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Tree size and relative clade age influence estimation of speciation rate shifts

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The development of methods to estimate rates of speciation and extinction from time-calibrated phylogenies has revolutionized evolutionary biology by allowing researchers to correlate diversification rate shifts with causal ecological factors. We use rigorous simulations to evaluate the statistical performance of three widely used modelling approaches - BiSSE, BAMM and MEDUSA - in relation to detection of speciation rates shifts. We simulated sets of trees with each tree having a single increase in speciation rate. We varied the location of shifts, the degree of increase in speciation rate and the total age of the tree. We then used BiSSE, BAMM and MEDUSA to estimate rate shifts. For BiSSE, we assigned different character states for the lineages with different simulated speciation rates. We show that all methods are better at detecting rate shifts when the change in speciation rate is higher, but had high Type II errors (non-detection of rate shifts). While the algorithms more accurately identified rate shifts close to the root of the tree, both perform poorly when the rate shift occurred more recently. All methods performed better with increase in the overall number of tips and the number of tips in the clade with rate shift, both of which are correlated with tree age and speciation rate asymmetry. We discuss the implications of this study for the use and development of methods for hypothesis testing based on diversification rate shifts.

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Abstract

The development of methods to estimate rates of speciation and extinction from time-calibrated phylogenies has revolutionized evolutionary biology by allowing researchers to correlate diversification rate shifts with causal ecological factors. We use rigorous simulations to evaluate the statistical performance of three widely used modelling approaches - BiSSE, BAMM and MEDUSA - in relation to detection of speciation rates shifts. We simulated sets of trees with each tree having a single increase in speciation rate. We varied the location of shifts, the degree of increase in speciation rate and the total age of the tree. We then used BiSSE, BAMM and MEDUSA to estimate rate shifts. For BiSSE, we assigned different character states for the lineages with different simulated speciation rates. We show that all methods are better at detecting rate shifts when the change in speciation rate is higher, but had high Type II errors (non-detection of rate shifts). While the algorithms more accurately identified rate shifts close to the root of the tree, both perform poorly when the rate shift occurred more recently. All methods performed better with increase in the overall number of tips and the number of tips in the clade with rate shift, both of which are correlated with tree age and speciation rate asymmetry. We discuss the implications of this study for the use and development of methods for hypothesis testing based on diversification rate shifts.

Introduction

Much as the advent of phylogenetics (Hennig, 1965) led to a spectacular revolution in evolutionary biology, the arrival of mathematical methods to estimate divergence times from molecular phylogenies has offered unprecedented novel insights into macroevolutionary patterns and processes. More recently, a seminal innovation has been the development of tools to estimate rates of speciation and extinction from time-calibrated phylogenies (Nee, May & Harvey, 1994). Until such methods became available, our understanding of macroevolutionary patterns and processes of diversification (net result of speciation minus extinction) largely relied on the fossil record, which is incomplete for most taxa (Benton, Wills & Hitchin, 2000; Quental & Marshall, 2010) and virtually non-existent for many soft-bodied life forms (Donoghue & Purnell, 2009) However, the possibility of using phylogenies of extant taxa to shed light on macroevolutionary history is appealing, and there has been a phenomenal interest in applying such methods to understand fundamental questions such as how the mode and tempo of diversification have been influenced by trait evolution (especially ‘key innovations’, e.g. Hunter & Jernvall, 1995; Hodges & Arnold, 1995; Sahoo et al., 2017), biogeography (e.g. Kozak, Weisrock & Larson, 2006; Wahlberg et al., 2009; Dunn et al., 2009), climate change (e.g. Jansson & Davies, 2008; Dunn et al., 2009; Ezard et al., 2011), etc.

Analyses testing the effect of a trait or trait variant on diversification hitherto relied on comparisons of species richness of sister clades (e.g. Mitter, Farrell & Wiegmann, 1988; Zeh, Zeh & Smith, 1989). The method cannot distinguish between speciation and extinction, is prone to Type II error (non-detection of significant differences), and it is not straightforward to utilize information from clades with mixed character states (Maddison, Midford & Otto, 2007). The most recent analytical models estimate rates of speciation and extinction both across time and lineages, which form the basis for hypothesis testing. These estimates are based on information about clade age and species richness (e.g. Paradis, 2012), as well as from topology and branch lengths (Maddison, Midford & Otto, 2007; Alfaro et al., 2009; Rabosky, 2014). Thus, these models allow inferences of speciation and extinction rate differences associated with lineages, traits, time or diversity (Laurent, Robinson-Rechavi & Salamin, 2015). The BiSSE (Binary State Speciation and Extinction; Maddison, Midford & Otto, 2007) modelling approach has been especially popular for hypothesis testing because it estimates speciation and extinction rates associated with character states, i.e state-dependent diversification rates.

While BiSSE only models binary discrete character states (for example presence or absence of a trait; two states a trait), extensions of BiSSE can handle other types of data. For instance MuSSE (Multiple SSE; (FitzJohn, 2012) can deal with multiple discrete character states, while QuaSSE (Quantitative SSE; FitzJohn, 2010) allows testing the effect of quantitative traits. GeoSSE (Geographic SSE; Goldberg, Lancaster & Ree, 2011) tests region-dependent diversification, while BiSSE-ness (BiSSE-node enhanced state shift; Magnuson-Ford & Otto, 2012) and Cladogenetic SSE (ClaSSE; Goldberg & Igić, 2012) integrate cladogenetic and anagenetic trait evolution. BiSSE and its derivatives have been employed for hypothesis testing in a wide range of taxa and evolutionary scenarios. All above models are typically used by researchers to test how a change in character state has led to a shift in the rates of extinction or speciation. Beaulieu & O'Meara (2016) proposed the HiSSE (Hidden States SSE) model, which attempts to identify unmeasured ('hidden') factors impacting diversification rates of a known trait or character state.

In contrast to the BiSSE family of models, character-independent diversification models attempt to identify the number and location of rate shifts in speciation and extinction across the tree, without *a priori* information on character states. Once the locations of rate shifts are found, the researcher can test for associations with traits of interest. BAMM (Bayesian Analysis of Macroevolutionary Mixtures; Rabosky, 2014) is the most widely used of these models.

MEDUSA (Modeling Evolutionary Diversification Using Stepwise Akaike Information Criterion; Alfaro et al., 2009), is another popular modelling framework to estimate rate shifts. The MEDUSA algorithm incrementally assigns rate shifts to all possible branches of the tree, and uses stepwise AIC (Akaike Information Criterion) to determine the number and location(s) of rate shifts that best fit the data. As in the case of BAMM, rate shifts estimations are agnostic of character states of lineages.

