

Species occurrence as a function of both emergent biological traits and environmental context

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Introduction

How do species pools change over time as species are recruited or go extinct? When are ecotypes enriched or depleted? How does global and regional environmental context affect the distribution of species ecotypes (e.g. guilds) in a regional species pool?

A regional species pool is the set of species which form communities in a specific region; local communities are subsets of the regional pool. The composition of a regional species pool changes over time due to speciation, migration, extinction. Local scale processes like resource competition only affect the regional species pool if all communities are affected.

Valentine and Bambach how they presented guilds in paleobiology. Bush and Bambach presented an ecocube to describe what how marine invertebrates partition space and resources (Bambach et al., 2007; Bush and Bambach, 2011; Bush et al., 2007). Unique combinations represent what possible ecotypes are observable. The distribution of ecocube occupancy is then normally analyzed as raw counts of unique combinations or using ordination methods and the change in disparity over time is estimated (Bambach et al., 2007; Bush and Bambach, 2011; Bush et al., 2007).

One of the greatest challenges with analyzing species occurrence data is the inherent incompleteness of any sample (Foote, 2001; Foote and Sepkoski, 1999; Lloyd et al., 2011; Royle and Dorazio, 2008; Royle et al., 2014; Wang and Marshall, 2016). In the modern, only presences are certain as an absence can be caused by both the species being truly absent or the species never having been sampled (Royle and Dorazio, 2008; Royle et al., 2014). For paleontological data in the context of this study, the incomplete preservation of fossil communities combined with the incomplete sampling of what fossils there are means that the true times of origination or extinction may not be observed (Foote, 2001; Foote and Sepkoski, 1999; Wang et al., 2016; Wang and Marshall, 2016)

Smits (2015) found several systematic differences in mammal species durations associated with various species traits. Omnivorous taxa were found to have, on average, a greater duration than other dietary categories. Additionally, arboreal taxa were found to have a shorter duration than other locomotor categories.

An unresolved question from Smits (2015) is whether the greater extinction risk faced by arboreal is
28 constant over time or if there was a change in extinction risk at the Paleogene/Neogene boundary.
Specifically, the question is whether the extinction risk arboreal taxa increased in the Neogene,
30 driving the loss of arboreal taxa and average extinction risk of arboreal taxa down.

There are no observed massive cross-taxonomic turnover events in the North American record,
32 unlike the Neogene record Europe (Alroy, 1996, 2009; Alroy et al., 2000; Eronen et al., 2015; Janis,
1993).

34 The effect of climate on diversity and the diversification process has been the focus of considerable
research with many analyses favoring diversification being more biologically-mediated than
36 climate-mediated (Alroy, 1996; Alroy et al., 2000; Clyde and Gingerich, 1998; Figueirido et al.,
2012). Scale of analysis makes a big difference in interpretation of results, both temporal and
38 geographic. For example when the mammal fossil record analyzed at small temporal and geographic
scales a correlation between diversity and climate are observable (Clyde and Gingerich, 1998).
40 However, when the record is analyzed at the scale of the continent and the Cenozoic there is no
correlation with diversity and climate (Alroy et al., 2000). This results, however, does not go
42 against the idea that there may be short periods of correlation and that this correlation change or
reverse direction over time; instead this result means that there is no single direction of correlation
44 between diversity and climate (Figueirido et al., 2012). In the case of a fluctuating correlation
between diversity and climate it is hard to make the argument of an actual causal link between the
46 two without understanding the ecological differences in mammalian fauna over time; when this
analysis is based on diversity or taxonomy alone no mechanisms are possible to infer. After all,
48 taxonomy conflates many potential factors that could affect diversification into a single variable; by
separating the effects of shared common ancestry (i.e. phylogeny) from species ecology the subtle
50 differences in the diversification process can be observed (Smits, 2015).

There are many global climatic events that may have influenced the distribution of mammal
52 ecotypes regionally, if not globally (Zachos et al., 2008, 2001). PETM. The Mid-Miocene climactic
optimum. The general cooling throughout the Cenozoic and the development of ice-caps in the

Neogene. The Oligo-Miocene boundary. The transition from the Paleogene to the Neogene in North America is typically described as the “opening-up” of the landscape as partially forested environments were replaced by savannah and grasslands (Blois and Hadly, 2009; Janis, 1993; Janis et al., 2000; Strömberg, 2005).

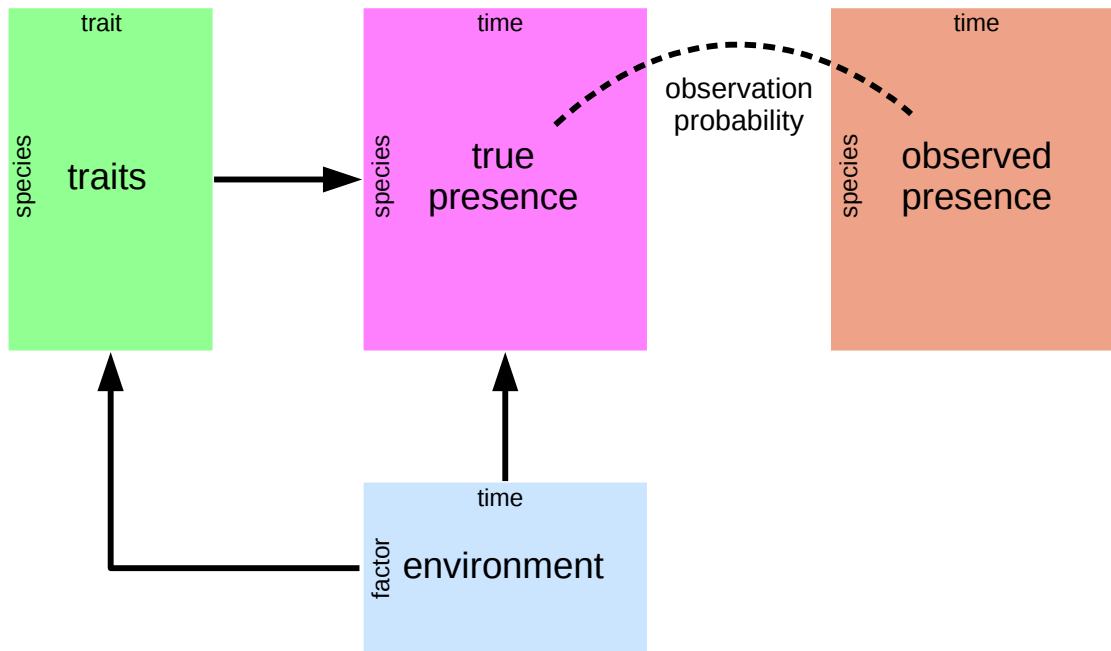


Figure 1: Conceptual diagram of the paleontological fourth corner problem. The observed presence matrix (orange) is the empirical presence/absence pattern for all species for all time points; this matrix is an incomplete observation of the “true” presence/absence pattern (purple). The estimated true presence matrix is modeled as a function of both environmental factors over time (blue) and multiple species traits (green). Additionally, the affect of environmental factors on species traits are also modeled as traits are expected to mediate the effects of a species environmental context. This diagram is based partially on material presented in Brown et al. (2014) and Warton et al. (2015).

Fourth-corner modeling an approach to explaining the patterns of either species abundance or presence/absence as a product of species traits, environmental factors, and the interaction between traits and environment CITATION. In modern ecological studies, what is being modeled is species

occurrences at localities distributed across a region CITATION. In this study, what is being modeled is the pattern of species occurrence over time for most of the Cenozoic in North America (Fig. 1). These two approaches, modern and paleontological, are different views of the same three-dimensional pattern: species at localities over time. The temporal limitations of modern ecological studies and difficulties with uneven spatial occurrences of fossils in paleontological studies means that these approaches are complimentary but reveal different patterns of how species are distributed in time and space.

The major species trait included in this study is species ecotype, defined as the combination of species dietary category (e.g. carnivore) and locomotor category (e.g. arboreal). This trait is a descriptor of a species' ecological guild, similar to the unique combinations of the ecocube used in analysis of marine invertebrates (Bambach et al., 2007; Bush and Bambach, 2011; Bush et al., 2007). Importantly, the probability of a species ecotype being present was modeled as a function of environmental factors (Fig. 1). Species mass was also included as a species trait, but primarily just to control for that effect on species occurrence.

The environmental factors included in this study include estimates of global temperature and the changing floral groups present in North America across the Cenozoic. Why are these factors important? What are the hypotheses associated with environmental context?

Materials and Methods

Taxon occurrences and species-level information

All fossil occurrence information was downloaded from the Paleobiology Database. Occurrences (PBDB) were restricted to all Mammalia sampled in North America between the Maastrichtian and Gelasian stages. Taxonomic, stratigraphic, and ecological metadata for each occurrence was included. The raw data is available for download at <http://goo.gl/2slgeU>.

This raw data was then sorted, cleaned, and manipulated programmatically prior to analysis.

Species taxonomic assignments given by the PBDB were updated for accuracy and consistency. For example, species classified in the order Artiodactyla were reclassified as Cetartiodactyla. These re-assignments follow Smits (2015) and were Janis et al. (2008, 1998) and the Encyclopedia of Life WEBSITE. Additionally, Taxa who’s life habit was classified as either volant (i.e. Chiroptera) or aquatic (e.g. Cetacea) were excluded from this analysis because of both differences in fossilization potential and applicability to the study of terrestrial species pools.

The life habit and dietary categories provided through the PBDB were coarsened to increase per ecotype sample size; this coarsening follows the same procedure as Smits (2015). Additionally, life habit category was further modified to break-up the vague “ground-dwelling” category; re-classifying these species by ankle posture gives more precise information about that species’ environmental context. Ground-dwelling taxa were reassigned following ? by species taxonomic context. Species ecotype is defined as the interaction between life habit and diet categories. Ecotype categories with less than 10 species having ever been that combination were excluded, yielding a total of 18 of 21 possible ecotypes.

