Joint inversion of proxy system models to reconstruct paleoenvironmental time series from heterogeneous data

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# Abstract

Paleoclimatic and paleoenvironmental reconstructions are fundamentally uncertain because no known proxy is a direct record of a single environmental variable of interest; all proxies are sensitive to multiple forcing factors. One productive approach to reducing proxy uncertainty is the integration of information from multiple proxy systems with complimentary, overlapping sensitivity to environmental one or more target variables. Most such analyses are conducted in an ad-hoc fashion, either through qualitative comparison to assess the similarity of single-proxy reconstructions or through step-wise quantitative interpretations where one proxy is used to constrain a variable relevant to the interpretation of a second proxy. Here we propose a formal framework for the integration of multiple proxies via the joint inversion of proxy system models. The “Joint Proxy Inversion” (JPI) method provides a statistically robust approach to producing self-consistent interpretations of multiproxy datasets, allowing full and simultaneous assessment of all proxy and model uncertainties to obtain quantitative estimates of past environmental conditions. Other benefits of the method include the ability to use independent information on climate and environmental systems to inform the interpretation of proxy data, to fully leverage information from unevenly- and differently-sampled proxy records, and to obtain refined estimates of proxy model parameters that are conditioned on paleo-archive data. Application of JPI to the marine Mg/Ca and δ18O proxy systems at two distinct timescales demonstrates many of the key properties, benefits, and sensitivities of the method, and produces new, statistically-grounded reconstructions of Neogene ocean temperature and chemistry from previously published proxy data. We suggest that JPI is a universally applicable method that can be implemented using proxy models of wide-ranging complexity to generate more robust, quantitative understanding of past climatic and environmental change.

# Introduction

Paleoenvironmental reconstructions, including reconstructions of past climate, provide a powerful tool to document the sensitivity of Earth systems to forcing, characterize the range of natural responses associated with different modes of global change, and identify key mechanisms governing these responses. Throughout the vast majority of the planet’s history, however, estimates of environmental conditions can only be obtained through proxy reconstructions. Proxy data are, as their name implies, indirect recorders of the environmental conditions we hope to estimate, and the estimates they provide are plagued by substantial, often poorly characterized, uncertainty.

The simplest proxy reconstructions typically focus on a single environmental variable of interest, inverting experimental or natural calibration datasets to obtain quantitative estimates of that variable and treating residual variance in the calibration as ‘noise’. In reality, however, no proxy system exists that is sensitive only to a single paleoenvironmentally-relevant variable, the majority of this noise reflects the uncharacterized influence of other environmental variables on the proxy system. Fossil leaf assemblages exhibit characteristic variability that can be associated with mean annual air temperature, but also appears to be influenced by annual temperature range and diverges among floras separated by long periods of independent evolution (REF). The saturation state of alkenones produced by marine phytoplankton is a sensitive recorder of water temperature, but characteristics of alkenones preserved in marine sediments appear to also be strongly affected by physiological factors, seasonality of production, and selective degradation (Conte et al. 1998, Conte et al. 2006). Even recently emerging clumped isotope techniques, which are in theory a direct recorder of the temperature of carbonate mineral formation, can be affected by factors such as growth-rate effects, carbonate system disequilibrium, and poorly constrained, potentially variable offsets between the environment of carbonate formation and more commonly targeted atmospheric temperature conditions (Passey et al. 2010, Saenger et al. 2012, Affek et al. 2014). Failure to recognize and consider the sensitivity of proxies to multiple environmental factors leads to two important problems in traditional proxy interpretations. First, considering only a single environmental variable in our interpretations maximizes the uncertainty in our reconstructions, which could be reduced if the influence of other variables is described and constrained. Second, unacknowledged sensitivity to multiple variables creates potential for biased proxy interpretations if variation in these variables is non-random over the period being reconstructed.

