Climatic niches in phylogenetic comparative studies: a review of challenges and approaches

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Abstract Studying the evolution of climatic niches through time in a phylogenetic comparative framework combines species distribution modeling with phylogenies. Phylogenetic comparative studies aid the understanding of the evolution of species' environmental preferences by revealing the underlying evolutionary processes and causes, detecting the differences among groups of species or relative to evolutionary pattern of other phenotypic traits, but also act as a yardstick to gauge the adaptational potential under climate change. Because several alternatives exist on how to compute and represent the climatic niche, we here review and discuss the current state of the art and propose a best practice to use in comparative studies. Moreover we outline the common evolutionary models and available model-fitting methods and describe the procedure for ancestral niche reconstruction with the intention to give a broad overview and highlight the most advanced approaches for optimal niche-related comparative studies.

Introduction

Phylogenetic comparative studies use a wide range of methods to explore patterns and processes linked to phylogenetic trees and species traits (Pennell and Harmon, 2013). These studies uncover how a certain trait evolves among different taxa, how evolution of one trait influences another, whether a trait represents adaptation to the environment etc. In this review we focus exclusively on studies testing hypotheses about species' climatic niches evolution through phylogeny.

The aim of such studies is typically not only to suggest the trajectories of niche evolution, but rather to test specific hypothesis about the timing of appearance, causation or evolutionary processes responsible for observed patterns. Such studies aim to discover, for instance, whether shifts in the climate niche occur at the same time as shifts in a particular trait (such as C3/C4 photosynthesis: Edwards and Smith, 2010), whether it was a key driver for developing specific life-histories (e.g. cactus life-form: Edwards and Donoghue, 2006), or whether temporal and/or spatial fluctuation of climate caused species to evolve and diversify (Evans et al., 2009). Furthermore, linking climate niche evolution to population demography through time could reveal whether major niche shifts occur in small or large populations (Jakob et al., 2010). The analyses are based on current trait values, the phylogenetic relationship between species and an evolutionary model. Climate niche is treated as if it was a phenotypic trait and the analysis of, say, temperature values follows the same logic as evolutionary analysis of body mass. The actual reconstruction of ancestral trait values is unnecessary for testing correlations between characters. Being an integral part of the procedure, ancestral states along the phylogeny are implicitly inferred but not actually presented. However, other hypotheses might require reconstruction of ancestral values, such as tests of niche overlap between specific ancestral nodes, pinpointing the exact time of appearance of certain values, identifying reversals in evolutionary progression or visualization of trait changes through time.

Given that understanding the evolution of species' niches through time attracts extensive interest and is highlighted as a priority research question in paleoecology (Seddon et al., 2014), we discuss and propose guidelines for optimal use of species distribution and climatic data in comparative studies.

The aim of this review is to (1) introduce the concepts relating niche space to its evolution through time, (2) discuss and propose the optimal niche representation to be used in phylogenetic comparative studies, (3) introduce most common evolutionary models (4) describe the methods for ancestral reconstruction and discuss future directions of the field.

Climate niche in space and time

Hutchinson (1957, 1978) defined a species' fundamental niche as all combinations of environmental conditions where a species can persist and maintain a viable population in the absence of predators or competitors (Kearney and Porter, 2004). Although the ecological niche is not strictly a heritable phenotypic trait for which these methods were developed, niche characteristics are defined and constrained by species physiology, which *is* heritable, and as such can be analyzed in a phylogenetic framework (Kozak and Wiens, 2010a).

Biologists are generally interested in the "fundamental niche", which represents species physiological limits and is the actual evolvable trait, although what we actually observe in nature is the "realized niche". Unfortunately we are currently unable to determine the fundamental niche without manipulative experimental studies, so we are bound to analyse the realized niche, a restricted section where a species lives, limited by biotic interaction or dispersal limitation (Jackson and Overpeck, 2000; Soberón and Nakamura, 2009).

It is currently impossible to tell how closely the realized niche approximates the fundamental niche, and for this reason it is difficult to guess whether the observed change really demonstrates niche evolution, or if this change is merely a shift of the realized niche within the species' fundamental niche (e.g. due to changed biotic interactions: Graham et al., 2004; Dormann et al., 2010). High within-species plasticity (e.g. in mammals, Réale et al., 2003) may lead to changes in realised habitats as biotic and/or abiotic conditions change.

A further complication is introduced by the existence of no-analog climate conditions at different time slices, e.g. in the past (Williams et al., 2001) or future (Williams et al., 2007, see Fig.1), which indicates that only a portion of a species' fundamental climatic niche (termed "potential niche") actually exists in the world at a given time. Therefore, whole sections of fundamental niche might be unobserved because they are nonexistent in space at that time (Fig. 1). Moreover, in the presence of facilitative biotic interactions or mutualism, species' niche could even extend beyond the fundamental niche (e.g. in lichens or corals; see Fig. 1, Bruno et al., 2003; Afkhami et al., 2014). Given the tremendous complexity of confounding factors it seems incredibly difficult to be certain how to interpret the observed change in the climate niche. Distinguishing evolutionary change from shifts within unknown niche limits certainly merits attention, and comparative studies could potentially disentangle one from another: if a trait tightly linked to physiology changes along with the niche (assuming this change is at the genetic level, i.e. it goes beyond phenotypic plasticity), this could indicate the species is adapting to new environmental conditions, and hence its niche is evolving. For example, Edwards and Smith (2010) found that the origin of C4 photosynthesis in grasses coincided with shifts to drier environments. Without considering the exact mechanism, or excluding other hypotheses, it should be reasonable to interpret this finding as species adaptation to novel climate conditions (i.e. evolutionary change of the fundamental niche). In this review we consider the "realized" niche, since this is the most common situation for which we have data although we acknowledge it is far from a consistent approximation of the fundamental niche, and encourage using direct physiological estimates of climatic tolerance whenever available.

