

Response to referees' comments

Journal: NPG

Title: Estimation of sedimentary proxy records together with associated uncertainty

Author(s): B. Goswami et al.

MS No.: npg-2014-49

MS Type: Research Article

Dear Editors,

We thank very much both anonymous reviewers for their helpful comments and constructive criticism. Please find below our responses to all comments by the two referees. For the sake of clarity, we have italicized the referees' comments in the text below.

We hope that our responses have covered the various issues raised by the referees.

With best regards,
on behalf of all co-authors,

Bedartha Goswami

Anonymous Referee #1

In the manuscript "Estimation of sedimentary proxy records together with associated uncertainty" Goswami et al. demonstrate how to derive proxy records with associated uncertainties based on the corresponding archives depths and its age estimation. Using a Bayesian framework they propagate the age uncertainty, calibration uncertainty and the proxy's variance to estimate the expected proxy values as well as their uncertainty. Therefore the proposed method can improve the reliability of the proxy and provides a better uncertainty measure.

Clearly this work is novel and a natural, but still clever, extension of S. F. M. Breitenbach et al. COPRA paper (Climate of the Past 8, 1765-1779, 2012). One would hope that the authors will provide their method ready to use in a similar software package. The representation of the paper is throughout and the more tedious calculations are summarized in the appendix. Therefore scientists with some background in Bayesian statistics can easily check the method while the main text is free of lengthly mathematical arguments so that it still is accessible to researchers from a more applied field.

We thank the referee for the kind and supportive comments. We indeed plan to release an open-source implementation of our Bayesian proxy estimation approach very soon. However, rather than creating a separate package for our method alone, we want to include it as being a part of a future COPRA version (available at: <http://tocsy.pik-potsdam.de/copra.php>). Till then, a hands-on working implementation of our approach can be easily made available by the authors on request.

In my opinion one of the strong points of the paper is that the authors must have spent some time thinking about how to present their arguments. In Sec. II they provide the basic theory of their method and first of all clarify for which data sets their method can be used and in 2.2 list all the necessary assumptions behind their method. As a consequence researchers can assess their own data sets and immediately realise that they are missing for example the C14 calibration curve. In this sense the clear presentation could also be thought of as a tutorial for

researchers in the field or laboratories on what data is needed for more advanced time series analysis.

We are grateful to the referee for the encouragement. We had put in a lot of hard work on how to best present our work without going into formidable mathematical details and with the use of suitable schematics along with a structured argument. We are therefore very happy that we managed to present our ideas with clarity.

The method developed in Sec. II is tested in Sec. III using a simulated stalagmite proxy and a simulated lake sediment core. Using simulated data for testing is good practice since direct comparisons between truth (the simulation) and the estimates are possible. Moreover the two examples chosen come with different uncertainties: while the lake core needs C14 calibration, the stalagmite is dated using U/Th and does not have age uncertainty. Consequently the reader realises the impact of the C14 calibration on the final uncertainty. Finally they apply their method using a real time series from Lake Lonar in central India. This analysis is quite interesting since two measurements are recorded after 1950 and therefore the "post-bomb" calibration has to be used along the "pre-bomb" calibration for the earlier measurement points. The discussion of the analysis is given in Sec. IV. While for the Lonar record they show that the C14 uncertainty plays a minor role for the overall uncertainty, the data analysis is used to demonstrate how to check the major sources of uncertainty. Following their analysis by setting C14 uncertainty to 0 in certain parts of the record one can evaluate whether it is worthwhile to get more data points in some particular part of the record to reduce the uncertainty.

Overall the paper is well written, addresses a major problem in time series analysis of proxy records and the Bayesian propagation method is a novel contribution to the field. The authors do not fall into the trap of overselling and clearly state for what kind of records their method can be applied. In addition one would hope that they continue their work and incorporate discrete proxy variables and measurement errors in the depths observations as well. I do recommend publication of the manuscript as it is.

We thank the referee for this recommendation. We feel that the method presented in this study has the potential to provide valuable insights to paleoclimate, and in particular Quaternary, research and we are hopeful that our revised version meets the standards of publication.

Anonymous Referee #2

General comments:

The manuscript by Goswami et al. deals with an important yet often overseen problem - namely how the dating uncertainties affect the interpretation of paleoclimatic proxy records. The work highlights how the nature (variability) of the proxy signal itself adds to the final uncertainty of the age model – also an issue rarely realized by researchers working with proxy datasets. The text is exceptionally well structured and neatly written. The authors provide a step-by-step algorithm estimating the probability of a data point having a certain calendar age. I am looking forward to an open source, easy to use program, which can assist me with such a task.

