

Tempo and Mode in Plant Breeding System Evolution

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APPENDIX A: MODEL RELATIONSHIPS AND FORMULATION

The central technical difficulty in phylogenetic models of cladogenetic character change is accounting for “hidden” speciation events—lineage bifurcations that do not produce a node in the reconstructed phylogeny because one or both daughter clades go extinct before the present or are otherwise not sampled. Previous treatments either ignored hidden nodes by relying on branch length transformations (Mooers et al. 1999; Pagel 1999), or they summarized the effects of hidden nodes by estimating speciation and extinction rates before modeling state changes (Bokma 2002, 2008). The best existing model of character state-dependent diversification for discrete traits (BiSSE; Maddison et al. 2007) does, however, incorporate hidden speciation events directly when computing the likelihood of the observed tip states and tree shape. In this framework, cladogenetic character change can be treated as a Poisson process—just as anagenetic change, speciation, and extinction are—without further assumptions about how its occurrence should scale with phylogenetic branch lengths or nodes.

The model we use to analyze anagenetic and cladogenetic breeding system shifts, ClaSSE with two character states, is equivalent to the BiSSE-ness model (Magnuson-Ford and Otto 2012), a recent extension of BiSSE. We find the ClaSSE parameterization more convenient for our purposes, but the two models produce identical likelihood values for corresponding sets of rates. It is also straightforward to generalize ClaSSE to more than two states. The formulation is given below, and the implementation is available in the *R* package *diversitree* (FitzJohn 2010). With three character states, ClaSSE can then be viewed as a generalization of GeoSSE (Goldberg et al. 2011), a model for the evolution of a character representing geographic range. The relationships among these models are summarized in Table A1.

ClaSSE formulation

We define λ_{ijk} to be the rate of speciation for which a parent lineage in state i produces one daughter lineage in each of states j and k , μ_i to be the rate of extinction from state i , and q_{ij} to

be the rate of transition within a lineage from state i to j , or 0 when $i = j$. For $j \neq k$, one of the parameters λ_{ijk} and λ_{ikj} is set equal to zero because they describe the same process and so can not be estimated separately.

As in BiSSE (Maddison et al. 2007) and all its model relatives, let $D_{Ni}(t)$ be the likelihood that a lineage in state i at time t gives rise to the clade N that is observed, and let $E_i(t)$ be the likelihood that a lineage in state i at time t goes extinct by the present time. The time-evolution of these quantities in the ClaSSE model is described by

$$\frac{dD_{Ni}}{dt} = - \left(\sum_{j,k} \lambda_{ijk} + \sum_j q_{ij} + \mu_i \right) D_{Ni} + \sum_j q_{ij} D_{Nj} + \sum_{j,k} \lambda_{ijk} (D_{Nj} E_k + D_{Nk} E_j) \quad (\text{A1})$$

$$\frac{dE_i}{dt} = - \left(\sum_{j,k} \lambda_{ijk} + \sum_j q_{ij} + \mu_i \right) E_i + \sum_j q_{ij} E_j + \mu_i + \sum_{j,k} \lambda_{ijk} E_j E_k, \quad (\text{A2})$$

where summations over j and k cover all character states. The initial conditions come from the tips of the tree, at $t = 0$: $D_{Ni}(0) = 1$ if the tip is in state i and 0 otherwise, and $E_i(0) = 0$. Computations proceed backwards from the tips towards the root, integrating Eq. A1–A2 along the branches of the tree. At each node C , the likelihoods for its two descendant clades N and M are merged with

$$D_{Ci}(t_C) = \frac{1}{2} \sum_{j,k} \lambda_{ijk} (D_{Nj} D_{Mk} + D_{Nk} D_{Mj}). \quad (\text{A3})$$

At the root, the overall likelihood of the tree and tip states, given the model parameters, is obtained as the sum of the likelihoods for each state weighted by the conditional probability of the root being in the corresponding state (FitzJohn et al. 2009).

Table A1: Relationships among parameters in ClaSSE and other models of the same family. For the parameters of each model indicated (first column), the equivalent parameters in ClaSSE are given (second column), along with a brief description of their meaning (third column). ClaSSE parameters not specified for a model are removed, i.e., fixed equal to zero.

