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Statistical classification of mineral chemistry: identification of mineral facies by random forest method

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Assemblage, modal composition, and spatial distribution of minerals within rocks are important to recognize the petrogenesis of the rocks. Although many attempts have been done to obtain such information of minerals by statistical and empirical methods (e.g. Kikuchi, 1991; Launeau et al., 1994; Togami et al., 1998, 2000; Maloy and Treiman, 2007; Tsuji et al., 2009), these methods are successful only when the mineral assemblages in the rocks are known, that is, rock types are limited. To overcome this limitation, we tried to classify mineral facies for unlimited rock types.

We employed the random forest (RF) method (Breiman, 2001), which is a kind of the ensemble learning method based on classification trees generated by bootstrap sampling, to classify mineral facies from their chemical compositions. Over 3500 chemical compositions of 72 mineral groups from Deer, Howie and Zussman's "Rock-forming minerals" book series (e.g. Deer et al., 2001) were prepared for supervised data for the RF method. The data contain 38 variables of weight-percent of oxide components such as SiO_2, Al_2O_3 and so on. All Fe and Mn were converted into FeO* and MnO*, respectively.

The result of the RF analysis shows that the total error rate of the classification by 38 components of oxides is only 7.9-8.3% in both weighted and non-weighted classifying of supervised data and the only 9 major oxides, SiO_2, TiO_2, Al_2O_3, FeO*, MnO*, MgO, CaO, K_2O, and Na_2O are important to classify the mineral facies. Further RF analysis only by these 9 major oxides successfully classify the mineral facies in the error rate of 8.0-8.6%, almost same when using all the 38 oxides. This implies that the mineral facies for unknown compositions of minerals can be predicted only by the 9 major oxides with the RF classifier. We will show how RF mineral classifier works to predict the mineral facies from the data in some literatures and chemical maps by an electron probe microanalyzer.

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