

Do they? How do they? WHY do they differ? On finding reasons for differing performances of species distribution models

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Species distribution models (SDMs) are increasingly being used to address a diverse range of applied and theoretical questions (Guisan and Thuiller 2005, Jeschke and Strayer 2008). Also known as ecological niche models, bioclimatic envelopes, habitat models and resource selection functions, SDMs are correlative models that use environmental and/or geographic information to explain observed patterns of species occurrences. Their expanding use means that models are now being fitted to new forms of data, including a recent focus on modelling occurrence records from museums or herbaria (Graham et al. 2004). For some applications, such as climate change or invasive species research, model predictions are extended beyond the geographic or environmental region from which training samples were drawn (Araújo et al. 2005). SDMs are also being used in a variety of fields including evolutionary biology, where they are used to study topics such as speciation or hybrid zones (Kozak et al. 2008) and epidemiology, where they are used to predict the spread of disease (Peterson et al. 2002). As a result of these diverse uses of SDMs that have been spurred on by advances in geographic information systems (GTS, Foody 2008) and data analysis (Breiman 2001a), new modelling methods continue to be implemented. Model complexity has generally increased over time from simple environmental matching (e.g. BIOCLIM, Busby 1991; DOMAIN, Carpenter et al. 1993) to fitting more complex non-linear relationships between species presence and the environment (e.g. generalised additive models, GAM, Hastie and Tibshirani 1990, Yee and Mitchell 1991; and maximum entropy modelling, MaxEnt, Phillips et al. 2006). Recent emphases on machine-learning and Bayesian methods indicate that new methods will continue to be developed (Latimer et al. 2006).

This wide array of methods, data types and diverse research questions imply firstly, that there are many different requirements of modelling methods, and secondly, that when choosing a method, knowledge is required about which method is best suited to the available data and the intended application. However, the criteria and advice that would enable informed choice of method are currently

scattered throughout the literature, and are incomplete. This makes it hard for most users to know whether it is worth adopting newer methods and for newcomers to know where to start.

How could species distribution modelling as a research field provide clearer advice as to what methods are best for a given application? To date research has focused on studies that compare model performance across multiple methods, address specific solutions to a given statistical or sampling issue, or provide detailed treatments of particular models. Some attempts have also been made to link ecological theory to choice of method (Table 1). While this research has provided information and guidance necessary for selecting relevant methods, it is our opinion that we need more syntheses of existing knowledge, more advice from statisticians and computer scientists expert in the algorithms, and a broader suite of evaluation methods that target not just whether there are differences in predictive performance, but why these differences occur. This forum piece focuses on the third of these, and aims to demonstrate the effectiveness of asking why.

There are various approaches for assessing why models differ in predictive performance, including developing strong theoretical knowledge of how a method works, testing multiple parameter settings for the method and observing effects on outputs, and using data with known characteristics to test model fit and prediction. The latter can be sets of data with known properties e.g. drawn from a known distribution, created from a known equation (Bio 2000, Moisen and Frescino 2002) or simulated (artificial) species (Austin et al. 2006). Simulated species are particularly useful if relevant features such as population processes, competition, or typical landscape properties can be included (Tyre et al. 2001, Reineking and Schröder 2006, Meynard and Quinn 2007, Kearney et al. 2008). While we encourage the use of any approach that gives insight into why methods differ, here we choose to use a simulated species within a real landscape.

We evaluate three applications of distribution modeling: 1) understand the relationships between the species and its environment; 2) predict which parts of the landscape are

Table 1. Examples of existing approaches addressing a variety of methodological, theoretical, statistical and applied questions.

Category	Aim	Examples
Comparative studies	To quantify whether methods perform differently (in terms of model fit or prediction) and to search for any general patterns in the differences	Moisen and Frescino 2002, Seguardo and Araújo 2004, Reese et al. 2005, Elith et al. 2006, Hernandez et al. 2006, McPherson and Jetz 2007a, b, Graham et al. 2008, Loiselle et al. 2008
Specific methods for treating specific problems	To use an appropriate method for data (or for a problem) that has characteristics violating assumptions of common models	Models for data with imperfect detection (MacKenzie et al. 2002); models for zero-inflated data (Martin et al. 2005); models that deal with spatial autocorrelation (Dormann et al. 2007); subsampling data or accounting for its bias
Detailed treatments of methods	To explain a method clearly and inform users of its characteristics, strengths and weaknesses for ecological analyses	Generalised additive models (Yee and Mitchell 1991), MaxEnt (Phillips and Dudik 2008), Resource Selection Functions (Manly et al. 2002)
Linking ecological theory to choice of method	To ensure the selected model is consistent with known ecological theory	Methods appropriate for modelling realistic species environment relationships (Austin 2002); quantile regression for modelling limiting factors (Huston 2002); multiplicative models for modelling interactions and overriding limitations (McCune 2006)

more or less suitable for the species by creating a map of relative suitabilities; 3) extrapolate to environmental conditions outside those in the sample space. Because simulated species provide known species-environment relationships and spatial distribution we can evaluate differences among methods in relation to the truth and gain insight into why these differences exist.

Simulating the species and sampling it

We created a simulated plant species and mapped it onto a landscape in southern Australia. The species responds to three variables: wetness, aspect (“southness”) and geology and prefers wet and south-facing (shaded) sites and fertile substrates. We created an interaction between the response to wetness and the summed responses to southness and geology, and weighted the terms so that wetness dominated the final distribution (eq. 1 and Fig. 1, top panel). Note from Fig. 1 that the responses to continuous variables are non-linear; details of how each component (SI.wetness etc.) was specified is presented in Supplementary material Appendix S1.

Suitability of a cell

$$= \text{SI.wetness} * 0.5 * (\text{SI.southness} + \text{SI.geology})$$

where SI = suitability index (Supplementary material) (1)

The predictor variables (wetness, southness and geology) existed as real mapped data; the species’ response to them was invented. The mapped distribution based on these relationships shows the suitability (scaled 0 to 1) of each grid cell for the plant (Fig. 2, top left). Whilst these data could be modelled as suitabilities, most species data exist as presence-only or presence-absence records, so we made a presence-absence realisation of the species. We used the suitability value in each grid cell of the map as the success rate for one sample of the binomial distribution, i.e. a cell with a suitability of 0.6 has a 60% chance of being occupied (rbinom function in R; R Development Core Team 2006). The binomial realisation is consistent with an interpretation of species relationships that says: “if the environment is only

partially suitable for the species, in some cases the species will occur there and in some it will not”. Our presence-absence realisation of the simulated species occupied 12% of the cells in the study region (Supplementary material Fig. S2a).