Table 1: Species trait assignments in this study are a coarser version of the information available in the PBDB. Information was coarsened to improve per category sample size and uniformity and followed this table.

| This study | | PBDB categories |
|------------|-----------------|---|
| Diet | Carnivore | Carnivore |
| | Herbivore | Browser, folivore, granivore, grazer, herbivore. |
| | Insectivore | Insectivore. |
| | Omnivore | Frugivore, omnivore. |
| Locomotor | Arboreal | Arboreal. |
| | Ground dwelling | Fossorial, ground dwelling, semifossorial, saltatorial. |
| | Scansorial | Scansorial. |

Table 2: Posture assignment based on taxonomy

| Order | Family | Stance |
|------------------------|------------|-------------|
| | Ailuridae | plantigrade |
| | Allomyidae | plantigrade |
| Continued on next page | | |

Table 2 – continued from previous page

| Order | Family | Stance |
|------------------------|-------------------|-------------|
| Dinocerata | Amphicyonidae | plantigrade |
| | Amphilemuridae | plantigrade |
| | Anthracotheriidae | digitigrade |
| | Antilocapridae | unguligrade |
| | Apheliscidae | plantigrade |
| | Aplodontidae | plantigrade |
| | Apternodontidae | scansorial |
| | Arctocyonidae | unguligrade |
| | Barbourofelidae | digitigrade |
| | Barylambdidae | plantigrade |
| | Bovidae | unguligrade |
| | Camelidae | unguligrade |
| | Canidae | digitigrade |
| | Cervidae | unguligrade |
| | Cimolodontidae | scansorial |
| | Coryphodontidae | plantigrade |
| | Cricetidae | plantigrade |
| | Cylindrodontidae | plantigrade |
| | Cyriacotheriidae | plantigrade |
| | Dichobunidae | unguligrade |
| | | unguligrade |
| | Dipodidae | digitigrade |
| | Elephantidae | digitigrade |
| | Entelodontidae | unguligrade |
| | Eomyidae | plantigrade |
| Continued on next page | | |

Table 2 – continued from previous page

| Order | Family | Stance |
|------------------------|-----------------|-------------|
| Lagomorpha | Erethizontidae | plantigrade |
| | Erinaceidae | plantigrade |
| | Esthonychidae | plantigrade |
| | Eutypomyidae | plantigrade |
| | Felidae | digitigrade |
| | Florentiamyidae | plantigrade |
| | Gelocidae | unguligrade |
| | Geolabididae | plantigrade |
| | Glyptodontidae | plantigrade |
| | Gomphotheriidae | unguligrade |
| | Hapalodectidae | plantigrade |
| | Heteromyidae | digitigrade |
| | Hyaenidae | digitigrade |
| | Hyaenodontidae | digitigrade |
| | Hypertragulidae | unguligrade |
| | Ischyromyidae | plantigrade |
| | Jimomyidae | plantigrade |
| | Lagomorpha | digitigrade |
| | Leptictidae | plantigrade |
| | Leptochoeridae | unguligrade |
| | Leptomerycidae | unguligrade |
| | Mammutidae | unguligrade |
| | Megalonychidae | plantigrade |
| | Megatheriidae | plantigrade |
| | Mephitidae | plantigrade |
| Continued on next page | | |

Table 2 – continued from previous page

| Order | Family | Stance |
|------------------------|---------------------|-------------|
| Mesonychia | Merycoidodontidae | digitigrade |
| | | unguligrade |
| | Mesonychidae | digitigrade |
| | Micropternodontidae | plantigrade |
| | Mixodectidae | plantigrade |
| | Moschidae | unguligrade |
| | Muridae | plantigrade |
| | Mustelidae | plantigrade |
| | Mylagaulidae | fossorial |
| | Myodontidae | plantigrade |
| | Nimravidae | digitigrade |
| Notoungulata | Nothrotheriidae | plantigrade |
| | | unguligrade |
| | Oromerycidae | unguligrade |
| | Oxyaenidae | digitigrade |
| | Palaeomerycidae | unguligrade |
| | Palaeoryctidae | plantigrade |
| | Pampatheriidae | plantigrade |
| | Pantolambdidae | plantigrade |
| | Periptychidae | digitigrade |
| | | unguligrade |
| | Phenacodontidae | unguligrade |
| Primates | | plantigrade |
| | Procyonidae | plantigrade |
| | Proscalopidae | plantigrade |
| Continued on next page | | |

Table 2 – continued from previous page

| Order | Family | Stance |
|-------|-------------------|-------------|
| | Protoceratidae | unguligrade |
| | Reithroparamyidae | plantigrade |
| | Sciuravidae | plantigrade |
| | Sciuridae | plantigrade |
| | Simimyidae | plantigrade |
| | Soricidae | plantigrade |
| | Suidae | digitigrade |
| | Talpidae | fossorial |
| | Tayassuidae | unguligrade |
| | Tenrecidae | plantigrade |
| | Titanoideidae | plantigrade |
| | Ursidae | plantigrade |
| | Viverravidae | plantigrade |
| | Zapodidae | plantigrade |

Species mass information was gathered from multiple different sources where a plurality of the body size estimates are from the PBDB. Body part measurements for many species are also available through the PBDB. Just as with Smits (2015), these measurements and corresponding regression equations were used to get mass estimates for more species. Additional mass estimates and body part measurements were sourced from numerous publications and the Neogene Old World Database; see the supplementary material to Smits (2015) for details. Mass was log-transformed and then mean-centered and rescaled by dividing by two-times its standard deviation; this insures that the magnitude of effects for both continuous and discrete covariates are comparable (Gelman, 2008; Gelman and Hill, 2007).

Table 3: Regression equations used in this study for estimating body size. Equations are presented with reference to taxonomic grouping, part name, and reference.

| Group | Equation | log(Measurement) | Source |
|--------------|------------------------------|-----------------------|-----------------|
| General | $\log(m) = 1.827x + 1.81$ | lower m1 area | Legendre (1986) |
| General | $\log(m) = 2.9677x - 5.6712$ | mandible length | ? |
| General | $\log(m) = 3.68x - 3.83$ | skull length | ? |
| Carnivores | $\log(m) = 2.97x + 1.681$ | lower m1 length | ? |
| Insectivores | $\log(m) = 1.628x + 1.726$ | lower m1 area | ? |
| Insectivores | $\log(m) = 1.714x + 0.886$ | upper M1 area | ? |
| Lagomorph | $\log(m) = 2.671x - 2.671$ | lower toothrow area | Tomiya (2013) |
| Lagomorph | $\log(m) = 4.468x - 3.002$ | lower m1 length | Tomiya (2013) |
| Marsupials | $\log(m) = 3.284x + 1.83$ | upper M1 length | ? |
| Marsupials | $\log(m) = 1.733x + 1.571$ | upper M1 area | ? |
| Rodentia | $\log(m) = 1.767x + 2.172$ | lower m1 area | Legendre (1986) |
| Ungulates | $\log(m) = 1.516x + 3.757$ | lower m1 area | ? |
| Ungulates | $\log(m) = 3.076x + 2.366$ | lower m2 length | ? |
| Ungulates | $\log(m) = 1.518x + 2.792$ | lower m2 area | ? |
| Ungulates | $\log(m) = 3.113x - 1.374$ | lower toothrow length | ? |

All fossil occurrences from 64 to 2 million years ago (Mya) were binned into 31 2 million year (My) bins. This temporal length was chosen because it is approximately the resolution of the North American mammal fossil record.

Environmental and temporal covariates

The group-level covariates in this study are descriptors of species' environmental context, specifically global temperature estimates and Graham's floral intervals CITATION. Global temperature across most of the Cenozoic was calculated from Mg/Ca isotope record from deep sea carbonates (Cramer et al., 2011). Mg/Ca based temperature estimates are preferable to the frequently used $\delta^{18}\text{O}$ temperature proxy (Alroy et al., 2000; Figueirido et al., 2012; Zachos et al., 2008, 2001) because Mg/Ca estimates do not conflate temperature with ice sheet volume and depth/stratification changes; this makes it preferable as an estimate of global temperature for macroevolutionary and macroecological studies (Ezard et al., 2016).

Two aspects of the Mg/Ca-based temperature curve were included in this analysis: mean and range. Both were calculated as the mean of all respective estimates for each 2 My temporal bins. Both

mean and range were then rescaled as above: subtract mean, divide by twice the standard deviation.

The other major set of environmental factors included in this study are Graham’s Cenozoic plant phases CITATION. Graham’s plant phases are holistic descriptors of the taxonomic composition of which plants were present at a given time and their relative modernity, with younger phases representing increasingly modern taxa CITATION. Graham CITATION defines four intervals from the Cretaceous to the Pliocene, though only three of these intervals are included in this analysis. Graham’s plant phases CITATION was included as a series of “dummy variables” encoding the three phases included in this analysis. This means that the first phase is synonymous with the intercept and phases

Modelling species occurrence

Two different models were used in this study: a pure-presence model and a birth-death model. Both models at their core are hidden Markov model where the latent aspect of the process has an absorbing state (Allen, 2011). The difference between these two models is if the probability of a species origination and survival are considered equal or different (Table 4). Something that is important to realize is that while there are only two state “codes” in a presence-absence matrix (i.e. 0/1), there are in fact three states in a birth-death model: never having originated, extant, and extinct. The last of these is the absorbing state, as once a species has gone extinct it cannot re-originate (Allen, 2011); this is made obvious in the transition matrices as the probability of an extinct species changing states is 0 (Table 4). See below for parameter explanations (Tables 6, and 7).

Data augmentation

All presence/absence observations are incomplete. The hidden Markov model at the core of this analysis allows for observed absences to be used meaningfully to estimate the number of unobserved species. Of specific concern in this analysis is the unknown “true” size of the dataset; how many species could have actually been observed? While many species have been observed, the natural

| | | State at $t + 1$ | | |
|--------------|---------------|------------------|----------|---------------|
| | | 0_{never} | 1 | $0_{extinct}$ |
| State at t | 0_{never} | $1 - \theta$ | θ | 0 |
| | 1 | 0 | θ | $1 - \theta$ |
| | $0_{extinct}$ | 0 | 0 | 1 |

(a) Pure-presence

| | | State at $t + 1$ | | |
|--------------|---------------|------------------|--------|---------------|
| | | 0_{never} | 1 | $0_{extinct}$ |
| State at t | 0_{never} | $1 - \phi$ | ϕ | 0 |
| | 1 | 0 | π | $1 - \pi$ |
| | $0_{extinct}$ | 0 | 0 | 1 |

(b) Birth-death

Table 4: Transition matrices for the pure-presence (4a) and birth-death (4b) models. Both of these models share the core machinery of discrete-time birth-death processes but make distinct assumptions about the equality of originating and surviving (Eq. 2, and 3). Note also that while there are only two state “codes” (0, 1), there are in fact three states: never having originated 0_{never} , present 1, extinct $0_{extinct}$ (Allen, 2011).

incompleteness of all observations, especially in the case of paleontological data, there are obviously many species which were never sampled (Royle and Dorazio, 2008; Royle et al., 2007).

Let N be the total number of observed species, M be the upper limit of possible species that could have existed given a model of species presence, and N^* is the all-zero histories where $N^* = M - N$.

This approach assumes that $\hat{N} \sim \text{Binomial}(M, \psi)$ where \hat{N} is the estimated “true” number of species and ψ is the probability that any augmented species should actually be “present.” Because M is user defined, this approach effectively gives ψ a uniform prior over N to M (Royle and Dorazio, 2008). For this study, $M = N + \lfloor N/4 \rfloor$.