Representing the climatic niche

To test hypotheses about the climatic niche in phylogenetic comparative methods, it is necessary to infer the present climate niche of extant species. There is no standard protocol and the way the niche is represented varies widely among studies. For example, some authors represent the niche with climate niche models (Graham et al., 2004; Yesson and Culham, 2006a,b; Eaton et al., 2008; Dormann et al., 2010), others use raw climate data (Evans et al., 2005; Ackerly et al., 2006), some combine the two approaches (Fig. 3, Evans et al., 2009; Smith and Donoghue, 2010), and others represent the niche with ordination techniques (principal component analysis, outlying mean index: Eaton et al., 2008; Boucher et al., 2012; Bystriakova et al., 2011). Here we define the optimal climate niche representation for the most common circumstance, where data derive from occurrence data and the hypothesis to be tested is specific to that region. In this case, niches based on **raw** data consist only of climate values extracted at species locations: generally the mean of those values is representing the niche (e.g. mean annual temperature, total annual precipitation). Climate niche models, a subset of species distribution models, are the most frequently used approach to represent the niche (Franklin and Miller, 2009; Peterson et al., 2011). Algorithms relate a species' geographical locations to climate characteristics in order to describe its environmental niche (Guisan and Zimmermann, 2000; Kozak et al., 2008, a review of prediction ability of numerous modeling algorithms is provided by Elith et al. 2006). Modeling the niche to get insights of the functional relationship between a species and its environment is statistically preferable to the use of raw data (Peterson et al., 2011), because it accounts for the fact that species occurrences in an area might be determined by habitat availability and is not only a function of species preferences. For instance, a higher abundance in valleys compared to mountain tops could be due to a higher availability of valleys in that area, despite species' higher preference for mountains (see Fig. 3 c,d and examples below).

Niche statistics

The niche is a multidimensional entity and as such difficult to analyze phylogenetically as a whole. In general, it is decomposed into its marginal components (e.g. annual precipitation), each of which is examined separately along the phylogenetic tree. Most if not all variables describing the climate niche are continuous and the statistic most commonly chosen to represent them is the mean (e.g. mean annual precipitation). As some authors acknowledged, the mean may or may not be the most informative descriptor of the niche (see Fig. 3d, Graham et al., 2004). Different solutions have been proposed, particularly among studies where ancestral climate niche was reconstructed along the phylogeny. Graham et al. (2004) and Hardy and Linder (2005) proposed to consider the upper and lower niche limits separately, in order to infer the whole range of conditions of the ancestral niche, the so called "MaxMin" coding, which was used in a number of later studies (Yesson and Culham, 2006a,b; Lo Presti and Oberprieler, 2009; Lawing and Polly, 2011; Töpel et al., 2012). Instead of using maximum and minimum, which could be outliers, Vieites et al. (2009) proposed to consider 95% confidence values. In any case, mean, minimum or maximum temperature still do not fully describe the distribution of species climatic tolerances. To tackle this issue Evans et al. (2009) proposed the "predicted niche occupancy" (PNO) profiles: histograms obtained by combining response curves from niche models with climate layers of actual species distribution in geographic space. With this approach, each climate variable is represented by a histogram, which is especially appropriate for species whose niche variables are multimodal or, more generally, do not approximate a normal distribution. Working with histograms (or rather, empirical densities) requires sampling from the distribution of values and thus repeating the same analysis for each sampled value.

Analyzing the whole distribution of preferences is certainly more desirable than using single values. It would, however, be more appropriate to consider response curves obtained from niche models in parameter space, rather than combining them with geographic space. This avoids spurious results arising when large areas with low suitability are present in geographic space: the total sum of suitabilities (as used in Evans et al., 2009) could still be higher for those suboptimal conditions, only because of their high frequency in geographic space. This is illustrated in Fig. 3c, where a great portion of sites with the temperature of 9-10°C are not occupied by the species, therefore the probability of species occurrence at that temperature is relatively low (see Fig. 3d), but the sum of those probabilities in space will be high because there are many sites with that temperature. On the other hand, a temperature of 12-13°C is highly suitable (probability of 0.8), but there are so few sites with these conditions that the sum of suitabilities is low, despite the species' high preference for those sites. The statistical model would pick it up and discriminate between use and availability (the maximum in Fig. 3d), while the histogram of suitability in geographic space (PNO) will be biased towards common environmental conditions. Therefore, model output allows an unbiased representation of preferences, irrespective of geographic availability (Hurlbert, 1978; Manly et al., 1993; Matthiopoulos et al., 2011). This is relevant also when considering large-scale climate change and the existence of no-analog climates in different time periods - climate conditions that cover large areas today might have been very restricted at a different time, and vice versa.

In principle, the same resampling scheme can be used for multivariate distributions (as in Boucher et al., 2012), obviating the need to study each climate variable separately. However, given the no-analog conditions, the problem of assuming the same correlation structure between variables for different time periods arises again, an issue still waiting to be solved.

Ecological variability

Species are often polymorphic; populations of the same species may live, for example, on different types of soil, or along a wide gradient of temperature (Pearman et al., 2010). The approach described above, where species' climatic preferences are expressed with empirical densities, automatically takes into account the ecological variability within species by resampling from climatic values based on species' preferences. Theoretically the same approach could be employed for categorical variables, with preferences determining the probability of drawing from each character state (e.g. in case of higher species' preference for soil-type A compared to B). This way ecological variability can be taken into account in any comparative analysis. Another method to accommodate polymorphism in discrete characters is through the quantitative genetic threshold model (Felsenstein, 2005), which models a discrete character as a continuous trait and is described in more detail in Box 1. See also Hardy and Linder (2005) and Hardy (2006) for additional methods and discussion on this topic.

Evolutionary analyses

How did the niche evolve among different species? Under which processes? What were the drivers? Are niches conserved or labile? What was the ancestral niche like? These are some of the most intriguing questions in comparative studies about climatic niches. We next describe the available methods to tackle some of them: we discuss the utility of phylogenetic conservatism tests, describe the most common evolutionary models, explain the procedure to infer the ancestral climatic niche and end with a summary and recommendations of best approaches.

As the name suggests, phylogenetic tree is the backbone of phylogenetic comparative studies. A detailed description on building a phylogeny is beyond the scope of this review, and we refer the interested readers to Holder et al. (2003); Bininda-Emonds (2004) and Roquet et al. (2012). At the coarsest level, a distinction can be drawn between phylograms (trees with branch lengths proportional to molecular distance), and chronograms (or ultrametric trees, with branch lengths proportional to time). Unless the aim of the study specifically requires the use of a phylogram, the general consensus is to use ultrametric trees because niche evolution is assumed to be proportional to time. Although sophisticated methods are continually reducing uncertainty, phylogenies still remain only hypotheses of how species evolved (Webb et al., 2002). Alternative trees often have almost the same support, which is problematic because for instance, niche reconstruction on different trees may produce different results. Therefore the best way to incorporate phylogenetic uncertainty is to carry out the analyses on a sample of plausible phylogenetic trees instead of using the single best phylogeny.

Phylogenetic niche conservatism

Phylogenetic niche conservatism (PNC) is the tendency of species to retain their ancestral niches through time (Boucher et al., 2014). The most common way to assess the PNC is by measuring the phylogenetic signal: a measure indicating whether a trait evolves according to the null expectation of neutral drift model. There is still disagreement and it remains a debated topic at which similarity level phylogenetic signal can be interpreted as phylogenetic niche conservatism (Losos, 2008a; Wiens et al., 2010).

