

# A New Method for Integrating Ecological Niche Modeling with Phylogenetics to Estimate Ancestral Distributions

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**Abstract.**—Ancestral range estimation and projection of niche models into the past have both become common in evolutionary studies where the ancient distributions of organisms are in question. However, these methods are hampered by complementary hurdles: discrete characterization of areas in ancestral range estimation can be overly coarse, especially at shallow timescales, and niche model projection neglects evolution. Phylogenetic niche modeling accounts for both of these issues by incorporating knowledge of evolutionary relationships into a characterization of environmental tolerances. We present a new method for phylogenetic niche modeling, implemented in R. Given past and present climate data, taxon occurrence data, and a time-calibrated phylogeny, our method constructs niche models for each extant taxon, uses ancestral character estimation to reconstruct ancestral niche models, and projects these models into paleoclimate data to provide a historical estimate of the geographic range of a lineage. Models either at nodes or along branches of the phylogeny can be estimated. We demonstrate our method on a small group of dendrobatid frogs and show that it can make inferences given species with restricted ranges and little occurrence data. We also use simulations to show that our method can reliably reconstruct the niche of a known ancestor in both geographic and environmental space. Our method brings together fields as disparate as ecological niche modeling, phylogenetics, and ancestral range estimation in a user-friendly package. [Ancestral range estimation; ancestral state reconstruction; biogeography; Dendrobatidae; ecological niche modeling; paleoclimate; phylogeography; species distribution modeling.]

Biogeography is a complex science that seeks to characterize organismal distributions through both space and time. However, investigating the interplay between these two dimensions has proved challenging. As a result, the field of biogeography has been largely split into two subfields—ecological biogeography (concerning the roles of present-day processes in shaping biodiversity) and historical biogeography (which deals with processes on greater timescales), with little effort made to integrate them (Wiens and Donoghue 2004; Crisci et al. 2009). Developments over the last few decades have begun to bridge the gap between ecological and historical biogeography by considering the extant ranges of organisms, defined by their present-day ecologies, in the context of their evolutionary histories, which are shaped by thousands to millions of years of global environmental change (Ronquist 1997; Avise 2000; Graham et al. 2004; Carstens and Richards 2007; Smith and Donoghue 2010; Landis et al. 2018).

Modern historical biogeography methods generally characterize the focal group's contemporary ecologies or distributions in some way and then use phylogenies to infer past changes. Though methods that characterize distributions as continuous variables have been developed (Lemmon and Lemmon 2008; Lemey et al. 2010), discrete-area methods are in wider use. These comprise the family of methods known as “ancestral range estimation,” which is essentially an offshoot of ancestral character estimation (=ancestral state reconstruction; see Maddison 1994; Schluter et al. 1997; Joy et al. 2016), in which extant taxa at the tips of

phylogeny are assigned a “range” made up of one or more discrete “areas,” and the most likely range at each node is reconstructed via some model of lineage diversification through space and time (see Lamm and Redelings 2009 for an overview). Important ancestral range estimation methods include dispersal-vicariance analysis (Ronquist 1997), the dispersal-extinction-cladogenesis model (Lagrange) (Ree et al. 2005; Ree and Smith 2008), and BayArea (Landis et al. 2013). Software packages such as BioGeoBEARS (Matzke 2013) and RASP (Yu et al. 2015) implement and expand upon these tools in user-friendly frameworks. These methods' characterization of areas as discrete units can be useful in abstracting geography over very large timescales: their use may diffuse signals from paleogeographical estimates that are likely to be artificially precise, as uncertainty only increases for deeper time periods. However, for shallower timescales, where paleoclimate and paleogeography are clearer, the use of discrete areas may be overly coarse—underpowered compared to the precision of available data.

As such, a continuous characterization of species' ranges, couched in rasterized estimates of both present-day and ancient environments, may be more pertinent at shallow timescales or when greater precision is desired. There are a number of theoretical advantages over discrete areas in these situations. For one, a continuous range characterization can accommodate small or unusual distributions due to ecological and local-scale effects, while discrete areas assume uniform taxon occupation of that area, and may often be larger than the taxon ranges they represent. Further, a

continuous range characterization drawn from a species' distribution itself (when it can be precisely estimated) avoids bias that stems from user-defined discrete areas, which may not be biologically relevant to the taxon or time period at hand. Finally, characterizing a species' range in terms of continuous environmental variables "untethers" it from geography, allowing finer detection of ancient dispersal to or between areas nonintermediate to those of a node's two descendants. Again, these characteristics may be undesired for certain systems, or unnecessary over deeper timescales due to concerns over false precision, but for shallower timescales, they could lead to improvements in ancestral range estimation.

Ecological niche modeling (=species distribution modeling; see [Elith et al. 2006](#); [Elith and Leathwick 2009](#); [Peterson et al. 2011](#)) offers an ideal framework for continuous characterizations of species' distributions in terms of environmental variables. Ecological niche models (ENMs) take the form of raster map layers in which each pixel, analogous to a point on a landscape, is associated with a continuous value of suitability for the species in question. Occurrence data for that species as well as climate raster data are used as inputs; in brief, the niche modeling algorithm samples the climate at each occurrence point and creates a model of the taxon's climatic tolerances. The model is projected across the geographic area, creating a map of habitat suitability. Popular ENM algorithms include Bioclim ([Nix 1986](#)), Maxent ([Phillips et al. 2006](#)), and BIOMOD ([Thuiller et al. 2009](#)). Ecological niche modeling methods consider a species' distribution in terms of its occupied *environmental* space rather than *geographical* (E-space vs. G-space; see [Peterson et al. 2011](#)), thus satisfying the criterion wherein a nonintermediate ancestral range may be estimated for a pair of descendants.

ENMs are commonly projected into paleoclimatic models to infer the potential past distributions of the species in question ([Chan et al. 2011](#); [Svenning et al. 2011](#)). However, organisms evolve in tandem with the Earth's continually shifting geography. Paleo-niche models are calibrated with present-day taxon occurrence data, and thus do not account for potential physiological changes in the focal taxon that may have occurred through evolution. At shallow timescales such as the Last Glacial Maximum (~25 kya), this may not be a serious issue, but as paleoclimatic data becomes higher in quality for deeper times ([Brown et al. 2018](#)), model projection schemes will have to account for this by integrating niche modeling with phylogenetics.

