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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

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This is the authors' Response to Referee John Miller (hereafter "JM"), by R. Wehr and S. R. Saleska (hereafter "WS").

JM: Congratulations on writing a terrific paper: well researched, well written and very much needed. I have just a few questions and comments.

WS: We thank the referee for his compliments and for taking the time to review our paper.

JM: How can we, or should we, consider variability in CO2 and $\delta$13C arising not from instrumental noise but from the environment? As pointed out in Miller and Tans, in



some real- world situations, assignment of analytical uncertainties to CO2 and $\delta$13C may result in poor goodness of fit, i.e. a large value of reduced-chi square, suggesting that analytical CO2 and $\delta$13C uncertainties are too small. This is of course important because small CO2 and $\delta$13C uncertainties will lead to too small slope and intercept uncertainties. Note that while not so common now, as analytical precision improves, instances where natural variability significantly exceeds instrumental precision will need to be dealt with more. In MT2003, we attempted to deal with this by starting with an initial estimate of the best fit line, although we used a GMR instead of fitexy (for speed, and because we only knew the analytical uncertainties). We then proceeded to scale the standard deviations of the x and y residuals to produce a reduced chi-square value of 1; finally fitexy was used to calculate the slope and intercept uncertainties. Nonetheless, a problem persists, which is that the slope of the best fit line depends on the initially assigned x and y uncertainties. I'm very interested to hear your ideas of how to address this. (Maybe I'm missing something obvious, like using an OLR regression as a starting point.)

WS: As you know, York's method deals with the situation in which there is a linear relationship between the true values of X and Y (i.e. of CO2 and d13C) but those values are measured with error. Natural variability may sometimes be describable as measurement error; that is, as a stochastic process that intervenes between the quantity of interest and the measurement of that quantity. For example, the eddy covariance method uses a single-point measurement to estimate the gas flux through a large 2D plane overlying an ecosystem, and most of the noise in the estimation comes not from the instrumental measurement uncertainty but from the natural (turbulence-driven) variability in the flux past that single point relative to the flux through the whole 2D plane. If the natural variability in X and the natural variability in Y are describable as measurement error and can be characterized independently (along with any correlation between them), then York's method can be applied and is likely to be very useful.

On the other hand, it is often the case that the natural variability is not well character-

ized, or that it is not well described as additional measurement error. In this case, we argue that one cannot proceed to determine the best-fit line, or even to define what "best-fit" means. In general, one can view natural variability as variation in the true X-Y relationship due to the influence of other factors that are not controlled for. So a Keeling plot with natural variability is like many true mixing lines all superimposed on the same plot (one line for each set of influencing factors). It is therefore pertinent to consider which true line one is looking for. To define that line is, in effect, to characterize the natural variability in X and Y.

If one is interested not in the X-Y relationship per se (i.e. not in an intercept or slope), but simply in predicting the most likely value of Y given X for the particular data that were sampled and put on the plot, then OLS is the proper fit to use. If differences among the various fit methods are not large enough to matter to the scientific question being posed, then OLS is again a sensible choice, owing to its simplicity.

If it would be helpful for context, we would be happy to include a brief discussion of the above points in the manuscript.

Regarding the approach you mention from MT2003, it seems that the slope you end up with must depend on your arbitrary choice of how to apportion the variability into X and Y. That seems to be what you are saying when you say that "the slope of the best fit line depends on the initially assigned x and y uncertainties". Any meaningful approach will require independent information on how to apportion the natural variability between X and Y.

JM: P4 l8. Note for future reference that the Keeling plot equation is valid not just for a single source (or sink), but delta_s can be interpreted as a the flux- weighted source (sink) signature.

WS: That is a good point. We will remove the word "single" from this sentence.

JM: Eq. 3. The derivation of this was not obvious. It's not critical to the argument, but



since you have an appendix, can you add this?

WS: Yes, we will be happy to add the derivation of Eq. 3. It consists merely of writing the definition of the correlation coefficient in terms of the covariance, and then the definition of the covariance in terms of means and expectations, and so it is probably short enough to be included in the main text.

JM: P7 l5. I am surprised by (and skeptical of) an instrument with 0.01 ppm and 0.01 per mil uncertainty. Can you provide a reference in the literature for this, especially since this is characterized as 'common instrumentation'?

WS: The 0.01 ppm and 0.01 permil uncertainties are attributed to "the best existing laser spectrometer" rather than common instrumentation, but we recognize that this point is confusing because of the placement of the phrase "including some corresponding to common instrumentation" (which was meant to apply to the whole list). We will move that phrase to avoid the confusion. The spectrometer referred to has a precision of 0.016 ppm and 0.02 permil under optimal conditions, and we will add its citation (Wehr et al, 2013, Agricultural and Forest Meteorology, 181,69–84). We will also clarify that 0.01 and 0.01 are slightly better than said spectrometer (we chose to round down to 0.01 because our aim was to bracket the range of conditions that researchers are likely to encounter, and spectrometer precision is likely to continue to improve).

JM: P7l8. Change 'latter' to 'last'.

WS: Ok, we will make this change.

JM: P7l34 and Table 2. I'm confused as to why CO2 ranges from 100 to 5000 are relevant and why CO2 uncertainties greater than 1 are relevant. I understand that soil chambers could give such high CO2 enhancements, but as seen from the table, uncertainties become very small. Perhaps you could add a column of 100 ppm in Table 1 and then summarize the rest of the Table2 results in the text.

WS: We included those ranges and uncertainties for comparison to Kayler et al 2010,

where it is argued that high CO2 values are often accompanied by high uncertainties. We agree that the 5000 ppm column is unnecessary, but for the highest CO2 uncertainty (20 ppm), there are non-negligible biases even for a CO2 range of 1000 ppm. We can condense the table substantially by eliminating the 5000 ppm column and then putting the Keeling and Miller/Tans results side by side rather than on top of one another.

JM: P8. L1. Why are the MT results a bit better at these high values? Or maybe better to say, why are the KP biases occasionally significant?

WS: This question is the subject of the following paragraph in the manuscript (beginning on P8 L4).

JM: P8l29. Factor of 2 seems a bit too generous. The biggest offset from Monte Carlo I see is 0.67.

WS: We can say that "the agreement is nonetheless within 33%."

JM: P8l35. What are the 'adjusted data points'?

WS: The adjusted data points are the fit method's estimation of the 'true' data points that were measured with error in order to produce the measured data points. We will add this explanation to the manuscript.

JM: P9.l7 Isn't G simply reduced chi-square? If so, why introduce a new term for this?

WS: G is the weighted reduced chi-square. In our revised manuscript, we will state that this is the goodness of fit metric being used, and we will use the variable chi-square in place of G.

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