Here we want to highlight how testing for PNC by measuring phylogenetic signal can be potentially misleading and special caution is needed when interpreting the results. For instance, no phylogenetic signal is a pattern where species niches appear to be independent from phylogenetic relationship among them (Losos, 2011). This is usually interpreted as no niche conservatism, as it can arise when the niche evolved more than expected from random evolution. Niche diverged to such an extent that the similarity among closely related species is lost (Fig. 1c). Another cause leading to the same pattern is convergence, when species belonging to separate clades adapt to the same types of environment, and therefore the pattern of niche values distribution among clades is similar (Fig. 1c, Kraft et al., 2007). Again, this is seen as no niche conservatism. But a highly problematic and less obvious cause of observing no phylogenetic signal is *perfect* conservatism: if the evolution is extremely conserved, all species will have the same or very similar niches, and no phylogenetic signal can be detected (Fig. 1d, Revell et al., 2008; Kozak and Wiens, 2010b). This occurs under strongly stabilizing selection, where all species evolve towards the same optimum value (Revell et al., 2008; Kozak and Wiens, 2010b), or when strong biological constraints bound the niche values to a narrow interval (Revell et al., 2008; Losos, 2011). Hence no signal could indicate either divergent evolution, strong stabilizing selection with one optimum (i.e. stasis), or bounded evolution. Therefore, the same pattern can be caused by completely different processes, which cannot be distinguished among each other by measuring the level of phylogenetic signal alone. To identify whether the niche evolved under, e.g., directional selection or genetic drift, the recommended approach is to fit different evolutionary models to data, rather than measuring the phylogenetic signal (Revell et al., 2008; Cooper et al., 2010).

Furthermore, the detection of a phylogenetic signal depends on the size of the phylogenetic tree and the section analyzed (Fig. 1e). It is extremely important to interpret the patterns only according to the climatic/temporal boundaries within which they were identified; niche lability in a strictly tropical species does not preclude PNC at larger scales (Losos, 2008b; Wiens, 2008).

To summarize: (a) phylogenetic signal and niche conservatism are patterns which do not necessarily reveal the underlying processes (Losos, 2011; Crisp and Cook, 2012); (b) completely different processes can lead to the same pattern (see Revell et al., 2008); (c) the detection of patterns is context-dependent (Fig. 1e).

Therefore, a better approach to assess niche conservatism among different clades is to test for mechanisms and evolutionary processes.

Models of evolution

Evolutionary models describe and approximate the natural processes responsible for trait evolution (Fig. 4). Fitting various models to the data permits to test hypotheses about the processes driving evolution of particular trait (e.g. the climatic niche). Before actually fitting models to the data, it is advisable to first identify plausible evolutionary processes based on prior biological knowledge, and afterwards proceed to fit only the corresponding models (Fig. 5). By fitting all the models without distinction one runs the risk of selecting a model with good statistical fit, but biologically improbable premises (as demonstrated in Wiens et al., 2007). The model with best fit is chosen in most cases through likelihood ratio tests (LRT, Johnson and Omland, 2004). Model selection criteria such as Akaike information criterion (AIC, Akaike, 1973) or Schwarz criterion (BIC, Schwarz, 1978) provide several advantages; they can compare multiple models simultaneously, rank them, give relative supports and are not influenced by the hierarchical order in which the models are compared (Burnham and Anderson, 2002; Johnson and Omland, 2004; Posada and Buckley, 2004).

Nonetheless, recent criticism about information theoretic approaches cast a doubt on their ability to discern the correct model. As Boettiger et al. (2012) and Slater and Pennell (2013) argue, in comparative studies *predictive approaches* are more robust and powerful means for model selection. While information theoretic approaches select the model which maximizes the posterior probability of the observed values, predictive approaches prefer the model which best predicts the observed values through simulation (Slater and Pennell, 2013). In this approach the models are first fitted and parameters for each model of evolution are estimated, and subsequently used to simulate new data. The models are then evaluated based on how closely they predicted the observed data. This procedure is available in the R-package “geiger”(Harmon et al., 2008), so far to test for early burst, Brownian motion and rate shift models. Package “pmc” (Boettiger et al., 2012) allows a simulation based method to choose between models fitted in“geiger”, “ape” (Paradis et al., 2004) and “ouch” (King and Butler, 2009). Given that complex models have a higher number of parameters, the phylogenies have

Evolutionary models for continuous characters

The simplest evolutionary model is the **Brownian motion model** (BM, Cavalli-Sforza and Edwards, 1967; Felsenstein, 1985, 1988). Under this model the traits are evolving randomly in any direction from the mean at each instant of time, with a net change of zero. The probability of character change is thus proportional to branch length, and the correlation among trait values at the tips of the tree decreases linearly with increasing phylogenetic distance between species (i.e. the more closely related the species, the more similar their traits are, Hansen and Martins, 1996). Exactly the same correlation structure is also expected when traits evolve under some other processes, such as directional or stabilizing selection with fluctuating optimum or punctuated change (periods of stasis alternated by abrupt changes, Hansen and Martins, 1996; O'Meara et al., 2006; Thomas and Freckleton, 2011). The assumptions of BM are violated if the values of a trait are near their biological limits and therefore cannot decrease or increase independently of the current value, or if the trait is under stabilizing selection (O'Meara et al., 2006). In those cases trait evolution is better described by the **Ornstein-Uhlenbeck model** (OU, Hansen, 1997; Butler and King, 2004; Estes and Arnold, 2007), an extension of BM which has an additional term describing the "pull" towards an optimum value (known as mean-reversion rate in finanical mathematics). When the value of this constraint equals zero, the model is equal to BM. On the other hand, the higher the pull towards an optimal value is, the lower the correlation among closely related species will be, as all species evolve towards the same optimum.

Another process of great evolutionary importance is "adaptive radiation", which traces back to Simpson (1944). According to this process, species traits initially evolve rapidly and then slow down as the niche space becomes filled, which is basically opposing the idea of gradual evolution as described by simple BM (Harmon et al., 2003, 2010; Slater et al., 2010). It is modeled as BM with decelerating rates of evolution through time, a model commonly known as **early-burst (EB)** or **ACDC** (accelerating versus decelerating rates of character evolution, Blomberg et al., 2003), which can also be tested with **Pagel's δ** (Pagel, 1997; Pagel et al., 1999). Another way of detecting the pattern of decelerating evolutionary rates is to infer rate shifts through phylogeny, as described in Eastman et al. (2011), or by calculating the morphological disparity index (MDI, Harmon et al., 2003).

