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Application of independent component analysis to geochemistry

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One of the ultimate goals of geochemistry is to extract and understand the independent sources and processes that create the geochemical observations. Principal component analysis (PCA) has been regarded to be one of the most efficient ways to deduce them from the observations, and has been used widely in various kinds of geochemical studies. However, it has a fundamental problem: principal components are independent only when the data distribution follows the Gaussian distribution, which is not in general the case. Independent Component Analysis (ICA) is the method to deconvolve a data set into independent components that maximize the non-Gaussianity of the projected distribution of the data, and has developed in Information Science in the last 15 years or so (see, e.g., Hyvarinen et al., 2001). Although this method is suitable for the geochemical purposes raised above and is thought to be very useful, the application is almost none or very rare so far. In this paper, we will discuss the usefulness of ICA for geochemistry, and try to demonstrate several examples in which ICA works to deduce important features inherited in the observed data. One of such examples is the isotopic compositional space of oceanic basalts (Iwamori and Albarede, 2007). Isotopic variations in oceanic basalts indicate possible interactions among several distinct mantle components, such as DMM, EM, FOZO, C, HIMU, etc. Increasing number of data for various isotopic systems now allows us to systematically search the structure hidden in the multivariate compositional space by ICA. Based on ICA, we have explored the isotopic compositional space of the oceanic basalts from Atlantic and South Indian Oceans, based on the data from literature and GEOROC database. We show that the two independent compositional vectors/directions (referred to as independent components or ICs) are involved to create the variations with five isotopic ratios of Pb, Sr and Nd. One of the two ICs clearly divides OIBs and MORBs, while another IC distinguishes the geographical distribution including DUPAL anomaly. This feature supports that the two ICs are indeed independent. We also show that the conventional mantle end-components are not appropriate to represent the compositional space. Instead, two independent processes that create the compositional space are proposed to explain the observations. Since the average composition of the oceanic basalts is similar to that of a DMM, around which MORBs and OIBs are roughly symmetrically distributed in the IC space, we argue that these processes occur as two dominant but independent differentiation processes within the depleted mantle domain. Considering these nature, one IC is likely to be produced by recycling and stirring of MORB and its residue, while another IC is possibly created by the subduction zone processes. According to the ICs, the criterion of DUPAL anomaly is re-defined. As a result, distribution of the enriched region is modified, showing that the enriched signature disperses into the northern hemisphere. By tracing the detected subduction-related signature, we are able to trace the mantle flow in the past, which bring new insights into the studies of mantle dynamics and the evolution of the Earth.