BIOINFORMATICS APPLICATIONS NOTE Vol. 30 no. 15 2014, pages 2216–2218
doi:10.1093/bioinformatics/btu181

Phylogenetics

Advance Access publication April 10, 2014

geiger v2.0: an expanded suite of methods for fitting macroevolutionary models to phylogenetic trees

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Associate Editor: David Posada

ABSTRACT

Summary: Phylogenetic comparative methods are essential for addressing evolutionary hypotheses with interspecific data. The scale and scope of such data have increased dramatically in the past few years. Many existing approaches are either computationally infeasible or inappropriate for data of this size. To address both of these problems, we present `geiger v2.0`, a complete overhaul of the popular R package `geiger`. We have reimplemented existing methods with more efficient algorithms and have developed several new approaches for accomodating heterogeneous models and data types.

Availability and implementation: This R package is available on the CRAN repository http://cran.r-project.org/web/packages/geiger/. All source code is also available on github http://github.com/mwpennell/geiger-v2. `geiger v2.0` depends on the `ape` package.

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Supplementary information: Supplementary data are available at *Bioinformatics* online

Received on February 24, 2014; revised on March 31, 2014; accepted on April 1, 2014

1 INTRODUCTION

In the past few decades, phylogenetic trees have become a key component of evolutionary research. This development has been fueled by the increased availability of robust time-calibrated phylogenies for many groups, in addition to an expanding number of statistical techniques for inferring patterns and processes from comparative data (reviewed in Pennell and Harmon, 2013). Among the many R packages developed for phylogenetic and comparative data (e.g., Paradis *et al.*, 2004), `geiger` (Harmon *et al.*, 2008) has been a primary utility for making macroevolutionary inferences from phylogenetic trees.

However, in the ~6 years since the initial release of `geiger`, the data available for comparative biology have changed substantially. For some groups, we now have phylogenies and corresponding trait data with thousands (and even tens of thousands) of species (e.g. Jetz *et al.*, 2012). `geiger v2.0` is a complete overhaul of the previous release (Harmon *et al.*, 2008), designed to scale up comparative methods to large datasets. To do so, we have taken two complementary tacks. The first is to improve algorithms and implementations to increase computational efficiency of existing methods. The second is to expand the suite of statistical approaches to allow for heterogeneity in both models and data types across the phylogeny.

In this applications note, we briefly describe the methods now in `geiger`, with a particular focus on novel implementations and algorithms. Most of these methods have been previously published elsewhere in some form, and we refer readers to the relevant publications for full explanations (for an overview of the main features of the package, see Appendix 1 in Supplementary Material).

2 METHODS

2.1 Fitting simple models of character evolution using maximum likelihood

Fitting and comparing models of trait evolution can provide insight into many macroevolutionary questions (Pennell and Harmon, 2013). The two 'workhorse' functions in `geiger` for fitting models of trait evolution using maximum likelihood, `fitContinuous` and `fitDiscrete`, have both been completely reimplemented. The previous version of `fitContinuous` calculated the likelihood of a set of continuous characters (e.g. body size) having evolved under a model using a variance–covariance (vcv) matrix approach. This involves inverting the vcv matrix, which is extremely computationally intensive, making the method infeasible for large trees. FitzJohn (2012) demonstrated that using a 'pruning'-based algorithm (Felsenstein, 1973) allows for much more efficient likelihood calculations. This algorithm is used in the `diversitree` package (FitzJohn, 2012). [For related algorithms, see Freckleton (2012) and the `phylolm` package (Ho and Ané, 2014)]. The approach has now been extended to all the models in `fitContinuous`. In addition to improving the efficiency of the algorithm, we have improved numerical optimization procedures and implemented a novel method to simultaneously estimate model parameters and an additional term to account for measurement error.

For the case of modeling discrete characters, the most commonly used models are the Mk models (Pagel, 1994), which can be fit to data with

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the function `fitDiscrete`. We have rewritten this function for `geiger v2.0`, again using an alternative, more efficient algorithm for calculating the likelihood of observing trait values under a model (FitzJohn *et al.*, 2009). In the new version of `fitDiscrete`, the computational time required for the likelihood calculation scales approximately linearly with the number of character states, whereas the previous version scaled superlinearly (see Appendix 2 in Supplementary Material for details). This improvement allows for more complex models to be efficiently fit to large phylogenies.

