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Climate of the Past Discussions

Interactive comment on "OPTiMAL: A new machine learning approach for GDGT-based palaeothermometry" *by* Yvette L. Eley et al.

Anonymous Referee #1

Received and published: 4 August 2019

The study by Eley et al. enriches the discussion on GDGT temperature calibrations by describing a novel machine learning approach. Previous calibrations including Bayspar relied on the reduction of GDGT abundance data into one dimension (TEX86) and used only a subset of the commonly quantified GDGTs. Compared to these prior approaches, the strength of Eley et al's approach lies in the development of a distance parameter of the full GDGT diversity. This approach has great potential for identifying anomalous GDGT distributions. However, I agree with some of the criticisms raised by J. Tierney and H. Yang. Specifically, I think the authors should state more clearly the cons and pros of Optimal relative to Bayspar. In my view, the approaches taken in Bayspar and Optimal are complementary: From what I understand Bayspar is concerned with finding a regional TEX86-temperature calibration by subsampling the

modern dataset, Optimal seems to find the best fit to the whole modern dataset but ignores regional differences. A more balanced discussion should highlight these differences. Further, applying both approaches to the same paleorecord may yield novel information. Below I make recommendations for improving this study:

i) I missed a thorough exploration of the outliers, for example the large number of grey outlier data points in figure 13. Identifying patterns (e.g. similar depositional environments or similar environmental parameter space) in the distribution of outliers could advance our understanding of anomalous distributions.

ii) The agnostic approach of Optimal is both its greatest strength and weakness. Optimal implicitly ignores some of the things that we do know about GDGT distributions besides temperature-dependence. One important aspect that is not covered by Optimal is the existence of temperature-independent and regionally varying patterns of GDGT distributions and calibration slopes (see Fig. 5 of Pearson & Ingalls, 2013, Annu. Rev., and many papers concerning regional calibrations). Regionality is addressed to some degree by Bayspar and thus it would be worth exploring if the differences between Bayspar and Optimal could be attributed to regional effects. Further, addressing regionality as a source of noise could significantly reduce uncertainty and the issue of overfitting.

iii) The final test of a proxy should be its application to a paleorecord. I recommend the authors test Optimal against established approaches (e.g., TEX86L/H, Bayspar, UK37, Mg/Ca) on both a deep-time (e.g., Eocene) and a recent (e.g., Pleistocene) temperature record. I believe that Optimal can become an important part of the GDGT toolbox if the above criticisms are addressed. I thank the authors for thinking about this problem in a novel way and pushing the field in a new and promising direction.

Additional comments below:

Line 20: Rather "site of deposition" than site of formation.

Line 43: from “dialkyl” to “dibiphytanyl”

Line 45-46: Bacteria are not known to produce isoprenoidal GDGTs. You could also make this distinction by substituting “dialkyl” with “dibiphytanyl”.

Line 53: Based on new structural data by Liu et al. 2018, Organic Geochemistry, the “crenarchaeol regioisomer” is no longer considered to be a regioisomer of regular crenarchaeol. Consider renaming to “crenarchaeol isomer”.

Line 78-80: The original work on Red Sea GDGTs should be cited here (Trommer et al. 2009, Organic Geochemistry). This sentence may need to be rephrased. Trommer et al. suggested salinity as an indirect effect on TEX86 through its influence on community composition. Therefore, the actual difference between Red and Arabian Sea GDGT distributions may be the existence of an endemic population.

Line 96: Unclear what “GDGT productivity environment” means: The habitat of Thaumarchaeota or the productivity of Thaumarchaeota?

Line 110-111: I think “not helped” is a little harsh. BIT, MI and RI have valid use cases.

Line 125-127: A bigger issue than the small number of cultures is the fact that all cultured planktonic species belong to the same genus, Nitrosopumilus, which is not necessarily representative for all Thaumarchaeota.

Line 134-139: Elling et al. 2015 is not the only culture study on temperature response. Qin et al. 2015 (cited in line 127) also studied temperature response and found non-linear temperature response. This study should be discussed here.

Line 162: Consider using more precise language than “wildly”

Line 280: Is this a linear correlation?

Line 261: Missing citations for seasonality. Add Hurley et al. 2016, PNAS, for growth rate dependency.

Line 262: Trommer et al., 2009, Organic Geochemistry, was one of the first studies to suggest an effect of ecosystem composition. Consider

Line 265: Not sure I understand why std errors are compared to standard deviations.

Line 340: Missing parenthesis after 2006.

Line 507: What is the rationale behind using >0.5 as cutoff?

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