Fortunately, the groundwork for phylogenetic niche modeling (=phyloclimatic modeling) has already been laid. [Hugall et al. \(2002\)](#) and [Rice et al. \(2003\)](#) made some of the earliest efforts at integrating ENMs with phylogenies, but we consider [Graham et al. \(2004\)](#) to be the first true phylogenetic niche modeling study. They constructed niche models of *Epipedobates* poison frogs with Bioclim and used the minimum and maximum values of each climate variable for each species as continuous characters for ancestral character estimation, then constructed ancestral climate envelopes at each

node and projected them into present-day climate data. Other, subsequent studies characterized niche evolution by comparing the niches of sister species ([Kozak and Wiens 2006](#); [Eaton et al. 2008](#); [Anciães and Peterson 2009](#)) or correlating niche similarity with phylogenetic similarity ([Knouft et al. 2006](#)). A pair of studies by [Yesson and Culham \(2006a,b\)](#) took a similar approach to [Graham et al. \(2004\)](#), and the former additionally projected ancestral niches into paleoclimatic data—the first study known to us to have visualized ancestral niches in their appropriate time period.

The next major advance in phylogenetic niche modeling was by [Evans et al. \(2009\)](#), who examined niche evolution in *Oenothera* primroses. Unlike [Graham et al. \(2004\)](#) and [Yesson and Culham \(2006a,b\)](#), they used Maxent, which had begun to supplant older niche modeling algorithms, to generate ENMs for each extant taxon. They then integrated suitability values with respect to each climate variable—for example, they binned and summed the habitat suitability values for every cell with a given mean annual temperature value, then repeated across other temperature values. They used this technique to discuss niche evolution in terms of individual climate variables, without visualizing the ancestral niche models in geographic space. This method was further enumerated by [Smith and Donoghue \(2010\)](#) and later made available in the R package *phyloclim* ([Heibl and Calonge 2018](#)), which has been used in a variety of studies (e.g., [Jakob et al. 2010](#); [Nyári and Reddy 2013](#); [Kolanowska et al. 2017](#)).

To date, *phyloclim* is the only widely available tool for phylogenetic niche modeling, and further development in the field has mostly flagged. A few recent studies have used techniques similar to those of [Yesson and Culham \(2006a,b\)](#) to infer ancestral niches from Bioclim niche models, and projected them into the past ([Töpel et al. 2012](#); [Rödger et al. 2013](#)) or present ([Li et al. 2017](#)) climates, but methodological innovation in phylogenetic niche modeling since [Evans et al. \(2009\)](#) has been limited. Further, cases where researchers project ancestral niches into paleoclimate data are rare ([Yesson and Culham 2006a](#); [Töpel et al. 2012](#); [Rödger et al. 2013](#) are the only examples we know of). We think this aspect of phylogenetic niche modeling is particularly important, as a spatial visualization of past distributions is far more intuitive than a separate treatment of each climate variable. Projecting the ancestral niche into past climates allows us to estimate an answer to the glaring question, "Where did this lineage originate?"

Here, we propose a new method for phylogenetic niche modeling which can be seen as an extension of, or successor to that of, [Graham et al. \(2004\)](#), and a companion to the [Evans et al. \(2009\)](#) method implemented in *phyloclim*, though we note that our derivation of this method was independent of either. We take advantage of recent innovations in paleoclimatic data for niche modeling ([Brown et al. 2018](#)) that allow us to project and visualize ancestral niche models in past climates. Our primary innovations are in more precise quantification of taxon responses to climate

as skew-normal rather than uniform distributions, the ability to seamlessly project and visualize ancestral niches into paleoclimate data, and the implementation of the method in an R (R Core Team 2020) package, which we call *machuruku*, the Quechua word for “ancient.”

## MATERIALS AND METHODS

### *Step 1: Constructing and Parsing Niche Models for Extant Taxa*

The first step of our method is to construct present-day ENMs for a set of taxa with associated occurrence data. A modified Bioclim (Nix 1986; Hijmans et al. 2017) model is constructed for every taxon in the current climate. Bioclim samples occurrences for the highest and lowest values of each climate variable and then uses these values to construct a hyperdimensional envelope of suitable E-space. We then parse each niche model, characterizing the response of each taxon to each climate variable independently as a skew-normal distribution using the “snormFit” function from the R package *fGarch* (Wuertz et al. 2019). Using a skew-normal distribution much more accurately approximates the shape of a thermophysiological reaction norm, usually an asymmetrical bell-shape (Angilleta et al. 2003; Klepsatel et al. 2013), than simply using the maximum and minimum occupied values. It is also less sensitive to outliers and provides a continuous scale of habitat suitability for each climate variable, rather than a single suitability value between, as in a uniform distribution. Specifically, we retain the mean, standard deviation, and skewness of each taxon’s response to each climate variable; these are used as input for the second part of our method.

Bias due to spatial autocorrelation of samples or to correlated climate variables is a concern when constructing ecological niche models. The user has the option to spatially rarefy occurrence data to reduce bias due to spatial autocorrelation (Boria et al. 2014), as well as to detect and remove correlated or low-importance climate variables before generating niche models (e.g., see Brown and Carnaval 2019). Reduction and removal of such variables are important for mitigating overparameterization. As the number of climate variables used to construct the ENM increases, suitable E-space shared among localities typically decreases, resulting in artifactually narrow models that overestimate the presence of true biological constraints (Brown and Carnaval 2019). The variable reduction is performed by generating ENMs using boosted-regression trees (Elith et al. 2019) as implemented in the function “humboldt.top.env” from the R package *humboldt* (Brown and Carnaval 2019).

### *Step 2: Estimating Ancestral Niche Models*

The contemporary response parameters for all taxa and a corresponding time-calibrated phylogeny containing those taxa are used as inputs for the second

step. A continuous ancestral character estimation is performed on each climate response value over the input phylogeny, using the “ace” function from the R package *ape* (Paradis et al. 2004), under maximum likelihood with a Brownian motion (BM) model of evolution. “Ace” estimates ancestral character states for both continuous and discrete characters, as well as the associated uncertainty. The climate response values estimated at each node can then be combined back into ancestral Bioclim niche models, which is accomplished in the third step (below).

This step can output reconstructed climate response parameters for each node, but this may not be appropriate for the research question at hand. Specifically, if one intends to project ancestral models into a paleoclimate, it is unlikely that the branching time of any one node exactly matches the time period of the paleoclimate data. To this end, one can opt to provide a “time-slice” corresponding to the age of their paleoclimate data. The method detects which branches exist at that time-slice and interpolates each climate response value along those branches using the following equation from Revell (2013) and Felsenstein (1985):

$$\hat{a} = \frac{\frac{x_i}{v_i} + \frac{x_j}{v_j}}{\frac{1}{v_i} + \frac{1}{v_j}},$$

where  $\hat{a}$  is the interpolated maximum likelihood estimator at the chosen time-slice,  $x_i$  and  $x_j$  are the values at the nodes at either end of the branch, and  $v_i$  and  $v_j$  are the phylogenetic distances from either node to the time slice. This equation assumes a linear evolutionary change along the branch, but absent any knowledge of rate heterogeneity in the phylogeny, we think this is a fair assumption. When a particular time-slice is chosen, only ancestral climate response parameters for the branches present at that time-slice are returned. These can then be combined into ancestral niche models and projected into paleoclimate data corresponding to the time-slice.

