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Inferring state-dependent diversification rates using approximate Bayesian computation

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Abstract

1. State-dependent speciation and extinction (SSE) models are a popular framework for quantifying whether species traits have an impact on evolutionary rates and how this shapes the variation in species richness among clades in a phylogeny. However, SSE models are becoming increasingly complex, limiting the application of likelihood-based inference methods. Approximate Bayesian computation (ABC), a likelihood-free approach, is a potentially powerful alternative for estimating parameters.
2. Here, we develop an ABC framework to estimate state-dependent speciation, extinction and transition rates from phylogenetic trees in BiSSE (binary state dependent speciation and extinction), GeoSSE (geographic state dependent speciation and extinction) and MuSSE (multiple state-dependent speciation and extinction) models. Using different sets of candidate summary statistics, we then compare the inference ability of ABC with that of using likelihood-based maximum likelihood (ML) and Markov chain Monte Carlo (MCMC) methods to identify the combinations that best capture the complex relationships between rates of diversification and species traits.
3. Our results show the ABC algorithm can accurately estimate state-dependent diversification rates for most of the model parameter sets we explored. The inference error of the parameters associated with the species-poor state is larger with ABC than in the likelihood estimations only when the speciation rate (λ) is highly asymmetric between states in all three models.
4. We suggest that the combination of normalized lineage-through-time (nLTT) statistics and phylogenetic signal constitutes efficient summary statistics for the ABC method.
5. By providing an efficient algorithm and a set of suitable summary statistics, our work aims to contribute to the use of the ABC approach in the development of complex SSE models, for which a likelihood is not available.

KEYWORDS
approximate Bayesian computation, diversification, extinction, speciation, state-dependent, summary statistics

1 | INTRODUCTION

Detecting the factors that underlie variations in diversification rate is a major topic of research in evolutionary biology, as it may reveal the causes of unevenness of species richness among clades and geographical regions. Numerous studies highlight the important role of traits in shaping speciation and extinction rates. For example, the presence of the nectar spur in flowering plants (angiosperms), which facilitates pollination and reproductive success, is associated with rapid diversification in the clades of spurred species (Armbruster, 2014; Fernández-Mazuecos et al., 2019). Traits such as this are hypothesized to affect evolutionary processes by determining the interactions between species, as well as how species respond to the environment (Li & Wiens, 2022; Wiens, 2017).

Over the past years, phylogenetic comparative methods to test evolutionary hypotheses have been developed rapidly (Adams, 2013; Miles & Dunham, 1993). A widely used class of phylogenetic tools are state-dependent speciation and extinction (SSE) models, which aim to investigate how species traits shape variation in diversification and richness, and to infer the rates of evolutionary processes (speciation, extinction and transitions between character states; Maddison et al., 2007). BiSSE (binary-state speciation and extinction) is the original SSE model and has been expanded to consider quantitative (QuaSSE, Fitzjohn, 2010), geographic (GeoSSE, Goldberg et al., 2011) and multiple categorical states (MuSSE, Fitzjohn, 2012a, 2012b). However, these models have been shown to suffer from a high risk of false-positives, which are likely to attribute differential diversification rate to trait-dependence. In order to reduce this Type I error in the SSE models, Beaulieu and O'Meara (2016) introduced the HiSSE (hidden-state-dependent speciation and extinction) model incorporating the effect of hidden states, which further promotes the subsequent development of state-dependent diversification models. More recently, Herrera-Alsina et al. (2019) introduced the SecSSE (several examined and concealed states-dependent speciation and extinction) framework accounting for multiple traits (observed and hidden) and multiple trait states. Around the same time, Nakov et al. (2019) introduced the MuHiSSE (multi-character hidden state-dependent speciation and extinction) model, which is a multi-state variant of HiSSE. These models have been applied in numerous empirical studies to identify the correlation between trait states and diversification rates (Onstein et al., 2017; Pyron & Burbrink, 2012; Rolland et al., 2014).

The most commonly used methods for estimating parameters in the current SSE models are likelihood-based inference approaches, such as maximum likelihood (ML) estimation. In recent years, researchers have explored the power of parameter estimations of existing models (Rabosky & Goldberg, 2015) and strived to improve the accuracy of the likelihood computing approaches (Laudanno et al., 2021; Louca & Pennell, 2020). An alternative is the Bayesian inference method, for example through Markov chain Monte Carlo (MCMC), which provides the full posterior distributions of parameters and allows for the incorporation of prior knowledge. However, these Bayesian methods still require the computation of the likelihood, which may be difficult or impossible for more complex models, for example models where the diversification rates depend on both clade diversity and traits.

In such cases, approximate Bayesian computation (ABC) is a powerful alternative for estimating parameters (Beaumont, 2019; Csilléry et al., 2010). ABC is a simulation-based Bayesian approach to find the parameters that can generate data close to the target (observed data) by evaluating the similarity of a set of summary statistics between simulated and observed data (Tavare et al., 1997). A series of efficient ABC algorithms have been expanded based on the simple rejection algorithm, such as incorporating Markov chain Monte Carlo (MCMC) (Marjoram et al., 2003), population Monte Carlo (PMC) (Beaumont et al., 2009) and sequential Monte Carlo (SMC) (Toni et al., 2009). However, it may be challenging in ABC-MCMC and ABC-PMC to achieve convergence and explore high-dimensional parameter space. ABC-SMC combines the strengths of these two methods and performs better in such cases. The algorithm systematically improves the approximation of the posterior distribution through a series of intermediate distributions, which allows it to converge to the posterior faster, reducing the usage of computational resources and offering improved parameter estimation in complex models. The developments of ABC methods have facilitated the application of ABC approaches in a broad field of studies. However, while these methods have been widely used in different fields, including ecological and evolutionary studies (Beaumont, 2010; Janzen et al., 2015), the applications in trait evolution or diversification analysis are still very limited, especially to study the effect of trait dynamics on diversification rates.

Key to the performance of ABC methods is the choice of the summary statistics, which should cover the maximum amount of the information in the data (Sirén & Kaski, 2020). The posterior distribution can be biased if the summary statistics fail to include important aspects of the data. However, using a too large vector of summary statistics can increase the dimension and cause redundancy. For SSE models, efficient summary statistics should ideally capture information on two aspects: the topology and the branch lengths of the phylogenetic tree on the one hand and the distribution of traits across the tips of the tree on the other hand. Currently, few statistics have been synthesized to describe the dynamics of binary or multi-state categorical traits along phylogenies. Phylogenetic signal is a potentially powerful statistic, which evaluates how phylogenetic distance shapes the distribution of traits among species, as well as the frequency of trait changes along a phylogeny. The Fritz and Purvis' *D* statistic was derived to measure phylogenetic signal particularly for binary traits (Borges et al., 2019; Fritz & Purvis, 2010). In addition, a set of statistics (e.g. normalized Lineage Through Time (nLTT)) employed in phylogenetic ABC analyses of diversification (Janzen et al., 2015), as well as statistics applied to measure the phylogenetic diversity (mean pairwise distance (MPD) (Tsirogiannis & Sandel, 2014), mean nearest taxon distance (MNTD) (Webb et al., 2002)), can also be extended to measure the distribution of a trait along phylogenies by separately analysing species with the same trait state. However, the performance of these summary statistics in trait state-dependent

models is yet to be evaluated. In recent years, the development of random forest and neural network methods enables the comparison of the importance of summary statistics, facilitating selection of informative statistics and improving the efficiency of likelihood-free inference methods (Lajaaiti et al., 2023; Raynal et al., 2019).

We use the ABC-SMC framework to estimate parameters in three state-dependent models (BiSSE, GeoSSE and MuSSE), and test the inference performance by comparing the inference error of the parameters using the ABC-SMC algorithm and two likelihood-based approaches: maximum likelihood estimation (MLE) and Markov chain Monte Carlo (MCMC). Importantly, we investigate the performance of a set of phylogenetic and trait-related summary statistics to select the most efficient combination for estimating evolutionary rates of state-dependent models, which may aid broader ABC development as well as other likelihood-free methods in SSE models where the likelihood cannot be (easily) computed.

