessment and removal

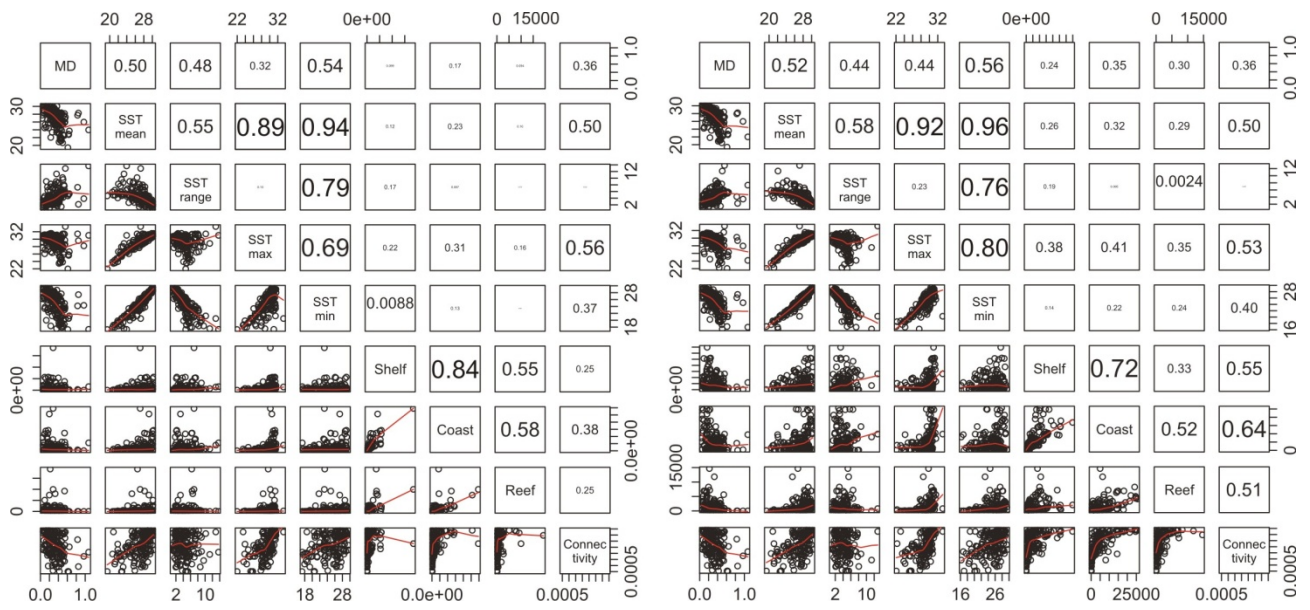
Although boosted regression trees (BRT) are generally considered a robust technique not requiring *a priori* selection of explanatory variables, recent research evidenced that removal of collinearity remains a desirable choice reducing the risk of biased predictions also for techniques based on boosting (Dormann et al., 2012). As suggested by Dormann et al., 2012, we have made an *a priori* selection for explanatory variables showing a Pearson correlation coefficient  $|r| > 0.7$ .

Figure S1 shows the absolute values of Pearson correlation coefficient calculated between each pair of the explanatory variables obtained with both locations of different size and locations defined as areas within a 600km radius. In both cases, strong collinearity (i.e.  $|r| > 0.7$ ) was detected for SST variables and between shelf area and coast length. In particular, mean SST was strongly collinear to the minimum and the maximum SSTs. In addition, minimum SST was strongly collinear to SST range. For this reason, we decided to remove the minimum and the maximum SST from our analysis *a priori* while keeping mean SST and SST range. The choice is motivated by the fact that highest values of  $|r|$  were always detected between mean SST and the other variables, thus suggesting that alone, the mean SST already contains most of the information about the extremes (i.e. minimum and maximum SST). Regarding the collinearity detected between shelf area and coast length, we decided to remove the shelf area from the explanatory variables because previous research evidenced a negligible role of this variable as determinant of reef fish richness (Bellwood et al., 2005)

For the structural equation model, collinearity among variables may be handled by modeling them as indicators of a unmeasured latent (Mitchell, 1992). However, recent research evidenced that the employment of latent variables does not outperform the pre-selection procedure (Dormann et al., 2012). For this reason and in order to keep the structural equation analysis conform to BRT, the same *a priori* selection of explanatory variables was employed.

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**Figure A1.** Plot of the correlations between pairs of explanatory variables obtained for locations of different size (left panel) or standard areas within a radius of 600km. Number are proportional to absolute values of the Pearson correlation coefficient.

## Appendix 3

### Model calibration

Boosted regression trees were fitted using the gbm library in R (Ridgeway, 2007) and additional functions provided by Elith et al. (2008). The technique allows for the specification of 4 main parameters: bag fraction (*bf*), learning rate (*lr*), tree complexity (*tc*) and the number of trees (*nt*).

*bf* is the proportion of samples used at each step, *lr* is the contribution of each fitted tree to the final model; *tc* is the number of nodes of each fitted tree determining the extent to which statistical

interactions were fitted and *nt* represents the number of trees corresponding to the number of boosting iterations.

Once the first three parameters are set, the optimal *nt* may be estimated using a Cross-Validation (CV) procedure allowing to identify the number of trees minimizing a loss function, i.e. deviance (*D*) reduction.

