

1 **Running head:** REVERSIBLE-JUMP INFERENCE OF ADAPTIVE SHIFTS

2 A novel Bayesian method for inferring and interpreting the
3 dynamics of adaptive landscapes from phylogenetic comparative
4 data

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9

ABSTRACT

10 Our understanding of macroevolutionary patterns of adaptive evolution has greatly increased with the
11 advent of large-scale phylogenetic comparative methods. Widely used Ornstein-Uhlenbeck (OU)
12 models can describe an adaptive process of divergence and selection. However, inference of the
13 dynamics of adaptive landscapes from comparative data is complicated by interpretational difficulties,
14 lack of identifiability among parameter values and the common requirement that adaptive hypotheses
15 must be assigned *a priori*. Here we develop a reversible-jump Bayesian method of fitting multi-optima
16 OU models to phylogenetic comparative data that estimates the placement and magnitude of adaptive
17 shifts directly from the data. We show how biologically informed hypotheses can be tested against this
18 inferred posterior of shift locations using Bayes Factors to establish whether our *a priori* models
19 adequately describe the dynamics of adaptive peak shifts. Furthermore, we show how the inclusion of
20 informative priors can be used to restrict models to biologically realistic parameter space and test
21 particular biological interpretations of evolutionary models. We argue that Bayesian model-fitting of
22 OU models to comparative data provides a framework for integrating of multiple sources of biological
23 data—such as microevolutionary estimates of selection parameters and paleontological
24 timeseries—allowing inference of adaptive landscape dynamics with explicit, process-based biological
25 interpretations.

26

INTRODUCTION

27 The phenotypic adaptive landscape has been widely used as the conceptual foundation for studying
28 phenotypic evolution across micro- to macroevolutionary scales (Arnold et al. 2001). The concept has
29 been applied to microevolutionary studies of selection (Lande and Arnold 1983), studies of
30 paleontological time-series (Simpson 1944, 1953; Hunt et al. 2008; Reitan et al. 2012) and to stochastic
31 models of trait evolution fit to phylogenetic comparative data (Hansen 1997; Butler and King 2004;
32 Hansen et al. 2008; Uyeda et al. 2011; Eastman et al. 2013). Consequently, the adaptive landscape has
33 the potential to unite micro to macroevolution into a single cohesive theoretical framework (Arnold
34 et al. 2001; Hansen 2012). However, a major disconnect between microevolutionary and
35 macroevolutionary formulations of adaptive landscapes is that microevolutionary studies typically
36 examine static landscapes, whereas macroevolutionary patterns result from the dynamics of adaptive
37 peak movement over long evolutionary timescales (Gavrillets 2004; Hansen 2012). While
38 macroevolutionary models fit to phylogenetic comparative data almost certainly describe the
39 cumulative dynamics of adaptive landscapes, these phenomenological models are disconnected from
40 adaptive landscapes at shorter timescales, and thus, become difficult to interpret in terms of biological

41 processes. Synthesis will require a unification of theory and data across scales that allows inference of
42 the dynamics of the movement of adaptive landscapes directly from macroevolutionary data (Uyeda
43 et al. 2011).

44 Existing models of adaptive evolution at macroevolutionary scales typically rely the
45 Ornstein-Uhlenbeck (OU) model of trait evolution (Hansen 1997; Butler and King 2004), which has a
46 strong connection to the concept of adaptive landscapes (Lande 1976). Fitting OU models to
47 macroevolutionary data allows researchers to test hypotheses regarding the existence of distinct
48 phenotypic optima between groups of species (Butler and King 2004; Beaulieu et al. 2012) and more
49 generally, infer evolutionary regressions between phenotypic traits and predictor variables (Hansen et al.
50 2008; Hansen and Bartoszek 2012). Hansen (1997) introduced the method to phylogenetic comparative
51 methods as a means to test specific adaptive hypotheses—such as the hypothesis that phenotypic optima
52 for browsing vs. grazing horses are different. Butler and King (2004) extended this method to test
53 among competing adaptive hypotheses and provided a widely used implementation as an R package
54 (`ouch`). However, `ouch` and other software typically require *a priori* assignment of adaptive hypotheses
55 to the phylogeny, with optima “painted” onto branches according to the researcher’s pre-existing
56 hypotheses (but see Ingram and Mahler 2013). Following model-fitting by maximum likelihood, model
57 selection is used among hypothesized scenarios and the best-fitting model is chosen (Butler and King
58 2004). However, it can be difficult to ascertain whether the specific hypothesis chosen by the researcher
59 is a good hypothesis, or simply better than the tested alternatives. Furthermore, to infer the dynamics
60 of adaptive landscapes themselves, we do not wish to assume a limited set of hypotheses *a priori*, but
61 to estimate the dynamics of phenotypic optima directly from the data. This of course does not mean
62 that we want to throw away biologically informed hypotheses. Rather, we seek a framework for
63 evaluating whether *a priori* hypotheses adequately describe the statistical patterns in the data.

64 Incorporating biological realism into comparative models remains a challenging goal.
65 Statistical models fit to phylogenies are inherently phenomenological, and may be consistent with
66 multiple biological interpretations. For example, Brownian motion (BM) processes can result from
67 neutral genetic drift of trait means, neutral drift of adaptive peaks, or drifting adaptive zones (Lande
68 1976; Felsenstein 1985, 1988). Rate tests derived from these models have generally rejected genetic
69 drift as a model for macroevolutionary patterns (Turelli et al. 1988; Lynch 1990; Hohenlohe and Arnold
70 2008), and simple drift of adaptive peaks seems inconsistent with observed microevolutionary and
71 macroevolutionary data (Estes and Arnold 2007; Uyeda et al. 2011). As with BM models, OU models
72 have an explicitly microevolutionary interpretation in terms of the process of stabilizing selection and
73 genetic drift on static adaptive landscapes (Lande 1976). Alternatively, these optima may represent
74 adaptive zones within which adaptive peaks drift stochastically, or even broad ranges around which

75 dynamically evolving adaptive zones evolve (Hansen 1997). The boundaries between these latter
76 interpretations can become fuzzy, and while a tendency for a species to return to an optimal state is
77 suggestive of adaptive evolution, it remains unclear how fitted models reflect evolutionary processes
78 and patterns. Because of this difficulty, previous authors have tended to use terms such as “adaptive
79 regimes” or “selective regimes” to describe optima fit via OU modeling. These terms only vaguely
80 connect model parameters to the process of adaptive evolution. More specific interpretations of these
81 models will require methods that can more explicitly connect to microevolutionary and paleontological
82 data.

83 We present a Bayesian framework for studying adaptive evolution using multi-optima OU
84 models that attempts to provide solutions to these challenges. We implement a reversible-jump
85 algorithm that jointly estimates the location, number and magnitude of shifts in adaptive optima from
86 phylogenetic comparative data (Green 1995; Huelsenbeck et al. 2000, 2004; Eastman et al. 2011, 2013;
87 Rabosky et al. 2013). We use simulations to demonstrate the effectiveness of this method at identifying
88 the location of shifts and estimating parameters. Furthermore, we demonstrate how the method can be
89 used to compare specific hypotheses, and how informative priors can be incorporated from different
90 data sources to test mechanistic interpretations of phylogenetic patterns of trait divergence. We
91 incorporate these methods into a flexible software package, `bayou`, for the R statistical environment (R
92 Core Team 2014).

93 Our approach has a number of distinct advantages over existing methods. First, the
94 reversible-jump framework will produce a full posterior of credible models and parameter values and
95 therefore incorporates uncertainty in regime number, placement and parameter estimates. This is
96 particularly important when modeling OU processes, as these models often have flat ridges on
97 likelihood space, particularly for the correlated parameters α and σ^2 (Ho and Ané 2013). However,
98 some parameter values along these ridges are inconsistent with particular biological interpretations of
99 the model. A natural way of restricting model exploration to interesting regions of parameter space is
100 to place priors on the parameters. We compare model fits between biologically informed *a priori*
101 hypotheses of adaptive evolution against the full posterior of credible models using marginal
102 likelihoods. From these comparisons, we can conclude whether a particular hypothesis captures the
103 relevant signal of adaptive peak movement in the data. Furthermore, we show how alternative priors
104 and parameterizations of OU models based on different biological interpretations can be compared, and
105 suggest how additional sources of data may be incorporated into analyses. By using informative priors,
106 we can incorporate data on microevolutionary biological processes (e.g. strength of natural selection,
107 population size, genetic variance) and/or constrain the dynamics of the model to be consistent with
108 patterns observed at other biological scales (e.g. stasis, rapid evolution over short timescales, etc.). By

109 doing so, we obtain a clearer picture of what our comparative models are actually measuring and how
110 we can interpret macroevolutionary patterns.

111 METHODS

112 We model phenotypic evolution across phylogenies as an Ornstein-Uhlenbeck (OU) process, which is a
113 mean-reverting continuous-time stochastic process with three parameters describing per unit time
114 magnitude of uncorrelated diffusion (σ^2), the rate of adaptation (α) and the optimum value of the
115 process (θ) according to the stochastic differential equation:

$$d\bar{z} = \alpha(\theta - \bar{z}) + \sigma dW \quad (1)$$

116 where dW is a continuous-time Wiener process and \bar{z} is the trait mean. If $\alpha = 0$, the process
117 reduces to a Brownian motion model of trait evolution. The parameter α is measured in inverse time
118 units while the parameter σ^2 is in units of squared trait units per unit time. An easier way to interpret
119 α is by reparameterizing the value as the phylogenetic half-life (Hansen et al. 2008), which is defined as
120 $\ln(2)/\alpha$ and is measured in time units. It can be interpreted as the amount of time it takes for the
121 expected trait value to get halfway to the phenotypic optimum. Small values of phylogenetic half-life
122 (i.e. large values of α) also have the effect of eroding covariance between species following speciation. A
123 model with a phylogenetic half-life much greater than tree height will thus resemble a BM process,
124 whereas a phylogenetic half-life much shorter than the youngest split on a phylogeny will resemble a
125 white noise process (i.e. residual trait values are completely uncorrelated). We will refer to both α and
126 phylogenetic half-life throughout the manuscript, as doing so will make certain patterns more clear and
127 interpretable. In addition, a useful compound parameter for OU processes is the stationary variance
128 $[V_y = \sigma^2/(2\alpha)]$, which is the equilibrium variance of an OU process evolving around a stationary
129 optimum θ .

