Global Marine Isochore Estimates Using Machine Learning

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Abstract The thickness normal to deposition (isopachs) and vertical thickness (isochores) of geological units is important for assessing various geologic processes. We present the first marine global sediment isochore estimates for five geological periods dating from middle Miocene (15.97 Ma) to present. We use sparsely distributed sediment depth vs. age observations from the Deep Sea Drilling Project and global maps of biological, oceanographic, geographic, and geological variables as training features in a k-nearest neighbor regressor to estimate isochores. Results are compared to isochore estimates generated by applying a constant depositional rate from recent estimates of global total sediment thicknesses. Both models of isochore thickness exhibit consistent error. Results from a machine learning approach show major advantages, including results that are quantitative, easily updatable, and accompanied with uncertainty estimation. Final predictions can provide first-order constraints on sediment deposition with geologic time, which is of timely importance for assessing past climate variability.

Plain Language Summary Maps displaying the thickness of sedimentary units are useful for a variety of reasons such as assessing how Earth’s climate and depositional systems (e.g., river deltas) have changed through geologic time. In this study, we use a machine learning approach to estimate how thick time bound (present day to 15.97 million years) geological units are. To produce these global thickness estimates, we used depth-age observations from an international deep-sea drilling collaboration, the Deep Sea Drilling Project. Our machine learning approach uses these observations and complementary data sets, such as water depth and latitude, to estimate unit thicknesses where previous observation has not been made. We then compare the machine learning approach to an independently empirically based method. The model skill calculated by comparing observed and predicted values for each model is approximately the same; however, there are major advantages of using a machine learning approach. Major advantages of using a machine learning approach include the ability to easily update final predictions with new data and calculated uncertainty estimates in the final prediction. Predictions of unit thicknesses can help to indicate where sediment is more likely to accumulate and be preserved in geologic time. Since sediment is capable of sequestering large amounts of carbon from the atmosphere, understanding the regions of preservation is important for studying past and future climate change.

1. Introduction

Isochores are the technical term used to describe the true vertical thickness between geologic units, whereas, a commonly used term throughout literature, isopachs describes the true stratigraphic thickness, that is, unit thickness perpendicular to dip. The difference between the terms isochores and isopachs is generally negligible for most deep marine settings where dip angles are less than 10° (Dikkers, 1985). Here we use the technical term, isochore; however, the term isopach may be used throughout the literature to describe the same sediment unit thicknesses.

The accumulation and erosion of marine sediment through geological time occurs via global and regional processes and is mediated by climate, tectonics, and volcanism (Engwell et al., 2015; Straub et al., 2020). Understanding sedimentary process variability in both time and space requires geospatially estimating isochores, which represents the vertical thickness of sedimentary units bound by chronostratigraphic horizons. Regionally, isochores are used to estimate hydrocarbon maturation for economic exploitation, assess potential for geological hazards such as submarine slope failure (Hill et al., 2017), and infer the geologic history of
the Earth (Grall et al., 2018; Scheuer et al., 2006). Global-scale isochores may also be used to better constrain the contribution of marine sedimentation to carbon sequestration as a function of geologic time (Burdige, 2007; Cartapanis et al., 2018). Despite the clear value of a comprehensive marine isochore estimates, the sparseness of marine subsurface data has resulted in only limited, primarily qualitative published global-scale isochore estimates (Klawonn et al., 2014; Straume et al., 2019).

Here we use observed chronostratigraphic unit thicknesses and machine learning algorithms (MLA) to generate and validate the first estimate of global marine isochores, with associated uncertainties, representing geologic periods from the middle Miocene (15.97 million years) to present. This study addresses four primary objectives: (1) provide quantitative, easily updateable, observation-based methodology to estimate global marine isochores; (2) benchmark machine learning estimated global marine isochores using an independent methodology; (3) provide first order comparison of our isochores to previous regional and global isochores; and (4) assess how future predictions of isochores can be improved.