2 | METHODS

2.1 | Trait-dependent simulation

Our main simulations were based on the BiSSE (binary state dependent speciation and extinction) model which simulates diversification dynamics according to a birth-death model where traits shape diversification rates. The model considers an evolving binary trait with two states, 0 and 1 (e.g. presence or absence of a specific trait). It assumes that the per lineage rates of speciation (λ_0, λ_1) and per lineage extinction (μ_0, μ_1) depend on the trait state of a species. It also allows transitions between states (q_{01}, q_{10}). We generated our simulations by conditioning on the crown age and both crown lineages surviving to the present (Herrera-Alsina et al., 2019). We simulated 'observed' phylogenetic trees and trait states at tips, under eleven parameter scenarios considering symmetric (equal rates between trait states) or asymmetric (rates differ between trait states), speciation, extinction and transition rates (Table 1). To simplify the analysis, we set only one (Scenario S1–S7) or two (Scenario S8–S11) of the three pairs of rates to be asymmetric in each scenario. For each scenario, we simulated 25 replicates with the ancestral state being 0 and 25 replicates with the ancestral state being 1. In total, we therefore produced 11 scenarios × 50 replicates = 550 (S1–S11 in Table 1) phylogenetic trees with trait data as observed data for parameter inference. We compared the differences in the distribution of richness and phylogeny-related statistics for 50, 200 and 500 replicates to check whether 50 replicates are sufficient for each scenario. We found that 50 replicates are sufficient, as the distributions of the metrics look very similar to those for 200 and 500 replicates (Figure S1). In addition, the values of the rates were selected based on values used by Herrera-Alsina et al. (2019). For computational convenience, these were adjusted to generate trees with a realistic number of species to avoid extremely small or large trees. In addition, we assume that the net diversification rate in State 0 is always higher than in State 1, with higher speciation or lower extinction rate. We set a constraint with a maximum of 1000 species in total for each observed tree, and for trait dependence to make sense (i.e. we would not expect to do an SSE-analysis when only one state is observed), we imposed the constraint that at least one species is present for each state at the end of the simulation. The simulation was discarded and rerun if the data was beyond the constraints. To ensure that the constraint does not affect the analysis results, we performed 5000 simulations for each parameter set without this species number constraint. We found more than 95% (more than 99% for parameter sets S2, S3, S4, S5) of the simulations were within this constraint.

In addition, we examined a broader and more random parameter space. Similar to the space above, we considered three scenarios with either asymmetric speciation, asymmetric extinction or asymmetric transition rates, respectively. For each scenario, we randomly sampled 100 parameter combinations from a uniform distribution for the asymmetric rates. Therefore, for this parameter space in total, 300 phylogenetic trees were used for parameter inference (S12, S13 and S14 in Table 1). In the main text, we focus on the analysis of the above parameter space. The analysis of the broader space is shown in the supplementary material.

We also considered the GeoSSE (geographic state dependent speciation and extinction, Goldberg et al., 2011) model, which is a geographical version of BiSSE that allows taxa to simultaneously occur in two different geographical regions (States 1 and 2), which means species are allowed to diversify through within-region speciation (λ_1, λ_2), between-region speciation (λ_{12}), extinction (μ_1, μ_2) and transition (q_{12}, q_{21}). We set one symmetric scenario and three asymmetric scenarios in speciation, extinction and transition rates, respectively. Similarly to the BiSSE case, we simulated 50 replicates as observations for each scenario (G1–G4 in Table 1).

Finally, we considered the MuSSE (multiple state-dependent speciation and extinction) model, which is also an extension of BiSSE, in this case allowing more than two character states (Fitzjohn, 2012a, 2012b). We focused on simulations with one trait and three possible states (1, 2 and 3). To simplify the analysis, we assumed that species can transition to other states with the same transition rate q (M1–M3 in Table 1).

2.2 | Maximum likelihood estimation

The three SSE models all allow likelihood calculation (Fitzjohn, 2012a, 2012b; Maddison et al., 2007), where the likelihood indicates the probability of observing the trait data on the phylogenetic tree with given parameters. Parameters can then be estimated using maximum likelihood estimation (MLE), which yields a point estimate. The likelihood is calculated based on a set of ordinary differential equations (Maddison et al., 2007).

The simulations and likelihood calculations for the BiSSE and MuSSE models were performed using the R package *secsse*. For the GeoSSE model simulations, we used the R package *diversitree* (Fitzjohn, 2012a, 2012b). The reason for using the *secsse* package is that the SecSSE model reduces exactly to BiSSE and MuSSE when there are no hidden states and the examined states are set as binary

TABLE 1 Parameter sets used to generate the observed data via simulations of the (A) BiSSE (S1–S14), (B) GeoSSE (G1–G3) and (C) MuSSE models (M1–M3).

Scenario	Speciation rate state 0 (λ_0)	Speciation rate state 1 (λ_1)	Extinction rate state 0 (μ_0)	Extinction rate state 1 (μ_1)	Transition state 0 to 1 (q_{01})	Transition state 1 to 0 (q_{10})
(A) BiSSE						
S1	0.6	0.6	0.05	0.05	0.05	0.05
S2	**0.6**	**0.3**	0.05	0.05	0.05	0.05
S3	**0.6**	**0.12**	0.05	0.05	0.05	0.05
S4	0.6	0.6	**0.05**	**0.1**	0.05	0.05
S5	0.6	0.6	**0.05**	**0.25**	0.05	0.05
S6	0.6	0.6	0.05	0.05	**0.05**	**0.1**
S7	0.6	0.6	0.05	0.05	**0.05**	**0.25**
S8	**0.6**	**0.3**	0.05	0.05	**0.05**	**0.1**
S9	**0.6**	**0.3**	0.05	0.05	**0.1**	**0.05**
S10	**0.6**	**0.3**	**0.05**	**0.1**	0.05	0.05
S11	**0.6**	**0.3**	**0.1**	**0.05**	0.05	0.05
S12	**U (0.2, 0.8)**	**U (0.2, 0.8)**	0.05	0.05	0.05	0.05
S13	0.6	0.6	**U (0.01, 0.2)**	**U (0.01, 0.2)**	0.05	0.05
S14	0.6	0.6	0.05	0.05	**U (0.01, 0.2)**	**U (0.01, 0.2)**

Scenario	Within-region Speciation state 1 (λ_1)	Within-region Speciation state 2 (λ_2)	Between-region Speciation (λ_{12})	Extinction rate state 1 (μ_1)	Extinction rate state 2 (μ_2)	Transition state 1 to 2 (q_{12})	Transition state 2 to 1 (q_{21})
(B) GeoSSE							
G1	0.5	0.5	0.5	0.1	0.1	0.2	0.2
G2	**0.75**	**0.5**	**0.25**	0.1	0.1	0.2	0.2
G3	0.5	0.5	0.5	**0.1**	**0.2**	0.2	0.2
G4	0.5	0.5	0.5	0.1	0.1	**0.2**	**0.1**

Scenario	Speciation rate state 1 (λ_1)	Speciation rate state 2 (λ_2)	Speciation rate state 3 (λ_3)	Extinction rate state 1 (μ_1)	Extinction rate state 2 (μ_2)	Extinction rate state 3 (μ_3)	Transition state (q)
(C) MuSSE							
M1	0.6	0.6	0.6	0.05	0.05	0.05	0.05
M2	**0.6**	**0.3**	**0.1**	0.05	0.05	0.05	0.05
M3	0.6	0.6	0.6	**0.05**	**0.1**	**0.2**	0.05

Note: Parameter pairs with asymmetric values (different rates between states) are in bold. S1–S7 are the seven BiSSE scenarios used in the main text, with only one pair of rates asymmetric, including a symmetric scenario as control (Scenario 1), and two asymmetric scenarios for each pair of rates. S8–S11 consider two pairs of rates to be asymmetric. S12–S14 explore a broader parameter space, with randomly sampled parameters from uniform distributions for each pair of asymmetric rates. G1–G4 are four GeoSSE scenarios with only one pair of asymmetric rates. M1–M3 are three MuSSE scenarios used with only one pair of asymmetric rates.

or multi-state, and the code is easily modified to models beyond BiSSE and MuSSE. Therefore, it can accurately generate BiSSE and MuSSE simulations and estimates and facilitate further testing in the more complex conditions, for example with hidden or quantitative states.

2.3 | Likelihood-based Bayesian MCMC

We developed a Metropolis–Hastings Markov chain Monte Carlo algorithm (Hastings, 1970), which is a foundational MCMC method that allows for sampling from a target probability distribution. For the BiSSE model, we tested two sets of prior distributions: (1) uniform prior distributions U(0, 2) for speciation and extinction rates and U(0, 1) for transition rates; (2) exponential prior distribution Exp(2) for all the rates. However, because we aim to test the parameter estimation performance without the influence of additional prior information, we focus on the analyses with the uniform prior. Therefore, for GeoSSE and MuSSE models, we only used uniform prior distributions for all the parameters. The algorithm constructs a Markov chain, a sequence of random parameter

values, where the next state depends only on the current state. To obtain a stable and convergent MCMC chain, we ran 1,000,000 iterations after 100,000 iterations of burn-in. For each data set, we used an unconstrained model and estimated all the parameters regardless of the symmetry of the generating rates in BiSSE and GeoSSE models. For the MuSSE model, we estimated state-dependent speciation and extinction rates as well as a single transition rate.

