# Supplementary Material

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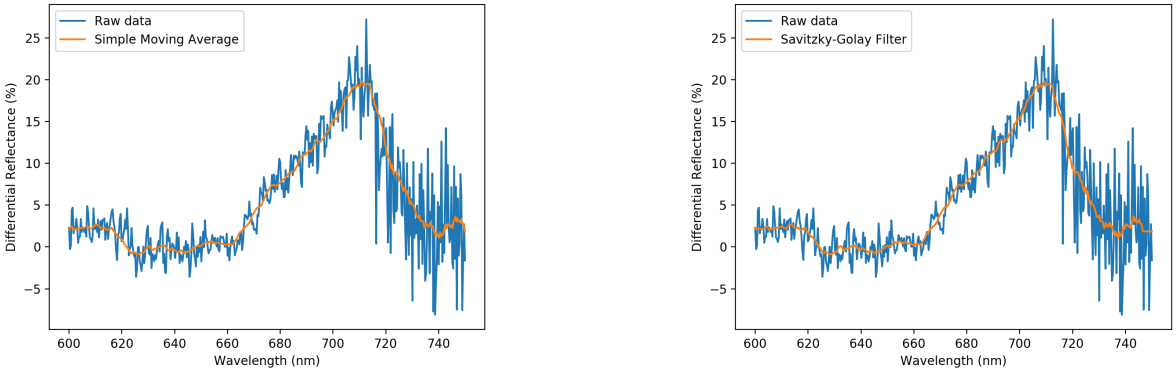
To assess whether using standard signal preprocessing techniques such as simple moving average or Savitzky-Golay filter would improve the performance of dimension reduction, we apply simple moving averages and Savitzky-Golay filter to the data before dimension reduction. For both simple moving average and the Savitzky-Golay filter, we used a window size of 21 data-points. For the Savitzky-Golay filter, we fit a cubic order polynomial to the data in the filter window. An example of the reflectance data after the preprocessing filters have been applied is shown in Figure 1.




(a) Simple average filter

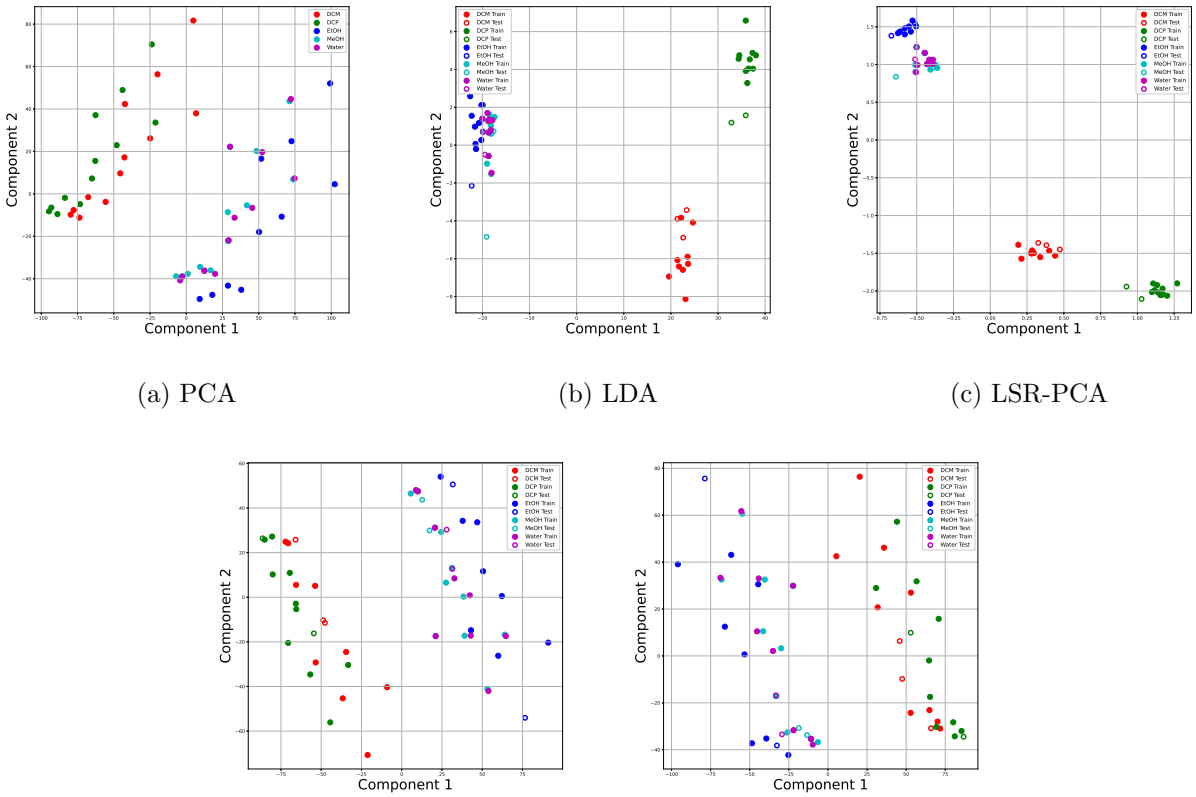
(b) Savitzky-Golay filter

Figure 1: An example of the reflectance data after applying the data processing filters.