BiSSE ^a or MuSSE ^b		
λ_i	λ_{iii}	speciation for state i
μ_i	μ_i	extinction for state i
q_{ij}	q_{ij}	anagenetic transition from state i to j
BiSSE-ness ^c		
λ_0	$\lambda_{000} + \lambda_{001} + \lambda_{011}$	speciation for state 0
λ_1	$\lambda_{111} + \lambda_{101} + \lambda_{100}$	speciation for state 1
p_{0c}	$(\lambda_{001} + \lambda_{011})/(\lambda_{000} + \lambda_{001} + \lambda_{011})$	cladogenetic state change from state 0
p_{1c}	$(\lambda_{101} + \lambda_{100})/(\lambda_{111} + \lambda_{101} + \lambda_{100})$	cladogenetic state change from state 1
p_{0a}	$\lambda_{001}/(\lambda_{001} + \lambda_{011})$	asymmetric cladogenetic change from state 0
p_{1a}	$\lambda_{101}/(\lambda_{101} + \lambda_{100})$	asymmetric cladogenetic change from state 1
μ_0	μ_0	extinction for state 0
μ_1	μ_1	extinction for state 1
q_{01}	q_{01}	anagenetic transition from state 0 to 1
q_{10}	q_{10}	anagenetic transition from state 1 to 0
GeoSSE ^d		
s_A	$\lambda_{112}, \lambda_{222}$	speciation within region A
s_B	$\lambda_{113}, \lambda_{333}$	speciation within region B
s_{AB}	λ_{123}	between-region speciation
x_A	μ_2, q_{13}	extinction/extirpation from region A
x_B	μ_3, q_{12}	extinction/extirpation from region B
d_A	q_{21}	dispersal/range expansion from region A
d_B	q_{31}	dispersal/range expansion from region B

^aBinary State Speciation and Extinction, Maddison et al. 2007

^bMulti-State Speciation and Extinction, FitzJohn in press

^cBiSSE-node enhanced state shift, Magnuson-Ford and Otto 2012

^dGeographic State Speciation and Extinction, Goldberg et al. 2011

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APPENDIX B: ALTERNATIVE MODEL FITTING

We also conducted a maximum likelihood, rather than Bayesian, analysis of breeding system evolution and lineage diversification in Solanaceae. Results are summarized in Table B1, for comparison with Table 1. Relative support for the six models is similar when judged with AIC rather than Bayes factors. Maximum likelihood parameter estimates are also similar to those from Bayesian inference, except for the reversible models allowing state-dependent diversification (*classe-rev* and *bisse-rev*).

The source of this difference in parameter estimates is bimodality in the likelihood surface. A single clear peak exists under the irreversible forms of ClaSSE and BiSSE. This same peak also appears in their reversible forms, although it is very narrow along the additional axes of λ_{CCI} (for *classe-rev*) and especially q_{CI} . The reversible models also show a second peak, corresponding to a set of parameter values that allows substantial regain of SI, and correspondingly higher rates of (anagenetic) SI loss, SC speciation, and SC extinction, and lower rates of SI speciation and SI extinction. This second peak is lower but broader than the first, particularly along the λ_{CCI} and q_{CI} axes. The two sets of parameter values corresponding to the two peaks collapse, however, to unimodal posterior distributions of net diversification for each state ($\lambda_{III} + \lambda_{IIC} - \mu_I$ and $\lambda_{CCC} + \lambda_{CCI} - \mu_C$) and of net state change ($q_{IC} + \lambda_{IIC} - q_{CI} - \lambda_{CCI}$).

The relative support for each of these two peaks in the reversible models depends on the model-fitting methodology. Maximum likelihood identifies the first, taller peak, and so the rate estimates under *classe-rev* and *bisse-rev* are similar to those under the irreversible forms of those models (Table B1). Bayesian inference gives more weight to the peak with the greater area under it, which in this case is the second peak. Rate estimates under *classe-rev* and *bisse-rev* thus include a moderate amount of SI regain (Table 1). Even so, the *classe-irr* model is preferred overall, consistent with the independent evidence that SI has not been regained in this family, and with the important role of cladogenesis in the loss of SI.

Table B1: Model fitting results in a maximum likelihood framework. Compare with Table 1, which shows conclusions under Bayesian inference. Relative model supports are similar under the two statistical frameworks, with classe-irr being preferred over all. Parameter estimates are also similar, except for classe-rev and bisse-rev.

