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Predictive modelling of the 3D chemical composition of soil using kriging based methods

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Many problems in environmental and soil research require techniques that quantify the soil micro-environment. It has become increasingly apparent that we need novel micro-analytical techniques to compliment well established methods that study soils at macro-spatial scales. Despite tremendous progress in this field over the last decade, quantitative methods have developed within separate disciplines and operate at different spatial scales hampering their integration. In the present study, we develop and implement a geostatistical method, that enable integration of a 3-D non-invasive technique to characterise soil structure (X-ray CT) with a 2-D spectroscopic method that characterises the spatial distribution of chemical elements on surfaces (SEM-EDX), in order to predict the spatial distribution of chemicals in 3D soils. To achieve this, five different kriging based interpolation techniques including two regression kriging methods, a linear regression and a regression tree kriging, and three cokriging based methods were implemented and their predictive performance was compared and tested on three different chemical, Carbon, Silicon and Calcium, which were measured on the surface of a soil slice. Two of the cokriging methods were based on two variables (one chemical as principal variable and the physical variable as secondary variable), while the third cokriging methods incorporated all four variables i.e. all three chemical and the physical structure. An intermediary step in the kriging methods is to model the sample variograms and cross-variograms of the variables involved in the study. While this is straight forward in the case of ordinary kriging by using a standard non-linear fitting procedure, for cokriging, this is less evident requiring the implementation of a linear model of coregionalization for two or more variables. In general, Carbon and Silicon was approximately correctly predicted by the first four methods, with Carbon occupying the pore space and Silicon being present on the solid component. In turn, presence of Calcium concentration was best predicted by the regression tree kriging method. As indicated by the two diagnostic statistics, the mean error and the mean squared error, among all five methods, the regression tree kriging had the best predictive performance, while the cokriging based on all four variables gave some inconsistent results, this last method requiring further investigation, including a more accurate fit of the coregionalization model.