Data imputation is the process of estimating missing data for partially observed covariates (Gelman and Hill, 2007; Rubin, 1996), this is simple in a Bayesian context because data are also parameters (Gelman et al., 2013). Augmented species also have no known mass so a mass estimate must be imputed for each possible species (Royle and Dorazio, 2012). This procedure assumes that mass values for augmented species are from the same distribution as observed species. The distribution of observed mass values is estimated as part of the model, and new mass values are then generated from this distribution. This approach is an example of imputing data missing completely at random (Gelman and Hill, 2007; Royle and Dorazio, 2012). Because log mass values are rescaled as a part of this study, the body mass distribution is already known ($\mathcal{N}(0, 0.5)$); augmented species body mass just simply drawn from this distribution.

In addition to body mass information, the augmented species need an ecotype classification. Because

Table 5: Observation parameters

| Parameter | dimensions | explanation |
|------------|--------------|--|
| y | $N \times T$ | observed species presence/absence |
| z | $N \times T$ | “true” species presence/absence |
| p | T | probability of observing a species that is present at time t |
| m | N | species log mass, rescaled |
| α_0 | 1 | average log-odds of p |
| α_1 | 1 | change in average log-odds of p per change mass |
| r | T | difference from α_0 associated with time t |
| σ | 1 | standard deviation of r |

these species are completely unknown, they were all classified as “augmented,” an additional
168 grouping indicating their unknown biology. This classification has no biological interpretation.

Observation process

170 The type of hidden Markov model used in this study has three characteristic probabilities:
probability p of observing a species given that it is present, probability ϕ of a species surviving from
172 one time to another, and probability π of a species first appearing (Royle and Dorazio, 2008). In
this formulation, the probability of a species going extinct is $1 - \pi$. For the pure-presence model
174 $\phi = \pi$, while for the birth-death model $\phi \neq \pi$.

The probability of observing a species that is present p is modeled as a logistic regression was a
176 time-varying intercept and species mass as a covariate. The effect of species mass on p was assumed
linear and constant over time and given a prior reflecting a possible positive relationship; these
178 assumptions are reflected in the structure of the model Equation 1. The parameters associated with
this part of the model are described in Table 5.

$$\begin{aligned}
y_{i,t} &\sim \text{Bernoulli}(p_{i,t}z_{i,t}) \\
p_{i,t} &= \text{logit}^{-1}(\alpha_0 + \alpha_1 m_i + r_t) \\
r_t &\sim \mathcal{N}(0, \sigma)
\end{aligned} \tag{1}$$

Table 6: Parameters for the model of presence in the pure-presence model

| Parameter | dimensions | explanation |
|-----------|------------------|---|
| z | $N \times T$ | “true” species presence/absence |
| θ | $N \times T - 1$ | probability of $z = 1$ |
| a | $T - 1 \times D$ | ecotype-varying intercept; mean value of log-odds of θ |
| m | N | species log mass, rescaled |
| b_1 | 1 | effect of species mass on log-odds of θ |
| b_2 | 1 | effect of species mass, squared, on log-odds of θ |
| U | $T \times D$ | matrix of group-level covariates |
| γ | $U \times D$ | matrix of group-level regression coefficients |
| Σ | $D \times D$ | covariance matrix of a |
| Ω | $D \times D$ | correlation matrix of a |
| τ | D | vector of standard deviations for each ecotype a_d |

180 Pure-presence process

For the pure-presence model there is only a single probability dealing with the presence of a species
182 θ (Table 4a). This probability was modeled as multi-level logistic regression with both species-level
and group-level covariates (Gelman et al., 2013; Gelman and Hill, 2007). The parameters associated
184 with pure-presence model are presented in Table 6 and the full sampling statement in Equation 2.

The species-level of the model (Eq. 2) is a logistic regression with varying-intercept that varies by
186 ecotype. Additionally, species mass was included as a covariate associated with two regression
coefficients allowing a quadratic relationship with log-odds of occurrence. This assumption is based
188 on the known distribution of mammal body masses where species with intermediate mass values are
more common than either small or large bodied species. These assumptions are also reflected in the
190 choice of priors for these regression coefficients.

The values of each ecotype’s intercept are themselves modeled as regressions using the group-level
192 covariates associated with environmental context. Each of these regressions has an associated
variance of possible values of each ecotype’s intercept (Gelman and Hill, 2007). In addition, the
194 covariances between ecotype intercepts, given this group-level regression, are modeled (Gelman and
Hill, 2007).

196 All parameters not modeled elsewhere were given weakly informative priors (Gelman et al., 2013)

CITATION STAN MANUAL STATISTICAL RETHINKING. Weakly informative means that

198 priors do not necessarily encode actual prior information but instead help regularize or weakly
 constrain posterior estimates. These priors have a concentrated probability density around and near
 200 zero; this has the effect of tempering our estimates and help prevent overfitting the model to the
 data (Gelman et al., 2013) CITATION STAN MANUAL STATISTICAL RETHINKING.

$$\begin{aligned}
 y_{i,t} &\sim \text{Bernoulli}(p_{i,t}z_{i,t}) & \alpha_0 &\sim \mathcal{N}(0, 1) \\
 p_{i,t} &= \text{logit}^{-1}(\alpha_0 + \alpha_1 m_i + r_t) & \alpha_1 &\sim \mathcal{N}(1, 1) \\
 r_t &\sim \mathcal{N}(0, \sigma) & \sigma &\sim \mathcal{N}^+(1) \\
 z_{i,1} &\sim \text{Bernoulli}(\rho) & b_1 &\sim \mathcal{N}(0, 1) \\
 z_{i,t} &\sim \text{Bernoulli}(\theta_{i,t}) & b_2 &\sim \mathcal{N}(-1, 1) \\
 \theta_{i,t} &= \text{logit}^{-1}(a_{t,j[i]} + b_1 m_i + b_2 m_i^2) & \gamma &\sim \mathcal{N}(0, 1) \\
 a &\sim \text{MVN}(u\gamma, \Sigma) & \tau &\sim \mathcal{N}^+(1) \\
 \Sigma &= \text{diag}(\tau)\Omega\text{diag}(\tau) & \Omega &\sim \text{LKJ}(2)
 \end{aligned} \tag{2}$$

202 Birth-death process

In the birth-death model, $\phi \neq \pi$ and so each of these probabilities are modeled separately but in a
 204 similar manner to how θ is modeled in the pure-presence model (Eq. 2, Table 4b). The parameters
 associated with the birth-death presence model are presented in Table 7 and the full sampling
 206 statement, including observation (Eq. 1), is described in Equation 3.

Similar to the pure-presence model, both ϕ and π are modeled as logistic regressions with
 208 varying-intercept and one covariate associated with two parameters. The possible relationships
 between mass and both ϕ and π are reflected in the parameterization of the model and choice of
 210 priors (Eq. 3).

The intercepts of ϕ and π both vary by species ecotype and those values are themselves the product

Table 7: Parameters for the model of presence in the pure-presence model

| Parameter | dimensions | explanation |
|---------------|------------------|---|
| z | $N \times T$ | “true” species presence/absence |
| ϕ | $N \times T$ | probability of $z_{-,t} = 1 z_{-,t-1} = 0$ |
| π | $N \times T - 1$ | probability of $z_{-,t} = 1 z_{-,t-1} = 1$ |
| a^ϕ | $T - 1 \times D$ | ecotype-varying intercept; mean value of log-odds of θ |
| a^π | $T - 1 \times D$ | ecotype-varying intercept; mean value of log-odds of θ |
| m | N | species log mass, rescaled |
| b_1^ϕ | 1 | effect of species mass on log-odds of ϕ |
| b_1^π | 1 | effect of species mass on log-odds of π |
| b_2^ϕ | 1 | effect of species mass, squared, on log-odds of ϕ |
| b_2^π | 1 | effect of species mass, squared, on log-odds of π |
| U | $T \times D$ | matrix of group-level covariates |
| γ^ϕ | $U \times D$ | matrix of group-level regression coefficients |
| γ^π | $U \times D$ | matrix of group-level regression coefficients |
| Σ^ϕ | $D \times D$ | covariance matrix of a^ϕ |
| Σ^π | $D \times D$ | covariance matrix of a^π |
| Ω^ϕ | $D \times D$ | correlation matrix of a^ϕ |
| Ω^π | $D \times D$ | correlation matrix of a^π |
| τ^ϕ | D | vector of standard deviations for each ecotype a_d^ϕ |
| τ^π | D | vector of standard deviations for each ecotype a_d^π |

212 of group-level regression using environmental factors as covariates (Eq. 3); this is identical to the

pure presence model (Eq. 2).

$$\begin{aligned}
y_{i,t} &\sim \text{Bernoulli}(p_{i,t} z_{i,t}) & \Sigma^\phi &= \text{diag}(\tau^\phi) \Omega^\phi \text{diag}(\tau^\phi) \\
p_{i,t} &= \text{logit}^{-1}(\alpha_0 + \alpha_1 m_i + r_t) & \Sigma^\pi &= \text{diag}(\tau^\pi) \Omega^\pi \text{diag}(\tau^\pi) \\
r_t &\sim \mathcal{N}(0, \sigma) & \rho &\sim \text{U}(0, 1) \\
\alpha_0 &\sim \mathcal{N}(0, 1) & b_1^\phi &\sim \mathcal{N}(0, 1) \\
\alpha_1 &\sim \mathcal{N}(1, 1) & b_1^\pi &\sim \mathcal{N}(0, 1) \\
\sigma &\sim \mathcal{N}^+(1) & b_2^\phi &\sim \mathcal{N}(-1, 1) \\
z_{i,1} &\sim \text{Bernoulli}(\phi_{i,1}) & b_2^\pi &\sim \mathcal{N}(-1, 1) \\
z_{i,t} &\sim \text{Bernoulli}\left(z_{i,t-1}\pi_{i,t} + \sum_{x=1}^t (1 - z_{i,x})\phi_{i,t}\right) & \gamma^\phi &\sim \mathcal{N}(0, 1) \\
& & \gamma^\pi &\sim \mathcal{N}(0, 1) \\
\phi_{i,t} &= \text{logit}^{-1}(a_{t,j[i]}^\phi + b_1^\phi m_i + b_2^\phi m_i^2) & \tau^\phi &\sim \mathcal{N}^+(1) \\
\pi_{i,t} &= \text{logit}^{-1}(a_{t,j[i]}^\pi + b_1^\pi m_i + b_2^\pi m_i^2) & \tau^\pi &\sim \mathcal{N}^+(1) \\
a^\phi &\sim \text{MVN}(U\gamma^\phi, \Sigma^\phi) & \Omega^\phi &\sim \text{LKJ}(2) \\
a^\pi &\sim \text{MVN}(U\gamma^\pi, \Sigma^\pi) & \Omega^\pi &\sim \text{LKJ}(2)
\end{aligned} \tag{3}$$

