How predictable is extinction? Forecasting species survival at million-year timescales

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# Supplement to Materials and Methods

## Data Specifications

### Binning fossil occurrences

The estimated age of each occurrence is based on the core-specific age-model that observation is from and can be overly precise. To alleviate this overprecision, we coarsened our temporal information in an effort to limit the effects of between-core heterogeneity in age. The occurrence histories of each species was then summarized as a series of binary codes indicating the presence or last occurrence of that species. For every occurrence of a species, except the last, that species existence and survival is recorded as a 0. The last occurrence of that species is considered the bin in which the taxon has gone extinct – and is recorded as 1. This protocol means that we are reading the fossil record “as written,” a practice that is potentially dangerous as it is an overconfident statement of preservation and may be shortening the actual durations of the studied species (Alroy 2010; Alroy 2000; Alroy 2014; M Foote 1997; M Foote and Sepkoski 1999; Michael Foote 2001; Michael Foote and Raup 1996; Lloyd et al. 2012; C. R. Marshall 1995; Wang and Marshall 2016). However, this practice is common with marine microfossil data due to their exceptional preservation rate (Ezard, Thomas, and Purvis 2013; Ezard and Purvis 2016; Ezard et al. 2011; Liow et al. 2010). In fact, with marine microfossils collected from cores a bigger problem may be over extending the duration of a species due to mixing and smearing within the cores (Mekik and Anderson 2018; W. Broecker et al. 1999; Mekik 2014; Peng and Broecker 1984).

### Covariate transformation and standardization

Prior to analysis, geographic range was then log-plus-one transformed and standardized by mean-centering the data and then dividing by the standard deviation of the distribution of geographic ranges. This standardization means that a regression coefficient associated with each covariate describes the change in extinction probability per change in standard deviation of that covariate, that coefficients associated with similarly standardized covariates will be directly comparable in magnitude, and that the intercept term corresponds to the expected value of the outcome at when geographic range is its average value (Gelman and Hill 2006). Change in geographic range between observations was measured from the standardized geographic range values and was not standardized separately.

Temperature was also transformed and standardized the in the same manner as geographic range. The change in temperature between an observation and its previous observation was measured from the standardized temperature values and was not standardized separately.

## Model Specifications

In survival analysis, the hazard function describes the instantaneous rate of extinction of a species given its age and covariate information. The hazard function is defined as the conditional probability of a species going extinct by the end of the -th interval given that it survived up until and the relevant covariate information for all 1 My intervals (Tutz and Schmid 2016). For the discrete time intervals , extinction is defined as . The discrete time hazard function is defined as

The hazard function (Eq. [eq:hazard]) is easily reparameterized as a logistic regression by defining that where is a logit inverse-link function and is the probability of a taxon going extinction during interval (Tutz and Schmid 2016). is then modeled as with any regression. In this case, we opted for a hierarchical/mixed-effects model with multiple non-nested varying intercepts and slopes (Gelman and Hill 2006).

Our covariates matrix is a matrix where is the total number of observations and is the total number of covariates. The first column of is entirely 1’s as it corresponds to the intercept term in the regression model. The next two columns of are two aspects of geographic range as continuous covariates: geographic range during interval , and the difference between the geographic range at and . Change in geographic range was calculated from the transformed and standardized geographic range values; this means that change in geographic range is in units of changes in standard deviations. The final two columns are two aspects of global temperature: mean temperature during interval , and the lag of mean temperature (i.e. mean temperature during interval .) As with change to geographic range, the lag of temperature is based on the transformed and standardized temperature estimates.

The matrix of time and phylum varying regression coefficients describing the effects of the covariates on a species’ risk of extinction is called – a by matrix, were is the number of time temporal intervals and is the number of phyla. The elements of this matrix, the regression coefficients, are themselves modeled as being multivariate normally distributed with vector of means describing the average intercept and regression coefficient estimates of each phylum . These phylum averages are themselves modeled as multivariate normally distributed with mean vector describing the overall average regression coefficients, including the intercept. has length and is ordered intercept, range coefficient, change in range coefficient, temperature coefficient, temperature lag coefficient.

The effect of species age on the log-odds of species extinction is modeled as a non-nested random intercept (Tutz and Schmid 2016). This term describes how the log-odds of extinction varies along a species duration, and how this effect can differ between the phyla. is a by matrix, where is the age at observation of a species and is its phylum. is modeled as following a multivariate normal distribution with phylum means being the vector and covariance matrix . The covariation between the elements of vector are modeled as a multivariate normal distribution with a mean vector of all 0s and covariance matrix .

To complete the generative model, we need to assign final priors to the “top-level” parameters. In general, we favored weakly informative priors which help regularize our estimates. In the case of a regression coefficient, this means a Normal distribution with mean 0 and a standard deviation of 3. For our scale parameters (e.g. standard deviations), we used half-Cauchy distributed priors with heavy tails but the majority of probability density near 0.

Our top-level intercept was given a more diffuse prior than our regression coefficients, which reflects our greater degree of uncertainty about its value. Our top-level regression coefficient for the effect of geographic range was given an informative prior reflecting the overwhelming amount of evidence that species with a larger than average geographic range have a lower risk of extinction than species with an average or less than average geographic range. In the context of this analysis, this means that we are again using a weakly informative prior but instead of centering the density around -1 (i.e. larger than average geographic range decreases extinction risk).

