Another Pipeline in Local Partial Least Squares Regression (LPLS) Methods: Assessing the Impact of Wavelet Transform Integration

Antoine Deryck[a], Andreas Niemöller[b], Vincent Baeten[a], Juan Antonio Fernández Pierna[a]

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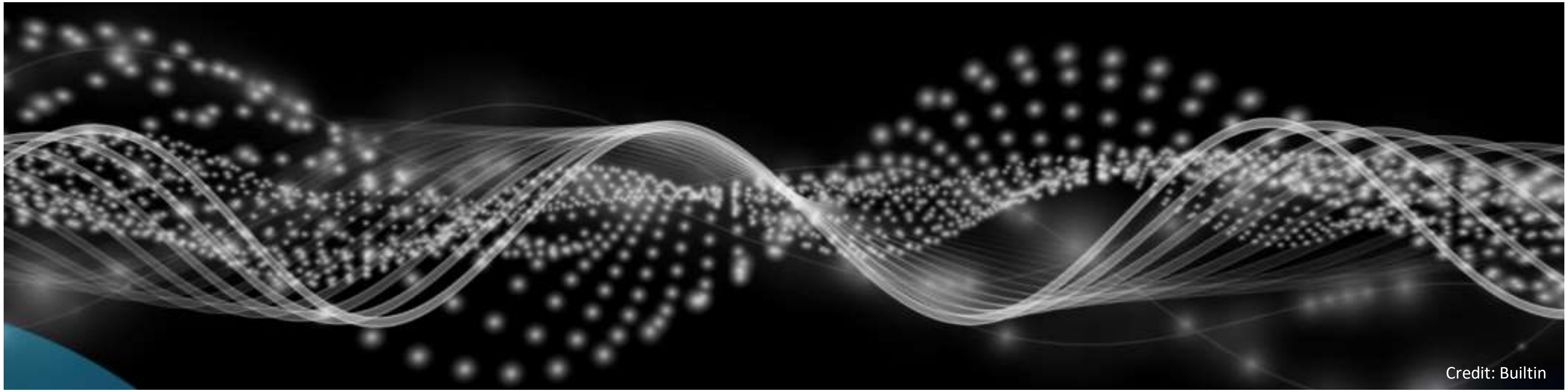