For the model calibration step, we tested different combinations of *bf* (0.5, 0.55, 0.6, 0.65, 0.7, 0.75, 0.8, 0.85), *lr* (0.01, 0.005, 0.001) and *tc* (from 1 to 20). These combinations derived mainly from the range of the parameters suggested by Elith et al. (2008) for *bf* and *lr*. For *tc*, given the expected complexity working at a global scale with interacting variables, we explored a range of variation that exceeds what is usually used (between 1 and 20).

For each combination of the parameters we performed 5-folds CV to derive the optimal *nt* and obtain an estimate of the prediction error. Because results from CV can vary according to the bag fraction and depending on the random selection of points for the folds, this procedure was repeated 10 times for each model, and overall mean was calculated for the predicting error and the optimal number of trees (Leathwick et al., 2006). From the mean prediction error, we computed, for each model, the overall mean CV- $D^2$  (i.e. the cross validated proportion of the deviance explained). Models were then ranked according to their CV- $D^2$  values and the models showing a  $\Delta$ CV- $D^2$  higher than 0.005 compared to the best model were excluded.

In the case of locations of different sizes, this procedure allowed us to select 13 combinations of *bf*, *lr* and *tc* which performed the best (Table S1) while, considering locations as areas within a fixed radius of 600km 6 best models were identified (Table S2).

In both cases, the predictive performances of the best models were considered analogous and we selected the models ranking first (i.e. location of different sizes: *bf*=0.85, *tc*=2, *lr*=0.01; 600km radius: *bf*=0.85, *tc*=3, *lr*=0.005) because they were the best compromise between predictive performance and complexity of the model (i.e. the number of trees to be fitted) thereby representing the most efficient solutions.

The best models can be considered analogous in terms of their predicting performances. In general, *lr* = 0.01 and *lr* = 0.005 performed better than both the slower and faster solutions explored.

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**Table A1.** Results of the procedure used for model calibration using explanatory variables extracted from locations of different size. *bf*: bag fraction; *tc*: tree complexity; *lr*: learning rate; CV-PE: mean predictive error over 10 replicates of 5-folds cross-validation (CV); CV- $D^2$ : mean cross validated proportion of the deviance explained over 10 replicates of 5-folds CV;  $\Delta$ CV- $D^2$ : mean loss of deviance explained compared to the best model over 10 replicates of 5-folds CV; *nt*: mean optimal number of trees estimated over 10 replicates of 5-folds CV.

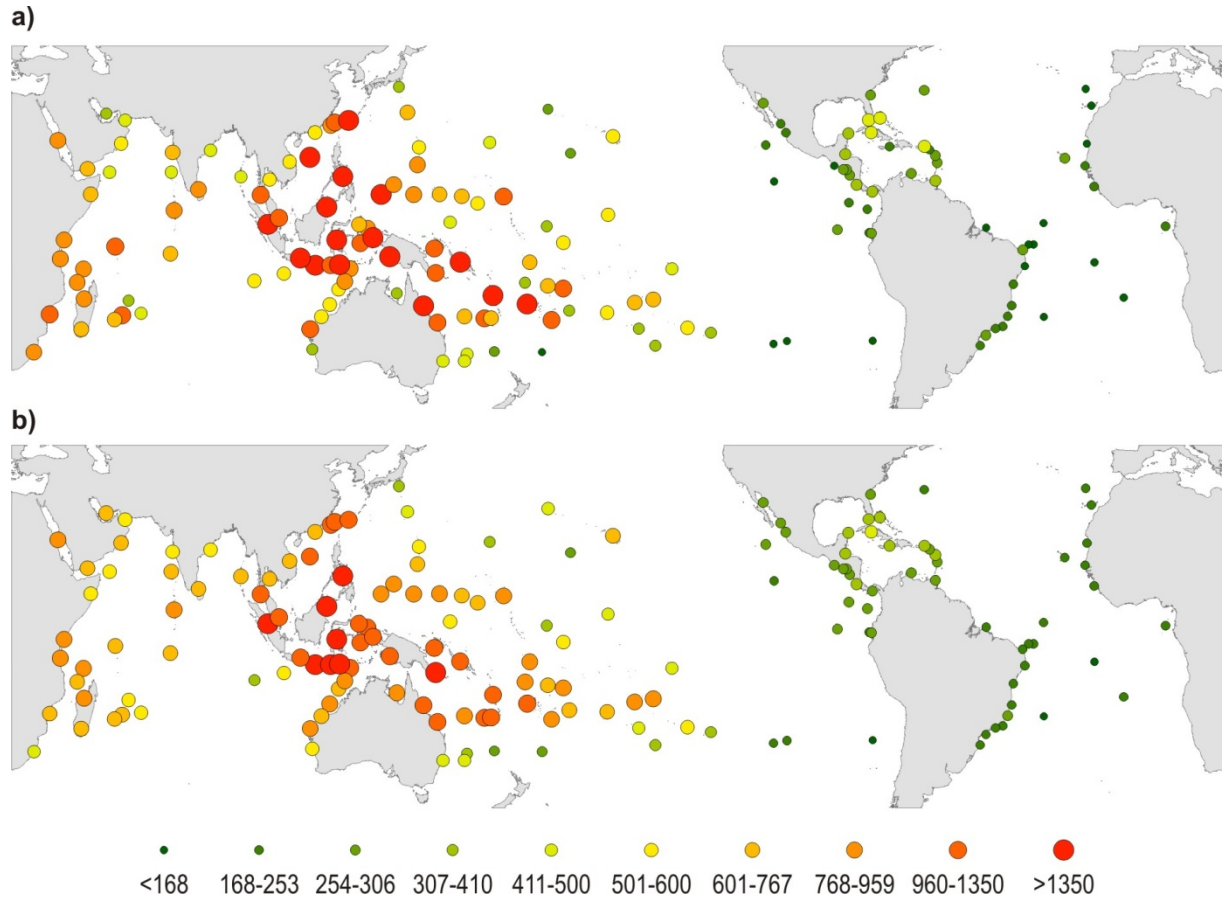
<i>bf</i>	<i>tc</i>	<i>Lr</i>	CV-PE	CV- $D^2$	$\Delta$ CV- $D^2$	<i>nt</i>
0.85	2	0.01	59.91	0.7944	0	1700
0.75	2	0.01	60.36	0.7928	0.0016	2100
0.70	3	0.005	60.42	0.7927	0.0018	4650
0.55	4	0.005	60.55	0.7922	0.0022	4150
0.75	3	0.005	60.69	0.7917	0.0027	4150
0.55	3	0.01	60.82	0.7913	0.0031	2450
0.65	2	0.01	60.82	0.7913	0.0031	3350
0.80	4	0.01	60.92	0.7909	0.0035	1850
0.60	4	0.01	60.93	0.7909	0.0035	2750
0.60	3	0.005	60.94	0.7909	0.0035	5000
0.55	3	0.005	61.08	0.7904	0.0040	4850
0.60	2	0.01	61.11	0.7903	0.0041	2450
0.85	3	0.005	61.31	0.7896	0.0048	3650
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
0.50	1	0,001	74.39	0.7447	0.0497	10000
0.55	1	0,001	75.88	0.7396	0.0548	10000
0.85	1	0.0005	82.87	0.7156	0.0788	10000
0.80	1	0.0005	83.49	0.7165	0.0809	10000
0.70	1	0.0005	83.97	0.7118	0.0829	10000
0.75	1	0.0005	84.41	0.7103	0.0841	10000
0.60	1	0.0005	84.75	0.7092	0.0852	10000
0.50	1	0.0005	84.76	0.7091	0.0853	10000
0.65	1	0.0005	85.08	0.7080	0.0864	10000
0.55	1	0.0005	86.45	0.7033	0.0911	10000