Box 1: continued

A further option is to perform the node height test: EB occurs when the standardized independent contrasts of trait values are higher deeper in the tree than among more recent nodes in the phylogeny (Freckleton and Harvey, 2006). Although the model of adaptive radiation is generally well supported in paleontology, it has not been often observed in comparative studies (Harmon et al., 2010). Slater and Pennell (2013) argue the inability of detecting EB may be because of lack of power of currently employed methods, rather than the absence of such pattern in nature. Several other models describing adaptive radiation exist which assume a decrease of evolutionary rates as a function of the number of competing lineages (Mahler et al., 2010), or are refinements of Price's **niche-filling** models (Price, 1997; Harvey and Rambaut, 2000; Freckleton and Harvey, 2006). Adaptive radiation can also be fitted with a stabilizing selection model where different clades in the tree evolve towards different optima (multiple-optimum OU model Butler and King, 2004).

Similarly, to investigate the tempo of evolution – whether traits evolved rapidly immediately after speciation events followed by a long period of stasis – it is necessary to fit **punctuational** or **speciational** models of evolution, where the evolutionary change is a function of speciation events and is independent of branch lengths (Gould and Eldredge, 1972; Huey and Bennett, 1987; Pagel, 1997; Pagel et al., 1999; Pagel, 2002). This type of evolution can also be detected by testing for a cladogenetic component of trait evolution with Bayesian MCMC test (Bokma, 2008). Models can also assign different rates of trait evolution to different parts of a tree (O'Meara et al., 2006; Thomas et al., 2006; Eastman et al., 2011; Venditti et al., 2011; Beaulieu et al., 2012; Revell, 2012). It is possible to identify the location of a rate shift in the phylogeny with R-packages "phytools" (evol.rate.mcmc Revell, 2012), or "geiger" (rjmcmc.bm).

Different evolutionary models for continuously varying trait can be fitted with R-package "geiger" (Harmon et al., 2008), "ouch" (Butler and King, 2004), 'ouwie" (Beaulieu et al., 2012), whereas Mahler et al. (2010) model can be fitted by fitDiversityModel in phytools.

Discrete characters

Statistical models describing the evolution of discrete characters are based on continuous-time Markov process, equivalent to the Brownian motion model for continuous characters (Schluter et al., 1997; Cunningham et al., 1998; Pagel et al., 1999; Ronquist, 2004). The earliest and simplest such model is the Jukes-Cantor model proposed for nucleotide substitution with equal transition rates (Jukes and Cantor, 1969; Galtier et al., 2005).

Box 1: continued

Kimura (1980) extended it to a two-rate model to allow the transition rates between nucleotides to differ. Today this family of models are known as Mk models, Markov models which can assume k states. (Lewis, 2001). The central feature of the model is the rate matrix, which contains the instantaneous transition rates between different character states (Pagel, 1997; Pagel et al., 1999). With a 3-states trait, this transition matrix is a 3 × 3 matrix with forward and backward transition rates represented on the off-diagonals (Revell, 2014). The model can assume different rates among characters (the rate A→ B may differ from B → C), and the direction of change (the forward transition A → B may differ from the backward direction B → A). Until recently, the transition rates were fixed and applied to the entire phylogeny, without the possibility, for instance, to assume a different rate of A → B transition on different parts of the tree. This is now possible with the R package "corHHM", which handles the different rate classes as hidden character states (e.g. fast and slow; Beaulieu et al., 2013). Another innovative way to model the evolution of discrete characters is through the "threshold" model, first described by (Wright, 1934), in which the discrete trait is practically transformed to a continuous character, an unobserved trait called "liability" with fixed thresholds (Felsenstein, 2012; Revell, 2014). For example, a trait with two states (A, B) can be represented by a continuous scale liability axis with an arbitrary threshold (e.g. at 0), so that when the liability assumes negative values, the trait is in state A, otherwise in state B. The threshold model is biologically reasonable because it models a discrete character as a continuous trait where the probability of the character to change states decreases with time: the longer the time after the character crossed the threshold and moved to another state, the less probable it is the return to previous state, in contrast to Mk model, in which the amount of time at a certain state does not influence the probability of change (Felsenstein, 2002). The threshold model is implemented in R package "phytools" (Revell, 2012) and permits ancestral reconstruction of discrete characters under BM and OU models of evolution. Several other R packages are available for reconstruction of discrete traits under both joint and marginal methods, allowing multistate characters and different transition rates: diversitree (FitzJohn, 2012), geiger (Harmon et al., 2008), ape (Paradis et al., 2004), as well as other software such as MESQUITE, BayesTraits and SIMMAP (Bollback, 2006). J. Felsenstein's webpage (http://evolution.genetics.washington.edu/phylip/software.html) provides an overview of other available phylogeny software.

to be large enough to allow a reasonable inference of the evolutionary model (Boettiger et al., 2012). Thanks to the increasing availability of molecular data, phylogenetic trees are growing to include many thousand species (Bininda-Emonds et al., 2007; Smith and Donoghue, 2008; Thuiller et al., 2011; Jetz et al., 2012). With such a variety of life forms it becomes reasonable, even necessary, to assume and test much more complex models of evolution than a simple Brownian motion.

Integrating fossil records Incorporating known ancestral values dramatically improves the inference of the evolutionary model, in particular by allowing the detection of directional evolutionary trends, which are virtually unobservable with extant taxa only (Oakley and Cunningham, 2000; Finarelli and Flynn, 2006; Albert et al., 2009; Slater et al., 2012). Substantial improvements were shown for model detection for all tested models (BM, AC/DC and OU: Slater et al., 2012). Integrating prior information by directly assigning values to specific ancestral nodes in the phylogeny is now possible and technically straightforward (e.g. in R-packages “phytools” and “geiger”; Slater et al., 2012). Constraining values from wandering too far from the optimum value can be achieved by simulating “bounded evolution” by varying the “pull” parameter of the OU model, which in turn determines the width around the optimum, or by setting absolute limits (as proposed by Revell, 2007; Revell et al., 2008). Given that the interpretation of results in comparative methods largely depend on the model of evolution, it will be important to integrate all available prior knowledge from paleosciences, continue developing realistic evolutionary models, as well as establishing reliable techniques to choose among them.

Ancestral niche reconstruction

Rapidly developing statistical reconstruction methods permit the estimation of ancestral trait values based on its present-day value, the phylogenetic relationship among species and an evolutionary model. Therefore the inference of the best evolutionary model should be an integral part of the reconstruction procedure. If a model is not specified, most reconstruction methods will follow a BM model by default, and their output will be identical or very similar (see Table 2).