2.4 | ABC-SMC estimation

We performed a sequential Monte Carlo algorithm (ABC-SMC) to estimate parameters for each observed data. The algorithm we used was derived from the original ABC-SMC algorithm introduced by Toni et al. (2009) (Box 1). To compare the ABC results with the likelihood-based approach, we did the ABC analysis under the same assumptions of prior distributions as the MCMC (see above). The algorithm starts by sampling a series of parameter sets (particles) θ from the prior distribution $\pi(\theta)$, and then simulates datasets with these parameters and computes the difference in summary statistic ($D(SS)$) between the observed data (P_0) and the simulated data (P). The simulated data were generated over a timespan matching the crown age of the observed data, with randomly sampled root state. The process was repeated until this difference was smaller than a threshold ϵ. We used an iteratively adaptive method choosing ever-decreasing thresholds for each iteration, by specifying the median values of the summary statistic distance from the previous iteration, which means the decreasing thresholds depend on the position of the accepted particles in the previous iteration. This is more efficient than using a given linearly or exponentially decreasing pattern. We used 500 particles per iteration and the algorithm was assumed to generate a converged posterior at an acceptance rate of 1 in 500. The ABC and MCMC algorithms used in this study were implemented in the R package *DivABC*, which is available on Github (https://github.com/xieshu95/DivABC).

2.5 | Summary statistics

We tested the usefulness and efficiency of a set of summary statistics for improving ABC performance. For the BiSSE model, we used six summary statistics to describe the branching dynamics and trait evolution along the phylogeny, which are as follows: (1) nLTT (normalized lineage-through-time) (Janzen et al., 2015), (2) MPD (mean pairwise distance) (Tsirogiannis & Sandel, 2014), (3) MNTD (mean nearest taxon distance) (Webb et al., 2002), (4) Colless index (Colless & Wiley, 1982), (5) tip ratio and (6) phylogenetic signal D (Fritz & Purvis, 2010). nLTT is a summary statistic that calculates the sum of the absolute differences between the normalized LTT curves of two phylogenies (Janzen et al., 2015). It is known to be efficient in phylogenetic analyses of diversification,

BOX 1 The ABC SMC algorithm.

S1: Initialize thresholds ϵ_1

S2: Set iteration $t = 1$

For particle $i = 1,\ldots, N$

Repeat

Sample ${\theta_1}^i$ from the prior $\pi(\theta)$.

Simulate phylogeny ${P_1}^i \sim {\theta_1}^i$.

Calculate distance ${D_1}^i(SS) = |SS({P_1}^i) - SS(P_0)|$.

until ${D_1}^i(SS) < \epsilon_1$

Calculate weight: $w_1^i = 1/N$

Calculate threshold for next iteration: ϵ_2 = median $\{{D_1}^1(SS), {D_1}^2(SS) \ldots {D_1}^N(SS)\}$

S3: $t = 2,\ldots,T$

For particle $i = 1,\ldots, N$

Repeat

Sample ${\theta_t}^i$ from population $\{\theta_{t\text{-}1}\}$ with weight w_{t-1}^i, and perturb ${\theta_t}^i \sim N(0, 0.01)$.

Simulate phylogeny ${P_t}^i \sim {\theta_t}^i$.

Calculate distance ${D_t}^i(SS) = |SS({P_t}^i) - SS(P_0)|$.

until ${D_t}^i(SS) < \epsilon_t$

Add ${\theta_t}^i$ to the population $\{\theta_t\}$

Calculate weight: $w_t^i = \frac{\pi(\theta_t^i)}{\sum_{j=1}^{N} w_{t-1}^j N(\theta_{t-1}^j, \theta_t^i)}$

Normalize the weights.

Calculate threshold for next iteration: ϵ_{t+1} = median $\{{D_t}^1(SS), {D_t}^2(SS) \ldots {D_t}^N(SS)\}$

where N is the total number of the particles needed for generation t, and T is the total number of iterations before the algorithm stops. $\epsilon_1 \ldots \epsilon_T$ means the sequence of decreasing tolerance threshold from iteration 1 to T. θ_t^i means the particle i of iteration t, and w_t^i is the weight of this particle. P_0 is the observed data and ${P_t}^i$ is the simulated data with the particle θ_t^i, and $SS(P_t^i)$ is the calculated summary statistic of the simulation.

which has been shown a better performance than classic statistics (e.g. phylogenetic diversity (PD); Faith, 1992) in different types of birth–death models (Janzen et al., 2015). The original nLTT statistic does not capture trait information, so we developed a method to calculate the nLTT statistic of each trait state by trimming branches from the phylogenetic tree with the other trait state at the tip. We calculated the nLTT statistics for the entire tree ($nLTT_{total}$), for the trimmed tree with only state 0 ($nLTT_0$), and the trimmed tree with only state 1 ($nLTT_1$). As illustrated in Figure 1, for the same phylogenetic tree, different trait distributions at the tips can lead to differences in $nLTT_0$ or $nLTT_1$. MPD and MNTD are metrics that have been commonly used to measure phylogenetic diversity (Webb, 2000), and the Colless index is a widely used statistic to measure the balance of phylogenetic trees (Colless, 1995). Furthermore, we calculated the state-specific MPD, MNTD and Colless index in the same way as calculating $nLTT_0$ or $nLTT_1$ based

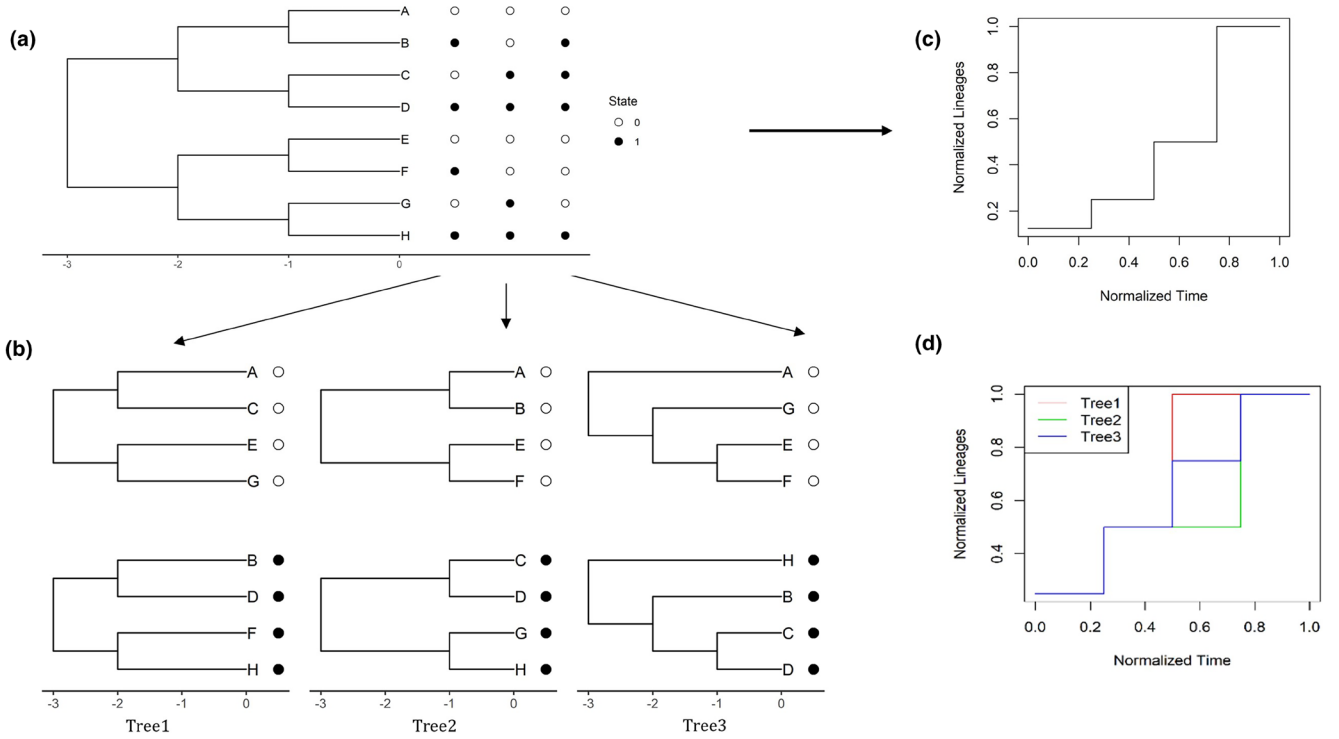

FIGURE 1 Hypothetical example of transforming an entire phylogeny with binary tip states into two trimmed trees with a single state by pruning the tips with the same states. (a) Example of a (balanced) tree with eight extant species at the present time, and three potential trait distributions at tips (other trait distributions are possible, but we show only three for the example). Blank circles represent State 0, and filled black circles represent State 1. (b) Two reduced trees for each state depending on the trait distribution at the tips (a). (c) The plot of the nLTT for the entire phylogenetic tree in (a). (d) The plot of the nLTT for the trimmed trees with a single state in (b), and here we show only the nLTT plot for one of the states, because the plot for the other state is equivalent in the example.

on the trimmed tree with a single state. The tip ratio between binary states was calculated as the number of species with a species-rich state divided by the number of species with a species-poor state:

$$\text{Tip ratio} = \frac{\max\left(N_{\text{state 0}}, N_{\text{state 1}}\right)}{\min\left(N_{\text{state 0}}, N_{\text{state 1}}\right)}$$

Another summary statistic we examined is *D* (Fritz & Purvis, 2010), which measures the phylogenetic signal of a given phylogeny with binary trait states. The method for computing statistic *D* is described in the Supporting Information.