214 Posterior inference and model adequacy

Programs that implement joint posterior inference for the above models (Eqs. 2, 3) were
216 implemented in the probabilistic programming language Stan CITATION. The models used here
both feature latent discrete parameters in the large matrix z (Tables 5, 6, 7; Eqs. 1, 2, 3). All
218 methods for posterior inference implemented in Stan are derivative based which causes
complications for actually implementing the above models because integers do not have derivatives.
220 Instead of implementing a latent discrete parameterization, the posterior probabilities of all possible
states of the latent parameters z were estimated (i.e. marginalized).
222 Species durations at minimum range-through from the FAD to the LAD, but the incompleteness of

all observations means that the actual time of origination or extinction is unknown. The

224 marginalization approach used here means that the probabilities all possible histories for a species
are calculated, from the end members of the species having existed for the entire study interval and
226 the species having only existed between the directly observed FAD and LAD to all possible
intermediaries CITATION STAN MANUAL.

| | Time Bin | | | | | | | |
|-----------|----------|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Observed | 0 | 0 | 0 | 1 | 0 | 1 | 1 | 0 |
| Certain | ? | ? | ? | 1 | 1 | 1 | 1 | ? |
| Potential | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 0 |
| Potential | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 0 |
| Potential | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 0 |
| Potential | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 |
| Potential | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 1 |
| Potential | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 |
| Potential | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Potential | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

Figure 2: Conceptual figure of all possible occurrence histories for an observed species. The first row represents the observed presence/absence pattern for a single species at eight time points. The second row corresponds to the known aspects of the “true” occurrence history of that species. The remaining rows correspond to all possible occurrence histories that are consistent with the observed data. The process of parameter marginalization described in the text

228 The combined size of the dataset and large number of parameters in both models (Eqs. 2, 3),
specifically the total number of latent parameters that are the matrix z , means that stochastic
230 approximate posterior inference is computationally very slow even using HMC. Instead, an
approximate Bayesian approach was used: variational inference. A recently developed automatic
232 variational inference algorithm called “automatic differentiation variational inference” (ADVI) is

implemented in Stan and was used here CITATION. ADVI assumes that the posterior is Gaussian
234 but still yields a true Bayesian posterior; this assumption is similar to quadratic approximation of
the likelihood function used in maximum likelihood inference CITATION. The principal limitation
236 of assuming the joint posterior is Gaussian is that the true topology of the log-posterior isn't
represented; this is a particular burden for scale parameters which are bound to be positive (e.g.
238 standard deviation).

After fitting both models (Eqs. 2, 3) using ADVI, model adequacy and quality of fit was assessed
240 using a series of posterior predictive checks CITATION CITATION. Because all Bayesian models
are inherently generative, simulations of new data sets is “free” CITATION. By simulating many
242 theoretical data sets using the observed covariate information the congruence between predictions
made by the model and the observed empirical data can be assessed. By combining multiple
244 posterior predictive tests of congruence between empirical and simulated values of interest, the
holistic adequacy of the model can be analyzed CITATION.

246 An example posterior predictive check used in this study was comparing the observed average
number of observations per species to a distribution of simulated averages; if the empirically
248 observed value sits in the middle of the distribution than the model is adequate in reproducing the
observed number of occurrences per species.

250 Posterior simulations for time series are start with the values at $t = 1$ and then just simulating
forward.

252 Given parameter estimates, diversity and diversification rates are estimated through posterior
predictive simulations. Given the observed presence-absence matrix y , estimates of the true
254 presence-absence matrix z can be simulated and the distribution of possible occurrence histories
can be analyzed. This is conceptually similar to marginalization where the probability of each
256 possible occurrence history is estimated (Fig. 2).

The posterior distribution of z gives the estimate of standing diversity N_t^{stand} for all time points as

$$N_t^{stand} = \sum_{i=1}^M z_{i,t}. \quad (4)$$

258 Given estimates of N^{stand} for all time points, the estimated number of originations O_t are be
estimated as

$$O_t = \sum_{i=1}^M z_{i,t} = 1 | z_{i,t-1} = 0 \quad (5)$$

260 and number of extinctions E_t estimated as

$$E_t = \sum_{i=1}^M z_{i,t} = 0 | z_{i,t-1} = 1. \quad (6)$$

Per-capita growth D^{rate} , origination O^{rate} and extinction E^{rate} rates are then calculated as

$$\begin{aligned} O_t^{rate} &= \frac{O_t}{N_{t-1}^{stand}} \\ E_t^{rate} &= \frac{E_t}{N_{t-1}^{stand}} \\ D_t^{rate} &= O_t^{rate} - E_t^{rate}. \end{aligned} \quad (7)$$

262 Results

Comparing the fits of the pure-presence and birth-death models

264 Comparison of the posterior predictive performance of the pure-presence and birth-death models
reveals a striking difference in quality of the models' fits to the data (Fig. 3 and 4). The birth-death
266 model is clearly able to reproduce the observed average number of occurrence, in contrast to the
pure-birth model which greatly underestimates the observed average number of occurrences. The
268 interpretation of these results is that the results of the birth-death model are more representative of
the data than the pure-presence model, though further inspection of the posterior parameter
270 estimates can provide further insight into why these models give different posterior predictive

results (Gelman et al., 2013).

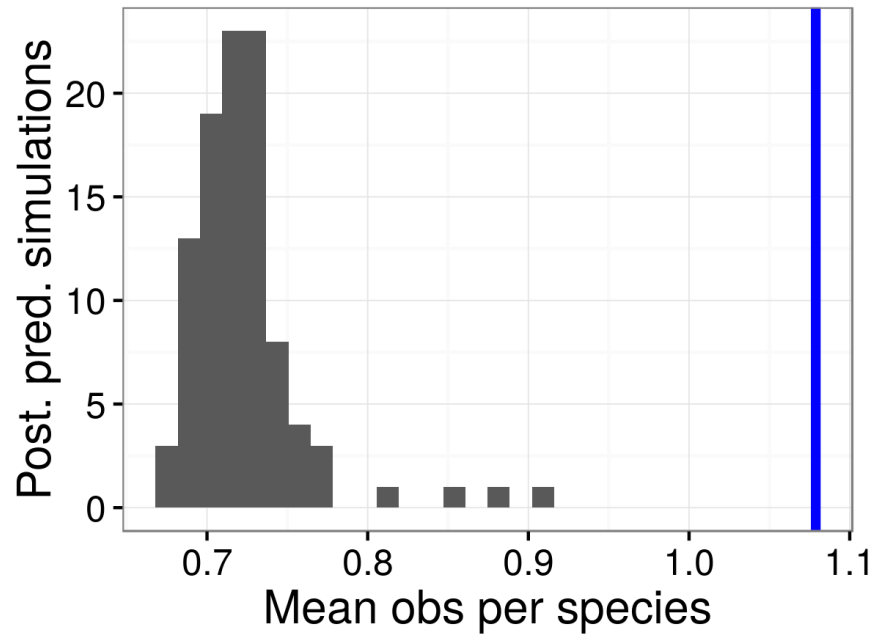


Figure 3: Comparison of the average observed number of occurrences per species (blue line) to the average number of occurrences from 100 posterior predictive datasets using the posterior estimates from the pure-presence model.

272 Posterior results take one of two forms: direct inspection of parameter estimates, and downstream
estimates of diversity and diversification rates.

274 Analysis of diversity

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280 Database publication XXX.

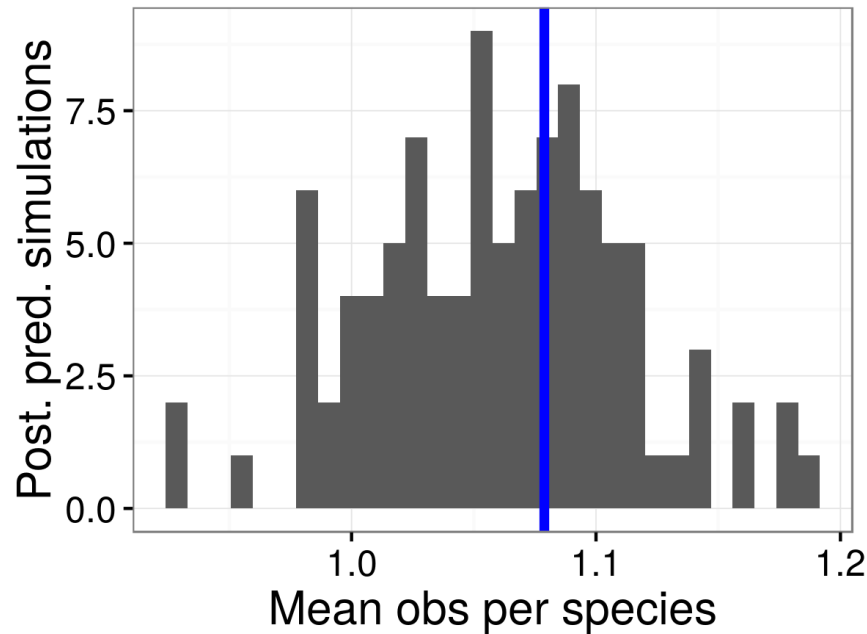


Figure 4: Comparison of the average observed number of occurrences per species (blue line) to the average number of occurrences from 100 posterior predictive datasets using the posterior estimate from the birth-death model.

References

- Allen, L. J. S. 2011. An introduction to stochastic processes with applications to biology. 2nd ed. Chapman and Hall/CRC, Boca Raton, FL.
- Alroy, J. 1996. Constant extinction, constrained diversification, and uncoordinated stasis in North American mammals. *Palaeogeography, Palaeoclimatology, Palaeoecology* 127:285–311.
- . 2009. Speciation and extinction in the fossil record of North American mammals. Pages 302–323 in R. K. Butlin, J. R. Bridle, and D. Schluter, eds. *Speciation and patterns of diversity*. Cambridge University Press, Cambridge.
- Alroy, J., P. L. Koch, and J. C. Zachos. 2000. Global climate change and North American mammalian evolution. *Paleobiology* 26:259–288.
- Bambach, R. K., A. M. Bush, and D. H. Erwin. 2007. Autecology and the filling of ecospace: Key metazoan radiations. *Palaeontology* 50:1–22.

