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ultrasphere and ultrasphere-harmonics: Python packages for Vilenkin–Kuznetsov–Smorodinsky polyspherical coordinates and hyperspherical harmonics methods in array API

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Summary

Spherical harmonics, which are the solutions to the angular part of the laplace equation, have been widely used in various fields of science and engineering. Spherical harmonics in 3D are well-known Especially, hyperspherical harmonics, which are spherical harmonics in higher dimensions, have been applied to many-body problems in quantum mechanics (Fock, 1935), representation of crystallographic textures (Bonvallet et al., 2007), description of 3D models (Bonvallet et al., 2007), representation of brain structures (Hosseinbor et al., 2013), representation of the Head-Related Transfer Function, which characterizes how an ear receives a sound from a point in space (Szwajcowski, 2023), and so on.

Statement of need

`ultrasphere` is a Python package for Vilenkin–Kuznetsov–Smorodinsky polyspherical coordinate systems (Vilenkin & Klimyk, 1993). `ultrasphere-harmonics` implements hyperspherical harmonics methods for any type of polyspherical coordinates based on `ultrasphere`. The main goal of these packages is to provide a unified framework for implementing spherical harmonics techniques in arbitrary dimensions and coordinate systems. This would allow researchers to easily extend their work to higher dimensions, for example, from 2D to 3D and further to 4D, without having to duplicate code for each dimension. To demonstrate this, we implemented code for solving acoustic scattering from a single sound-soft sphere using any type of polyspherical coordinates as a command-line application.

Spherical expansion methods are sometimes computationally expensive, especially in higher dimensions. To address the recent diversification of HPC environment, our api is made to be compatible with the array API standard (Meurer et al., 2023), which enables writing code which runs on multiple array libraries (e.g., NumPy(Harris et al., 2020), PyTorch(Paszke et al., 2019)) and multiple hardware (e.g., CPU, GPU). Our packages fully support vectorization to leverage the performance of these libraries.

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