Interactive comment on “Multi-annual changes of NO\textsubscript{x} emissions in megacity regions: nonlinear trend analysis of satellite measurement based estimates” by I. B. Konovalov et al.

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Received and published: 30 July 2010

Response to the comments of the anonymous referee No. 3

We thank the reviewer for the generally positive evaluation of our paper and useful comments. All the questions and comments are carefully addressed in the revised manuscript. Below we describe our point-to-point responses.

Comment: In Equation 5, the symbols are not explained, the difference between w and \(^{\wedge}\) w is not provided. Further, the summation starts at 1 and runs over the total number of neurons, whereas in the next page (p.10941, l.19) N could also be equal to zero. To my understanding, when N = 0 the trend is reduced to the linear one, correct?

In the revised manuscript, the notations in Eq. 5 are slightly changed to make them more consistent with other equations. Indeed, the case N=0 corresponds to a linear trend. Eq.5 is generalized for this case by means of “dummy” parameters which equal zero when N=0.

Comment: The errors \(\epsilon_i\) are assumed to satisfy the normal distribution. Could you specify what are the initial values assumed for these errors?

Unfortunately, we are not sure that we understood this question correctly. In fact we do not assume any initial (or other) values for these errors but these values are generated automatically using the standard routine “gasdev” provided in Numerical Recipes by Press et al. This routine generates random values from the Gaussian distribution. We made sure that uncertainty intervals obtained in our experiments do not depend on the starting value of the parameter of this routine. The corresponding remark is added to paper.

Comment: How the sampling is impacted by accounting for the uncertainty of the convolution scale \(s_c\) (p.10942, l.11-15)?

The assumed errors in the estimate of the convolution scale \(s_c\) are sampled completely independently from errors in \(x_e\), that is, no information passes between generators of these two kinds of errors.

Comment: Do you fit a parametric distribution to the sample of \(x_e\) obtained by the Monte Carlo method described in lines 9-17 of page 10942?

No, there is no need to fit a parametric distribution in our case, because the uncertainty intervals (corresponding to a chosen level of statistical significance) can be calculated directly from the samples of \(x_e\) obtained from the Monte-Carlo experiment. Specifically, given a set of samples of \(x_e\) generated in the Monte Carlo experiment, we find (by means of a simple iterative procedure) the interval which includes at least 68.3 percent of the samples \(x_e\).
Comment: The authors choose to work with a level of significance of 0.683. How would the results be impacted if a higher level of significance (0.90 or 0.95) is assumed?

We work with the level of significance of 0.683 because of the strong noise in input data. Even if this is a relatively low level of statistical significance, we believe that our results are meaningful. In fact any probabilistic estimation cannot give 100 percent of statistical significance, and in this sense, it can only help in approaching "the truth" rather than in obtaining it. We expect that our estimates can be considered by experts together with other relevant data (from, e.g., bottom-up emission inventories), while paying attention to their possible uncertainties. While confidence intervals evaluated in this study correspond roughly to one standard deviation of $x_e$, the uncertainty intervals at the 0.95 significance level would correspond to about two standard deviations of $x_e$. Accordingly, if the level of significance were 0.95, the uncertainty intervals would be about two times larger (this follows from the properties of the normal distribution, but we have checked it directly in our Monte-Carlo experiment). The nonlinearities revealed in the study are not significant at the 95 percent significance level. A corresponding remark is added in the revised manuscript.

Comment: The method for the evaluation of the statistical significance level for the non-linear trend is not easy to track. It is not clear to me when the non-linear trend differs in a statistically significant way from the linear one. I would say that if the values of the linear trend lie within the area defined by the 68.3 significance level applied on the non-linear trend values distribution, then the difference between linear and non-linear trends is not statistically significant. A short discussion on this very important definition should be included in the manuscript.

We use a different criterion: the nonlinearity is considered as statistically significant if there are at least two different periods such that the corresponding confidence intervals of the rates of inter-annual changes (shown in Figs. 6, 7 by green dashed lines) do not intersect. In other words, the trend of $NO_x$ emissions is nonlinear if there are statistically significant variations of the rate of emission changes, because the linear trend is characterized by a constant rate. For example, the rate of interannual changes of $NO_x$ emissions in Paris is $-1.1 (\pm 2.2)$ percent per year between 2001 and 2002 and $-7.3 (\pm 2.9)$ between 2007 and 2008. The corresponding confidence intervals $[-3.3; 1.1]$ and $[-10.1; -4.3]$ do not intersect. A corresponding discussion is included in the revised manuscript.

Comment: In page 10941, a way to determine the number of neurons $N$ is presented. To my understanding, neurons should be removed as long as the leave-one-out error remains constant or decreases, but not when it increases. If this is true, then please state it clearly in the manuscript. Further, a network with more weights might be prone to overfitting and one with less weights might be inadequate to model the trend function. How are you sure that over- or under-fitting does not occur in this case?

Normally, the leave-one-out error (validation error) first decreases as the number of neurons increases and then it increases (when the neural network becomes overfitted). However, as it was noted in the reviewed manuscript, “the differences between estimates obtained with different numbers of neurons are frequently too insignificant”, and so the leave-one-error does not provide a practical criterion for choosing $N$. We further specified that “we choose the smallest value of $N$ such that a corresponding nonlinear trend (if it is detected) is significantly different from a linear trend but is not significantly different from trends obtained with a larger numbers of neurons.” If the nonlinearity is statistically significant, then the network is probably not overfitted. Indeed, overfitting, by definition, means that a network reproduces the noise rather than some general functional relationships between the considered quantities, and the noisy variations cannot be statistically significant. Furthermore, while minimizing the number of neurons, we also minimize the risk of overfitting. On the other hand, we try to make sure that the network is not underfitted; that is why we try networks with different numbers of neurons.

Comment: I believe that the article would benefit from a schematic picture, including the different steps necessary in order to derive the trends. To avoid lengthening the
A schematic diagram illustrating different steps of our algorithm is provided in the revised manuscript (Fig. 5). We are not sure that a special technical supplement is really needed because the method is, in our opinion, already adequately presented in Section 3.2.2 (and we believe that the presentation is improved in the revised manuscript, thanks to the comments of the reviewers). As to the technical realization of the algorithm, it is entirely based on standard routines from the “Numerical recipes”.

Comment: Please explain what is the meaning of the uncertainty intervals shown on p. 10944, l.20-25, and Fig.9.

The uncertainty intervals reported on p. 10944 are the same as in Fig.7 of the reviewed manuscript. They were evaluated by means of the Monte-Carlo experiment discussed in Section 3.2.2. The uncertainty intervals shown in Fig. 9 are the standard deviation of the slope of a linear fit. This standard deviation is evaluated analytically in a standard way. This point is clarified in the revised manuscript.

Finally, the typos and misspells revealed by the Reviewer are corrected in the revised manuscript.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 10925, 2010.