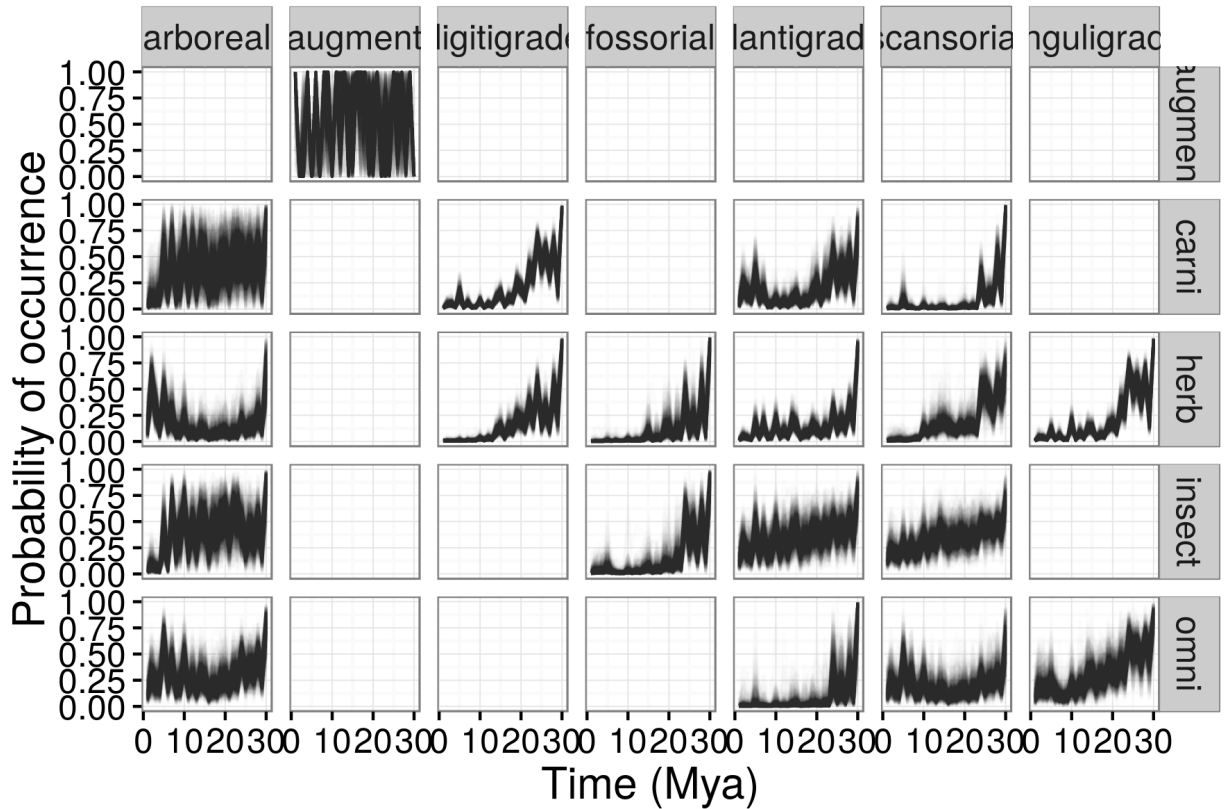


Figure 5: Probability of a mammal ecotype occurring over time as estimated from the pure-presence model. Each panel depicts 100 random samples from the model's posterior. The columns are by locomotor category and rows by dietary category; their intersections are the observed and analyzed ecotypes. Panels with no lines are ecotypes not observed in the dataset.

Blois, J. L., and E. A. Hadly. 2009. Mammalian Response to Cenozoic Climatic Change. Annual
 294 Review of Earth and Planetary Sciences 37:181–208.

Brown, A. M., D. I. Warton, N. R. Andrew, M. Binns, G. Cassis, and H. Gibb. 2014. The
 296 fourth-corner solution - using predictive models to understand how species traits interact with
 the environment. Methods in Ecology and Evolution 5:344–352.

Bush, A. M., and R. K. Bambach. 2011. Paleoeologic Megatrends in Marine Metazoa, vol. 39.
 298

Bush, A. M., R. K. Bambach, and G. M. Daley. 2007. Changes in theoretical ecospace utilization in
 300 marine fossil assemblages between the mid-Paleozoic and late Cenozoic. Paleobiology 33:76–97.

Clyde, W. C., and P. D. Gingerich. 1998. Mammalian community response to the latest Paleocene

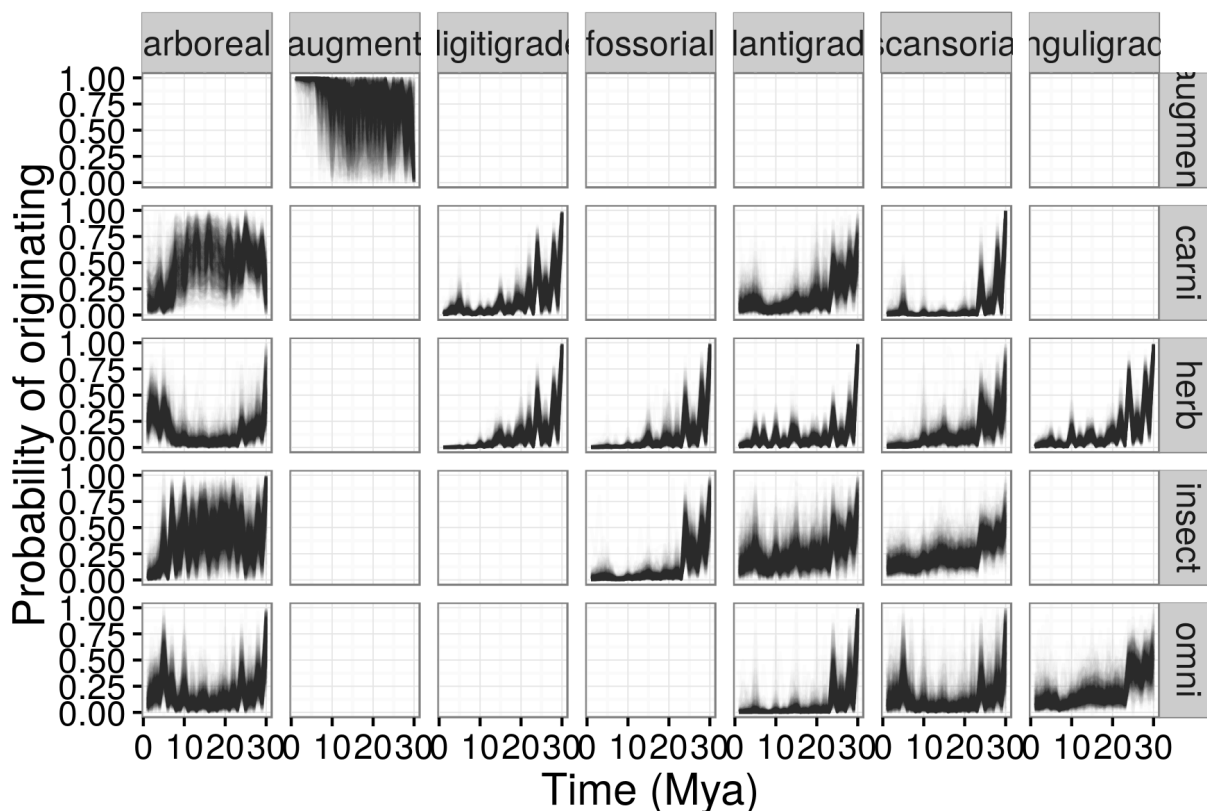


Figure 6: Probability of a mammal ecotype origination probabilities at each time point as estimated from the birth-death model. Each panel depicts 100 random samples from the model's posterior. The columns are by locomotor category and rows by dietary category; their intersections are the observed and analyzed ecotypes. Panels with no lines are ecotypes not observed in the dataset.

thermal maximum: an isotaphonomic study in the northern Bighorn Basin, Wyoming. *Geology* 26:1011–1014.

Cramer, B. S., K. Miller, P. Barrett, and J. Wright. 2011. Late Cretaceous-Neogene trends in deep ocean temperature and continental ice volume: Reconciling records of benthic foraminiferal geochemistry ($\delta^{18}\text{O}$ and Mg/Ca) with sea level history. *Journal of Geophysical Research: Oceans* 116:1–23.

Eronen, J. T., C. M. Janis, C. P. Chamberlain, and A. Mulch. 2015. Mountain uplift explains differences in Palaeogene patterns of mammalian evolution and extinction between North America and Europe. *Proceedings of the Royal Society B: Biological Sciences* 282:20150136.

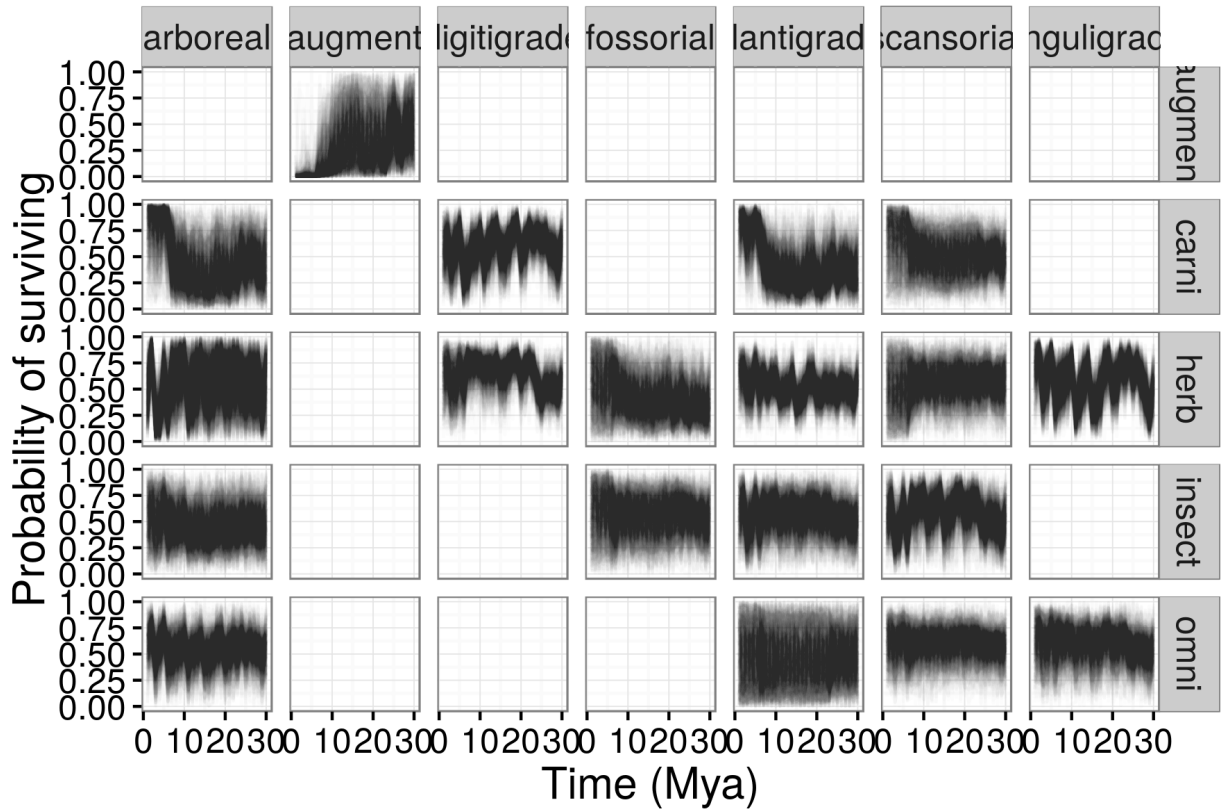


Figure 7: Probability of a mammal ecotype survival probabilities at each time point as estimated from the birth-death model. Each panel depicts 100 random samples from the model's posterior. The columns are by locomotor category and rows by dietary category; their intersections are the observed and analyzed ecotypes. Panels with no lines are ecotypes not observed in the dataset.

