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Review of the manuscript:
"Improving the thermocline calculation over the global ocean"

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Summary:
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This paper presents a new method to diagnose both the MLD and the thermocline characteristics (thickness, depth, strength), from observed ocean profiles of temperature and salinity. Based on Argo profiles, a new climatology of MLD and thermocline variables is constructed using this method. It is compared with previous similar climatologies of MLD to validate the approach, and then the results about the new thermocline fields (depth and thickness) are discussed.

General comments:
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This work is innovative because it proposes a new method that can be applied to get both the MLD and the thermocline characteristics at the global scale for the first time. This topic of ocean stratification is quite important and had several noticable studies lately (eg Sallee et al 2021), because of its potential impact on climate evolution. For those reasons, it would make sense that this rather method/data paper could be published in OS. However, when reading the paper, many serious problematic points appeared in the presentation of the method and results, showing that there is somehow a lack of knowledge about the MLD/stratification problems (unprecise method presentation, no word at all about barrier layers, comparing different types/family of MLD for validation, no introduction/references/discussion of the 3 layer hypothesis, a quite weak discussion of the results...). After having hesitated to reject the paper I must say, I would still advice a major revision of this work because the topic is relevant and actual, even if I think that the task is big to come to a publishable version. I give below precise comments about the modifications I suggest. There are especially 4 major points (and part of those points may also be developped in the detailled comments section) that, for me, must be adressed seriously before any possible publication.

Major points to address:
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1) You should clarify the description of the method :
I have questions about the details of your method, which is the base/heart of the paper. It is very important that the method is presented clearly and univoquely, here it is not the case for me at least. There are several detailed points to address (next section of the review, fig1, eqn 1, l99-100, l143-144) about this hereafter. Here is how I see the process of your method from a T/S profile :

- get the depth D1 of vertical max of N2 from the density profile
- multiply D1 by two to get the depth D2 over which we make the coming fit (D2 = 2*D1)

- evaluate the direction of vertical T change --> how do you do this ? It looks not present in your python code (?) and it must be explained here, is it by computing the difference T(0)-T(D2) ? something else ?
- amend the sigmoid function sign according to previous test
- normalise the temperature data between 0 and 1
- the fit : non-linear adjustment of the sigmoid function f = +/- (1/(1+exp(-a*(x-b)))), to find the best a and b parameters, along with a goodness of fit coeff R^2
- get MLD by threshold on the T sigmoid (0.2 degC from 10m), get also MTD by threshold of 0.2 degC from the deepest level value of our interval (i.e. at D2 right ?)

If this process is right, then what you basically do is to fit a sigmoid on the temperature profile. Then you will diagnose a temperature-MLD (or isothermal layer depth) + its thermocline, and not an isopycnal layer depth + pycnocline.

. Then I do not understand why you diagnose your working depth interval (ie D2) from the density profile, logically it could be done directly from the temperature profile by searching the max of grad(T), because it is the pattern you basically look for and on which you perform a fit ?

. Also by doing this, you will end up with a sigmoid that is not centered on the N2 max, i.e. your b parameter in the sigmoid fit will be different from zero, because your thermocline is rarely exactly at the depth of the N2-max (as shown in fig1f cf detailed comments). This is not what is in the text when saying l. 99 that you "locate the most stratified point in the center of the sigmoid function".

2) The area/conditions of validity of your method should be clarified, with possible evolution toward application on density profiles :

There are detailed comments below for lines 143-152. This part should be re-written I would advice, and the context of Barrier Layer should be presented as it is strongly linked to this part and it is never mentionned. Your method diagnose MLD from temperature profiles as presented here, so obviously, you will miss the density-MLD (B04 or HT09) in all BL areas, which are quite numerous despite what you say in several places of your text. But this is not a problem according to me. To get a correct density-MLD, you should simply apply your method also to the density profiles, which have also often a 3-layer shape (even more than temperature, and no density inversion occur while you may have temperature inversions). This may make a bigger paper, but as it is now I have wondered why you stick to thermocline only, trying to say that it is nearly same as pycnocline (which is not true in many areas), while it seems that you have everything to do the computation directly to get the pycnocline also. Then when you compare with previous climatologies, you should compare what is comparable, if you have a temperature-based MLD (as it is now) then you should compare with a temperature-based MLD also (eg a 0.2 degC threshold MLD compared to 10m). Otherwise you will end up discussing Barrier Layers (BL) and compensated layers issues which have been discussed previously in papers and may not be the goal of your work (which seems to validate your new dataset of MLD and Thermocline or pycnocline if ever).

