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Discussions

Interactive comment on "The long-solved problem of the best-fit straight line: Application to isotopic mixing lines" *by* Richard Wehr and Scott R . Saleska

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This is the Authors' Response to Anonymous Referee #1 (hereafter "AR1"), by R. Wehr and S. R. Saleska (hereafter "WS").

AR1: The manuscript by Wehr and Saleska re-introduces a non-linear iterative method to determine slope and intercepts of mixing line relationships. Isotopic mixing line relationships have been analyzed in previous studies (notably Zobitz et al. 2006 and Kayler et al. 2010). The current study expands on the previous two by introducing a "long-solved" method. Overall the paper is well written and readable. A strength of the manuscript is that it very acutely emphasizes the disconnect between the geoscience and environmental science - and arguably the mathematical science - communities.

Technical advances in one area don't seem to percolate over the the other area (as highlighted in the second paragraph of the introduction). Illuminating this tension between translatability across disciplines is a strength of the paper.

WS: We thank the referee for these supportive comments, and for taking the time to review our manuscript.

AR1: There are few weaknesses to the paper which could be addressed by revision.

WS: We appreciate the referee's suggestions and will incorporate them into our revised manuscript as described below.

AR1: First, there is a lack of recognition of the importance of OLS and other regression methods. OLS, GMR, ODR, as well as Maximum Likelihood Estimation are essentially a linear problem and are amenable to several different approaches in mathematics - OLS is a topic in a Calculus sequence. The York method, best I can tell, is a non-linear iterative method - which perhaps may contribute to its unfamiliarity across disciplines.

WS: We agree on "the importance of OLS and other regression methods", and had intended that the manuscript acknowledge their wide use while making clear that their overuse (in cases where their assumptions do not apply) is an explicit motivation for the paper. Regarding the contrast between methods, yes, the general LSE solution for the slope and intercept cannot be written analytically, and so York's method finds it numerically, by iteration. The OLS, GMR, and ODR slopes and intercepts are special cases of the general LSE solution that can be solved for analytically. We can mention this distinction in our revised manuscript.

AR1: Second, I also think some more careful tracking of the timing of the key studies cited is important. Zobitz et al 2006 was written in response to previous studies by Pataki et al 2003. Kayler et al 2010 addressed minimizing bias for large CO2 ranges - and addressed some of the issues raised in the previous two studies. A consistent finding both in Zobitz et al 2006 and Kayler et al 2010 is that OLS is appropriate for sufficiently large CO_2 ranges and is highly biased at low CO_2 ranges. Given that, the authors of the current manuscript don't present a pressing need to move away from OLS in favor of a more complicated linear fitting method. What is the current state of the art in the measurement method? How imperative to determine mixing line parameters with samples of low CO_2 ranges? Addressing some of the importance and need of this method will help increases its applicability, and the tradeoff for using a relatively more complex fitting routine than what is provided on all statistical software programs (R, SAS, etc).

WS: We like the referee's suggestion to add mention of the timing/context/motivation of the cited studies, and we will do so in our revised manuscript. Zobitz et al 2006 actually reported that OLS was negligibly biased for all measurement conditions (but the random error increased at low CO_2 ranges). On the other hand, Kayler et al 2010 reported that the OLS Keeling plot intercept was negligibly biased (i.e. by less than about 0.1 permil) for CO_2 ranges above roughly 50 ppm but non-negligibly biased for CO_2 ranges below roughly 10 ppm. The particular numbers depend on the measurement precisions (as illustrated by our tables); however, in Kayler et al 2010, various precision scenarios seem to have been amalgamated in their Table 1, so that for a given set of measurement precisions, it is not clear whether non-negligible OLS bias emerges at a CO_2 range of 100 ppm or 10 ppm. That is an important issue because Keeling plots with CO_2 ranges below 50 ppm are not unusual – indeed the real data example that we will include in our revised manuscript (see below) involves hundreds of Keeling plots made from nighttime air sampling in a forest, and most of those Keeling plots have a CO_2 range below 50 ppm (for quite a few, the range is even below 25 ppm). So prior to the present manuscript, it was unclear whether it was acceptable to use OLS under some fairly common conditions. Moreover, the primary conclusion of Kayler et al 2010 was actually that GMR is better than OLS for very high CO_2 ranges such as might be encountered in soil measurements ("The combination of geometric mean regression and the Miller–Tans mixing model provided the most accurate and precise estimate of $d13C_R$ when the range of CO_2 is >1,000 umol mol-1."). The main goal of our paper

is to inform readers that there is a single general fit method (York's) that is best in all measurement scenarios, so that they do not need to make a choice among imperfect methods or to switch between those methods depending on the conditions. We will add a paragraph to the introduction clarifying the above points, thereby adding motivation for the use of York's method.

Having said all that, we recognize that OLS is more accessible and familiar to researchers, and we do not argue that researchers must abandon OLS. Indeed, a second goal of our paper is to accurately detail the range of conditions in which OLS can safely be used to approximate the York solution (hence the tables with biases under various conditions). It turns out that under most practical conditions, OLS is an acceptable approximation to the York solution, while under some conditions, it is not. We will clarify this point in the Results and discussion section. When in doubt, researchers will now have a general method that they can use without risking introducing bias.

More broadly, the isotopic mixing line is being used here as a practical example to illustrate the York method, which might prove even more valuable to other applications, quite apart from our own line of research. We would like to add a paragraph briefly presenting a separate potential application of York's solution, which is quite common across disciplines: the comparison of measurements of the same quantity by two different instruments that differ in their precisions (such as when replacing an old instrument with a new one).