130 Multi-optima OU models are modifications of the standard OU model in which adaptive
131 optimum, θ , varies across the phylogeny according to discrete shifts in adaptive regimes (Hansen 1997;
132 Butler and King 2004). However, unlike most previous implementations, we do not fix the number of
133 shifts or their locations on the phylogeny. Instead, we implement a reversible-jump algorithm that
134 estimates the number, location and magnitude of shifts in adaptive optima, while jointly sampling OU
135 parameters. Although we focus on shifting values of θ across the phylogeny, our method can be
136 extended to allow other parameters to differ among regimes (i.e. α and σ^2 , Beaulieu et al. 2012).

137 *Reversible-jump Model*

138 We consider a fully resolved phylogeny with N taxa. We follow Hansen (1997) and Butler and King
139 (2004) and model a multi-optima OU model with discrete adaptive states $\boldsymbol{\theta} = \{\theta_0, \dots, \theta_K\}$, where θ_0 is
140 the optimum at the root and K is the number of shifts between adaptive optima. The locations of
141 shifts between adaptive states is given by a vector of shift locations mapped onto the phylogeny
142 $\mathbf{L} = \{L_1, \dots, L_K\}$ with each L_i corresponding to beginning of an adaptive regime assigned to the
143 optimum θ_i . Given these parameters, the distribution of tip states \mathbf{Y} is multivariate normal with an
144 expectation:

$$E[\mathbf{Y}|Y_0, \alpha, \mathbf{L}, \boldsymbol{\theta}] = \mathbf{W}\boldsymbol{\theta}$$

145 where Y_0 is the root state and \mathbf{W} is a matrix of weights used to calculate the weighted average of
146 adaptive optima, discounted by an exponentially decreasing function that depends on the rate
147 parameter α and the elapsed time since the species evolved under a given adaptive optimum (For a full
148 explanation and derivation, see Hansen 1997; Butler and King 2004). The elements of the
149 variance-covariance matrix for \mathbf{Y} are:

$$Var[Y_i|Y_0, \sigma^2, \alpha] = \frac{\sigma^2}{2\alpha} [1 - e^{-2\alpha t_{0,i}}]$$

150 and

$$Cov[Y_i, Y_j|Y_0, \sigma^2, \alpha] = e^{-\alpha t_{ij}} \frac{\sigma^2}{2\alpha} [1 - e^{-2\alpha t_{0,ij}}]$$

151 where $t_{0,i}$ is the time from the root to species i , t_{ij} is the total time separating species i and j , and $t_{0,ij}$
152 is the total time separating the root and the most recent common ancestor of species i and j .

153 To calculate the likelihood, we assume that $Y_0 = \theta_0$. Alternatively, the likelihood can be
154 calculated assuming a stationary distribution or by estimating Y_0 . However, we found that assuming a
155 stationary distribution resulted in poor mixing when α was small (which is typical during the
156 beginning stages of the MCMC). We use a pruning algorithm to speed computation and calculate
157 conditional likelihood (as in FitzJohn 2012). We use a reversible-jump algorithm to search among
158 varying shift numbers (extitK) and shift locations (\mathbf{L}) (Green 1995; Huelsenbeck et al. 2000, 2004;
159 Eastman et al. 2011; Rabosky et al. 2013). The reversible-jump framework of Green (1995) uses a
160 Metropolis-Hastings algorithm to explore models with varying dimensionality through the course of the
161 MCMC. The amount of time the MCMC spends in a given model is proportional to its posterior
162 probability, thus providing inference on the best supported regime shift placements and magnitudes,
163 while accounting for model uncertainty in all estimated parameters. Proposals in the MCMC are

164 accepted with the general probability:

$$R = \min(1, \text{LikelihoodRatio} \times \text{PriorRatio} \times \text{ProposalRatio} \times \text{Jacobian})$$

165 The proposal ratio and the Jacobian together compose the “Hasting’s ratio”, which is dependent on the
166 specific proposals used, as described below.

167 *Proposals*

168 The proposals to the parameters α , σ^2 and θ_i do not change the dimensionality of the model, and can
169 therefore be updated using standard MCMC proposal mechanisms. We update the parameters α and
170 σ^2 using a multiplier proposal mechanisms, while θ_i parameters are updated using a sliding-window
171 proposal (described in Eastman et al. 2011).

172 The dimensionality of the model can change via either a birth or a death step, which adds or
173 subtracts a regime shift from the model, respectively. A branch is chosen from the phylogeny at
174 random. If the branch currently contains a shift, then a death step is proposed. If the branch does not
175 contain a shift, a birth step is proposed. During a birth step, a location for the shift is drawn from a
176 uniform distribution over the length of the branch. The value of the adaptive optima before and after
177 the shift are simultaneously updated according to the following proposal. A random uniform number
178 (u) between (-0.5,0.5) is drawn. New values of θ are obtained by splitting the value of this random
179 uniform number proportionally to the amount of branch length across the entire tree inherited by each
180 optimum after splitting:

$$\theta'_j = \theta_j - u\delta r'_{j+1}$$

181

$$\theta'_{j+1} = \theta_j + u\delta r'_j$$

182 Where r'_j is the proportion of the branch lengths across the tree that will evolve under θ'_j and r'_{j+1} is
183 the proportion of branch lengths that will evolve under θ'_{j+1} , and δ is a tuning parameter. Thus,
184 whichever optimum inherits the most branch length will have the most conservative proposal, while the
185 optimum that inherits smaller amounts of branch length will have more liberal proposals (i.e. its value
186 will change the most). The new optimum θ'_{j+1} cascades down the phylogeny until it reaches a tip, or a
187 pre-existing shift. The acceptance ratio for the move from parameter set $\Theta_K \rightarrow \Theta_{K+1}$ is then (Green
188 1995; see Online Appendix I for the derivation, which follows Jialin 2012):

$$A(\Theta_K, \Theta_{K+1}) = \frac{p(\mathbf{Y}|\theta_{K+1})p(K+1)(K+1)p(\theta'_i)p(\theta'_{i+1})\delta}{p(\mathbf{Y}|\theta_K)p(K)(2N-2-K)p(\theta_i)} \quad (2)$$

189 Death steps operate in reverse, collapsing two regimes into a single regime. The new value of
190 this proposed regime is a weighted average of the previous two regimes according to the equation:

$$\theta'_j = \theta_j r_j + \theta_{j+1} r_{j+1}$$

191 Consequently, proposed values of optima during death steps are deterministic weighted averages, and
192 the acceptance ratio is simply the inverse of equation (2).

193 In addition to birth and death proposal mechanisms for adding and subtracting regime shifts,
194 we allow shifts to slide along branches without changing the number of parameters in the model with
195 two different proposal mechanisms. The first (*slide1*) allows the position of the shift to move within a
196 branch via a sliding-window proposal mechanism. Proposals are reflected back at the nodes so that the
197 proposed shift location remains on the same branch. A second proposal allows shifts to slide up or
198 down onto neighbouring branches (*slide2*). When this move is proposed, the total number of allowable
199 shifts are counted across the tree for all K shifts. Moves are not allowed to branches that already
200 contain shifts, or tipward at the tips and rootward at the root. Each allowable move has an equal
201 probability of being chosen. For example, a shift surrounded by three empty branches (two tipward and
202 one rootward) has three times the probability of being chosen for the proposal than a shift surrounded
203 by only one empty branch and two branches with existing shifts. Once a branch with a shift is chosen,
204 one of the available neighbouring branches is chosen with equal probability. The proposed location of
205 the shift on the new branch is drawn from a uniform distribution and regimes are cascaded tipward
206 until reaching an existing shift.

207 The proposal probability for the regime birth-death move was set at a fixed value (in our study
208 we used $\phi_{bd} = 0.45$). The remaining proposal probability was divided between the five other proposal
209 mechanisms: the two sliding shift proposals (*slide1* and *slide2*) and proposals to α , σ^2 and θ . We
210 placed equal proposal weight on updating α and θ , which were set to 3.5 times the proposal weight of
211 updates to σ^2 and the two sliding shift proposals. We chose these values based on preliminary
212 explorations which indicated that these proposal probabilities resulted in roughly equal effective sample
213 sizes for all parameters. Thus, for $0 < K < K_{max}$, we set $\phi_\alpha = \phi_\theta = 0.1925$ and
214 $\phi_{\sigma^2} = \phi_{slide1} = \phi_{slide2} = 0.055$. When $K = 0$, both *slide1* and *slide2* are disallowed, and the proposal
215 probabilities for these two moves are divided evenly between the updates to α , σ^2 and θ .

216 Each shift in our model leads to a unique adaptive optimum. In other words, we do not allow
217 convergence of adaptive regimes in our reversible-jump model (though such models may be fit in bayou
218 with a fixed number of parameters without a reversible-jump proposal). This is because satisfying the
219 “detailed balance condition” of the reversible-jump MCMC requires both forward and reverse proposals

220 to calculate the acceptance probability (Green 1995). However, under convergent regimes, a new shift
221 added to the tree can actually reduce the number of shifts (K) by replacing multiple downstream
222 transitions to θ_i in a single move. Since the reverse move would require several proposal steps rather
223 than one, satisfying the detailed balance condition is substantially more complex. It is likely that clever
224 proposal mechanisms can be designed to adequately explore across models with and without convergent
225 regimes with sufficient mixing, but we leave this to future work. Regardless, our primary goal is not to
226 estimate the amount of convergence (which remains quite challenging for single-trait datasets, but see
227 Mahler et al. 2013), but instead to provide a flexible Bayesian framework for exploring among
228 alternative hypotheses and for incorporating prior information to test specific biological interpretations
229 of comparative models. Furthermore, the amount of convergence can be assessed post-hoc by the degree
230 of overlap among regimes, or by comparing the marginal likelihoods among fixed convergent regimes.

231 *Priors*

232 We placed a prior on the number of shifts between adaptive regimes using a conditional Poisson
233 distribution, with a maximum number of shifts equal to half the number of tips in the phylogeny.
234 Informative priors for this distribution may be taken, for example, from the duration of chronospecies
235 or genera in the fossil record. These may suggest the typical duration of a static adaptive regime.
236 Alternatively, a given adaptive hypothesis may suppose only a few adaptive shifts across a radiation of
237 species.

238 We placed a normal prior on adaptive optima. Setting a prior on adaptive optima allows us to
239 avoid fitting models in unrealistic regions of parameter space that allow species to track unrealistically
240 distant adaptive optima. For example, if we are studying primate body size evolution, it may be
241 reasonable to take the prior for the adaptive optima of body sizes by using the distribution of body
242 sizes across all terrestrial mammals. Alternatively, we may place the prior based on how distant the
243 optima will be from any extant species. Thus, the prior on the optima would be based on both the
244 observed range of phenotypes in the data being studied plus the prior belief in how distant any given
245 species is from its adaptive optimum. In our model, shifts between adaptive regimes can occur in any
246 region of parameter space. Future implementations could penalize unreasonably large shifts between
247 adaptive regimes by modeling shifts in optima as a compound point process. Landis et al. (2013)
248 proposed fitting models that include these so-called “Levy processes” that model rare jumps in
249 phenotypic space where the rate and magnitude of jumps follow a regular stochastic process model.
250 Integrating Levy models and OU models would add considerable realism to models of phenotypic
251 evolution and allow statistical inference on the rates and distribution of the shifts themselves, but is
252 beyond the scope of the current paper.

