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Machine Learning and Mass Balance Methods for the Quantifying Carbon Capture Capacity of Nickel Deposits from Whole-rock Geochemistry: Strengths, Weaknesses, and Best Practices

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The mining of serpentinite-hosted nickel deposits generates tailings that can be used as feedstock for carbon sequestration. The presence of brucite, even in minor amounts, offers significant offsets of greenhouse gas emissions associated with mining. Brucite is found throughout the Decar nickel district of Central British Columbia, Canada, in the range of 0-12 wt% and is hosted in variably serpentinized peridotite. However, brucite (especially in minor amounts) is not readily discerned from conventional core logging practices and brucite-bearing tailings are underutilized. Here we have investigated the accuracy, versatility and best practices for predicting brucite abundance in dill core of the Baptiste nickel deposit (part of the Decar nickel district) from pre-existing mineral exploration whole-rock geochemistry data through machine learning and mass balance methods.

Mass balance methods aim to calculate the mineral proportions that best explain the measured whole-rock chemistry, and may incorporate thermodynamic constraints. They are better suited for extrapolation than supervised machine learning (i.e., empirical methods). Attaining a very high degree of accuracy is considered necessary because minor brucite abundances (0-4 wt%) are characteristic of the most common of ultramafic rocks (harzburgite), while high abundances (0-12%) are generally found in rarer dunite. However, achieving the desired accuracy of less than +/- 1 wt% brucite in diverse rock types through mass balance methods is not pragmatic due to the combination of geological uncertainties (mineral chemistry variability within and between serpentine types), mathematical uncertainties (underdetermined systems of equations), and analytical uncertainties (unmeasured analytes and non-stoichiometric mineral phases).

Supervised machine learning can circumvent the previously described uncertainties and achieve the required degree of accuracy within a restricted range of host rock. The greatest risks are extrapolating the models beyond training data, bias from non-representative training populations, and overfitting models. Here we show that machine learning extrapolations are sensitive to differences in the degree of serpentinization between training and test samples, that the risk of overfitting to noise is reduced by optimizing the fit to “validation data”, and that fit bias towards rarer brucite-rich samples can be reduced by considering mean absolute error, rather than mean square error as the optimization (loss) function.