Determination of Silicon in Wheat Leaves with ATR-FTIR and Chemometrics

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Introduction

Because of the importance of crops such as wheat, barley, rice, and other grasses that accumulate Si, understanding the relationship between this element and plant science is the focus of numerous scientific efforts. Si quantification is a difficult and costly task, and destructive wet chemistry methods are commonly used. With the recent development of chemometric tools, analysis of silicon in complex matrices have has been proved feasible.

Methods

Three groups of wheat plants were cultivated using both greenhouse and controlled growing chambers in hydroponic beds. These groups were different by their silicon supply, which was through NaSiO3. Samples from the leaves of plants from all three groups were analyzed using ATR-FTIR, spectra were pre-processed by calculating the mean of three samples and performing a baseline correction.

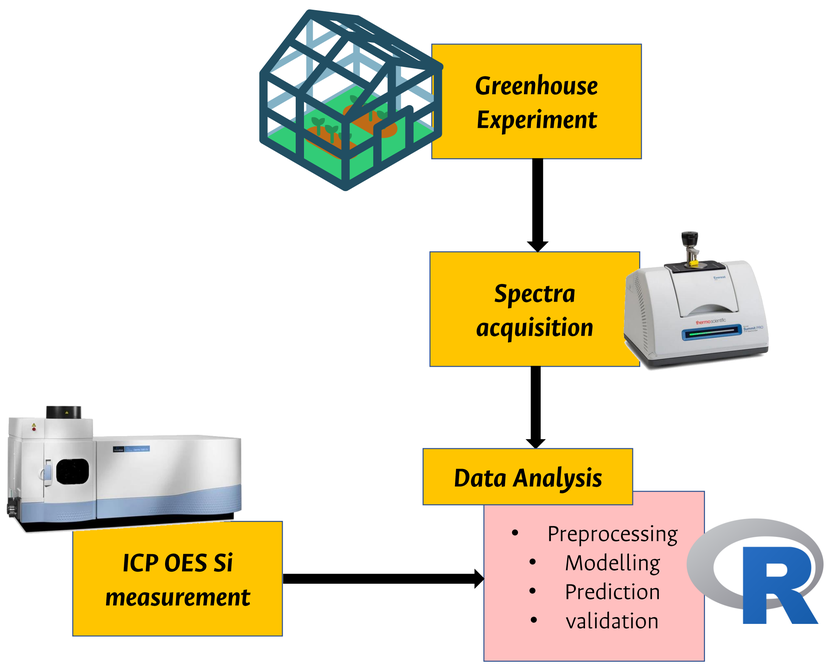

Diagram 1: Overview flowchart showing the steps of the analysis protocol

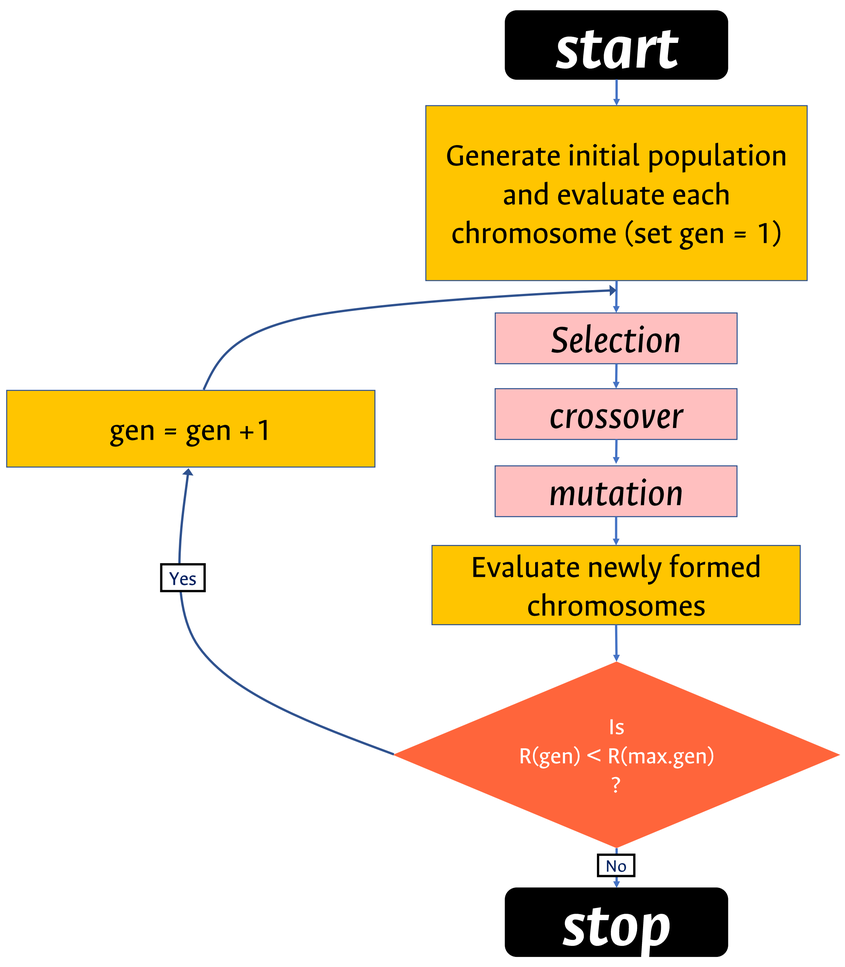

Diagram 2: Genetic algorithm for variable selection

Results

Baseline correction

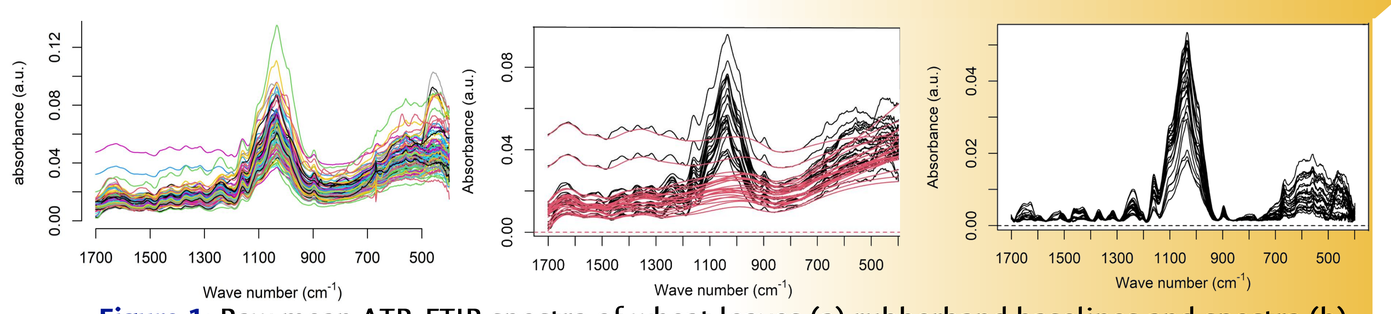

Figure 1: Raw mean ATR-FTIR spectra of wheat leaves (a) rubberband baselines and spectra (b) corrected spectra (c)