As in model-fitting, the methods for continuous and discrete traits are slightly different. Climate variables are most commonly expressed on a **continuous** scale and ancestral climate niches can be reconstructed following the methods for continuous characters. Squared-change parsimony (or weighted squared-change parsimony) was initially the most widely used method. The optimal values for ancestral characters are found when the sum of their squared changes over the whole phylogenetic tree reaches the minimum value (Maddison, 1991; Garland et al., 1997). Weighted squared-change parsimony takes into account branch lengths (i.e. evolutionary time), so that the resulting reconstruction corresponds to BM evolution (Maddison, 1991; Webster and Purvis, 2002). Another widely used method was Felsenstein's (1985) independent contrasts (IC). Although weighted squared-change parsimony and IC both implicitly assume a BM model of evolution, those two methods will yield slightly different reconstructed values for all nodes except the basal, because independent contrasts use "local" optimization (only daughter nodes are considered to infer the value of the ancestor), as opposed to "global" optimization used in squared-change parsimony (Maddison, 1991; Garland et al., 1997; Webster and Purvis, 2002). Nowadays more commonly used methods are maximum likelihood (ML) (Schluter et al., 1997; Cunningham et al., 1998), generalized least squares (GLS) (Grafen, 1989; Martins and Hansen, 1997; Pagel et al., 1999; Martins, 1999) and Bayesian approaches (Pagel et al., 2004). Ancestral traits, and hence also climate niches can be estimated using R-packages "ape", "phytools" and "phyloclim" (Heibl et al., 2013) and other software as MESQUITE (Maddison and Maddison, 2001), BayesTraits (Pagel and Meade, 2007) or COMPARE (Martins, 2004). Table 3. summarizes the approaches used in climatic niche reconstruction studies, indicating methodological improvements over time.

One could represent climate preferences as **discrete** characters (e.g. by categorising temperature values into "arid" and "mesic" conditions). Performing this categorization *after* the reconstruction of continuous climate variables allows more precision and avoids spurious results due to arbitrarily chosen thresholds. Maximum parsimony reconstructs the ancestral values by minimizing the number of changes needed to reach the observed present-day values (Pagel et al., 1999; Pedersen et al., 2007). Maximum likelihood and Bayesian methods are broadly grouped into "joint" or "global" and "marginal" or "local" reconstructions. Joint reconstruction finds the states which jointly maximize the likelihood over the whole phylogeny. In contrast, marginal reconstruction singles out the state with the highest likelihood at each node separately, which can be useful to test a specific hypothesis at a certain node in the tree (Pagel, 1999). Models which describe the evolution of discrete characters are based on the Markov-transition process of the probability of the character (see Box 1, Pagel et al., 1999).

Reconstruction procedures take into account evolutionary models by transforming the branch lengths, the path separating species pairs from their common ancestor in the phylogenetic tree. For instance, according to early burst model, evolution is faster closer to the root of the tree, therefore after transformation those branches will be longer compared to the branches closer to the tips where the rate of evolution is slowing down. Reconstructing the values according to a specific model of evolution in R can be done in two steps: first, it is necessary to transform the phylogenetic tree according to the previously tested best fitting model (e.g. rescale function in “geiger”), and afterwards this rescaled tree can be used for ML-based ancestral niche reconstruction under the default BM model of evolution (e.g. ace function in “ape”). The obtained ancestral values correspond to values evolved according to the evolutionary model used to transform the tree. Accordingly, weighted squared change parsimony or independent contrasts can fit different models of evolution in a computationally efficient way, by employing appropriate transformations of the phylogeny (see Table 1).

Regardless of the character type or method of choice, estimating trait history on a sample of possible phylogenetic trees instead of using only the single best tree allows to incorporate phylogenetic uncertainty in the analysis. Reconstructed estimates of all trees are then averaged and their distribution provides uncertainty estimates. This procedure is not limited to Bayesian analysis, but can be applied to any ancestral reconstruction method (Donoghue and Ackerly, 1996; Martins and Hansen, 1997; de Villemereuil et al., 2012).

Visualizing and validating the ancestral range and climatic niche If the aim of niche reconstruction was exploring the unfolding of evolutionary changes through time, we may want to visualize the ancestral climatic niche in an abstract multidimensional climate space (e.g. Veloz et al., 2012). On the other hand, to visualize the historical distribution and appreciate the extent of range shift through time, ancestral niche is often projected to a geographic map along with the current climatic niche (e.g. Yesson and Culham, 2006a; Lawing and Polly, 2011; Töpel et al., 2012). This may be problematic because environmental variables today are most likely correlated differently among each other than they were in the past (Boucher et al., 2012), given that non-analog climate conditions were already present at different time steps even on a short time scale, such as in the Quaternary (Jackson and Overpeck, 2000; Williams and Jackson, 2007). Therefore, projecting the ancestral niche to today’s world and vice-versa will not accurately represent the ancestral range, as parts of the range may be missing while some other areas might be wrongly assigned. It practically shows where the ancestor would live today, but not necessarily where it actually lived in the past. The ideal solution would be to project to paleoclimate maps, but because they become less reliable the further one goes back in time, it is difficult to infer the correct ancestral range solely with SDMs, without fossil records. Fossil records are scarce for most species and are often biased with respect to climate, topography, species size and abundance, yielding fewer traces of rare and small-sized animal species especially in wet tropical climates (Kidwell and Flessa, 1995). Still, whenever available they are a valuable indicator of a species' past distribution as they are generally buried within the species' range so spatial displacements between past and present are likely due to a range shift of species (Kidwell and Flessa, 1995). Fossil records of species occurrences can prove that species were present in the study area at the specific time (Vieites et al., 2009), and/or in the predicted ancestral range.

Known ancestral climatic values from paleodata add valuable information and should either be used to aid a better approximation of evolutionary models by constraining specific nodes to known values, as previously seen, or be employed for validating the reconstructed niche values. Validation may be more important when current data already yield a well-constrained model. In contrast, poorly defined models may profit from integrating paleoclimate data into the estimation process.

Summary and recommendations

Here we summarize and propose tentative guidelines for optimal use of species occurrence and climatic data in phylogenetic comparative studies.

Niche representation

- When present-day climate niches are inferred from spatial occurrences, niche models are a better choice than raw data.

- Each climatic variable should ideally be expressed by species preference for the full range of values (i.e. empirical densities), instead of being summarized by the mean or other point estimates (e.g. mean temperature).

Ancestral niche reconstruction

- Before reconstructing the niche, a best-fitting evolutionary model should be estimated for each climatic variable.

- Known paleoclimate data can either be used to improve the evolutionary model inference or to validate the reconstructed values.
- Evolutionary changes are best visualised in an abstract climatic space.
- Ancestral species range should be projected to a paleoclimate map.

