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To: Roger Powell, University of Melbourne

Dear Professor Powell,

Thank you for submitting your manuscript entitled "Robust Isochron Calculation" to *Geochronology*. Having considered your paper, the four reviews and your response to the reviews, I have decided that your manuscript is suitable for publication in *Geochronology* after moderate to major revision. In addition to the reviewer comments, I would like to add a few thoughts of my own.

1. I agree with reviewers 3 and 4 that your paper needs to become accessible to a wider readership. I am concerned that there are only a handful of people in the geochronology community who will be able to understand the current version of your paper, or run your `Python` code. The impact of your work would greatly increase if you could explain your algorithm in plain English. Please note that I am not asking you to remove the mathematical details of the robust regression algorithm from your paper. In fact it is important that those details are retained. But much of this could be moved to the appendices.
   In your response to reviewer 4, you wrote that "Clearly it was a mistake to sweep as many of the equations as possible into the Appendix!". I disagree, and think that you could move even more content to the appendices, as long as you add enough links to them in the main text.
2. The algorithm in your paper is not the first to apply robust statistics to isochron regression. In fact, robust isochron regression is already implemented in Ken Ludwig's popular `Isoplot` add-in to `MS-Excel`. Unfortunately, the `Isoplot` user manual does not provide any details about this implementation. However, Ludwig (2003) does mention your earlier paper on the subject (Powell et al., 2002), and a personal communication from you. Does this mean that `Isoplot`'s robust regression algorithm is based on your bootstrap algorithm? I would love to read more about this in your paper. In any case, I think that you should discuss the merits and limitations of these competing algorithms in a revised version of your paper. A side-by-side comparison of the different algorithms on the same dataset would be particularly helpful.
3. In your response to reviewer 3, you wrote:

   > "the 95% confidence limit on the ages is 3.97 to 4.03 Ma with HUBER , but 3.91 to 4.09 Ma under YORK , a significant increase in reliability with HUBER."

   Precision is not the same as reliability! This brings me to an important point that was only briefly touched by the reviewers, but I think should be addressed in the revision. In your paper, you refer to isochrons that exhibit excess scatter (MSWD$\gg$1) as 'errorchrons'. Ludwig (2003) proposes five ways to deal with these. The first is to ignore the excess dispersion; the second is to inflate the errors by a factor of $\sqrt{\text{MSWD}}$; the third is to ignore the analytical uncertainties altogether; the fourth is to quantify the dispersion as a separate free parameter; and the fifth is robust regression. Your paper only mentions options 1, 2, 3 and 5. However I would argue that the fourth

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option ('model-3 regression') is the best way to deal with excess scatter (Vermeesch, 2018).

The great appeal of maximum likelihood estimation is that it provides clear tests for its underlying assumptions. No such tests are available for robust regression. On the surface, the ability of your algorithm to fit errorchrons may seem like a strength. But this robustness comes at a cost, in that is no longer possible to tell the difference between 'good' and 'bad' datasets. This creates a 'garbage in, garbage out' problem. Can you explain how to deal with this?

The 'errorchron' moniker is widely used in geochronology. But I think that its negative connotation is undeserved. A high precision TIMS errorchron can have greater scientific value than a low precision LA-ICP-MS isochron. What matters is not whether the data are overdispersed or not, but rather *how much* overdispersion there is. This is exactly what model-3 regression aims to achieve. In the case of isochrons, the excess scatter can either be attributed to the initial (non-radiogenic) isotope ratios, or to diachronous isotopic closure.

The dispersion has scientific value. For example, Rioux et al. (2012) estimated the dispersion of high precision TIMS U–Pb data to estimate the residence time of zircon in a magma chamber. A robust algorithm would have completely missed this information. As technology improves, overdispersed datasets will become ever more prevalent. For example, new noble gas mass spectrometers achieve an order of magnitude improvement in $^{40}Ar/^{39}Ar$ age precision. This has revealed that even the best reference materials are not homogeneous (Heizler, 2012). So in my opinion, geochronologists might want to abandon the 'cult of MSWD' and embrace dispersion rather than banish it.

I am not asking you to provide a comprehensive overview of model-3 regression in your paper. But I do think that it is important that the revised manuscript (a) addresses the 'garbage in, garbage out' problem, and (b) warns the users that any scientifically valuable dispersion will be lost.

4. Please rewrite and extend your abstract. The late Albert Tarantola once pointed me to the following text, which I found very useful:
   `https://www.caam.rice.edu/~symes/CAAM600/abstract_scrutiny.pdf`

Geochronology normally gives authors four weeks to complete the revision. But I would be happy to extend this to eight weeks if you need it. Please do not hesitate to contact me if you have any questions.

Sincerely yours,

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*References

Heizler, M. Higher Precision: Opening A New ^{40}Ar/^{39}Ar Can Of Worms. In *AGU Fall Meeting Abstracts*, 2012.

Ludwig, K. R. Mathematical–statistical treatment of data and errors for ^{230}Th/U geochronology. *Reviews in Mineralogy and Geochemistry*, 52(1):631–656, 2003.

Powell, R., Hergt, J., and Woodhead, J. Improving isochron calculations with robust statistics and the bootstrap. *Chemical Geology*, 185(3-4):191–204, 2002.

Rioux, M., Lissenberg, C. J., McLean, N. M., Bowring, S. A., MacLeod, C. J., Hellebrand, E., and Shimizu, N. Protracted timescales of lower crustal growth at the fast-spreading East Pacific Rise. *Nature Geoscience*, 5(4):275–278, 2012.

Vermeesch, P. `IsoplotR`: a free and open toolbox for geochronology. *Geoscience Frontiers*, 9:1479–1493, 2018.