To provide the data set for modelling we sampled from the simulated presence-absence distribution by taking 1000 sites at random; these included 115 presences and 885 absences and together comprise what we will call the presence-absence (PA) sample. This number of sites is somewhat arbitrary, but is enough to fit models well, and is consistent with some real data sets used in modelling. Other protocols such as stratified sampling across environmental gradients could be used instead of random sampling. The PA sample is visualised in Fig. 3a. Note that, consistent with the full data set (Fig. 3b), samples at high wetness are relatively rare. For methods only requiring presence data, the presence records in the PA sample were used as presence-only (PO) data. In the online supplement (Supplementary material Appendix S5) we describe additional data samples, in which 1000 or 3000 pseudo-absences were selected and combined with the PO data, to test the effect of using presences with pseudo-absences instead of true absence data.

Modelling and evaluation methods

We chose five algorithms to demonstrate what simulated data can show about differences between methods. For the PA data we selected a generalised linear model (GLM; McCullagh and Nelder 1989) as a standard regression model and two more recent methods, boosted regression trees (BRT; Friedman et al. 2000) and random forests (RF; Breiman 2001b). For the PO data, we used MaxEnt and GARP as featured in recent comparisons (Peterson et al. 2007, Phillips 2008). MaxEnt, GARP and RF are machine learning (ML) methods. The version of BRT used here is a ML method reinterpreted into a statistical paradigm. More details and references for all algorithms are given in the online supplement. These methods were selected because they allow a number of contrasts including comparison of

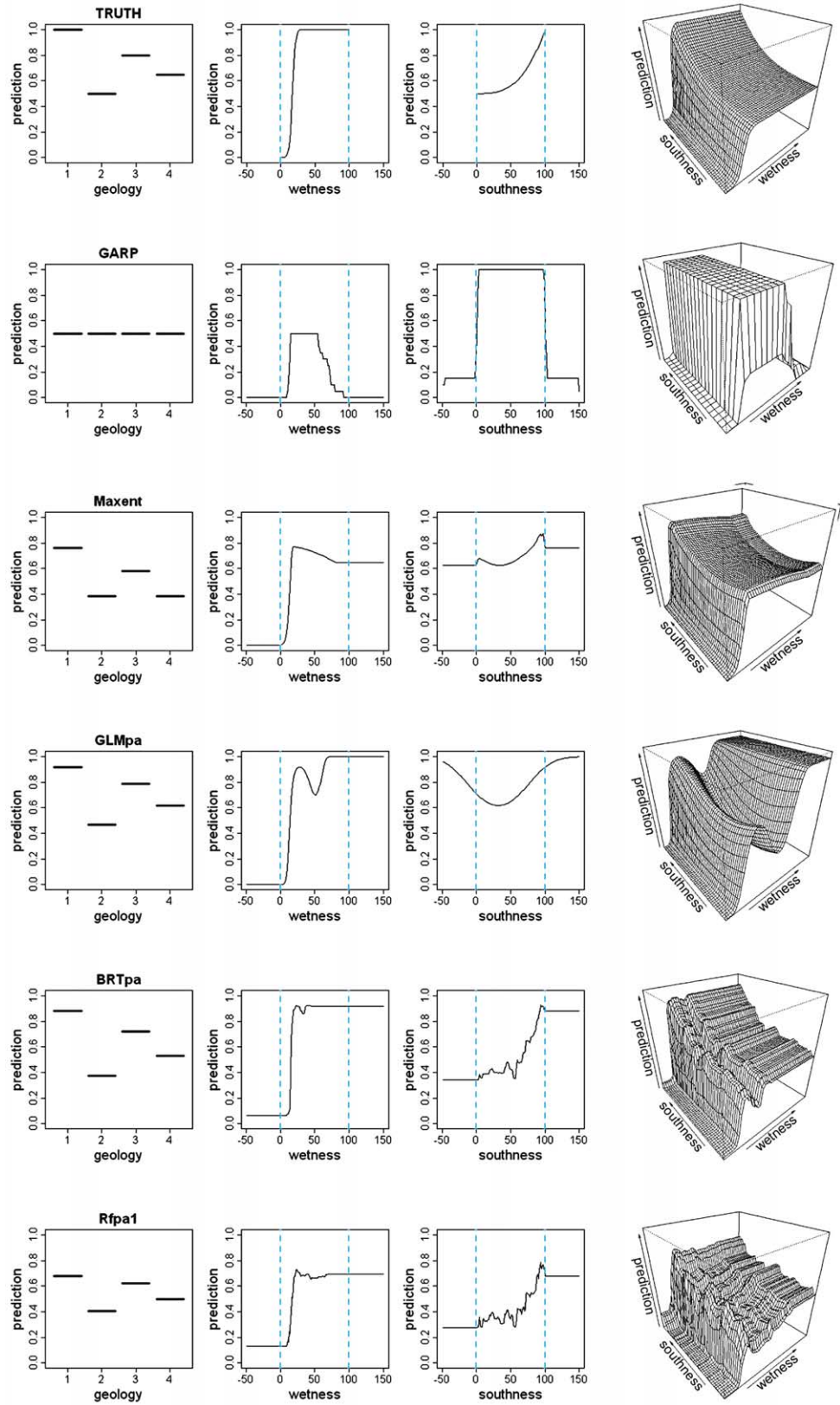


Figure 1. Partial responses to the 3 variables (left) and over co-varying wetness and southness (3D plots, right). The true responses (top panel) were generated by using the equations that define the simulated species to predict to the evaluation strip, then plotting the results (see Elith et al. 2005 for details). The blue vertical lines show the extent of the variable values in the mapped region; outside these the models are extrapolating. The range on the wetness and southness axes of the 3D plots is that within the blue lines of the 2D ones, and predictions range from 0 to 1.