2. Methods

2.1. Machine Learning Prediction of Isochores

Determining the vertical thickness between chronostratigraphic horizons requires either direct (e.g., age-dated sediment samples) or indirect (e.g., age-estimated seismic horizons) observations. For most regional (i.e., basin-scale) analyses, where seismic data exist and a continuous time reflector of an age associated boundary also exists, isochore thicknesses can be determined by inverting travel times to the unit bounding reflectors with a seismic velocity model (e.g., Calvert et al., 2008; Scheuer et al., 2006). In regions where seismic data or direct observations are unavailable, sparse or poorly constrained, other methods are required. Techniques commonly used to estimate spatial distribution of a particular property include interpolation methods that assume spatial autocorrelation such as kriging or nearest neighbor. These methods perform best when observational data are uniformly distributed across the prediction domain and/or a small number of well-constrained variables are responsible for the spatial variability of the estimated value (Li & Heap, 2008). Conversely, MLAs quantitatively predict unconstrained spatial variables and associated uncertainties with more complete spatial coverage than those provided by other interpolation techniques as predictions are made in predictor space instead of physical (i.e., geographic) space; this allows for more accurate predictions where observed data are exceptionally sparse or nonuniformly distributed (Dutkiewicz et al., 2015; Lee et al., 2019; Martin et al., 2015; Wei et al., 2010).

Our isochore estimates were created using the Global Predictive Seabed Model (GPSM Level 0), which is designed for the MLA prediction of regional and global marine geological variables (Lee et al., 2019). GPSM Level 0, as implemented in this study, uses the k-nearest neighbor regressor (KNR) to evaluate correlations between observed isochore thicknesses and a variety of physical parameters, or predictors, mapped at the 5-arc minute global scale; for example, sea surface particulate inorganic carbon, bathymetry, biomass estimates. These relationships are then implemented via KNR algorithm to predict global isochore thicknesses, at a grid resolution of 5-arc minutes, for five geological time periods ranging from present to late Miocene (0–1.8, 1.8–2.58, 2.58–5.33, 5.33–11.63, and 11.63–15.97 Ma).

Isochore observations (Figure 1a) are sourced from a data set published by the DSDP (Legs 1–96), which represents the largest curated database of age-depth control points for global marine sediments (Deep Sea Drilling Project, 1989). Other ongoing drilling campaigns such as the Ocean Drilling Program (ODP) and International Ocean Discovery Program (IODP) are not yet included, as the age data file structure of these later drilling campaigns is less accessible.

The specific age-depth observations in the data set are not at consistent depths and/or geologic time period boundaries; therefore, for each DSDP hole, we linearly interpolated between age-depth points to determine the depth to the top and bottom of a defined period of interest (Imhof et al., 2011). We estimate the uncertainty in this interpolation technique by withholding the 1.8 million year observations and then interpolating these observations. We then compare the interpolated observations to the true observed depth-age values for the 1.8 million year isochore observations. The uncertainty in this interpolation method is 8.8 m for the Calabrian–present isochore, which is less than the final prediction uncertainty. As no other depth-age isochores observations are explicitly recorded in reasonable abundance, we cannot determine the true
uncertainty in the interpolation technique for each isochore. However, we suspect it to be less than the prediction uncertainty.

We then calculated the depth difference between our interpolated depth-age points for the beginning and end of each geologic interval of interest to obtain isochore thicknesses. We used age intervals associated with established geological ages and epochs (Table 1), due to their global geologic familiarity and relevance, but the technique is applicable for any finite geologic time interval. Where there is more than one observation in a 5 × 5-arc minute grid cell, the median observed thickness is assigned to represent that grid cell. Table 1 shows a complete list of the number of raw and binned observations. A global plot and histogram of these binned observations and the maximum age of interest encountered downhole is shown in Figure 1. The gridded thicknesses were converted to centimeters (to avoid calculating values <1 m as a negative log number) and transformed to logarithmic base 10 units. A log transformation was performed because the observed data spans many orders of magnitude (centimeters to hundreds of meters). This transformation technique

Figure 1. (a) Isochore observations after binning at 5 × 5-arc minute from the Legs 1–96 of the Deep Sea Drilling Project. Colors indicate the maximum isochore age at each location. Age-coded data are used to create respective isochore predictions (Figure 2). (b) Histogram of observed data after binning. Colors represent the different respective isochore age intervals. The last bin on the histogram represents any value greater than 400 m.
has been used previously in other MLAs to address sparsity in the observed data distribution (Wong et al., 2013).