One productive approach to resolving the second issue is the development and use of proxy system models in the interpretation of proxy data (Evans et al. 2013). These models represent an attempt to mathematically describe the complex of environmental, physical, and biological factors that control how environmental signals are sampled, recorded, and preserved in proxy measurements. Several recent reviews and perspectives are available discussing the concepts underlying proxy system models and different ways that they have been applied to proxy interpretation, ranging from substitution for empirical calibrations in inverse estimation of environmental signals to formal integration within climate model data assimilation schemes (Evans et al. 2013). A growing number of proxy system models and modeling systems are being developed (e.g., Tolwinski-Ward et al. 2011, Stoll et al. 2012, Dee et al. 2015), and useful models span a range of complexity from empirically-constrained regressions to fully mechanistic, theory-based formulations. Key to any such model is accurate representation of uncertainty in each model component, which allows even relatively simple, potentially incomplete models to be used to obtain reconstructions with quantifiable uncertainty bounds.

Reducing the uncertainty of quantitative paleoenvironmental reconstructions requires adding constraints to proxy interpretations, as exemplified by the increasingly common development of multi-proxy reconstructions. In situations where two or more proxies share sensitivity to common or complimentary environmental variables, it stands to reason that the information provided by each can be used to refine interpretation of the multi-proxy suite. In practice, a variety of approaches have been used. Commonly, multi-proxy integration has been qualitative and focused on confirmation: trends reconstructed using one proxy system are cross-checked against a second, providing increased confidence in the reconstruction where the patterns match and further investigation where they don’t (e.g., Keating-Bitonti et al. 2011, Grauel et al. 2013). In other cases, proxies have been combined quantitatively, but usually in a stepwise fashion: one proxy system is used to estimate an environmental variable to which it is sensitive, and those reconstructed values are then used to constrain the interpretation of a second proxy formed at the same time (e.g., Fricke et al. 1998, Lear et al. 2000). Although it provides a simple strategy to combining complimentary proxy information, this approach does not fully leverage overlapping information that may be contained in multiple systems that respond to common forcing, is not conducive to robust quantification of uncertainty, and requires that both proxies sample coeval paleoenvironmental conditions.

Here we propose a general approach to proxy interpretation that leverages the benefits of proxy models and provides a formal statistical framework for proxy integration. The method, which we call Joint Proxy Inversion (JPI), cast in a Bayesian inferential framework, uses Markov Chain Monte Carlo methods to invert a hierarchy of proxy-system and environmental time series models. These models are simultaneously conditioned on proxy data and calibration datasets to obtain posterior estimates of the target paleoclimate time series with quantifiable uncertainty that accounts for all model components. We first describe the framework as applied to joint inversion of the marine Mg/Ca and δ18O proxy systems. We choose this system not because it is particularly challenging, but because it represents a well-established and widely-used multi-proxy system where diverse examples of proxy integration are available. We then present applications of JPI to two such datasets recording paleoceanographic conditions at two different timescales. These applications provide a platform allowing us to illustrate and discuss merits and limitations of JPI relevant to its broader application.

# Methods

Bayesian inversion of proxy system models has been demonstrated previously, for example to estimate site-specific model parameters (Tolwinski-Ward et al. 2013). JPI extends this approach to the simultaneous inversion of multiple proxy system and environmental time series models, conditioned on multiproxy data, to generate estimates of the posterior distribution of model parameters including the target paleoenvironmental time series.

## Data

Proxy and proxy model calibration datasets were compiled from published work (Fig. 1). Estimates from fluid inclusions, calcite veins, and echinoderm fossils (Lowenstein et al. 2001, Dickson 2002, Coggon et al. 2010) were combined with information on modern seawater Mg/Ca (de Villiers & Nelson 1999) to represent variation in seawater Mg/Ca since 110 Ma. For simplicity, and because of the relatively low sensitivity of the other paleoenvironmental variables to seawater Mg/Ca estimates, we use interpreted seawater Mg/Ca estimates given by these authors instead of developing formal models for each Mg/Ca proxy system. Because uncertainty exists in the form of the partitioning function between seawater and echinoderm carbonate, our dataset includes both the original estimates from Dickson (2002) and the reinterpreted estimates of Hasiuk and Lohmann (2010). The uncertainty associated with each estimate was approximated from the primary publication, and ranged from 0.03 mmol/mol for modern seawater to ~0.5 mmol/mol for some of the proxy estimates (1 σ, see data and code available at <https://github.com/SPATIAL-Lab/JPI_marine>).