### *Step 3: Visualizing Ancestral Niche Models in Past Climates*

The final step in our method is to convert ancestral climate response parameters into ancestral niche models. The reconstructed means, standard deviations, and skewnesses are used to construct a skew-normal distribution for each taxon’s response to each climate variable using the “dsnrm” function in the R package *fGarch* (Wuertz et al. 2019). Using the paleoclimate layer as the independent variable, the suitability of each pixel is calculated as the dependent variable. Skew-normal distributions may be “clipped” by additionally reconstructed 95% confidence limits, which may produce more restrictive and precise models. Additionally, these reconstructed 95% confidence limits may be used to characterize the suitability response as a uniform distribution, producing broader, more inclusive models. All reconstructed models can then be projected

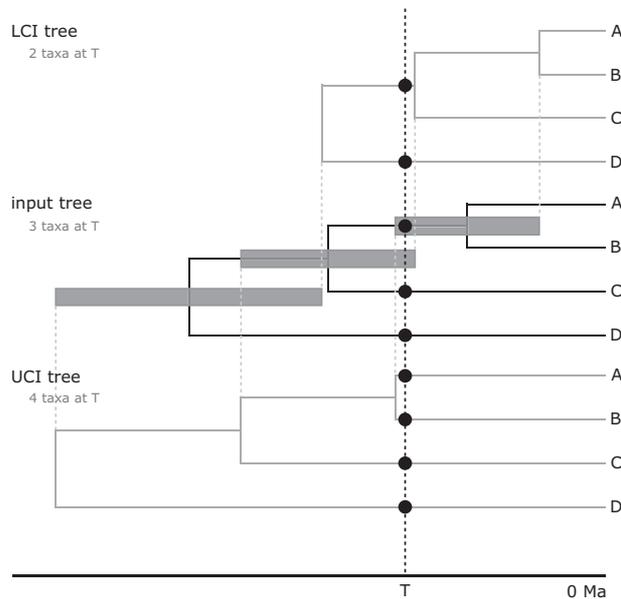


FIGURE 1. Pictorial representation of how “time-slicing” affects taxon selection when interpolating ancestral character estimations along branches, and how variable node heights can affect taxon selection when using a time-slice. The trees shown also demonstrate the first of our two utilities for characterizing uncertainty in divergence time estimation. Starting with the median (input) tree, with provided 95% HPD intervals (gray bars), the lower confidence interval (“LCI”), and upper confidence interval (“UCI”) trees are created from the 95% HPD values (dotted gray lines). In this case, the number of taxa “retained” at the time slice (dotted black line) differs for each tree (black dots). For the LCI tree, only two taxa are retained; for the input tree, three are retained; and for the UCI tree, four are retained.

into corresponding paleoclimatic data layers to visualize suitability for that lineage in paleogeographic space, though any model can be projected into any climatic layer.

#### *Accounting for Uncertainty*

The outputs of Bayesian phylogenetics programs characterize uncertainty in divergence time estimation by presenting a posterior distribution of trees with varying node heights. Optimally, our method would integrate over this distribution, but it is impossible to summarize and visualize ancestral niche models over many trees. This is because, assuming node heights (much less topologies) vary between trees, a node in one tree does not necessarily represent the same taxon/species as the same node in another tree. In the case of a time-slice through multiple trees, the time-slice will intersect with different branches for each tree, and thus different “branch-taxa” will be recovered (Fig. 1). Even if the same branches are intersected, they will be intersected at different places. Thus, ancestral niche models created for different trees may not be combined, only compared, as they represent different taxa.

However, it still may be necessary to account for uncertainty in divergence times. We enable the user to do this by constructing or sampling a limited number of

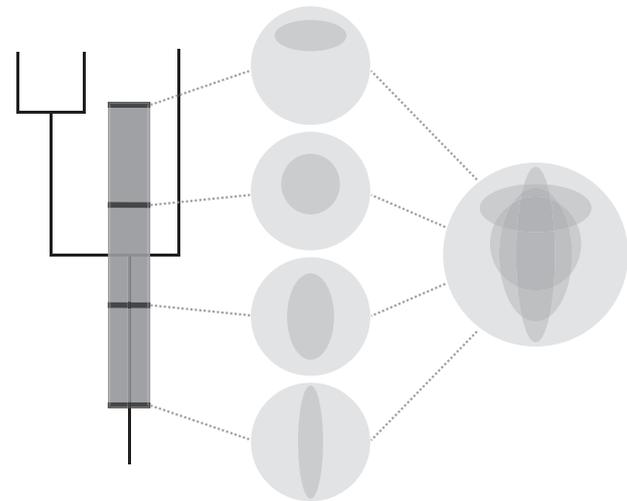


FIGURE 2. Cartoon representation of our method for quantifying uncertainty in ancestral character estimation. The tree’s node bar represents the uncertainty in a generic “niche” parameter reconstructed at that node, characterized by a 95% confidence interval. In this case, the confidence interval is evenly sampled four times, represented by horizontal black lines across the node bar. Each sample corresponds to a separate estimate of the “niche” parameter, which is then shown projected into “G-space.” Circles of lightest gray represent total available habitat. The “niches” are then summed into an ensemble, where overlapping (darker) areas are of the highest suitability, e.g., the highest probability of occurrence for the ancestor at that node.

trees representing the tails and center of the distribution of node heights and then using these trees as separate inputs for the main pipeline. We include two utilities for this, the first of which constructs two additional trees from a single input tree that is itself the summary of a posterior distribution of trees, such as output from the BEAST 2 utility TreeAnnotator (Bouckaert et al. 2014). The additional trees’ node heights are set equal to the upper and lower highest posterior density (HPD) limits of the input tree’s node heights, respectively. Because these trees are effectively chimeric, we use the “force.ultrametric” function from *phytools* (Revell 2012) to reinstate ultrametricity. The second utility directly samples the posterior distribution of trees. It first calculates the tree height for all trees in the posterior, then calculates the average and HPD limits of the height distribution, and finally finds those trees with heights closest to those three values.

Another source of uncertainty in our analyses comes from our usage of ancestral character estimation (Schluter et al. 1997; Losos 1999). Our method can account for this uncertainty by using the 95% confidence limits for each reconstructed parameter at each node, returned by the “ace” function. The range defined by the confidence limits is evenly sampled a user-specified number of times (Fig. 2). Each corresponding set of sampled values for all climate response parameters can be thought of as an individual niche model. In the final step of the method, these sample-models are summed on a per-taxon basis and reweighted according to the number of samples so that the highest suitability value possible remains 1.

