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spant: An R package for magnetic resonance spectroscopy analysis

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Software

- Review
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Summary

Magnetic Resonance Spectroscopy (MRS) allows the measurement of small molecules (metabolites) in the body without the use of harmful radiation. Based on the same basic principles and technology behind Magnetic Resonance Imaging (MRI), most modern MRI scanners are also capable of acquiring MRS — making the technique highly suited to a number of clinical applications (Oz et al. (2014)). Despite the success of MRS in the research environment, clinical translation has proven slow due to a number of technical and practical reasons, with challenges associated with reliable data processing and analysis having particular importance (Wilson et al. (2019)). The `spant` (SPectroscopy ANalysis Tools) package has been developed to: (1) provide open-source implementations of traditional and modern MRS processing and analysis techniques for routine analysis (Near et al. (2021)) and (2) aid the development, validation and comparison of new algorithms and analysis pipelines.

Statement of need

Traditional MRS analysis was dominated by the use of proprietary software, either supplied by scanner manufactures or offline tools such as LCModel (Provencher (1993)) and jMRUI (Naressi et al. (2001)). In more recent years there has been a steadily increasing trend toward the use of open-source methods — with some early examples including TARQUIN (Reynolds et al. (2006); Wilson et al. (2011)) and AQSES (Poullet et al. (2007)). This trend is set to continue with the recent transition of LCModel to an open-source license, and an acceleration in the development of new open-source methods and packages such as Vespa (Soher et al. (2011)), Gannet (Edden et al. (2014)), FID-A (Simpson et al. (2017)), Osprey (Oeltzschner et al. (2020)), suspect (Rowland (2021)) and FSL-MRS (Clarke et al. (2021)). The availability of the MRSHub (https://mrshub.org/), a new community orientated software sharing and support platform, and the recent development of the NIfTI MRS file format (Clarke & Wilson (2021)), to aid data sharing and interoperability, are set to further enhance the ecosystem of open-source MRS analysis tools.

The vast majority of recently developed open-source MRS analysis tools have been written in either MATLAB or Python. Whilst all languages have strengths and weaknesses, R is particularly suited to the interactive exploration and batch processing of large and complex datasets — typical of MRS and neuroimaging studies. For example, the acquisition and storage of high dimensional datasets, including three spatial axes, chemical shift and coil axes are becoming more common for MRS. For a typical study, these scans may be acquired at multiple time-points for multiple participants split across one or more groups (e.g. control and treatment) - requiring both single subject and group level analyses.

The spant package was developed to combine traditional and modern MRS data processing techniques with strengths of R, including: plotting/visualization, statistics, machine learning and data wrangling. Furthermore, spant may be used to conveniently combine MRS results with other imaging modalities, due to the availability of a wide range of R packages focused on image processing (Muschelli et al. (2019)) and support for the NIfTI data format (Whitcher et al. (2011); Clayden et al. (2021)). spant also supports the majority of common MR vendor data formats allowing complete pipelines to be developed, from raw time-domain samples to metabolite quantities derived from spectral fitting.

spant is part of the MRSHub, demonstrating its acceptance and interest from the MRS community. At the time of writing, spant has been used to develop and validate two new MRS spectroscopy analysis algorithms: RATS (Wilson (2019)) and ABfit (Wilson (2021)), and has also been used to study cancer (Franco et al. (2021)), Alzheimer's Disease (Montal et al. (2021)) and psychosis (Fisher et al. (2020)) — confirming its suitability for both MRS methods research and clinical studies.

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