The skill of KNR implemented with GPSM in predicting the presented isochore thickness values is quantitatively evaluated in two ways: (1) the absolute median error between 10-fold cross validation of observed and predicted values and (2) the $R^2$ value calculated from a least-squares best fit through the 10-fold cross validation of observed vs. predicted points. For the KNR, absolute median error is determined through robust 10-fold cross validation, wherein 10% of the observed data is withheld and 90% is used to predict the removed 10% (Alpaydin, 2010). This process is repeated 10 times until all observations have been withheld and predicted. The resultant median value of the absolute residual between the 10-fold cross validation of observed and predicted values is the absolute median error metric.

The predictors used are updated versions of those described in Lee et al. (2019) and represent a wide variety of present-day chemical, physical, oceanographic, and geological variables. Feature selection determines which predictors will be used in the final prediction; the feature selection method used for the isochore predictions is similar to the univariant methodology described in Lee et al. (2019) with minor differences. Foremost, predictors that are 90% co-correlated among the sampled observation locations are discarded. In this feature selection method, we use each predictor individually to predict each individual isochore. We then rank these individual predictors according to the resultant 10-fold cross validation error determined by comparing the observed and KNR predicted isochore values. We additionally perform the prediction using as our only predictor a grid of uniform random noise (URN). Assuming the URN has no correlation with observed data, we use the prediction error from using the URN as the threshold for predictor selection—no predictor is used that has a higher error than the URN grid.

This methodology ensures the final selection of predictors is entirely based on the observed data. For the ensemble feature selection processes, we use the features selected from the univariant feature selection method in ensemble mode, where we iteratively run the combination of $n$ features (e.g., 1; 1,2; 1,2,3). The $n$ combination of features with the lowest possible median 10-fold cross validation error are used in the final KNR prediction. The final number of predictors used for each isochore prediction is shown on the validation plots of Figures 3a–3e. While each isochore prediction selects different sets of predictors, common selected predictors among all isochores include empirically calculated latitude, mission average of particulate inorganic carbon from Aqua MODIS satellite, bathymetry from SRTM +15, and invertebrate biomass estimates from Wei et al. (2010).

Further details and assumptions regarding the observed data, predictors, KNR, and uncertainty are available in the supporting information.

2.2. Empirically Calculated Isochores

The only global estimate of isochore thickness similar to our predictions is the recently released GlobSed which reports sediment thickness between the seafloor and crustal boundary (Straume et al., 2019). The GlobSed sediment thickness estimate can be related to elapsed geologic time using an updated estimate of the crustal age from Müller et al. (2019). Entirely independent from our MLA predictions, we use the
GlobSed sediment thickness estimate (Straume et al., 2019) and the crust age from Müller et al. (2019) to calculate isochores for the same geologic time periods of our predictions, hereafter referred to as GlobSed+. This allows us to compare both model results from GPSM Level 0 and GlobSed+ to observed DSDP data.

For the GlobSed+ estimate, there is no 10-fold cross validation performed; therefore, we calculated the absolute median error as the residuals of the final estimated and observed data. In the final prediction using GPSM, grid cells that hold observations are represented with those observations, not the predictions at those locations. As the 10-fold cross validation error within KNR represents the error in predictive skill and is not truly comparable to the error estimate for GlobSed+, we calculate another error metric only to compare GlobSed+ and KNR results. In this case, we do not replace predictions with observations at the locations with observed data. We then calculate the KNR error between the observed and predicted values. The residual error calculated in this way is lower than 10-fold cross validation error and not significantly different than the 10-fold cross validation error. These errors are referenced in Table 1 as the residual error in estimation for KNR. A complete description of the calculations used to produce the GlobSed+ isochores is available in the supporting information.

3. Results

The KNR model (Figure 2) exhibited the greatest predictive skill in the Calabrian—present isochore with a median error of ~15 m and an $R^2$ value of ~0.4 as shown on Table 1. By comparing the median observed value to the median 10-fold cross validation error, the isochore with the least predictive skill is Gelasian. We find that the most volume of sediment preserved is during the Langhian–Serravallian and the least during the Gelasian. These volumes correlate with the most and least amount of elapsed time.

