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Regression techniques for estimating soil organic carbon contents from VIS/NIR reflectance spectra

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Soil reflectance spectroscopy is regarded as a promising approach to efficiently obtain densely sampled soil organic carbon (SOC) estimates at various spatial scales. The estimates are usually based on a statistical modeling approach since physical models are mostly not applicable owing to the manifold influences on soil spectra by different soil constituents and properties.

Different multivariate statistical methods exist to estimate SOC concentrations in soil samples using visible and near infra-red (VIS/NIR) reflectance spectra. All these techniques face the challenge of generating accurate predictive models with a disproportionate large number of variables compared to the number of observations in such datasets, and in addition highly correlated independent variables. This often results in overfitting and may at the same time reduce the predictive power of such models.

In this study, we conduct a rigorous assessment of the predictive ability of different regression techniques (stepwise regression, robust regression with feature selection, lasso, ridge regression, elastic net, principal component (PC) regression, partial least squares (PLS) regression). We apply datasets from different environments to include a wide variety of soils and to investigate the effects of different SOC variances and concentrations on model performance. Our hypothesis is that the predictive ability of regression techniques can be significantly improved by using more advanced techniques such as PLS regression. We discuss our findings with respect to the applicability of SOC estimation from VIS/NIR reflectance spectra in different environments.