Foram Mg/Ca and δ18O data were compiled from three Ocean Drilling Program (ODP) sites: site 806, Ontong Java Plateau (Bickert et al. 1993, Lear et al. 2003, Lear et al. 2015); site 1123, Chatham Rise (Elderfield et al. 2012), and site U1385, Iberian Margin (Birner et al. 2016). Data from site 806 constitute a low-resolution record from ~18 Ma to present, with an average sampling resolution of 1 sample per 240 and 180 kyr for Mg/Ca and δ18O, respectively, prior to 800 ka. Mg/Ca measurements were made on the benthic infaunal foraminifer *Oridorsalis umbonatus*. δ18O data represent a mix of benthic species, predominantly *Cibicidoides* spp, and we adopt the inter-species offset corrections applied by Lear et al. (2003) to correct data from other species to *Cibicidoides*-equivalent values. For the other two sites, data were extracted for the overlapping period of record (1.32 – 1.23 Ma), and comprise a set of higher-resolution records (sampling resolution between 1 per 110 and 1 per 1,700 years) spanning two glacial/interglacial cycles. Mg/Ca measurements were made on tests of the infaunal foraminifer *Uvigerina* spp at both sites, and δ18O data are from either *U.* spp (site 1123) or *Cibicidoides wuellerstorfi* (site U1385). Variance in the foram data, e.g., due to analytical effects and sample heterogeneity, was not estimated independently but rather treated as a model parameter and conditioned on the calibration and proxy data.

Calibration datasets were compiled to constrain the Mg/Ca and δ18O proxy system models. Mg/Ca calibration data for *O. umbonatus* are from the compilation of Lear et al. (2015), and include both modern coretop samples and samples from Paleocene and Eocene sediments of ODP site 690B. Data from site 690B include an adjustment for differences in cleaning procedures used for those samples (Lear et al. 2015). For *U.* spp we use the compilation of Elderfield et al. (2010) which consists of core-top samples exclusively. Each Mg/Ca datum is accompanied by a bottom water temperature (BWT) estimate based on syntheses of observational data (modern) or δ18O thermometry (paleo), the latter assuming ice-free conditions. We adopt both sets of estimates directly, applying a normally distributed uncertainty to the BWT values with a standard deviation of 0.2 and 1 °C for the modern and paleo data, respectively, to approximate the different quality of these estimates. For δ18O we used the compilation of Marchitto et al. (2014) including new and published coretop data for the genera *Cibicidoides* and *Uvigerina* (Shackleton 1974, Grossman & Ku 1986, Keigwin 1998). Estimates of BWT and δ18O of seawater from the original authors were adopted with an estimated uncertainty of 0.2 °C (1 σ) for BWT; as for Mg/Ca we do not attempt to constrain the uncertainty in the relationship between temperature and δ18O fractionation between seawater and calcite directly, but treat it as a model parameter.

The age of each pre-modern datum was taken from the primary source. Age uncertainties, where known, can be incorporated in the JPI analysis framework by treating ages as random variables rather than as fixed values and/or including proxy model components representing processes governing the time-integration of observations. To reduce the complexity of the current analysis we do not include such a treatment for any of the datasets. We note in the discussion several cases where including age uncertainty would produce a more robust analysis.

## Proxy models

The proxy system models used here are comprised of simple, empirically constrained transfer functions relating proxy data to contemporaneous environmental variables, and as such can be considered “observation models” in the terminology of Evans et al. (2013). The simplest model is that for seawater Mg/Ca proxy data, where, as noted above, we consider the interpreted data directly, giving:

. (1)

Here *MgCaswp*(*i*) is the *i*th proxy estimate, *N* represents the normal distribution, *MgCasw* is the paleo-seawater Mg/Ca value, and *tswp* and *σswp* are the age estimate and uncertainty associated with a proxy estimate.