We thank the referee for the encouraging and insightful comments. We also plan to release an open-source, easy-to-use implementation of the method outlined in our manuscript so that it becomes accessible to paleoclimatologists. However, rather than creating a separate package for

our method alone, we envision our Bayesian proxy estimation approach as being a part of a larger, more holistic framework of proxy estimation such as COPRA (available at: <http://tocsy.pik-potsdam.de/copra.php>). We are working on including our work in a future COPRA version. Till then, a hands-on working implementation of our approach can be easily made available by the authors on request.

The only problem I see is the choice of exemplary data for a dataset provided by the authors (Lonar Lake data). It appears, that the authors do not feel at ease with XRF measurements and their arguments could have been much stronger if applied to quantitative instead of qualitative data. My comments concerning problems of XRF data (actually never even mentioned as such in the text!) are listed below together with specific comments.

We apologize for not making it clear in our manuscript as to the details of the XRF datasets that we used from Lonar Lake. Thank you for pointing this out. In the current revised version, we have included the details of the XRF measurements and have also explained our choice of Al and Ca as paleoclimate proxies in both the main text and in a newly included subsection in the Appendix. We provide the details of these revisions in the following paragraphs.

I like the proposed approach and appreciate the elegant simplicity of its presentation. I would like to see this work published. However, it requires some changes from its present state – either providing a different example or a solid clarification for used one.

We are thankful to the referee for this recommendation, and for raising critical issues regarding the motivation of the exemplary datasets from Lonar lake and their interpretations thereof. We provide our response to these points in the text below, We have also revised our manuscript, as per the suggestions of the referee, to include a detailed description of the datasets.

Specific comments:

Page 1025, line 3: change 'allow us to investigate' to 'allow us investigating'

We have not made the change suggested above as we feel that the change would result in grammatically odd-sounding sentence.

Page 1025, line 15; page 1038, lines 11-13: how do the authors know what exactly Ca and Al stand for? They take for granted that Ca represents groundwater inflow and Al surface erosion – and this is the first time ever these data are reported. I assume that for a proof of concept it is better to use a dataset that is settled and has already been published. At least, the authors should explain in full what their interpretation of XRF data is based on.

We are especially sorry that our earlier manuscript glossed over the details of the nature of Lonar Lake datasets. The dataset linking the Ca to groundwater inflow (evaporitic carbonate (CaCO_3) formed during periods of low lake level) and Al to surface erosion (lithogenics brought in by rain events) has already been tested, established, and published in Basavaiah et al. 2014). We have, in our revised version, included the following text in Section 3.2 "Holocene proxies from central India" of the text:

"For the proxy records, we take the Ca-area proxy for groundwater inflow and Al-area proxy for surface erosion from the same archive at Lonar. The links of both the Ca to groundwater inflow (evaporitic carbonate (CaCO_3) formed during periods of low lake level), and that of the Al to surface erosion (lithogenics brought in by rain events) have been validated in Basavaiah et al. (2014).

These were obtained from a continuous down-core X-Ray Fluorescence (XRF) (Avaatech XRF Core Scanner III) scanning of the Lonar lake sediment core surface. The relative abundances of the elements (Ca, Al, Ti, Si, and K) were recorded at every 5 mm with the X-PIPS SXP5C-200-1500 detector from Canberra while the tube voltage was kept at 10 kV (Prasad et al., 2014)."

Page 1026, line 4: change ‘unobservable climatic variables’ to ‘past physical variables that cannot be directly measured’

We have made the corresponding change in the text.

Page 1027, line 3: add ‘ever’ after ‘first’

We have made the corresponding change in the text.

Page 1030, line 22: add ‘(age reversals)’ after ‘outlying values’

We have made the corresponding change in the text.

Page 1030, line 25: Please do not mix ‘age’ and ‘date’. ‘Age’ is an interval while ‘date’ is an exact time point in the past. Even if informally speaking ‘radiocarbon date’ is fine, in order to get the exact point in the past you need to calibrate it – and here the problem you deal with in this paper starts. . . I suggest changing ‘radiocarbon dates’ to ‘radiocarbon ages’ or ‘radiocarbon dating points’.

We have changed all occurrences of radiometric “dates” to “ages” or “dating points” as suggested.

Page 1037, line 17: if DWF stands for ‘depth-spanning weight function’ do you really need ‘the weight function DWF’?

