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Machine-learning analysis of reservoirs of trace metals and metalloids (Pb, Cu, Zn, Sb) in igneous rocks

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Data mining is a vital analytical method for detecting patterns, trends, relationships, and anomalies in elemental distribution within rocks. As geological data volumes continue to grow, data mining has become increasingly important for advancing scientific understanding of Earth's materials. This study aims to identify reservoirs of metals and metalloids (Pb, Cu, Zn, As, Sb) elements using the global geochemical database of Gard et al. (2019), using eXtreme Gradient Boosting (XGBoost) machine learning (ML) model. These elements are of importance in economic geology—as they may be leached from rocks and precipitated in ore deposits— and in environmental geochemistry —as their natural fluxes may merge with the man-made fluxes to contaminate or decontaminate the environment.

After training the Pb concentration on the 40 input elemental features, screened by the data mining approach, XGBoost achieved a correlation coefficient (r^2) of 0.85 and 0.74 in predicting lead concentration from the unseen test dataset of volcanic and plutonic samples, respectively. The regression results show an excellent agreement between predicted and actual lead concentration values, showing the effectiveness of ML to predict lead concentrations. Additionally, data mining enabled us to assess the importance of each input element in predicting the lead concentration.

In plutonic rocks, the most important features are Rb and K_2O, identifying clearly K-feldspar as the most important Pb carrier. Some Pb is related to Th, likely in accessory minerals that carry radioactive elements. These could include allanite (that may be also a host of REE, such as Lu) or zircon. In rocks that lack K-feldspar, Pb could be concentrated in pyroxenes. The ML results agree well with case studies on mineral and chemical content of rocks and minerals around the world and with published data on partitioning of Pb among minerals and melts.

Gard, M.G., Hasterok, D., Halpin, J., 2019: Global whole-rock geochemical database compilation. Earth Syst. Sci. Data 11, 1553–1566.