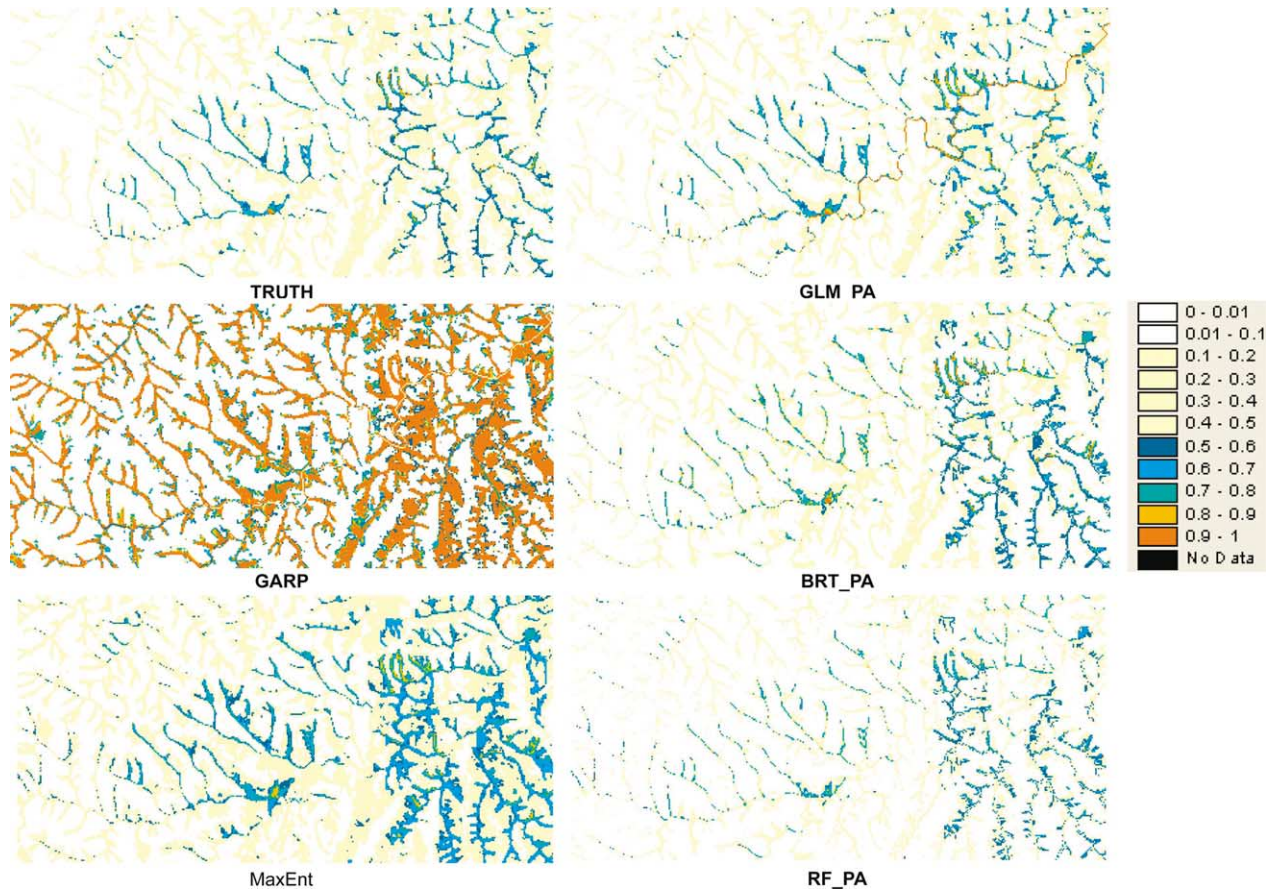


Figure 2. Mapped distributions of the virtual species (top left) and predictions of relative suitabilities from the methods detailed in the text, legend: white < 0.1 , cream 0.1–0.5, blue-light, blue-green-orange-vermilion at steps of 0.1 from blue (0.5–0.6) to vermilion (0.9–1).

models developed on PA compared with PO data, comparison of MaxEnt and GARP, and comparison of two methods using ensembles of trees, BRT and RF. Each of the methods is assumed capable for at least some of our three posed applications, and they have all been used for related tasks.

For details of model building methods see Table 2 and Supplementary material Appendix S2, S3 and S4. In those appendices the settings for some methods are tested in detail; this reflects our need to explore the effect of a range of settings for some methods, either because we were relatively inexperienced with that method or because the recommended settings did not produce good results.

The first of our applications was to understand the relationships between the species and its environment. The second – mapped predictions – would also benefit from knowledge of the modelled relationships, for understanding differences between the maps. However, not all methods provide visualization of fitted functions, so we created a second set of environmental grids with an evaluation strip inserted, following Elith et al. (2005). The strip is a simple data arrangement that holds two of the three environmental variables at a constant value (here, a value achieving maximum suitability for the species) whilst varying the value of the third environmental variable across its numerical range. To visualise interactions (and to check that results do not depend on the value at which variables are held constant), pairs of variables can be covaried. For

this, we included a comprehensive set of combinations of wetness and southness for each of the four classes of geology. Predictions were made to the evaluation strip and then plotted, to illustrate the partial response to one or two variables while holding other variables constant. This method is analogous to the partial plots from standard regression methods (see Elith et al. 2005 for details). To determine how the models extrapolate we included values for variables in the evaluation strip that were outside the variable range in the study area for both wetness and southness. We acknowledge that this approach only measures one aspect of extrapolation, and that other possibilities exist including creating landscapes or evaluation data with new combinations of variables. The simple test of extrapolation outside limits will suffice here, as a first exploration of extrapolation behaviour.