AR1: Third, the results of this paper relied on subsampling of simulated data, which does limit the applicability of their results. I suggest the authors provide a case study of non-simulated data, comparing the two York method to OLS, GMR, ODR etc. Simulations are great for emphasizing the theoretical underpinnings of a method, however the addition of real measured data would enhance the applicability and impact of the simulation results.

WS: As mentioned above, we have a real data set that we will add to the manuscript:

precise (0.05 permil and 0.02 ppm) nighttime air sampling on the tower at the Harvard Forest Environmental Measurements Site. Given that our simulated data results show the York method to be unbiased, we can suppose that the bias in GMR (or OLS) is given by the difference between the GMR (or OLS) intercept and the York intercept. The 429 nights in our dataset (with one Keeling plot per night) allow us to clearly see the dependence of the biases on the CO2 range – and by adding additional noise to the real data, we also get an indication of the dependence of the bias on the instrument precision. We find that OLS is a very good approximation to the York solution for our particular instrument precision, while GMR is a poor one. With noise levels typical of lower-cost instruments, we find that even OLS becomes a poor approximation for CO2 ranges less than 10 ppm, in agreement with our simulated data results. These results using real data are shown in the figure attached to this response; the grey area in the figure is the area in which bias would be negligible for practical purposes (i.e. < 0.1 permil).

AR1: P1 L21: "Much of it was outdated before it was written" is a very vague sentence.

WS: Taken in isolation, it is vague, but this sentence is the deliberately suspenseful setup for the two sentences that follow, which make the point that the solution sought by the literature in question was already known in 1969. In context, we feel that the sentence is not vague, and that it adds to the readability of the manuscript.

P1 L26: Point made that York's solution is unknown, but impact is not an indication of quality - I think it just got dwarfed, highlights the need for interdisciplinary collaboration.

WS: We are glad that the referee agrees with us on this motivational point.

AR1: P2 L9: Delete "but the debate is immaterial" This is a general sentence that is unprovable and opinion.

WS: We meant to convey the idea that when a convenient, general solution is available, it is not necessary to choose among special-case solutions. But perhaps we do not

need to make that point here, and so we will delete this phrase.

AR1: P3 L1: Please clarify if the Hirsch and Gilroy citation applies to all the quoted phrases in this sentence or only one (clarify)

WS: We will clarify by writing: "Adding confusion to the literature is the fact that OLS, ODR, and GMR are each known by other names (York, 1966; Hirsch and Gilroy, 1984): OLS is called. . .".

AR1: P4 L27: Given the fact you need an initial guess slope, is the convergence of the method sensitive to the initial guess value, or does it converge globally?

WS: The method will require more iterations to converge to the desired accuracy level when the initial guess is poorer, but the value of the initial guess has little impact on the convergence speed unless the guess is extreme. As stated in the manuscript, "This guess can be very rough and still sufficient. . . If desired, a good initial guess slope can be obtained from an OLS fit".

AR1: P7 L24: "For CO2 ranges less than 50 ppm . . ." This sentence reads very awkwardly and to follow the logic.. Please rephrase

WS: We can rephrase the sentence thusly: "For CO2 ranges less than 50 ppm, the GMR bias is non-negligible (> 0.1 ‰) unless the measurement uncertainty in δ is extraordinarily low ($\leq$ 0.01 ‰)."

AR1: P8 L22: Now I am confused. Does the York method give an exact solution (as in OLS, GMR) or is it a nonlinear iterative method as described on page 4?

WS: We see that the meaning of 'exact' was unclear. York's general LSE solution is exact in that no approximation is involved in its derivation, unlike the preceding approach of Deming (1943), which dropped terms from a Taylor expansion. As mentioned above, York's solution is also a numerical, iterative solution, in contrast to the special-case LSE solutions (OLS, ODR, and GMR), which can be written analytically (i.e. in closed form). In practice, there is no difference in exactitude between the numerical approach of York and the analytical approach of OLS, ODR, and GMR; all are limited only by machine precision. This will be clarified in the revision.

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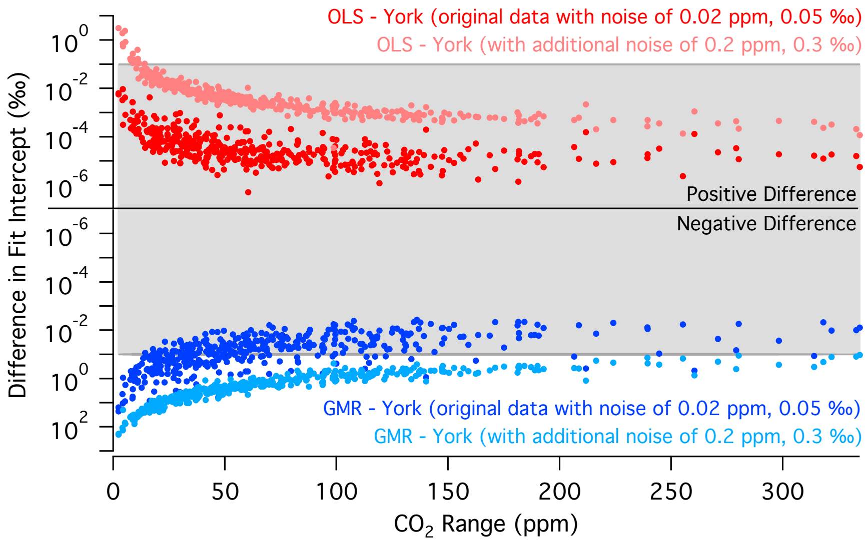

Fig. 1.