Reviewer’s report

Title: A biplot correlation range for group-wise metabolite selection in mass spectrometry

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Reviewer: Jeff Xia

Reviewer's report:

In this manuscript, Park et al described a new method named BCR or biplot correlation range to address the limitations of FDR used in selection of significant biomarkers in metabolomics. Biplot is a very useful graphical approach for feature selection and data interpretation in chemoinformatics (and metabolomics). Further improvement on this presentation could potentially improve its performance & utility.

My concerns are mainly on the lack of detailed benchmarking and comparisons (with several different methods) to demonstrate convincingly the performance and improvements made by BCR. In particular, as BCR seems can "always" find more significant features, it is important to see how it deals with "overfit" (i.e. those identified features are false positives or not predictive). This can be achieved in cross validation in classification. Alternatively, authors can also create "null" data sets (i.e. no significant features) to show that BCR will not contribute to identification of those false patterns. BCR will not be considered "validated" without giving these baseline performance measures. This needs to be addressed in this manuscript, and cannot be in the "future directions" as mentioned in the end of the manuscript.

More specific comments:

1) In the abstract, last sentence "The results show that BCR provides means to identify metabolites contributing to class separation in a manner that can complement a statistical method by false discovery rate in complex data analysis for predictive health and personalized medicine."
   => I have difficulty understanding the exact contributions by BCR. The "complement" is too vague. Please be explicit on two points - what is the progress made, and how it is achieved

2) P12, L19 "These features, illustrated as filled circles in the solid ellipsoid, greatly contribute to the group label in a covariance (magnitude) sense. Since the selected features are treated equally as long as they are within the top 5% criterion, post-analysis such as ordering them by correlation, covariance, p-values, or variable importance projection (VIP) values will be possible"
   => It is critical for the authors to compare these with other common approaches (mentioned here) to show how similar or difference (i.e. how they are complementary as claimed)

3) BCR is "implemented MATLAB package is available from authors upon request."
   => This is actual a key contribution of this manuscript. To improve reproducible analysis and wide application of the method, I strongly urge the authors to make it publicly available (i.e put it to GitHub
with good documentation).

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