We model foram Mg/Ca (*MgCaf*, including both calibration and proxy data) as a function of seawater chemistry and bottom water temperature:

, (2)

where *α1-3* and *τMgCaf* are the parameters and precision (1/σ2) associated with the transfer function, respectively, and other parameters are analogous to equation 1. In the absence of theoretical constraints, we assign normally distributed priors to the *α* parameters based on Bayesian regression of the expression for the mean in equation 2 against the calibration datasets. For *Oridorsalis* we assume paleo-seawater Mg/Ca of 1.5 mmol/mol in the Paleocene and Eocene for these initial estimates, and the prior estimates are *α1* ~ N[1.5, σ = 0.1], *α2* ~ N[0.1, σ = 0.01], and *α3* ~ N[-0.02, σ = 0.03]. For *Uvigerina* these distributions are *α1* ~ N[1.02, σ = 0.1] and *α2* ~ N[0.07, σ = 0.01], and the prior estimated for *α3* from the *Oridorsalis* data set was used because no calibration data were used that represented non-modern *MgCasw*. For both genera, the prior estimate on the precision of the foram Mg/Ca model, *τMgCaf*, is the gamma distribution Γ[shape = 2, rate = 1/30], which approximates the precision of the independent regressions.

Foram calibration and proxy δ18O values (*δ18Of*) are modeled similarly, with:

. (3)

Here *δ18Osw* is the modeled seawater isotope composition and *β1-3* are the transfer function coefficients. In this analysis we treat the scale conversion factor between the SMOW and PDB reference scales (Shackleton 1974) as implicit in the transfer function intercept term (*β1*), which is relevant only in comparing our posterior parameter estimates to other work. Prior estimates of the model parameters were obtained and specified as for Mg/Ca; these are *β1* ~ N[3.32, σ = 0.02], *β2* ~ N[-0.237, σ = 0.01], *β3* ~ N[0.001, σ = 0.0005] for *Cibicidoides* and *β1* ~ N[4.05, σ = 0.06], *β2* ~ N[-0.215, σ = 0.02], *β3* ~ N[-0.001, σ = 0.001] for *Uvigerina*. Because the amplitude of high-frequency (i.e. below the resolution of our model) *δ18Osw*variance in the long record from site 806 increased substantially with the onset of modern, 100 kyr glacial cycles, we modeled *τδ18Of*(*i*) separately for proxy data younger than 800 ka (prior on *τδ18Of* ~ Γ[6, 1]) and for all other proxy and calibration data (prior on *τδ18Of* ~ Γ[3, 1/30]). The former estimate is based on the observed proxy variance since 800 ka, whereas the former approximates the precision of the calibration relationships.

## Environmental models

The paleoenvironmental variables driving the observed proxy signals are represented as time series using a correlated random walk model. This parameterization is desirable in that it is minimally prescriptive (i.e. no preferred state or pattern of change is proscribed) but allows incorporation of constraints on (and extraction of inference about) two basic characteristics of the underlying environmental systems – namely their rates and directedness. The correlated random walk for variable *Y* is expressed as:

, (4)

where:

. (5)

In short, the variable follows a random walk in which the next value in the time series is a function only of the current value and a normally distributed error term *ϵY*, which has a temporal autocorrelation of *φY* and precision *τy*. This gives three independent parameters, *φY*, *τy*, and an initial value of *Y* at the beginning of the time series.

For seawater Mg/Ca, which is thought to evolve gradually in response to long-term tectonic and biogeochemical forcing (Wilkinson & Algeo 1989), we simulate the time series at 1 Myr steps from 110 Ma to present. Although the foram proxy data used here span only the interval from ~18 Ma to present, extending the seawater model over this longer temporal domain was necessary in order to generate a stable time series, conditioned on sparse seawater Mg/Ca proxy data, that spanned both the proxy records and the Paleogene-aged Mg/Ca proxy calibration data. Given that the modeled quantity is a ratio, we treat the error term in this time series model as a proportion, such that the change in *MgCasw* between two time steps is *MgCasw*(*t-1*) \* *ϵMgCasw*. We adopt priors that imply relatively slow change and strong temporal trends (*φMgCasw* is given by a uniform distribution, U[0.9, 1]; *τMgCasw* ~ Γ[100, 0.01]). We use a weak prior on the initial state of *MgCasw* at 110 Ma, U[0.75, 2], consistent with independent interpretations of Cretaceous proxy data (Coggon et al. 2010).