253 Finally, we assign an equal probability of each branch having a shift, with no more than one
254 shift allowed per branch. A more realistic model may allow the probability of shifts between regimes to
255 occur proportional to the length of the branch, and to allow multiple shifts per branch. We leave these
256 enhancements to future work. Shifts may occur anywhere on a branch with a uniform probability
257 distribution, thereby allowing uncertainty in the location of the shift to affect estimation of other
258 parameters.

259 *Simulation study*

260 To assess the performance of the method given the assumptions we have made above, we conducted a
261 simulation study. Phylogenies were simulated under a pure-birth process using the R package TreeSim
262 (Stadler 2011) with 64 tips (except for when the effect of sample size was being examined, see below)
263 and a constant birth rate of 0.1. For all simulations, the resulting phylogenies were scaled to unit
264 height and starting parameters were drawn from the prior distribution to initialize the chain. Two
265 independent chains were run for at least 200,000 generations, with a thinning interval of 20 and the
266 first 60,000 generations discarded as burnin. We estimated Gelman's R-statistic for each parameter,
267 which compares the within- to between-chain variance to evaluate convergence (Gelman and Rubin
268 1992). Values of R close to 1 indicate that the two chains are not distinguishable, whereas high values
269 (we used a cutoff of $R = 1.1$) indicate non-stationarity of the chains.

270 We tested the performance of the method across a range of parameter values varying a single
271 parameter at a time and using broad, weakly informative priors. For the standard simulation we used
272 $\alpha=3$ (phylogenetic half-life = 23.1% of the total tree height), $\sigma^2 = 3$ (stationary variance = 0.5), $K =$
273 9 (10 selective optima including the root) and a root value of 0. Shifts were randomly placed on
274 available branches at regular intervals separated by 0.1 units of tree height. At each shift, new optima
275 were drawn from a normal distribution with mean = 0 and sd = 3. Each parameter was varied
276 independently for a series of simulations while all others were held constant at the above values.
277 Parameters were examined over the following ranges: Phylogenetic half-life ($\ln(2)/\alpha$; in units of tree
278 height) = (0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.75, 1, 2, 10), $\sigma^2 =$ (0.1, 0.5, 1, 2, 3, 5, 10, 25, 50), clade
279 size = (32, 64, 128, 256, 512, 1064) and $K =$ (1, 5, 7, 8, 9, 10, 11, 13, 20, 50).

280 We used the simulation-based posterior quantile test of Cook et al. (2006) to validate our
281 implementation. This powerful method relies on the distributional properties of Bayesian posteriors
282 when simulation parameters are drawn from the prior distribution. Specifically, if the software and
283 model are correctly formulated, then posterior quantiles should contain the true parameter value in the
284 corresponding percentage of simulations (e.g. a 50% posterior quantile will contain the true parameter

285 value in 50% of the simulations). Although validation using the posterior quantile test does not
286 guarantee that an implementation is correct, it is a highly sensitive method of testing the null
287 hypothesis that the software is working correctly (Cook et al. 2006). Parameters were simulated from
288 the prior distribution, which were set as follows: $P(\alpha) \sim \text{LogNormal}(\ln \mu=0.25, \ln \sigma=1.5)$; $P(\sigma^2) \sim$
289 $\text{LogNormal}(\ln \mu=0.25, \ln \sigma=0.1)$; $P(\theta_i) \sim \text{Normal}(\mu = 0, \sigma = 3)$; $P(K) \sim \text{Conditional Poisson}(\lambda = 10,$
290 $K_{max} = 32)$. Data were simulated for each set of parameters on a simulated phylogeny (following the
291 same simulation parameters described above) and posterior distributions were estimated. The quantile
292 of the true parameters are determined within the estimated posterior distribution. If the posterior
293 distribution is estimated correctly, then the distribution of these quantiles across simulations should
294 follow a uniform distribution (Cook et al. 2006). We tested each of the parameters α , σ^2 , K and θ_0
295 (the root optimum) for deviations from a uniform distribution using a Kolmogorov-Smirnov test.
296 Significant deviations would indicate that the method incorrectly estimates the posterior distribution.

297 We used these same simulations from the posterior quantile test (in which simulation
298 parameters were drawn from the prior distribution) to evaluate the performance of the method in
299 assessing the location of shifts and magnitude of shifts. Thus, we assessed the power of the method to
300 detect shifts across a broad range of possible parameter combinations. Posterior probabilities were
301 calculated for each branch by counting the proportion of posterior samples with a shift on that branch,
302 after excluding the burn-in phase. Consequently, a posterior probability of 0.5 would indicate that half
303 the posterior sample contained that shift on a given branch. We then plotted the posterior probability
304 of each branch against two values. The first we term “regime divergence” and is defined as the log of
305 the ratio between the shift magnitude and the stationary variance of the OU process. The second we
306 term the “scaled age” of the shift, which is the log of the ratio between the age of the shift (in time
307 units before present) and the true phylogenetic half-life value. We expect a relationship between these
308 two ratios and our power to detect shifts because 1) higher values of regime divergence indicate a more
309 dramatic shift relative to the variation within a selective regime and 2) the scaled age is a measure of
310 how recent the shift is relative to the speed of the OU process. A very low scaled age value would
311 indicate that very little time has elapsed for the descendants of this shift to adapt to the new regime,
312 thus resulting in low power to detect the shift. Conversely, high values would indicate that ample time
313 has elapsed for species to equilibrate on their new adaptive optimum. We estimated a contour plot of
314 the posterior probability values for all branches across simulation against regime divergence and scaled
315 age by kriging. In addition to the above analyses, we conducted a number of additional simulations to
316 assess the power of the method to accurately recover shift number, magnitude and location, including
317 an extensive prior sensitivity analysis for the prior on the number of shifts. A detailed description of
318 these simulations can be found in the Online Appendix III.

319 *Testing specific biological interpretations of evolution*

320 One of the strengths of OU models is that the process and parameters describe the dynamics of
321 adaptive evolution in biologically interpretable quantities. However, whether or not we can interpret
322 OU models fit to the deep timescales of phylogenetic comparative data as—for example—stabilizing
323 selection and genetic drift, has generally been addressed with only qualitative arguments. The utility
324 (and in some cases drawback) of the Bayesian approach is that it allows/requires the use of priors on
325 parameter values. We use this feature in `bayou` to allow the specification of informative priors on
326 parameter values that correspond to particular biological interpretations of the OU process. For
327 example, rather than specifying a prior on α and σ^2 , we may instead have prior information on
328 phylogenetic half-life or stationary variance. Reparameterization of the model in this way would
329 provide a useful way to incorporate prior information on the width of niches, adaptive peaks, adaptive
330 zones or the rate of adaptation toward a phenotypic optimum.

331 We use the quantitative genetic model of Lande (1976), who showed that genetic drift around a
332 stationary Gaussian adaptive peak results in a OU process with parameters:

$$\Delta\bar{z} = \frac{h^2 V_P}{\omega^2 + V_P} (\theta - \bar{z}) + \sqrt{\frac{h^2 V_P}{N_e}} dW \quad (3)$$

333 where h^2 is the trait heritability, V_P is the phenotypic variance, ω^2 is the width of the adaptive
334 landscape, and N_e is the variance effective population size. We allow specification of this model in
335 `bayou` and use informative priors on these parameters to constrain the model to realistically reflect this
336 particular biological interpretation. Note that the branch lengths of the phylogeny should be expressed
337 in number of generations in order to fit such a model. Furthermore, we assume that all parameters are
338 constant across the phylogeny, an assumption that is likely to be violated.

339 To test the utility of this method, we compared models fit using either an unconstrained
340 standard OU parameterization (OU_{Free}) or a quantitative genetic Lande model parameterization (QG)
341 with priors taken from compilations of empirical estimates typical for linear body size traits on the log
342 scale [Table 1; similar to the approach of Estes and Arnold (2007), but in an explicitly Bayesian
343 framework]. While the priors for the OU_{Free} model were chosen to have a majority of the prior density
344 centered on values of parameters typical of comparative data, effort was made to make them broad
345 enough to also have a some significant prior density on the values generated under Lande-model priors.
346 As before, we simulated 64-taxa trees, but scaled trees to 50 million years old and a generation time of
347 5 years. Simulated data were drawn by drawing parameter values from either the QG or OU_{Free} prior
348 distributions. We included normally distributed measurement error in both the simulation and

349 estimation of the data, with a error variance of $\sigma_\epsilon^2 = 0.05^2$.

350 To compare model fits to the simulated data, we estimated marginal likelihoods under each
351 model using stepping-stone sampling of models fit to either the OU_{Free} or QG parameterizations (Fan
352 et al. 2011). These marginal likelihoods were then used to compute Bayes Factors for model selection
353 (Kass and Raftery 1995). Briefly, the stepping-stone method runs a sequence of MCMC simulations to
354 estimate “power posterior” distributions sequentially stepping from a reference distribution (we used
355 uncorrelated multivariate distributions with parameters estimated from the posterior distribution) to
356 the posterior distribution (Fan et al. 2011). Each power posterior is used as an importance density to
357 estimate a series of ratios of normalizing constants, the product of which provides the ratio of the
358 known reference distribution and the marginal likelihood (Xie et al. 2011). We used a total of 12 steps
359 along the path from the reference distribution to the posterior for each stepping-stone MCMC and ran
360 each step for 500,000 generations. This was done for 10 datasets simulated from the prior for each
361 model. Distributions of Bayes Factors were then compared across model fits to evaluate the degree of
362 support for a specific biological interpretation of the model under different simulation parameters.

