

Interactive comment on “Improved real-time bio-aerosol classification using Artificial Neural Networks” by Maciej Leśkiewicz et al.

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We would like to thank the Reviewer for evaluation of our manuscript. The detailed answers to the questions are as follows:

Reviewer #3

In this paper the authors present a method for bio-aerosol classification using labelled-laboratory data. The authors are correct in noting the need to improve and document such methods for improved bio-aerosol research. However before publication is considered, I feel the following points should be addressed. Presently it is unclear how anyone might replicate these results.

Minor points: The formatting of references is wrong? Please check with the Copernicus

guidelines and change from (xx)(xx) format to (xx;xx;xx...)

- The formatting of references was corrected.

There is a range of grammatical issues that need revising before publication. I have listed some below but would suggest the authors re-read the paper and change accordingly, removing any vague descriptions that require support with numerics or information to enable replication of experimental conditions. E.g: Line 76: 'This paper focuses on the application of ANN for real time discrimination of bio-aerosols basing on single particle fluorescence characteristics.' Please change 'basing' to 'based'

- Corrected

Line 108: 'The concentration of the aerosols was adjusted with vibration frequency of [the] vortex.'

- Corrected

Line 176: In order to determine whether it is time to stop teaching,. This is too informal. I would suggest rewriting in terms of the fitting process.

- In our opinion "teaching" process is appropriately used phrase and is widely applied in ANN related literature. We used "overfitting" in context of data not the learning process.

Specific Points: In table 2 the authors use the term 'own collection'. I'm a little concerned this does not provide enough information to enable replication of results. Where was the sample obtained? How old? Also the terms 'regular shop' and 'pharmacy' raise similar concerns. Which Pharmaceutical brand?

- The description and full information on the samples was added to the table 2.

Would it be possible to present size and shape information for each specie in a separate table?

- The missing data were added to the table 2.

Line 119: Please list the bands of fluorescence recorded. You have done so in Table 1 but you should reference this table in the text on this line to avoid confusion.

- The table has been referenced in the text just above.

Line 127: 'An Important aspect of the data acquisition process was monitoring the rate of generation of aerosol, which should be stable (not too high or spontaneous). 'Please define how this is quantified. What is 'too high'? How would this experiment be repeated?

- The BARDet's measurement window is 20us, but the data are integrated and recorded every 2 ms. It gives up to 100 averaged aerosol characteristics per 2 ms. It does not strongly influence the result if one aerosol type is measured, however, we tried to avoid such measurements. - The sentence in the manuscript was clarified (Lines: 335-337) as follows: "The data acquisition process started after stabilization of aerosol generation rate which was measured by the device. It was important to not exceed one particle per 2 ms of data integration time at 20 us measurement window."

Line 130: 'It is important to note that fact because of its statistical value for the further analysis'. What statistical value?

- The sentence was removed.

Section 3.2.1.2: What comparisons have been made, if any, between the bespoke implementation of the ANN in this work with what should be identical performance in existing software packages? How do we know the implementation of the bespoke ANN is correct? Please provide evidence.

- The presented ANNs were not compared to existing packages. We believe that our implementation of ANNs is correct since they produce correct results on approximated mathematical functions.

Major points: It is difficult to contextualise the input data being used. Please provide a visualization of some example spectra.

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- An exemplary characteristics were added as a figure 2.

To the best of the reviewers understanding, each particle will be classified at multiple levels of the decision tree. For example each particle will be classified as FM7, Rib, NT, LCB, or group 1 etc. and then should the particle be identified as group 1, the particle will then get classified again as UDP, PNP, group 4 etc.

- Yes. In practice separation is done not by one confusion matrix (ANN) but by all of them in sequence (22 ANN's combined in a decision tree). For example, if ANN classifies unknown substance into any of 22 groups it means that decision process is not ended but from that moment another ANN classifies this substance. That's why there are substances which only needs one ANN to make a classification (e.g. FM7), but there are also such which needs 6 ANN (e.g. BWF) to do that. Main difference between this two examples is that 98.5% of all FM7 particles are classified correctly but BWF has only 54.8% detected particles. However in both cases system recognize aerosol type every time with no mistake.

