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Interactive comment on "U-Th-Pb discordia regression" *by* Pieter Vermeesch

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I would like to thank Dr. Samperton for his positive review. Most of his comments are easy to address apart from one remark about the $^{238}U/^{235}U$-ratio, which prompted me to confront a bigger issue that I had avoided in the original manuscript.

> Page 1, Lines 3-4: "The $^{206}Pb/^{238}U$ and $^{207}Pb/^{235}U$ decay systems are routinely combined to improve accuracy". May be more appropriate to have something along the lines of "...are routinely combined to improve the assessment of accuracy"?

It is true that, in many geological applications, the ^{238}Pb–^{206}Pb and ^{235}Pb–^{207}Pb clocks are simply plotted together to assess concordance, after which a simple weighted mean $^{206}Pb/^{238}U$ age is calculated. However, Ludwig (1998) showed that the clocks can

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also be combined to estimate a hybrid (concordia or isochron) age, which in theory is more accurate than either the $^{206}Pb/^{238}U$ or $^{207}Pb/^{235}U$ age. The aim of the U-Th-Pb isochron paper is to explore this application further but including the $^{208}Pb/^{232}Th$ clock as well. So in this case I maintain that "improving acccuracy" is a more appropriate term than "improving the assessment of accuracy".

> Page 1, Lines 28-31: "Nevertheless, it manages to fit the data very well. The method should work even better for low-Th phases such as carbonates." These sentences are far too subjective and informal, please rewrite.

I will add two new datasets to the paper, including a carbonate example (Parrish et al., 2018) and an allanite example (Janots and Rubatto, 2014). By comparing conventional common-Pb corrections for these data with the new Total-Pb/U-Th algorithm, the improvement in precision and accuracy will be much clearer to the reader. See Figures 1 and 2 of this response letter for further details.

> Technically, the proportions are a function of the Th/U-ratio, age, AND the $^{238}U/^{235}U$ ratio. Here and later in the manuscript the author assumes the mean terrestrial zircon $^{238}U/^{235}U$ value (137.818, without uncertainty) of Hiess et al. (2012). While for many (most?) applications of the algorithm this assumption is possibly acceptable, insofar as broadening the general applicability of this approach I think it is worth stating this point explicitly.

The reviewer is correct that the $^{238}U/^{235}U$ ratio affects the $^{207}Pb/^{206}Pb$ ratio. However as long as all the analyses are cogenetic (which is a requirement for isochron regression), departure of the $^{238}U/^{235}U$ ratio from the Hiess et al. (2012) values actually does not hurt the accuracy of the isochron age. This is because, in Equation 12 of the original manuscript, $^{238}U/^{235}U$ is multiplied with the common-Pb ratio β. So as long as

$^{238}U/^{235}U$ and β do not vary between aliquots, an overestimation of one translates into an underestimation of the other without affecting t.

So the uncertainty of the $^{238}U/^{235}U$ ratio (U in Equation 12) only matters for the error propagation of β. It is not easy to address this issue with the maximum likelihood formulation of the original manuscript, in which U occurs in a product with γ. If the uncertainty of U is to be propagated, it is no longer possible to reformulate the sum of squares S in terms of the Th/Pb misfit parameter M (Equation 23). Similarly, the analytical uncertainty of the measured $^{232}Th/^{238}U$ ratio (W in Equations 12-14) is also difficult to propagate.

The solution to both of these problems is straightforward in theory, but complicated in practice. Recalling the general equation for the sum-of-squares (Equation 11 of the original manuscript):

$$S = \Delta^T \left(J^T \Sigma J\right)^{-1} \Delta$$

we can replace Equations 12 (for J) and 13 (for Σ) with

$$\Sigma = \begin{bmatrix} s[X]^2 & s[X,Y] & s[X,Z] & s[X,W] & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} \\ s[Y,X] & s[Y]^2 & s[Y,Z] & s[Y,W] & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} \\ s[Z,X] & s[Z,Y] & s[Z]^2 & s[Z,W] & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} \\ s[W,X] & s[W,Y] & s[W,Z] & s[W]^2 & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} & 0_{n\times1} \\ 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & s[\lambda_{35}]^2 & 0 & 0 & 0 \\ 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0 & s[\lambda_{38}]^2 & 0 & 0 \\ 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0 & 0 & s[\lambda_{32}]^2 & 0 \\ 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0_{1\times n} & 0 & 0 & 0 & s[U]^2 \end{bmatrix}$$