Although BiSSE, BAMM and MEDUSA have been immensely popular, researchers have only recently begun critically evaluating their performance within a statistical framework. For instance, May & Moore (2016) used extensive simulations to understand the statistical behaviour of MEDUSA, and showed that the algorithm is prone to a very high rate of false inferences of rate shifts (ca. 30% on average), and that the estimated diversification parameters were biased. The probability of rate shift detection in MEDUSA depends on the number of terminals in the tree (Laurent, Robinson-Rechavi & Salamin, 2015). BiSSE has been shown to be severely affected by tree size (number of terminals) (Davis, Midford & Maddison, 2013; Gamisch, 2016) and tip-ratio bias (i.e. ratio of terminals with one character state versus another). Moore and colleagues (Moore et al., 2016) showed that the accuracy of BAMM is strongly affected by the priors specified, and that the of estimates of diversification rate parameters are unreliable. Using empirical datasets, Rabosky & Goldberg (2015) found that the BiSSE is prone to high Type I error rates, wherein diversification-neutral traits are often found to be significantly associated with speciation rate. Surprisingly, such false associations appear to also be detected for traits with weak phylogenetic signal (Rabosky & Goldberg, 2015). Unsurprisingly, estimation of extinction rates from extant taxa appears to be particularly error prone - many authors have argued that the current analytical methods are not reliable for this purpose (Rabosky, 2010; Laurent, Robinson-Rechavi & Salamin, 2015; May & Moore, 2016, but see Stadler, 2013; Beaulieu & O'Meara, 2016).

In this study, we use rigorous simulations to evaluate the statistical performance of BiSSE, BAMM & MEDUSA in relation to detection of speciation rates shifts. We varied the location of shifts, the degree of increase in speciation rate and overall tree age. We show that all methods perform poorly under some conditions, and we provide recommendations to users and developers of such methods.

Materials and Methods

(1) Simulation of phylogenetic tree with single diversification rate shift

(1a) General procedure

The basic workflow of the simulation process is outlined in **Figure 1**. To obtain a phylogeny with a single shift in speciation rate, we first simulated two trees - a *basetree* and a *subtree* wherein the *subtree* had a greater speciation rate (λ_1) compared to that of the *basetree* (λ_0) - and then replaced a *basetree* clade with the *subtree*. A subtree of a given age (S_{age}) was grafted onto the *basetree* following pruning of a randomly chosen *basetree* clade with approximately the same age (S_{age} ±0.65) (**Figure 1**), using a custom written function (**available on Figshare**). Details of the *subtree* and *basetree* simulations are described in the next section. The relative age of the *subtree* in relation to the overall tree was varied by varying the age of the *subtree*. This procedure was followed to generate a large number of composite trees (20000) with different relative *subtree* ages, overall tree (*basetree*) ages and relative speciation rate (*speciation rate asymmetry*) (**Table 1**).

(1b) Tree simulation

We used the forward algorithm in R (R Development Core Team, 2016) package *TESS* (Höhna, May & Moore, 2015) to simulate trees. The package implements tree simulation based on a global, time-dependent birth-death process conditioned either on number tips or age of the tree (Höhna, May & Moore, 2015). Since simulation of branching process conditioned on number of tips can lead to bias in the diversification rate (Hartmann, Wong, and Stadler 2010), we simulated phylogenies by conditioning on age using the function *tess.sim.age*, which simulates trees given the age (*basetree* age B_{age} & S_{age}) and diversification rate parameters (speciation rate-λ and extinction rate-μ). As this method produces trees with varying tip numbers, we simulated 1000 trees each time and used the function *tess.nTaxa.expected* from the same package to select the best tree out of the 1000 trees. This was done by comparing the expected number of tips for every 1 unit time with the simulated tree using a correlation test. The tree with the maximum correlation coefficient was chosen as the best tree. We also corroborated the results using a backward simulation procedure using the *Treesim* package (Stadler, 2011) **(Supplemental Figure S1**).

(1c) Systematic simulation of composite trees with diversification rates shifts of varying subtree age

We first adopted values of B_{age} of 25 units and λ_0 (speciation rate of *basetree*) of 0.27, and varied speciation rate asymmetry (λ_1/λ_0) by altering *subtree* speciation rate (λ_1), while keeping extinction rates constant across both). Thus, there was no rate shift when the speciation rate asymmetry was 1, and higher values indicate a greater degree of speciation rate increase in the *subtree*. We simulated 100 composite trees each for λ_1/λ_0 ratios from 1.1 to 2 with an interval of 0.1. This was repeated for a S_{age} ranging from 20 - 60% of *basetree* age (Table 1). Simulated trees were subsequently used for the diversification analysis.

To check the robustness of the inferences with respect to B_{age} and λ_0 we also conducted the simulations as outlined above for (B_{age}=25, λ_0=0.22;;B_{age}=15; λ_0=0.27) with λ_1/λ_0 ratios ranging from 1.1 to 2.5.

(2) Estimation of diversification rate parameters and power of modelling approaches

We used BiSSE, BAMM and MEDUSA to estimate diversification rate parameters (λ_0, μ_0, λ_1 and μ_1) of the simulated composite trees and detect rate shifts. The probability of detection of a rate shift, i.e. power, for a given combination of Bage, S_{age}, λ_1 and λ_0 was calculated as the proportion of trees in which a significant rate shift was detected.

(2a) BiSSE

We assigned a character to be present only in the *subtree*. This was automated in the algorithm based on the different tip labels assigned to the *subtree* after the tree simulation process. Therefore, diversification rate estimates of the BiSSE model will reflect the actual speciation and extinction rate estimates of the *subtree* (i.e. λ_1 and μ_1*)* and *basetree (*λ_0 and μ_0*)*. We then compared the unrestricted full model ($\lambda_1 \neq \lambda_0$; $\mu_0 \neq \mu_1$; q01≠q10) to a model with restricted speciation rates ($\lambda_1 = \lambda_0$) using likelihood ratio tests (LRT). If LRT $P<0.05$, the rate shift was considered to have been detected, while the rate shift was not considered detected if $P \geq 0.05$.

(2b) BAMM

We performed BAMM analyses with the default parameter settings using the control file available from the BAMM website (http://bamm-project.org/quickstart.html#control-file accessed: May 2016). We ran the MCMC analysis for 2 million iterations and checked for convergence using ESS metrics (>200) for a sample trees for each subtree age category. The *bammdata* object was generated using the *getEventData* function from the *BAMMtools* package after discarding the first 10% of samples as burnin. The *bammdata* object was then used to calculate the diversification rates.