The errors between the GlobSed+ estimate and the observed data are shown in Table 1. The errors between the KNR and GlobSed+ models are between ~1 and 10 m of one another (GlobSed+ estimates are plotted in Figure S2). GlobSed+ has a lower median error than the KNR results (~1 m less) in only one isochore, Calabrian–present. In the Gelasian isochore, KNR results exhibit lower error than GlobSed+ estimate. For the earliest three isochore estimates, the KNR prediction exhibits diminishingly smaller error than the GlobSed+ estimate.

4. Discussion

A qualitative assessment and comparison of GlobSed+ and KNR MLA reveals results from GlobSed+ with similar sedimentary depositional patterns as the KNR results, with thicker deposits along continental shelves and thinner deposits in the deep sea (Figure S2). However, GlobSed+ consistently predicts greater sediment thicknesses than KNR, potentially a result of assuming a time-averaged sedimentation rate over long time intervals. Quantitatively, the errors between observed data and model predictions (KNR and GlobSed+) are generally similar; however, there are major advantages to using an MLA over an empirical model. KNR results do not rely on time averaging over the full age of the sediment column, a substantial limitation of the GlobSed+ approach. Additionally, MLA isochore predictions can be easily updated as more observational data become available. Conversely, updating the GlobSed+ isochores would require an update of the full crust age grid or the total sediment thickness grid. Updates to the KNR result require only more data and can be accomplished almost automatically. Finally, the presented KNR method yields an uncertainty estimation (Figure S3), whereas equivalent uncertainty values cannot be calculated for empirical methods like GlobSed+.

Despite the uncertainties being relatively high for the KNR methodology, the resultant global predictions of the spatial variability of isochore thickness are sufficient to infer first-order processes of sediment deposition through geologic time. Here, we discuss those processes compared to previous studies and/or hypotheses.

In general, each isochore prediction indicates thicker sediment deposits along the continental shelves that thin into the deep sea (Figure 2). This is consistent with frequently observed clinoforms in cross-margin seismic lines exhibiting deposition on continental shelves proximal to terrestrial sediment sources (e.g., deltas) that is substantially greater than slow deep-sea deposition dominated by biologically and eolian-driven sedimentation. Furthermore, global isochore predictions exhibit areas of elevated sedimentation, possibly resulting from increased productivity, as a result of equatorial upwelling of nutrients. This phenomenon is
Figure 2. (a–e) Respective isochore predictions in meters using a k-nearest neighbor regressor (KNR) machine learning algorithm. Adjacent plots show respective standard deviation in the k-nearest neighbors (i.e., proxy for uncertainty) in each isochore prediction.
particularly conspicuous in the late Miocene isochore (Tortonian–Messinian) in equatorial regions as compared to the other locations and geologic time intervals. A distinctive increase in isochore thickness along the eastern equatorial Pacific current during Tortonian–Messinian is observed in the results and is consistent with the hypothesis of vigorous upwelling and resulting high accumulation rates of biogenic material (Zhang et al., 2017).

KCN isochore predictions can be compared on regional scales to previous isochore estimates/observations. We highlight two regions—the Northern Mid-Atlantic Ridge (MAR) and the Indus River Delta near the Arabian Sea. For all time periods, the Northern MAR region shows consistently thick isochores. Within the Northern MAR region, we suspect increased sedimentation as a result of drift deposits which are known to be prominent at high latitudes along flanks and ridges or as a result of tectonic activity associated with transverse trenches (Litvin, 2013). Further, in comparing the Northern and Southern MAR, we find that the southern MAR has much smaller preserved thickness estimates through time. These sedimentary thickness predictions are broadly consistent with the northern and southern transects discussed in Litvin (2013).