*An Empirical Examination of Niche Evolution in the  
Ameerega bassleri Group*

We used our method to examine an empirical case of niche evolution in a small, range-limited dendrobatid frog group. The *Ameerega bassleri* species group is composed of three charismatic and aposematic poison frogs, localized to the east Andean versant of the Peruvian Amazon: *A. bassleri*, *Ameerega yoshina*, and *Ameerega pepperi*. The three species are separated based on morphological, call, and molecular differences and have small, nonoverlapping ranges (Brown and Twomey 2009). Divergence time estimation suggests that the three species began to diverge 2–4 Ma, probably in the late Pliocene (Guillory et al. 2020). Given that they occupy different ranges in a topographically and climatically heterogeneous area, and that amphibians have low vagility and respond closely to changes in their environment, we might expect to see niche evolution in this species group.

We used the comprehensive *Ameerega* phylogeny from Guillory et al. (2020), trimmed to include only the *bassleri* group as well as *Ameerega silverstonei*, an outgroup taxon with a similar range. This tree was constructed using ultraconserved elements (Faircloth et al. 2012), the coalescent-based method ASTRAL-III (Zhang et al. 2018), and time-calibrated in BEAST 2 (Bouckaert et al. 2014). We accrued a total of 67 occurrence points for the four *Ameerega* species from field notes, museum specimens, and the primary literature (Supplementary Table S1 available on Dryad at <https://dx.doi.org/10.5061/dryad.wh70rxwk0>). We spatially rarefied the occurrence data at a distance of 10 km, reducing spatial autocorrelation while also reducing our data set to 29 occurrence points. Our data sets for certain species were extremely small—we retained only three points for *A. silverstonei*, for example. Fortunately, Bioclim can construct ENMs given very limited occurrence data.

For climate data, we used current climate layers as well as paleoclimate layers from Paleoclim (Brown et al. 2018). We selected the *mis19* (Marine Isotope Stage 19; Pleistocene; ~787 ka), *mpwp* (Mid-Pliocene Warming Period; Pliocene; ~3.264 Ma), and *M2* (Marine Stage M2; Pliocene; ~3.3 Ma) paleoclimate data sets from Paleoclim at a spatial resolution of 2.5 arc-minutes (~5 km). All layers were trimmed to an extent surrounding the ranges of the four species, focused on central Peru. We determined which climate layers had the greatest contributions to the species' niches with the boosted-regression tree method described above. For each species, we selected the five layers with the highest contribution to their ENM and removed all other layers from the analysis (surmising them to be correlated with more important ones, and thus unnecessary). The seven layers retained were bio1 (mean annual temp.), bio9 (mean temp. of driest quarter), bio10 (mean temp. of warmest quarter), bio11 (mean temp. of coldest quarter), bio12 (annual precip.), bio15 (precip. seasonality), and bio19 (precip. of coldest quarter). Expert examination

confirmed that the niche models characterized the species' suitable habitat fairly accurately, despite the small number of points.

Ancestral character estimation of niche parameters was performed for each of the three time-slices above (0.787, 3.264, and 3.3 Ma). The 0.787 Ma time-slice captured four ancestral taxa, while the other time-slices captured two. We performed analyses while accounting for uncertainty with 20 samples of the reconstructed climate response parameters' 95% confidence intervals. Following this step, we projected each ancestral niche model into its corresponding paleoclimate data set.

*Method Validation Using Simulated Niches*

Estimating the accuracy of our method requires simulation because we cannot know real ancestral niches exactly for comparison. We used an extant-taxon niche model from our empirical data as our "known ancestral niche." An estimated niche retains the nuances of a real data set (i.e., the synergies between several climate variables and a species' actual distribution). We simulated forward-time niche evolution along a tree and then used our method to work backwards from the output to reconstruct the original niche (Fig. 3). We then compared the simulated ancestral niche to the known. We performed 12 treatments under various conditions. We used three manually constructed four-taxon phylogenies to exhibit different "radiation schemes" (Fig. 3). In theory, more niche divergence will occur between taxa that diverged earlier. To that end, we used an "Early Radiation" tree, where all taxa diverged near the tree's root, a "Late Radiation" tree, where all crown-group taxa diverged near the tree's tips, and a "Steady Radiation" tree, where taxa diverged at equal intervals along the tree. To test the effect of tree age, wherein more niche evolution is likely to occur for older trees, for each radiation scheme we used two tree heights: one set to the age of our M2 paleoclimate data (3.3 Ma), and the other the age of our *mis19* data (0.787 Ma). Finally, for each of these six trees, we ran forward-time simulations with both BM and Ornstein–Uhlenbeck (OU) models of evolution.

We initiated each treatment with a niche model of *A. bassleri* calibrated in present-day climate with the seven climate variables used in the empirical study described above (bio1, bio9, bio10, bio11, bio12, bio15, and bio19) (Fig. 3a). This provided biologically realistic climate response parameters for use in our forward-time simulations and avoided using output from our method as input for the simulations. We used *A. bassleri* as the starting taxon because we had the most occurrence data points for it ( $n=37$ ). We used the "fastBM" function from the R package *phytools* (Revell 2012) to simulate the evolution of each climate response parameter independently along each of the six trees, using either BM or OU as the model of evolution. The starting value of each parameter was the corresponding value for the known *A. bassleri* niche model. For BM,

