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Atmospheric Chemistry and Physics Discussions



# *Interactive comment on* "Nonlinear relationships between atmospheric aerosol and its gaseous precursors: Analysis of long-term air quality monitoring data by means of neural networks" *by* I. B. Konovalov

**I. B. Konovalov**

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I would like to thank Prof. Jari Kaipio for his generally positive evaluation of my paper and useful critical comments.

My point-to-point response to critical comments is given below.

1. No doubt, the novelty of the method used in my study does not consist in the mere fact of using neural networks, but in the way of their using. While neural networks have been used very extensively in variety of researches and applications, I am really (and unfortunately) not aware of any studies where they have been successfully used with the purpose to derive some interpretable information on relationships between

observed variables, except my own previous study concerning relationships between ozone and its precursors. This point will be further clarified in the Introduction.

I agree that when the model is referred to as being the "black box", it is usually assumed that the parameters of that model have no clear physical meaning. And I do not pretend that my models are exceptional in that sense. It is important to note, however, that the fact that neural networks are black boxes is generally believed to impose rather strong limitations to possibilities of understanding and utilizing the information they learn. Let me cite, for example, the review of atmospheric applications of neural networks by Gardner and Dorling [Atmospheric Environment, 32, 2627-2636, 1998] (whom I, in fact, did not intend to criticize): "If the problem that the multilayer perceptron is applied to one of prediction, or classification, or the exact nature of the input-output relationships is not important, then the "black box" limitation is of no consequence. If the multilayer perceprton is being applied to problems where the desire is to increase the knowledge of a physical process, then the "black box" limitation will restrict the usefulness of the multilayer perceptron". They refer also to unsuccessful attempt of McCann [Forecasting Techniques, 7 525-534, 1992] to understand what the neural network has learnt after it has been trained to predict thunderstorms, who concludes that it is "practically impossible to understand the "black box". Accordingly, one of the main goals of my study was to try to overcome the black box limitation for the concrete situation, rather than to argue that the neural networks are improperly considered as being "black boxes". This issue will be also addressed in the Introduction in more detail.

2. I agree that the standard practice in neural network applications is to divide the data into three subsets: training, validation and testing subsets. On the other hand, I would like to note that the goals of applications of neural networks in my study are, obviously, rather exceptional from the point of view of the standard practice. Generally speaking, if I want to use the standard tool in some non-standard way, would it be reasonable to use "blindly" the standard methodology of work with it? I would rather answer "no". In my opinion, it is more important that the methodology satisfies to the goals of the

concrete study, rather than to the general practice. To be more specific, the testing subset is usually used for assessing the quality of the neural networks from the point of view of their predictive capabilities. In my study, the use of testing subset would merely mean that the derivatives of interest are assessed under conditions which the neural networks have not "seen" before, on the training stage. In other words, the neural networks does not contain any information about those conditions, except that they will be able to extrapolate the relationships for those conditions. As a result, the evaluations of derivatives for those conditions will inevitably be much more uncertain than for conditions which the networks have already seen. The similar situation is with the validation subset, which is used in the training procedure in very indirect way (for "early stopping" of training). Indeed let us consider an imaginary simplified situation, when the neural network is trained with just two inputs, x and y, and it is desired to assess derivatives of the output, z, with respect to y at the given point (x1, y1). To do that, it is necessary first to estimate value of z1 in the reference point (x1,y1) and then value z2 at the close point (x1, y1+dy). The estimate of the derivative (z2-z1)/dy will incorporate uncertainties of estimations of both z1 and z2. There is a well know experimental fact that the neural networks perform better with the training subset than with validation or testing subsets. Accordingly, if the point (x1, y1) belongs to the training subset, the estimation of the derivative will be more accurate than if it does not (assuming, of course, that the accuracy of estimation of z2 will remain the same). Thus, it seems not surprising that I have found that the results for validation subset are more diverse than that for the training subset. The key point is how to insure that estimation of z2 will be reasonably accurate and, accordingly, the estimations of derivatives will not be spurious. The first action taken in my study in this direction is to employ the early stopping method. The second, and perhaps, more important action is to perform averaging of the outputs of the large ensemble of individually trained networks with different configurations and different initial guesses regarding values of weights. I would like to note that such averaging also is not performed in standard practice, and moreover, I strongly believe, that such averaging could provide the good quality of neural network models even without early stopping. These issues will also be discussed in more detail in the revised paper. Finally, I would like to emphasize that the plausibility of evaluations of derivatives is insured by the fact (which is emphasized in the paper too) that two models constructed with different databases collected in different environment exhibit a number of common essential features of the relationships between aerosol and its precursor. In my opinion, this fact provides a very good reason to believe that those common features reflect the real physical-chemical processes, rather than some drawbacks of the methodology.

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Interactive Comment