and

$$J = \begin{bmatrix} 1_{n,n} & 0_{n\times n} & 0_{n\times n} \\ 0_{n\times n} & 1_{n\times n} & 0_{n\times n} \\ 0_{n\times n} & 0_{n\times n} & 1_{n\times n} \\ -U\beta\gamma & -\alpha\gamma & 0_{n\times n} \\ -t_{1\times n}e^{\lambda_{35}t} & 0_{1\times n} & 0_{1\times n} \\ 0_{1\times n} & -t_{1\times n}e^{\lambda_{38}t} & 0_{1\times n} \\ 0_{1\times n} & 0_{1\times n} & -t_{1\times n}e^{\lambda_{32}t} \\ -\beta W\gamma & 0_{1\times n} & 0_{1\times n} \end{bmatrix}$$

respectively. Unfortunately, taking matrix derivatives of S is difficult to do by hand for this generalised formulation. In well behaved cases, R's optimisation function manages to calculate them numerically. But the numerical stability of these solutions is significantly poorer than that of the original algorithm.

An additional advantage of the new formulation is its ability to accommodate a second type of overdispersion model. Section 5 of the original manuscript parameterised the overdispersion in terms of the concordia intercept age. With the generalised formulation of the maximum likelihood problem, it is also possible to attribute the excess dispersion to the common Pb composition. In this case we replace Equation 44 of the original manuscript with the following alternative:

$$J_\omega = \begin{bmatrix} -UW\gamma \\ -W\gamma \\ 0_{n\times n} \end{bmatrix}$$

Again, the numerical stability of this formulation is not as good as that of the original algorithm. If I find a way to increase this stability, then I will use the new algorithm. Otherwise I will stick with the original version and be more clear about its limitations.

throughout the manuscript a quantitative blank correction is not addressed, which is fine, but if so a statement should be made here that the equations as currently formulated assume a trivial Pb blank component.

I will add a line to clarify that the data are assumed to have been blank corrected.

Couldn't you pull a representative carbonates dataset to demonstrate this point explicitly? I'd be interested to see this.

A carbonate example will be added to the revised manuscript. See Figure 1 of this response letter.

You mention in passing that data are "overdispersed if... MSWD $\gg$1". However, I think it worth stating a more general point about the acceptable MSWD range as a function of the number of degrees of freedom (i.e., data points), a la Wendt and Carl (1991). I think it worth citing Wendt and Carl (1991) here, as well as presenting a general formula for the range/uncertainty on the MSWD itself, beyond stating the oversimplification that data are overdispersed when MSWDÂż1.

I will add a reference to Wendt and Carl (1991). However it is also important not to overly rely on MSWDs and p-values. It is possible for a precise dataset with an MSWD value of 100 to be more valuable than an imprecise dataset with an MSWD of 1. What matters is not so much whether a dataset is overdispersed or not, but rather *how* dispersed it is. This key point is addressed in Section 5 of the paper.

You should cite R for those not in the know

I will add the requested citation.

References

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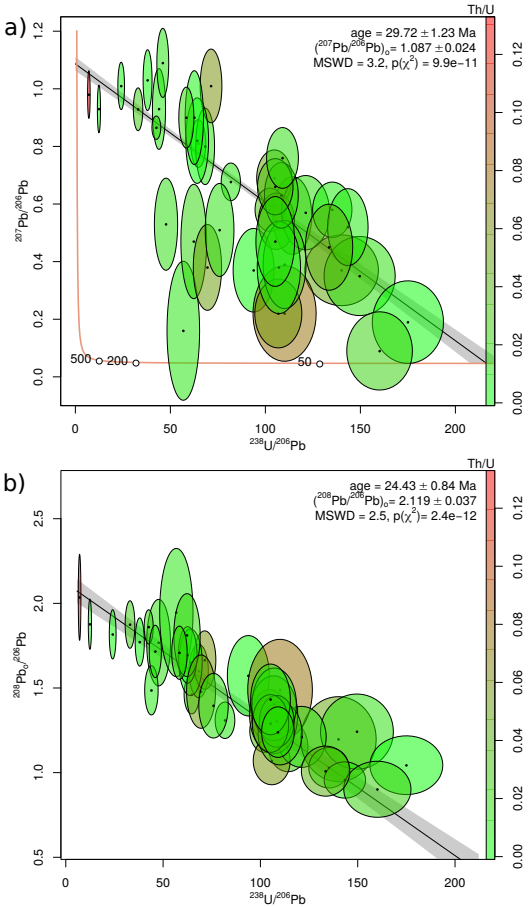