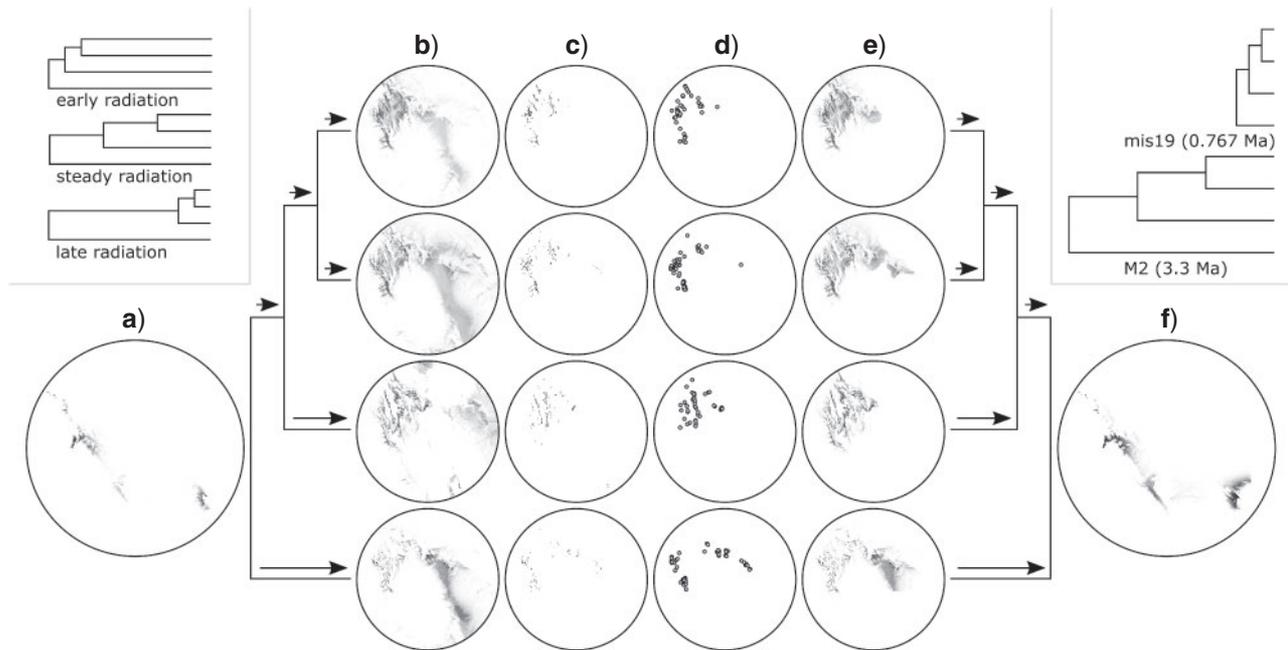


FIGURE 3. Schematic illustrating the simulation procedure we used to validate our approach. a) Known, starting niche in paleoclimate. Darker color indicates higher suitability. b) Artificial evolution of the niche up the tree to the present day. Top-left inset shows different radiation schemes used; top-right inset shows tree heights used. c) Models are converted to binary with a 50% suitability threshold. d) 50 random points are sampled from the binary models. e) Niche models are constructed from the occurrence points and projected into present-day G-space. f) The ancestral niche is reconstructed at the root of the tree, again using the radiation and tree-height schemes shown in both insets.

we controlled the magnitude of change that a parameter is allowed to evolve by using corresponding  $\sigma^2$  values taken from the previously described empirical ancestral niche reconstruction of the *bassleri* group. For OU, we used the “compar.ou” function from the R package *ape* (Paradis et al. 2004) to fit an OU model to the *bassleri* group phylogeny for each climate response parameter, then used the resulting values of  $\alpha$ ,  $\sigma^2$ , and  $\theta$  as input to “fastBM” for the forward-time simulations. We performed 100 forward-time simulations for all 12 treatments to account for random variation in the simulated niche models.

For each simulation, we projected each of the four descendant niche models into the current climate (Fig. 3b). We transformed each niche model into a binary model, where pixels with above 0.5 suitability are given a value of 1, and those with below 0.5 a value of 0 (Fig. 3c). We then used the “rasterToPoints” function from the *raster* R package (Hijmans et al. 2019) to sample 50 random occurrence points from each of these binary models (Fig. 3d).

We then used our own method to reconstruct the starting, known *bassleri* niche model at the base of the tree from the occurrence points of the four simulated descendant taxa. We constructed and parsed present-day niche models from each taxon (Fig. 3e). We then used the resulting climate response values in the ancestral character estimation step (Fig. 3f).

We compared the reconstructed niche at the root node in both E-space and G-space. For our E-space

comparison, we compared the area shared by the known and simulated response curves for each climate variable, quantifying niche overlap outside of G-space. We used the “dsnrm” function from *fGarch* to reconstruct each curve from its mean, standard deviation, and skewness and rescaled each curve so that its area summed to one. This allows direct comparison of the shapes of the known and simulated curves; otherwise, the calculation would be biased toward the “larger” curves. This has been shown to improve predictive performance in past studies (Broennimann et al. 2012; Brown and Carnaval 2019). For each value of  $x$ , we found the lowest value of  $y$  between either curve, then integrated this “shared” curve using the “sintegral” function from the package *Bolstad2* (Curran 2013). This estimated the shared response curve area for that particular climate variable, equivalent to Schoener’s D (Schoener 1968), a common niche overlap metric. We averaged the estimates for each climate variable in a single simulation, and finally averaged the 100 estimates of all simulations in a treatment. We performed pairwise Wilcoxon rank-sum tests between each treatment to assess whether the mean shared response curve area differed significantly between different treatments.

For the G-space comparison, we sought to quantify how the real and simulated niches overlapped in real space. For all simulations, we projected the reconstructed root node model (corresponding to the starting *A. bassleri* model) into the corresponding paleoclimate data. We then rescaled each simulated model to

vary from 0 to 1 in suitability to enable unbiased comparison, and then summed the models to form an ensemble composed of all 100 simulated models for each treatment. We compared the occupied G-space of the ensemble and the starting *A. bassleri* model, also projected into paleoclimate, using the Schoener's D metric. We performed a Niche Divergence Test (Brown and Carnaval 2019) by quantifying the niche equivalence between the ensemble model and the starting *A. bassleri* model using the "humboldt.doitall" function in the R package *humboldt* (Brown and Carnaval 2019) based on 100 iterations of equivalence and background statistics. If the Niche Divergence Test results in a significant value, this indicates that the niches of two species that share common accessible environmental space are not equivalent, lending support for the hypothesis that their fundamental niches are not the same and statistically different.

## RESULTS

### Empirical Study

Given what is known about the modern distributions of the *bassleri* group, their phylogeny, and the nature of past climates in the Peruvian Andes, we recover both reductions and expansions in the evolving niche of this group of frogs. It is important to note that the niches displayed represent the niche as realized in geographical space, but without limits due to biotic interactions or geographical barriers. The modeled niche of the ancestor to the *bassleri* group (Fig. 4a) shows that it was strictly limited to the southeastern versant of the Peruvian Andes, followed by a potential migration northward during the Mid-Pliocene Warming Period, only a few dozen millennia later (Fig. 4c). Niche reductions are seen in the three daughter species in the Pleistocene (Fig. 4e–g, blue), followed by more recent niche expansions (Fig. 4i–k). Without climate data for the period from