We select the bounds, resolution, and prior distributions for the bottom water temperature and δ18O time series models based on the properties of each record. For site 806 we use a time step of 50 kyr from 18 Ma to present, adequate to allow the time series model to adapt across the range of surpa-orbital timescales represented in the sample distribution. Prior estimates of the error term parameters were chosen to allow sampling across a range of weak to moderate autocorrelation states and error variances that were consistent with first-order interpretations of the proxy data (*φ* ~ U[0, 0.4] for both proxies; *τBWT* ~ Γ[20, 2]; *τδ18Osw* ~ Γ[10, 0.2]). We use weakly informative uniform priors for initial values at 18 Ma (*BWT*(-18) ~ U[3, 8], *δ18Osw*(-18) ~ U[-1, 1]). For the higher-resolution Pleistocene records, we bound the models between 1.32 and 1.235 Ma and adopt a time step of 1 kyr, accommodating orbital-scale changes in the parameter values. We adopt the same prior distributions for *τBWT* and *τδ18Osw* as in the long-term model, but use a broader prior on *φ* (U[0, 0.8] for both environmental variables) based on the expectation that temporal autocorrelation in temperature and seawater δ18O trends will be stronger at timescales of 1 kyr than at 50 kyr.

## Model inversion

The equations above were coded in the BUGS language (Lunn et al. 2012) and Markov Chain Mote Carlo was used to generate samples from the posterior distribution of all model parameters conditioned on the proxy and calibration datasets. The analysis was implemented in R version 3.5.1 (R Core Team 2018) using the rjags (Plummer 2018) and R2jags (Su & Yajima 2015) packages. Three chains were run in parallel. Convergence was assessed visually via trace plots and with reference to the Gelman and Rubin convergence factor (Rhat; Gelman & Rubin 1992) and effective sample sizes reported by rjags.

For the site 806 analysis, chains were run to a length of 1e6 samples with a burn-in period of 10e5 samples and thinning to retain a total of 5,000 posterior samples. All parameters showed strong convergence (Rhat << 1.05, effective sample size > 3,500) with the exception of some parts of the seawater Mg/Ca time series and the initialization period of the *BWT* and *δ18Osw* time series (i.e. prior to the first proxy observation). The long run and burn-in periods were dictated by the *MgCasw* time series values, which exhibited very strong autocorrelation as a result of their ‘stiff’ time series behavior and weak data constraints. Qualitative assessment showed no perceptible covariance between seawater MgCa and other parameters in the posterior samples; as a result, we do not believe the weaker sampling from the *MgCasw* posterior has a significant impact on our results or interpretations. The entire analysis took approximately 15 hours running on three cores of a Windows desktop computer.

For the Pleistocene data we conducted three different analyses, the first two inverting data from each site independently and the third inverting both records together. Because of the short time interval covered by these analyses we did not model the seawater Mg/Ca explicitly, but estimated paleo-seawater Mg/Ca values, where needed, from the posterior distributions of an independent inversion of the sweater Mg/Ca proxy data. Chains were run to 5e5 and 7.5e5 samples for the single- and multi-site analyses, respectively, using a burn in period of 1e4 samples and thinning to retain 5,000 posterior samples. All parameters showed strong convergence (Rhat << 1.05) and effective samples sizes were >4,000 for most parameters and >2,000 for all parameters excluding the initialization period of the time series (i.e. prior to the first observation). Total analysis time ranged from <1 hour (site 1123) to ~4 hours running three chains in parallel.