Ezard, T. H. G., A. Purvis, and H. Morlon. 2016. Environmental changes define ecological limits to species richness and reveal the mode of macroevolutionary competition. *Ecology Letters* 19:899–906.

Figueirido, B., C. M. Janis, J. A. Pérez-Claros, M. De Renzi, and P. Palmqvist. 2012. Cenozoic climate change influences mammalian evolutionary dynamics. *Proceedings of the National Academy of Sciences* 109:722–727.

Foote, M. 2001. Inferring temporal patterns of preservation, origination, and extinction from taxonomic survivorship analysis. *Paleobiology* 27:602–630.

Foote, M., and J. J. Sepkoski. 1999. Absolute measures of the completeness of the fossil record.

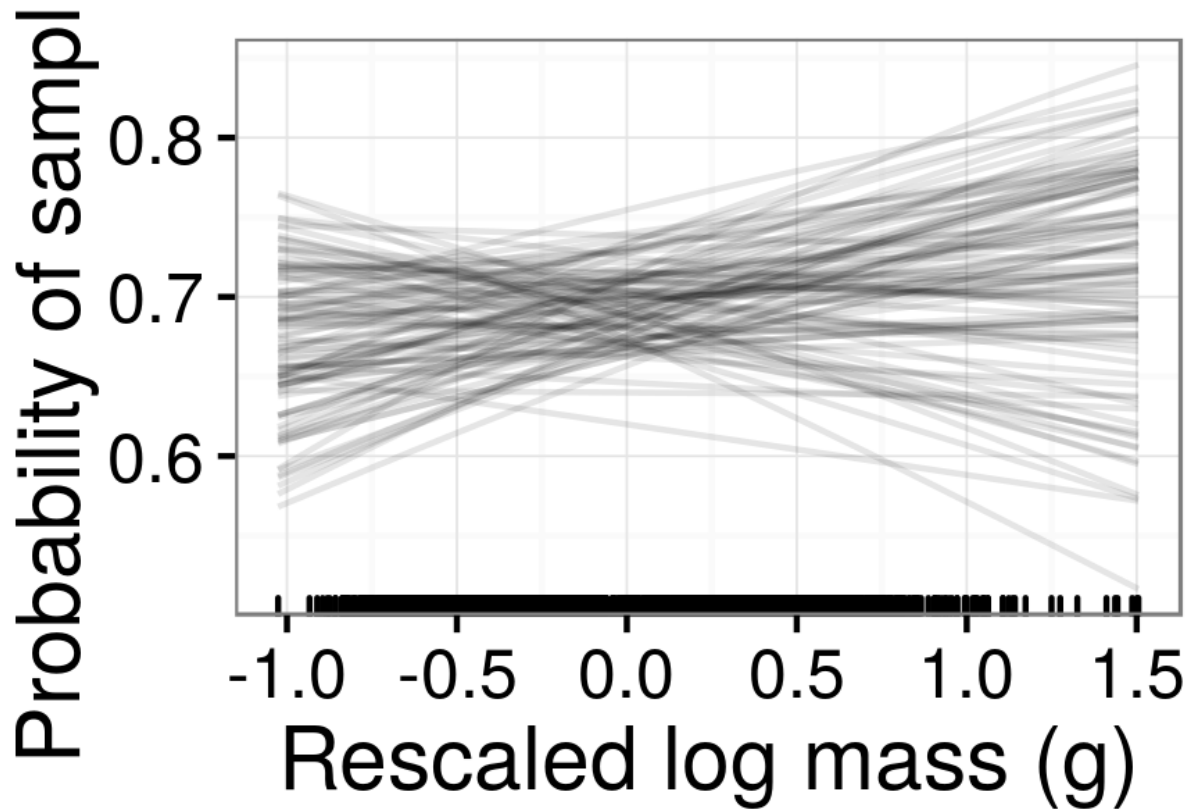


Figure 8: Estimates of the effect of species mass on probability of observing a present species (p). Mass has been log-transformed, centered, and rescaled; this means that a mass of 0 corresponds to the mean of log-mass of all observed species and that mass is in standard deviation units. Estimates are from the pure-presence model.

Nature 398:415–7.

Gelman, A. 2008. Scaling regression inputs by dividing by two standard deviations. *Statistics in Medicine* pages 2865–2873.

Gelman, A., J. B. Carlin, H. S. Stern, D. B. Dunson, A. Vehtari, and D. B. Rubin. 2013. *Bayesian data analysis*. 3rd ed. Chapman and Hall, Boca Raton, FL.

Gelman, A., and J. Hill. 2007. *Data Analysis using Regression and Multilevel/Hierarchical Models*. Cambridge University Press, New York, NY.

Janis, C. M. 1993. Tertiary mammal evolution in the context of changing climates, vegetation, and tectonic events. *Annual Review of Ecology and Systematics* 24:467–500.

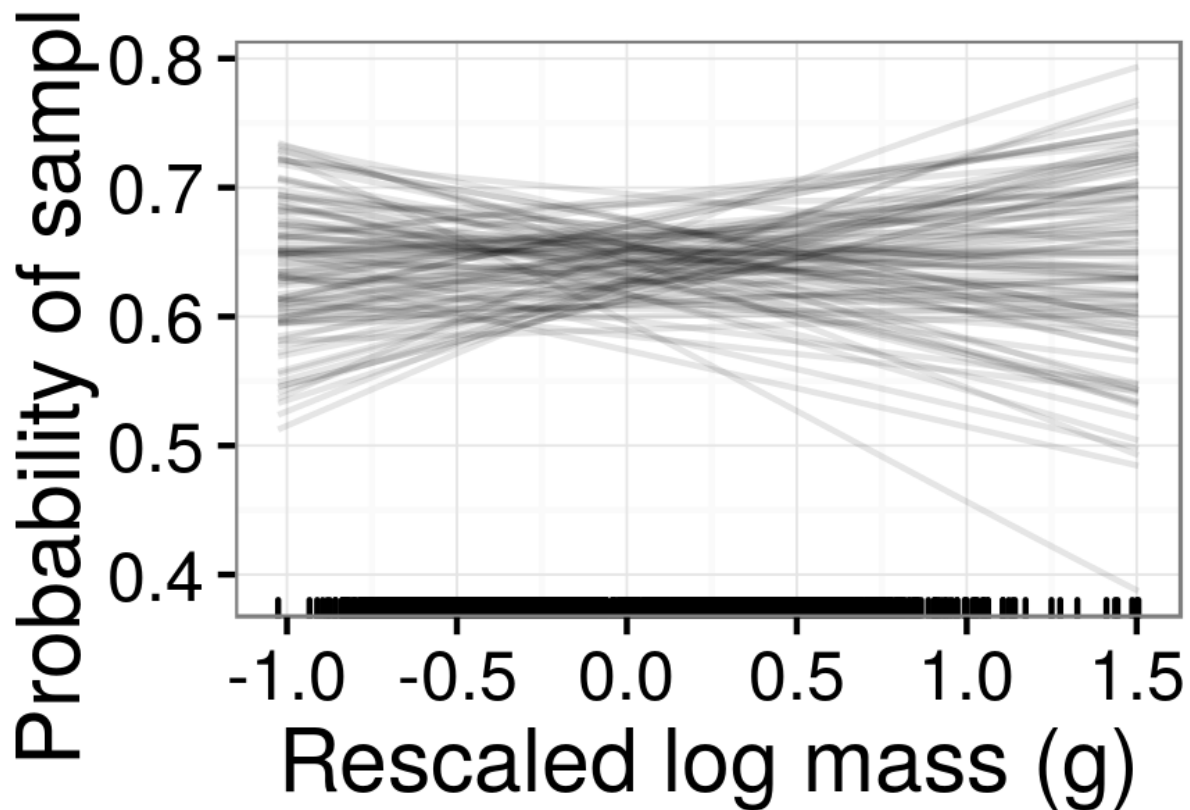


Figure 9: Estimates of the effect of species mass on probability of observing a present species (p). Mass has been log-transformed, centered, and rescaled; this means that a mass of 0 corresponds to the mean of log-mass of all observed species and that mass is in standard deviation units. Estimates are from the birth-death model.

Janis, C. M., J. Damuth, and J. M. Theodor. 2000. Miocene ungulates and terrestrial primary

productivity: where have all the browsers gone? *Proceedings of the National Academy of Sciences* 97:7899–904.

Janis, C. M., G. F. Gunnell, and M. D. Uhen. 2008. *Evolution of Tertiary mammals of North America*. Vol. 2. Small mammals, xenarthrans, and marine mammals. Cambridge University

Press, Cambridge.

Janis, C. M., K. M. Scott, and L. L. Jacobs. 1998. *Evolution of Tertiary mammals of North*

America. Vol. 1. Terrestrial carnivores, ungulates, and ungulatelike mammals. Cambridge University Press, Cambridge.