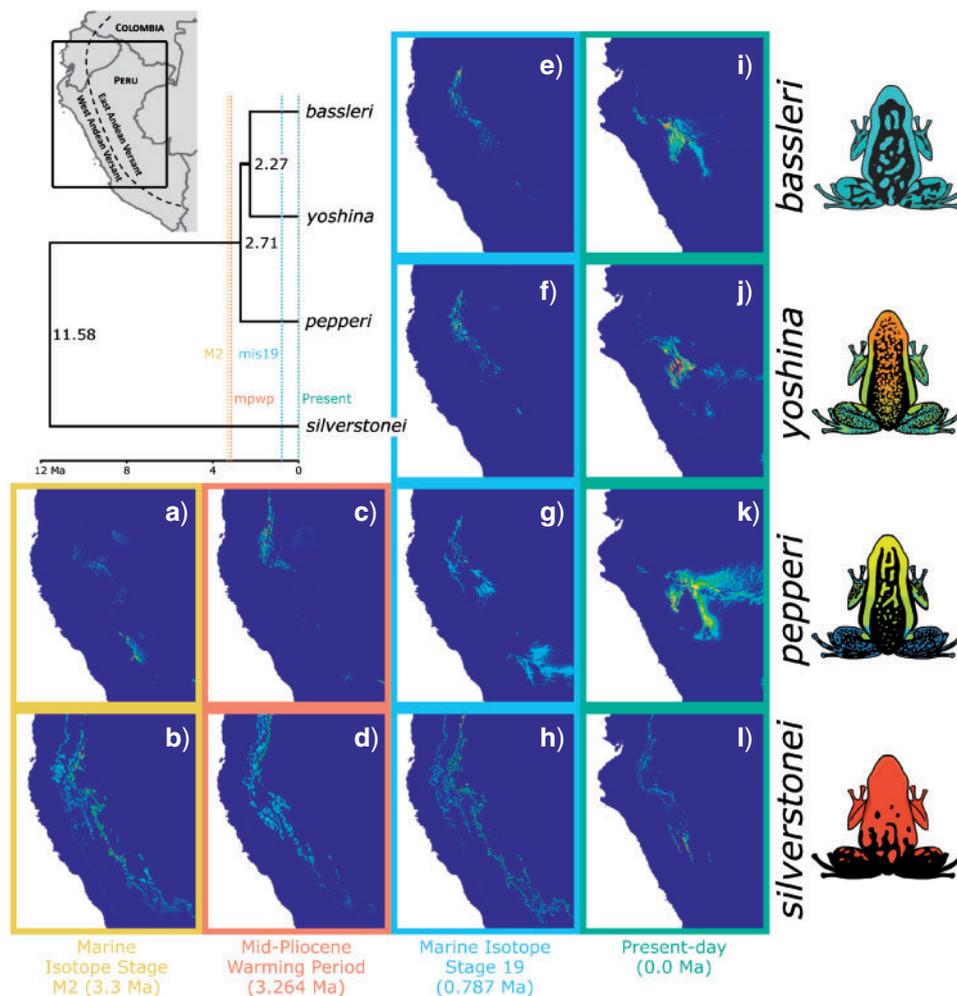


FIGURE 4. Ancestral niche reconstruction of the *Ameerega bassleri* group, with *Ameerega silverstonei* as an outgroup taxon. Models are projected into the area corresponding to what is now Peru. Each color-coded column corresponds to a time-slice of the same color. The tree used is shown at the top left along with divergence times and a timescale in millions of years ago (Ma). A map inset at top left shows the borders of the raster layers used in the context of political boundaries and Andean geography. Subplot labels (a–l) are referred to in the text. Frog illustrations by WXG.

TABLE 1. Results of niche divergence tests

Scenario			Niche similarity (D)	P value
MIS19	Early	OU	0.238	<b>0.009</b>
		BM	0.532	0.198
Pleistocene	Late	OU	0.175	<b>0.009</b>
		BM	0.492	0.307
	Steady	OU	0.251	<b>0.009</b>
M2 Pliocene	Early	BM	0.582	0.336
		OU	0.335	0.129
	Late	BM	0.547	0.257
		OU	0.341	0.198
	Steady	BM	0.622	0.544
		OU	0.355	0.188
		BM	0.530	0.357

Notes: Niche overlap was quantified between the “true” niche and an ensemble of 100 simulated niches using the Schoener’s D metric of niche similarity. A significant P value (bold) signifies that the simulated and known niches were significantly different.

OU = Ornstein–Uhlenbeck; BM = Brownian motion.

2.71 to 2.27 Ma, we cannot assess the niches of the two lineages that existed after the speciation of *A. pepperi* but before the divergence of the clade containing *A. bassleri* and *A. yoshina* (Fig. 4).

By contrast, *A. silverstonei*, which is distantly related to the *bassleri* group as the sister taxon to all other *Ameerega* species, but similar in habitat, distribution, and appearance, shows only niche reduction since the Pliocene. Suitable habitat is shown along the eastern versant of the Peruvian Andes in the Pliocene (Fig. 4b,d), steadily reducing in suitability and occupancy until the small present-day distribution is reached (Fig. 4h,l).

#### Simulation and Validation

Overall, our method was able to recover a simulated niche from artificially evolved descendants with high accuracy. Across all treatments, the average response curve match was 73.18%. The main consistent pattern found was that our method performed better when BM was used to simulate evolution up the tree, rather than an OU model; the average match for all BM treatments was 76.89%, while for OU it was 69.48% (Fig. 5a). Pairwise Wilcoxon rank-sum tests found that all BM treatments were significantly different from all OU treatments (Fig. 5b). Other treatment factors (radiation scheme and tree height) only negligibly affected response curve match. The main exception was the BM/M2/Early Radiation simulation, which had the highest average match (78.31%) and was significantly different from all other treatments (Fig. 5b).

The Niche Divergence Tests demonstrated that in most cases the simulated niches were functionally equivalent to the true niches (Table 1). One notable exception was the OU models of Pleistocene niche evolution. All three of these simulations were significantly different from the true niches.

## DISCUSSION

### Niche Evolution in the *Ameerega bassleri* Group

Our empirical analysis of niche evolution in the *A. bassleri* group of Neotropical poison frogs demonstrates the merits and potential utility of our method. The *bassleri* group, at least beginning in the Pliocene (the earliest timeframe we have paleoclimatic data available for), seems to have undergone niche/range reductions, migrations, and finally niche/range expansions during its evolution. The geographic origins of this group appear to be south of its constituent species’ present-day distributions, in the southeastern versant of the Peruvian Andes. This is in accordance with findings from the overall phylogeny of *Ameerega* frogs, which shows that most of the species occupying branches closest to the root node of the phylogeny (i.e., *Ameerega ingeri*, *A. boliviana*, *A. silverstonei*, and the *bassleri* and *parvula* groups) inhabit limited ranges along this slope in a general south-to-north pattern (Guillory et al. 2020). It is also consistent with a highland origin for *Ameerega* diversity, contra Roberts et al. (2006) (see Guillory et al. (2020)).

The timeframe denoted by our oldest paleoclimate layer (M2), the Marine Isotope Period M2, is approximately 3.3 Ma in the Late Pliocene, and corresponds to a period of incomplete glaciations across both hemispheres (Dolan et al. 2015). The cooler climate is perhaps responsible for the restricted range of the ancestor of the *bassleri* group at this time (Fig. 4a). The Mid-Pliocene Warming Period (*mpwp*), the most recent period of Earth’s history with a warmer climate than today (Hill 2015), and occurring only a few dozen millennia later than M2, saw a northward range shift for this lineage (Fig. 4c). It is unsurprising that such a rapidly shifting climate induced such distributional change, as it is probable that little niche evolution occurred in the time between these periods, so the frogs may have been forced to “follow” suitable climates northward in an example of niche conservatism (e.g., Kozak and Wiens 2006). It is possible that range shifts in tandem with niche conservatism fomented the rapid speciation of the original lineage into three species as some lineages remained in climatically stable regions while others continued to migrate. In the Pleistocene, the ancestors of the *bassleri* group underwent another range reduction, presumably due to cooling temperatures (Fig. 4e–g). Since then, they have undergone range expansions (Fig. 4i–k). Our present-day climate models of each taxon correspond well to what is known of their present distributions.