Concluding remarks

Analysing the evolution of climatic niches integrates species distribution modeling, phylogenies, evolutionary models as well as elements of paleosciences. Such a complex research question requires careful consideration of each component to minimize potential bias and information loss. We primarily focused and discussed the most appropriate methods to represent the climatic niche through species distribution modeling and outlined the procedure for ancestral niche reconstruction. This research field has a lot to gain from improvements in other areas, particularly from developing new evolutionary models, which would better approximate processes on macroevolutionary scale. Available paleodata has the potential to greatly improve the detection of evolutionary models (Slater et al., 2012), and we expect the future efforts in this interdisciplinary field to focus especially on a better integration of phylogenetic, paleontological and climatic data.

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Tables

Table 1: Reconstruction outcome from different methods for continuous characters. Under default conditions - untransformed ultrametric tree and/or no model specification - all methods will produce roughly the same ancestral states, as all assume Brownian motion model of evolution. Note: independent contrast (IC) method will yield the same ancestral state estimates as the other methods only when each node of the tree is separately re-rooted during the reconstruction process (Maddison, 1991; Garland et al., 1997). Weighted squared-change parsimony (WSqCP) and independent contrasts can also assume different models of evolution by reconstructing the trait values on a transformed phylogeny. Bayesian estimate can lead to a different result under the same model due to different prior distributions for model parameters.

IC [untransformed tree]	≈	WSqCP [untransformed tree]	=	ML [BM]	=	GLS [BM]	≈	Bayesian [BM]
IC [OU tree]	≈	WSqCP [OU tree]	=	ML [OU]	=	GLS [OU]	≈	Bayesian [OU]

Table 2: A proposal of best practice and data format for phylogenetic comparative studies

	Best choice	**Alternative**
Phylogeny	Sample of trees Chronogram	Single tree Phylogram/topology
Climate niche from occurrence data	Modelled data	Raw data
Climate niche from experimental data	Direct measures	-
Niche statistics	Empirical distribution	Point values
Evolutionary model	Selected according to prior knowledge, followed by model selection based on fit	No selection
Ancestral niche projection	To paleoclimate maps, if reliable	To present-day maps
Validation	Fossil records	-

Table 3: List of studies reconstructing the ancestral climate niche in chronological order. The fields with missing values indicate either that the tests were not performed or no information is available in the text. An overview of R packages implementing comparative phylogenetic methods is available in O'Meara (2012).

Study	Phylogeny	N°of species	Niche representation	Reconstruction method	Model selection/ additional indices	Software
Rice et al. (2003)	Phylogram	19	Modelled mean and st. error	GLS (BM)	Randomization	Compare
Graham et al. (2004)	Phylogram	2,3,5	Raw min/max values	ML/GLS (BM)	LR	
Hoffmann (2005)	Phylogram	15	Raw distribution	SqCP		MacClade
Edwards and Donoghue (2006)	Phylogram	9, 8	Mean climatic and physiological parameters	GLS (BM,OU_1)		Compare
Yesson and Culham (2006b)	Topology	21	Mean/st.dev/min/max of raw data	SqCP	Randomization	Mesquite
Yesson and Culham (2006a)	Chronogram	45	Mean/st.dev/min/max of raw data	SqCP	Randomization	Mesquite
Eaton et al. (2008)	Phylogram	19,23,39	PC axes centroids	SqCP (BM)		Mesquite
Crisp et al. (2009)	Chronogram/ phylogram	11064 in 4 trees	7 biomes	SqCP, ML (Mk1)	Randomization	Mesquite

Table 3: continued

Evans et al. (2009)	Chronogram	20	Modelled distribution	ML (BM)	MDI[1]	R[2]
Lo Presti and Oberprieler (2009)	Chronogram	147	Raw mean, min, max values	SqCP	QVI, K	Mesquite
Smith and Beaulieu (2009)	Chronogram, phylogram	301,351, 889,3174	PC axes	GLS (BM)	Disparity ratios, rates of evolution (AIC_c)	R, Brownie
Verbruggen et al. (2009)	Chronogram	52	Raw mean/min/max	ML	λ,K, LR	R[3]
Vieites et al. (2009)	Chronogram	80	Raw mean, 95% CI	ML (BM)	λ,K,δ, LR	Mesquite
Edwards and Smith (2010)	Chronogram sample	1230, 299	C3/C4 physiology, mean climate values	IC/ML (BM), ML (OU2)	AICc	Phylocom, LASRdisc, Brownie
Jakob et al. (2010)	Chronogram sample	12	Modelled distribution	GLS (BM)		R[4]

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[1] Morphological Disparity Index calculated in R package Geiger

[2] geiger

[3] ape, geiger

[4] phyloclim

Table 3: continued

Smith and Donoghue (2010)	Chronogram sample	19	Modelled distribution	ML (BM)	Niche overlap/ similarity/equivalency	
Boucher et al. (2012)	Chronogram sample	51	OMI	JL (OU3)	AICc	R[5]
Bystriakova et al. (2011)	Phylogram	53	Mean values/OMI centroids	ML (BM)	Permutation	R[6]
Holstein and Renner (2011)	Chronogram	24	Biomes	ML (Mk1)	Randomization	Mesquite
Rivera et al. (2011)	Phylogram	5	Raw mean	GLS (BM)		Compare
Heibl and Renner (2012)	Chronogram sample	43	Biomes	ML, Bayesian RJMCMC (Mk1)	AICc	Bayestraits
Kellermann et al. (2012)	Chronogram	92, 95	Cold/dessication resistance	ML (BM)	K,λ, Moran's I	R[7]
Schnitzler et al. (2012)	Chronogram sample	89	Raw mean values	PIC (BM,OU)	λ,AIC$_c$	R[8]

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[5] ade4, ape, geiger, picante, diversitree

[6] ape

[7] picante, geiger

[8] ape

Table 3: continued

Töpel et al. (2012)	Chronogram	38	Min, max values	ML (BM)		R[9]
Ahmadzadeh et al. (2013)	Chronogram sample	8	Modelled	ML (BM)		R [10]
Koecke et al. (2013)	Chronogram	19	Modelled distribution	ML (BM)	MDI	R[11]
Nyári and Reddy (2013)	Chronogram	29	Modelled distribution	ML (BM)	MDI	R[12]
Wiens et al. (2013)	Chronogram	117	Raw mean values	GLS (OU_1)	AIC,λ	Compare, R[13]
Guerrero et al. (2013)	Chronogram	73, 96, 25, 24	Raw mean, min, max values	GLS (BM,OU_1)	AIC	Compare, R[14]
Jara-Arancio et al. (2014)	Chronogram	17,25	Biomes,raw median values	MP,ML,GLS (OU)	AICc	Mesquite,R[15],Compar

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[9] ape
[10] phyloclim
[11] Phyloclim
[12] Phyloclim, Phyloch
[13] ape,geiger
[14] geiger
[15] OUCH

Figure legends

Figure 1: Climatic space represents all the combinations of two climatic variables existing at a certain time, which may differ at different times in history (t1, t2). The fundamental niche of a species includes all the possible conditions where a species could persist, some of which may lie outside conditions currently existing in the world. The intersection of the two represents the potential niche, which the species would fill in the absence of biotic interactions and dispersal limitations. The realized niche is the segment actually occupied by the species; it may occasionally extend towards climatic conditions outside its fundamental niche if facilitative biotic interactions are present. Adapted from Jackson and Overpeck (2000).

