Comments on
Comparison of Multi-response prediction methods
JCHEMLAB_2019_163

General comments This paper reports results from a well-conceived simulation study of five prediction methods based on underlying linear models. The two envelope method are relatively new and, to my knowledge, have not been studied in the Chemometrics literature. I expect that all of the past work on envelopes is from a theoretical perspective and that this paper is the first to conduct a head-to-head comparison with other methods. Nor do I know of any studies that measure the effects of response correlations on the performance of any of the five methods. For these reasons I judge this paper to be timely, novel and likely of interest to many in the Chemometrics community and perhaps Statistics as well.

The paper made me wonder about comparative results in other simulation settings, and I expect other readers may have a similar reaction. After reflection, however, I caution against significantly expanding the study in this paper.

Page 4: Represented by "##" a the end of the page

Page 4, PLS In the paragraph on PLS, I suggest mentioning that the accompanying orthogonality and length constraints are key in producing the PLS solution. For instance, changing the inner product in the length constraint to be the same as that in the orthogonality constraint results in an entirely different solution.

Page 4: Below the first line of Envelopes

Page 4, Envelopes In the paragraph on PLS, please mention also that the response envelope must be a reducing subspace of $\Sigma_{y|x}$.

Page 20: Discussed in discussion

Page 5, line 7 Why 97.5%? If there is a clear rationale for this choice, please state it.

Page 7: Above the R-code

Page 6, Common parameters Were the informative and uninformative response and predictor components generated independently prior to rotation? Please state how they were generated.

Page 6: Some discussion on the maximum correlation we can obtain from using specific parameters in the simulation is discussed.

γ **and** η Please give some intuition on how the values of these parameters translate into high correlations or collinearity. For instance, what does the value 1.2 mean?

Page 11, lines 6-7 from the bottom The envelope objective functions are not convex and can occasionally get caught in a local optimum,

The text is the observation for the simulation results. In the case of real dataset, the outlier situation is not visible and we have discussed them on the example section.

resulting in "weird" output. This is not worrisome for hands-on data analysis, but can affect simulation studies that produce automated output. I expect that is the reason for the unexpected predictions mentioned on these lines.

Page 20: We have now pointed out this in the discussion

Impact of $p > n$ The methodology used to adapt envelopes to settings in which $p < n$ is in effect the same as that used by PLS: reduce by principal components, run the method, and then back transform to the original scale. The minor relative impact of p shown in Figure 7 suggests that this adaptation method is useful. I suggest that this be pointed out in the discussion of Figure 7.

Corrected.

Page 14, Error Model, line 3 . . . interaction of Method with "gamma"?

Page 20: Since we are not is position to conclude the statement with our simulation, we have removed it from the text.

Page 19, highlighted sentence It does seem possible that a single latent response component might have given a slight edge to simultaneous envelopes. But as state elsewhere in the paper, the Xenv method is the same as the Senv method when the number of response components is assumed to be 4. In view of the performance of Xenv, I doubt that changing the number of response components would matter much. Indeed, I am a bit surprised that Senv didn't do better with one component. I expect that a limiting factor here might be the number of responses, 4 in this case. To be clear, I'm not suggesting that additional simulation results be included, but it does seem appropriate to un-highlight the sentence.