Credit: Builtin

A little bit of context

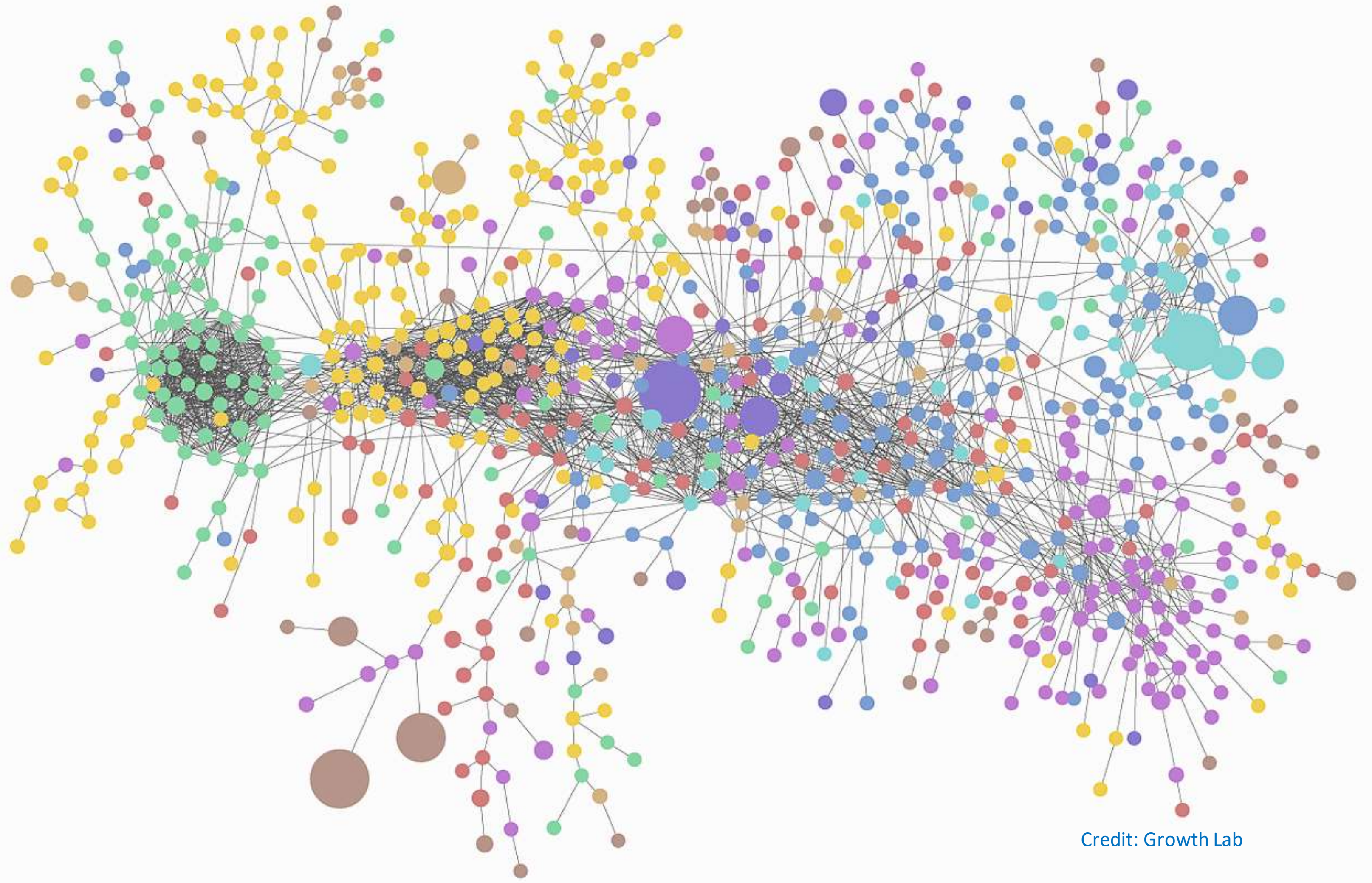
New analytical tools and technologies

↓

More and more data collected, including much more complexity

↓

Limitations of classical methods such as PLS (based on the study of global variability)