For example, should a particle from group 2 be misclassified and placed into group 1, which will happen about 12% of the time, how does this error propagate down the tree? Will it be evenly distributed amongst UDP, PNP, group 4 etc. or will it be heavily weighted towards one class?

- Error should be distributed according to confusion matrix of the group where particle is classified. There are 22 groups/ANN's/confusion matrices. In paper only 2 were presented as an examples.

With the exception of the level 0 ANN, I assume that each of the ANNs are trained only on a subsection of the data. This needs to be clarified. For example the ANN for group 1, is trained in absence of the data from group 2 etc.

- It is done exactly like that. - To clarify the text to the reader the following sentence in lines 504-516 was added: "In practice separation is done not by one confusion matrix

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(ANN) but by all of them in sequence (22 ANN's combined in a decision tree). For example, if ANN classifies unknown substance into any of 22 groups it means that decision process is not ended but from that moment another ANN classifies this substance. However, each new ANN is trained using only subsection of the data excluding the data from other groups.”

On line 245 it is stated that it is impossible to produce a single neural network to perform classification of all 48 classes. Need to be clear whether this means that it is impossible because of the number of classes, or that it is possible to create a single neural network but the classification error is unreasonably high.

- Our intention was to reporting that it is impossible to distinguish all substances using one ANN, not to create such single ANN. - In the manuscript it was as follows: “First attempts were made to distinguish all substances using only one neural network model. The tests revealed that it is impossible due to the huge number of samples (48 aerosols) and only a few of them presented significantly different fluorescence spectra.” - To clarify the text in lines 487-488 where additional explanation was added: “. . .that allow accurate characterization. The remaining substances are then misclassified. Therefore, we decided to use a. . .”

Would it be possible to produce a contour confusion matrix plot for the full 48 classes, for a single ANN and for the approach suggested in the manuscript, or to provide adjusted rand score or percentage of particles correctly classified to demonstrate whether better classification can be attained using the tree of ANNs as opposed to a single ANN?

- Such network and comparison has been made but authors decided not to present such single ANN, just mentioned about it in the text. Also presentation of 48 substances ANN would be hard to follow due to large number of data.

How was the decision tree created? I.e. how it was decided which individual classes would be placed into group 1 through 3?

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- The process of creation of decision tree was described in the manuscript as follows: "It was achieved after many trials of matching substances, which were not well separated, into new groups and checking if they are good enough on ROC graphs. Consequently, this procedure was also applied to those new groups." - New groups had been tested by creating for them new ANN's and checking by ROC graphs which one separates substances better. Many of them had been trained before the best ones were found. The Final ANN's were learned after dozens of trials.

The authors have indicated on line 203 that the hyper-parameters of the ANNs have been randomly selected until the desired/best result is reached. In terms of reproducibility, it would be helpful to specify the range of parameters which were tested and which of these options produced the best results. Also did each of the 22 networks utilise the same hyper parameters, or was this optimisation conducted for each of the 22 networks?

- It is impossible to reproduce learning process. Even if exactly the same parameters are chosen the learning process will generate each time different result according to randomly chosen initial weights. The range of parameters is typical for backpropagation algorithm and is well documented in the literature. Therefore, authors decided to perform random parameters procedure demonstrated in the paper.

There is no discussion on either data or software availability. The authors need to consider the default Copernicus publishing rules and provide text that would allow others to request access to both the data and software. If this is restricted, it should be stated with the reasons why. https://www.atmospheric-measurement-techniques.net/about/data_policy.html

- The following sentence was added in the manuscript "The experimental aerosol data can be provided upon request. The software for automatic data analysis cannot be commonly provided at this moment since it is a subject of negotiations with a company."