Estimation of mass transfer and protolith composition for mafic metamorphic rocks using machine learning

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Geochemical compositional data obtained from rocks and soils are essentially multi-dimensional, and consist of a large number of element concentrations and isotope ratio compositions of several tens of dimensions. The “current” rock composition we can obtain is that of the protolith affected by the geochemical process. Therefore, in order to evaluate the geochemical process from the "current" rock composition, it is necessary to quantitatively estimate the composition of the protolith.

In previous studies on protolith estimation, the type of protolith was identified by discrimination diagrams, yet, quantitative estimation of the protolith composition was not performed. On the other hand, in recent years, the use of machine learning has been increasing in the geochemistry field due to technological advances in programming languages and machine learning (eg, Kuwatani et al., 2014; Harsterok et al., 2019). However, there has been no application of machine learning to the problem of quantitative estimation of geochemical composition data, and it is necessary to establish a new method.

In this study, we aimed to quantitatively evaluate geochemical processes by estimating the composition of basalt, which is the protolith of metamorphic rocks. Geochemical processes of metamorphic rocks include weathering and metamorphism. Elements transferred by these processes are Rb, Ba, Sr, Ce, etc., and elements are not transferred are Nb, La, P, Nd, Zr, Ti, Y, etc. (e.g., Ludden 1979; Uno et al., 2014; Kessel et al., 2005). Therefore, Rb, Ba, Sr, and Ce were defined as mobile elements, and Nb, La, P, Nd, Zr, Ti, and Y were defined as immobile elements.

The chemical composition of basalt, which is the protolith of metamorphic rocks, was used as the teaching data of the machine learning model. The chemical compositional data were compiled from PetDB. A machine learning model was constructed in which the input variable was the concentration of immobile elements and the output variable was the concentration of mobile elements. Since the concentration of immobile elements does not change between metamorphic rocks and protoliths, it is possible to estimate the "mobile element concentration of protoliths" by giving the "immobile element concentration of metamorphic rocks" as an input variable to the machine learning model. LightGBM, an ensemble of decision trees, was used as the machine learning algorithm.

As a result, it was possible to construct a model that estimates the Rb, Ba, Sr, and Ce concentrations of protolith within an error of 10% to 20%. When metamorphic rocks are actually applied to the model, a significant difference is derived between the “metamorphic rock composition” and the “estimated protolith composition”, and this significant difference is considered to be the amount of mass transfer by geochemical processes during metamorphism. Therefore, the machine learning model, constructed by decision trees with LightGBM algorisms, is effective for estimating the mobile element concentration from the immobile element concentration. Our model can quantitatively evaluate geochemical processes during metamorphism when applied to compositional data of metamorphic rocks.

Keywords: Machine Learning, Fluid rock interaction, Metamorphism, Mass transfer, Protolith estimation