Model	λ_{III}	λ_{CCC}	λ_{IIC}	λ_{CCI}	μ_I	μ_C	q_{IC}	q_{CI}	$\ln L$	ΔAIC
classe-irr	2.6	4.9	0.46	—	2.6	5.1	1e-7	—	-937	0
classe-rev	2.6	4.9	0.28	0.04	2.9	4.9	1e-6	1e-7	-936	3.4
bisse-irr	3.1	5.2	—	—	2.6	5.4	0.48	—	-949	23.4
bisse-rev	3.0	5.3	—	—	2.7	5.3	0.31	0.05	-942	7.7
mk-irr	4.2	—	—	—	4.1	—	0.12	—	-985	91.4
mk-rev	4.2	—	—	—	4.1	—	0.17	0.09	-947	16.3

Maximum Likelihood Rate Estimates on Simulated Trees

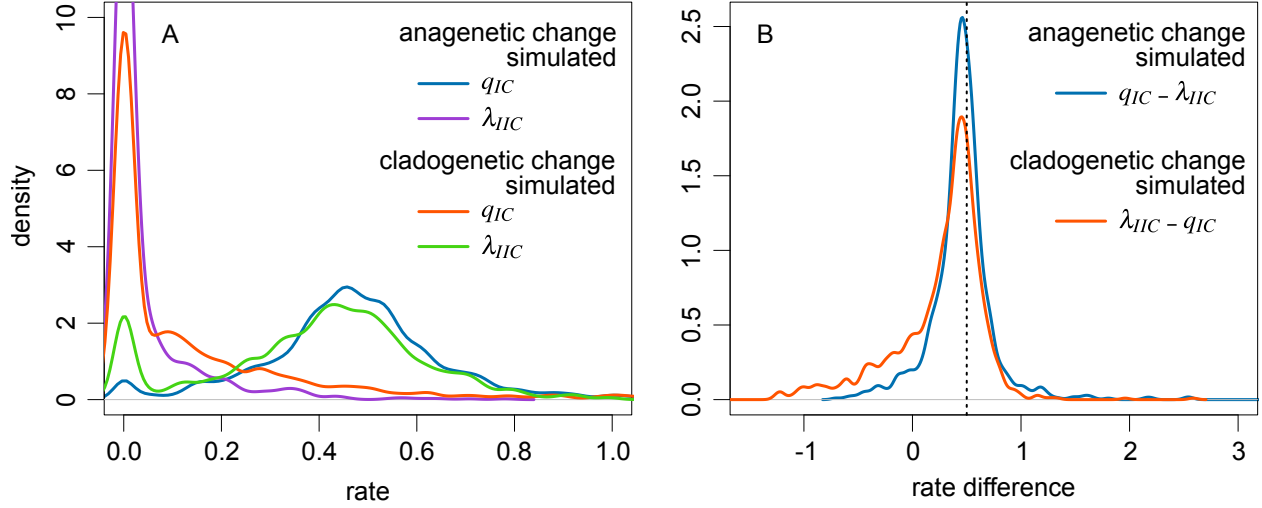


Figure S1: Maximum likelihood estimates of character change rates on simulated trees. Trees were simulated with unidirectional character change that was either purely anagenetic (blue, purple; $\lambda_{III} = 3$, $\lambda_{CCC} = 5$, $\lambda_{IIC} = \lambda_{CCI} = 0$, $\mu_I = 2.41$, $\mu_C = 5.24$, $q_{IC} = 0.5$, $q_{CI} = 0$) or purely cladogenetic (orange, green; same parameter values except for $\lambda_{III} = 2.5$, $\lambda_{IIC} = 0.5$, $q_{IC} = 0$). For 1000 trees under each of these two simulation scenarios, smoothed histograms are shown for rate estimates obtained by fitting the classe-irr model. (A) Estimates of anagenetic (q_{IC}) and cladogenetic (λ_{IIC}) character change rates. Values displayed to the left of zero are merely an artifact of smoothing; rate estimates are constrained to be non-negative. (B) Estimates of the difference between anagenetic and cladogenetic character change rates. The vertical dotted line marks the true value of this difference.