Credit: Growth Lab

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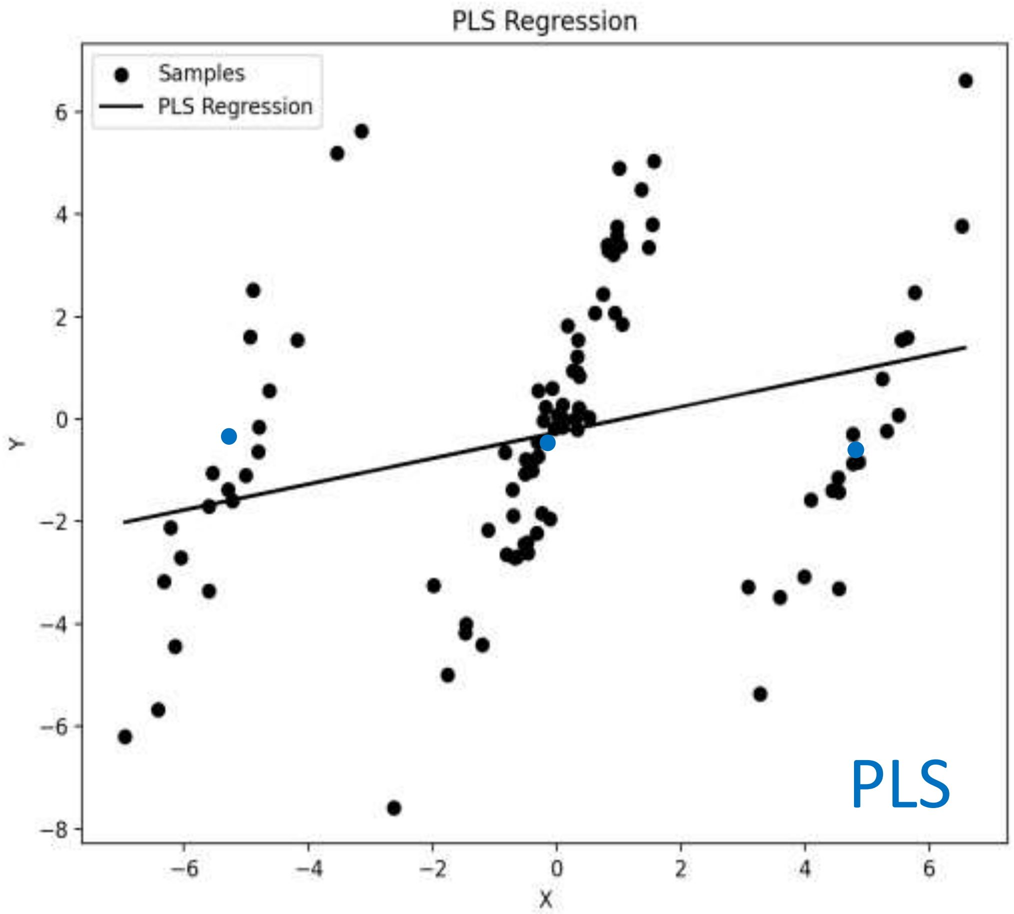
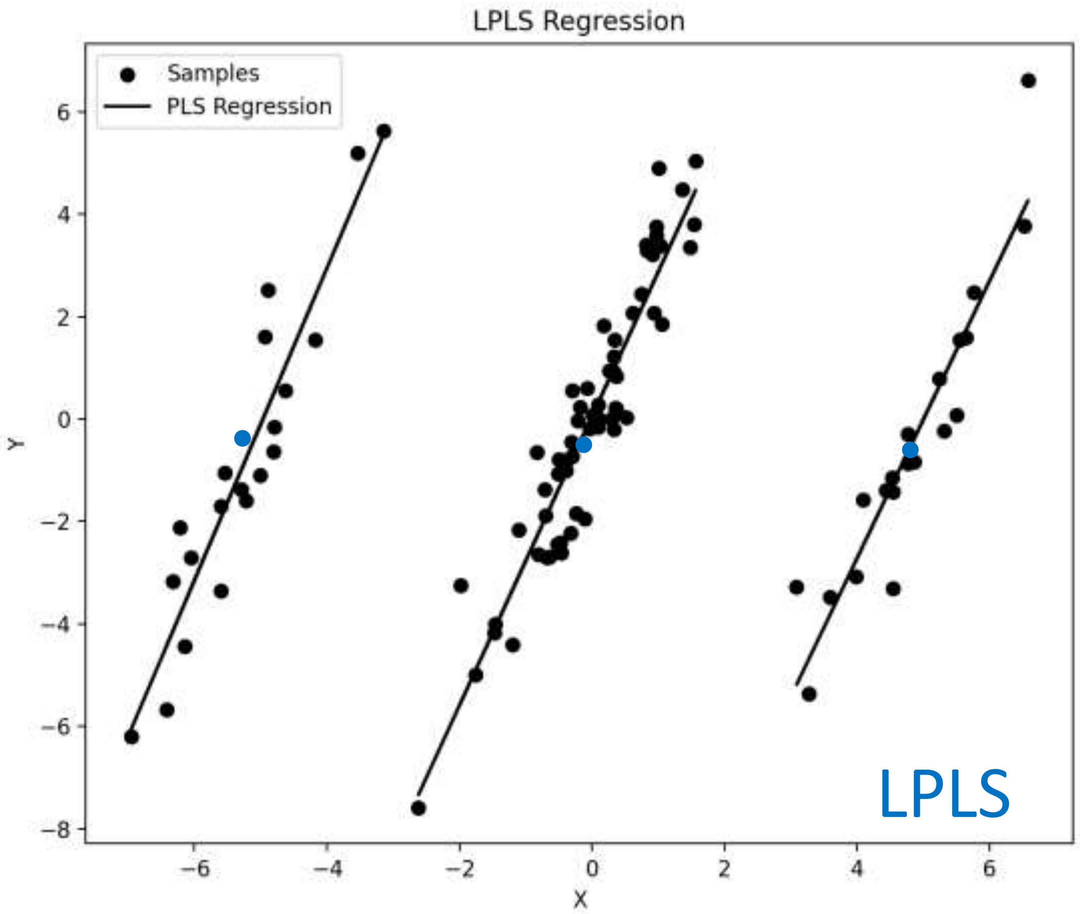
LPLS Algorithms





