Statistical Methods: Prediction of Soil Parameters through Near Infrared Spectroscopy

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Abstract

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1 Introduction

Through soil analyses or soil testing one can get certain chemical and physical information about the used soil like the concentration of soil organic carbon (SOC) or the pH-value. With these Measurements, known as soil parameters, it is possible to optimize plant growth or to assist in solving soil-related problems.

However the direct measurement of soil parameters is very costly and error-prone. Therefore methods for fast and cheap determination of these parameters play a fundamental and vital role in particular fields like agriculture, geochemistry and ecology.

At the beginning of the 1960s Karl Norris for the first time in history used Near Infrared Spectroscopy (NIRS) to predict and calculate moisture content from seed extracts through a multivariate calibration approach. His work had a huge impact in agricultural an non-agricultural fields since NIRS proved to be a significant timesaver and cheap alternative to other methods.

In the last few years NIRS applications experienced a massive growth. This would have not been possible without better computing capabilities and progress in multivariate methods as the prediction of soil parameters out of a measured soil spectrum requires a large amount of statistical computations.

2 Fundamentals

2.1 Soil Parameters

Let A be any substance in a given soil sample with volume $V \in [0, \infty)$ and let $n_A \in [0, \infty)$ be the amount of A in the sample. Then the molar concentration c_A is given by

$$c_A := \frac{n_A}{V}$$

Now let c_0 be the molar concentration of this sample. We define the amount-of-substance fraction (ASF) p_A of A as

$$p_A := 100\% \cdot \frac{c_A}{c_0}$$

In this elaboration we concentrate on three main soil parameters that are given by existing NIRS-measurements. The first two parameters p_{SOC} and p_{N} are ASFs relating to soil organic carbon (SOC) and nitrogen in the soil sample. SOC is the carbon in this sample which is bound in an organic compound. The third parameter is the pH-value that is used to specify the acidity or basicity of an aqueous solution. It is based on the concentration of hydronium ions $c_{\mathrm{H_3O^+}}$.

$$\mathrm{pH} := -\log_{10} c_{\mathrm{H_3O^+}} = -\frac{\ln c_{\mathrm{H_3O^+}}}{\ln 10}$$

2.2 NIRS

In NIRS one uses electromagnetic waves, also known as light, with a wavelength from 780 nm to 3000 nm. This area is called the near infrared region and is the most energetic one of the infrared light.

An emitted light wave with a certain wavelength λ can interact with a soil sample in three ways. It can be reflected, absorbed or transmitted. For most soil samples measuring the transmittance of light waves is not sensible. So the measurement of the spectrum is reduced to the reflectance since absorptance cannot be directly determined.

Reflectance $\varrho(\lambda)$ of a surface referring to a wavelength λ of a light wave is given by the amount of radiation power P_r that is reflected from a surface divided by the initial power P_0 of this light wave.

$$\varrho := \frac{P_\mathrm{r}}{P_0}$$

3 Model Selection

4 Simulation

5 Conclusion

A Prediction Parameters

B R Source Code

References