Finally, to evaluate a method's ability to predict habitat, mapped predictions were visually and quantitatively assessed. Summary statistics were calculated across predictions in all 80 000 cells, and then used to compare the presence-absence realisation and the true suitabilities. Analyses using presence-absence data as truth focussed on: 1) the area under the receiver operating characteristic curve (AUC; Hanley and McNeil 1982); 2) the remaining per-observation deviance (i.e. the variation left unexplained, as measured by the mean binomial deviance across sites; Elith and Leathwick 2007); 3) the point biserial correlation coefficient (a Pearson correlation, Elith

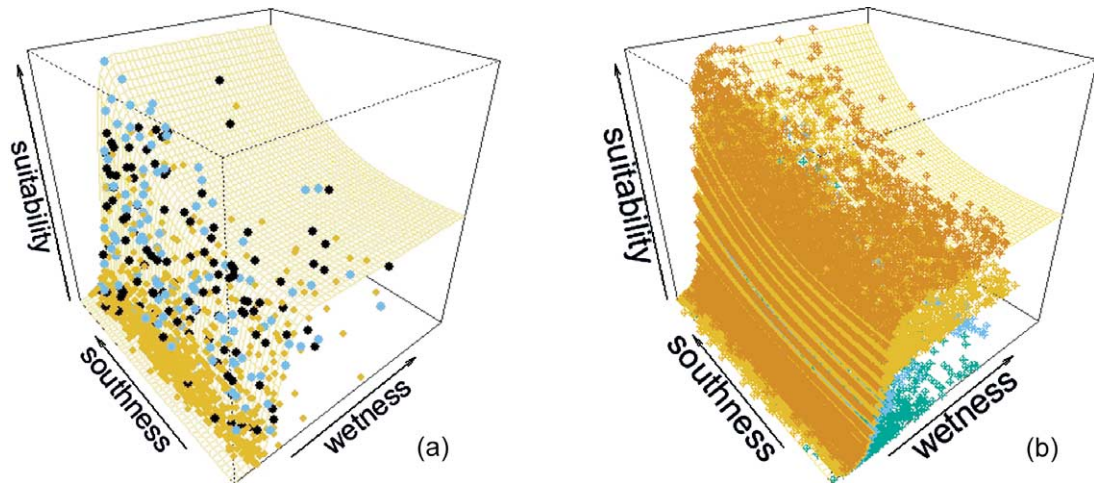


Figure 3. (a) The data samples for presence-absence models. Samples are shown at their original true suitability value (vertical axis), but were converted to presence (blue) or absence (orange) as described in the text. (b) The location of all 80 000 grid cells in environmental space. The pale yellow mesh shows the full suitability surface from the simulated species, for geology class 1. The points of varying colours show sites in the four geology classes. Note the few sites with high wetness values.

et al. 2006, COR.pa); and 4) elements of the confusion matrix for predictions converted to binary values, using a threshold described later. Predictions were compared with true suitabilities with a Pearson correlation coefficient (COR.si).

It is important to use more than one metric to assess model performance because each quantifies a different aspect of predictive performance (see Murphy and Winkler

1987 and Pearce and Ferrier 2000 for interesting discussions of this topic). Amongst the measures tested against PA observations, AUC measures the ability of predictions to discriminate between observed presence and absence, regardless of the absolute value of the predictions. COR.pa also measures discrimination, but includes consideration of the actual value of the prediction, and how it compares to the observation. Deviance puts more emphasis on the

Table 2. Details of model fitting procedures and settings.

Method	Name for model	Data	Settings and notes on further tests
Genetic algorithm for ruleset prediction	GARP	PO	Used v 1.1.6. Details in Supplementary material Appendix S2 on tests to compare effects of different settings. Results presented here from: species data = 115 PO samples plus pseudo-absences selected by GARP. 50% data used for training, 50% for extrinsic evaluation. Created 500 models each with a convergence limit of 0.01 and 1000 maximum iterations. Allowed all rule types. From the 500 models chose 20% with mid extrinsic omission error and from those 20 with mid commission error. Final prediction is mean of these. For predicting to evaluation strip projected to grids with strip inserted.
Maximum entropy	MaxEnt	PO	Used ver. 3.2.1 from the command line. Modelled the 115 PO samples and allowed MaxEnt to select a random 10000 background samples (the default). All other settings were the defaults except: flagging geology as a categorical variable, providing a separate set of grids to project to that contained the evaluation strip, and using the "-d" flag (see help file for MaxEnt). The -d flag forces MaxEnt to calculate the probability distribution over the background samples alone (rather than the default, which calculates it over the joint background and presence data), and providing it with the best chance to be well calibrated. For predicting to evaluation strip projected to grids with strip inserted.
Generalised linear models	GLM.pa	PA	Used R ¹ and function GLM. Created all possible subsets of models with the options for each variable being: exclude, or (if continuous): linear, quadratic or cubic fits. Used AIC to select the best model.
Boosted regression trees	BRT.pa	PA	Used R ¹ and function GBM with custom scripts of Elith et al. 2008 to build an ensemble of regression trees. Selected tree complexity of 3, learning rate of 0.001, using prevalence-stratified cross-validation to determine optimal number of trees (4250). See Supplementary material Appendix S4 for details.
Random forests	RF.pa	PA	Used R ¹ and function random forest to build an ensemble of classification trees. Tests of a range of settings are presented in Supplementary material Appendix S3. Model presented here had 500 trees with one variable randomly selected from the 3 candidates at each split. No class weights.

¹R Development Core Team 2006.

model calibration i.e. on whether predictions reliably predict frequencies of occurrence.

Results

Relationship of species to environment

Figure 1 shows the modelled responses to the 3 variables when others are held at their optima, and in the right column, the response to co-varying wetness and southness for geology class one. Here we analyse the results for the ranges of the variables in the data – i.e. within the blue vertical lines of Fig. 1. In the later section “Extrapolation” we deal with predictions outside the range of the data.

We would not expect any of the methods to fully retrieve the species environment relationship of the simulated species because a relatively small sample of a binary realisation of the data was used to build the models (Fig. 3a). Nonetheless, several of the methods were able to fit reasonably accurate functions. This was an easier task for the methods using smoothed functions (GLM and MaxEnt), given that the true relationships were smooth.

All methods except GARP modelled geology correctly (Fig. 1, left column). GARP’s modelled response to geology varied across different data samples, runs, and summaries of the data (Supplementary material Appendix S2). GARP might be expected to model categorical data properly because it uses logistic rules, but the implementation is a genetic algorithm version of logistic regression and has not been coded to properly deal with unordered categorical variables (Elith unpubl. and Peterson pers. comm.). However, the atomic rules provide some opportunity to model geology correctly, and in some cases (Supplementary material Fig. S3 and S6) the result was better than the one presented.