To simplify the analysis, we did not test all the permutations among these six metrics, but manually selected the most relevant combinations (Table 2). We used the $\text{nLTT}_{\text{total}}$ as the main measurement of the branching dynamics. However, this metric is insufficient for inferring diversification variance between states because of the lack of trait information. Therefore, we combined $\text{nLTT}_{\text{total}}$ with different pairs of trait-related statistics, respectively. Finally, we compared the performance among the combinations to filter the most powerful statistics. The calculations of nLTT, MPD, MNTD and Colless index are implemented in the R package *treestats*, which is available on Github (github.com/thijsjanzen/treestats). The

TABLE 2 Selected summary statistic combinations and their abbreviations.

Combination	Summary statistic	Abbreviation
(*A*) *BiSSE*		
1	*D*	*D*
2	$\text{nLTT}_{\text{total}}$	nLTT
3	$\text{nLTT}_{\text{total}}$+*D*	nLTT-*D*
4	$\text{nLTT}_{\text{total}}$+tip ratio	nLTT-Ratio
5	$\text{nLTT}_{\text{total}}+\text{MPD}_1+\text{MPD}_2$	nLTT-MPD
6	$\text{nLTT}_{\text{total}}+\text{MNTD}_1+\text{MNTD}_2$	nLTT-MNTD
7	$\text{nLTT}_{\text{total}}+\text{colless}_1+\text{colless}_2$	nLTT-Colless
8	$\text{nLTT}_{\text{total}}+\text{nLTT}_1+\text{nLTT}_2$	nLTTs
9	$\text{nLTT}_{\text{total}}+\text{nLTT}_1+\text{nLTT}_2+D$	nLTTs-*D*
10	$\text{nLTT}_{\text{total}}+\text{MNTD}_1+\text{MNTD}_2+D$	nLTT-MNTD-*D*
11	$\text{nLTT}_{\text{total}}+\text{MNTD}_1+\text{MNTD}_2+\text{nLTT}_1+\text{nLTT}_2+D$	nLTTs-MNTD-*D*
(*B*) *GeoSSE/MuSSE*		
1	$\text{nLTT}_{\text{total}}+\text{nLTT}_1+\text{nLTT}_2+\text{nLTT}_3+D_{12}+D_{13}+D_{23}$	nLTTs-D_{subtree}
2	$\text{nLTT}_{\text{total}}+\text{nLTT}_1+\text{nLTT}_2+\text{nLTT}_3+D_{1\text{-}23}+D_{2\text{-}13}+D_{3\text{-}12}$	nLTTs-D_{merge}
3	$\text{nLTT}_{\text{total}}+\text{nLTT}_1+\text{nLTT}_2+\text{nLTT}_3+\text{M}$	nLTTs-M

phylogenetic signal *D* is calculated using the function *phylo.d* from the R package *caper*.

For GeoSSE and MuSSE models, we focused on the combination of nLTT statistics and phylogenetic signal (shown to perform well for BiSSE). However, the phylogenetic signal *D* is only applicable to binary trait data and therefore not suited for MuSSE or GeoSSE. We therefore used two methods to transform the multistate data into binary data to calculate the *D* statistic. One of the methods generates subtrees containing only two states and cuts off all the branches of the remaining trait states ($D_{subtree}$). The other fixes one trait state and merges all the rest of the trait states into one (D_{merge}). In addition, we also applied a newly proposed summary statistic *M* (Yao & Yuan, 2025), which can be used to calculate phylogenetic signal across multiple traits. The phylogenetic signal *M* is calculated using the function *phylosignal_M* from the R package *phylosignalDB*.

3 | RESULTS

We compared the inference error of the different inference methods by calculating the relative distance between the estimations using the ABC, MCMC and MLE approaches and the true (generating) values. To ensure a fair comparison, in the main text, we use the medians of the posterior distributions representing the estimations from the ABC and MCMC algorithms to compare with the point estimation of MLE. In addition, the comparisons of the full posterior distributions are given in the Supporting Information. We find that the results are consistent between the two approaches. Since we have more scenarios for BiSSE to analyse the effect of different levels of trait dependence on parameter estimation, we focused on the first seven scenarios and divided the scenarios into three groups according to the asymmetry of different rates, which are (1) asymmetry in speciation (scenarios S1, S2 and S3); (2) asymmetry in extinction (scenarios S1, S4 and S5); (3) asymmetry in transition (scenarios S1, S6 and S7). We did not run all types of analyses for GeoSSE and MuSSE. For these two models, we focused on comparing inference performance between ABC, MCMC and MLE, as well as on assessing the performance between three summary statistic combinations.

Our general conclusion is that the ABC method performs well in estimating all parameters of the three models for most of the scenarios we investigated, and is comparable with MCMC and MLE methods with minor differences. The Bayesian inference methods only lead to relatively larger inference errors when the speciation rates are highly asymmetric between states (e.g. $\lambda_1/\lambda_0 = 5$ in BiSSE), but in this case, the error occurs only in the rates associated with the state with fewer species. For the performance of summary statistics in estimating parameters of the BiSSE model, we found that using only the nLTT statistics in the ABC approach can lead to accurate estimates of state-dependent speciation and extinction rates, but produces a relatively larger inference error in estimating transition rates between states. However, the inference accuracy can be significantly increased by adding the summary statistic *D*. In addition, the combinations of nLTT statistics and phylogenetic signal also perform well in estimating rates in GeoSSE and MuSSE models. We will now discuss our results in detail.

3.1 | Statistics of the observed data

For the BiSSE model, we calculated six properties of the observed trees: the tree size (as measured by the total number of species on the observed phylogenetic tree), tip ratio (the ratio of the diversity between the species-rich state and the species-poor state), the number of tips with each state, phylogenetic signal and nLTT across all the observed datasets in scenarios S1–S7 (350 trees) (Figure 2). The observed phylogenetic trees generated under the seven scenarios show different patterns. Overall, the mean and the standard deviation of the species richness with state 0 are similar among scenarios due to the control of the rates with state 0, except when transition rates are highly asymmetric (S7). Species richness with State 1 decreases with an increasing level of asymmetry in speciation (S2 and S3), extinction (S4 and S5) and transition rates (S6 and S7), which in turn cause smaller tree size and larger tip ratio (Figure 2), where larger tip ratio values imply a higher degree of unbalance of tip states. The bimodal distributions in the richness-related statistics are mainly attributable to different trees being generated from different root states (Figure S3). Although there is overlap in some dataset characteristics between scenarios, we find that some scenarios show strong overlap for some statistics but strong differences for others, confirming that the scenarios are sufficiently different from each other.

3.2 | ABC with different summary statistics

Using different groups of summary statistics shows a large difference in the performance of parameter estimation of ABC in the BiSSE model (Table 3). The nLTT statistic alone can accurately estimate speciation and extinction rates, except when the generating rates of speciation greatly vary between binary states (i.e. scenario S3) (Figure 3, Figures S4–S6). However, the inference errors and the variance in transition rates among replicates are always large (Figure 3, Figures S4–S6), due to the lack of trait dynamic information along phylogenetic trees. The combination of nLTTs and nLTT-MNTD improves the overall inference accuracy, especially in estimating speciation rates when there is high asymmetry in speciation (Table 3 and Figure 3), while the other combinations including nLTT (i.e. nLTT-MPD, nLTT-colless and nLTT-ratio) show no significant improvement in estimations over using nLTT alone (Table 3).