3) As stated above, you should compare climatologies with at least same family of criterion :

Your criterion is a threshold criterion of 0.2 degC on a fitted temperature profile. You should then compare it to the 0.2 degC threshold criterion of B04 also on temperature profiles not to the 0.03 kg/m3 density criterion, or you will mix several source of differences, especially salinity effects (cf lines 175-182). B04 and HT09 are shallower than your temperature-MLD mostly in the BL areas and high latitudes, which makes sense. B04 is deeper than HT09 which also makes sense as HT09 is a mix of several criteria and takes the smaller one, and this has also been already noticed in HT09 paper. Here you want to validate your MLD method, not discuss where salinity plays or not, for me it is another problem that has been tackled in many Barrier layer papers already. So you should compare your temperature based MLD with a similar temperature based MLD (eg deboyer 2004 0.2 degC threshold). Then if you want to have a part to see where your temperature MLD is biased compared to a density MLD, you should first cite the BL papers, and then make a comparison that should well correspond to BL areas as is seen in your figures already.

4) An extended discussion about what you expect to diagnose as your thermocline is necessary, along with presenting in introduction what you talk about with this 3 layer hypothesis. Will you give the permanent thermocline or the seasonal one ? is it just below the MLD or not ? is it a mix of those 2 features ? (see helber et al JGR 2012, sprintall cronin EOS2001, Johnston Rudnick JPO 2009...)

Other detailed points to address :
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l. 22-23 : the ocean surface layer density and extent of the MLD is also determined by salinity in all "Barrier Layers" area which are present all over the tropical ocean (e.g. Sprintall and Tomczak JGR 1992, de Boyer Montegut et al JGR 2007). This should be mentionned here, as the total areas where salinity drives the stratification and MLD is actually not small at all (maybe about 20% of the total ocean surface when checking maps visually in the 2 references above).

l. 26 : "The characteristics and ... (coast-ocean gradients)" --> I think this sentence does not bring much information actually but could be kept as a transition. However, I would have said "spatially" instead of "latitudinally and longitudinally". Also, I do not really get the meaning of the term "coast-ocean gradients" here. It may be worth explaining further or being more precise, or else remove it.

l. 29 : I advice the change: "heat flux" --> "net heat flux"

l. 59 : "MTD" : I could not find the definition for this before (guess it is for "Maximum Thermocline Depth")

l. 62 : I am surprised that I could not find any trace of the Jiang et al 2016 publication via google, may be my mistake, but talking about maximum curvature method, I also though of the paper by Lorbacher et al JGR 2006, and would have liked to see how the Jiang paper would compare to that one, with the possibility of citing also the Lorbacher paper as being before in time, if it suits the situation of course.

l. 79 : you could also tell what quality control flag you use for selecting the acceptable DMQC data, only the flag 1 ? both flag 1 and 2 ? (of course you removed the 3 and 4 QC flags data I suppose)

Figure 1 (and equation (1) of sigmoid):
- from the description of your algorithm, you multiply the depth of density stratification maximum by 2 to get the max depth on which you fit you sigmoid, but on this figure, you do not show profile on this complete depth in (a) to (d) panels (e and f look quite ok to me). For exemple, in panel (a), the max stratif N2 (center of sigmoid) appears to be at 80 meters depth, so we could have expected that you show the profile on the whole depth of the sigmoid fit (ie 160m, but you stop your plot around 140m), and same in b,c, and d. Is there a reason for that ? if not, I think it could be somehow better to see the whole depth on which the fit occurs.
- in panels b and f at least, it looks like the max of N2 is not the center of the sigmoid, with the limits of the thermocline you diagnose being even below this depth fro panel f. This is apparently in contradiction with the algorithm you describe, or I may have missed something (as said in your texte you multiply by two the N2 max depth so that your sigmoid is centered at the max of N2, no ?). This may show the difficulty of mixing a density diagnostic (max of N2) with a temperature one (fit on T profile) because the 2 are not always linked, and their maximum gradient can often be at a different

depth. This may also be linked to the fact that your actual sigmoid is not necessarily symetric with the max of N2, which is necessary because you fit on T-profile, not on density-profile. Indeed, if I believe the formula found in the python code of Romero 2022, it is "1/(1+exp(-a*(x-b)))", so you should give this formula in your equation (1) so that readers know exactly what variables you fit (ie a and b here), and that your final sigmoid is not necessarily centered on the max of N2, but centered on the max of grad(T) as you make the fit on T, not on density.