Figure 2: A hypothetical illustration of different degrees of phylogenetic signal. (a) Situation where trait values follow the expectations of a BM model of evolution (i.e. traits similarity is proportional to shared evolutionary history among species). (b) Strong phylogenetic signal is found when the trait values among closely related species are more similar than would be expected from BM. (c) A situation with no or low phylogenetic signal as a consequence of over-dispersion or convergence to habitat-specific trait values. Closely related species are not more similar than species drawn at random. (d) No phylogenetic signal as a consequence of trait stasis or convergence of all the species to the same trait value. (e) A signal (or its absence) may be restricted to a specific clade of a phylogenetic tree.

Figure 3: Climate niche representation. Niches are inferred by combining a) species distribution maps with b) climatic layers (temperature, precipitation, etc). c) The simplest niche representation that combines those data can be plotted as a histogram, with grey bars being the number of species occurrences at a certain temperature and white bars representing the entire area. Alternatively, niches can be statistically modeled, as shown in diagram d). The parameters finally obtained from those two approaches, in this example the mean values, may differ. Fig d) illustrates why the mean value is not necessarily the optimal statistic; instead reconstructing the whole distribution is preferable.

Figure 4: Evolutionary processes shaping the evolution of species traits are approximated by evolutionary models. Some processes, such as adaptive radiation or speciational processes can be approximated or tested by a number of slightly different models. See Box 1 for abbreviations and details.

Figure 5: Fitting the evolutionary models to data. Based on prior biological knowledge plausible evolutionary processes responsible for shaping the evolution of species traits are identified, and the corresponding evolutionary models are fitted to the data (see Fig. 4 for a readable version of this step). The model that fits best to the data (trait values and phylogeny) is commonly selected with likelihood ratio test (LRT), or with model selection criteria such as Akaike information criterion (AIC) or Schwarz criterion (SC=BIC).

Figures

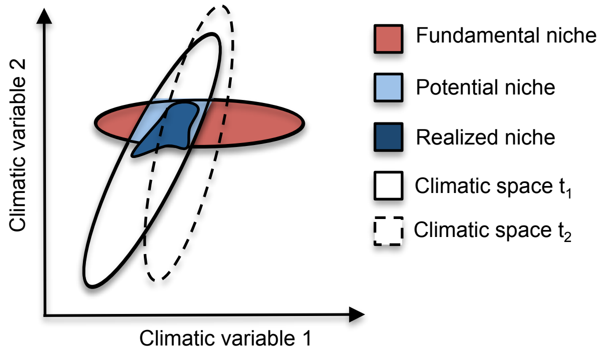

Figure 1:

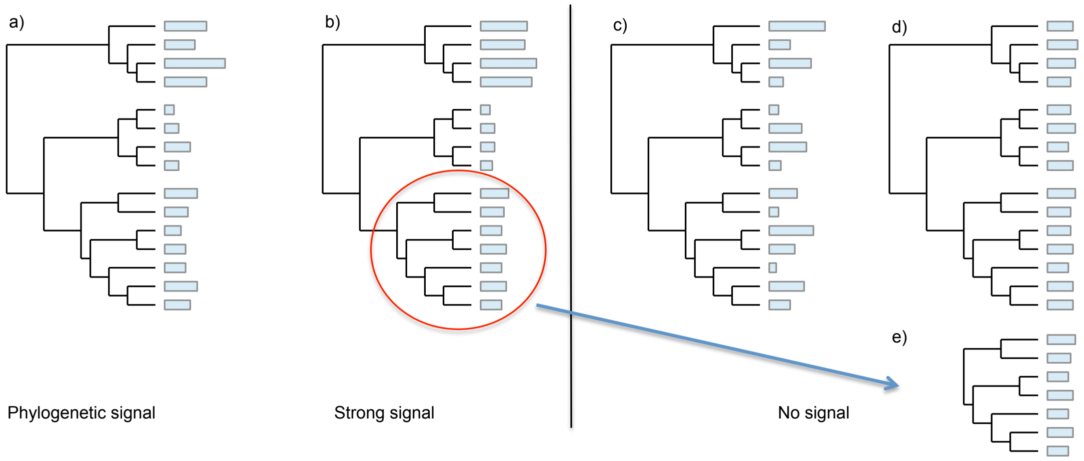

Figure 2:

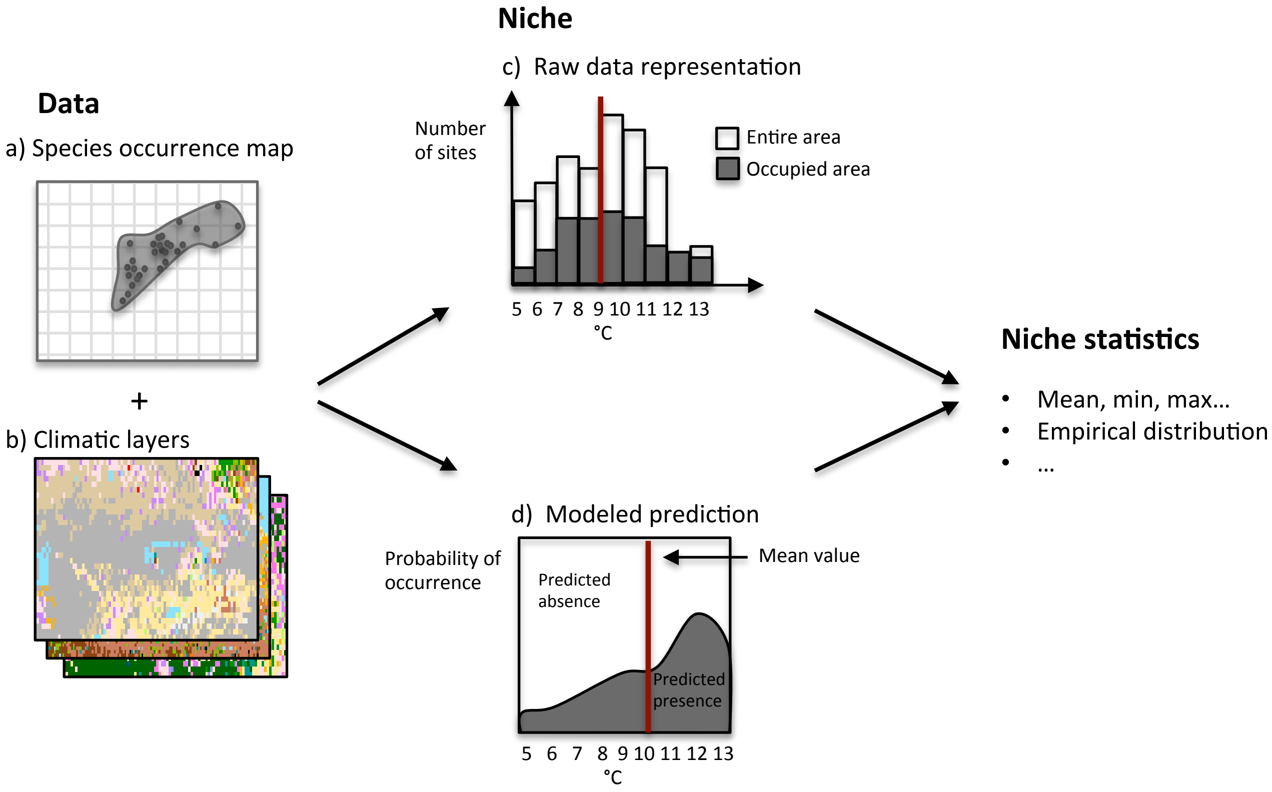
Data
a) Species occurrence map
+
b) Climatic layers
Niche
c) Raw data representation
Number of sites
Entire area
Occupied area
5 6 7 8 9 10 11 12 13
°C
d) Modeled prediction
Probability of occurrence
Predicted absence
Predicted presence
Mean value
5 6 7 8 9 10 11 12 13
°C
Niche statistics
• Mean, min, max…
• Empirical distribution
• …

