Clim. Past Discuss.,
https://doi.org/10.5194/cp-2019-60-RC2, 2019

Climate of the Past Discussions

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

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Received and published: 12 September 2019

I think TEX86 is wickedly charming. We all have heard about the misdeed of TEX86, but also realized that often times TEX86 is the only thing that could help us to learn about the ocean temperatures, especially in the greenhouse climates. This proxy has probably already passed its pessimism stage, and currently in the realism phase. Eley et al is a timely contribution to help us better understand this important proxy. They applied the cutting-edge machine-learning tools to improve the SST estimates using GDGTs, with the concept of identifying nearest neighbors in the global core-top dataset. This is innovative, but I do have some concerns detailed below. I suggest moderate revision of the MS before it can be accepted by CP.

Although this was not explicitly explained in the MS, I assume the authors used the percentage of each individual GDGT, when [GDGT-0]+[GDGT-1]+[GDGT-2]+[GDGT-3]+[Cren]+[Cren']=100%. If this is the case, these 6 variables are not independent from each other. Instead, they are often dominated by the variations of [GDGT-0] and [Cren], the two major GDGTs. To show this, I did a simple calculation of the T&T15 global core-top dataset, which yielded an average [GDGT-0]+[Cren] of 88% of all GDGTs. This means that the variability of [GDGT-1], [GDGT-2], [GDGT-3] or [Cren'] that you see might be largely explained by the changes of [GDGT-0] or [Cren]. This is one of the reasons that TEX86 only considers the minor GDGTs, and uses a ratio. Ratios are good, as demonstrated by numerous cases in geochemistry.

With that being said, I agree with the authors that by using a subset of GDGTs like the TEX86, we are losing some information. We also discussed this in the Rind Index paper of Zhang et al., 2016. We realized that Ring Index values are dominated by [GDGT-0] and [Cren], as illustrated in Fig. 2. So the real difference between OPTIMAL and TEX86 (and any TEX86 calibrations, BAYSPAR, Kim or Liu) is not 6 dimensions vs. 1. If the authors would like to, they can try something like use 2 subgroups of GDGTs - major and minor ones, with the total of each equals 100%; or some other forms of 6 ratios, normalizing GDGTs to one in the major, and one in the minor category. There's still going to be some dependency between the 6 variables, but they are closer to the 6 dimensions than the original treatment. If they decide not to pursue these alternatives, I'd like to see that at least they acknowledge the interdependency of GDGT% data.

Another issue is the extrapolating from the modern calibration data set. Nobody likes extrapolations. But there are these mesocosm studies from NIOZ that demonstrated the response of GDGTs to ~40oC temperatures. The archaea found in hot spring continues to increase their ring numbers until ~100oC. I agree that we might not know the absolute temperature above ~30oC very well, but I wouldn't call them "inappropriate use" that "impacts the confidence". In fact, the beauty of TEX86 is that it works in greenhouse climates and tropics when Uk'37 maxes out, carbonates are diagenetically

altered and seawater Mg/Ca is difficult to constrain.

There are minor problems but I'll save that for the next version, assuming some of them will be fixed in the revision.

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