363 *Test Case: Chelonian carapace evolution*

364 The wide variation in body sizes across extant chelonians (tortoises and turtles) has been hypothesized
365 to result from a number of causes, including gigantism resulting from marine and island habitats that
366 are thought to remove evolutionary constraints on body size (Arnold 1979). Jaffe et al. (2011) explored
367 the evolution of the length of the carapace (i.e. the dorsal shell) in a phylogeny of 226 extant chelonians
368 using traditional likelihood approaches by fitting multi-optima OU models to the data using `ouch`
369 (Butler and King 2004). The best-fitting model in Jaffe et al. (2011) assigned four separate regimes to
370 freshwater, mainland-terrestrial, island-terrestrial, and marine species of turtles (which they called the
371 ‘OU2’ model; we will refer to the model as the $OU_{habitat}$ model). This model was compared to a
372 limited set of alternative hypotheses, including BM, a single-optimum OU model, and several models
373 which collapsed various combinations of the four regimes in the $OU_{habitat}$ model. From these results,
374 Jaffe et al. (2011) concluded that there was a strong signal in the data supporting a shift to larger size
375 optima in chelonians in marine and island habitats. Parameter estimates from the study suggest that
376 body size evolves slowly toward these new optima, with phylogenetic half-lives on the order of 15-20
377 million years (7-10% of tree height). This same dataset served as a test case for a reversible-jump
378 algorithm that explored the potential for shifts in BM rate parameters (Eastman et al. 2011). The
379 relaxed BM model (rBM) uses a reversible-jump framework to find shifts in evolutionary rates in a
380 manner very similar to `bayou`. For the Jaffe dataset, Eastman et al. (2011) found shifts in evolutionary

381 rates between several groups of turtles and tortoises, including increased rates in Testudinidae
382 (tortoises) and Emydidae (pond turtles). Note that we discovered an error in the acceptance ratio of
383 the rBM model in previous versions of the R package `auteur` (Eastman et al. 2011). We provide the
384 corrected acceptance ratio for the rBM model in Online Appendix II, which has been updated for the
385 implementation of the rBM model in the R package `geiger` (versions 1.99 and greater, Harmon et al.
386 2008). Because the Eastman et al. (2011) model detects rate-shifts not mean-shifts, it is not well-suited
387 for testing hypotheses about directional adaptation in a clade to an optimal state. We instead fit a
388 related, recently developed model of phenotypic shifts in a BM framework that combines "jumps" or
389 mean-shifts with a standard BM (bm-jump model, Eastman et al. 2013). Note that this model is
390 distinct from the models implemented in `bayou`, because mean-shifts under the bm-jump model come
391 from a distinct distribution and are best thought of as temporary shifts to high rates of evolution. By
392 contrast, OU models use the same α parameter to control the rate of adaptation to a new optimum
393 before and after a shift, and therefore cannot combine rapid jumps in mean with BM-like evolution.

394 We use the Jaffe et al. (2011) dataset to demonstrate the utility of `bayou`, and to compare to
395 existing approaches. We analyzed the $OU_{habitat}$ model in `bayou` by constraining the location of shifts
396 and regimes to be the same as the model of Jaffe et al. (2011), except we allowed the location of the
397 shift to move freely along the branch (rather than constraining it to occur at the nodes). We replicated
398 maximum likelihood estimates for the $OU_{habitat}$ model to obtain comparable estimates of parameters
399 using the R package `OUwie` (Beaulieu et al. 2012). We then compared this to an unconstrained `bayou`
400 model that allows shifts to be assigned freely among the various branches. Note that these models are
401 not nested, because in the $OU_{habitat}$ model regimes are convergent, whereas in the unconstrained
402 model, each shift is given its own unique adaptive regime. Priors on the parameters in all runs were
403 assigned as follows: $P(\alpha) \sim \text{LogNormal}(\ln \mu = -5, \ln \sigma = 2.5)$; $P(\sigma^2) \sim \text{LogNormal}(\ln \mu = 0, \ln \sigma = 2)$; $P(\theta_i)$
404 $\sim \text{Normal}(\mu = 3.5, \sigma = 1.5)$; $P(k) \sim \text{Conditional Poisson}(\lambda = 15, k_{max} = 113)$.

405 We compared these models by comparing the posterior probabilities of shifts on each branch in
406 the `bayou` unconstrained run to the locations of the shifts in the $OU_{habitat}$ hypothesis. Furthermore, we
407 evaluated overall model support for the constrained vs. the unconstrained model by using
408 stepping-stone sampling using the method of Fan et al. (2011) to estimate Bayes Factors. Note that
409 Bayes Factors can be sensitive to prior specification, especially when one model has a very specific prior
410 specification (e.g. the location and number of shifts are fixed, as in the $OU_{habitat}$ model) and the
411 alternative has a very vague prior (as in the unconstrained `bayou` model). Specifically, vague priors are
412 expected to produce lower marginal likelihoods than more specific priors, and thus these tests favor
413 constrained models. Furthermore, the $OU_{habitat}$ model has fewer parameters than the unconstrained
414 `bayou` model with the same number of shifts due to evolutionary convergence.

415 In addition to comparing the unconstrained and constrained model in a Bayesian framework,
416 we compared our method to the method of Ingram and Mahler (2013) as implemented in the R package
417 **SURFACE**. Our unconstrained model is analogous to the forward-addition procedure of **SURFACE**, and
418 thus we compare parameter estimates and shift locations in both the forward and reverse steps of the
419 **SURFACE** algorithm independently. These two methods differ in that the **SURFACE** algorithm of Ingram
420 and Mahler (2013) relies on stepwise-AIC rather than Bayesian reversible-jump methods to find the
421 location of shifts. While stepwise-AIC methods attempt to find the single, best-fitting model, our
422 method integrates over uncertainty in regime placement and returns a posterior of shift locations that
423 well-describe the data. Finally, we fit the BM-jump model of *auteur*, which fits jumps to a background
424 of constant-rate BM (Eastman et al. 2013). As we described above, this is similar to the **bayou** model,
425 but differs in that jumps are realized instantaneously rather than approaching at a rate determined by
426 α . Thus, these two models may be expected to find similar shift locations and have relatively
427 comparable parameter estimates. As with the **bayou** implementation, we place a conditional Poisson
428 prior on the number of shifts (“jumps”) at $\lambda = 15$.

429

RESULTS

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Simulation study

431 Under most simulation conditions, convergence was reached within 500,000 generations (i.e. Gelman
432 and Rubin’s R reached below 1.1 for all parameter values). When convergence failed to occur within
433 this time frame, it tended to be when shift magnitudes were large relative to the stationary variance of
434 the process (i.e. high regime divergence). This results in steep likelihood peaks and a tendency to get
435 trapped under non-optimal configurations of shifts. A potential solution to this issue, besides running
436 longer and more chains, would be to use Metropolis-Coupled MCMC, which improves mixing by
437 implementing “heated” chains that explore the likelihood surface more efficiently. Interestingly, these
438 instances in which mixing is poorest and convergence is most problematic are the instances in which
439 the model finds the strongest support for regime shifts and estimates their location most reliably
440 (although it may get caught in less parsimonious likelihood peaks than the simulated model).
441 Nonetheless, the model effectively identifies the presence of adaptive peaks shifts, although it may have
442 difficulty determining the exact order of shifts among branches in these instances.

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444 Overall, simulations indicated that parameters are estimated with reasonable accuracy. The
445 diffusion rate parameter σ^2 tends to be slightly underestimated, especially for low phylogenetic half-life
values (i.e. values less than most of the splits in the tree) and overestimated when phylogenetic

446 half-lives are much longer than tree height (Figure 1, A & D). However, for half-life values ranging
447 from around 0.1-2 times tree height, σ^2 is estimated reasonably with a slight bias toward
448 underestimation (Figure 1, D). Phylogenetic half-life tends to be overestimated over most of this range
449 as well (Figure 1, B & E). These two effects balance out, however, and produce reasonable estimates of
450 stationary variance. Increasing number of tips greatly improves estimates of both σ^2 and α and reduces
451 bias (Figure 1, J & K). For small numbers of tips (e.g. 32), there is a tendency to fit models with
452 higher values of phylogenetic half-life (more BM-like) models. This is likely because many shifts occur
453 on branches leading to singletons, resulting in very little power to distinguish the effect of rate
454 parameters (α and σ^2) from shifts (θ).

455 We show that inference becomes problematic when the ratio of the number of tips to the
456 number of shifts decreases below 4, and recommend at a minimum ~ 50 tips. The number of estimated
457 shifts seems are particularly sensitive to the prior when using the conditional Poisson as the prior,
458 despite some influence of the data on the estimation of the number of shifts (Figure 1, C, F, I & L;
459 Online Appendix III). When the number of shifts are large, the method generally results in
460 underestimation of the true number of shifts. This is particularly true when more permissive priors are
461 used (e.g. negative binomial or discrete uniform, Online Appendix III). However, even when the
462 number of shifts is not reliably estimated, parameter estimates for α , σ^2 and branch-specific posterior
463 probabilities were not substantially affected until the number of shifts was large (e.g. 20 shifts on a
464 64-128 taxa phylogeny, Figure 1, G-I; Online Appendix III).

465 Inferences based on branch-specific posterior probabilities were not affected by mis-estimation
466 of the total shift number, as long as the prior allowed a sufficient number of shifts to explain the true
467 model (Online Appendix III). Rather than producing a large number of strongly supported
468 false-positives, strong priors with a large number of expected shifts (e.g. conditional Poisson with
469 $\lambda = 20$) resulted in diffusely elevated branch posterior probabilities across all branches when no high
470 magnitude shifts were present. By contrast, when the prior allows only a few shifts, complex models
471 are poorly fit and the models tend to collapse to BM-like models with mis-estimated parameters. Thus,
472 priors that favor complex models have little effect on inference of shift location and magnitude, whereas
473 conservative priors tend only to fit models with very few shifts, and severely mis-estimate parameters
474 for complex models (see Online Appendix III).

475 Branches on which a shift was simulated have much higher posterior probabilities than
476 branches in which no shift occurred in the true simulation model, even when the number of shifts is
477 over or under-estimated (Figure 2). This is particularly true for small σ^2 and low phylogenetic half-life
478 (Figure 2A & B). This is because low values of σ^2 results in very little trait variation within regimes
479 relative to the divergence between regimes (high regime divergence), and low values of phylogenetic

480 half-life result in rapid adaptation to regimes (high scaled age). As phylogenetic half-life approaches 1
481 (i.e. the tree height), the power to detect shifts is reduced nearly to 0 under the simulation parameters
482 we examined. The number of tips did not significantly affect the posterior probability of correctly
483 identifying a shift (Figure 2D). This is likely because the expected number of tips evolving under a
484 randomly placed adaptive regime increases slowly with increasing number of tips, meaning that adding
485 tips does relatively little to improve estimates of shift parameters (i.e. assuming equiprobable shift
486 locations among branches—regardless of the phylogeny size—results in approximately 50% of randomly
487 placed shifts being placed on terminal branches that contain only one descendant, Ho and Ané 2013).
488 Furthermore, as the number of tips increased, the prior probability of a given branch having a shift
489 decreased. When errors were made and branches with a true shift were assigned low posterior
490 probabilities, this was generally because the shift was assigned with high posterior probability to a
491 neighbouring branch.