Analyses of this nature may also be supplemented by population genetic analyses to test for evidence of range expansion/retraction, migration, and introgression that corresponds to the suggestions provided by ancestral niche modeling (Csilléry et al. 2010; Gehara et al. 2013; He et al. 2013; French et al. 2019). Of course, any comparative analysis will be hampered by incomplete taxon sampling, which we see here by lacking 28 of the other described species of *Ameerega* while including the outgroup *A. silverstonei*. We also benefit from

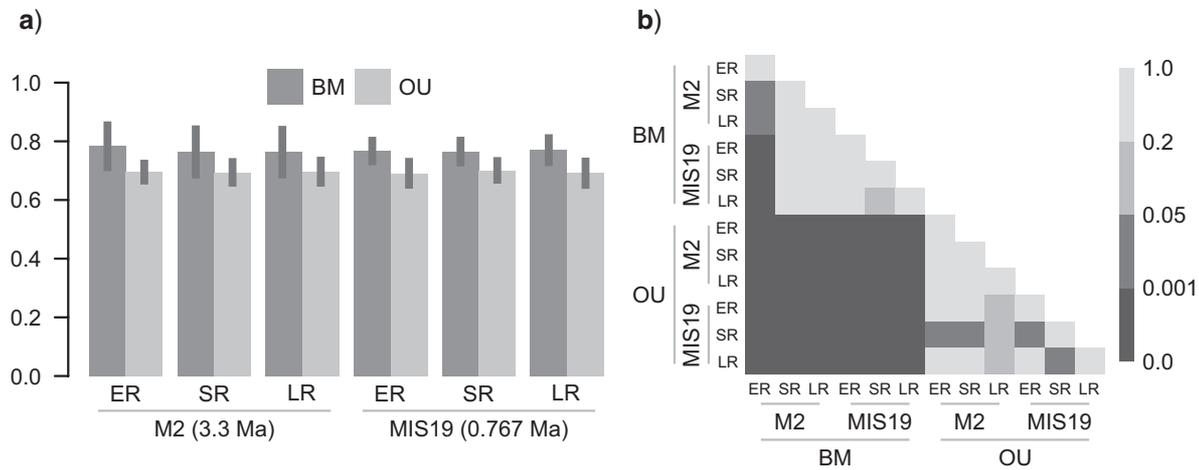


FIGURE 5. Results of the simulation-validation study. a) Average response curve matches across 100 simulations for each of the 12 treatments. A value of 1.0 represents a perfect match. ER = early radiation; SR = steady radiation; LR = late radiation. BM = Brownian motion; OU = Ornstein-Uhlenbeck. Error bars represent  $2 \times$  stdev of the sample. See [Supplementary Table S2](#) available on Dryad for exact values. b) Half-matrix displaying  $P$  values resulting from pairwise Wilcoxon rank-sum tests of the differences between the averages shown in a). The lower the  $P$  value/darker the cell, the more significant the difference. See [Supplementary Table S3](#) available on Dryad for exact values.

having a recently diverged lineage as our study group, which takes advantage of our relatively recent ( $\sim 3$  Ma) paleoclimatic data.

#### Method Validation Via Simulations

We intentionally used species with limited ranges in our empirical study, and as the basis for our simulations, to test the robustness of our method, especially with regards to how well it can reconstruct very specific niches accurately. When the comparison is divorced from geography, solely pertaining to the relationship of the taxon to the environment (E-space), we found that the simulated reconstructions on average shared around 75% similarity to the known. We found that only the model of evolution (BM vs. OU) seemed to affect the accuracy of our method in reconstructing the simulated niche, with BM generally performing  $\sim 74\%$  better than OU ([Supplementary Table S2](#) available on Dryad; Fig. 5a). This is expected since our method itself uses BM to reconstruct the ancestral niche. However, the only slight drop in accuracy when estimating a simulated niche from data derived from a different model of evolution is promising. Radiation scheme and tree height in general did not affect the accuracy of our method, though theoretically more recent radiations and shorter tree heights would produce more accurate results since less change in the niche can accumulate in shorter time spans and branches. It is likely that we would have seen a difference if we had used trees with larger differences in height (ours were 3.3 Ma and 0.767 Ma), but we were limited by the ages of our paleoclimate data. Much of the difference in the response curves of the known, starting niche, and the simulated ancestral niche seems to stem from shifts in standard deviation during the random simulations, which can either expand

or shrink the simulated response curve. This can greatly restrict the amount of area shared by the curves.

Results from Niche Divergence Tests between the “true” niche and the simulated niches show that our method has high predictive performance in many different situations (early vs. late vs. steady radiations) and among different tree ages (Pleistocene vs. Pliocene radiations). However, our method was not perfect and consistently reconstructed significantly different niches that were simulated over shorter periods using an OU model of evolution (Table 1). These results also suggest that the significant differences between the simulation means (Fig. 5) in many cases might not be biologically informative, potentially overstating the differences between the E-space occupied among our reconstructed niches and the true scenarios. The Niche Divergence Test looks at the shape and density of a species’ niche in 2D environmental space and uses a Monte Carlo resampling technique to assess significance. As such, it accurately quantifies the finer nuances of a species’ niche while accounting for spatial processes ([Brown and Carnaval 2019](#)).

These results demonstrate that, at least under these circumstances, our method is robust. However, it would be careless to assume that this applies to all situations. We expect our methods to perform more poorly in situations where fundamental niches evolve rapidly, particularly when these changes are preceded by a period of extended niche stasis ([Wiens et al. 2019](#)). Under this scenario, our method would estimate the process as a gradual continuum, and error in niche predictions would be highest at the point of rapid change. A broader concern for all correlative niche predictions is reconstruction of fundamental niches from contemporary distributions and their associated climates ([Brown and Carnaval 2019](#)). This is particularly challenging for taxa with limited dispersal potential

in areas of high climate dynamism and includes issues characterizing nonanalogous climates not present in contemporary times (Qiao et al. 2017). As such, reconstructed niches can only represent a subset of the true fundamental niche and if greatly undersampled, reduce the size of areas predicted suitable for ancestors.

### *Overcoming Uncertainty and Bias in Phylogenetic Niche Modeling*

Any method that brings together such disparate types of data as phylogenetic niche modeling will be riddled with assumptions, uncertainty, and bias. We contend that these issues do not invalidate our method, and have taken steps to address many of these concerns. Something as nebulous as the ancestral distribution of a lineage can never truly be known for certain, absent voluminous fossil data (lacking for most organisms, entirely for dendrobatid frogs in our case). In that sense, our method is intended more as a hypothesis generator than a hypothesis tester.