We have made the corresponding change in the text.

Paragraph 3.1: I realize that the authors use here a synthetic record but why given as “X %o” ? Presumably, it is supposed to represent a synthetic ^{18}O record (as suggested by Fig 4) – then please state it clearly. Or else, just call the synthetic dataset “Proxy value” to avoid confusion. Adding a temporal resolution of synthetic data set would also helpful.

We thank the reviewer for pointing this out and agree that the usage of the “%o” in the figures can lead to an unnecessary ambiguity. We have therefore changed the labels of the proxy axes in Figures 4 and 5 to simply “Proxy Value” as suggested.

We have also included an additional sentence in Section 3.1 “Synthetic examples” regarding the temporal resolution of the generated synthetic proxy datasets: “Also, the proxy datasets were generated annually, i.e., with a proxy value for every year.”

Paragraph 3.2: The authors admit that they use unpublished data and without spending a word on how they where actually measured they take for granted what the data stand for and how to interpret them. This choice is the weakest point of the manuscript and has further consequences for their argumentation. Additionally, it shows the authors’ poor understanding of data they are working with – a pretty ironic turn in their paper as they are trying to help paleoclimatologists to understand the dangers lurking behind incautious application of age models. Please see my comments below.

This is a critical issue and we thank the referee for raising this point. We concede that we failed to provide the details of the XRF measurements for the Lonar Lake dataset and that this could create serious issues for interpreting the results. We rectify this issue in our revision by including the necessary details about the proxy datasets in Section 3.2 "Holocene proxies from central India" (see response above). However, we would also like to stress that both the proxies used have been validated as being representative of the groundwater inflow and surface erosion in the Lonar lake catchment (Basavaiah et al., 2014). The water content, grain size and porosity of the sediments can impact upon the XRF data (Tjallingii et al. 2007; Weltje and Tjallingii, 2008) especially for lighter elements like Al but not for heavier elements like Ti. Moreover, Al and Ti show a high correlation coefficient of 0.81 indicating that the effect (if any) on Al is minor. We further note that in Lonar core the Al (cps) are not related to water content which under normal circumstances is higher near the core top. Checks on limited core samples (Menzel et al., 2014) show that Al is higher in samples with higher lithogenic content. In the absence of long term monitoring data, the proxy (elemental or isotopic) variability cannot be quantitatively linked to monsoon rainfall. There is no additional advantage to quantifying the scanning XRF data – their qualitative link to lithogenic content is sufficient at this stage.

The text in the manuscript (Section 3.2) has been accordingly revised as given below:

"The Al counts were found to be strongly correlated with the Ti, Si and K counts obtained from the XRF scanning (see Appendix B2). Due to this, and combined with the findings of Basavaiah et al. (2014) where they show the relation of the Al abundance to catchment erosion as well as the lithogenic contents, we choose this as a representative proxy for the Lonar lake surface erosion. We note that due to the difficulties of representing errors of XRF measurements, we consider the proxy observations along depth to be error-free. This however, does not change the fundamental objective of our analysis, which is to estimate the final proxy uncertainties in an analytical fashion and investigate how they are impacted by proxy-depth variability. If the proxy measurements were to have error, these would simply be added to the final errors as is indicated by Eq. A15."

Page 1040, line 6-7: what do the authors mean by 'proxy measurement error were in order of parts per million'? Unless they mean a 'dating error' (and just made a tipping mistake) there is a problem. Similarly, page 1045, line 19-20: 'the proxy measurement error is already at the instrumental limits of precision'.

We sincerely apologize for this mistake. We have removed the text 'proxy measurement error were in order of parts per million'. For the second instance, we have changed the corresponding text in the manuscript to:

"... and the proxy measurement error is already set to zero in our analysis."

I recon - from the unit used (cps, counts per second) – the authors are using XRF (X-Ray Fluorescence) measurements. XRF scanners provide the bulk intensities of major elements (e.g. Al, Si, K, Ca, Ti, Fe). The data are given as e.g. Ca area, which refers to the intensity of the element, measured as mentioned in cps or alternatively total counts. Traditionally XRF data are reported as 'XRF Ca-intensity (cps)' or 'XRF Al-intensity (cps)'... etc... Now, coming back to the original question, how do the authors come from cps to % XRF measurements are qualitative -- therefore it is extremely difficult (though not impossible) to estimate the error of the measurement. One of the more tedious methods is scanning the same core (or epoxy block for that matter) several times – still this will provide again only qualitative information. Preparing additional discreet set of samples and running a quantitative measurement on e.g. ICP-OES or ICP-MS will be the most time consuming but also most appropriate way to calibrate XRF data. Nowadays, XRF data are mostly used as a 'quick & dirty' method to have a first look into the composition of the sediment and for identification of interesting intervals – basically first screening. E.g.: Are there any cycles, or abrupt changes? What is the amplitude of change, shape of the curve? Are there any similarities to reference records like ice cores? This is the