- as an illustration, I would advice to also show a typical exemple of a profile when your method does not work so well as it happens quite in several extended places, i.e. when the 3-layer shape is not valid for temperature (R2 below 0.7 or 0.5), this should happen a lot in high latitudes beta-ocean with many interleaving features and several temperature inversions, or maybe in cases of remnant layers when restratification occurs by steps during spring at mid latitudes.

l. 119 : "HT03" should be "HT09" I think

l. 120 : here it would be better to (re)precise also the reference depth of B04 as the scope of the paper is about methods to diagnose MLD and stratifications, e.g. "... a threshold of 0.03 kg.m-3 compared to the reference value at 10 m depth in the density..."

l. 121 : "...de MLD..." should be "...the MLD..."

l. 136-137 : from your figure legend lon/lat data, I have profiles a, b and f in southern hemisphere, and d and e in northern, so you should correct something somewhere to be sure where we are.

l. 140-141 : Your conclusion is somehow a scientific overstatement. You cannot draw a general conclusion from a sample of 6 profiles among 2 millions or more. This analysis is not scientifically reproductible. If you take another 6 profiles, you may have a completely different conclusion. So it cannot be used for a general conclusion. Such exemples of profiles are nevertheless important to be shown so that the reader can realize some of the main details of the method illustrated in different situations (for exemple the fact that in austral the max of N2 is not at same depth as the max of thermocline, cf remark above for figure 1 also). I would advice that you temper your conclusion saying that this figure is an illustration of how the method works, and of the fact that it seems to work well (but this will be quantified afterward in the paper actually).

l. 143-144 : Again, for me this statement is not exact or misleading (and same at l.99-100). From fig 1. and formula in your python code, we can see that your sigmoid is not necessarily symetric with the max of N2 being the central point of the sigmoid (not central if b param is not zero in your sigmoid, cf also major point to address). Eventually I do not see exactly why you need to show that your method should be applied with caution in salinity dominated region. This is basically obvious from your method : you diagnose the isothermal layer depth (or temperature-MLD) because you work on the T-profile only, so of course in every Barrier Layer areas, you should end up with a too deep temperature-MLD compared to a density-MLD, and this may happen in all high latitude areas (beta oceans) and all tropical and mid latitude Barrier Layers areas (cf maps by sprintall tomczak JGR 1992 or deBoyer Montegut et al JGR 2007). Eventually your method is another way to compute the MLD (here based on temperature, but it could/should have been applied on density also) with one advantage that is to give also an estimate of thermocline depth and thickness which is a nice plus of your method of course.

Figure 2 and l. 144-152 : Here you show the T/S contributions to the stratification at the depth of the max-N2 (max density stratification). If we assume that this depth is most of the time at the base of the isopycnal mixed layer, then this analysis is very similar to the Barrier Layer (BL) mapsmentionned above. It is then surprising that all the historical BL in western equatorial paicifc are not more pronounced, but still they are present in your plot and should be noticed (As your map is not seasonal, only the permanent BL patterns are well evidenced, or as the diagnostic is not really the same there are small differences, but in fig 8 the shaded areas indeed occur in west equat pacif during jun to sept for exemple.)

l. 151-152 : This statement is misleading to me. Your present diagnostic does not tell you about the vertical thermal structure of the ocean. You may have a BL situation typically in the west equat pacif, where you have warm waters at the surface then a thermocline with decreasing temperature at about 60m and colder water below (a thermal classic three layer structure). Yet you also have fresh water eg in the top 20 or 30 meters, with a 1st pycnocline at this depth, dominated by salinity. What figure 2 tells us is just what happens at the depth of N2 max. This is rather the R2 that tells you if your T-profile is well fitted to a sigmoid and hence if it has a 3-layer shape. Eventually I wonder about the relevance and this figure in your work, or it needs to be better presented, within the context of BL I would say, and may be seasonally.

l. 193-195 : I do not really agree with this statement, and this is not what was shown in HT09 and from your map in fig S1c, where B04 density MLD is shown to over estimate the MLD in high latitudes. This also makes sense with the fact that the ocean has a very low vertical stratification at high latitude, which pushes for smaller density criterion to get the mixed layer, especially in winter. And even if Perralta-Ferriz and Woodgate 2015 used 0.1 kg/m3 (but based on a heuristic method for choice), they recognize that they had to use a smaller 0.03 kg/m3 for several of their winter profiles to avoid over estimation of MLD.
Also you show that B04 overestimate MLD in arctic ocean in winter (region 48 of fig 6 a b), and then at line193 you say that their 0.03 criterion underestimate the MLD in polar regions. This makes not sense to me.