In contrast, the statistic *D* is efficient in estimating transition rates in different scenarios, but leads to large bias and variation in estimating speciation and extinction rates when used on its own (Figure 3, Figure S4). Combining the statistic *D* with MNTD and

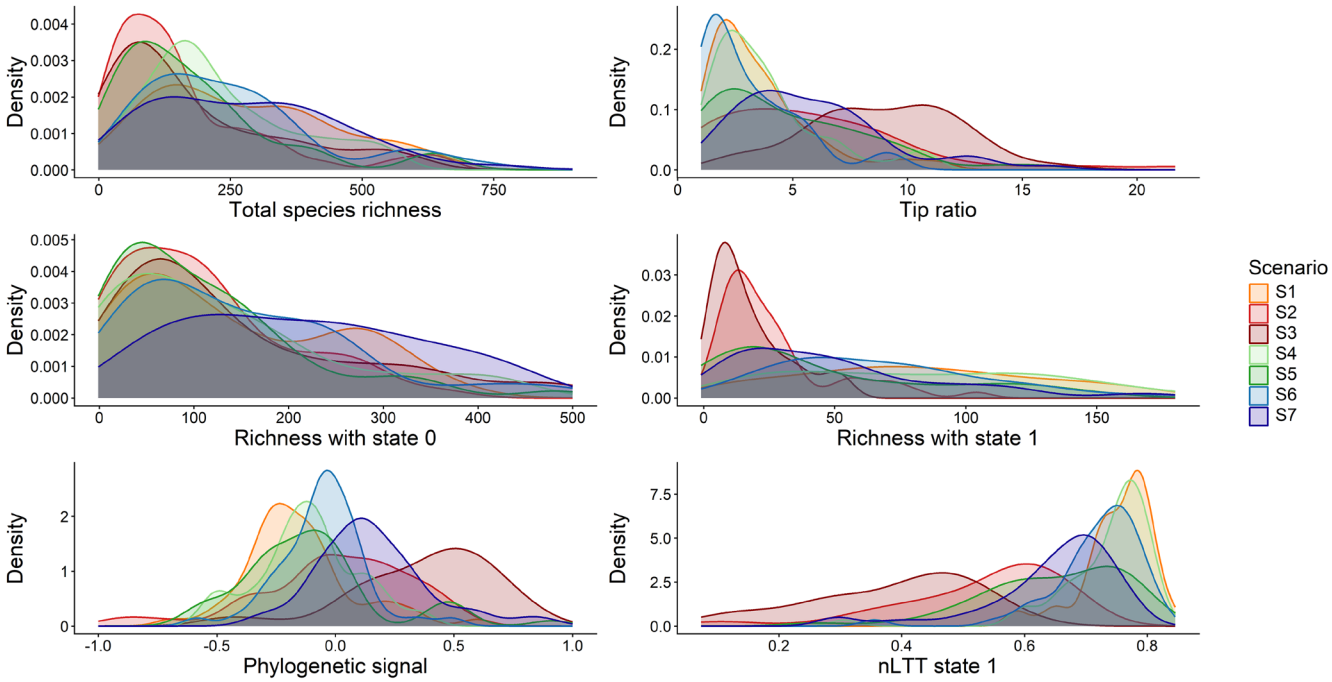

FIGURE 2 Main properties of the observed BiSSE datasets. Plots show the density distribution of different properties (total species richness, tip ratio, richness with State 0 and richness with State 1, phylogenetic signal and nLTT of State 1) across the different scenarios (indicated with different colours).

nLTT statistics (i.e. nLTT-*D*, nLTT-MNTD-*D*, nLTTs-MNTD-*D* and nLTTs-*D*) improves the estimation accuracy in transition rates in all scenarios compared with the other combinations without *D* (Table 3 and Figure 3). To statistically distinguish the differences in performance between different summary statistics, we measured the mean and the standard deviation of the Euclidean distance across all six parameters as statistical metrics (Table 3). The calculation of the Euclidean distance for each replicate is given in the supplementary. Overall, the best summary statistic combination is nLTTs-*D*, which includes both trait dynamic information from phylogenetic signal (as measured by *D*) and temporal trait information coming from the nLTT statistics (Table 3).

To evaluate the importance of each summary statistic and the sufficiency of the selected summary statistic combinations, we employed the ABC-Random Forest (ABC-RF) approach implemented in the *abcrf* R package (Raynal et al., 2019). ABC-RF produces a ranking of the contribution of each summary statistic for the estimation of parameters. While the method provides this ranking for individual parameters, it does not produce a combined ranking of the best summary statistics overall when considering all parameters. Thus, to gain a comprehensive ranking of the best summary statistics overall when considering all parameters, we normalized the importance of each summary statistic, and then calculated the average importance across all six parameters. The ABC-RF test shows a similar pattern that MNTD and nLTT statistics overall contribute more to parameter estimation than the others, and each summary statistic does not contribute equally to all parameters (Figure S7). The phylogenetic signal *D* is less important in estimating extinction rates, but ranks as one of the most informative predictors for transition rates. In addition, when evaluating the correlations between the summary statistics, we found that nLTT statistics have relatively strong positive or negative correlations with most of the other summary statistics, especially a strong positive correlation with MPD and a strong negative correlation with MNTD (Figure S8). This indicates that there is an overlap of information among these summary statistics. Conversely, *D* is independent of most of the statistics, as it shows relatively weak correlations (Figure S8).

3.3 | Inference with different methods (ABC, MCMC and MLE)

Of the 11 summary statistic combinations we considered in the BiSSE estimation, the combination of the phylogenetic signal summary statistic *D* and the nLTT statistics (i.e. nLTTs-*D*) was found to give the most accurate state-dependent rate estimations (Table 3 and Figure 3). Therefore, here we focus on comparing the ABC estimations of nLTTs-*D* with the estimations of MCMC and MLE. We measured the mean and standard deviation of Euclidean distance across all parameters as statistical metrics to evaluate the inference error (Tables 3 and 4).

According to the significance analyses across all parameter sets, the performance of the ABC method with efficient summary statistics is slightly below that of MLE, but above that of MCMC (Table 3). As for Bayesian inferences, there is no significant difference between ABC and MCMC for most of the scenarios (except Scenarios 5 and 7). In addition, significant differences between ABC

TABLE 3 Quantitative analysis of inference errors (estimate—true value) across parameters using ABC, MCMC and MLE for (A) BiSSE, (B) GeoSSE and (C) MuSSE.

Methods	Summary statistics	Euclidean distance mean (SD)
(*A*) *BiSSE*		
ABC	*D*	1.03 (0.374)[a]
	nLTT-Colless	0.932 (0.249)[b]
	nLTT-MPD	0.876 (0.258)[b]
	nLTT	0.757 (0.290)[c]
	nLTT-ratio	0.752 (0.238)[c]
	nLTTs	0.751 (0.287)[c]
	nLTT-MNTD	0.718 (0.238)[cd]
	nLTT-*D*	0.651 (0.325)[d]
	nLTTs-MNTD-*D*	0.538 (0.247)[e]
	nLTT-MNTD-*D*	0.532 (0.232)[e]
	nLTTs-*D*	**0.449 (0.225)[f]**
MCMC		0.503 (0.343)[ef]
MLE		0.333 (0.275)[g]
(*B*) *GeoSSE*		
ABC	nLTTs-$D_{subtree}$	0.380 (0.139)[a]
	nLTTs-D_{merge}	**0.351 (0.129)[ab]**
	nLTTs-M	0.362 (0.146)[a]
MCMC		0.309 (0.186)[b]
MLE		0.307 (0.238)[b]
(*C*) *MuSSE*		
ABC	**nLTTs-$D_{subtree}$**	**0.412 (0.198)[ab]**
	nLTTs-D_{merge}	0.434 (0.189)[ab]
	nLTTs-M	0.460 (0.197)[a]
MCMC		0.417 (0.213)[ab]
MLE		0.366 (0.281)[b]

Note: We calculate the Euclidean distance of errors for each parameter set, and then calculate the mean and standard deviation (in brackets) of Euclidean distance across all the parameter sets. Lower bias and lower Euclidean distances indicate better performance of the combination of summary statistics for parameter estimation (best performing summary statistic combination highlighted in bold). Pairwise comparisons were made using ANOVA followed by Tukey's HSD for multiple comparisons. The summary statistic combination with the highest Euclidean distance is named 'a'. Different superscript letters in each column indicate statistical significance ($p < 0.05$).

and MLE only occur when the speciation rates are largely asymmetric between states (Scenarios 2 and 3). In other cases, there is no significant difference between ABC and MLE (Table 4 and Figure 4). Zooming into the groups of scenarios with different levels of asymmetry in speciation, extinction and transition, we found that asymmetry in speciation rates had a greater influence on inference accuracy than asymmetry in extinction or transition rates (Figure 4, Figure S9). In the scenarios with asymmetric speciation rates, the inference error increases with a higher level of asymmetry (Figure 4 and Table 4), especially when the observed data are generated from a low-rate root state and later transferred to high-state branches, which may cause phylogenetic trees with small tree size but large tip ratio (Figure S10). However, the bias only occurs when estimating the rates of the species-poor state (e.g. λ_1, μ_1, q_{10} in Scenario S3) (Figure 4, Figure S9), and whether the root state of the simulations matches that of the observation does not affect the performance of the ABC approach (Figure S11).

The inference power of the Bayesian methods is sensitive to the selection of the prior distribution. By comparing the estimations using uniform and exponential prior distributions, we found that an informative prior does improve the accuracy of the Bayesian estimation methods (Figure S12). In addition, the variance in the Bayesian inference methods can be reduced greatly when using the median of the posterior distributions, although the errors are still present in estimating the species-poor state in scenario S3 (Figure 4, Figure S9). The analyses of scenarios with two pairs of asymmetric rates (Scenarios S8–S11 in Table 1) and the broader space with continuous asymmetric levels in speciation, extinction and transition (Scenarios S12–S14 in Table 1) show similar results (Figures S13 and S14). The inference error of speciation and extinction rates in State 1 (λ_1 and μ_1) in scenario S8 and S10 is relatively larger than the other scenarios because lower speciation rate and higher transition rate (S8) or high extinction rate (S10) in State 1 lead to larger richness difference between two states, resulting in a larger error of the species-poor state (State 1) (Figure S13).

