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Pushing forward population comparison tests in geochemistry: the take-home rerollR package

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Along with obtaining the most accurate data, obtaining the most precise measurements is often decisive to address the questions probed by modern geochemistry. However, uncertainty metrics and resulting confidence intervals (e.g. expressed around isotopic ratios and δ values) are not effectively standardized in our community. For example, while some favor the use of standard deviation or standard error, others advocate for the use of the more comprehensive standard u uncertainties (commonly in the form of expended U uncertainties). If this debate is important, the question of how to propagate these uncertainties to population-scaled questions is often largely overlooked. This is problematic, because addressing population-scaled questions has widely gained in popularity and feasibility during the last decades, and because this is a key aspect of many emerging applications of geochemistry, notably in ecology, paleontology, archaeology and biomedicine.

Quite often, questions addressed by geochemists at the population scale involve discussing differences (or an absence of differences) between studied populations of samples (or individuals). In such situations, methods such as t-test, Wilcoxon rank-sum test or randomization tests are pivotal. However, using such methods commonly imply to neglect intra-sample uncertainties, for example by processing only the mean δ values of the samples within the test. This is a good approximation in some situations, typically when intra-sample data uncertainties are small compared to intra-population data dispersion and homogeneous within the populations, and when the number of samples per population is high, but these conditions are not always met in real life geochemistry.

Using the power of post-hoc resampling and statistical distributions, the *rerollR* package (R-based) provides a quick and user-friendly way to account for individual uncertainties when comparing population of isotope data. In essence, this package uses individual uncertainties to recursively simulate alternate populations in a statistically representative manner. These simulated populations are compared using the test selected by the user (e.g. t-test) and the package delivers a metric and graph assessing test result's robustness. This open-access R package is designed to allow every geochemist, even with a minimal R experience, to improve their decision-making in addressing isotope population-scaled questions for any isotopic system.