We estimated speciation and extinction rates for the *subtree* (λ_1 and μ_1) as an average rate of the clade using the function *getCladeRates* in the *BAMMtools* package (Rabosky et al., 2014). We estimated λ_0 and μ_0 using the same function by specifying the common ancestor node of composite tree, but excluding the rates of the *subtree*. If BAMM reported >0 rate shifts, a significant rate shift in the *subtree* was considered to have been detected..

(2c) MEDUSA

We performed MEDUSA analyses using the function *medusa* available from the *geiger* package (Harmon et al., 2007) in R. We specified the model of tree evolution to be a *Yule* process as the model did not converge for *mixed* or *pure birth-death* process. Hence, the diversification rate parameters λ_0, λ_1, μ_0, μ_1 were not estimated by MEDUSA. A significant rate shift in the *subtree* was considered to have been detected if MEDUSA identified at least one rate shift.

Results

Rate shifts in a large proportion of simulated trees were not detected under certain conditions. The power (measured as the proportion of trees in which a significant shift was correctly detected) of all three methods was affected by speciation rate asymmetry (ratio of speciation rate of the *basetree* to that of the *subtree*) (**Figure 2**), relative subtree age (ratio of *subtree* age to *basetree* age) (**Figure 2**), overall age of the tree (**Figure 2**) and tip number (**Figures 3 & 4**).

Effect of speciation rate asymmetry

Power increased with increasing asymmetry. For BiSSE, the critical speciation rate ratio at which power reached 95% varied from 1.5 (λ_0 0.27, *basetree* age 25 and relative subtree age 60%; **Figure 2B**) to >2.5 (e.g. λ_0 0.27, *basetree* age 15 and relative *subtree* age 20%; **Figure 2C**). The corresponding range for BAMM was 1.6 (λ_0 0.27, *basetree* age 25 and relative *subtree* age 60%; **Figure 2E**) to >2.5 (e.g λ_0 0.22, *basetree* age 25 and relative *subtree* age 20%; **Figure 2D**), and that for MEDUSA was 1.4 (λ_0 0.27, *basetree* age 25 and relative *subtree* age 20%; Figure 2H) to 2.5 (λ_0 0.27, *basetree* age 15 and relative *subtree* age 20%; **Figure 2I**).

Effect of relative subtree age

For all combinations of relative speciation rate and root (=*basetree*) age, power increased as the *subtree* age increased, i.e. when the rate shift occurred earlier in time (**Figure 2**). For e.g., power was always greater for 60% relative *subtree* age (pink curve in **Figure 2**) compared to 50% (blue curve).

Effect of overall tree age

All three methods had greater power when the root age was 25 units compared to when it was 15 units (**Figure 2**, comparison of columns 1 & 2).

Effect of number of tips

In the analyses with the pooled dataset of all trees for a given method, power was positively correlated with the number of *subtree* tips as well as overall tree tips (**Figures 3 & 4**).

Estimates of diversification rates

Figure 5 depicts the diversification rate estimate error as ratios of estimated and actual diversification rates (speciation minus extinction) for BiSSE and BAMM for the different simulated scenarios. A ratio of 1 indicates no error, while greater deviance from 1 indicates greater error. For both BiSSE and BAMM, error tended to decrease with increasing relative *subtree* age, as well as with speciation rate asymmetry. BAMM had a stronger tendency to underestimate diversification rates compared to BiSSE. **Supplemental Figures S2-5** depict simulated diversification values (dotted red lines) against values estimated by the analyses.

Discussion

Previous studies have identified shortcomings specific to particular modelling approaches for estimation of rate shifts in phylogenies (Rabosky, 2010; Davis, Midford & Maddison, 2013; Laurent, Robinson-Rechavi & Salamin, 2015; Rabosky & Goldberg, 2015; Gamisch, 2016; Moore et al., 2016; May & Moore, 2016). We simulated large sets of trees varying in specific attributes, and analyzed these trees using three widely used modelling approaches. We are therefore able to assess the relative performance of the three methods, and identify problems that are common to these methods. Specifically, we simulated an evolutionary scenario where speciation and extinction rates remained constant throughout the tree (*basetree*), apart from an increase in speciation rate at a single node (*subtree*). We find that the power of the analytical method to detect the rate shifts was strongly influenced by rate asymmetry, relative *subtree* age and root age, all three of which are related to the number of tips (clade size). All three methods performed poorly in terms of estimation of speciation (**Supplemental Figure S2,S3**) and extinction rates (**Supplemental Figure S4,S5**) but there was a tendency for reduced error with increasing *subtree* size and speciation rate asymmetry (**Figure 5**).

Effect of speciation rate asymmetry:

Not surprisingly, power increased as the speciation rate asymmetry increased. All methods performed poorly when the *subtree* speciation rate increased by 50% or lesser relative to the *basetree*. However, even when the asymmetry was as high as 2.5, a significant proportion of rate shifts were undetected by all methods (Type II error, red curves in **Figure 1**). Interestingly, no method exhibited Type I error, i.e identification of non-existent rate shifts (rate asymmetry of 1) as significant rate shifts. This is in contrast to other studies (e.g. Rabosky & Goldberg, 2015) which reported high Type I error rates. The lack of Type I error in our study may be because we incorporated a simplistic evolutionary scenario with a single rate shift.

Effect of relative subtree age:

Rate shifts occurring in younger clades were difficult to detect. For instance, when the subtree age was 20% of the base tree age (red curves in **Figure 2**), MEDUSA and BAMM rarely detected the rate shifts, even when the rate asymmetry was 2. BiSSE performed marginally better, with power tending to reach 100% above a rate asymmetry of 2 (**Figure 2B**) or 2.5 (**Figures 2A,C**). Relative *subtree* age directly affects both the number of subtree tips and overall number of tree tips. We later discuss the possible effects of tip number in more detail.

Effect of overall tree age:

Across all methods, power increased as root age increased from 15 to 25 (Comparison of columns 2 & 3 in **Figure 2**). Given other parameters being the same, older trees will have a greater overall number of tips compared to younger trees. Furthermore, relative *subtree* age and rate asymmetry are both correlated with *subtree* tip number, which is in turn correlated with overall tip number.

Effect of number of tips:

Taking together results from all simulated datasets, power is positively correlated with the number of *subtree* tips (**Figure 3**) as well as with overall tree tips (**Figure 4**). Davis and colleagues (Davis, Midford & Maddison, 2013) and Gamisch (2016) showed that BiSSE analyses on trees with very few taxa (overall tree size) are prone to high Type II error. They simulated complex evolutionary scenarios with multiple increases and decreases in diversification parameters at random points across the tree, and only assessed the effect of overall tree size. Laurent and colleagues (Laurent, Robinson-Rechavi & Salamin, 2015) showed that MEDUSA also performs better when the number of tree tips increases. They inferred that there was no effect of overall tree size because diversification shifts in lineages of the same size were as likely to be detected in small or larger trees (their Figure 3b). Thus, *subtree* size could be more important than overall tree size. However, in our simulations variation in overall tree size is because of variation in *subtree* tree size. The three parameters - relative *subtree* age, overall tree size and *subtree* size - are all correlated with each other, and therefore their individual effects cannot be easily disentangled. It is possible that the effects of tree size reported in the above studies are related to differences in other parameters that were not explicitly varied in simulations.