**Table A2.** Results of the procedure used for model calibration using explanatory variables extracted within areas of fixed radius of 600km. *bf*: bag fraction; *tc*: tree complexity; *lr*: learning rate; CV-PE: mean predictive error over 10 replicates of 5-folds cross-validation (CV); CV- $D^2$ : mean cross validated proportion of the deviance explained over 10 replicates of 5-folds CV;  $\Delta$ CV- $D^2$ : mean loss of deviance explained compared to the best model over 10 replicates of 5-folds CV; *nt*: mean optimal number of trees estimated over 10 replicates of 5-folds CV.

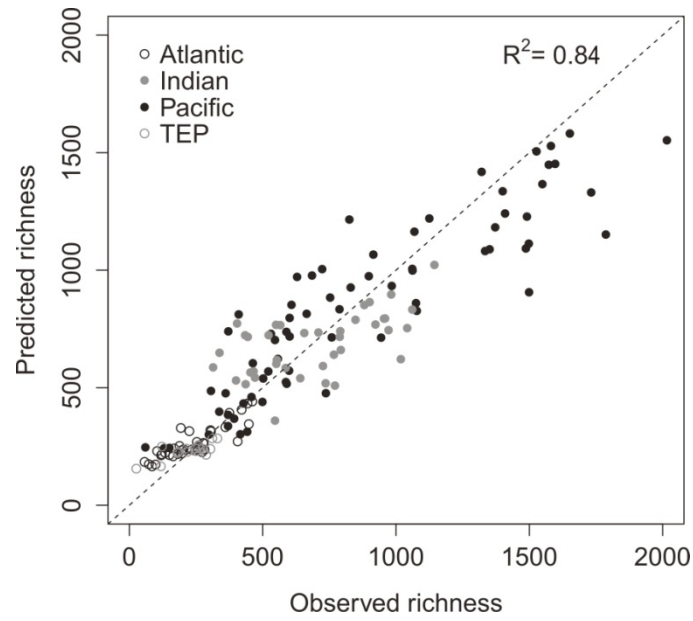
<i>bf</i>	<i>tc</i>	<i>Lr</i>	CV-PE	CV- $D^2$	$\Delta$ CV- $D^2$	<i>nt</i>
0.85	3	0.005	88.14	0.6971	0	1200
0.55	13	0.005	88.47	0.6959	0.0011	1500
0.85	4	0.005	88.58	0.6956	0.0016	1270
0.55	16	0.005	88.83	0.6948	0.0023	1520
0.50	5	0.005	89.38	0.6928	0.0042	1700
0.55	9	0.001	89.45	0.6926	0.0044	5270
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
0.60	1	0.0005	74.39	0.7447	0.0497	10000
0.80	1	0.0005	75.88	0.7396	0.0548	10000
0.85	1	0.0005	82.87	0.7156	0.0788	10000
0.80	1	0.0005	83.49	0.7165	0.0809	10000
0.70	1	0.0005	83.97	0.7118	0.0829	10000
0.75	1	0.0005	84.41	0.7103	0.0841	10000
0.60	1	0.0005	84.75	0.7092	0.0852	10000
0.50	1	0.0005	84.76	0.7091	0.0853	10000
0.65	1	0.0005	85.08	0.7080	0.0864	10000
0.55	1	0.0005	86.45	0.7033	0.0911	10000

