On the interpretability of O-PLS filtered models

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INTRODUCTION

Orthogonal PLS, introduced originally by Trygg and Wold in 2002 [1], is a patented algorithm that has received much attention for its perceived ability to simplify model interpretation. Since its introduction, it has been shown by Ergon [2] and Kemsley and Tapp [3] that results identical to the original O-PLS formulation can be obtained by post-processing conventional PLS models in a non-patented way. This demonstrated, unequivocally, that O-PLS models have predictive properties identical to their non-rotated versions. The authors did not, however, consider the interpretability of the models at length. This is the subject of this paper.

1   EXAMPLES

The effect of O-PLS on interpretability will be demonstrated using actual and synthetic data. Examples follow.

1.1 Near Infrared Spectra of Pseudo-gasoline mixtures

As a first example, we consider the NIR spectra of of pseudo-gasoline that is a mixture of five analytes (octane, benzene, toluene, o-xylene and p-xylene). Thirty samples are available and the constituent concentrations are known, thus, it is possible to estimate the pure component spectra of the analytes using Classical Least Squares (CLS) as shown in Figure 1. (This data set is distributed with PLS_Toolbox is available upon request.) Note that the pure components are highly overlapped.
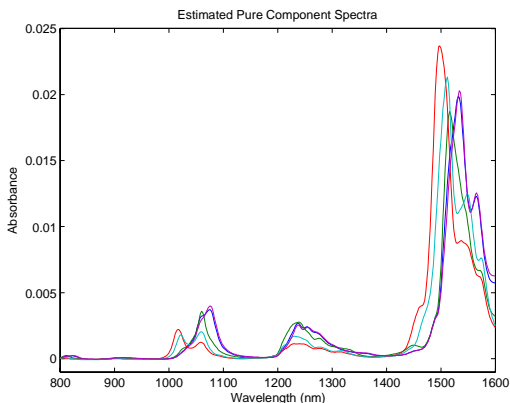
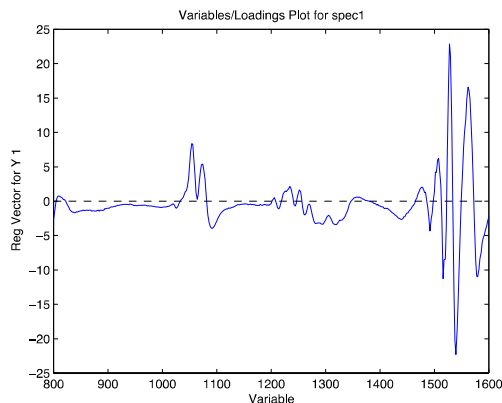

Figure 1. Estimated Pure Components   Figure 2. Conventional PLS Regression Vector

A PLS model is built for one component (o-xylene) with mean-centering and five Latent Variables (LVs). The regression vector for this model is shown in Figure 2. The model was then rotated and the non-predictive factors used to create a preprocessing filter. The regression vector based on this data is shown in Figure 3, along with the estimated pure component spectra. Clearly, the O-PLS filtered regression vector is more similar to the pure component than the conventional PLS regression vector. The O-PLS filtered regression vector, however, does

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contain negative portions. But in the case of spectra, even if the pure component estimate were not available, we would know that the negative portions could not be correct, and must be accounting for overlapped species. Furthermore, we know that NIR spectra is continuous and smooth, thus aiding our ability to mentally correct for any discrepancies in the O-PLS result.

1.2 Synthetic Data with Discrete Variables

Consider now a data set generated from 10 discrete variables with 5 sources of variation, with factors shown in Figure 4. The factor indicated with the thicker blue line is related to the property of interest. The O-PLS filtered regression vector is shown in Figure 5. In this case, O-PLS fails completely to recover the underlying factor, with the coefficients of some variables being relatively much too large (*e.g.* #2), some large negative when they should be positive (*e.g.* #6) and some large magnitude when they should be zero (*e.g.* #9). With no requirement that the coefficients should be continuous or of any particular sign, intuition cannot save the interpretation.
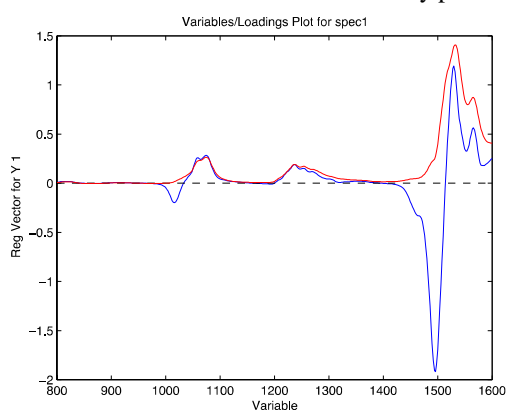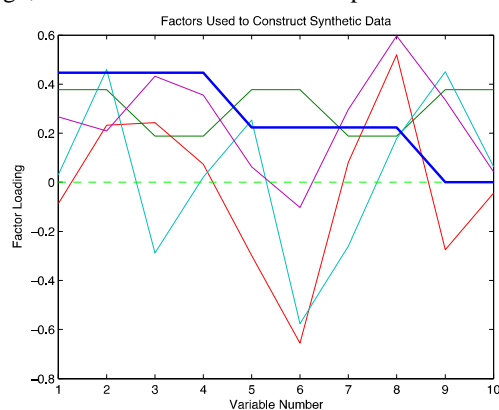

Figure 3. O-PLS Regression Vector
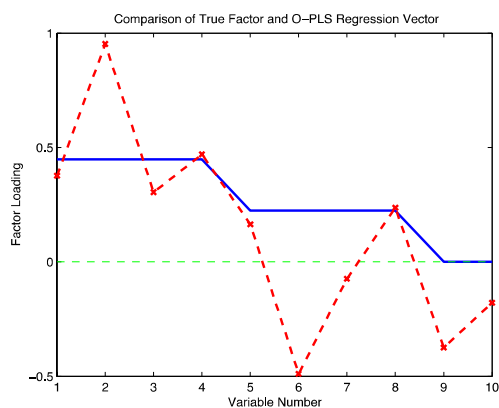

Figure 4. Synthetic Data with Discrete Variables

Figure 5. O-PLS Regression Vector and True Factor

1   CONCLUSION

The examples above illustrate that, while O-PLS may aid interpretation, chemical/physical insight can still be required to "complete the picture." In other instances, where little a priori information is available, O-PLS may provide misleading results. In this paper the situations where O-PLS will and will not aid interpretability are elucidated using additional examples and simulated data sets.

References

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