Our analyses show that the performance of BAMM is very similar to that of BiSSE and MEDUSA. Intriguingly, there was a strong correlation between BAMM estimated *subtree* and *basetree* speciation rates when the speciation rate asymmetry and relative subtree ages were low (**Supplemental Figure S3**), a pattern that was not found in the case of BiSSE. We are unable to explain this correlation, but note that this correlation disappeared as power increased, suggesting that the correlation is an artefact. All methods performed well when there is strong rate asymmetry and when the phylogeny being analyzed is large. However, the effects of tip number (both *subtree* and overall tree), and associated parameters such as relative *subtree* age, may be the most serious and universal issues for modelling approaches, and development of future methods should focus attention on rectifying these. In practice, a user intending to analyze diversification rate shifts only has information about overall tree size, and not the *subtree* size or relative *subtree* age. We provide the following recommendations when analyzing diversification rate shifts.

Recommendations:

We extend the recommendations of Davis and colleagues (Davis, Midford & Maddison) to BAMM and MEDUSA. Users should be extremely cautious when using BiSSE, BAMM or MEDUSA on small phylogenies and should avoid using small, incomplete phylogenies to test hypotheses of rate shifts. When testing hypotheses of change in speciation rates, we recommend that users explore results from multiple datasets, such that the relative age of the clade of interest with respect to the entire tree varies. In analyses of trait-dependent diversification rates, we also encourage readers to report results from traditional sister-group species richness comparisons such as the richness Yule test (Paradis, 2012), and recently developed non-parametric tests such as FiSSE (Rabosky & Goldberg, 2017).

Single versus multiple trait transitions

Trait-dependent methods such as BiSSE may perhaps perform better with multiple trait transitions over the tree. Further simulation is needed to ascertain how the number of transitions affects the power of trait-dependent methods. However, no method tested here is designed to be employed exclusively when there are multiple rate shifts. Therefore, inferences drawn here should be widely applicable.

Conclusions

Assessment of diversification parameters and rates shifts is rapidly becoming a standard procedure in studies involving molecular phylogenies. There is a strong demand for analytical tools that detect rate shifts with low Type I and II errors. Although many studies have reported glaring flaws with state-of-the-art modelling approaches, the number of studies employing them continues to increase. More studies are needed to understand the statistical performance of these methods, under what scenarios the results are reliable and when they should be interpreted with caution. Empirical datasets offer limited capabilities to rigorously test the statistical performance of such analytical tools. Simulation studies provide an alternative where individual parameters can be manipulated to illuminate the scenarios or parameter combinations that constitute serious challenges, and to aid development of methods to alleviate these problems. Estimation of extinction rates appears to be particularly prone to error. Although simple simulations such as ours are important steps, future simulation work should concentrate on mimicking more complex evolutionary scenarios, for e.g. with combinations of extinctions and speciation rates shifts.

Data availability

Data files and codes supporting the article can be accessed from Figshare via https://figshare.com/s/cb85b1db6a64328b36f9

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References

Alfaro ME., Santini F., Brock C., Alamillo H., Dornburg A., Rabosky DL., Carnevale G., Harmon LJ. 2009. Nine exceptional radiations plus high turnover explain species diversity in jawed vertebrates. *Proceedings of the National Academy of Sciences* 106:13410–13414.

Beaulieu JM., O'Meara BC. 2016. Detecting hidden diversification shifts in models of trait-dependent speciation and extinction. *Systematic biology* 65:583–601.

Benton MJ., Wills MA., Hitchin R. 2000. Quality of the fossil record through time. *Nature* 403:534–537. DOI: 10.1038/35000558.

Davis MP., Midford PE., Maddison W. 2013. Exploring power and parameter estimation of the BiSSE method for analyzing species diversification. *BMC Evolutionary Biology* 13:38.

Donoghue PCJ., Purnell MA. 2009. Distinguishing heat from light in debate over controversial fossils. *BioEssays: News and Reviews in Molecular, Cellular and Developmental Biology* 31:178–189. DOI: 10.1002/bies.200800128.

Dunn RR., Agosti D., Andersen AN., Arnan X., Bruhl CA., Cerdá X., Ellison AM., Fisher BL., Fitzpatrick MC., Gibb H., Gotelli NJ., Gove AD., Guenard B., Janda M., Kaspari M., Laurent EJ., Lessard J-P., Longino JT., Majer JD., Menke SB., McGlynn TP., Parr CL., Philpott SM., Pfeiffer M., Retana J., Suarez AV., Vasconcelos HL., Weiser MD., Sanders NJ. 2009. Climatic drivers of hemispheric asymmetry in global patterns of ant species richness. *Ecology Letters* 12:324–333. DOI: 10.1111/j.1461-0248.2009.01291.x.

Ezard TH., Aze T., Pearson PN., Purvis A. 2011. Interplay between changing climate and species' ecology drives macroevolutionary dynamics. *Science* 332:349–351.

FitzJohn RG. 2010. Quantitative Traits and Diversification. *Systematic Biology* 59:619–633. DOI: 10.1093/sysbio/syq053.

FitzJohn RG. 2012. Diversitree: comparative phylogenetic analyses of diversification in R. *Methods in Ecology and Evolution* 3:1084–1092.

Gamisch A. 2016. Notes on the statistical power of the binary state speciation and extinction (BiSSE) model. *Evolutionary bioinformatics online* 12:165.

Goldberg EE., Igić B. 2012. Tempo and mode in plant breeding system evolution. *Evolution* 66:3701–3709.

Goldberg EE., Lancaster LT., Ree RH. 2011. Phylogenetic inference of reciprocal effects between geographic range evolution and diversification. *Systematic Biology* 60:451–465.

Harmon LJ., Weir JT., Brock CD., Glor RE., Challenger W. 2007. GEIGER: investigating evolutionary radiations. *Bioinformatics* 24:129–131.

Hennig W. 1965. Phylogenetic systematics. *Annual Review of Entomology* 10:97–116.

Hodges SA., Arnold ML. 1995. Spurring plant diversification: are floral nectar spurs a key innovation? *Proc. R. Soc. Lond. B* 262:343–348. DOI: 10.1098/rspb.1995.0215.