LPLS Algorithms

- Better consideration of data complexity
- Robust to outliers
- Allow centralization of samples of different natures

- Difficult to interpret
- Increased computation time
- Technical constraints for implementation on handheld instruments

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ARTICLE | September 3, 1998

Optimization in Locally Weighted Regression

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Dataset reduction techniques

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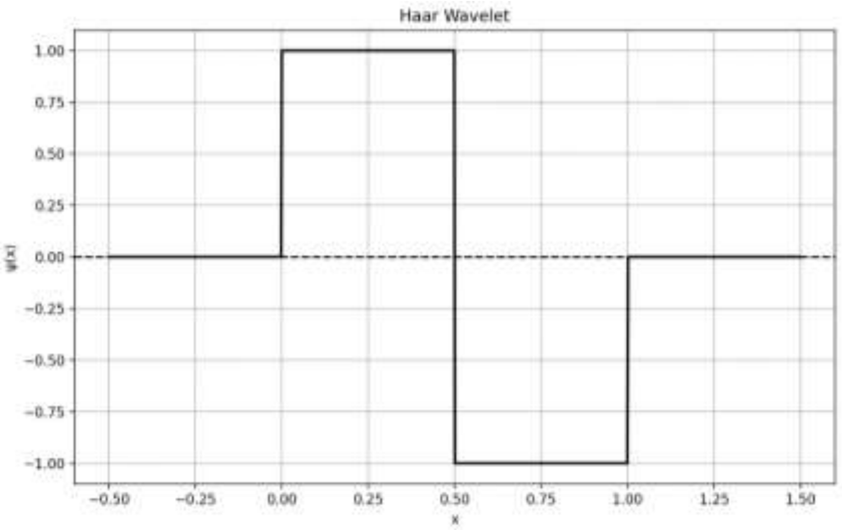
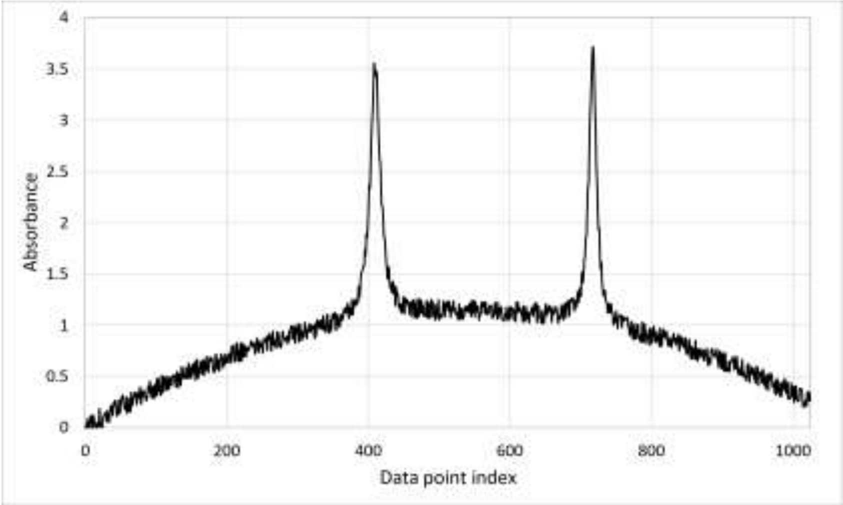
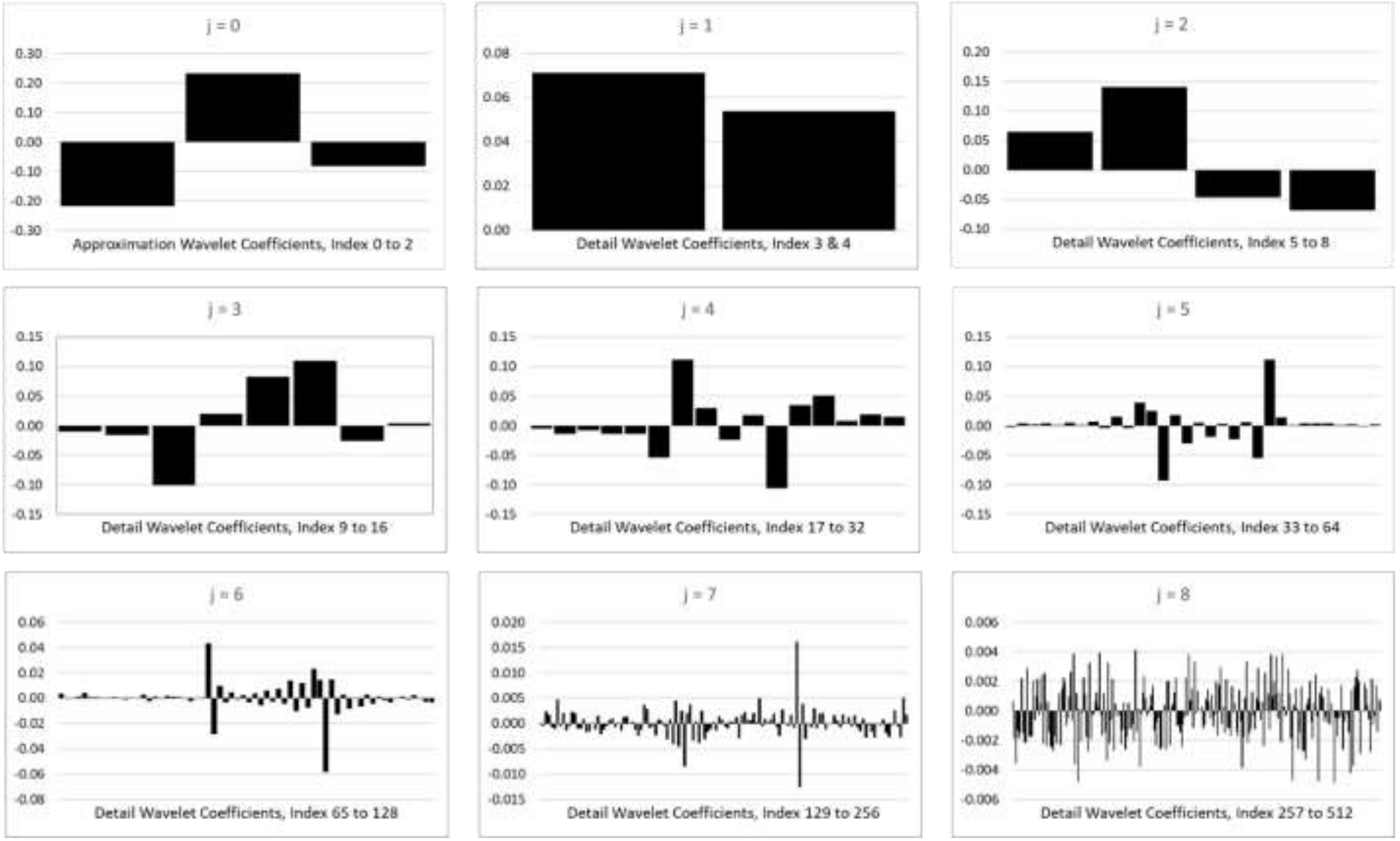
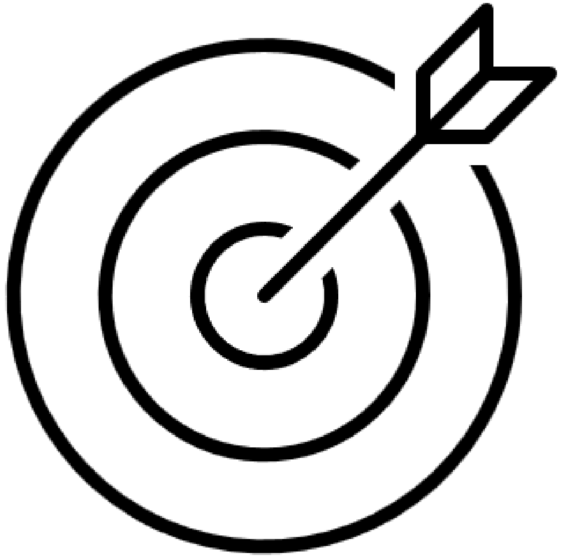
Wavelet Transform