492 Simulation of parameters from the prior distribution and subsequent simulation was carried
493 out for 1118 simulations run for 200,000 generations to evaluate posterior quantiles of the simulated
494 parameter values (Cook et al. 2006). A total of 938 of the simulation runs resulted in Gelman’s R
495 statistics less than 1.1 and were used in subsequent analyses. Posterior quantiles of the simulated
496 parameter values for the root (θ_0), the number of shifts (K) and σ^2 were not significantly different from
497 a uniform distribution, as expected if these parameters are estimated accurately and without bias.
498 Posterior quantiles for the α parameter deviated significantly from a uniform distribution ($p = 0.01$,
499 Table 2), tending to be slightly under-estimated ($\sim 54\%$ of true parameter values were estimated to be
500 in the upper 50% quantile of the posterior distribution). This significant deviation may have been
501 affected by issues with convergence rather than implementation error, as α tended to converge slower
502 than other parameters and runs that failed to converge ($\sim 16.1\%$ of simulation runs) had significantly
503 larger values of α ($p < 0.05$), suggesting that systematic removal of non-convergent runs could affect
504 the distribution of posterior quantiles. Regardless, the distribution for α was nonetheless qualitatively
505 quite similar to a uniform (Figure 4). Overall, the method appears to perform quite well at recovering
506 accurate posterior distributions for the estimated parameters.

507 Branches with shifts tend to have high posterior probabilities if the shift magnitude is high
508 relative to the stationary variance and when the age of the shift is much older than the phylogenetic
509 half-life (Figure 3). Specifically, a shift that is 1 phylogenetic half-life old and 1 standard deviation
510 from the stationary distribution away from the previous optimum will have an estimated posterior
511 probability of having a shift of around 0.2, or slightly more than twice the prior probability of a branch
512 having a shift (Figure 3).

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Modeling biological interpretations

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Models simulated under Lande model (QG) priors were decisively favored under a QG parameterization as opposed to an OU_{Free} in 9 out of 10 simulations, with exceedingly high Bayes Factors (Figure 5, mean = 4746.5, sd = 6166.4). Around half of these simulations failed to converge across chains (Gelman and Rubin's $R > 1.1$) after 500,000 generations, and therefore a total of 20 simulations were required to obtain 10 well-estimated Bayes factors. Models simulated under OU_{Free} priors typical of comparative data also resulted in decisive support in all 10 simulations against the Lande model, but Bayes Factors were not nearly as high as those simulated under the Lande model (Figure 5, mean = 46.6, sd = 15.7). The asymmetry results from the known effect of vague priors on Bayes Factors (Kass 1993) when compared to highly specific models. Even so, we observe that we can easily reject certain parameterizations and prior sets over alternatives.

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Chelonia carapace evolution

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The unconstrained bayou model identified a number of highly supported shifts in the posterior distribution (Figure 6). In particular, strong shifts were detected for increased carapace length in the clades that include softshell turtles (family Trionychidae), sea turtles (superfamily Chelonioidae), the genus *Batagur*, the Malaysian giant turtle (*Orlitia borneensis*) and two clades of tortoises (Figure 6). Decreases in size were found in the clade leading to tortoises and most modern turtles, as well as a few moderately support shifts across the tree, such as the tortoise clade including *Geochelone elegans* and *Geochelone platynota*. Posterior distributions of parameter values were much narrower than the prior distributions, and indicate substantial information in the data driving the estimation of these parameters. Phylogenetic half-lives were relatively short compared to the height of the tree (posterior median = 3.94 my) indicating that after accounting for adaptive regimes, very little phylogenetic covariance remained among species in the phylogeny. This is in contrast to the $OU_{habitat}$ model, which estimated significantly higher values of phylogenetic half-life and lower values of σ^2 (Figure 7).

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Support for the unconstrained bayou model over the Bayesian $OU_{habitat}$ model was very strong, with a $2 \ln BF = 15.24$ (Kass and Raftery 1995, ; Table 3). Only one shift (leading to sea turtles) identified in the $OU_{habitat}$ model was identified as strongly supported in the posterior of the unconstrained bayou model (Figure 6), while SURFACE and auteur's bm-jump model found more comparable shift locations. We conclude that while the $OU_{habitat}$ model is better than many models, it is not a representative model from the posterior distribution obtained from bayou. Instead, the hypothesis proposed by Jaffe et al. (2011) captures only a few of the relevant statistical features of the data. The $OU_{habitat}$ model also had higher estimates for both the phylogenetic half-life and for

545 stationary variance, likely because multiple adaptive regimes were combined into single adaptive
546 regimes, resulting in inference of broader adaptive zones, and a weaker rate of adaptation.

547 SURFACE runs identified most of the same shifts that were found in bayou, as well as
548 considerable amounts of convergence. However, more shifts were identified, likely due to the prior on
549 the number of shifts (SURFACE identified 33 shifts, while the prior on the number of shifts in the bayou
550 runs was only 15). Estimates of adaptive optima, θ , were extremely distant in the best-fitting SURFACE
551 models, and estimates of phylogenetic half-life were correspondingly considerably larger than the
552 estimates from bayou (Table 3).

553 DISCUSSION

554 *Bayesian Inference of Adaptive Regimes*

555 In this study, we have shown how Bayesian inference of adaptive regimes fit to multi-optima OU
556 models provides a flexible framework for testing evolutionary hypotheses. Bayesian OU models have
557 had limited application to trait evolutionary studies (but see Reitan et al. 2012, for layered OU models
558 applied to fossil timeseries data), but offer a number of distinct advantages over existing methods.

559 First, our method integrates over uncertainty in regime placement and allows inference of the
560 location, magnitude and number of adaptive shifts. Based on our simulation results we find that
561 inference on the number of shifts is more difficult as estimation of this parameter tends to heavily
562 influenced by the prior distribution. However, other parameters in the model are well-estimated and
563 the method correctly identifies the location of most shifts in the phylogeny so long as the number of
564 shifts is not large ($K > 25\%$ the number of tips). The probability of correctly identifying a shift
565 increases with the magnitude and age of adaptive regimes. Because low magnitude, recent shifts of
566 little effect can always be added to the model, inference should focus on the branch posterior
567 probabilities themselves rather than the total shift number (see Online Appendix III).

568 Second, the great advantage of OU models is their compatibility with our understanding of the
569 evolutionary process (Hansen 1997; Hansen et al. 2008). On the other hand, many of the statistical
570 properties of OU models can complicate inference resulting from inconsistent estimators and lack of
571 identifiability (which has been shown for the case when the root state is drawn from a stationary
572 distribution, see Ho and Ané 2013). We show how Bayesian implementation of these models allows a
573 full exploitation of the biological realism of OU models by allowing the use of informative priors that
574 constrain the model to biologically realistic values while simultaneously alleviating the some of the
575 statistical issues of OU model-fitting, such as the existence of likelihood ridges that extend into regions

576 of unrealistic parameter space. Furthermore, we demonstrate how the model can be used to explicitly
577 test alternative biological interpretations by testing alternative parameterizations of the models. Note
578 that no method, however, will retrieve an automatic determination of whether a model is correct or
579 not, only whether the correlative pattern and model is consistent with a given biological interpretation.
580 The discretion of the researcher is needed to adequately interpret the reasonableness of the results
581 produced by `bayou`.

582 Just as a clear understanding of the mechanisms behind molecular evolution have
583 revolutionized methods of phylogenetic inference (Kimura 1980, 1984; Felsenstein 1981), additional
584 sources of data can trigger effective, and informative, methods of inference for phenotypic traits
585 (Pennell and Harmon 2013). Our results demonstrate how models consistent with a quantitative
586 genetic interpretation can be identified statistically from other interpretations of OU models. Our
587 comparisons of simulated OU_{Free} vs. QG models are somewhat contrived in that parameters were
588 drawn directly using informative priors that were subsequently used as priors for model-fitting—an
589 optimal scenario that is unrealistic when fitting real data. Furthermore, priors for the QG model were
590 set to correspond to parameters estimated for body size data, a trait known to be unlikely to follow the
591 QG model over million-year timescales (Lynch 1990; Hansen 1997; Butler and King 2004; Uyeda et al.
592 2011). Consequently, it is unsurprising we can obtain such dramatic support for the generating model
593 when comparing QG and OU_{Free} parameterizations. Nevertheless, the QG model may be appropriate
594 to apply to traits that are known to be more constrained, have lower additive genetic variances, if
595 selection is known to be quite weak or if the underlying dynamics of adaptive landscapes are
596 well-described by the model of peak movement. The potential for incorporating prior information is
597 not limited to QG data. OU models have been effectively implemented to fit to fossil timeseries on
598 timescales intermediate between microevolutionary, and phylogenetic scales (Hunt 2007, 2008, 2013;
599 Reitan et al. 2012). The possibility of uniting these different data sources using either a single,
600 phylogeny-based modeling framework, or by using the results of models fit to fossil data to inform the
601 priors for comparative data (for example) provides rich avenue for unification of microevolutionary,
602 fossil and macroevolutionary data.

603 Some may view the reversible-jump framework proposed in this study to be a data-mining tool
604 that will lead to over-fitting of non-biologically relevant statistical noise. We agree that biologically
605 informed *a priori* hypotheses should not be thrown out in any analysis and should be preferred to *a*
606 *posteriori*, non-biologically based statistical models. However, we demonstrate one way to unite these
607 approaches by comparing biologically informed *a priori* hypotheses to the posterior distribution of the
608 unconstrained model. We tested the best-fitting model of a previous study (Jaffe et al. 2011) to
609 demonstrate how *a priori* hypotheses can be compared to *a posteriori* hypotheses obtained in the

610 reversible-jump framework. We find that the best-fitting model of chelonian carapace length evolution
611 found in Jaffe et al. (2011) captures only one of the highly supported optima-shifts in the posterior
612 distribution (Figure 6). The posterior obtained via reversible-jump inference is much more strongly
613 supported based on Bayes Factors even given the high penalty assigned to models with vague priors
614 (Kass 1993). Comparing biologically informed hypotheses to the posterior distribution of statistically
615 supported hypotheses provides a useful metric for determining the adequacy of our model in explaining
616 the data. Furthermore, we can generate additional hypotheses based on the inadequacy of the *a priori*
617 hypotheses to explain the existence of distinct adaptive regimes for certain clades. For example, in the
618 Chelonia dataset we examine here we find that there is a strongly supported adaptive shift in the
619 softshell turtles (Trionychidae) that is not captured by the $OU_{habitat}$ model of Jaffe et al. (2011).
620 Based on this observation, we can conclude that the simple freshwater-marine dichotomy does not
621 capture the underlying causal forces behind carapace length evolution. Instead, optimal body size may
622 be better explained by other factors. For example, a shift to a larger phenotypic optimum may be
623 accompanied by shifts to more aquatic lifestyles (irrespective of salinity) by releasing species from
624 constraints imposed by the physical environment. Furthermore, it has been hypothesized that larger
625 body sizes in chelonians may require higher environmental temperatures to enable high enough
626 mass-specific metabolic rates to sustain growth (Makarieva et al. 2005; Head et al. 2009). Thus, a
627 combination of an aquatic lifestyle and warm temperatures may favor shifts toward larger body sizes.