## Appendix 4

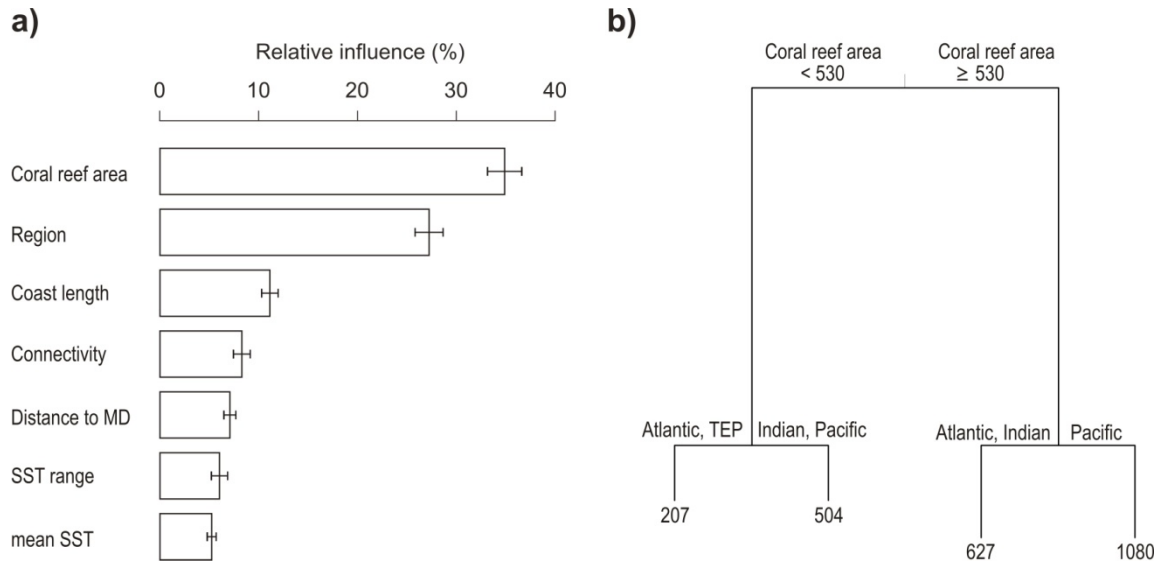
### Results obtained with standard buffer of 600km radius



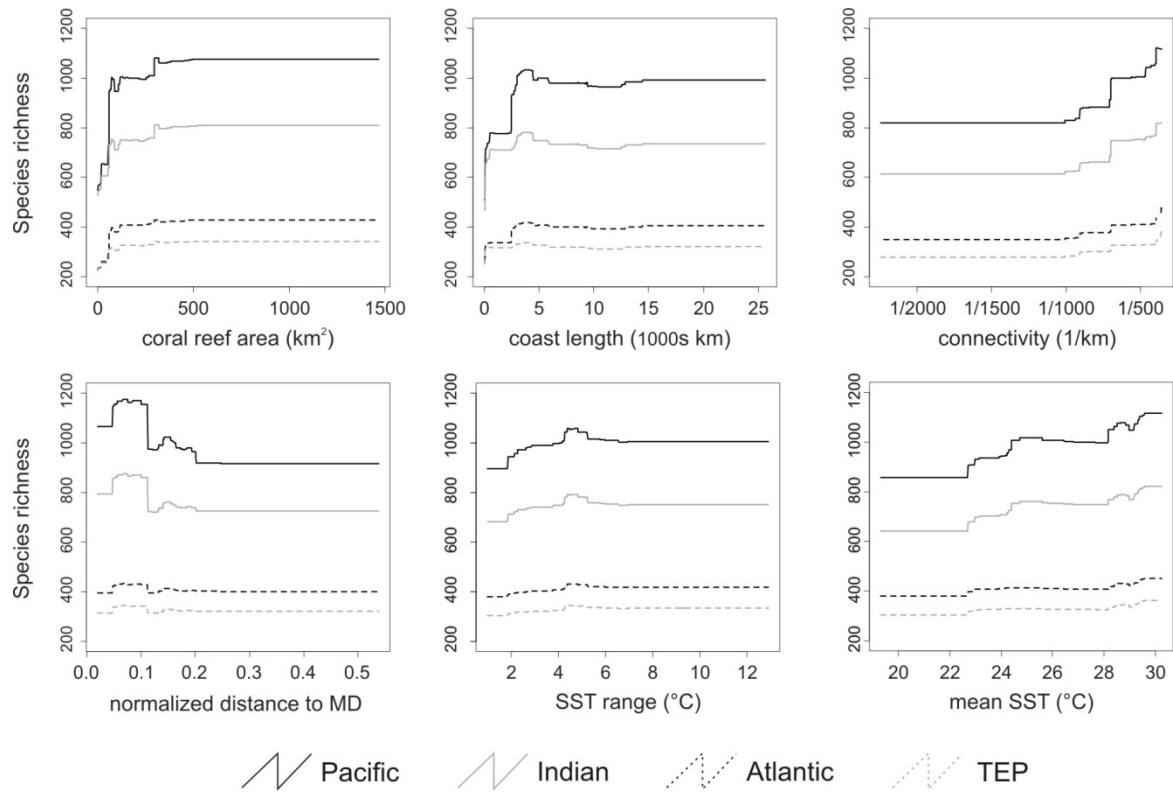
**Figure A3.** Maps of the observed richness of reef fishes (a) and the richness predicted by the BRT model (b). Colors and circle size represent 10 richness classes identified on the map of the observed richness with the quantiles method. The same scheme was later applied on the map of predicted richness.