# Results and Discussion

## JPI paleoenvironmental reconstructions

The paleoenvironmental reconstructions obtained by applying JPI to the site 806 data are similar, to first order, to the reconstructions from Lear et al. (2015; hereafter L15) on which our analysis was modeled (Fig. 2). Our reconstruction shows strong support for ~2 °C of bottom-water warming at site 806 during the mid-Miocene Climatic Optimum (centered here on ~15.5 Ma), and although abrupt cooling followed this event, water temperatures warmed again by ~1 °C into the late Miocene. A strong and sustained multi-Myr cooling trend began at the site just prior to 5 Ma and persisted throughout the remainder of the record. Our median temperature estimates are most similar to those obtained by L15 using their “NBB” calibrations, which was based on the same compilation of calibration data used here. Our estimates of seawater Mg/Ca match those obtained by L15 using polynomial curve-fitting throughout most of the common period of analysis. Prior to 40 Ma our estimates diverge, reflecting the incorporating additional data from the Cretaceous in our analysis, but this difference does not impact other interpretations given that L15 did not use the curve-fit estimates from this part of the record in their analysis. 95% credible intervals estimated from JPI average ca. 3 °C and 0.5 ‰, which is similar to the uncertainty bounds provided by L15 based on iterative estimation using different calibration functions. The width of the JPI CIs varies subtly across the time series, with somewhat narrower intervals during periods of dense sampling, e.g., in the late Pleistocene.

Short para on 1123 and U1385 results

## Time series properties

One visually striking difference between the JPI and L15 reconstructions is the higher BWT and δ18Osw variability implied by L15 (e.g., compare our Fig. 2 with their Fig. 7). As is common in traditional proxy interpretations, the L15 paleoenvironmental record treats each individual datum as an estimate of an independent environmental state, giving a reconstruction centered on ‘best estimates’ derived from each data point. In reality, however, the environmental states giving rise to multiple proxy samples are not independent if autocorrelation exists at the resolution at which the time series is sampled; for BWT and δ18Osw this is true over a broad spectrum of resolutions including those considered here. This is commonly implicitly acknowledged in the presentation of traditional proxy reconstructions by including a smoothed representation of the record, obtained using a (usually arbitrary) smoothing filter (e.g., Elderfield et al. 2012).

JPI, in contrast, explicitly considers temporal autocorrelation of the underlying environmental variables, treating each proxy observation as a sample arising from one or more underlying, autocorrelated environmental time series. The properties of the time series themselves, rather than being arbitrarily assumed, are estimated to be consistent with the statistical properties of the proxy models and the data, meaning that the record produced is optimized to reflect the actual information content of the data. For very certain proxy models or densely distributed data that record high-frequency variability the reconstructed time series will express short-term changes in the environment, whereas reconstructions based on uncertain models or smooth or sparsely-sampled data will tend toward greater smoothing and reflect the actual information content of the proxies with respect to the longer-term evolution of the mean state of the system. This is nicely illustrated by the comparison of JPI reconstructions for sites 1123 and U1385 (Fig. X) …

Another advantage of embedding time series models in JPI is that it offers an explicit framework for integration of differently-sampled proxy records. In most of the applications presented here, for example, foram δ18O values are more densely sampled than Mg/Ca. In a traditional, piece-wise interpretation of these proxy data, *δ18Osw* can only be estimated if paired oxygen and Mg/Ca data are available for a given core level. Thus, if Mg/Ca data are missing at a level either this value must be estimated, usually through linear interpolation between values for underlying and overlying samples, or the foram δ18O data excluded from the analysis. JPI eliminates the need to exclude or selectively interpolate data by linking all proxy measurements to a common set of underlying continuous time series. The temporal interpolation required to integrate data sampled at different times is conducted for each environmental variable, which are in reality the quantities that are related in time, as an integrated component of the analysis, allowing the proxy data to be (appropriately) treated as independent samples. One note of caution is warranted here: although JPI provides a formal and rigorous framework for integrating differently-sampled proxy datasets, there is still potential to for artefacts to emerge from the integration of datasets with very different sampling densities. For example…

Scaling of CIs w/ data density

## Proxy model properties

## Derivative analyses

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***, less so for BWT***