Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.15636

The isoWater R-package: Open-source software for isotope hydrology

GABRIEL BOWEN

University of Utah

Presenting Author: gabe.bowen@utah.edu

Stable isotopes of H and O in water have been used for nearly 70 years to advance our understanding of the global water cycle, hydrological processes, and water resources. Over that time, technological advances have supported dramatic increases in the production of data, creating new opportunities for applications at new scales and in new systems. This growth in the field has created a pressing demand for data sharing and reuse, as well as analysis tools that support work with large datasets and implementation of a ever-growing range of data analysis methods.

The isoWater R-package is an open-source software tool that grew organically in response to the research demands of the developers, and thus fits the "Geoscientists' Little Helpers" paradigm. I will present the story of the software's origins and capabilities. The package facilitates data access and analysis in isotope hydrology, and currently includes two main tool sets. The first supports querying and accessing data from the Waterisotopes Database (wiDB), an open, community-engaged, global compilation of water isotope data spanning all hydrological systems. These tools use RESTful web services to submit user-authored queries via the wiDB API and receive and unpack data objects directly into the R environment. The second tool set supports analysis of water isotope data for the common problem of water source determination using a family of Bayesian hierarchical modeling frameworks. Different implementations of these tools allow the source of one or more water samples to be characterized in terms of its isotopic composition (constrained by a Local Meteoric Water Line) or as a mixture of two or more endmembers; in both cases (potential) isotopic fractionation of the water sample(s) due to evaporation is considered.

The isoWater package and an introductory vignette are available in the CRAN repository (https://cran.r-project.org/package=isoWater), and development versions are hosted in a public GitHub repository (https://github.com/SPATIAL-Lab/isoWater). We welcome all community contributions, including requests for features, identification of issues, and pull requests.