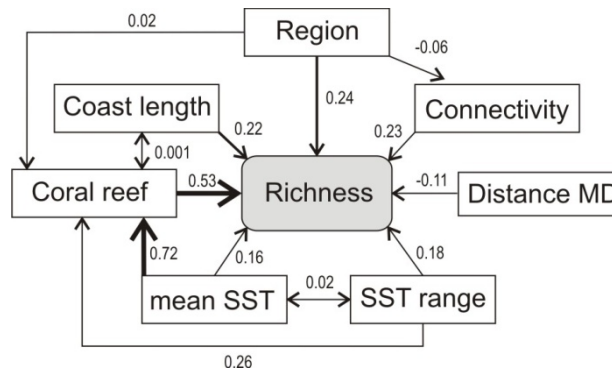
**Figure A4.** Relationship between observed species richness at each location and species richness predicted by the BRT model. Empty black circles: Atlantic Ocean; empty grey circles: Tropical Eastern Pacific (TEP); filled black circles: Pacific Ocean; filled grey circles: Indian Ocean.



**Figure A5.** a) Relative influence of the predictor variables as ranked by the final BRT model. Error bars represent 95% confidence intervals obtained from 1,000 bootstrap samples of the original dataset. b) First tree fitted by the BRT. The end points of the tree (nodes) represent mutually exclusive combinations of independent variables. At each node, a mean estimate of the dependent variable is calculated from the data points falling within that node. The final BRT model contains many trees.



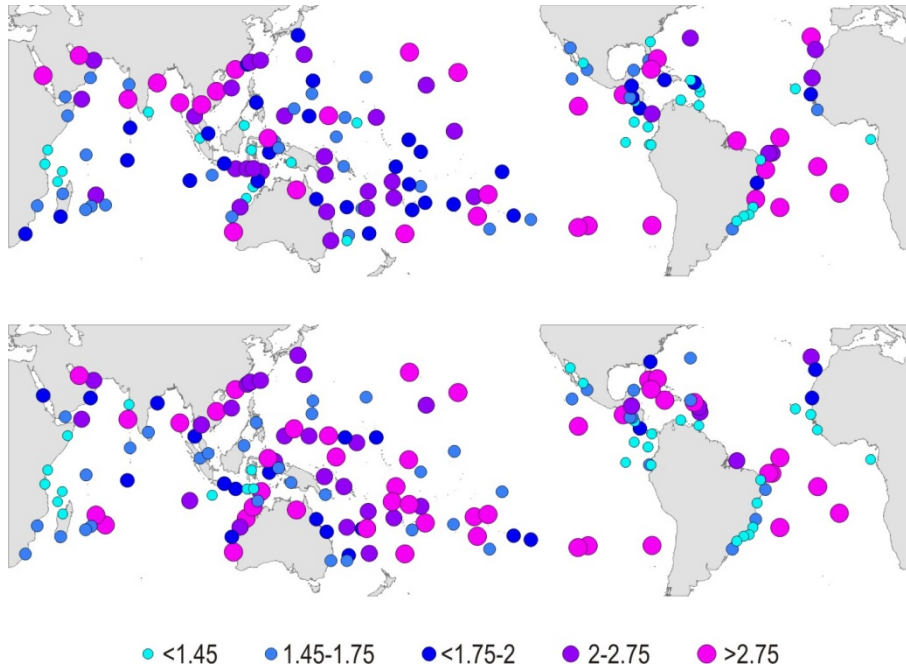
**Figure A6.** BRT model predictions of reef-associated fish richness according to several explanatory variables for different regions. Values for predictors other than those on the X-axis are held constant at their mean. Black lines: Pacific Ocean; grey lines: Indian Ocean; dotted black lines: Atlantic Ocean; dotted grey lines: Tropical Eastern Pacific.



**Figure A7.** Results of the structural equation model performed to assess direct and indirect effects of explanatory variables on reef fish species richness. Numbers represent standardized path coefficients. Arrows thickness is proportional to path coefficients. Since we detected spatial autocorrelation for our SEM model and this may inflate Type I error, we reported here all the path coefficient without considering p-values.