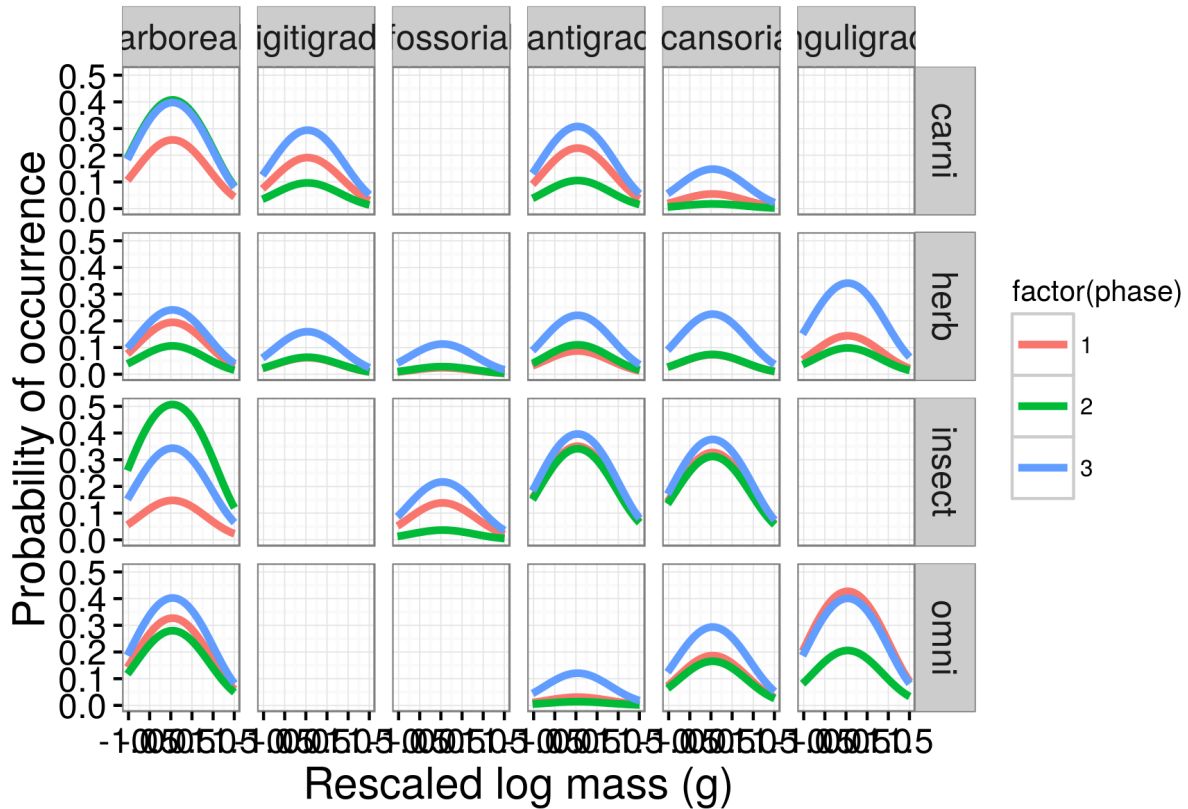


Figure 10: Mean estimate of the effect of species mass on the probability of a species occurrence for each of the three plant phases. The effect of mass is considered constant over time and that the only aspect of the model that changes with plant phase is the intercept of the relationship between mass and occurrence. The three plant phases are indicated by the color of the line. Mass has been log-transformed, centered, and rescaled; this means that a mass of 0 corresponds to the mean of log-mass of all observed species and that mass is in standard deviation units.

- 338 Legendre, S. 1986. Analysis of mammalian communities from the Late Eocene and Oligocene of Southern France. *Paleovertebrata* 16:191–212.
- 340 Lloyd, G. T., J. R. Young, and A. B. Smith. 2011. Taxonomic Structure of the Fossil Record is Shaped by Sampling Bias. *Systematic Biology* 61:80–89.
- 342 Royle, J. A., and R. M. Dorazio. 2008. Hierarchical modeling and inference in ecology: the analysis of data from populations, metapopulations and communities. Elsevier, London.
- 344 ———. 2012. Parameter-expanded data augmentation for Bayesian analysis of capture-recapture models. *Journal of Ornithology* 152:521–537.

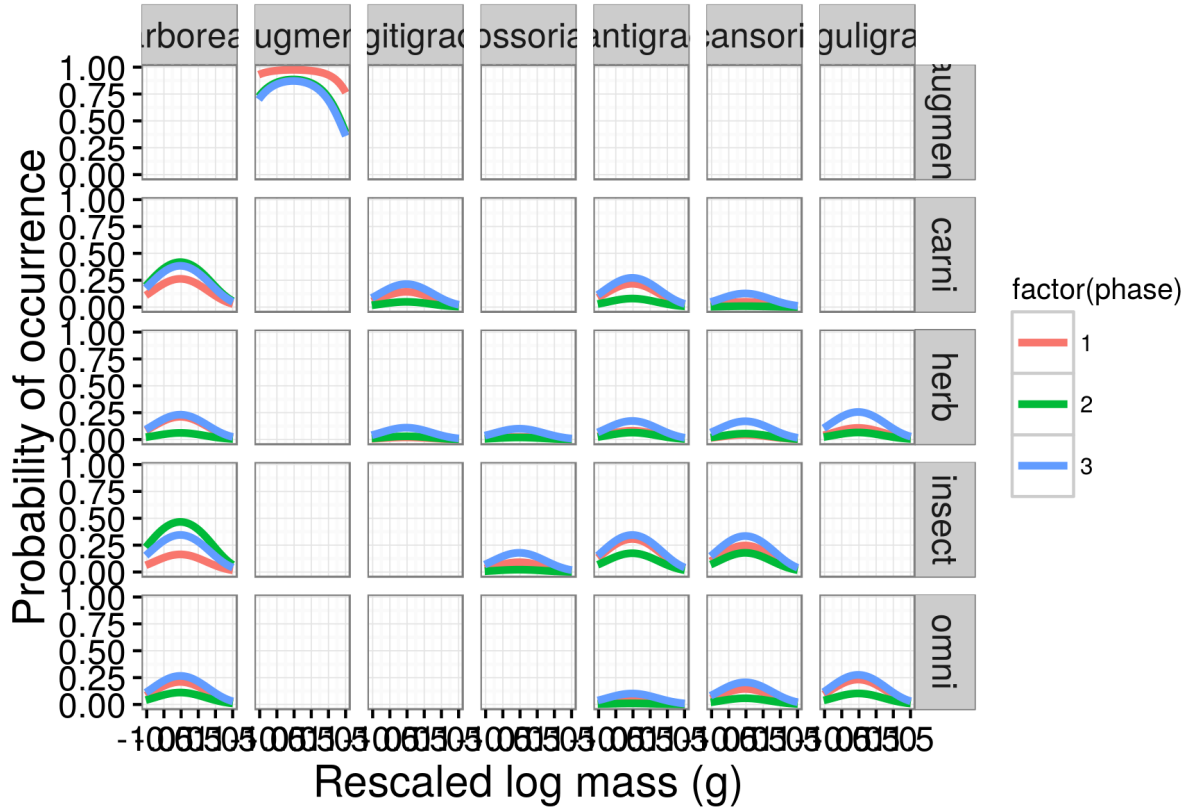


Figure 11: Mean estimate of the effect of species mass on the probability of a species originating for each of the three plant phases. The effect of mass is considered constant over time and that the only aspect of the model that changes with plant phase is the intercept of the relationship between mass and origination. The three plant phases are indicated by the color of the line. Mass has been log-transformed, centered, and rescaled; this means that a mass of 0 corresponds to the mean of log-mass of all observed species and that mass is in standard deviation units.

- 346 Royle, J. A., R. M. Dorazio, and W. a. Link. 2007. Analysis of Multinomial Models With Unknown
Index Using Data Augmentation. *Journal of Computational and Graphical Statistics* 16:67–85.
- 348 Royle, J. A., J. D. Nichols, M. Kéry, E. Ranta, and M. Kery. 2014. detection is of species when
Modelling occurrence and abundance imperfect 110:353–359.
- 350 Rubin, D. B. 1996. Multiple imputation after 18+ years. *Journal of the American Statistical
Assocaition* 91:473–489.
- 352 Smits, P. D. 2015. Expected time-invariant effects of biological traits on mammal species duration.
Proceedings of the National Academy of Sciences 112:13015–13020.

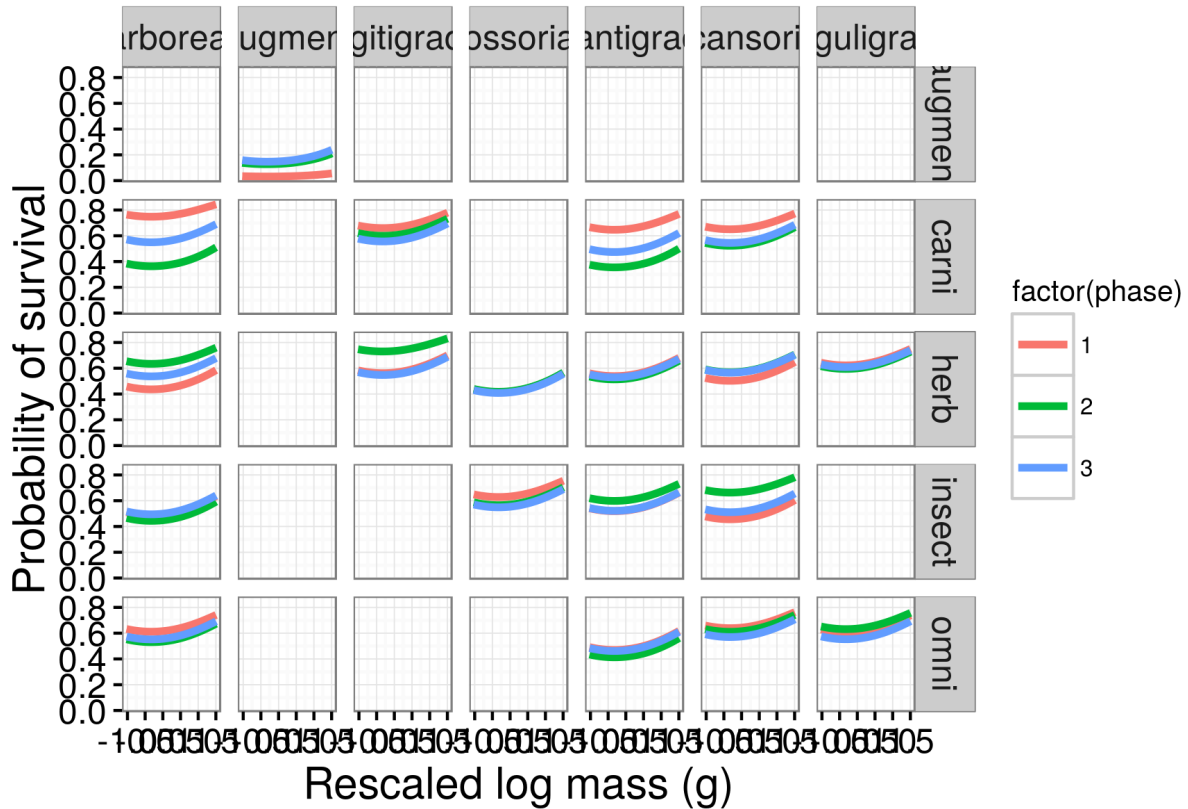


Figure 12: Mean estimate of the effect of species mass on the probability of a species survival for each of the three plant phases. The effect of mass is considered constant over time and that the only aspect of the model that changes with plant phase is the intercept of the relationship between mass and survival. The three plant phases are indicated by the color of the line. Mass has been log-transformed, centered, and rescaled; this means that a mass of 0 corresponds to the mean of log-mass of all observed species and that mass is in standard deviation units.

Strömberg, C. A. E. 2005. Decoupled taxonomic radiation and ecological expansion of open-habitat grasses in the Cenozoic of North America. *Proceedings of the National Academy of Sciences of the United States of America* 102:11980–4.

Tomiya, S. 2013. Body Size and Extinction Risk in Terrestrial Mammals Above the Species Level. *The American Naturalist* 182:196–214.

