Reviewer’s report

Title: On the utilization of deep and ensemble learning to detect milk adulteration

Version: 0 Date: 02 Apr 2019

Reviewer: Joseph Romano

Reviewer's report:

The authors present a study describing the use of three machine learning models (RF, gradient boosting, and CNNs) for detecting adulterations in milk samples. The paper describes an important and interesting application of machine learning, and is valuable in the context of this journal. As a reviewer, I feel the paper is marred by several issues that should be resolved before the study is ready for publication.

Stylistic issues:

- Various areas in the text need to be edited for English grammar and style. Not only do these affect the ease of reading, but they sometimes seem to actually affect the meaning intended by the authors. One example (I can't list them all): "Machine learning classifiers have been applied successfully in most diverse applications, including..." In this example, the word 'most' makes this sentence incorrect and less impartial than it should be. It should probably use the word "many".

- Mixing of tenses cause some confusion. For example, sentence 1 of Methods is in present tense, while sentence 2 is in past tense.

Scientific critiques:

- In ML, we usually want to use the simplest model that will return adequate performance. Is there a reason why you didn't use simpler models in your evaluation? It seems that the component-level measures (which you use with the ensemble methods only) would be good input for linear or logistic regression models, so I would expect to see these evaluated as well. If you have specific reasons NOT to use these models, you should explain those in the text.

- Your definition of bagging is flawed - it is not necessarily constrained to decision trees.
- It is important to justify your rationale for selecting ensemble and deep models to use for this *specific* task. Why did you choose these models for detecting adulterated milk? "Because they have been successful for many tasks" unfortunately isn't sufficient. Certain models perform better on different tasks (and vice versa) based on characteristics of the data. You *do* briefly justify the use of CNNs for spectral data, but you should do the same for ensemble methods.

- You consider "adulterated vs unadulterated" and multiclass (specific adulterations), but what about multiple adulterations in a single sample? Does illicit adulterated milk often contain multiple adulterations? This isn't necessarily within the scope of this study, but it should at least be discussed.

- An interesting extension of this work would be a metaclassifier application, where you combine the predictions of the CNN and the RF or GB models, potentially achieving better accuracy.

Other critiques:

- Some parts of the paper (especially the Introduction) require more complete citations supporting the authors' claims.

- The figure captions would be better if you included a bit more detail. As one example, for Figure 6, you say it is t-tests over pairwise AUC differences, but what do the values represent? t-statistic? p-value? something else? It doesn't look like p-values. Basically, I'm not sure what information I should be focusing on when I look at some of the figures, and I sometimes have a tough time finding the "main point" they are trying to convey. If a figure summarizes results, it helps to include your interpretation of the results in the caption.

- "Starch" is a common synonym for amylose, but it can be used to describe many compounds and solutions from many sources. Was the starch you used pure amylose, or a food product like corn starch or potato starch? You should specify.

- Figure 2 is interesting, but maybe would be better off as a supplemental figure.

- Some of the material in Methods should probably moved to the Background section (e.g., the explanation of types of ensemble learning models, among others).

- Watch capitalization of ADAM (which is an acronym) in the description of the CNN model.
- Your discussion of future work can be expanded. Please see the previous comments for suggestions (e.g., building a metaclassifier, using samples with multiple adulterations, using real-world samples, if available from the Laboratory mentioned).

If these issues can be addressed I would look forward to reviewing the revised manuscript - it is an interesting study with clearly demonstrated significance and scientific merit.

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