628 An important implication of our analysis is that the biological interpretation of a model may
629 change the posterior distribution of model fits. For example, species of turtles may cluster broadly into
630 adaptive zones defined based on aquatic or non-aquatic habits, and such transitions may be rare
631 enough that OU model with a handful of shifts and weak parameters for α and σ^2 could adequately
632 describe evolutionary patterns. However, support for such a pattern does not exclude the possibility
633 that at shorter timescales, species evolve according to a pulsed pattern of shifts in adaptive optima
634 separate by million-year periods of phenotypic stasis [i.e. the pattern of stasis that lead to Eldredge
635 and Gould's (1972) proposal of punctuated equilibrium, but see Pennell et al. 2013]. If such a stasis
636 model were enforced through informative priors, we would expect high values for α and σ , as well as
637 more numerous shifts. Both evolution within these broad adaptive zones and intervals of stasis may be
638 occurring simultaneously, and there may be statistical signals for both processes that are detectable in
639 phylogenetic comparative data. `bayou` provides a flexible means of fitting these biological
640 interpretations, and testing for specific processes and patterns of interest.

641 Our method helps alleviate many of the challenges inherent to fitting OU models to
642 phylogenetic comparative data. Inference of OU models is often challenging due to ridges in likelihood
643 space, which result in poor convergence and difficult to interpret parameter estimates. We emphasize

644 the importance of examining the full posterior distribution, rather than point estimates, when
645 interpreting model fits and the statistical signal of adaptive evolution in comparative data. For
646 example, Ingram and Mahler’s 2013 SURFACE method, as in `bayou`, searches for an optimal arrangement
647 of adaptive regimes across the phylogeny. However, because of ridges in likelihood space in the chelonia
648 dataset we examined, SURFACE gave highly unrealistic estimates of the values of the adaptive optima.
649 This is because there are a range of correlated values of α , σ^2 and $\theta_1, \dots, \theta_K$ that give essentially the
650 same likelihood. Thus, the ML estimate in SURFACE combines extremely distant optima (ranging from
651 -422.6 to 111.2; Table 3) with much weaker estimates of α (phylogenetic half-life of 92.6 vs. 3.94 in
652 `bayou`) to obtain very high log-likelihoods relative to other methods (Table 3, Figure 6). `bayou` avoids
653 these difficult to interpret results by using informative prior information to exclude biologically
654 unreasonable models. Although this introduces some subjectivity, most biologists would agree that we
655 can reasonably reject the idea that any extant species of chelonians are adapting to an optimal
656 carapace length of $e^{111.2} = 1.96 \times 10^{43}$ km long (i.e. larger than the diameter of the observable universe).
657 Since fitted model parameters are correlated, unreasonable estimates of adaptive optima also affect
658 estimation of α , σ^2 and the location of shifts. By simply setting a reasonable prior on this one set of
659 parameters ($\theta_1, \dots, \theta_K$), we show that the estimation of α and σ collapses from a ridge to a narrow peak
660 of values (Figure 7). Thus, while both methods can infer the location of shifts in adaptive optima
661 without *a priori* specification, `bayou` allows for the inclusion of informative priors and returns a full
662 posterior of credible models; while SURFACE allows for convergent regimes (the “backwards” selection
663 step) which is currently not implemented in the reversible-jump framework of `bayou`.

664 Our analysis of simulations results gives considerable insight into best practices in fitting OU
665 models to phylogenetic comparative data. While `bayou` does not estimate the number of shifts with
666 much power, it is nonetheless possible to distinguish models with little statistical support for adaptive
667 peak shifts vs. models with strong evidence of optima shifts. For example, as the true model
668 approaches BM (i.e. high phylogenetic half-lives) or the number of shifts goes to 0, the posterior
669 support for any particular branch greatly decreases, eventually reaching the probability of a random
670 branch having a shift given the prior density (Figure 1; Online Appendix III). Thus, if no branch has
671 high posterior support relative to the prior density, we conclude there is little evidence for an adaptive
672 shift (regardless of the mean number of shifts inferred in the posterior distribution). In fact, there is
673 relatively little cost to placing a high prior on the number of shifts for inference of phylogenetic
674 half-life, σ^2 , and the location and magnitude of optima shifts, whereas conservative priors will often
675 result in mis-estimation of these parameters if the true model is complex. Therefore, we recommend
676 using priors that favor a moderate to large number of shifts rather than using more conservative priors
677 (see Online Appendix III). Furthermore, if the posterior for phylogenetic half-life includes values higher

678 than the phylogenetic tree height, this indicates that the model is very BM-like and it is unlikely that
679 shifts will be estimated. This is because optima shifts are expected to only weakly affect the
680 distribution of the data. As a simple heuristic, we obtained reasonable estimates of parameters when
681 the phylogenetic half-life is between the youngest split in the phylogeny and the total tree height.
682 Half-life values substantially less than the youngest split in the phylogeny indicate that after
683 accounting for optima shifts, residual variation within regimes is not phylogenetically correlated (white
684 noise). By contrast, phylogenetic half-lives much higher than tree height indicate strong phylogenetic
685 signal even after accounting for shared adaptive optima, which is suggestive of BM-like evolution.

686 A number of extensions are possible within our proposed method, and is a first step toward a
687 much more expansive suite of models. Using likelihood approaches, OU models have been expanded to
688 include randomly evolving continuous predictors (Hansen et al. 2008), multivariate evolution of
689 correlated traits (Bartoszek et al. 2012), varying α and σ^2 parameters across the tree (Beaulieu et al.
690 2012; Lapedra et al. 2013) and identification of convergent regimes (Ingram and Mahler 2013; Mahler
691 et al. 2013). Expanding these models to a Bayesian framework would carry many of the same
692 advantages we describe in this study. Furthermore, we emphasize the importance of developing models
693 that describe the dynamics of adaptive landscapes themselves, and suggest anchoring these models in
694 empirical datasets through the use of informative priors will greatly improve our understanding of
695 macroevolutionary dynamics.

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Table 1: Prior distributions for OU_{Free} and QG models used in simulation study modeling different biological processes. Models are simulated and fit to the data from these priors, intended to reflect values typical for linear $\ln(\text{body size})$ related measurements in a clade 50 my old that spans two magnitudes in size. Measurement error (ME) is simulated and fit to be $\sim\text{Norm}(\mu = 0, \sigma_\epsilon^2 = 0.05^2)$.

Parameter	Prior	Quantiles (1%, 50%, 99%)	Ref
Model: QG			
h^2	$\sim\text{Beta}(a = 15, b = 20)$	(0.25; 0.43; 0.62)	Mousseau et al. 1987
V_P	$\sim\text{LogNorm}(\ln\mu = -5, \ln\sigma = 0.8)$	(0.032 ² ; 0.082 ² ; 0.208 ²)	Uyeda et al. 2011
ω^2/V_p	$\sim\text{LogNorm}(\ln\mu = 4, \ln\sigma = 1.5)$	(1.67; 54.6; 1,790)	Estes and Arnold 2007
N_e	$\sim\text{LogNorm}(\ln\mu = 10, \ln\sigma = 2)$	(210; 22,000; 2.31E6)	Estes and Arnold 2007
Phy half-life (y)	-	(21.2; 459; 15,200)	
$\sqrt{V_y + \sigma_\epsilon^2}$	-	(0.05; 0.05; 0.079)	
Model: OU_{Free}			
α	$\sim\text{LogNorm}(\ln\mu = -3, \ln\sigma = 3)$	(4.6E-5; 5.0E-2; 53)	Hansen 2012*
σ^2	$\sim\text{LogNorm}(\ln\mu = 0, \ln\sigma = 2)$	(9.5E-3; 1; 105)	
Phy half-life (my)	-	(0.013; 13.9; 1,487)	
$\sqrt{V_y + \sigma_\epsilon^2}$	-	(0.069; 3.17; 210)	
Both models			
θ	$\sim\text{Norm}(\ln\mu = 0, \ln\sigma = 0.5)$	(-1.2; 0; 1.2)	
K	$\sim\text{CondPoisson}(\lambda = 15, K_{max} = 32)$	(7; 15; 25)	

*This prior on α puts about $\sim 20\%$ of the probability density on a phylogenetic half-life less than the average youngest splits in the simulated phylogenies (~ 1 my, white noise-like evolution) and $\sim 30\%$ of the probability density above the tree height (50 my, i.e. BM-like evolution).

Table 2: Posterior quantiles for parameter values and p-values from a Komolgorov-Smirnov test. Runs that did not converge were removed from the analysis.

	N	2.5%	25%	50%	75%	97.5%	p-value
Log Likelihood	938	0.03	0.26	0.53	0.76	0.98	0.17
Log Prior	938	0.02	0.30	0.57	0.80	0.98	0.00
α	938	0.02	0.26	0.54	0.78	0.99	0.01
σ^2	938	0.02	0.26	0.52	0.74	0.98	0.78
K	938	0.03	0.27	0.51	0.76	0.99	0.42
Root θ_0	938	0.02	0.22	0.51	0.76	0.98	0.29

Table 3: Comparison of model fits to *Chelonia* carapace length data (Jaffe et al. 2011). The range of θ values are taken from either the posterior distribution (for Bayesian analyses) or from the range of estimates for individual optima from the ML analyses.

