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Atmospheric Chemistry and Physics Discussions

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Interactive Comment

Interactive comment on "Technical Note: Review of methods for linear least-squares fitting of data and application to atmospheric chemistry problems" *by* C. A. Cantrell

C. A. Cantrell

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"Technical Note: Review of methods for linear least squares fitting of data and application to atmospheric chemistry problems" by C. A. Cantrell

Reviewer #1 The review suggests applying statistical tests (t-test, F-test) to show statistical significance of the fitted slope and intercept for the analysis in Figure 3. While these tests could be performed, it appears the reviewer missed the point. Because of the way the data were constructed, it is known that there is a linear relationship between x and y. This is true even when r2 is far from unity. The easily calculated r2 values were simply used in this case as an indicator of when standard least squares might be expected to fail. The r2 values are not being used to test for linearity between x and y. This statistic only tells us something about the fitted residuals for standard least-squares. It doesn't and is not expected to tell us anything about the statistics of the bivariate fits. Press et al.(p 630) state "...r is a rather poor statistic for deciding whether an observed correlation is statistically significant, and/or whether one observed correlation is significantly stronger than another." That said, the F statistic on the standard least squares fits shows that almost all of them are significant at the 95% confidence level (except for those with the three lowest r values). I have added some text in the discussion of Figure 3 to clarify this. The question of weights is an important one, and perhaps not covered as fully as it could be in this manuscript. I do have a demonstration on page 17 that shows that the fit parameters are not as sensitive to the weights as one might think. In that discussion, you'll note that a constant plus a percentage value was used to calculate the uncertainties (corresponding to baseline noise and signal noise). There is no guidance in the literature for the best method in selecting weights. It is up to the researcher to determine the uncertainties in their measurements. My experience has been that reasonable estimates of uncertainties will give good fits and that errors in these estimates are not catastrophic. I have added some text in the introduction of weights (pg 5), and in the discussion on page 17. The issues of "underweighting" high values using the inverse of the variance as the weight is a common misconception. Indeed the wi values are much smaller at high variable values, if the variance is determined as a fraction of the value (as in the discussion on page 17), but the formulas call for the wi values to be multiplied by the x and y values, somewhat normalizing this impact. This has the effect of weighting data the highest at values several times the detection limit (represented by the constant term) and gradually decreasing the weighting at higher values. Obviously, if the user is concerned about this, the data may be weighted in any fashion desired. Unity weights effectively weight the data proportional to their value. So, if the data span a range of 3 orders of magnitude, the higher values will be effectively weighted 3 orders of magnitude more than the lower ones. This is usually not desirable. I have added some text to the revised manuscript to help clarify this. The reviewer is correct in pointing out that the examples I have picked

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for demonstration of the application of bivariate least squares are somewhat complex and perhaps not easily interpreted (because of the multiple sources and sinks of these species and the potential for unknown processes), but the examples were picked because the correlation plots were noisy. For the suggested examples (j(O1D) or NO2), the measurements and the model will be in much better agreement, and there will be little difference between bivariate and standard least squares methods. The point is to show how the use of improper fitting procedures lead to incorrect slopes, rather than the interpretation of what the slopes mean. I prefer to leave the examples as they are.

Reviewer #2 I have dealt with the first comment about fitting when r values are small, above. The reviewer suggests adding and discussion the error estimates for the slope and intercept to the discussion of the sample formaldehyde and peroxy radical data fits. This is an excellent suggestion and has been done. A short paragraph discussing the implications of non-normal error distributions on calculation of slope and intercept error estimates has been added. A sentence discussing outlier elimination has been added. For completeness, the correlation coefficients for the formaldehyde and peroxy radical datasets have been added to the text.

Comments by T. Brauers First, I want to that Theo for the extended and useful comments on my paper. It is clear that he has thought about this topic quite a lot. In Point 1, it is suggested that a more thorough discussion of errors be included. It is stated that "weights must be based on statistical errors (precision) only, not on accuracy." I disagree with this statement. There is nothing in the derivation of the fitting procedure that limits what should be included in the weights. Better uncertainty estimates include all the sources of uncertainty. Thus, one should include the uncertainty in the calibration as well as all the other sources of uncertainty in the measurement to derive a realistic representation of the overall uncertainty of the observation. I also demonstrate in the paper that the fitted slopes do depend strongly on the selection of weights. In the second paragraph of Point 1, it is suggested that the error estimates of the slope and intercept be included, in agreement with Reviewer #2. These have been added to

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the text. In Point 2, the method of Press et al. (1992) called "maximum likelihood estimation" is summarized. I am quite familiar with this routine, and indeed it gives results identical to those of York et al. and Williamson et al. In the latest paper of York and colleagues (2004), there is a proof that the two methods are mathematically identical, including ability to calculate a goodness of fit parameter (see equation (6) in the revised manuscript). Thus, readers are welcome and encouraged to use the Press et al. routine or the other routines presented here. I have added some text and references to clarify this. In Point 3, the use of the Press et al routine, fitexy, is applied to the Pearson data. This demonstrates that fitexy does indeed perform well. It also shows the value of including other parameters (such as errors in the slope and intercept, and goodness of fit) in the table. I have modified Table 2 accordingly.

Comments by S. Beirle Dr. Beirle suggests adding a reference to "total least squares" and including the term "orthogonal regression" in the introduction. These have been done.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 6409, 2008.

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