The low suitability of dry areas (wetness < 15) was correctly captured by all methods (Fig. 1, second and fourth columns). At higher levels of wetness, where the data are more sparse, BRT modelled the overall shape of the response most accurately, followed by MaxEnt (slightly reduced amplitude), RF (smaller amplitude) and GLM (unnecessary complexity around wetness of 50) and last, GARP (small amplitude and wrongly predicted that high wetness was unsuitable). Whilst the general form of the fitted function was correct for BRT, it was overfitted to the sample, producing a dip in the response at wetness ~ 30. At this level of wetness the sample was sparse and happened to contain more zeros than would be expected for the suitabilities. RF showed even more overfitting (note the more uneven surface, Fig. 1, right column), which was only fractionally reduced by using more trees in the ensemble (Supplementary material Appendix S3).

Southness (Fig. 1, third and fourth columns) was difficult to model well, probably partly because the response included an interaction between southness and wetness, and also because it was less dominant than wetness in the suitability equation. RF, BRT and MaxEnt did best, GLM was reasonable but gave an increasing response at low values of southness and, without an interaction, could not capture the response to southness at high wetness (see right side of 3D plot). GARP did not

manage to model the true response or anything close to it, and this result was consistent across all tests (Supplementary material Appendix S2).

Mapped predictions; visual assessments

Differences between the methods were also evident based on the mapped predictions. We present the results as maps and plotted data so that any arbitrary impressions introduced by choice of legend in the map (Fig. 2, 4) can be checked against the plotted results (Fig. 5). Note that the COR.s1 in Table 3 acts as a summary measure of the plotted data in Fig. 5.

Because all methods predicted the response to low wetness correctly, they all correctly predicted absence at dry sites (the white areas on the maps, Fig. 2). Modelling this part of the response accurately meant that all methods produced a broadly correct mapped pattern. GARP tended to predict high values across any areas that had at least some suitability for the species, whereas the other methods predicted gradations in suitability more accurately (Fig. 2 and related close-up, Fig. 4). The overprediction can be traced to the errors in retrieving the true underlying species-environment relationships, and particularly the dominance given to the incorrectly modelled response to southness. In other words, why GARP overpredicts is partially answered; GARP could not retrieve the true relationships in the data. This is only a partial answer because we do not know what features of the algorithm cause this overprediction. Simulated data like these could be used to explore whether another simulated species or different settings for GARP improve model performance. We were unable to improve GARP model performance substantially when we used different settings or methods to combine individual GARP runs (Supplementary material Appendix S2). Nonetheless, the results of the different trials shown in the Supplementary material, are interesting in that they suggest that means of all runs of GARP are slightly better for these data than the subsets that are generally advised. They also demonstrate considerable run-to-run variation (where one run is 500 models and summaries thereof).

As expected, none of the methods perfectly retrieved the true mapped suitabilities; sample size, characterising the response with binary data rather than suitabilities, and algorithmic limitations all contribute to this result. MaxEnt recreated the general mapped pattern of the simulated species well and was only worse than the best method, BRT, with respect to calibration (Fig. 2, 4). Perfect calibration would have resulted in all records in Fig. 5 sitting on the diagonal, but a presence-only method cannot be perfectly calibrated unless information on the species prevalence in the region is available (but note that proportional calibration is possible for a PO method – records would follow a straight line, but the gradient and intercept would not be 1 and 0 respectively). In contrast, the three methods trained on the PA data should be properly calibrated. The results for these methods are all reasonable, with BRT predictions slightly less dispersed than RF and GLM (Fig. 2, 4, 5). We tested various settings for RF (seven combinations are presented in Appendix S4); the ones we present here are those that would have been selected from the out-of-bag