Variable	bayou	$OU_{habitat}$ (ML)	$OU_{habitat}$ (bayou)	SURFACE Fwd	SURFACE Bwd	bm-jump
No. of shifts	16*	16	16*	33	33	16*
No. of θ	17*	4	4*	33	13	-
lnL	-90.9*	-137.8	-137.1*	34.3	30.7	-97.3*
Marginal lnL	-143.6	-	-151.2	-	-	-
ln $2/\alpha$ (my)	3.94*	17.6	16.7*	92.6	85.2	-
σ^2 (per my)	0.0568*	0.0285	0.0298*	0.00325	0.00341	0.00381*
V_y	0.16*	0.36	0.36*	0.21	0.22	-
Range of θ	(2.08, 5.12)	(3.11, 4.82)	(3.23, 5.19)	(-422.6, 111.2)	(-387.9, 102.5)	-

*Median of posterior distribution

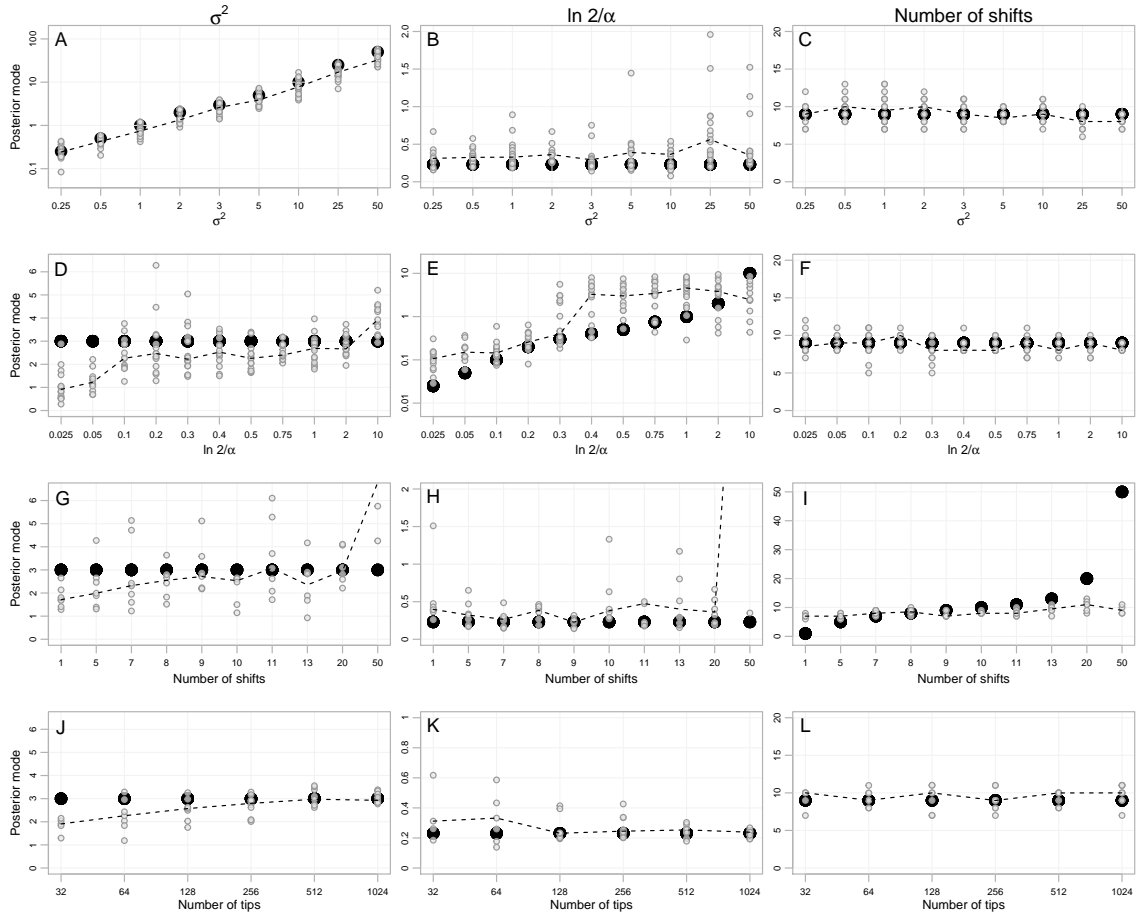


Figure 1: Results of simulation study varying the parameters σ^2 (row 1, A-C), phylogenetic half-life ($\ln(2)/\alpha$; row 2, D-F), the number of shifts on the phylogeny (K ; row 3, G-I) and the number of tips in the phylogeny (row 4, J-L). Solid black points indicate the true value used to simulate the data, dotted lines indicate the median posterior mode across simulations. Priors for parameters are as follows: $\alpha \sim \text{LogNormal}(\ln \mu = 0.25, \ln \sigma = 1.5)$, $\sigma^2 \sim \text{LogNormal}(\ln \mu = 0, \ln \sigma = 5)$, $\theta \sim \text{Normal}(\mu = 0, \sigma = 3)$, $K \sim \text{Conditional Poisson}(\lambda = 9, K_{max} = \text{ntips} / 2)$.

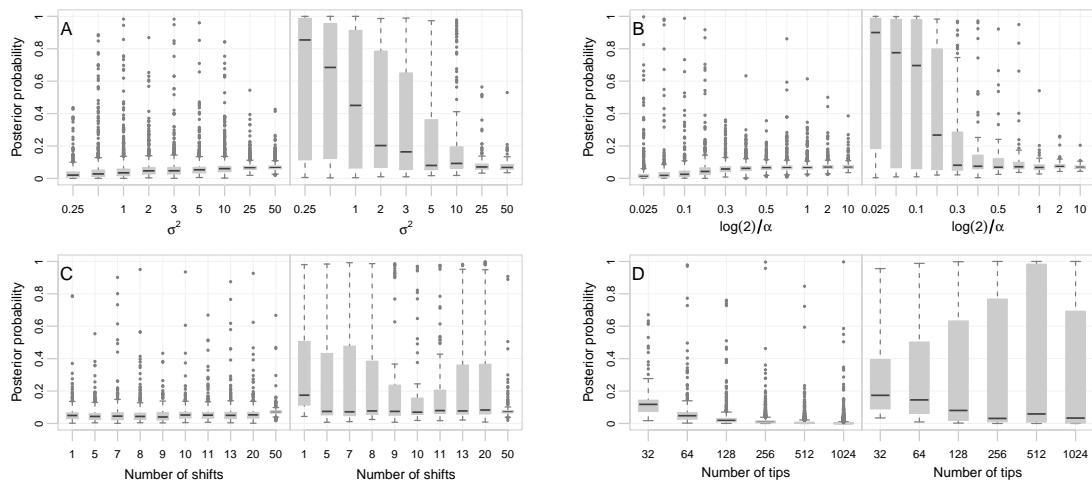


Figure 2: Estimation of branch posterior probabilities using the same simulations as in Figure 1 for varying values of (A) σ^2 , (B) phylogenetic half-life, (C) number of shifts (K) and (D) number of tips. For each plot, boxplots indicate the distribution of posterior probabilities of a shift occurring on branches that either contain no shift in the true model (left side of each panel) or contain a shift (right side). Locations of shifts were chosen randomly across the phylogeny, and magnitudes were determined by optima drawn randomly from a normal distribution.

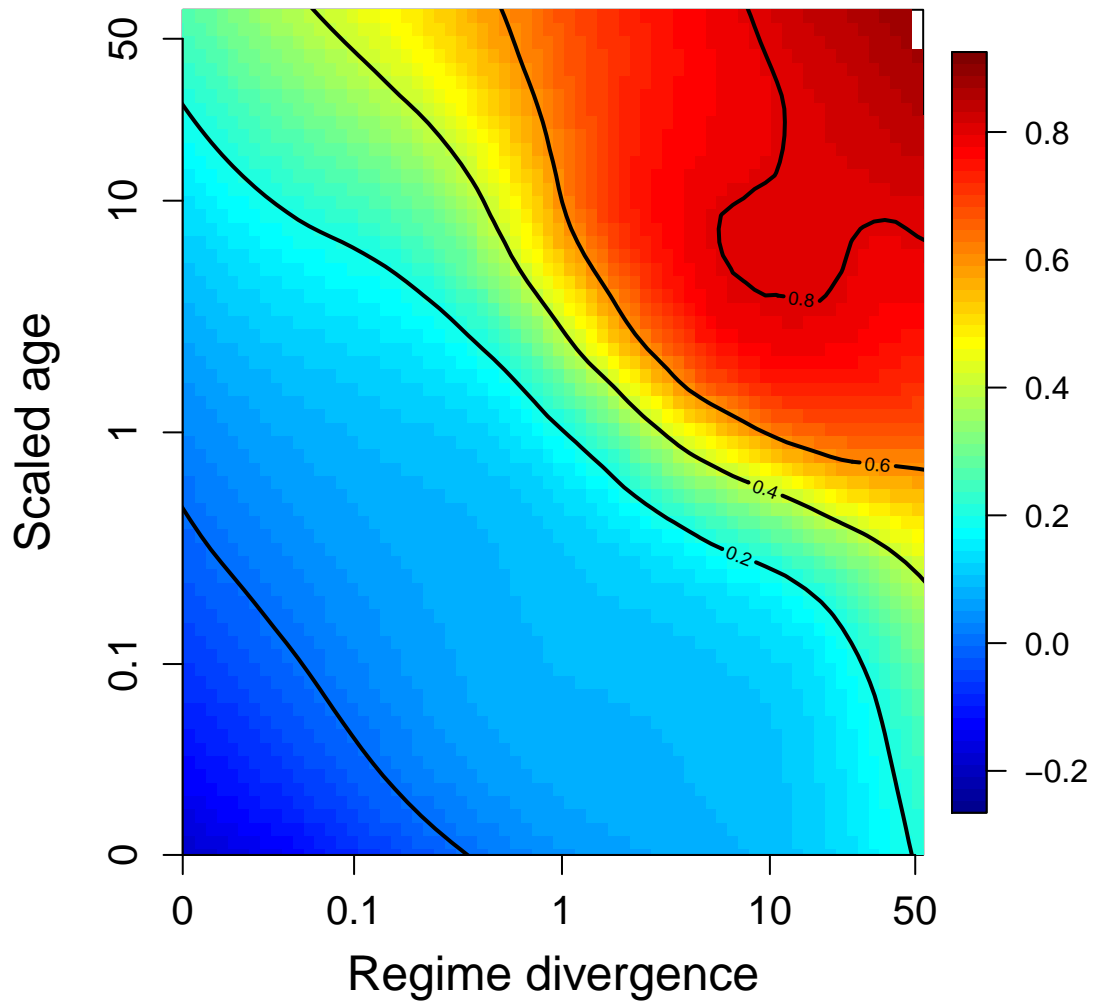


Figure 3: Relationship between regime divergence ($(\theta_2 - \theta_1)/\sqrt{V_y}$), the scaled age of the shift (*shift age/phylogenetic half-life*) and the posterior probability of detecting a shift. All branches from each 64-taxon tree were plotted to estimate this surface using ordinary kriging to visualize the relationship. Prior probability of a branch being selected is 0.0827. Branches without shifts were given a small divergence value ($\log(0.01)$) and correspond to the left-most data in the plot.