Objectives



Assessing the impact of wavelet transform within a LPLS pipeline (WLPLS)

Comparing its performance with the traditional LPLS pipeline (LPLS)

Comparing its performance with another data reduction technique within a LPLS pipeline: the LPLS on global PLS scores (LPLS-S)

Methodology

- 24,644 spectra of feed formulations (CRA-W database)
- Measured with FOSS XDS spectrometer (1100-2498 nm by 2 nm)
- Reference analytical methods for constituents (% total weight of the sample)

Constituents	N	Min	Max	Mean	Std
ASH	20,065	0.80	37.00	7.32	3.26
MOIST	23,392	2.04	16.70	11.36	1.82
PROT	22,371	6.80	62.30	20.47	8.10

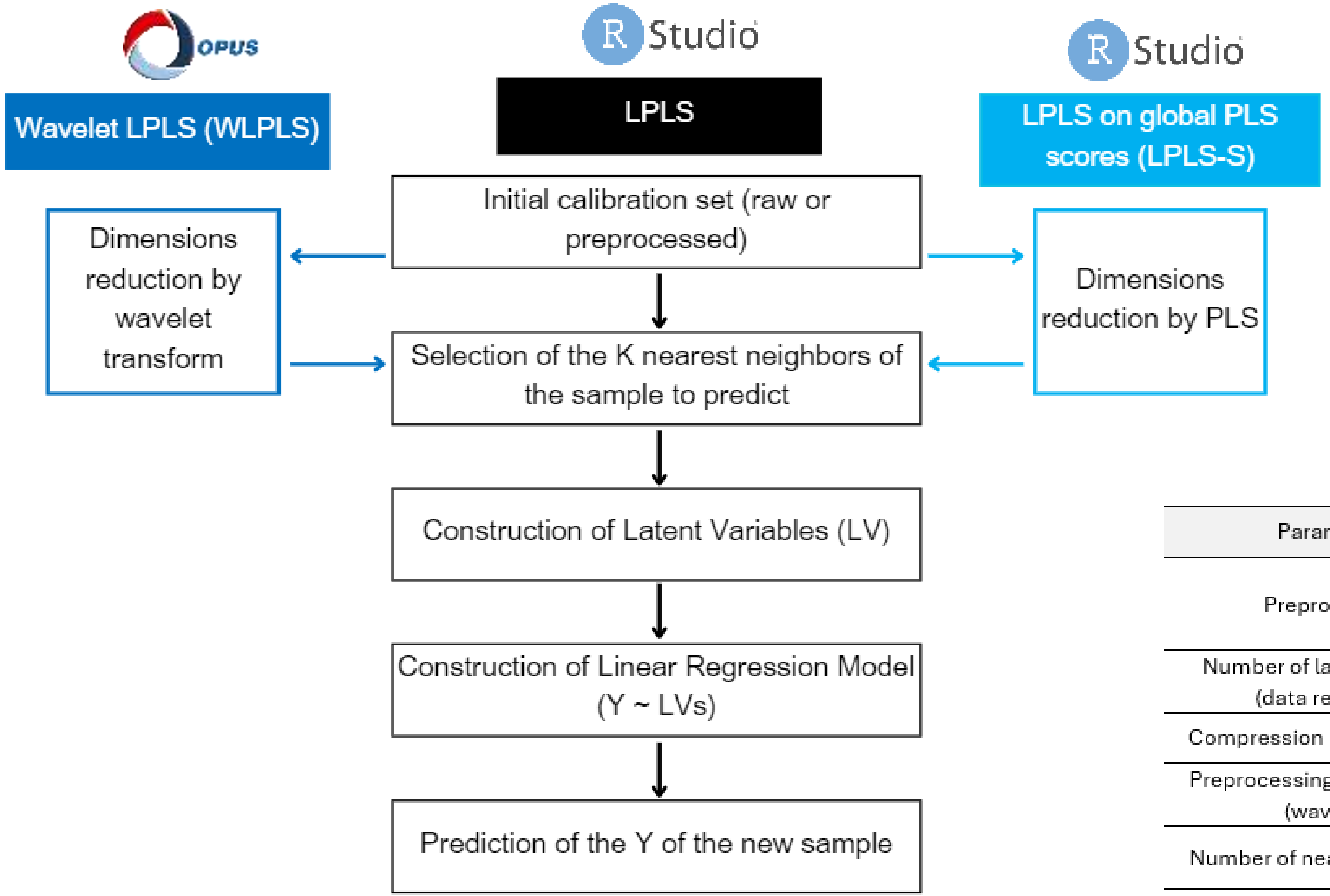
Parameters measured in % total weight of the sample