We did not notice any significant improvement using the aforementioned preprocessing techniques.

## Simulated optical vapor reflectance data

The vapors included in this dataset are also DCP, DMMP, EtOH, MeOH and water. The dataset consists of reflectance data at 15%, 25% and 50% of the saturation concentration for each vapor. The computational model studied the reflectance of the vapor at 4501 different wavelengths. This dataset contained 60 data points. For the supervised dimension reduction methods, 80% of the data points were used training and 20% of the data points were used for testing and evaluation of the dimension reduction. The results for the simulator optical vapor reflectance data using simple moving average and a Savitzky-Golay filter are shown in Figure 2 and 3. The results are similar to Figure 3 in in the paper.



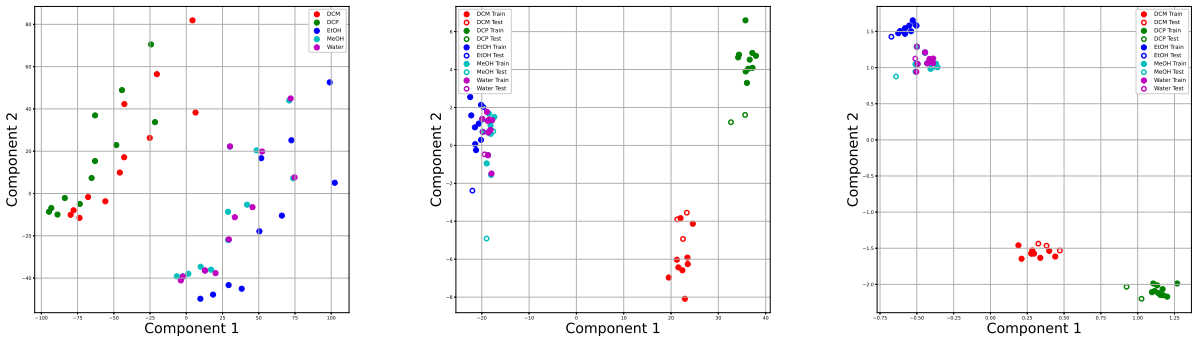

(a) PCA (b) LDA (c) LSR-PCA

(d) PLS (e) SPCA

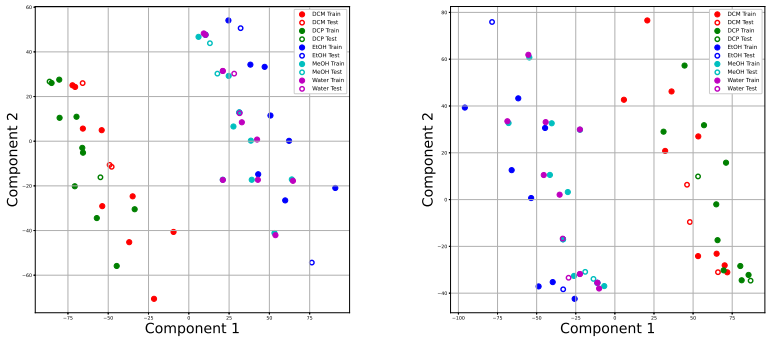
Figure 2: After preprocessing using simple moving average filter: projection onto two principal components for all five dimension reduction methods for the simulated Morpho didius butterfly wing data.

## Experimental data from different filters

In this dataset, we combined optical vapor data using two rugate filter substrates: the first substrate is coated with an oxidized surface and the other one is coated with a carbonized surface. The experiments used five different vapors, dichloromethane (DCM), DCP, EtOH, MeOH and water at 2%, 5%, 10%, 20% and 30% of the saturation concentration. There are a total of 50 data points. Each data point consists of differential reflectance at 438 wavelengths. For the supervised di- mension reduction methods, 80% of the data points were used training and 20% of the data points were used for testing and evaluation of the dimension reduction. The results after applying the simple moving average and the Savitzky-Golay filter is shown in Figures 4 and 5. The results are similar to Figure 4 in the paper.

