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Interpretable Machine Learning to Predict Mantle Metasomatism Worldwide

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Clinopyroxene major and trace element compositions document their physicochemical evolution and have been widely used to detect mantle metasomatism. Classical methods typically rely on one or several elemental ratios such as Ca/Al, Mg/Fe, La/Yb, and Ti/Eu to determine whether rocks or minerals have been metasomatized. Each of these methods proves useful at specific sites, but not at the global scale. In this study, we used machine learning methods to classify chemical compositions of clinopyroxenes from mantle xenoliths and examine their relationship with mantle metasomatism. We compiled major element data from 8,713 clinopyroxene samples (21,605 analyses) and trace element data from 1,235 clinopyroxene samples (2,967 analyses). Samples were labeled as “positive” if affected by patent metasomatism based on petrographic evidence, “negative” if they were unaffected by metasomatism, or left unlabeled if neither case applied. We then trained an XGBoost machine learning model which achieved higher accuracy than traditional methods using a limited number of elemental ratios. Our results identify a large number of locations with high mean probability of mantle metasomatism and show variability in the probability distributions observed across locations worldwide. These results show that metasomatism may be globally widespread, but the probability of metasomatism is not correlated with geophysical parameters (such as, crustal or lithospheric thickness, mantle *S*-wave velocity). Hence, the spatial distribution of metasomatism appears mainly driven by stochastic processes.