## Appendix 5

### Maps of uncertainty around model predictions



**Figure A8.** Maps of the uncertainty around BRT model predictions using locations of different size (upper map) and areas of 600km radius (lower map). Uncertainty was estimated as 95% confidence intervals of predictions obtained from models built on 1,000 bootstrap replicates of the original dataset. The confidence interval value was later standardized for the observed species richness in each location. The values mapped represents uncertainty around model predictions expressed as percentage of local species richness.

## Appendix 6

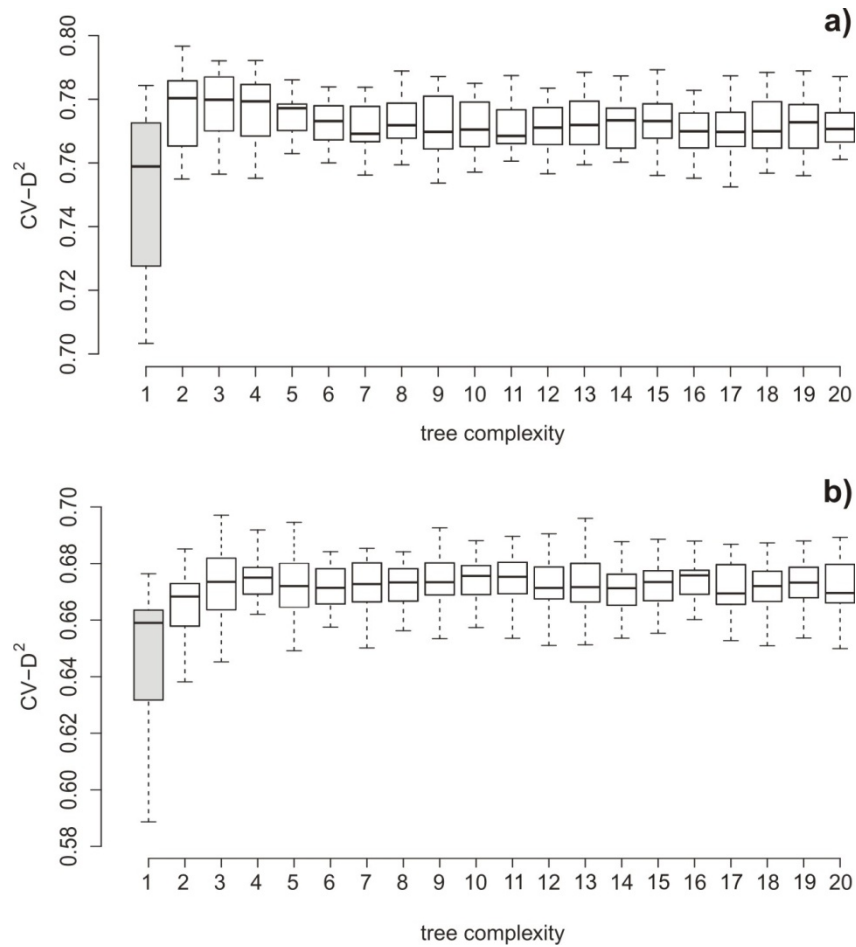
### Interactions between explanatory variables

The existence of interactions between explanatory variables was assessed by comparing the predictive performance ( $CV-D^2$ ) of BRT models considering all the possible combinations of model parameters ( $bf$ ,  $lr$ ,  $tc$ ) evaluated during the calibration procedure. In all cases models and regardless of the geographical definition of the locations employed, regression trees allowing for interactions between predictors (i.e.  $tc > 1$ ) performed better than models without interactions which always ranked worst (Figure S9).

The analysis of the interaction strengths for the best BRT models obtained with both location of different sizes and standard areas of 600km revealed that the Region factor was the most interacting variable (Table S3)

**Table A3.** Interaction strengths between pairs of the explanatory variables employed to build the BRT models. LDS: results obtained with locations of different size; 600km: results obtained with locations defined as standard areas of 600km radius.

	Distance MD	mean SST	SST range	Coast length	Coral reef area	Connectivity
<b>LDS</b>						
Region	2.56	0.09	0.38	0.40	0.64	0.10
Distance MD		0.02	0.13	0.15	0.05	0.01
mean SST			0.19	0.03	0.01	0.03
SST range				0.04	0.05	0.04
Coast length					0.01	0.08
Coral reef area						0.05
<b>600km</b>						
Region	1.78	0.07	0.13	1.82	2.67	0.08
Distance MD		0.00	0.01	0.15	0.02	0.01
mean SST			0.02	0.01	0.00	0.00
SST range				0.00	0.00	0.00
Coast length					0.00	0.04
Coral reef area						0.00



**Figure A9.** Cross validated deviance ( $CV-D^2$ ) explained by the models used for the calibration of BRT parameters according to the tree complexity range explored. The grey box-plot is referred to a tree complexity equal to 1, representing the performance of BRT models without interactions between predictor variables. White box-plots represent the performance of BRT models accounting for predictors interaction. Upper panel: results obtained with locations of different size; lower panel: results obtained with locations defined as standard areas of 600km radius.

## Appendix 7

### Spatial auto-correlation

Spatial auto-correlation violates the assumption of independently distributed errors in regression models, and, as a consequence, Type I errors of traditional tests might be inflated (Legendre, 1993; Kissling et al., 2007).