Höhna S., May MR., Moore BR. 2015. TESS: an R package for efficiently simulating phylogenetic trees and performing Bayesian inference of lineage diversification rates. *Bioinformatics* 32:789–791.

Hunter JP., Jernvall J. 1995. The hypocone as a key innovation in mammalian evolution. *Proceedings of the National Academy of Sciences of the United States of America* 92:10718–10722.

Jansson R., Davies TJ. 2008. Global variation in diversification rates of flowering plants: energy vs. climate change. *Ecology Letters* 11:173–183. DOI: 10.1111/j.1461-0248.2007.01138.x.

Kozak KH., Weisrock DW., Larson A. 2006. Rapid lineage accumulation in a non-adaptive radiation: phylogenetic analysis of diversification rates in eastern North American woodland salamanders (Plethodontidae: Plethodon). *Proceedings of the Royal Society of London B: Biological Sciences* 273:539–546. DOI: 10.1098/rspb.2005.3326.

Laurent S., Robinson-Rechavi M., Salamin N. 2015. Detecting patterns of species diversification in the presence of both rate shifts and mass extinctions. *BMC evolutionary biology* 15:157.

Maddison WP., Midford PE., Otto SP. 2007. Estimating a binary character's effect on speciation and extinction. *Systematic biology* 56:701–710.

Magnuson-Ford K., Otto SP. 2012. Linking the investigations of character evolution and species diversification. *The American Naturalist* 180:225–245. DOI: 10.1086/666649.

May MR., Moore BR. 2016. How Well Can We Detect Lineage-Specific Diversification-Rate Shifts? A Simulation Study of Sequential AIC Methods. *Systematic Biology*:syw026. DOI: 10.1093/sysbio/syw026.

Mitter C., Farrell B., Wiegmann B. 1988. The phylogenetic study of adaptive zones: has phytophagy promoted insect diversification? *The American Naturalist* 132:107–128.

Moore BR., Höhna S., May MR., Rannala B., Huelsenbeck JP. 2016. Critically evaluating the theory and performance of Bayesian analysis of macroevolutionary mixtures. *Proceedings of the National Academy of Sciences* 113:9569–9574.

Nee S., May RM., Harvey PH. 1994. The reconstructed evolutionary process. *Phil. Trans. R. Soc. Lond. B* 344:305–311. DOI: 10.1098/rstb.1994.0068.

Paradis E. 2012. Shift in Diversification in Sister-Clade Comparisons: A More Powerful Test. *Evolution* 66:288–295. DOI: 10.1111/j.1558-5646.2011.01429.x.

Quental TB., Marshall CR. 2010. Diversity dynamics: molecular phylogenies need the fossil record. *Trends in Ecology & Evolution* 25:434–441. DOI: 10.1016/j.tree.2010.05.002.

Rabosky DL. 2010. Extinction rates should not be estimated from molecular phylogenies. *Evolution* 64:1816–1824.

Rabosky DL. 2014. Automatic detection of key innovations, rate shifts, and diversity-dependence on phylogenetic trees. *PloS one* 9:e89543.

Rabosky DL., Goldberg EE. 2015. Model inadequacy and mistaken inferences of trait-dependent speciation. *Systematic Biology* 64:340–355.

Rabosky DL., Goldberg EE. 2017. FiSSE: A simple nonparametric test for the effects of a binary character on lineage diversification rates. *Evolution* 71:1432–1442.

Rabosky DL., Grundler M., Anderson C., Shi JJ., Brown JW., Huang H., Larson JG. 2014. BAMMtools: an R package for the analysis of evolutionary dynamics on phylogenetic trees. *Methods in Ecology and Evolution* 5:701–707.

R_Development_Core_Team. 2016. *R: A Language and Environment for Statistical Computing*. Austria.

Sahoo RK., Warren AD., Collins SC., Kodandaramaiah U. 2017. Hostplant change and paleoclimatic events explain diversification shifts in skipper butterflies (Family: Hesperiidae). *BMC Evolutionary Biology* 17:174. DOI: 10.1186/s12862-017-1016-x.

Stadler T. 2011. Simulating trees with a fixed number of extant species. *Systematic Biology* 60:676–684.

Stadler T. 2013. How can we improve accuracy of macroevolutionary rate estimates? *Systematic biology* 62:321–329.

Wahlberg N., Leneveu J., Kodandaramaiah U., Peña C., Nylin S., Freitas AVL., Brower AVZ. 2009. Nymphalid butterflies diversify following near demise at the Cretaceous/Tertiary boundary. *Proceedings of the Royal Society B: Biological Sciences* 276:4295–4302.

Zeh DW., Zeh JA., Smith RL. 1989. Ovipositors, amnions and eggshell architecture in the diversification of terrestrial arthropods. *The Quarterly Review of Biology* 64:147–168.

Figure 1

Flowchart of simulation process

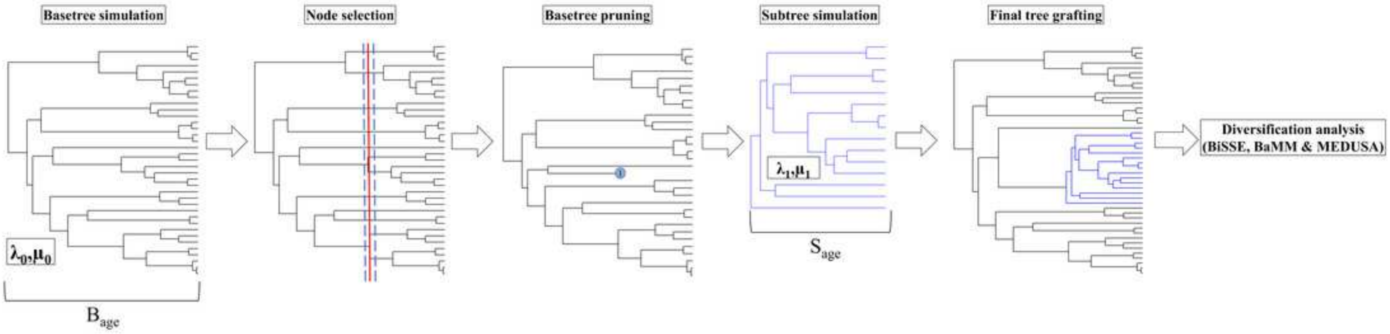

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Table 1(on next page)

Values of variables used in the simulation

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Variables	**Variable names**	**Values**
Basetree age	B_{age}	25 or 15
Subtree age	S_{age}	20,30,40,50,60 % of *basetree* age
Basetree speciation rate	λ_0	0.27 or 0.22
Subtree speciation rate	λ_1	0.27, 0.29,0.32, 0.35,0.37,0.40,0.43, 0.45, 0.48,0.51,0.54,0.56,0.59,0.62
Speciation rate asymmetry	λ_1 / λ_0	1-2.5
Basetree extinction rate	μ_0	0.05
Subtree extinction rate	μ_1	0.05

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Figure 2

Power of BiSSE, BAMM and MEDUSA in detecting simulated rate shifts

Power, measured as the proportion of shifts detected, for BiSSE (A, B & C), BAMM (D, E & F) and MEDUSA (G, H and I). X axes values are the simulated speciation rate asymmetry values. The first column (A, D and G) represents simulated scenarios of λ_0 0.22 and *basetree* age 25 units, the second column (B, E and H) represents λ_0 0.27 and *basetree* age 25 units, while the third column (C, F and I) represents λ_0 0.27 and *basetree* age 15 units.