2.2 Bayesian methods for fitting models of character evolution

A major addition to `geiger` is the implementation of several Bayesian methods for fitting models of trait evolution to comparative data. These include the Accomodating Uncertainty in Trait Evolution Using R (AUTEUR) approach of Eastman *et al.* (2011), which uses reversible jump Markov chain Monte Carlo machinery (Green, 1995) to move across multirate models of various complexities. The implementation of this method in `geiger v2.0` improves on the original by allowing model partitions to be constrained *a priori* and alternate models to be compared (Eastman *et al.*, 2013b). Additionally, `geiger` now includes the following: a method for fitting models to phylogenies including unresolved clades using Approximate Bayesian Computation (Modeling Evolution of Continuous Characters using Approximate Bayesian Computation, MECCA; Slater *et al.*, 2012b); a method for including fossil information as priors on node states (Slater *et al.*, 2012a); and a posterior predictive simulation approach for assessing the adequacy of common models of trait evolution (Slater and Pennell, 2013). These types of approaches, which allow for greater complexity both in models and data, will be essential to make robust evolutionary inferences from large comparative datasets.

2.3 Inferring shifts in the rate of lineage diversification

Alfaro *et al.* (2009) developed an approach, Modeling Evolutionary Diversification Using Stepwise-AIC (MEDUSA), to detect shifts in diversification rates from molecular phylogenies using a stepwise-Akaike Information Criteria (AIC) algorithm. A single-rate birth–death model is fit to the entire tree, and then the tree is partitioned into two rate classes, breaking the tree at all possible nodes. The partition that improves the fit of the model is then fixed and the process is repeated, breaking the tree into three partitions and so on, until a stopping criterion is reached. MEDUSA can be applied to both fully bifurcating and unresolved trees.

For this release of `geiger`, the MEDUSA algorithm has been improved in a number of ways. First, it has been recoded so that it is now orders of magnitude faster and scales well to large trees; this version of MEDUSA has already been applied to a phylogeny of all 9,993 extant bird species (Jetz *et al.*, 2012). Second, we used simulations to develop a threshold-AIC value as a stopping criterion (see Appendix 3 in Supplementary Material for details) to correct for multiple comparisons—the larger the phylogeny, the greater the threshold for accepting a new partition to the model [a similar approach was developed by Thomas and Freckleton (2012) for studying variation in rates of phenotypic evolution]. Last, we have developed tools for summarizing MEDUSA analyses across a distribution of trees, such as from a Bayesian posterior or from non-parametric bootstrapping, so that uncertainty in both topology and branch lengths can be accomodated.

3 CONCLUSION

In this note we provide a broad overview of the methods now available in `geiger`. We have not discussed some methods implemented in `geiger` (e.g. 'Congruification' for time-scaling large trees; Eastman *et al.*, 2013a) and many of the nuances of the methods described here have been left out. We refer readers to associated publications and the package documentation for more information.

It is an exciting time for macroevolutionary research. We now have access to datasets of unparalleled size and a wide variety of new statistical approaches with which to analyze them. We hope that the software presented here will help researchers address some fundamental and long-standing questions in macroevolution.

ACKNOWLEDGEMENTS

The authors are grateful to the large community of researchers—both method developers and users—who have been so generous with their time and expertise. The authors specifically thank Brian O'Meara, Liam Revell, Dan Rabosky, Carl Boettiger, Jeremy Beaulieu, Dan Wegmann and Simon Uribe-Convers who gave numerous helpful insights in the development of this work. The auhtors thank David Posada, Daniele Silvestro and two anonymous reviewers for comments on this note.

Funding: M.W.P. was supported by a Bioinformatics and Computational Biology Graduate Fellowship from the University of Idaho and a National Science and Engineering Research Council PGS-D Fellowship. This work was also supported by the National Science Foundation (DEB 0919499, 1208912 and 0918748).

Conflict of Interest: none declared.

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