For both GeoSSE and MuSSE, the ABC method performs well in estimating diversification and transition rates for most of the parameter sets. The three summary statistics combinations of nLTT statistics and phylogenetic signal perform identically with no significant difference between each other (Table 3), and can all thus efficiently extract the information on trait dynamics. This result is consistent with the importance test of the summary statistics using ABC random forest (Figure S17). In addition, the best performance of ABC is not significantly different to the performance of MCMC and MLE (Figure 5 and Table 3). Only when the speciation rate is highly asymmetric between states in the MuSSE model, the inference error of the extinction rate at the low-rate state is relatively larger when using Bayesian inference methods than when using MLE (Figure S16). We note that the test on MuSSE is under the simplification of equal transition scenarios. Considering unequal transition rates may exacerbate the inference errors.

3.4 | Effect of the statistics of observed data (tree size and tip ratio) on inference

We evaluated the relationships between tree size and tip ratio with inference error across all the observed datasets (Figures S18 and S19). As expected, smaller trees or trees with larger diversity differences between states tend to cause larger inference error, especially in extinction rates (Figures S18 and S19).

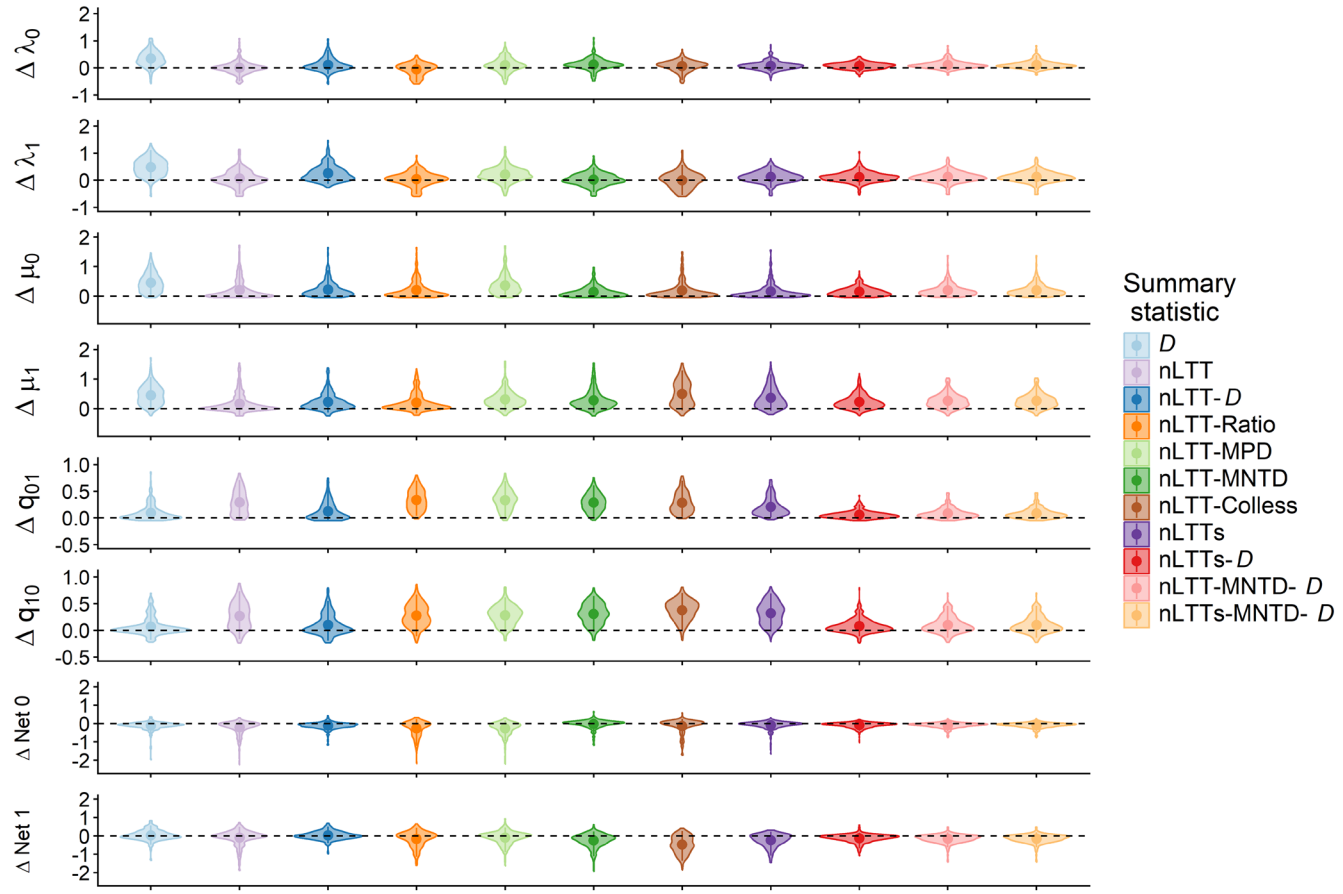

FIGURE 3 Parameter estimations of state-dependent speciation, extinction, transition and net diversification rates in the BiSSE model using the ABC method with different summary statistics. Plots show the residual inference error between estimated and (true) generating values. The dots and the whiskers indicate the medians and 95% intervals of the combined median posterior values across 350 parameter sets (Scenarios S1–S7 in Table 1). Dashed horizontal lines represent zero error to guide the eye. The colours indicate ABC results using different summary statistic combinations.

4 | DISCUSSION

The development of SSE models has recently accelerated, especially with advances in mathematical modelling techniques and the availability of empirical data (Holland et al., 2020). The main aim of this study was not to evaluate the power of existing likelihood methods of SSE models, which has already been done in previous studies (Davis et al., 2013; Holland et al., 2020). Instead, we used the likelihood-based MLE and MCMC estimations to compare with the performance of a new likelihood-free ABC approach, and to search for efficient summary statistics that cover the most comprehensive phylogenetic and trait information. Across all the scenarios we tested, the combination of the nLTT statistics and phylogenetic signal is sufficient to produce accurate estimations in ABC, which is on par with the likelihood estimations.

The nLTT statistic, which provides information of evolutionary dynamics over time, has been shown to be efficient and informative in phylogenetic analysis and diversification studies (Janzen et al., 2015; Richter & Wit, 2021; Saulnier et al., 2017), as well in island

TABLE 4 Quantitative analysis of inference errors (estimate—true value) across six parameters using ABC, MCMC and MLE for each scenario in BiSSE.

Scenarios	MLE	MCMC	ABC
S1	0.368 (0.307)^{a}	0.471 (0.343)^{a}	0.367 (0.187)^{a}
S2	0.306 (0.266)^{b}	0.545 (0.375)^{a}	0.541 (0.231)^{a}
S3	0.257 (0.204)^{b}	0.554 (0.354)^{a}	0.677 (0.256)^{a}
S4	0.342 (0.297)^{a}	0.463 (0.344)^{a}	0.410 (0.196)^{a}
S5	0.385 (0.247)^{b}	0.530 (0.330)^{a}	0.407 (0.170)^{b}
S6	0.241 (0.187)^{b}	0.375 (0.247)^{a}	0.323 (0.137)^{ab}
S7	0.430 (0.347)^{b}	0.585 (0.366)^{a}	0.420 (0.178)^{b}

Note: We calculate the Euclidean distance of errors across six parameters for each parameter set, and then calculate the mean and standard deviation (in brackets) of the Euclidean distance across all parameter sets. Pairwise comparisons were made using ANOVA followed by Tukey's HSD for multiple comparisons. The summary statistic combination with the highest Euclidean distance is named 'a'. Different superscript letters in each row indicate statistical significance ($p < 0.05$).