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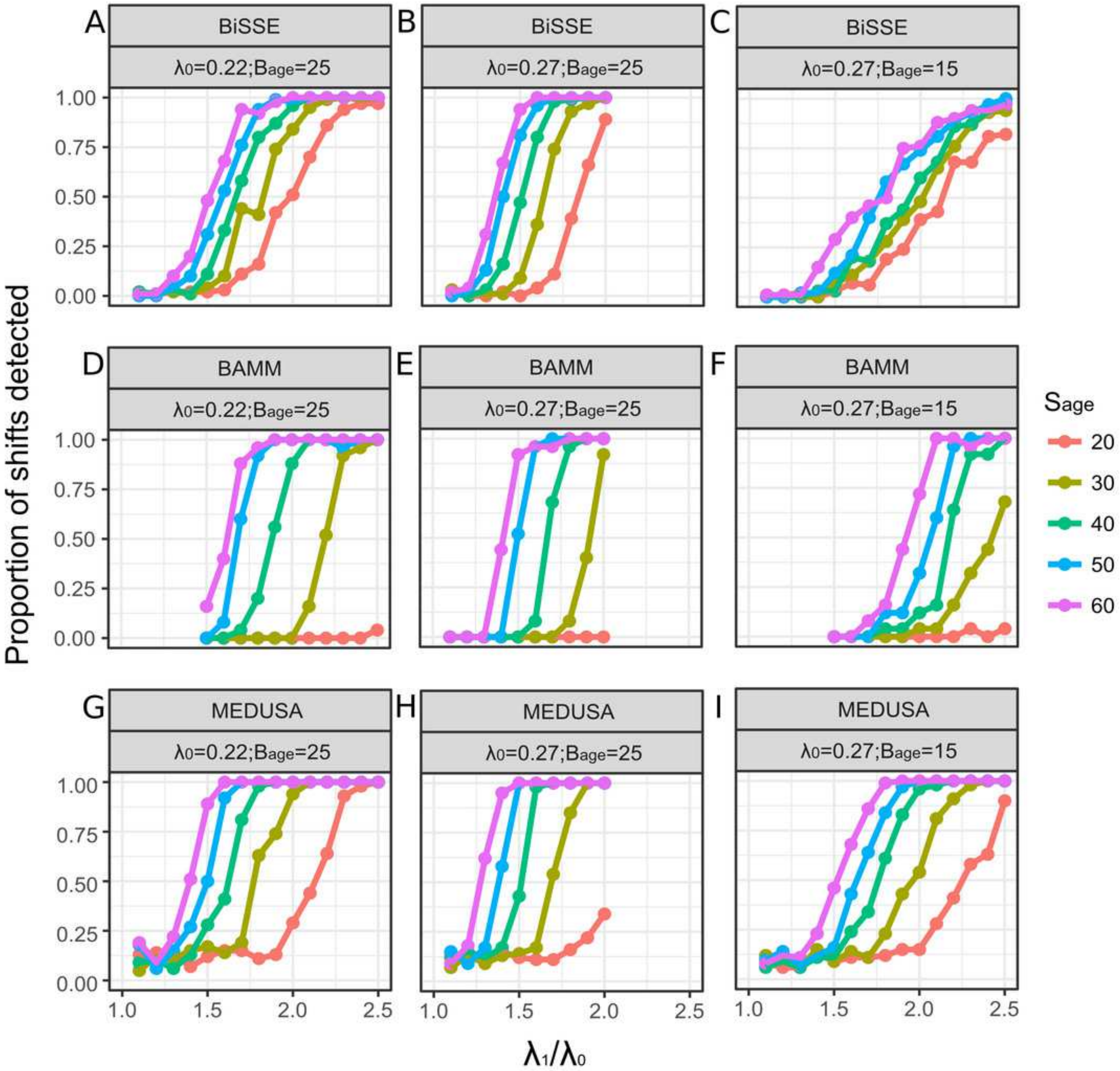
A
BiSSE
λ0=0.22;Bage=25
B
BiSSE
λ0=0.27;Bage=25
C
BiSSE
λ0=0.27;Bage=15
D
BAMM
λ0=0.22;Bage=25
E
BAMM
λ0=0.27;Bage=25
F
BAMM
λ0=0.27;Bage=15
G
MEDUSA
λ0=0.22;Bage=25
H
MEDUSA
λ0=0.27;Bage=25
I
MEDUSA
λ0=0.27;Bage=15
Proportion of shifts detected
0.00
0.25
0.50
0.75
1.00
1.0
1.5
2.0
2.5
λ1/λ0
Sage
20
30
40
50
60

Figure 3

Relationship between power and *subtree* size

Relationship between power, measured as the proportion of shifts detected, and *subtree* size for BiSSE (A, B & C), BAMM (D, E & F) and MEDUSA (G, H and I) analyses. Each plot represents values for a given combination of *basetree* and λ_0 conditions, and calculated by summing up the results of all analyses for this combination (i.e. all *subtree* ages and λ_1/λ_0 ratios). The first column (A, D and G) represents simulated scenarios of λ_0 0.22 and *basetree* age 25 units, the second column (B, E and H) represents λ_0 0.27 and *basetree* age 25 units, while the third column (C, F and I) represents λ_0 0.27 and *basetree* age 15 units.

