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Unmixing river sediments for the elemental geochemistry of their source-regions

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The geochemistry of river sediments is frequently used to infer processes occurring upstream such as chemical weathering and erosion. However, a quantitative scheme to relate downstream sediment geochemistry to the geochemistry of source-regions is lacking. Here, we describe an inverse methodology to 'unmix' fluvial sediments from higher-order river channels to produce a geochemical map of their source-regions. To test our scheme we consider a case-study in the Cairngorms mountain range, UK. We gathered 67 fine-grained (< 150 µm) sediment samples from the five major drainage basins including both trunks and tributaries, over an area spanning ~14,000 km^2. The elemental geochemistry of the sampled sediments was then measured by ICP-MS following mixed-acid digestion. Our goal is to produce a geochemical map of the ~14,000 km^2 study area using the 67 sediment samples we gathered. We start with the assumption (supported by previous studies) that downstream sediment geochemistry in our region is a conservative mixture of the source-region (e.g. weathering happens in-situ, not in-transit). Hence, it is possible to predict the downstream sediment geochemistry as a mixture of the source-region geochemistry, given the structure of the drainage network. This structure can be extracted from digital elevation data. We are therefore able to transform a geochemical map of the source-region into a prediction of the composition of sediments downstream. For each analysed element, we then seek the source-region geochemistry that best fits the point observations downstream, i.e. the 67 sediment samples. This optimisation problem is solved using the Nelder-Mead algorithm. We seek spatially smooth solutions. Synthetic examples, where we attempt to reconstruct a known synthetic input, indicate that our scheme is able to recover long-wavelength (>20 km) spatial geochemical patterns in the source-region. Predicted source-region compositions, generated by unmixing real data, are assessed using the independent G-BASE survey, which contains ~8,000 substrate samples across the studied region. This test shows that we can make meaningful predictions of major and trace elements including Mg, U, K, Sr, Ti. We propose that this scheme is a low-cost way to produce geochemical maps for use in environmental monitoring and geochemical exploration.