Wang, S. C., P. J. Everson, H. J. Zhou, D. Park, and D. J. Chudzicki. 2016. Adaptive credible intervals on stratigraphic ranges when recovery potential is unknown. *Paleobiology* 42:240–256.

Wang, S. C., and C. R. Marshall. 2016. Estimating times of extinction in the fossil record. *Biology*

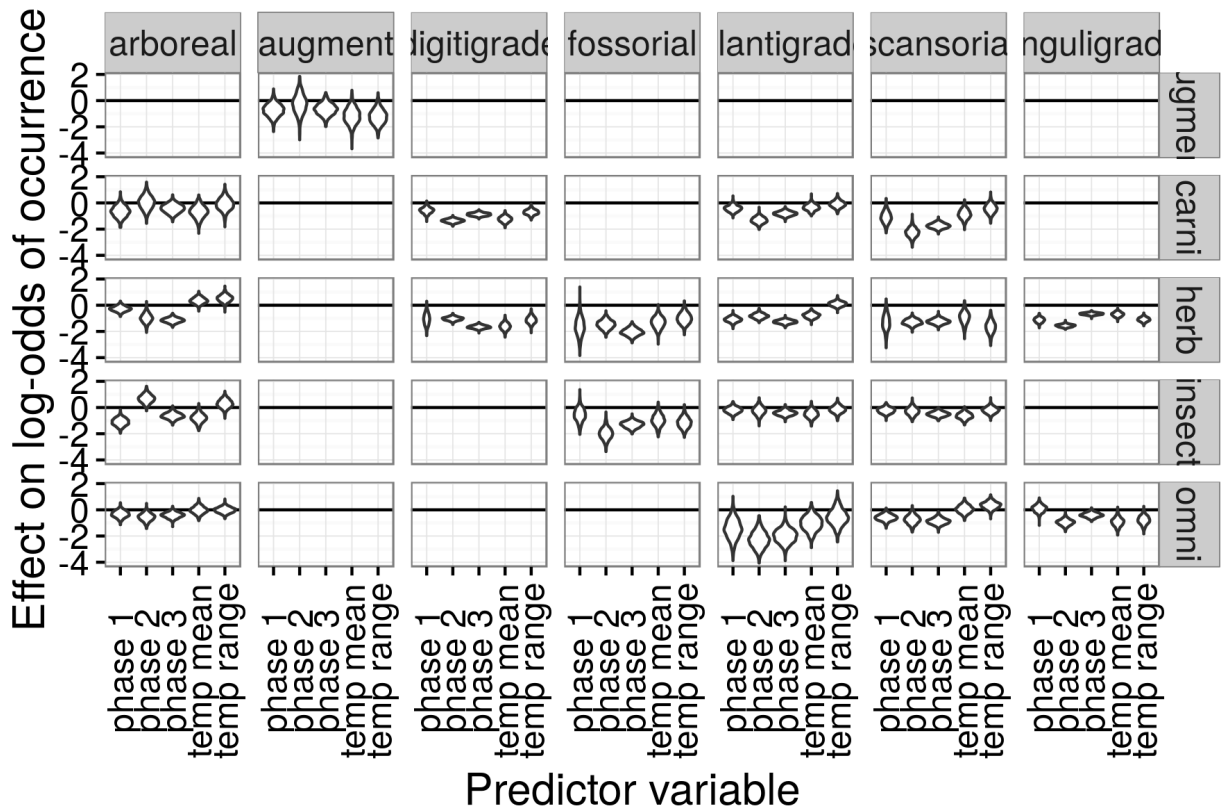


Figure 13: Estimated effects of the group-level covariates describing environmental context on log-odds of species occurrence. These estimates are from the pure-presence model.

Letters 12:20150989.

Warton, D. I., B. Shipley, and T. Hastie. 2015. CATS regression - a model-based approach to studying trait-based community assembly. *Methods in Ecology and Evolution* 6:389–398.

Zachos, J. C., G. R. Dickens, and R. E. Zeebe. 2008. An early Cenozoic perspective on greenhouse warming and carbon-cycle dynamics. *Nature* 451:279–283.

Zachos, J. C., M. Pagani, L. Sloan, E. Thomas, and K. Billups. 2001. Trends, rhythms, and aberrations in global climate 65 Ma to present. *Science* 292:686–693.

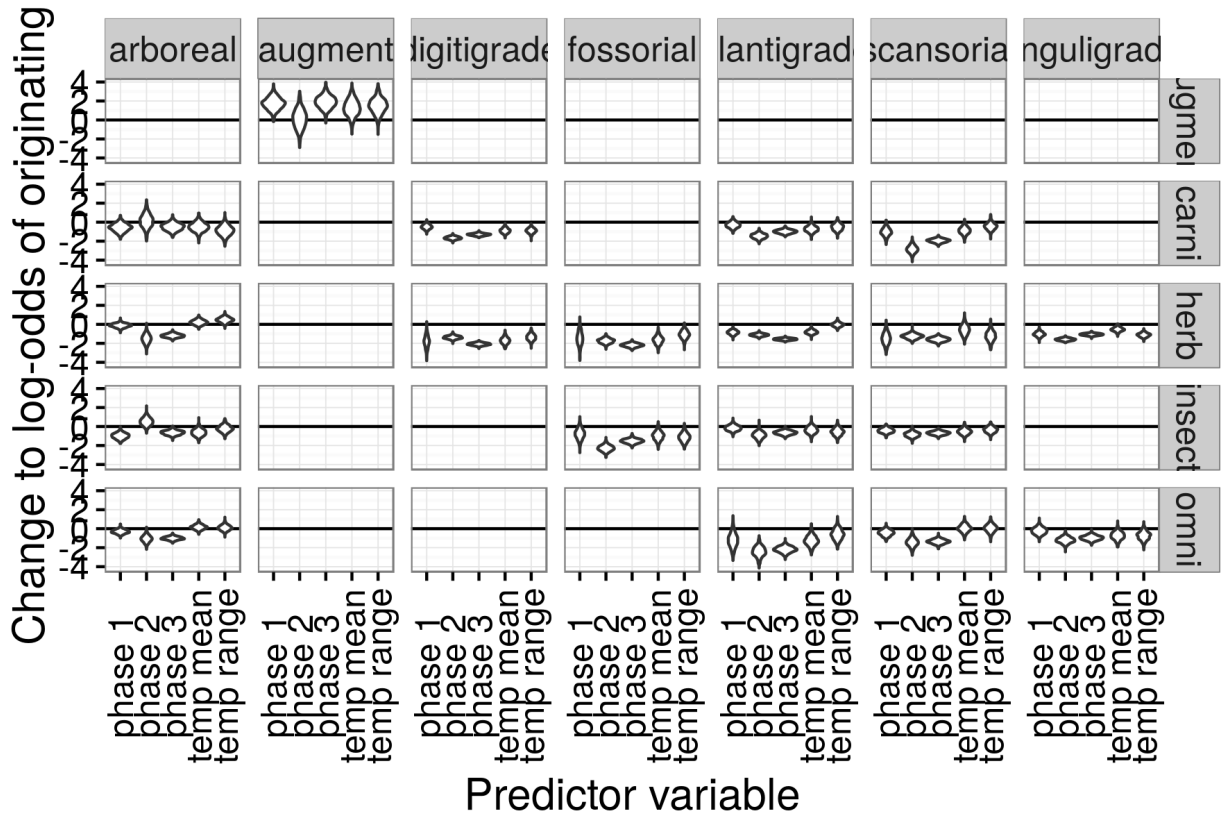


Figure 14: Estimated effects of the group-level covariates describing environmental context on log-odds of species origination. These estimates are from the birth-death model.

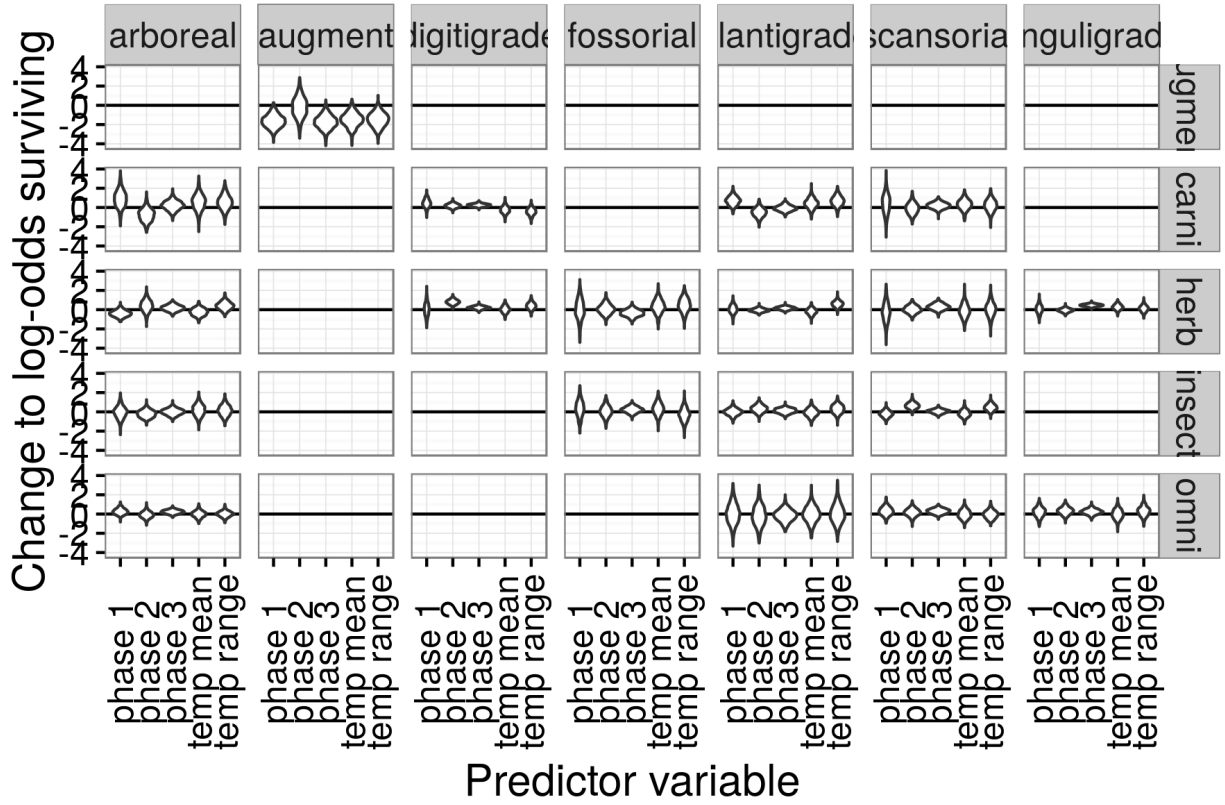


Figure 15: Estimated effects of the group-level covariates describing environmental context on log-odds of species survival. These estimates are from the birth-death model.