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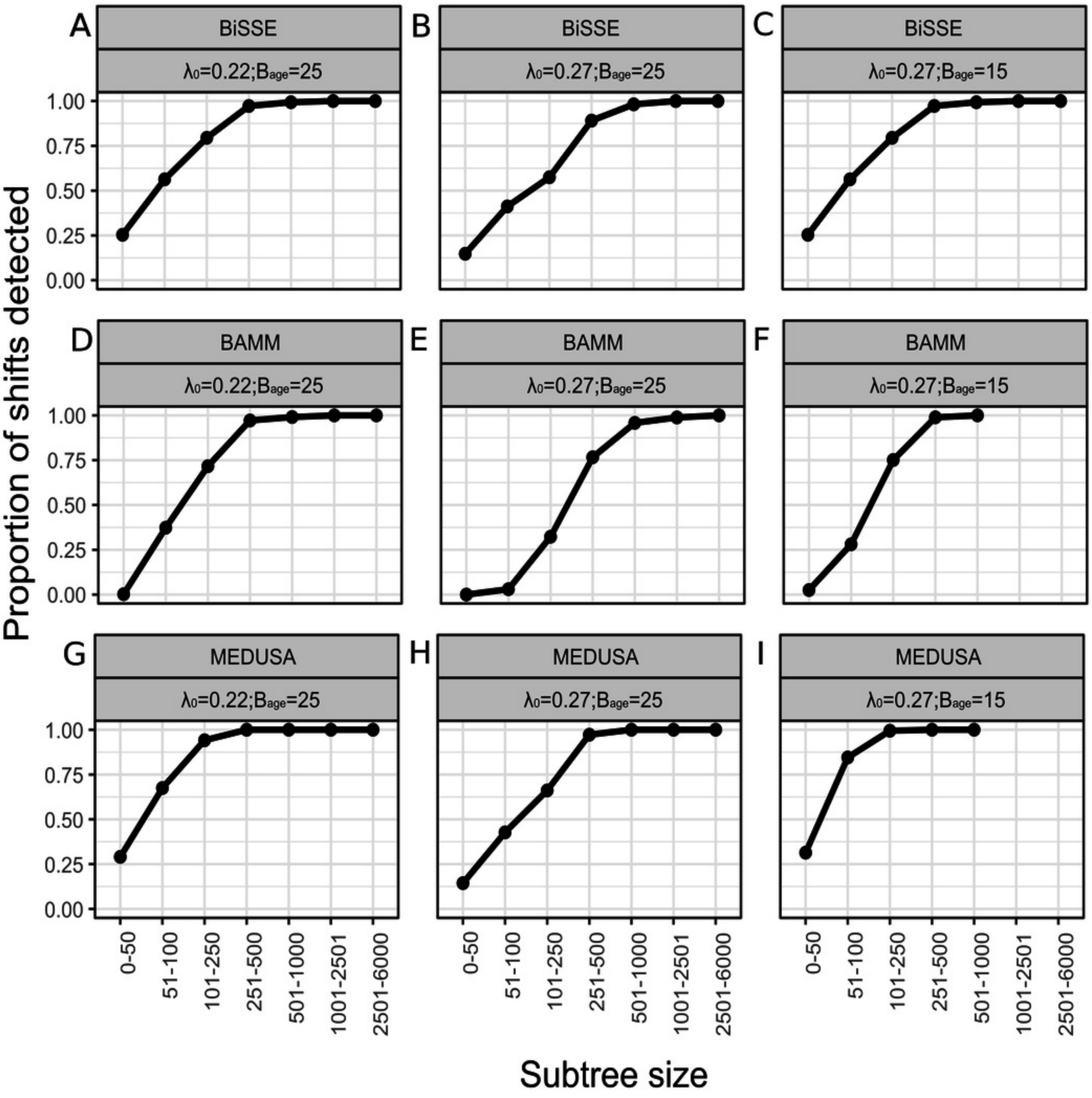
A
BiSSE
λ_0=0.22;B_{age}=25
B
BiSSE
λ_0=0.27;B_{age}=25
C
BiSSE
λ_0=0.27;B_{age}=15
D
BAMM
λ_0=0.22;B_{age}=25
E
BAMM
λ_0=0.27;B_{age}=25
F
BAMM
λ_0=0.27;B_{age}=15
G
MEDUSA
λ_0=0.22;B_{age}=25
H
MEDUSA
λ_0=0.27;B_{age}=25
I
MEDUSA
λ_0=0.27;B_{age}=15
Proportion of shifts detected
1.00
0.75
0.50
0.25
0.00
0-50
51-100
101-250
251-500
501-1000
1001-2501
2501-6000
Subtree size

Figure 4

Relationship between power and overall tree size

Relationship between power, measured as the proportion of shifts detected, and overall tree size for BiSSE (A, B & C), BAMM (D, E & F) and MEDUSA (G, H and I) analyses. Each plot represents values for a given combination of *basetree* and λ_0 conditions, and calculated by summing up the results of all analyses for this combination (i.e. all *subtree* ages and λ_1/λ_0 ratios). The first column (A, D and G) represents simulated scenarios of λ_0 0.22 and *basetree* age 25 units, the second column (B, E and H) represents λ_0 0.27 and *basetree* age 25 units, while the third column (C, F and I) represents λ_0 0.27 and *basetree* age 15 units.