reason why the error of the measurement is not as crucial as for quantitative measurements. Moreover, depending on the instrument used to measure the profile (AVAATECH, Itrax, etc. . .) and its settings, intensities of single elements might be too low to provide a reliable signal. Presented Al intensity seems to me too low to be really significant. I believe that by their nature XRF data are not an easy substance for statistic approaches (given the difficulties in estimating XRF measurement uncertainties), and in particular the Al data chosen by the authors are suboptimal to illustrate the proposed method. If the authors insist on using them – please provide all the limitations of the XRF measurement (similarly as you they did for their own method) and necessary background information to make sure you are not interpreting noise.

Based on the suggestion of the referee, we have now included the necessary details regarding the measurement process of the Al and Ca proxy datasets (see responses above). Furthermore, we have clarified that, due to the fact that the uncertainties of the XRF counts are not easily tractable, we choose to set them to zero. This does not change the fundamental results of applying our method to the Lonar lake datasets as the proxy measurement uncertainty comes in as an additive term in the final uncertainty of estimation as represented by the variance (c.f. Eq. A15). Moreover, we stress that the main objective of our paper is to analytically estimate the proxy-vs-time uncertainties (and how they relate to dating uncertainties), and further investigate the interrelations of proxy-depth variability with the final proxy uncertainties. In this regard, the choice of Al and Ca proxies helped us to gain certain critical insights on how proxy variance impacts proxy record estimation error.

We agree with the referee that the magnitude of the Al counts being low might raise a question on their reliability, but as shown in Prasad et al. (2014) and Basavaiah et al. (2014), the Al counts strongly correlate to other elemental abundances along the core (Fig. B1 of the revised manuscript, appended below in this response as well), as well as to the climatic variations in the area. We have tried to motivate our choice for Al in a subsection in the Appendix: “B2 Note on Al area as a surface erosion proxy”.

Page 1046, lines 16-20: here my comment boils down to the nature of XRF data. Yes, the variability of Al is indeed higher than that of Ca, at the same time the counts (cps) are very much lower – a strong indicator to treat the data with caution. If compared on the same scale Al will show as good as no changes at all so unless there is a good argument for using Al intensity this dataset is simply not convincing and the authors should employ a more robust/significant proxy.

The reviewer is correct that the scanning XRF data provide qualitative variability. However, as mentioned in the response above, we have linked the elements to environmental processes (Basavaiah et al., 2014). The XRF data (SOM-2 for XRF data in Prasad et al., 2014) show that the elements K, Ti, and Si are significantly correlated with Al ($r = 0.89, 0.81, 0.93$) for the whole core (c.f. Appendix B2 of our revised manuscript). Our investigations of modern catchment and lake surface sediments (Basavaiah et al., 2014) show that Al is contributed by catchment erosion and its distribution parallels the lithogenic content (brought in by surface erosion) in surface sediments. Therefore, we consider Al (or any other detrital indicator) to be a significant and robust proxy as it has been tested in modern environment. In palaeo-environment it has been tested against the present of other evaporite minerals (Anoop et al., 2013).

We stress that the primary results of our approach would not change if we were to change the Al proxy for another one. However, using the Al, and by comparing its results to that of the Ca proxy, we were able to illustrate how proxy-depth variability and proxy-time uncertainty are connected.

References:

Anoop, A., Prasad, S., Plessen, B., Basavaiah, N., Gaye, B.; Naumann, R., Menzel, P., Weise, S., Brauer, A. (2013). Palaeoenvironmental implications of evaporative gaylussite crystals from Lonar Lake, central India. *Journal of Quaternary Science*, 28, 4, 349-359.

Basavaiah, N., Wiesner, M.G., Anoop, A., Menzel, P., Nowaczyk, N.R., Deenadayalan, K., Brauer, A., Gaye, B., Naumann, R., Riedel, N., Stebich, M., Prasad, S. (2014) Physicochemical analyses of surface sediments from the Lonar Lake, central India – implications for palaeoenvironmental reconstruction. *Fundamental and Applied Limnology*, 184/4, 55-68.

