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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

Anonymous Referee #1

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General Comments 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.

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Discussion paper

Specific Comments There are few weaknesses to the paper which could be addressed by revision.

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.

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 CO2 ranges and is highly biased at low CO2 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 CO2 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).

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.

Technical corrections (P = page, L = line)

P1 L21: “Much of it was outdated before it was written” is a very vague sentence.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

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

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

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?

P4 L24: “For CO2 ranges less than 50 ppm . . .” This sentence reads very awkwardly and to follow the logic.. Please rephrase

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?

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