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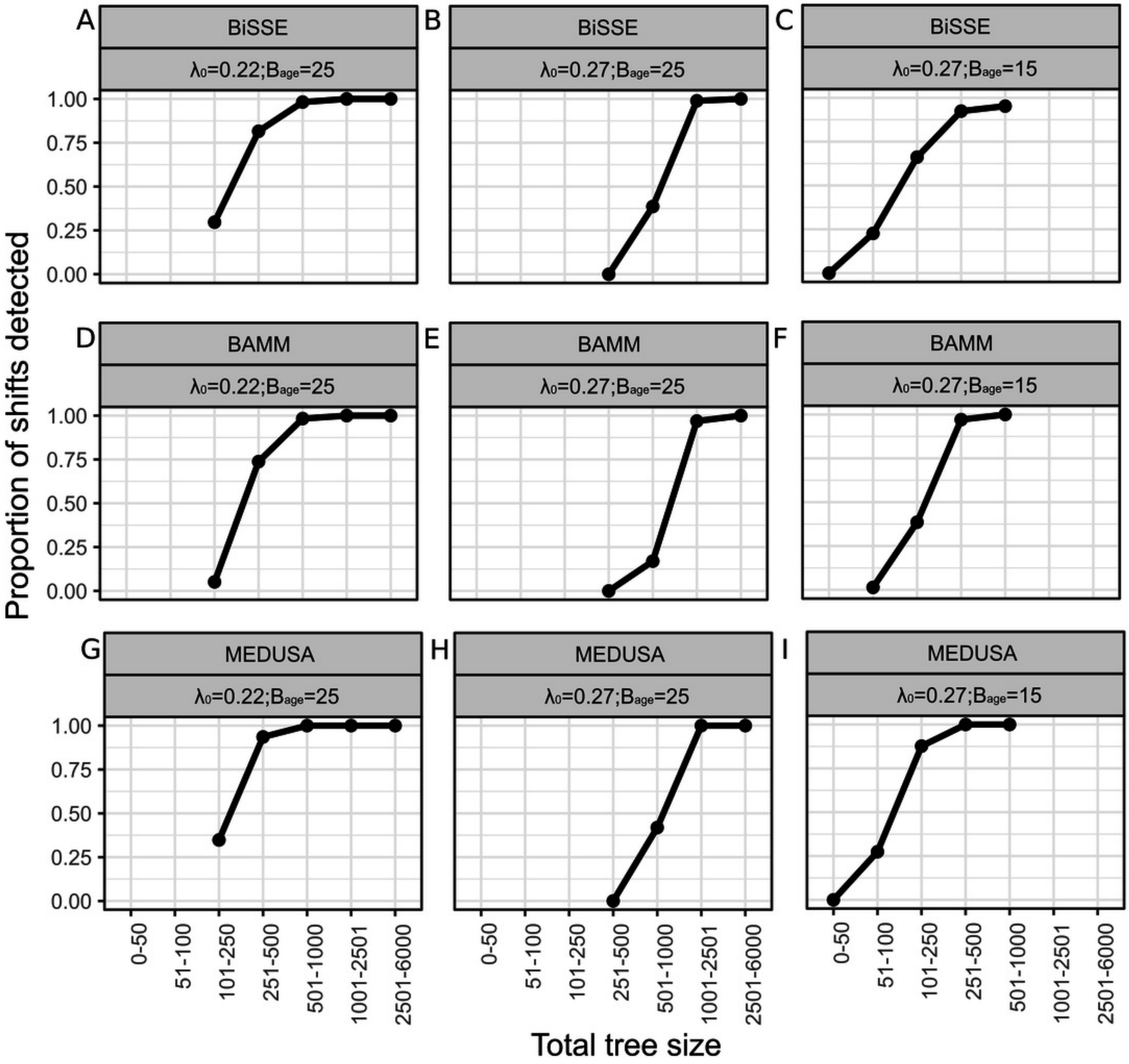
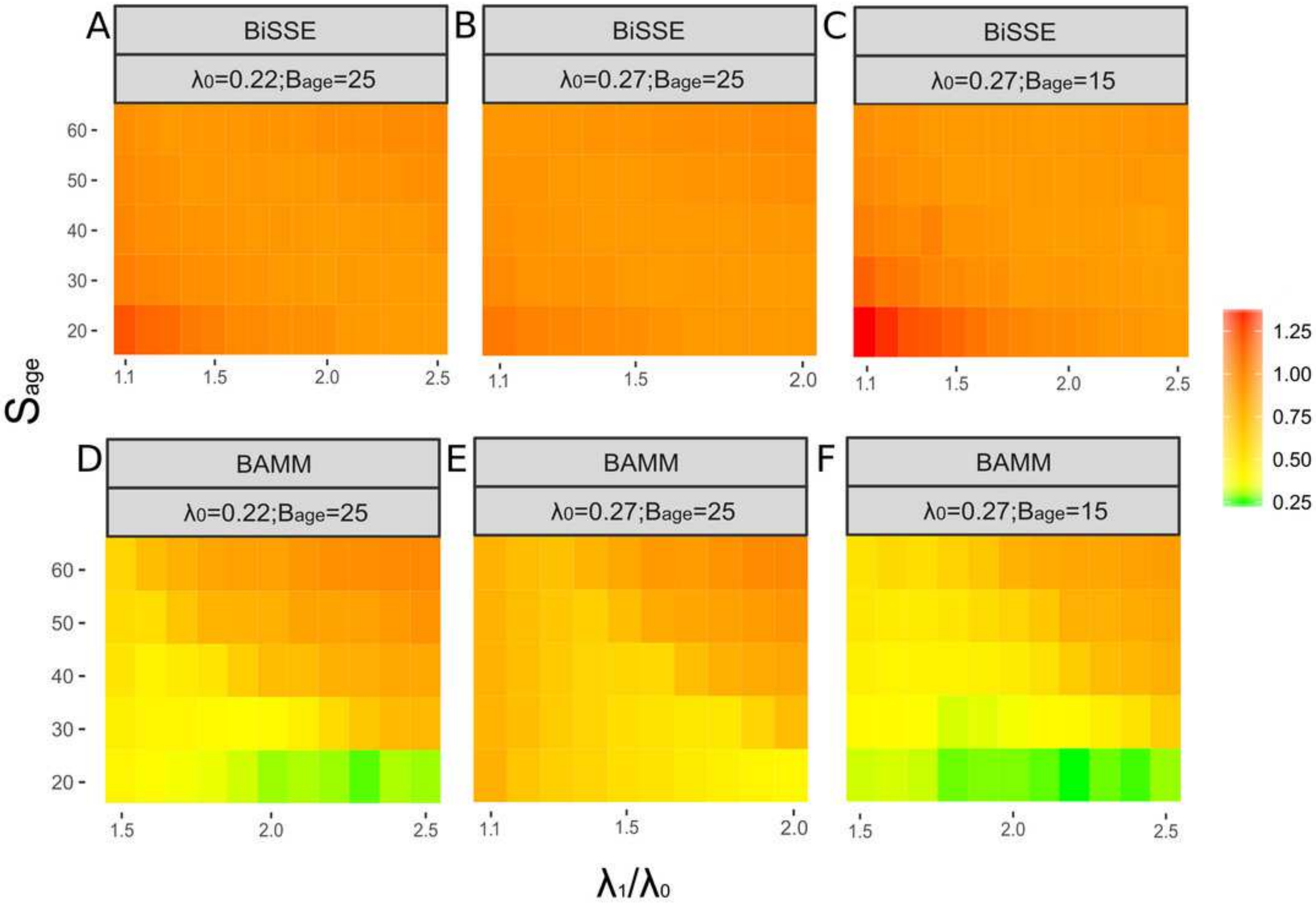

A
B
C
D
E
F
G
H
I
BiSSE
BAMM
MEDUSA
λ0=0.22;Bage=25
λ0=0.27;Bage=25
λ0=0.27;Bage=15
Proportion of shifts detected
1.00
0.75
0.50
0.25
0.00
0-50
51-100
101-250
251-500
501-1000
1001-2501
2501-6000
Total tree size

Figure 5

Error in estimation of diversification rates

Diversification rate estimate error, measured as the ratio of estimated and actual diversification rates (speciation minus extinction) for BiSSE (A, B & C) and BAMM (D, E & F) analyses. A ratio of 1 indicates no error, while greater deviance from 1 indicates greater error. X axes values are the simulated speciation rate asymmetry values and Y value represents relative *subtree* age. The first column (A and D) represents simulated scenarios of λ_0 0.22 and *basetree* age 25 units, the second column (B and E) represents λ_0 0.27 and *basetree* age 25 units, while the third column (C and F) represents λ_0 0.27 and *basetree* age 15 units.



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