Figure 6 : I advice to replace this one and fig S1 by a plot of the maps of differences between HT09/B04 and your method, at 2 relevant seasons at least, which makes 4 maps, and enables a more detailled analysis than the AR6-WGI regions (why choosing those?), that were not designed for MLD studies and are not really relevant for that (for exemple dividing the labrador sea deep convection region in 2 parts)

l. 204-205 : As a remark here, I would say again that your MLD method validation is not the main point fo your article. Basicaly, your method for MLD diagnostic is the 0.2 degC threshold on a temperature profiles (after a sigmoid fit, that is your plus so as to diagnose thermocline after), so it is nothing really new for me, and it should be validated with a previous climatology of the same type (a threshold of 0.2 degC from T profiles), and should work with no big surprise to me. The important and new part of your paper is the thermocline (or pycnocline if you add it) part that comes now indeed.

Figure 7 : In may an extended pattern of MTD reaches 350 to 400 m in north atlantic, while it is about 100m or less in MLD (linked to the about 300 m thickness in figure 8 also). At that time restratification already started form the MLD shift from April to May, then I wonder why you do not catch this restratification with your method. I would have expect to see the MTD not so far from the MLD in may when the restartification signal is there in MLD, why is it not the case ? Are you diagnosing the stratification below the MLD (which I doubt actually) or a stratification that corresponds to the permanent thermocline ? You must talk about this somewhere, and also you should define your view of the three layer more precisely, because this view corresponds to warm surface / permanent thermocline / deep cold ocean, but with your method that limits the fit to max of N2 depth * 2 we would think that you may not catch the permanent thermocline but the seasonal one (or trnasition layer after Johnston and rudnick JPO 2009, see also Helber et al JGR 2012 that tackled also a related topic). For such a discussion you can also rely eg on Sprintall & Cronin EOS 2001 (upper ocean vertical structure) for a basis.

l. 213-218 : this description does not really bring something new to the paper, and explanations are quite well known already

l. 220-221 : same remark as above, here if you have very close values of MLD and MTD (either small or even large), then it means the difference MLD-MTD is small and based on your sigmoid that is symetric, 2*diff (which is your thickness) is also small, nothing special that is worth noting for me here, or I missed something.

l. 239 : your term "mixing" here is not correct. the mixed layer is something different than the mixing layer and you should be aware of that when writing a MLD/thermocline paper I suppose. See Brainerd and Gregg DSR 1995 "mixed and mixing layer depth" to know about this point and make the difference between the 2.

l. 259-266 : precise RTQC and DMQC i do not think it has been done before.
Also I doubt when you say "a large number of cells would contain less than 3 values for monthly averages". I do not have the same result on my side, I have a map with number of argo profiles per 1 degree boxes annually and it is over 50 over nearly the whole ocean, which means on average over 4 profiles per month at least. So I have difficulties to understand from where you make this statement.

l. 267-269: Your argument is not correct here. Oceanographers have pushed for salinity measurements historically because the latter also plays a role eg in MLD and now that we have those data (with argo), you say "it is better to not have it and just use temperature" and for that you rely on a very good but very old paper (rao 1989) at a time, especially in indian ocean, when they had no choice at all about using temperature and/or salinity for diagnosing MLD. This has nothing related with a scientific choice. Also if you rely on temperature only you must face the BL problem that is more extended than compensated layers, and about which you must talk somewhere.

L. 271-272 : This is not convincing me. For me it is the temperature profile that is more complicate to fit with a sigmoid, as it can have many features (interleaving in high latitude, several inversions, fossil/remnant layers etc...), while the denisty profile do have a simple chape as the ocean is stable, so light waters are always above heavy ones, and the density profile is the one that have by default the shape of the sigmoid. If it is not the case for you, then you need to show precisely why this is not true and where. As I said before, I would expect that you do your method on density profiles also, so I really do not understand why it cannot work for those. You must discuss about this with clear evidences of the fact that fitting T is easier than fitting density.

l. 282 : see Helber et al JGR2012, they study the startification below the MLD and they have fields of stratification below the MLD as I remember.

l. 283-284 : repetition of sentence, problem of edition to correct

Conclusion : it should be extended, especially talking more about the real new point of your article which, again, is not the MLd for me, but the thermocline (and hopefully pycnocline) characteristics that you estimate here.

To finish, you never show a map of the thermocline strength, while you diagnose it (as slope at the center of the sigmoid for exemple), why not ? I think this is a new interesting field/variable that must also be shown and discussed here as it gives the strength of the link between the ocean surface and interior, it would be a plus of your paper.

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