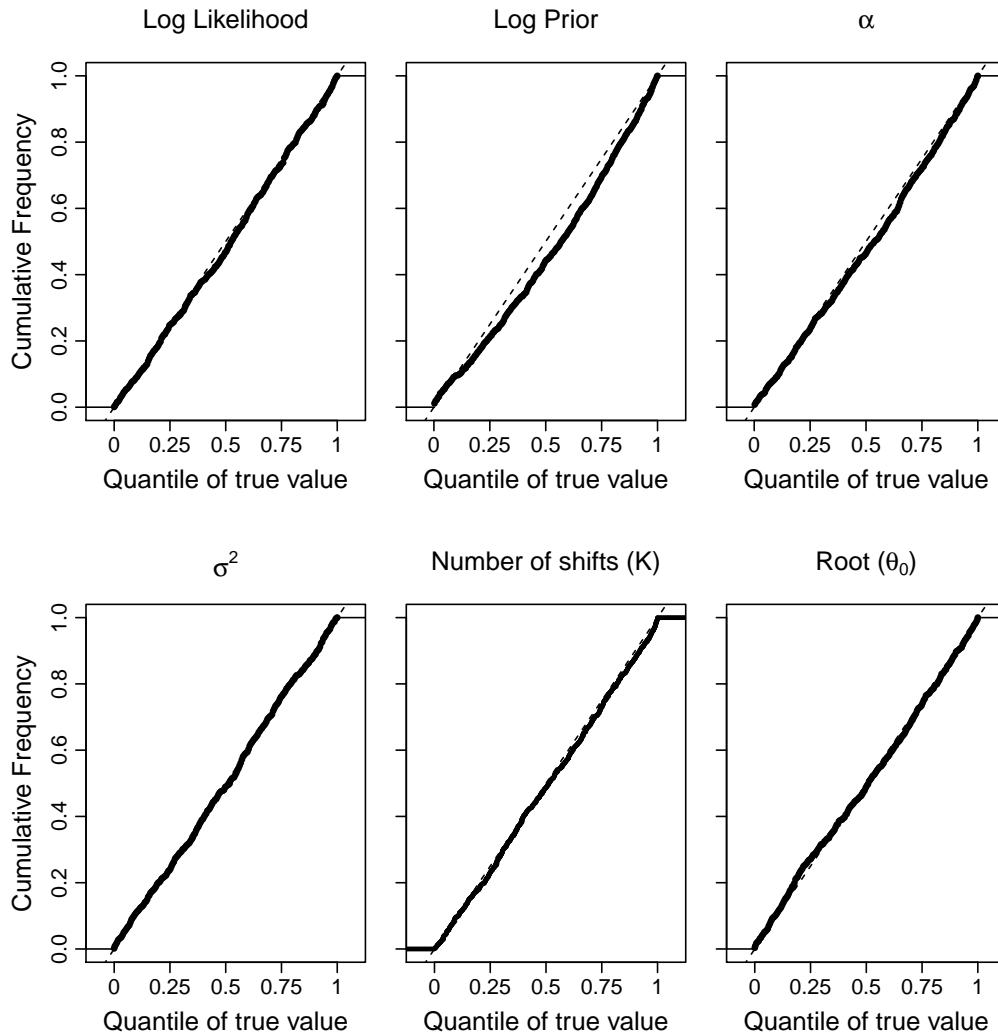


Figure 4: Cumulative distribution plots for posterior quantiles for selected parameters. If posteriors are estimated accurately, then the quantiles of true values of the parameters across simulated datasets should be uniformly distributed (Cook et al. 2006) and follow the dotted lines, which indicate the expected cumulative distribution function for a uniform distribution. Each MCMC was run for 200,000 generations and the first 30% of the samples were discarded as burnin. Runs in which Gelman's R failed to reach below 1.1 at the end of the run were removed. A total of 938 simulations were used after removing runs that did not reach convergence.

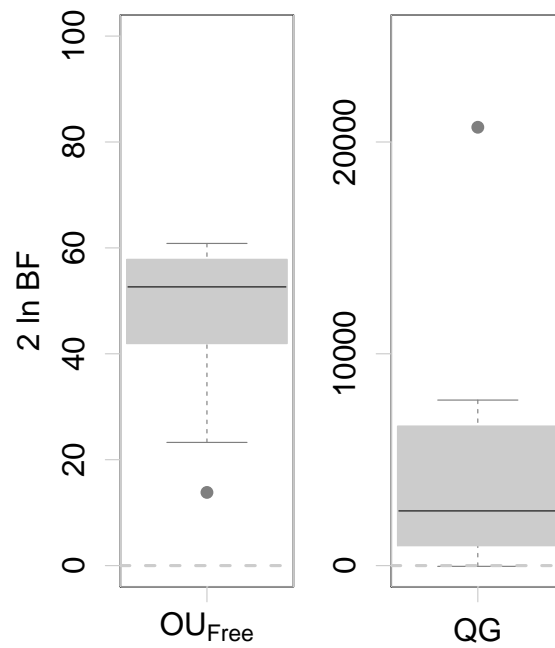


Figure 5: Model comparison for biological interpretations of OU models. Models were simulated either under diffuse priors typical of comparative data (OU_{Free} , left) or under realistic priors for the Lande model (QG , right). Both OU_{Free} and QG models were then fit to the data, and marginal likelihoods were estimated using stepping-stone modeling to obtain Bayes Factors (BF). $2 \ln BF$ are shown, with values above 0 (dotted gray line) indicating that the true model was favored. A total of 10 simulations were run under each model (see text for details).

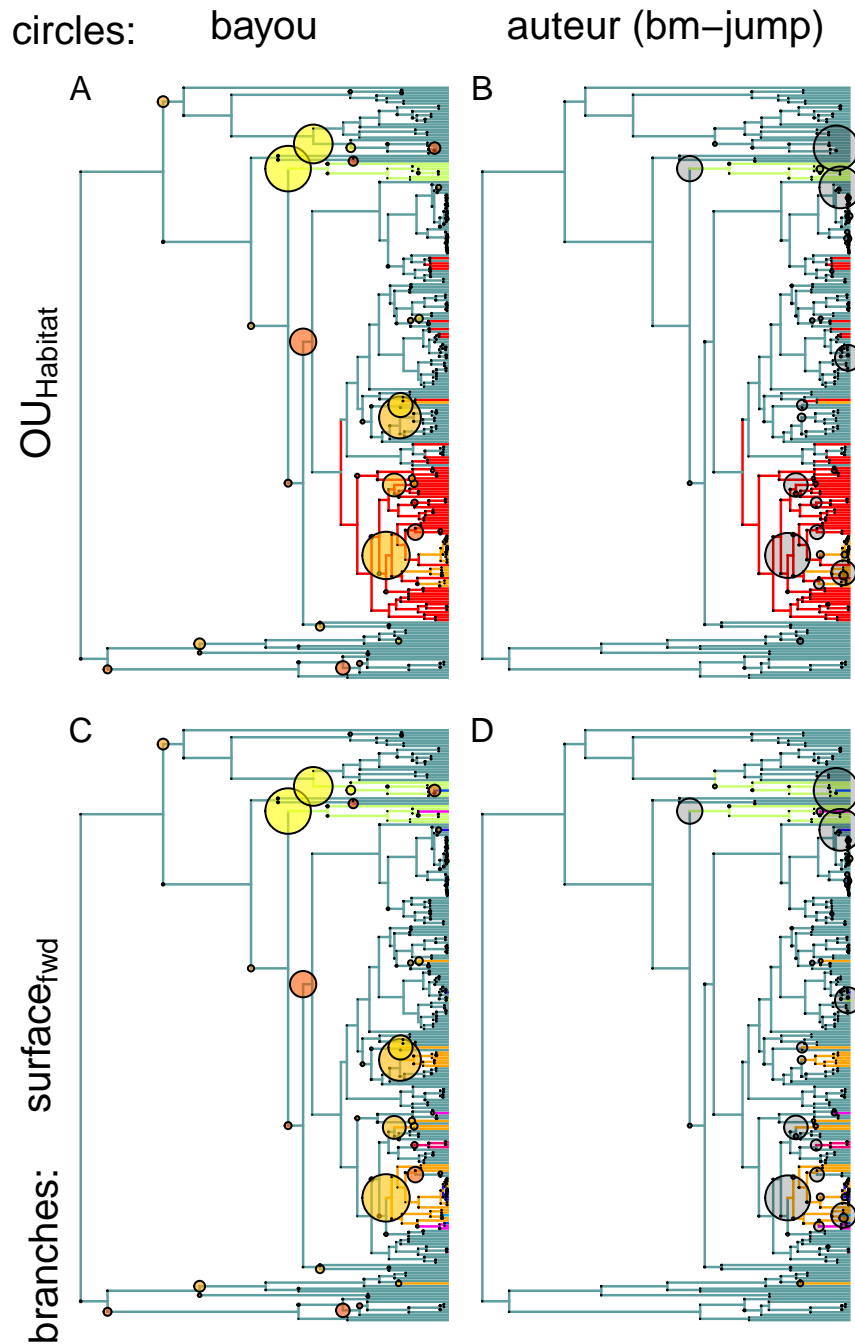


Figure 6: Model fits of multi-optima OU models using different methods. Circles at the nodes in A) and C) indicate by their size the posterior probability of shift locations from the reversible-jump model implemented in bayou, with the larger phenotypic values for optima being indicated by yellow and smaller optima indicated by red. Circles in B) and D) are the posterior probability of a shift in a constant-rate BM model with jumps fit using the bm-jump model in auteur. Branch painting in A) and B) is the $OU_{Habitat}$ model (which corresponds to the OU2 model of Jaffe et al. 2011). Regime paintings in C) and D) correspond to the best fitting model from SURFACE using forward stepwise addition (Ingram and Mahler 2013).

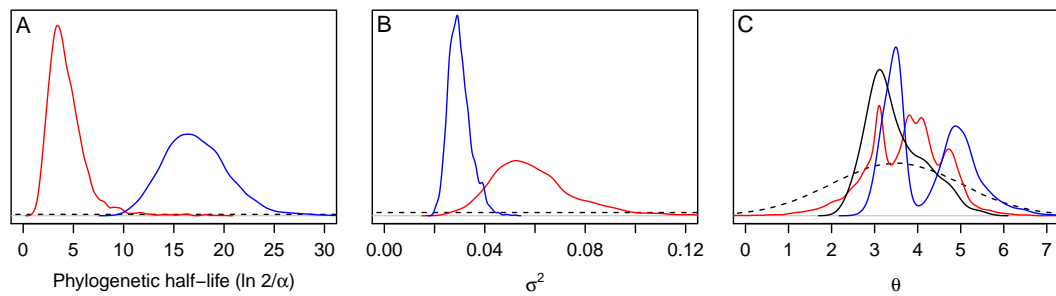


Figure 7: Posterior distributions for parameters estimated using `bayou` under a reversible-jump (Red) and fixed $OU_{habitat}$ (Blue) models to the chelonia carapace data. Parameters estimated include A) phylogenetic half-life B) σ^2 and C) the distribution of phenotypic optima (θ). Dotted lines indicate prior density, black solid line in C) indicates the distribution of phenotypes in the data.