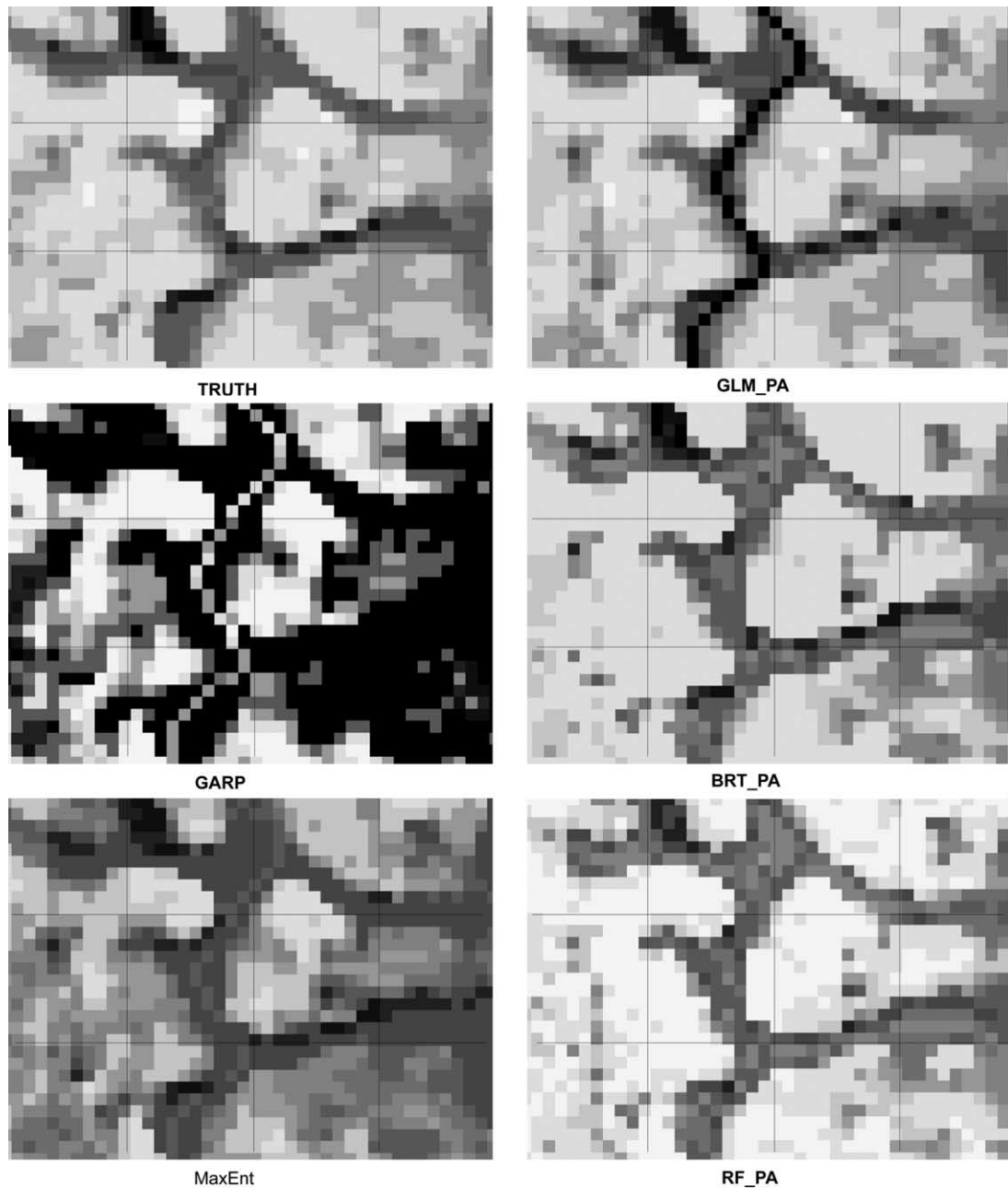


Figure 4. Close-up of predictions from Fig. 2. Choice of location was via random number selection for centre grid position. Predictions in greyscale, from white (zero) to black (one); fine grid lines are in the same position on each map.

error estimates, are consistent with those used in other published studies, and appear close to optimal (Supplementary material Appendix S4).

Before leaving the topic of calibration we note that, with PO data, MaxEnt calibration results may not always be as good as those presented here. Our simulated species was created to vary in suitability from 0 to 1. This range corresponds to that used in the MaxEnt logistic output (Phillips and Dudik 2008), so the MaxEnt predictions for this simulated species were reasonably well calibrated. However, if our truth was rescaled (say, by multiplying all suitabilities by 0.5), MaxEnt predictions would be more poorly calibrated (S. Phillips pers. comm.). This problem is not restricted to MaxEnt, as shown in Supplementary

material, Appendix S5, where BRT and GLMs are fitted with PO data. There the choice of the number of pseudo-absences, and the optional weighting of them, affected calibration. Together, these issues demonstrate an inherent problem for models using PO data; they cannot be well calibrated without information on species prevalence (Ward et al. in press).

Mapped predictions; quantitative analyses

The summary statistics presented in Table 3 focus on predictions as continuous values (i.e. in their default format, such as probabilities). These demonstrate some differences

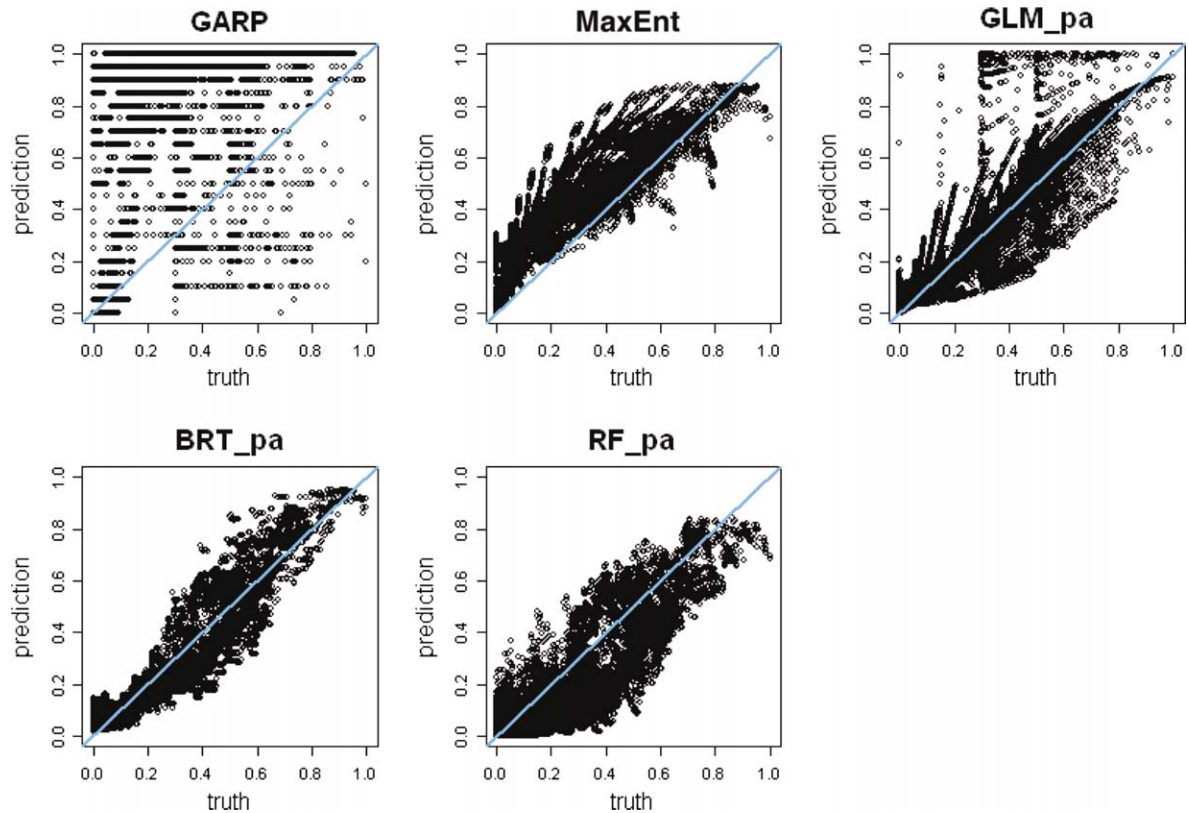


Figure 5. Predictions (y axis) versus the true suitability for all 80 000 grid cells in the maps in Fig. 2, covering five modelling methods described in Table 1. The blue diagonal line shows the 1:1 relationship.