Philip Menzel, Birgit Gaye, Praveen K. Mishra, Ambili Anoop, Nathani Basavaiah, Norbert Marwan, Birgit Plessen, Sushma Prasad, Nils Riedel, Martina Stebich, Martin G. Wiesner (2014). Linking Holocene drying trends from Lonar Lake in monsoonal central India to North Atlantic cooling events, *Palaeogeography, Palaeoclimatology, Palaeoecology*, Volume 410, Pages 164-178.

Prasad, S., Anoop, A., Riedel, R., Sarkar, S., Menzel, P., Basavaiah, N., Krishnan, R., Fuller, D., Plessen, B., Gaye, B., Röhl, R., Wilkes, H., Sachse, D., Sawant, R., Wiesner, M.G., Stebich, M. (2014). Prolonged monsoon droughts and links to Indo-Pacific warm pool: A Holocene record from Lonar Lake, central India. *Earth and Planetary Science Letters*, 391, 71-82.

Tjallingii, R., Röhl, U., Kölling, M., Bickert, T., 2007. Influence of the water content on X-ray fluorescence core-scanning measurements in soft marine sediments. *Geochem., Geophys., Geosyst.* 8. doi:10.1029/2006GC001393.

Weltje, G.J., and Tjallingii, R., 2008. Calibration of XRF core scanners for quantitative geochemical logging of sediment cores: theory and application. *Earth Planet. Sci. Lett.*, 274(3–4):423–438.

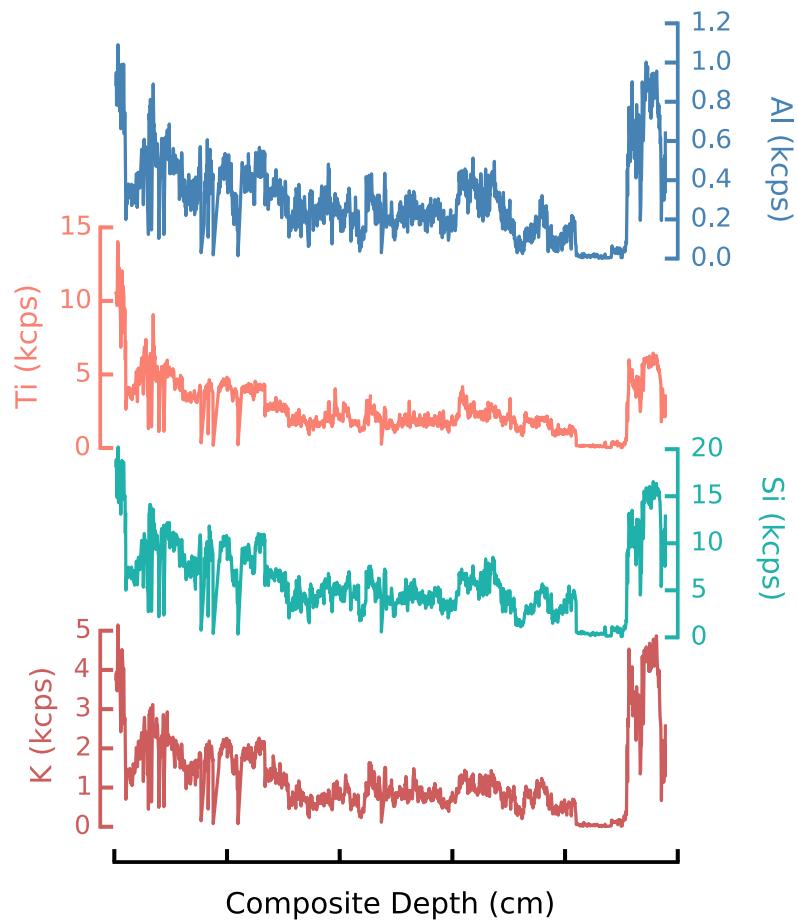


Fig. B1. Al counts as a representative proxy for Lonar lake. Al counts (top panel, in blue) are strongly correlated to the Ti (orange), Si (green) and K (red) counts obtained from XRF scanning of the Lonar lake sediment. This correlation with the other elements, combined with the fact that the Al counts arise due to the catchment erosion forms the basis of choosing it as a representative proxy for this analysis. This choice also helps us to illustrate the impacts of proxy- depth variability on the final proxy estimate uncertainties. (Color online.)