In an analysis by Clift et al. (2002), isopach thicknesses in seismic two-way travel time for the Indus River Delta near the Arabian Sea are mapped using seismic data. Although the units differ, the relative spatial trends in thickness exhibited by each can be compared. The KNR predictions and Clift et al. (2002) observations of thickness differ significantly, with KNR predictions tending to underestimate the observed thickness values by two orders of magnitude. KNR predictions were made at a coarser spatial resolution with no direct observations within/near this delta. Therefore, the prediction in this region was based entirely on DSDP observations from other regions of the world. The poor predictive skill can likely be attributed to lack of observations from parameter space similar to that of the Indus River Delta, that is, the Indus River Delta is unique our population of observations. Given MLAs are not explicitly dependent on spatial proximity to other points, the assimilation of new observed data would result in better predictive skill not only for the region in which they are acquired but also regions which are geologically (i.e., parametrically) similar. Further, poor predictive performance for the Indus River Delta may also be attributed to the lack of features (i.e., variables) that capture important factors controlling rapid sedimentation. Addition of features that represent these processes may also improve predictive capability.

Figure 3. (a–e) 10-fold cross validation plots in log10 centimeters generated from each isochore prediction (Table 1). The black line on each plot represents agreement between observed and predicted values (1:1 line). The gray line represents the least-squares best fit through the observed versus predicted data. The number of neighbors, final predictors, and $R^2$ value are shown to the bottom right of each validation plot.
An advantage of using MLA for prediction of isochores is that data from regional seismic analyses like Clift et al. (2002) could potentially be incorporated relatively easily into a new prediction of thicknesses with geologic time. Our MLA framework is not only geospatially agnostic (i.e., capable of using observations outside of the region of interest to arrive at predictions) but also scale agnostic, allowing for predictions over smaller spatial areas, such as the Indus River system, with higher resolutions, wherever observations and environmental predictor data at those smaller scales are available.

For a prediction reliant on only observed data such as KNR, the model skill in predicting isochores may be a result of the amount and distribution of observed data. KNR can only make predictions from the range of values that have been observed and thus the predictions are biased by the histogram distribution of the observed data. For example, the observed data for the Gelasian (1.8–2.58 Ma) isochore do not contain any thicknesses >200 m (Figure 1b); therefore, the prediction is constrained to a maximum predicted value of ~200 m.

Conversely, the Calabrian–present (0–1.8 Ma) isochore displays the greatest predictive skill and also has the largest range of isochore observations. This is likely one reason the KNR method has difficulty in predicting higher thicknesses estimates, as higher values are sparser for each isochore observational histogram. In the same way, the histograms are skewed towards lower isochore values, making smaller values more abundant in the final predictions. Augmenting the quantity and distribution of the data in parameter space (Figure 1b) will improve the accuracy of predicted isochores.

Future predictions can be improved in several ways. Foremost, observed data quantity and distribution (both geographically and parametrically) can be improved. Although much time and effort are likely required to curate and mine data from other deep-sea drilling campaigns, such as ODP and IODP, the abundance of data that could be added to the quantity and distribution of the observed data is likely immense given this accumulation of drilling campaigns spans from 1985–present. The addition of this observed data can also influence the predictors that are selected for the final prediction of each respective isochore resulting in improved predictions.

Further, updates, and additions of new predictor grids/variables that are relevant to the prediction of isochores can increase ability to predict isochores. If particular oceanographic, geological, and/or biological variables were known in geological time, potentially significant improvement in predictability is possible. Finally, there are several MLAs, some requiring a priori knowledge that could be utilized in the prediction of isochores.

5. Implications and Conclusions

We show here the first data-driven global estimates of marine sediment isochores for five geologic intervals. Global isochores can be used to indicate areas susceptible to submarine slope failure, infer the geologic history of the earth, and estimate the quantity of sediment preserved throughout geologic time. The latter may prove to be particularly useful for assessing the amount of carbon sequestered by marine sediments as a function of geologic time and hold important implications for global carbon budgets and long-term climate variability.

The methodology presented provides a framework within which isochore predictions can be easily updated with the assimilation of additional age-depth data (e.g., ODP and IODP). The inclusion of additional or updated observational data will result in more skilled predictions of sediment isochores with reduced uncertainty.

Data Availability Statement

All data sets supporting this research are publicly available at Lee et al. (2020). Detailed descriptions of the algorithms are available herein and within the supplemental material.

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