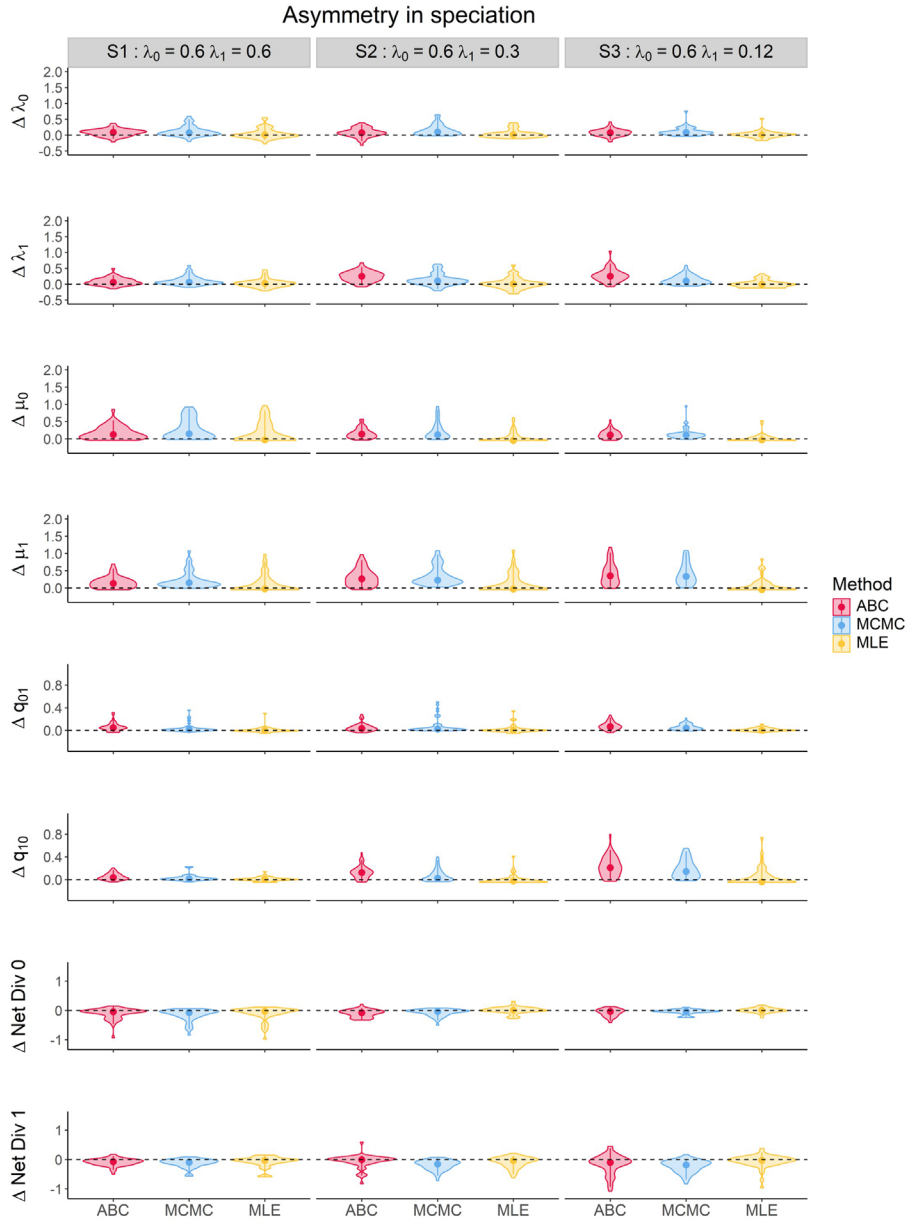

FIGURE 4 Parameter estimations of state-dependent speciation, extinction, transition and net diversification rates in the BiSSE model using the ABC, MCMC and MLE methods for scenarios with varying degrees of asymmetry in speciation (Scenarios S1–S3 in Table 1) in the generating rates. Plots show the residual inference error between estimated and (true) generating values. The dots and the whiskers indicate the medians and 95% intervals of the combined median values across 50 replicates for each single parameter set. Dashed horizontal lines represent zero error to guide the eye. Colours indicate different inference methods. The ABC results are estimated using the summary statistic combination nLTTs-*D* ($nLTT_{total}$, $nLTT_0$, $nLTT_1$ and *D*).

biogeography (Xie et al., 2023). However, the power of the statistic is limited in trait-related analysis when estimating transition rates due to the challenge and uncertainty of mapping trait evolution on phylogenies. nLTT for the whole tree can only capture the average diversification rates independent of traits, while adding nLTT for each state ($nLTT_0$ and $nLTT_1$) can improve the ability in capturing trait dependency in speciation and extinction rates (Figure 3), because of the information of branching times in the reduced trees. It is similar to the original sister-clade comparison method, which has been widely used in detecting the effect of traits on diversification rates before the establishment of the SSE models (Maddison et al., 2007; Mitter et al., 1988). Therefore, likewise, nLTT has the same limitation on detecting state shifts over time, leading to a poor estimation of transition rates between states (Figure 3). However, the phylogenetic signal statistic contains efficient information on trait evolution by comparing the observed trait distribution with the distributions simulated through continuous Brownian Motion patterns, compensating for the lack of information in nLTT statistics.

In this paper, we only tested the performance of 11 combinations among six summary statistics in the BiSSE model. However,

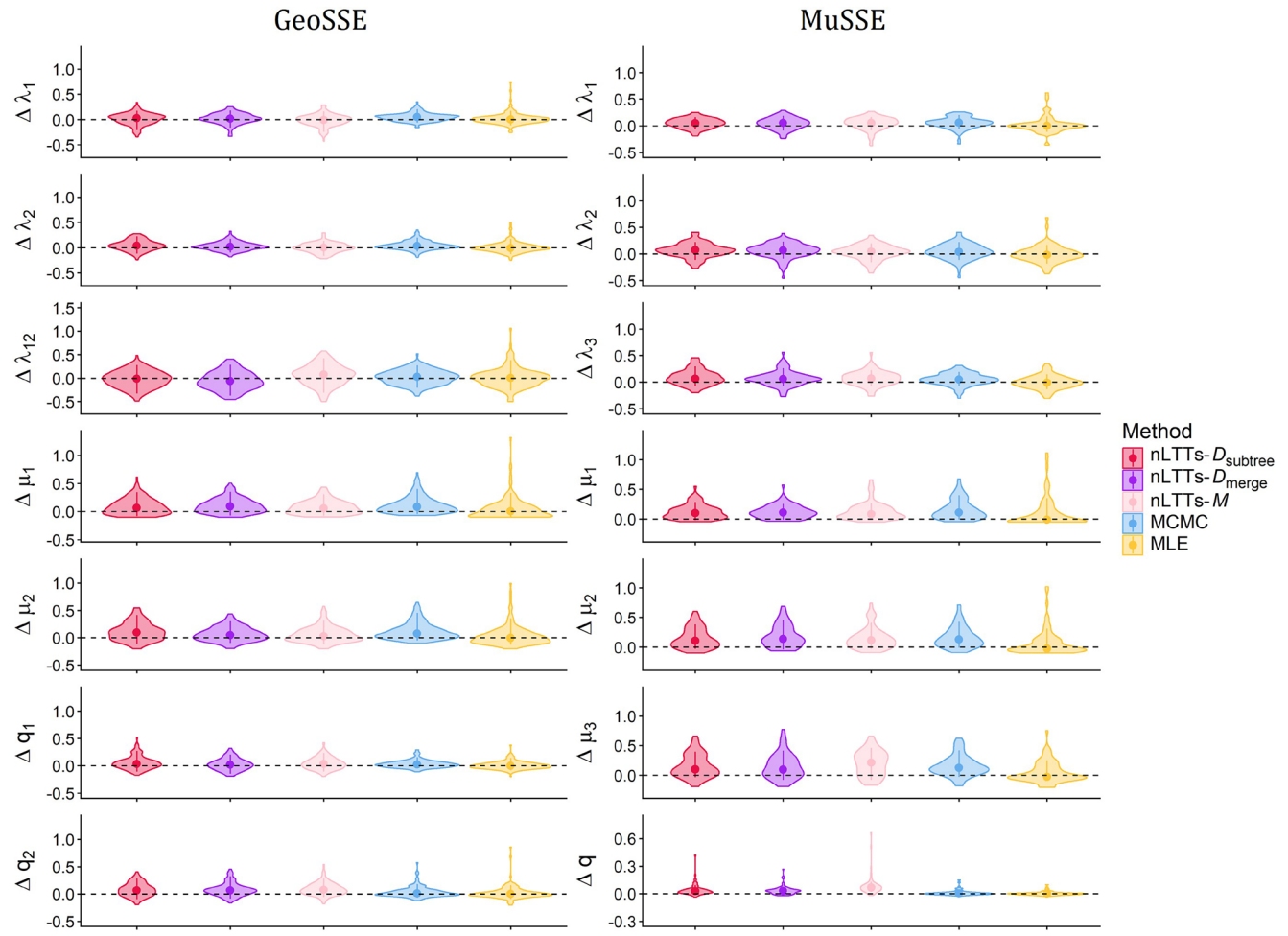

FIGURE 5 Parameter estimation of state-dependent speciation, extinction and transition rates in the GeoSSE and MuSSE models using MCMC, MLE and ABC with different summary statistics. Plots show the residual inference error between estimated and (true) generating values. The dots and the whiskers indicate the medians and 95% intervals of the combined median posterior across all the scenarios. Dashed horizontal lines represent zero error to guide the eye. The colours indicate different methods and summary statistic combinations.

there are a number of alternative statistics available in phylogenetics (e.g. phylogenetic diversity (*PD*) (Faith, 1992), *Laplacian spectrum* (Chindelevitch et al., 2021; Lewitus & Morlon, 2016) for tree shape). Recently, a few studies have proposed a number of summary statistics for detecting trait dynamics. Lajaaiti et al. (2023) applied multiple neural network architectures to estimate state-dependent diversification rates and compared the performance of deep learning methods with that of MLE, showing that the former provides a promising alternative for phylogenetic inference. However, the study focuses on summary statistics for describing the shape of phylogenetic trees (84 summary statistics) but less so on trait dynamics (one summary statistic (tip ratio)). Thereafter, Schwery et al. (2023) used a Bayesian approach to test the adequacy of trait-dependent diversification models with a number of summary statistics selected to capture trait distributions (e.g. FiSSE statistics) and the features of the phylogenetic tree (e.g. gamma statistics, Colless index, branch length). A few of the summary statistics that have not been included in our study are worth testing, but that does not mean that adding more summary statistics is necessarily better or recommended, because of the strong information overlap between statistics (Janzen & Etienne, 2024). A primary motivation for using summary statistics is to reduce the dimensionality of the observed datasets while retaining the most information for parameter estimation. Selecting an excess number of summary statistics, especially those that are highly correlated with one another, may lead to overfitting and redundancy, which reduce the efficiency and computability of the ABC algorithm (Blum et al., 2013; Jung & Marjoram, 2011). Therefore, apart from looking for alternative summary statistics, it is also important to choose and construct efficient combinations by weighting or transforming the statistics. The ABC random forest method provides a powerful solution for selecting summary statistics. However, the restriction of regression on one parameter at a time constrains its utility for multiple-parameter models, highlighting a potential direction for methodological development.

Apart from informative summary statistics, the inference power also depends on the amount of information in the data and the selection of the prior distribution. As expected, we found that small observed trees lead to high inference error in BiSSE estimations using both MLE, MCMC and ABC methods, which reemphasizes the results of previous studies that explored the accuracy and power of SSE

models (Davis et al., 2013; Gamisch, 2016). A large variance in speciation rates leads to a limited number of existing species in one state in simulated trees (particles) in ABC. Therefore, the summary statistics using trimmed trees (with either state) for trait analysis cause inference errors in the species-poor state, due to the lack of information on phylogenetic and trait dynamics in this state. In addition, the MLE method tends to estimate the extinction rate to be a value close to 0, which is a consistent issue in estimation using reconstructed trees due to the lack of information on extinction events (Louca & Pennell, 2021), while the Bayesian methods may fail to converge effectively to a narrow posterior distribution in estimating extinction rates, especially in the case of limited phylogenetic information in the data (Figure 4, Figure S9). However, our analyses show that the inference bias can be reduced by selecting a more informative prior distribution. The inference power may also be affected by the completeness of the dataset. In this study, we focus on demonstrating the feasibility of the ABC method and the summary statistics under completely sampled trees, but future studies could address the effect of sampling fraction on ABC, as was done for MLE by Mynard et al. (2023).

A typical issue with the power of the BiSSE model is high type I error. This problem has been addressed in a more complex model HiSSE and derived models (Beaulieu & O'Meara, 2016). However, in this study we aim to provide an ABC inference method to estimate parameters under the assumption that the model used is correct. Currently no summary statistic has been demonstrated to reliably capture the effects of unobserved traits on phylogenetic diversification, an important step towards the extension of the ABC method to hidden-state models. We cannot define summary statistics on traits that are unknown. Therefore, we tested the performance of the ABC approach and the summary statistics in BiSSE and two more complex models, GeoSSE and MuSSE, instead of models that include hidden/concealed traits, such as HiSSE or SecSSE. On the other hand, the computation speed of ABC is slower than that of MCMC and MLE, which takes more than twice as long as MCMC. Therefore, extending the application of ABC to hidden state models, where the parameter dimensionality is greatly increased, necessarily requires explicit consideration of scalability and computational runtime. A promising method is to integrate ABC with machine learning approaches to learn mappings from observed phylogenetic features to the latent effects of hidden states and provide informative summaries for likelihood-free inference. Recent advances in likelihood-free inference, such as neural network approaches (Lajaaiti et al., 2023; Lambert et al., 2023; Schwery et al., 2023), highlight the potential of simulation-based approaches for estimating parameters in complex diversification models. For instance, Lambert et al. (2023) have shown that neural networks can achieve similar or even higher accuracy than MLE when estimating BiSSE parameters; however, the performance highly depends on representation and network architecture. Future work should assess under what conditions neural networks may over- or underperform ABC. In any case, both ABC and machine learning methods offer important opportunities for further expansions of SSE models incorporating additional factors that affect evolutionary patterns (e.g. geography, ecology), where the likelihood equations become too complex to solve.

AUTHOR CONTRIBUTIONS

Shu Xie, Luis Valente and Rampal S. Etienne conceived the ideas and the methodology. Shu Xie performed the analysis and wrote the first draft. Luis Valente and Rampal S. Etienne contributed to the analysis and the revisions.

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CONFLICT OF INTEREST STATEMENT

The authors have no conflict of interest to declare.

PEER REVIEW

The peer review history for this article is available at https://www.webofscience.com/api/gateway/wos/peer-review/10.1111/2041-210x.70240.

DATA AVAILABILITY STATEMENT

Data generated and results obtained in this paper are archived on an open data repository hosted by Zenodo at https://doi.org/10.5281/zenodo.18080831 (Xie et al., 2025).

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

Figure S1. Properties of the observed datasets under different number of replicates, simulated under the BiSSE model.

Figure S2. Illustration of the calculation of Σd_{obs} and D under different phylogenetic patterns.

Figure S3. Main properties of the observed BiSSE datasets under different root states.

Figure S4. Parameter estimations of state-dependent speciation, extinction and transition rates in BiSSE model using the ABC method with different summary statistics for scenarios with varying degrees of asymmetry in speciation (scenarios S1, S2, S3 in Table 1) in the generating rates.

Figure S5. Parameter estimations of state-dependent speciation, extinction and transition rates in the BiSSE model using the ABC method with different summary statistics for scenarios with varying degrees of asymmetry in extinction (scenarios S1, S4, S5 in Table 1) in the generating rates.

Figure S6. Parameter estimations of state-dependent speciation, extinction and transition rates in the BiSSE model using the ABC method with different summary statistics for scenarios with varying degrees of asymmetry in transition rates (scenarios S1, S6, S7 in Table 1) in the generating rates.

Figure S7. The importance of summary statistics from ABC-RF for each parameter and overall variable importance among six parameters in BiSSE.

Figure S8. Correlation heatmap between summary statistics of all the observed datasets.

Figure S9. Parameter estimations of state-dependent speciation, extinction and transition rates in BiSSE using the ABC, MCMC and MLE methods for scenarios with varying degrees of (A) asymmetry in speciation (scenarios S1, S2, S3 in Table 1), (B) asymmetry in extinction (scenarios S1, S4, S5 in Table 1), (C) asymmetry in transition (scenarios S1, S6, S7 in Table 1) in the generating rates.

Figure S10. Parameter estimations of state-dependent speciation, extinction and transition rates in the BiSSE model under different root states using the ABC, MCMC and MLE methods for scenarios with varying degrees of asymmetry in speciation (scenarios S1, S2, S3 in Table 1) in the generating rates.

Figure S11. Parameter estimations of state-dependent speciation, extinction and transition rates in the BiSSE model using the ABC, MCMC and MLE methods for scenarios with varying degrees of asymmetry in speciation (scenarios S1, S2, S3 in Table 1) in the generating rates.

Figure S12. Parameter estimations of state-dependent speciation, extinction and transition rates in the BiSSE model using the ABC, MCMC and MLE methods for scenarios with varying degrees of asymmetry in speciation (scenarios S1, S2, S3 in Table 1) in the generating rates.

Figure S13. Parameter estimations of state-dependent speciation, extinction and transition rates in BiSSE using the ABC, MCMC and MLE methods for scenarios with asymmetry in two pairs of rates (scenarios S8, S9, S10 and S11 in Table 1) in the generating rates.

Figure S14. Parameter estimations of state-dependent speciation, extinction, transition and net diversification rates in BiSSE using the ABC, MCMC and MLE methods for scenarios with varying degrees of (A) asymmetry in speciation (S12 in Table 1), (B) asymmetry in extinction (S13 in Table 1), (C) asymmetry in transition (S14 in Table 1) in the generation rates.

Figure S15. Parameter estimation of state-dependent speciation, extinction and transition rates in the GeoSSE model using MCMC, MLE and ABC with different summary statistics.

Figure S16. Parameter estimation of state-dependent speciation, extinction and transition rates in the MuSSE model using MCMC, MLE and ABC with different summary statistics.

Figure S17. Overall variable importance among seven parameters in GeoSSE and MuSSE. Variables are ordered by importance, and larger values indicate greater contribution to predictive performance.

Figure S18. Relationship between phylogenetic tree size (total number of species) and the inference error in estimating state-dependent rates (estimated minus observed) for scenarios S1–S7 in BiSSE.

Figure S19. Relationship between the tip ratio and the inference error in estimating state-dependent rates for scenarios S1–S7 in BiSSE.

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