between the methods, with the extent of the difference varying with the statistic. Note that the first row in Table 3 (“Truth”) indicates the best possible performance for AUC, Deviance and COR.pa, because it measures the relationship between the true presence-absence realisation (sampled for modelling) and the true suitability. The AUC indicated that all models discriminated the broad patterns of presence and absence reasonably well, but there was some variation between methods. The broad success in discriminating between presence and absence locations probably results from the correct modelling of dry conditions, because all the pair-wise comparisons between predictions in these areas and ones in the wetter areas would have been correctly ranked. Measures that include consideration of the actual value of the predictions (all others) emphasise more clearly that MaxEnt, BRT and GLM all do well, followed by RF then GARP (Table 3). Note that it is difficult to make a fair comparison across all methods, because the 3 models fitted

to the PA data had more information than the PO methods, and this information allows the models to estimate probabilities and hence to be better calibrated. This particularly affects remaining deviance (Table 3). Nevertheless, for this exercise MaxEnt does well without this information (but see the earlier discussion about the scaling of suitabilities and its effects on calibration in MaxEnt). The fact that, for PA methods, the order of model performance is consistent across metrics shows that errors in prediction are related to both discrimination and calibration. Given that the general shapes of the fitted functions for RF are reasonable, it is likely that its reduced performance in these summary metrics results from the noisier fit compared with BRT (Fig. 1, right column) and the slightly poorer calibration.

It is possible that using predictions as continuous values unfairly discriminates against GARP, because GARP works by producing a presence-absence prediction, and non-binary predictions are achieved from summaries across multiple runs. Because of this, the predictions for all methods were thresholded and a test of binary predictions applied. We did this without biasing the results towards methods with good calibration, by using thresholds that gave the same prevalence across the landscape for all methods (following Phillips et al. 2006). This meant that we used a threshold of 1 for GARP (to get prevalence as close to truth as possible and to restrict the overprediction of GARP), then set others in relation to that. The results (Table 4) are consistent with other results, though the differences are less extreme. Note that this thresholding method likely disadvantages methods other than GARP

Table 3. Comparison of model results with truth, as realised by the presence-absence map (columns 2, 3 and 4) and the suitability values (column 5). For all statistics except deviance, higher is better.

Model	AUC	Remaining deviance	COR.pa	COR.si
Truth (suitabilities)	0.872	0.514	0.508	1.000
GARP	0.822	3.391	0.401	0.793
MaxEnt	0.861	0.612	0.467	0.922
GLM.pa	0.863	0.546	0.480	0.941
BRT.pa	0.862	0.537	0.485	0.954
RF.pa	0.834	0.736	0.448	0.875

Table 4. Comparisons among methods when predictions are reduced to binary results. Because GARP overpredicted, the highest possible GARP threshold (1) was used to convert GARP predictions to binary form, then thresholds were selected for all other methods that gave identical prevalence in the landscape (17.3%, compared with truth 11.9%). The values in the tables are the proportions of predictions that fell into each category (true negative etc.) when cross-tabulated with truth.

Prediction:	true negative	true positive	false negative	false positive
GARP	0.771	0.064	0.056	0.109
MaxEnt	0.778	0.071	0.049	0.102
GLM	0.780	0.073	0.047	0.100
BRT	0.780	0.073	0.047	0.100
RF	0.777	0.070	0.050	0.103

because others are likely to have lower optimal thresholds when set independently.

Information on BRT and GLM models fitted to the presence – pseudo-absence data are presented in Supplementary material Appendix S5. These show that in some (but not all) cases the fitted functions are reasonably accurate, and that across methods different ways of sampling and weighting the pseudo-absences have different effects on the discrimination and calibration of the models. We note that alternative implementations of BRT that are better suited to the presence/pseudo-absence data structure will be available soon (Ward et al. in press).

Extrapolation

The extrapolation behaviours of the models are presented in Fig. 1, in which the responses to the highest and lowest values for the wetness and southness, outside the blue dashed lines, are where the models are extrapolating to unsampled conditions outside the range of these variables in the mapped region. The nonsensical negative values of wetness and southness don't matter here – the important question is how the models would extrapolate beyond the sampled values of data. We had no prior knowledge of GARP behaviour, and in this example extrapolation was either a stepped decline (at extremes of southness) or a constant value. The selected rules in the best-subsets models would explain this behaviour, but they are not accessible in the desktop program so could not be analysed. Extrapolation patterns varied in GARP according to the dataset, the particular run, and the selected subsets (Supplementary material Fig. S3). By contrast, MaxEnt acts consistently and by default is “clamped” so it extrapolates in a horizontal line from the fit at the most extreme environmental value in the training data, both presence and background. As expected from the way polynomials behave, a GLM fitted with cubic and quadratic functions extrapolates by continuing the fitted trend beyond the last observation, sometimes with unwanted results. For example, here the projected increase in suitability at the lower values of southness is not sensible; north-facing (low southness) sites should be least suitable for the species. Classification and regression trees always extrapolate at a constant value from the last “known” site, as seen for BRT and RF.

Reflections on the simulation

Before considering the wider implications of this simulation, we want to first emphasise what it does not do. Whilst we built our simulated species to be somewhat ecologically realistic (the species is affected by more than one variable, and reacts to predictors in non-linear and non-additive ways), it is more simple than reality. We do not see that as a problem, though, if we appropriately restrict our conclusions to ones about the link between the algorithm, data and fitted functions. Other types of simulations could be used to test modelling abilities for other aspects of what influences species distributions in natural populations (e.g. interactions between species, sink and source habitats). We also only tested some of the many ways of fitting these methods – for example, a GLM can include interactions and use natural splines instead of polynomials to control behaviours at the extremes of the sample ranges. Finally, we did not attempt a comprehensive study, though we hope that our simulation inspires other explorations.

What then does this simulation demonstrate? First, knowing what an algorithm is doing can give insights into various features that are apparent in its predictions; it helps to answer why particular patterns are observed. We summarise in Table 5 some insights from this study, and some of the remaining open questions. Testing an algorithm's performance using a simulated species approach and multiple evaluation criteria reveals unique behaviours of the modelling methods we explored and therefore should help developers and modellers to understand and improve model performance. The systematic studies in Supplementary material Appendix S2, S3 and S5 demonstrate that carefully evaluating model performance across parameter settings reveals the effect of those parameters.

