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How Does Computational Pre-Processing Affect Spectral Analysis? An Investigation on Simulated Spectra

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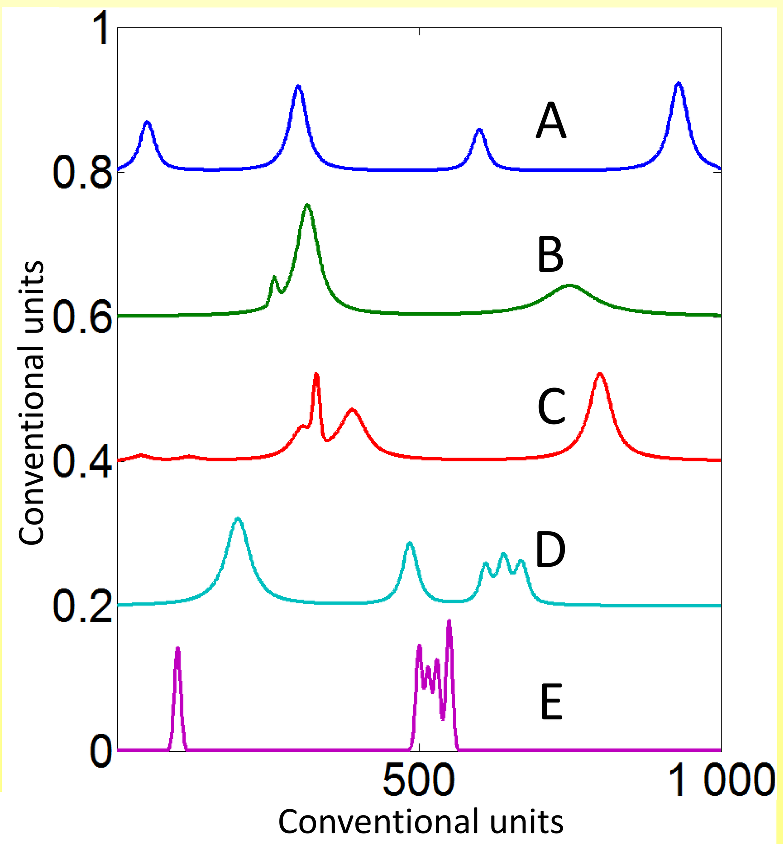
SCOPE OF THE WORK

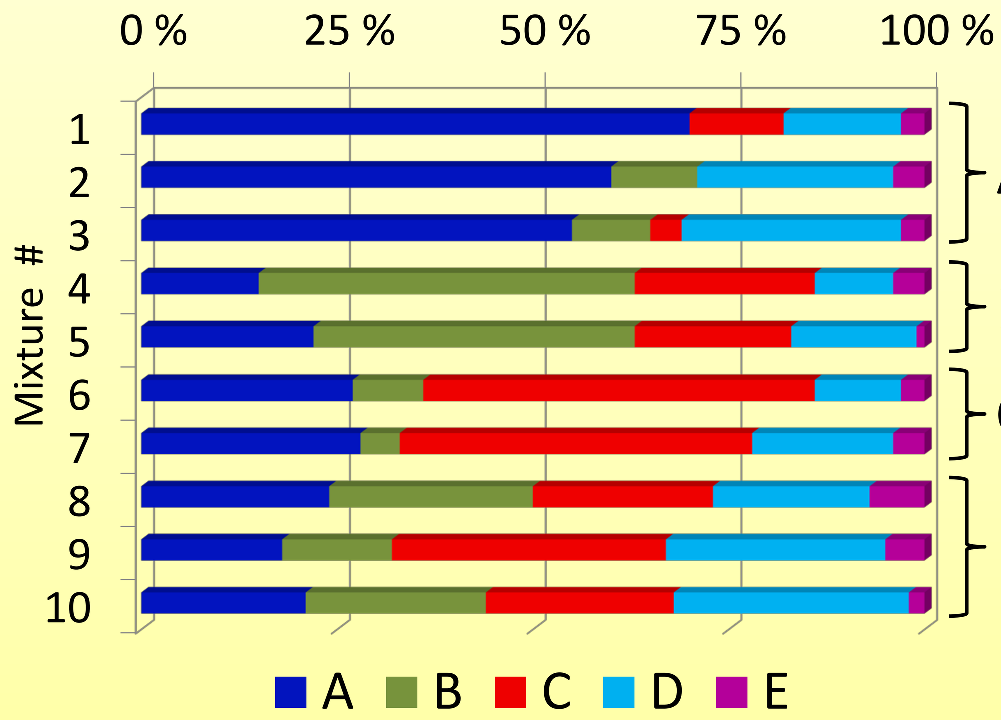
Spectral analysis is usually preceded by computational Pre-Processing (PP) to improve the signal and highlight the information of interest. However, little systematic study has been carried out on how the final result is affected by different PP methodologies, which are often chosen based on just common sense.