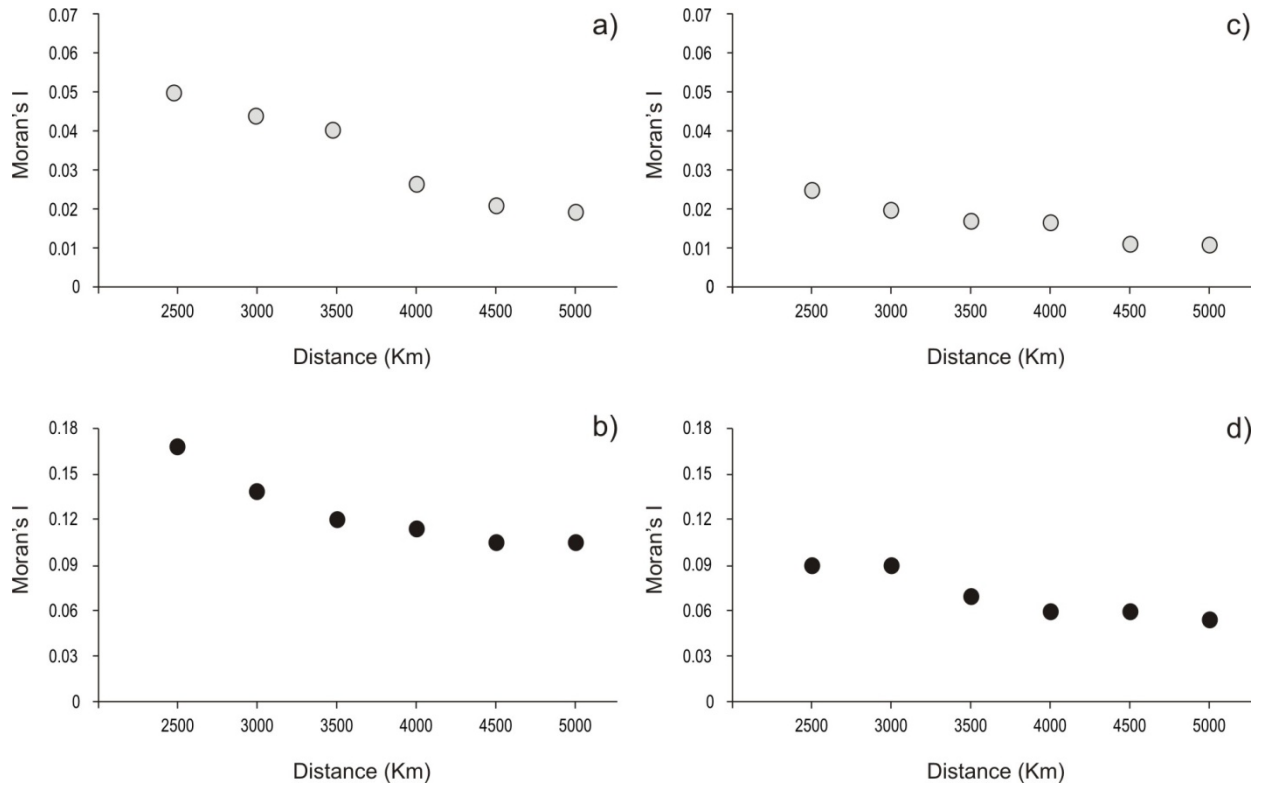
For this reason we assessed the spatial auto-correlation of both boosted regression tree (BRT) and Structural Equation Model (SEM). For BRT, we tested for spatial autocorrelation in the model residuals by computing the Moran's I for different spatial lag - i.e. from 2,500 km (the minimum radius allowing each location to have at least one neighbor location) to 5,000 km. Spatial pattern of the residuals was also mapped in order to highlight locations where overestimation or underestimation of the reef-associated fish richness occur (see main text).

Since Structural Equation models returns residuals in the form of a covariance matrix, these cannot be used to test spatial auto-correlation with classical tests, such as the Moran's I. To overcome this limitation, we assessed the spatial auto-correlation by obtaining the residuals from a OLS regression model performed on the same explanatory variables, which is analogue to a Structural Equation Models assuming only direct effects (Legendre, 1993; Kissling et al., 2008). Moran's I was then calculated on these residuals for the same spatial lags considered for BRT and a map was produced (Figure S10).