Second, our example clearly illustrates the value of evaluating models from several viewpoints. The summary statistics indicated which algorithm gave the best mapped predictions and, when taken together, the metrics gave some hints about why performance varied. AUC only measures rank so did not reveal the more extreme differences between methods that were more related to model calibration. We do not believe that this means that any of these statistics are misleading (Lobo et al. 2008), but simply that different statistics measure different aspects of performance, and that appropriate statistics relevant to the application of the model need to be selected. Being able to visualise fitted functions not only satisfied our application of exploring modelled relationships, but also allowed us to understand what caused differences among the methods and how different fitted functions influenced mapped predictions.

Third, comparing the results for the partial responses with the quantitative assessments gives some useful insights. For example, even though the GLM modelled unnecessary complexity in the wetness response (giving the wave-like forms in the 3D plots), the evaluation statistics implied it did nearly as well as BRT. This is in spite of the fact that BRT had a better controlled fit overall. The distribution of environments (Fig. 3b) gives the key; there are relatively few sites in the places where the GLM failed to model the true response. Similarly, the environmental distribution of the training data (Fig. 3a) explains why several methods (GLM, BRT and RF) tended to model a declining response (even if

Table 5. Information learnt from the case study, including explanations relating to “why”.

What	Why (demonstrated, postulated, or inferred)	What can be learnt?
Categories were modelled well with most methods	All algorithms, with the exception of GARP could identify the pattern correctly. GARP's logistic regression rules treat categories as ordered data. Atomic rules should be able to model categorical values but must not have done so in our example, or might have been overwhelmed by logistic rules.	Categorical data such as soil type or land-use can be used in most methods. Don't use categorical data with GARP, or present it as ordered categories or in binary format.
Wetness modelled reasonably but there was some variation across methods	Wetness was the dominant driver for the distribution so was probably the easiest to model correctly. All methods were capable of modelling non-linear trends but MaxEnt modelled amplitude imperfectly (i.e. it was not well calibrated) because it had no information on prevalence. When sampling was sparse (wetness ~30) GLM responds with a strong incorrect "trough" in predictions, a consequence of the complexity of fit allowed, and BRT and RF both overfit the response. MaxEnt did not model the detail in the sparse area, probably because the regularization was strong enough to model a smoother trend.	Presence-absence data gives more information for calibration than presence-only. Strong environmental trends are easiest to model. If there are "troughs" in fitted functions think about whether they make sense ecologically and look at data sparsity. Ignore small fluctuations in fitted functions for ensemble methods because they likely represent peculiarities of the sample, and watch for their effect on predictions. Produce error estimates to see where data sparsity creates uncertainty.
Southness harder to model	Southness was less dominant in the model, and interactions complicate the response. GLM is likely to have done better if we modelled the interactions.	It is possible to model weaker trends, but this varies more across methods. Need to test if GARP's tendency to overpredict stems from an inability to capture all but the strongest trends. Failing to allow interactions will compromise models.
Mapped predictions differ	Mapped predictions differ because the underlying fitted functions differ. Also some clues about why they differ can be gleaned from the various evaluation stats – e.g. models with higher unexplained deviance should produce maps less consistent with the true pattern.	Differences in maps can be understood by looking at underlying models. It would be useful to develop tools to link the map to the functions to show, for any grid cell, what part of the function is relevant. This would be part of the more comprehensive evaluation toolbox that is needed.
Extrapolations differ	Extrapolations differ because of how the functions are or are not constrained at the edges of the environmental response variables.	Knowledge is required about 1) what a method is doing when extrapolating into novel environments, and 2) what is sensible. Again, it would be useful to have tools to link maps to fitted functions for exploring what is behind the predictions.

only a small trough) to wetness at values early on the plateau of the true response – the samples are sparse in some parts of this environment, and several have been realised as “absence” in this particular sample. These results demonstrate that understanding the environmental distribution of the data in the region of interest, in the sample, and in regions that might be used for projection, is a critical part of understanding the implications for modelling and prediction.

Finally, the demonstration prompts a range of questions about what characteristics we want from models in certain situations. For example, when using species distribution models to predict how species ranges will shift with climate change or how they will extrapolate to new regions it is critical that we understand how the algorithm performs when projected into new environmental combinations not sampled by the training data. In other words, is the way that the algorithm extrapolates appropriate from an ecological perspective? Different behaviours are apparent in the implementations of the methods that we tested, but the choice as to which (if any) is correct is as much an ecological and/or a physiological question, as a statistical one. In fact, operationally there are more choices than we demonstrated – for example, GLMs can include natural splines in which knots can be specified and extrapolation controlled; MaxEnt has options to predict zero outside the range of

the data. For a full investigation of extrapolation or forecasting behaviour a much larger range of tests is required including prediction to new combinations of environments. The important point is that we need to first recognise what different modelling applications require of SDMs and then research the best means for achieving what they require. Understanding how the models work and devising evaluation criteria that are closely matched to the questions being asked can inform decisions about the best modelling approach.

Conclusion

We suggest that the SDM literature has not yet matured to the point that it provides clear guidance for selecting relevant methods. Additional model comparison studies may not be fruitful unless they start to ask why certain methods perform better than others. Deeper insights into the causes of varying model performance require an expansion of model evaluation approaches (Araújo and Guisan 2006), syntheses of existing knowledge, and contributions from experts. Given that applications of SDM have grown and are likely to continue to proliferate, insight into the characteristics of models that influence model performance is essential. For instance, there are applications

that do not satisfy the underlying assumptions of species equilibrium with environment (Dormann 2007) such as range shifts with climate, or species invasions into a new area. Likewise, there is an increased demand for models that capture realistic species-environment relationships for theoretical studies in both ecology (i.e. niche differentiation among related species) and evolution (i.e. trait conservatism and its influence on species distributions). For each case, what methods are particularly suitable for the intended use? By providing an example that we believe gives useful insight into model performance, we hope that both developers and users will increasingly question what their models are doing and whether that is most appropriate for the intended applications and outcomes.

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