This work addresses this issue through a simulation experiment in which fictitious spectra, corrupted by different types of noise, were processed by various combinations of PP techniques. K-means cluster analysis was then used to recognize the original spectra.

SIMULATED SPECTRA

Spectra were generated by first mixing signals A-E in 10 different proportions…



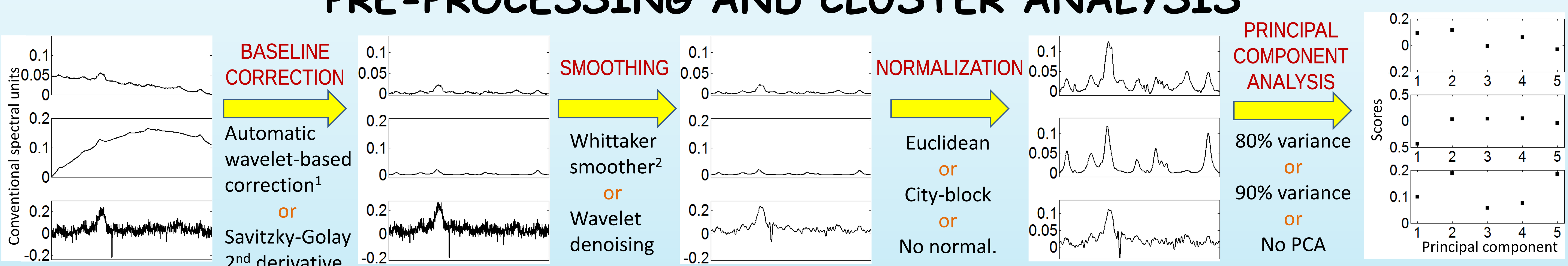


…and subsequently contaminating them with:

- **Baseline distortion**: linear or polynomial, baseline-to-signal ratio (BSR) from 0.5 to 8
- **Random noise**: signal-to-noise ratio (SNR) from 100 to 5
- **Intensity variation**: multiplication by 1, 2, 4 or 8

264 spectra were generated from each mixture, 2640 in total. These spectra simulate common issues encountered in spectral imaging.

PRE-PROCESSING AND CLUSTER ANALYSIS



All 216 combinations of the following techniques were tested (only one option per PP step is shown in this example figure)

K-MEANS CLUSTER ANALYSIS: Euclidean or City-block or Cosine

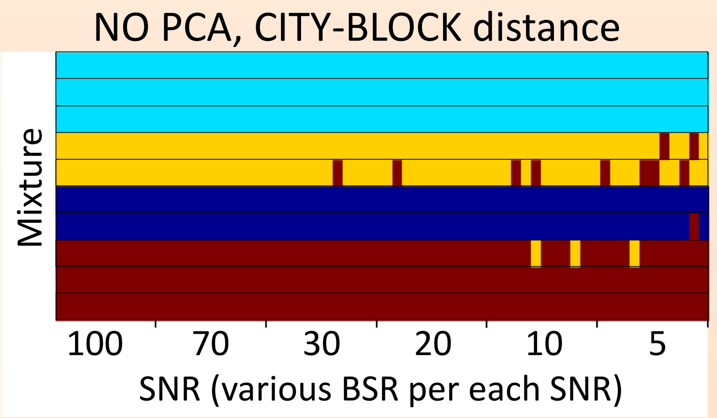
4 clusters or 10 clusters

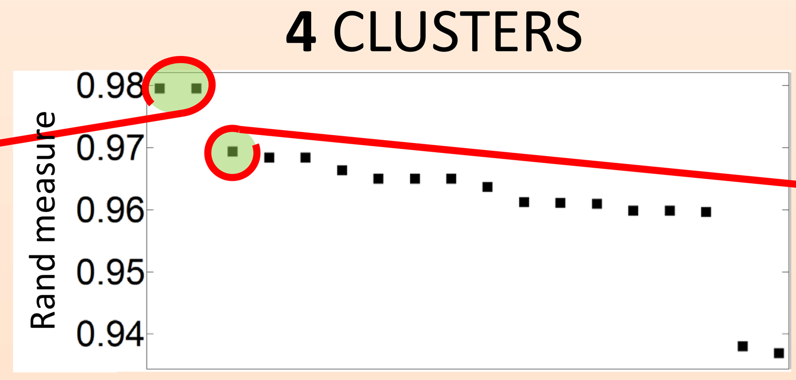
RESULTS

Best clusterings, according to the Rand statistic[3], visualized by color maps:
(a perfect clustering would consist of homogeneous horizontal stripes)

