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ATR – FTIR Chemometrics for Biological Samples

A thesis presented in partial fulfilment of the requirements for the degree of

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Abstract:

This project has used the analytical infrared reflectance technique of *Attenuated Total Reflectance Fourier Transform Infrared* (ATR-FTIR) spectroscopy, for the prediction of chemical components in a range of biological samples. Data collection was carried out on 40 hyperaccumulator samples, 56 chicken feed samples, 54 lamb faecal samples and 188 forage feed samples. Predictions were made using several different regression methods including: Ridge, Least Absolute Shrinkage and Selection Operator (LASSO), Elastic Net, Principal Components (PCR) and Partial Least Squares (PLS). The best methods were identified as LASSO, Elastic Net and PLS. Several spectral data pre-treatments were explored, the best of which combined Standard Normal Variant scaling (SNV) with a first-order Savitzky–Golay (SG) spectral derivative and smoothing filter. Several of the resulting models illustrated high quality predictions ($R^2 > 0.8$, Relative Performance Deviation (RPD) $\geq 2$). The SNV and SG pre-treatment almost completely reduces the contribution of strong water-based signals to the regression model, allowing the possibility of *in situ* prediction of forage feed composition with minimal sample preparation. ATR-FTIR spectrometers are available in a hand-held form, and the results of this research suggest that in situ forage quality analysis could be performed using mid–infrared (MIR) reflectance spectroscopy.
Preface:

A portion of this research thesis has been submitted to the Journal of Animal Feed Science and Technology for publishing. The article is titled “Mid-Infrared Reflectance Spectroscopy as a tool for forage feed composition prediction” and was authored by Josiah D. Cleland, Ellie Johnson, Patrick C. H. Morel, Paul R. Kenyon, Mark R. Waterland.
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Abbreviations:

PT Pre – Treatment
SG Savitsky – Golay filter
SNV Standard normal variate scaling
MSC Multiplicative Scatter Correction
DWT Discrete Wavelet Transform
AsLS Asymmetric Least Squares
PLS Partial Least Squares
PCR Principal Component Regression
PCA Principal Component Analysis
RR Ridge Regression
LASSO Least Absolute Shrinkage and Selection Operator
EN Elastic Net
NDF Neutral Detergent Fibre
ADF Acid Detergent Fibre
GE Gross – Energy
ME Metabolisable – Energy
OM Organic Matter
DOMD In vitro Digestible Organic Matter
PC Principal Component
ATR FTIR Attenuated Total Reflectance Fourier Transform Infrared
MIR Mid – Infrared
NIR Near – Infrared
FIR Far – Infrared
MPAES Microwave Plasma Atomic Emission Spectrometer
RMSEP Root Mean Squared Error of Prediction
RMSECV Root Mean Squared Error of Cross – Validation
SEP Standard Error of Prediction
SECV Standard Error of Cross – Validation
RPD Relative Performance Deviation
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