Fig. 1. a) SemiTotal-Pb/U isochron (conventional 207Pb-based common Pb correction) for Parrish et al. (2018)'s chalk data; b) Total-Pb/U-Th isochron (new 208Pb-based common Pb correction).

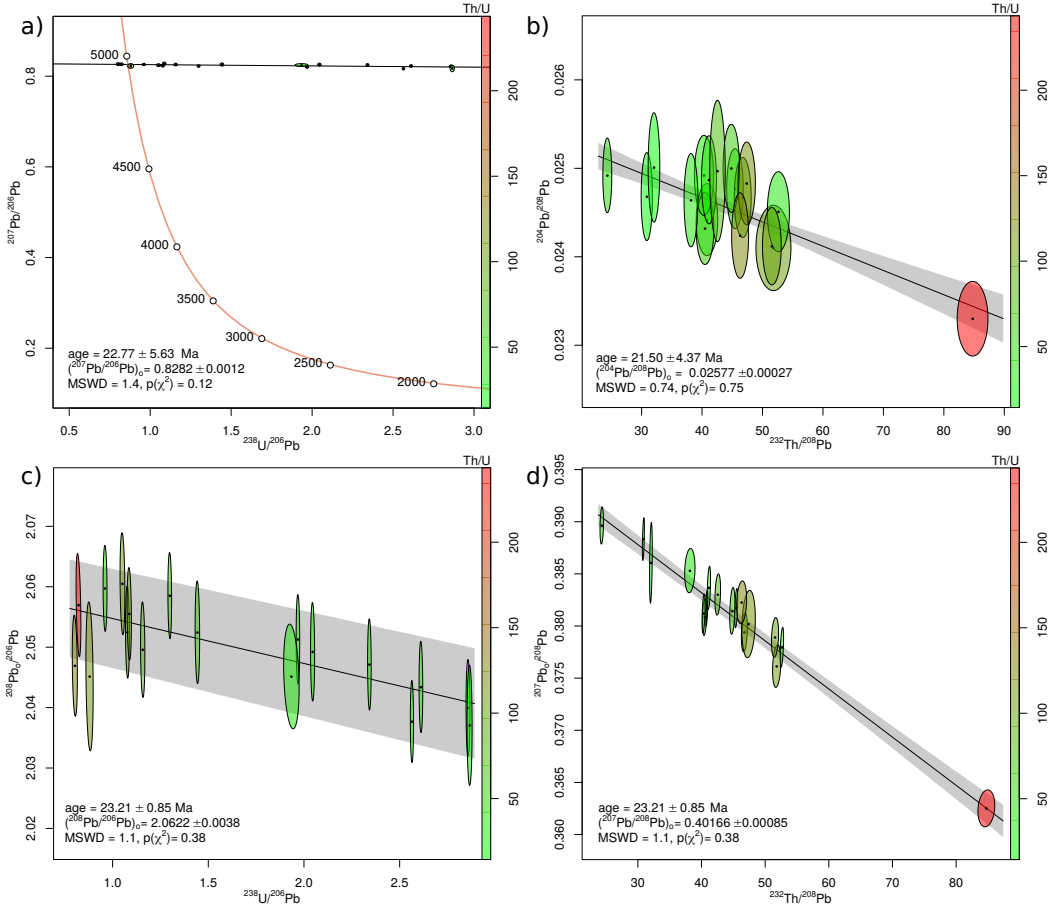

Fig. 2. a) Conventional SemiTotal-Pb/U isochron for Janots and Rubatto (2014)'s allanite data; b) 204Pb based Pb/Th-isochron; c) and d) new Total-Pb/U-Th isochron.

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