Our method assumes that the “true phylogeny” is the one given as input, though in reality, the true phylogeny is unknown. Dated phylogenies are also subject to considerable potential error (Drummond et al. 2006; Ho and Phillips 2009). We enable the user to produce additional trees with divergence dates corresponding to the upper and lower 95% HPD limits imposed on each node age or to sample directly from the posterior distribution for trees with heights closest to the average and 95% HPD limits of tree height. The user can separately optimize niche parameters across each phylogeny and then visualize ancestral niches; different ancestors (e.g., branches) may be recovered at particular time-slices given different divergence dates (see Fig. 1). It can be argued that optimizing niche parameters across the entire posterior distribution of dated phylogenies (the “tree cloud”) would more accurately characterize this uncertainty. This is unequivocally true, but given our method’s emphasis on visualization, we do not think it is a helpful feature to implement. We are not aware of a way to concisely visualize lineage-specific niche models constructed across a distribution of thousands of trees at a certain time-slice, given differences in topology and branch lengths.

Some issues stem from the construction of the original ENMs for each extant taxon, which are parsed into climate response parameters and estimated along the phylogeny. We use a Bioclim-based (Nix 1986) method, rather than other, more sophisticated methods, that is, the machine-learning algorithm Maxent (Phillips et al. 2006), which is in wider use today and generally regarded as more powerful than Bioclim (Elith et al. 2006). The primary reason for our use of Bioclim is that its simplicity enables us to easily parse its output for climate response values which can then be used in a continuous ancestral character estimation. Rödder et al. (2013) also point out some advantages of Bioclim over Maxent when it comes to modeling niches in paleoclimate: namely

that Bioclim makes fewer assumptions of constancy in the species–climate relationship, and that the Bioclim envelope can potentially include nonanalogous climates not available in present-day climate.

We do recognize that an ENM is only as good as the input data provided and how well the input samples reconstruct the species’ fundamental niche. We are currently working to expand our method to better account for the potentiality that contemporary distributions underestimate a species’ fundamental niche (Mercier et al. unpublished data). Challenges in producing accurate climate and paleoclimate data layers are beyond our purview. However, issues stemming from georeferenced occurrence data are familiar to evolutionary biologists. For many rare or range-limited species, there are very few occurrence points available; in that sense, our *Ameerega* data set represents something of a worst-case scenario; as before stated, we only retained three occurrence points for *A. silverstonei* after spatial rarefaction, and only marginally more for the other taxa. Another issue stems from spatial autocorrelation due to the biased nature of collecting biological samples. In short, occurrence points are generally not independent samples as assumed by niche modeling methods, because organismal samples (and their associated locality data) are generally collected in “convenient” ways, for example, along roads, near biological stations, or in protected wilderness areas. This introduces significant spatial autocorrelation (Boria et al. 2014). We include the ability to spatially rarefy occurrence points, which can improve niche models by reducing spatial autocorrelation.

Central to our method are concerns regarding ancestral character estimation (Losos 1999). In certain cases, the reconstructed states at different nodes may not be significantly different because of the very large confidence intervals associated with them. As such, the singular value returned by the algorithm (often the mean or median) may not be reflective of reality. We account for this uncertainty by enabling the user to evenly sample the confidence intervals of each niche parameter as many times as they like, and effectively treat each corresponding set of samples as separate ancestral niche models; in the last step, the models are summed and rescaled into an ensemble that better reflects the wide range of reconstructed niche values. We contend that sampling the niche parameter confidence intervals in this way (i.e., weighting all sampled parameters the same, even if they arise from the tails of the distribution) is the best approach because it is conservative. We would introduce artificial certainty into our final models by weighting each parameter according to its position along with the distribution. Finally, another potential issue with our method pertaining to ancestral character estimation is our treatment of niche parameters as independent values to be optimized. Given that many of the parameters are components of the same distributions (e.g., mean, standard deviation, and skewness), it may be pertinent to enable joint estimation of certain parameters in the future.

A final challenge for our method comes from limitations in the availability of paleoclimate data. Similar to estimating ancestral states in phylogenies, reconstructing paleoclimates becomes less precise further back in time. Currently available, reliable paleoclimate data that are suitable for constructing niche models (i.e., that correspond to the present-day climate layers usually used to construct ENMs) only go back a few million years at most and are thus irrelevant to older lineages. Further, paleoclimate simulations are models themselves with their own assumptions and errors, which should be considered when interpreting results. Lastly, accurate ancestral distribution estimates also need to consider physical changes in geography, in addition to paleoclimatic suitability. As such, this would constitute the removal of areas predicted outside of known geographic barriers.

#### *The Roles of Our Method and Phylogenetic Niche Modeling in Evolutionary Biology*

Though many studies have used *phyloclim* in their analyses, there has since been little innovation in phylogenetic niche modeling methodology. This is most likely due to a combination of factors. One is the perceived lack of informativeness from these types of analyses; a limitation of *phyloclim* is that it only provides ancestral niche estimates in environmental space, and then only for the response to a single climate variable at a time. It is difficult to draw generalized conclusions from such information, especially how it pertains to the actual geographic distribution of the ancestral lineages in question. However, the difficulty of performing phyloclimatic analyses in geographical space has also likely stymied the development of phylogenetic niche modeling methods. Principally, this is due to the dearth of high-resolution paleoclimatic data (further back than the Last Glacial Maximum) in an analogous format to the present-day climate layers commonly used in ecological niche modeling. Many phyloclimatic studies, such as Li et al. (2017), could have been improved by projecting their ancestral niche models into paleoclimatic rather than current climate data. Progress in developing paleoclimatic data for niche modeling studies, such as the resource Paleoclim.org (Brown et al. 2018), is continuing to mitigate this issue, though it is unlikely that accurate and high-resolution paleoclimate layers will ever extend past the early Neogene due to the uncertainties of deep time.

Our method has a variety of potential uses in evolutionary biology and phylogeography, including the inference of the potential geographic origins of lineages but extending beyond that as well. The method can potentially be used to infer niche differentiation or convergence through time within or between lineages by coupling it with niche comparison methods. The geography of speciation can be investigated by comparing the niches of sister species before, during, and after their divergence. Macroevolutionary methods

can be used to investigate the degree of phylogenetic signal and/or inertia in niche evolution. The method can also be used to investigate the responses of lineages to past climate change. Future studies may also merge population genetic and demographic analyses with our method, for example, by using ancestral niche models as resistance/conductance layers for demographic simulations and analyses (e.g., Prates et al. 2016).

Overall, our method advances phylogenetic niche modeling and opens its usage to the broader evolutionary biology community via an open-source R package entitled *machuruku*. *Machuruku* is intended for ease of use and is freely available from <https://github.com/wxguillo/machuruku>. We hope that this project rekindles interest in the field of phylogenetic niche modeling and assert that it represents an advance in both utility and usability in this area.

#### SUPPLEMENTARY MATERIAL

Data available from the Dryad Digital Repository: <https://dx.doi.org/10.5061/dryad.wh70rxwk0>.

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