60%
Spectral library

15%
Optimisation dataset

25%
Validation dataset

Methodology



Parameters	LPLS	LPLS-S	WLPLS
Preprocessing	1st derivative - window size of 13 / SNV / None	1st derivative - window size of 13 / SNV / None	1st derivative - window size of 13 / SNV / None
Number of latent variables (data reduction)	10 to 20	/	/
Compression level (wavelets)	/	/	5 / 6 / 7
Preprocessing of coefficients (wavelets)	/	/	SNV / None
Number of nearest neighbors	100 / 200 / 300 / 400 / 500 / 1000	100 / 200 / 300 / 400 / 500 / 1000	100 / 200 / 300 / 400 / 500 / 1000
Number of latent variables (rank model)	1 to 20	1 to 20	1 to 20

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LPLS: V. Centner, L. Massart, 1998, Optimization in Locally Weighted Regression, Analytical Chemistry 70 (1998), 19:4206-4211, https://doi.org/10.1021/ac980208r

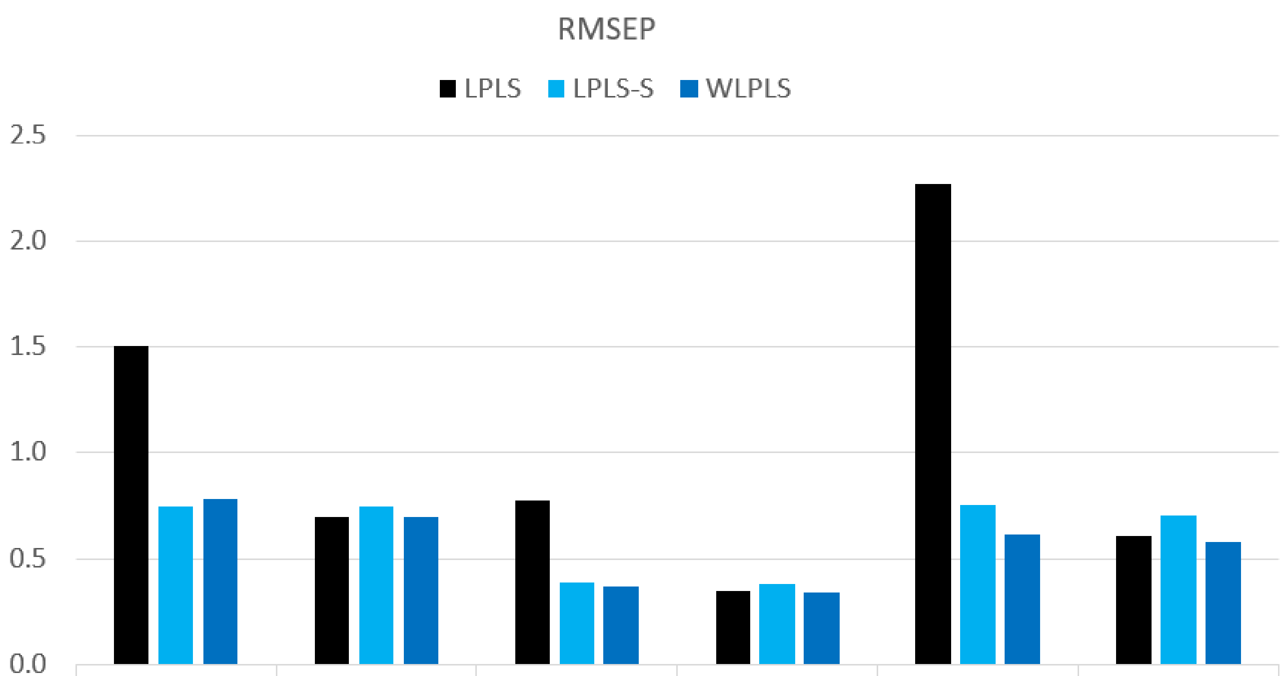
LPLS-S: G. Shen et al., 2019, Local Partial Least Squares Based on Global PLS Scores, Journal of Chemometrics 33 (2019), 5:e3117, https://doi.org/10.1002/cem.3117

Results

- The three LPLS pipelines gave high-quality predictions
- Small differences between pipelines for preprocessed data
- BUT significant differences for raw data (LPLS < LPLS-S and WLPLS)

RPD

	ASH	MOIST	PROT
PLS	2.733	3.699	9.109
LPLS	4.514	5.294	13.882
LPLS-S	4.370	4.849	11.444
WLPLS	4.504	5.358	13.935



	ASH RAW	ASH PREPRO	MOIST RAW	MOIST PREPRO	PROT RAW	PROT PREPRO
LPLS	1.505	0.698	0.772	0.346	2.269	0.608
LPLS-S	0.745	0.745	0.390	0.378	0.754	0.702
WLPLS	0.784	0.700	0.370	0.342	0.611	0.577

Discussion

LPLS	LPLS-S	WLPLS
• Significant computational power and time (not ideal for real-time analyses) • Usually requires preprocessing • Easily modifies library compositions without recalculations	• Reduces dataset to a few latent variables (e.g., 10-20 for a 700-point spectrum) • First PLS can remove noise (no further preprocessing required) • Relies on a simple data reduction technique • Changes in library composition require recalculation, affecting performance	• Reduces dataset to a few wavelet bands (e.g., 60-100 coefficients for a 700-point spectrum) • No need for spectral range selection or preprocessing • Less simple to understand and optimize • Adaptive through weighting of orthogonal coefficients • Easily modifies library compositions without recalculations

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Conclusion

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No method is universally better (dataset dependant)

WLPLS offers specific advantages BUT similar benefits may apply to LPLS-S and other methods not explored here

Pipeline selection should be based on dataset characteristics and research goals

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Further research and discussions

- Comparison of more algorithms applied to more datasets
- Why are local methods rarely used?
- Deep learning vs Local Methods?

Acknowledgments

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Thank you for your attention

Antoine DERYCK

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Knowledge and valorization of agricultural products Department

Quality and authentication of agricultural products Unit

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