

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 and have various applications, and many software packages have been developed for them. 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 (Hosseini et al., 2013), representation of the Head-Related Transfer Function, which characterizes how an ear receives a sound from a point in space (Szwajkowski, 2023), and so on. However, an attempt to develop a framework which allows codes to work on both 3D and higher dimensions has not been made. Therefore, we aim to provide a unified framework for implementing spherical harmonics techniques in arbitrary dimensions and coordinate systems. Our packages 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.

Statement of need

ultrasphere is a Python package for Vilenkin–Kuznetsov–Smorodinsky (VKS) polyspherical coordinate systems (Cohl, 2012; Vilenkin & Klimyk, 1993). ultrasphere-harmonics implements hyperspherical harmonics methods for any type of polyspherical coordinates based on ultrasphere. While spherical harmonics in 3D itself have been widely implemented in various software packages, such as Scipy (Virtanen et al., 2020), hyperspherical harmonics are rarely implemented, and software packages which supports arbitrary VKS polyspherical coordinates are not known. To remedy this, our packages allows to convert between Cartesian coordinates and VKS polyspherical coordinates, compute hyperspherical harmonics, elementary solutions to the Helmholtz equation, hyperspherical expansion of a function, and the translational coefficients of elementary solutions of the Helmholtz equation under arbitrary VKS polyspherical coordinates and dimensions. Our package especially utilizes NetworkX (Hagberg et al., 2008) to make use of the rooted tree representation of VKS polyspherical coordinates, which is known as “method of trees”. To illustrate the usage of our packages, example code for solving acoustic scattering from a single sound-soft sphere using any type of VKS polyspherical coordinates is implemented in ultrasphere-harmonics as a command-line application.

Spherical expansion methods are sometimes computationally expensive, especially in higher dimensions. To utilize HPC resources, which environment is recently diversified, 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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