Variable selection and modelling

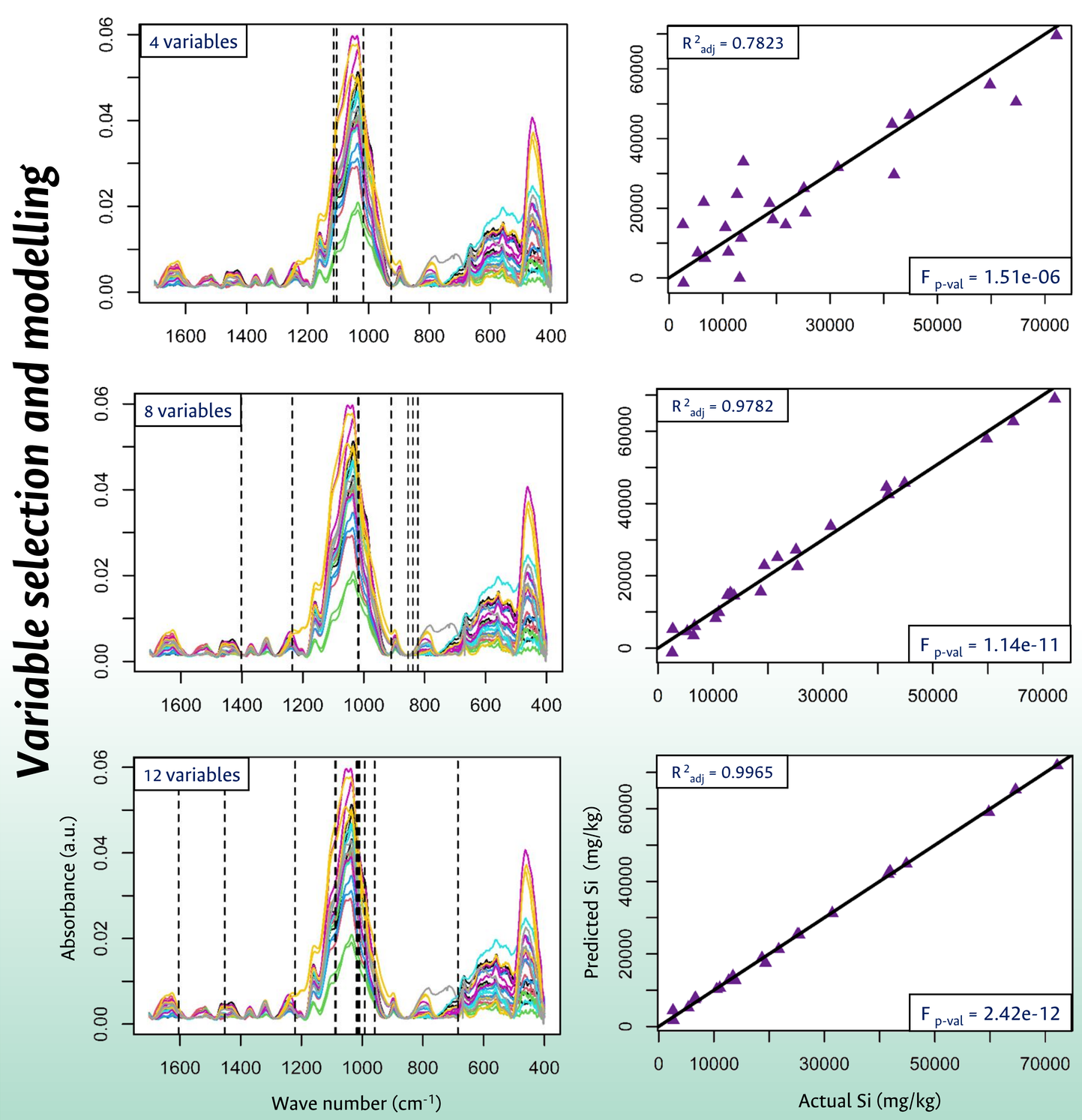

Figure 2: Spectra and variables selected by a genetic algorithm (left) calibration lines of predicted Si content vs ICP-OES measurements (right)

Cross- validation

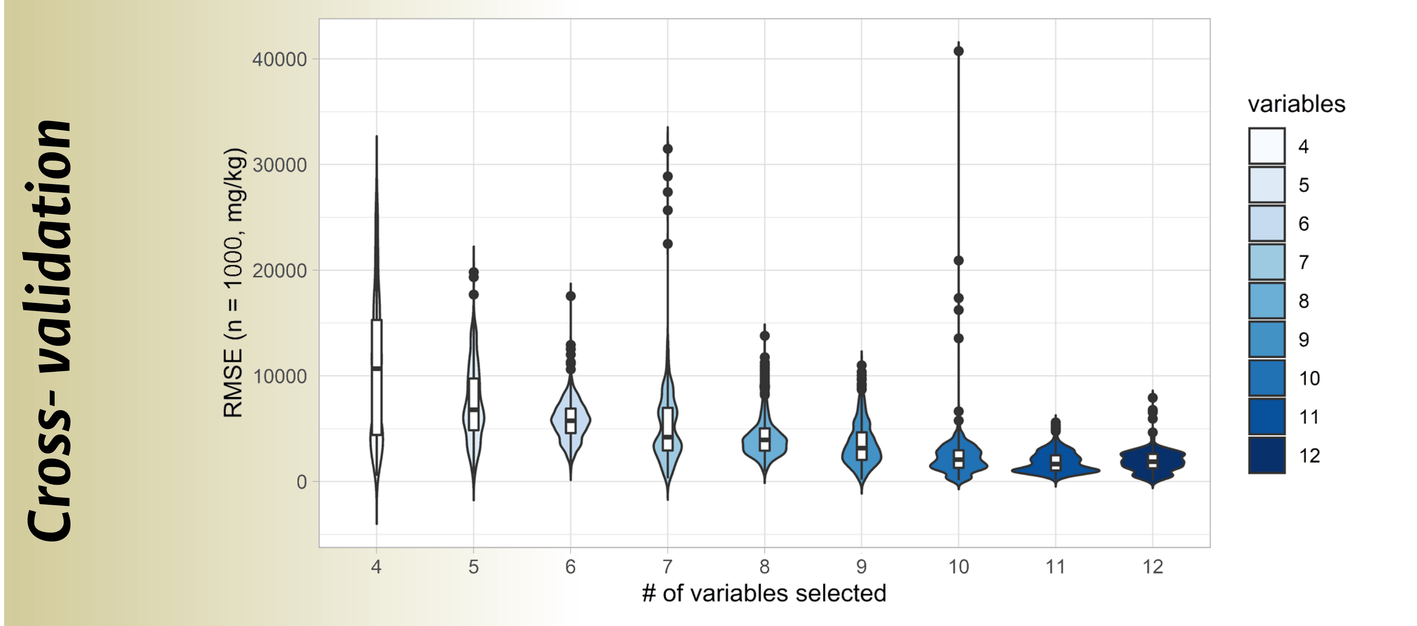

Figure 3: Cross validated error of prediction vs model complexity 100 iterations of 10 folds

Conclusion

Silicon quantification in a complex vegetal matrix such as wheat leaves was possible using ATR-FTIR and chemometrics. The models presented homoscedasticity (normal residuals around zero), significance (ANOVA, p-values), and good performance in prediction (CVRMSE < 1% wt.)

References

[1] Chen, H., Ferrari, C., Angiuli, M., Yao, J., Raspi, C., & Bramanti, E. (2010). Qualitative and quantitative analysis of wood samples by Fourier transform infrared spectroscopy and multivariate analysis. *Carbohydrate polymers*, *82*(3), 772-778.

[2] Varmuza, K., & Filzmoser, P. Introduction to multivariate statistical analysis in chemometrics. CRC press, 2016.