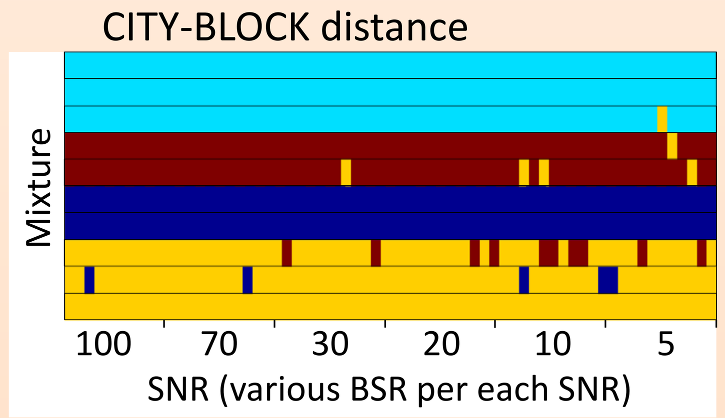
4 CLUSTERS

WAVELET baseline correction
CITY-BLOCK normalization
NO PCA, CITY-BLOCK distance



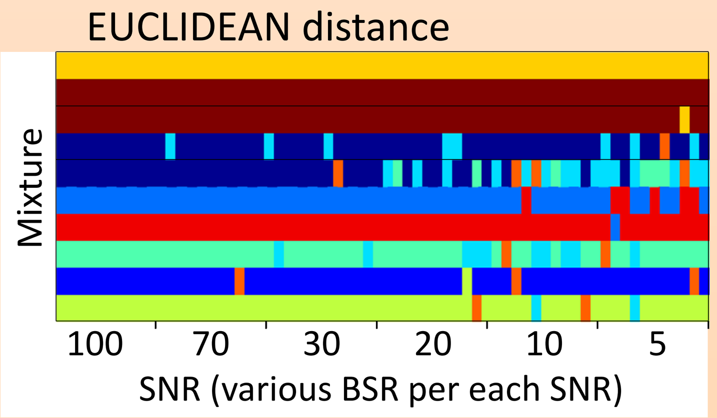


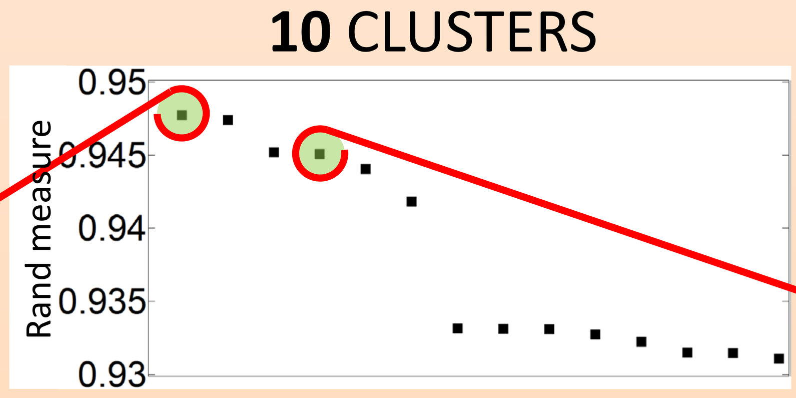
WAVELET baseline correction
EUCLIDEAN normalization
16 PCs (90% explained variance)
CITY-BLOCK distance



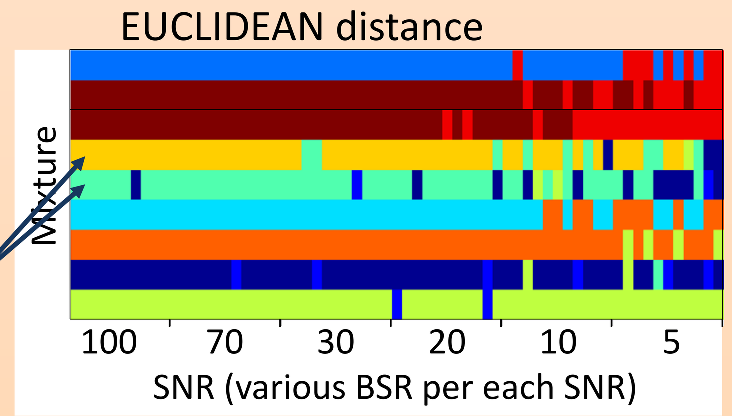
10 CLUSTERS

WAVELET baseline correction
EUCLIDEAN normalization
4 PCs (80% explained variance)
EUCLIDEAN distance





WAVELET baseline correction
CITY-BLOCK normalization
3 PCs (80% explained. variance)
EUCLIDEAN distance



Worse clustering of noisy spectra, but better distinction between mixtures 6-7 and higher silhouette coefficient

Further observations:

- No significant influence of the smoothing method was observed
- Good clustering can be achieved even when n. PCs < 5 (n. of components)
- Some PPs found in the literature[4] appear far from optimal in this study

CONCLUSIONS

For the proposed spectra, the best combinations of PP techniques to distinguish the relevant mixtures were found. The effect of each PP method was investigated.

These results can provide a guideline for a more effective spectral analysis and multivariate curve resolution.

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