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Compositional data analysis of geochemical soil data

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Abstract

Baseline mapping and the calculation of threshold values are often used to assess the quality of land based on land use categories such as residential or industrial sites. A threshold is often set to differentiate between concentrations of the element that naturally occur in the soil and concentrations that result from diffuse anthropogenic sources. Regional geochemistry soil databases are increasingly being used to determine these baseline environmental assessments. The key question raised in this presentation is whether the use of a single component baseline or threshold geochemical map can provide an accurate interpretation on its own. Implicit is the thought that single component geochemical maps represent absolute abundances. However, because of the compositional nature of the data due to the closed or constant sum problem, univariate geochemical maps cannot be compared directly with one another. As a result, any interpretation based on them is vulnerable to spurious correlation problems. This presentation examines what this means for baseline quality documentation and risk evaluation. Despite the limitation of relative abundances, individual raw geochemical maps are deemed fundamental to several applications of geochemical maps including environmental assessments. However, element toxicity is related to its bioavailable concentration, which is lowered if its source is mixed with another source. This may be more adequately dealt with if a single component map is not interpreted in isolation to determine baseline and threshold assessments. A range of alternative compositionally compliant representations based on log-ratio and log-contrast approaches are explored to supplement the classical single component maps for environmental assessment. Case study examples are shown based on the Tellus soil geochemical dataset covering Northern Ireland, UK.