Figure 3:

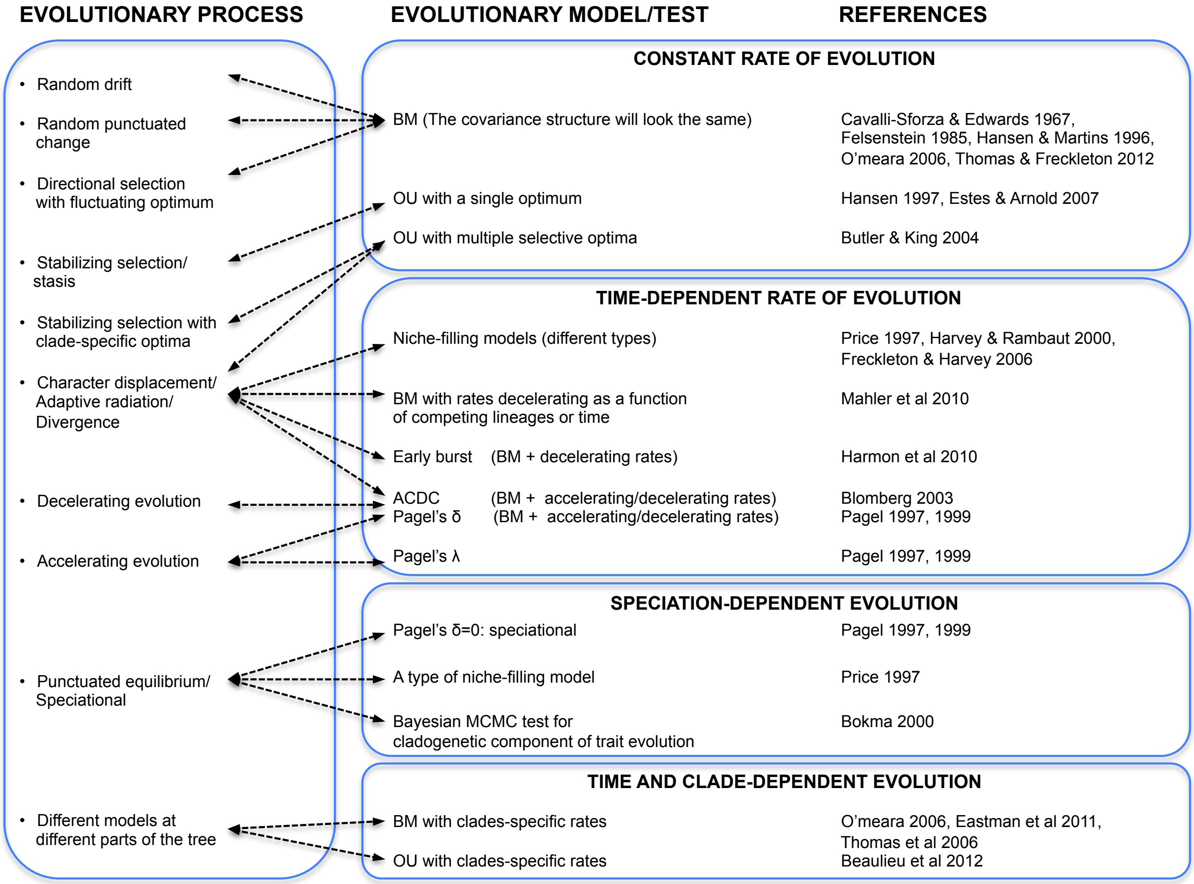

Figure 4:

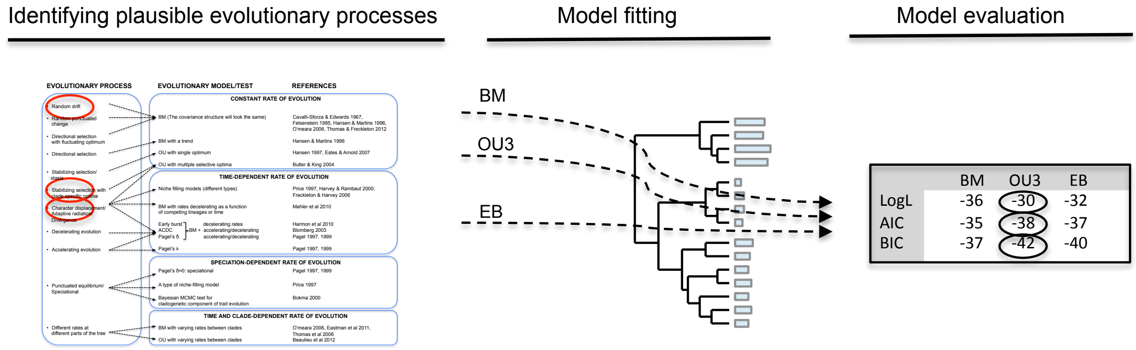

Figure 5: