

A flexible method for estimating tip diversification rates across a range of speciation and extinction scenarios

Supplementary Material 1

Implementing MiSSE

MiSSE is available within the R package *hisse* (Beaulieu & O'Meara, 2016). Some details of MiSSE's implementation differ from other SSE models also implemented in *hisse*. These differences are summarized here, but readers are encouraged to follow the example code available as Supplementary Material (SM2) when using MiSSE for their empirical analyses.

The main difference between MiSSE and other SSE models in *hisse* is how MiSSE models are fit. The user can set and fit MiSSE models individually with a standalone function (MiSSE, Table SM1.1). However, it is difficult to know how many different hidden states the models will fit for a given empirical tree. As of now, MiSSE can fit models with up to 26 hidden states each representing a given “rate class”, which defines a combination of turnover rates ($\tau = \lambda + \mu$) and extinction fraction ($\varepsilon = \mu / \lambda$). In total there are 676 (26^2) possible model combinations, each with a different combination of rate class number that range from a minimum of two diversification parameters (one hidden state) and a maximum of 52 (26 hidden states).

Performing an exhaustive search by fitting all possible models is not only computationally expensive, but also time-consuming. Furthermore, in general, the complexity of the models with the lowest AICc scale with the size of the tree, meaning that more complex models will tend to be more important in larger trees. In the same way, complex models with many rate classes are likely to be a poor fit for most small trees. To alleviate having to decide which set of models to fit, we developed an heuristic algorithm (function MiSSEGreedy) to search through a reasonably large set of models that terminates after the set of models evaluated no longer provide meaningful support in terms of AICc. The default search starts with a random selection of models. This first set is biased towards simpler models, as initial experimentation showed that these models usually have the lowest AICc for most trees. The subsequent model “chunks” are then models that are neighbors to the ones recovered with the best AICc values in the previous rounds. The path of the MiSSEGreedy search can be visualized with the function PlotMisseSpace. MiSSEGreedy will continue to fit new “chunk” of models until the lowest Δ AICc of the new “chunk” is higher than that specified by the user (Fig. SM1.1). The user is therefore advised to set the arguments “stop.deltaAICc” and “chunk.size” in a sensible way according to the size of the tree. Based on

preliminary tests, we recommend a ΔAIC of 10 for trees with up to 1000 tips, which is the current default setting.

Once MiSSEGreedy terminates, one can select the best fitted model or average across a set of models in relation to their Akaike weight to estimate the diversification parameters at the tips using a marginal reconstruction algorithm with the function `MarginReconMiSSE`. In addition to marginal probabilities of states at nodes, MiSSE will also return marginal probabilities for the tips. The states can be used as indexes for the estimates of speciation, extinction, and the orthogonal transformations of these rates, namely, net-diversification ($r = \lambda - \mu$), turnover ($\tau = \lambda + \mu$) and extinction fraction ($\varepsilon = \mu / \lambda$) returned by the model fit. A tip rate estimate for a given model, then, becomes the weighted average of the diversification rates with the marginal probabilities used as weights.

Table SM1.1: New functions implemented in R package *hisse* to fit, reconstruct, and visualize implementation of MiSSE models on phylogenetic trees.

Function name	Brief description
<i>PlotMisseSpace</i>	Imports from package <i>igraph</i> to plot a network showing which models have lower AICc weight in relation to their neighbors.
<i>MiSSEGreedy</i>	Uses greedy algorithm to fit a series of MiSSE models with different complexities in chunks. It will stop when delta AIC does not have significant improvement in the new chunk of models.
<i>MiSSE</i>	Standalone MiSSE function.
<i>MarginReconMiSSE</i>	Uses marginal reconstruction algorithm to reconstruct rates along the tree.
<i>plot.misse.states</i>	“Paints” the averaged rate reconstruction along the branches of the tree. However, inferences of rates through time should not be interpreted literally (see Discussion).
<i>PruneRedundantModels</i>	Prune models that are effectively identical in terms of likelihood and parameter estimates before model averaging.
<i>TipCorrelation</i>	Performs linear regression between phylogenetic independent contrasts of tip rates and continuous traits, with the option to prune out cherries (see Discussion).

We have also added functionality for eliminating redundant models within *hisse*. When calculating model weights, it is best not to include multiple copies of the same model (Burnham & Anderson, 2002). However, such cases can arise inadvertently. For example, a birth death model and a Yule model are essentially the same (other than in number of free parameters) if the best estimate for extinction rate is zero. In the case of MiSSE, where there can be many models compared, including multiple different models that are in fact identical (in terms of likelihood and parameter estimates) increases the Akaike weights for these models artificially. We thus prune these redundant models with the function `PruneRedundantModels`.

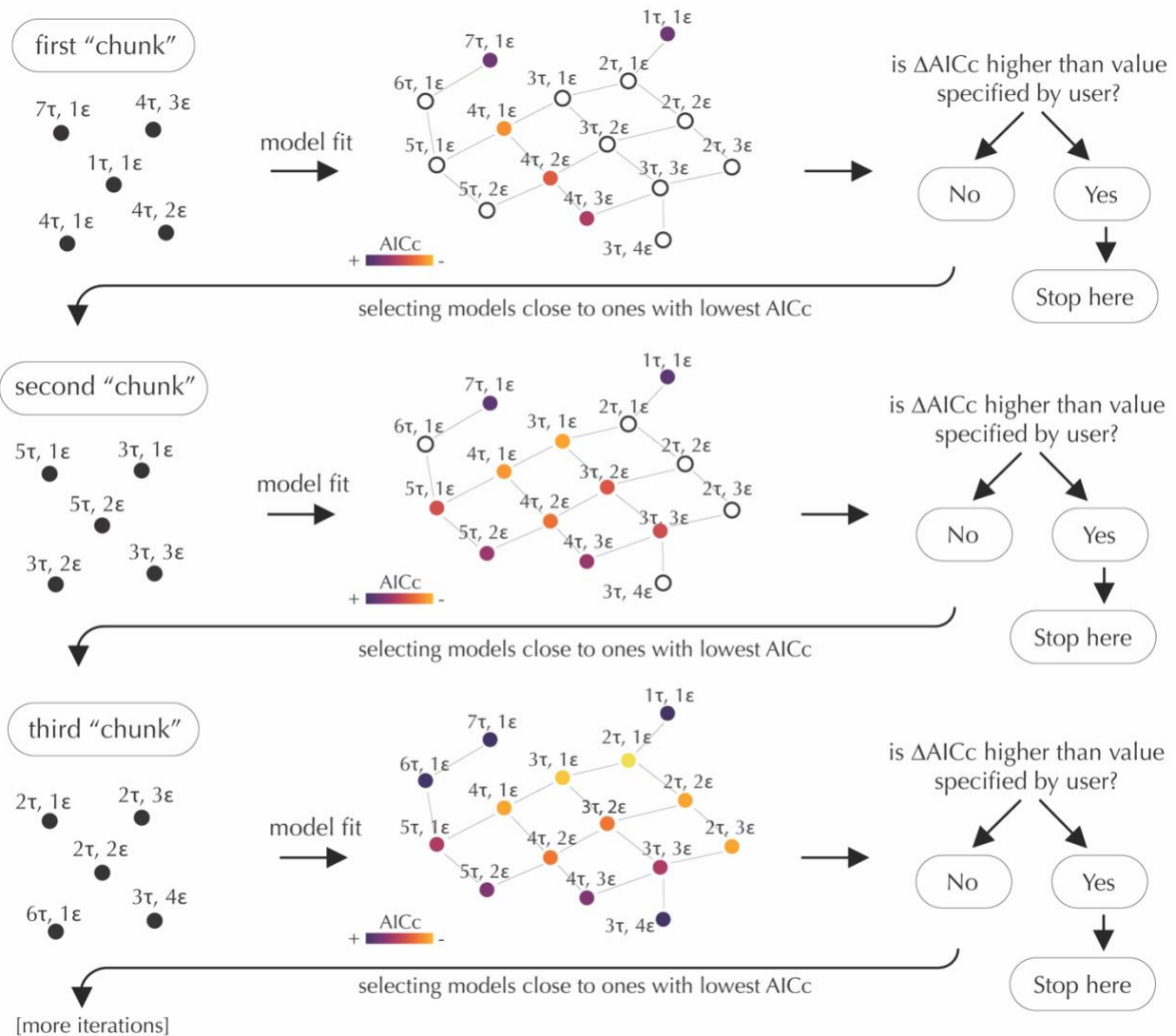


Figure SM1.1: Rationale behind MiSSEGreedy. The search start with a random set of simple models (first "chunk"). After AICc are calculated for this set, the search continues by fitting the models closest to the ones with lowest AICc in previous "chunks". The search continues until the

ΔAIC_c of the new chunk is higher than the threshold specified by the user. Here the search is represented by a “chunk” size of five, where five models are fitted at each time.

References

Beaulieu, J. M., & O’Meara, B. C. (2016). Detecting hidden diversification shifts in models of trait-dependent speciation and extinction. *Systematic biology*, 65(4), 583–601.

<https://doi.org/10.1093/sysbio/syw022>

Burnham, K.P., & Anderson, D.R. (2002). Model selection and multimodel inference: a practical information-theoretic approach. New York: Springer.