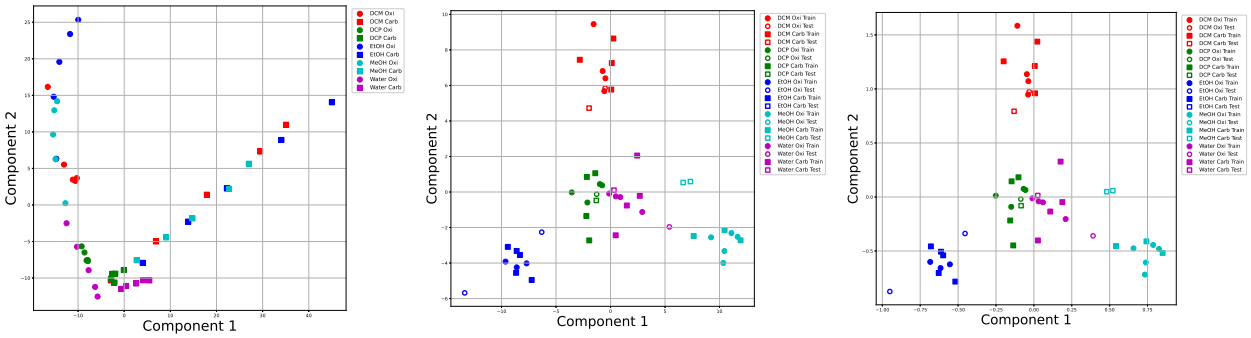



(a) PCA (b) LDA (c) LSR-PCA




(d) PLS (e) SPCA

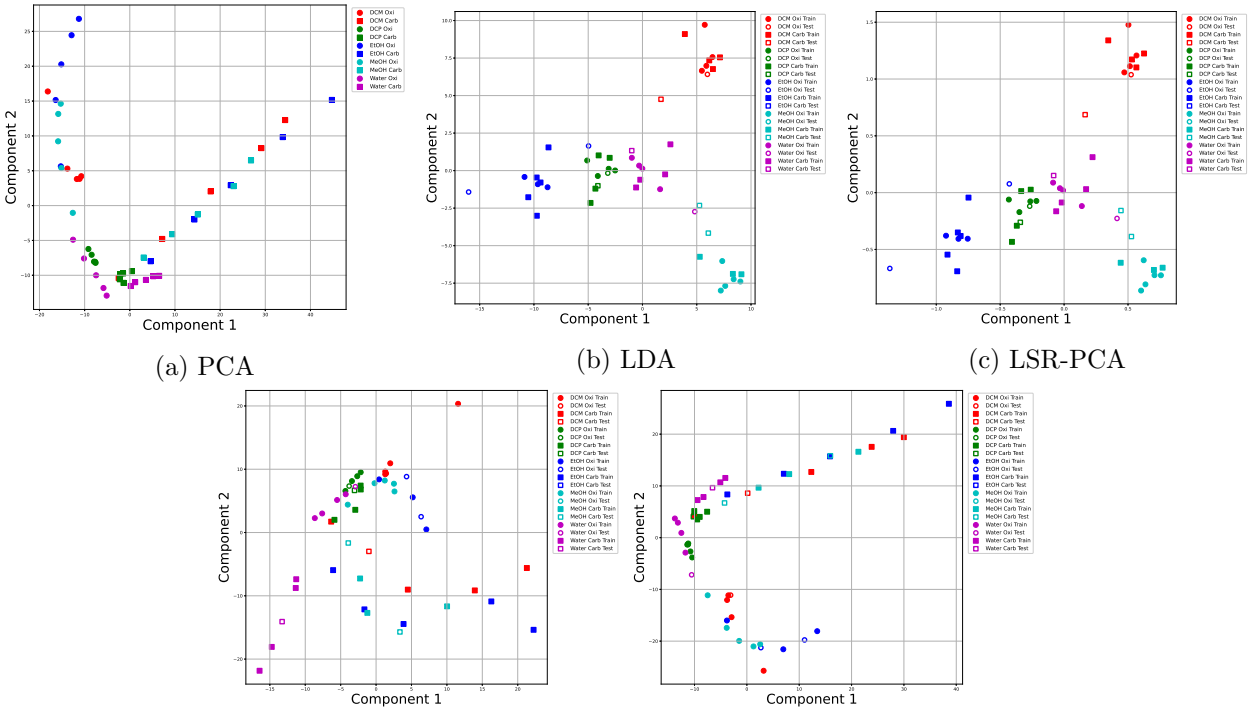
Figure 3: After preprocessing using the Savitzky-Golay filter: projection onto two principal components for all five dimension reduction methods for the simulated Morpho didius butterfly wing data.




(a) PCA (b) LDA (c) LSR-PCA

(d) PLS (e) SPCA

Figure 4: After preprocessing using the simple moving average filter: projection onto two principal components for all five dimension reduction methods for experimental results using two rugate filers..




(a) PCA (b) LDA (c) LSR-PCA

(d) PLS (e) SPCA

Figure 5: After preprocessing using the Savitzky-Golay filter: projection onto two principal components for all five dimension reduction methods for experimental results using two rugate filers..