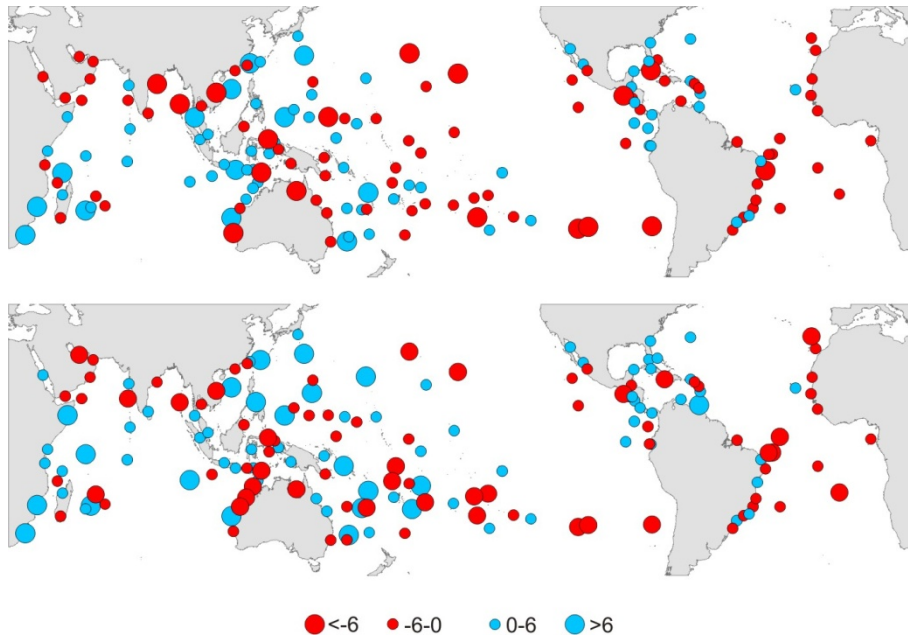
Residuals obtained from the BRT model did not showed any spatial auto-correlation for each spatial lag considered (see Figure S10). On the contrary, residuals obtained from the OLS model and assumed to be analogous to those of our SEM showed significant auto-correlation at each at the lag considered (Figure S10, S11). Since spatial auto-correlation tends to inflate Type I errors (i.e. the likelihood of rejecting the null hypothesis when this is actually true; Legendre, 1993), p-values may be considered reliable only for the detection of not significant effect. We then limited the interpretation of the SEM model to the path coefficients in order to delineate the potential for indirect effects, but we did not reported p-values on our path diagram (Kissling et al., 2008).

#### References

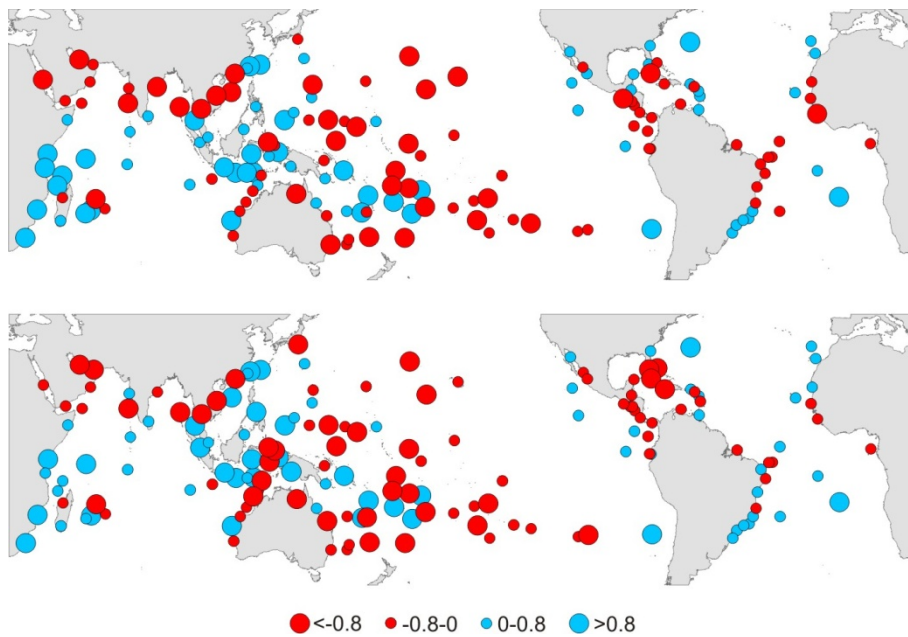
- Legendre, P. (1993) Spatial autocorrelation: trouble or new paradigm? *Ecology*, 74, 1659–1673.
- Kissling, W. D., & Carl, G. (2007). Spatial autocorrelation and the selection of simultaneous autoregressive models. *Global Ecology and Biogeography*, 17(1), 59-71.
- Kissling, W. D., Field, R., & Böhning-Gaese, K. (2008). Spatial patterns of woody plant and bird diversity: functional relationships or environmental effects? *Global Ecology and Biogeography*, 17(3), 327-339



**Figure A1.** a) Values of the Moran's I index of spatial correlation calculated on the residuals of the BRT model at different spatial lags (from 2500 km to 5000 km) using locations of different size; 2500 km represented the minimum distance to allow each location to have at least one neighbor. None of the test performed yield a significant spatial correlation. b) Values of the Moran's I index of spatial correlation calculated on the residuals of the SEM model at different spatial lags using locations of different size; c) values of the Moran's I index of spatial correlation calculated on the residuals of the BRT model at different spatial lags (from 2500 km to 5000 km) using locations of 600km radius; b) Values of the Moran's I index of spatial correlation calculated on the residuals of the SEM model at different spatial lags using locations of 600km radius. Black circles represents significant p-values (i.e. significant spatial autocorrelation) while grey circles represents not significant autocorrelation.



**Figure A10.** Maps of the distribution of the residuals deriving from the BRT model using locations of different size (upper map) or areas of 600km radius (lower map). Red circles indicates areas of overestimation (negative residuals) and blue circles are areas of underestimation (positive residuals)



**Figure A11.** Map of the distribution of the residuals of the OLS model as a proxy of the residuals of the SEM model using locations of different size (upper map) or areas of 600km radius (lower map). Red circles indicates areas of overestimation (negative residuals) and blue circles are areas of underestimation (positive residuals)