Instead of assigning a prior distribution for each of the covariance matrices in the model, we instead decomposed the covariance matrices (e.g. ) which allows us to assign independent priors for the scale and correlation aspects of covariance. The scale parameters were assigned half-Cauchy priors as described above in the context of all other scale parameters. The correlation matrices were assigned LKJ priors each with shape parameter set to 1. This choice of shape parameter produces a uniform distribution over possible correlation matrices. These priors are also slightly more interpretable than other common prior distributions for covariance matrices such as the inverse-Wishart distribution. This approach to assigning priors to a covariance matrix is recommended by the Stan Manual (Team 2017).

In total, our model can be expressed as:

with indexing the observation and bracket subscripts referencing the class of the th observation where is the time of the -th observation, is the phylum of the -th observation, and is the age of the -th observation.

## Model Parameter Estimation

We implemented our model (Eq. [eq:model] using the

rstanarm

package for the R programming language (Team 2017). This package provides an interface to the Stan probabilistic programming language for writing hierarchical/mixed-effects models in native R. Posterior estimates were obtained through Hamiltonian Monte Carlo, using 2000 steps divided equally between warm-up and sampling. In order to prevent divergent transitions adapt delta was increased to 0.999999; all other HMC/NUTS sampling parameters were kept at the defaults for rstanarm 2.18.2 (Gabry and Goodrich 2018).

To implement our VP model in

rstanarm

, where “data” is a data.frame object of all necessary data (response, covariates), is coded as:

form <- event ~   
 range + range\_diff1 + range\_diff2 + range\_diff3 +   
 temp + temp\_lag +   
 (1 + range + range\_diff + temp + temp\_lag | mybin/phylum) +   
 (1 | age/phylum),   
stan\_glmer(formula = form,  
 data = data,   
 family = 'binomial',  
 prior = normal(c(-1, 0, 0, 0, 0, 0), rep(1, 6), autoscale = FALSE),   
 prior\_intercept = normal(-2, 5, autoscale = FALSE),   
 prior\_aux = cauchy(0, 1, autoscale = FALSE),   
 chains = 4,  
 thin = 4,  
 adapt\_delta = 0.999999)

Similarly, our VP model can be implemented using the

brms

Stan interface (Bürkner 2017; Bürkner 2018) as:

priors <- c(set\_prior('normal(-2, 5)', class= 'Intercept'),  
 set\_prior('normal(0, 1)', class = 'b'),  
 set\_prior('normal(-1, 1)', class = 'b', coef = 'range'),  
 set\_prior('cauchy(0, 1)', class = 'sd'),  
 set\_prior('lkj(1)', class = 'cor'))  
form <- bf(event ~   
 range + range\_diff1 + range\_diff2 + range\_diff3 +   
 temp + temp\_lag +  
 (1 + range + range\_diff + temp + temp\_lag | mybin/phylum) +  
 (1 | age/phylum))  
brmfit <- brm(formula = form,  
 data = data,   
 family = bernoulli(),   
 prior = priors,  
 chains = 4,   
 thin = 4,  
 control = list(adapt\_delta = 0.999999)

Posterior convergence was determined using the general and HMC-specific diagnostic criteria: scale reduction factor (; target ), effective sample size (eff; target value eff/steps ), number of samples that saturated the maximum trajectory length for avoiding infinite loops (treedepth; target value 0), sample divergence, and the energy Bayesian Fraction of Mission Information (E-BFMI; target value ). For further explanation of these diagnostic criteria, see the Stan Manual (Team 2017).

# Supplement to Results

Here we present the parameter estimates for our from our VP model (Table 1). We choose to present the estimates from this model because it is our most inclusive model and its parameter estimates are indicative of parameter estimates from other models with a subset of those covariates included in this model.

First, we present the group-level estimates of our regression coefficients and intercept (Fig. [fig:param\_est]). Group-level effects are the average effects of that covariate over time and across taxonomic groups. These estimates make up the vector described above. In addition to the average effect of our covariates, we also included the estimate of the group-level intercept, which is the average log-odds of extinction for an average observation over time and across taxonomic groups.

Group-level parameter posterior estimates from our VP model (Table 1). The posterior distribution of our parameter estimates are presented as densities. Below each of these densities is marked the median estimate along with 50% and 80% credible intervals. Estimates are on the log-odds scale.

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Second, we present the population-level estimates for our regression coefficients along with the population-level intercept estimates (Fig. [fig:param\_est\_time\_group]. Our VP model allows for these our regression coefficients to vary over time and between taxonomic groups. Population-level estimates are those for a specific time interval and taxonomic group. In this case, the intercept estimate describes the log-odds of extinction for an average observation at that point in time and taxonomic group.

Population-level parameter posterior estimates from our VP model (Table 1). Posterior estimates are presented as a time series. The black line represents the median estimate of that parameter. In addition, the 50%, 80%, and 95% credible intervals are indicated. Estimates are on the log-odds scale.

Population-level parameter posterior estimates from our VP model (Table 1). Posterior estimates are presented as a time series. The black line represents the median estimate of that parameter. In addition, the 50%, 80%, and 95% credible intervals are indicated. Estimates are on the log-odds scale.

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