$S_n$FFT: A Julia Toolkit for Fourier Analysis of Functions over Permutations

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Abstract

$S_n$FFT is an easy to use software library written in the Julia language to facilitate Fourier analysis on the symmetric group (set of permutations) of degree $n$, denoted $S_n$, and make it more easily deployable within statistical machine learning algorithms. Our implementation internally creates the irreducible matrix representations of $S_n$, and efficiently computes fast Fourier transforms (FFTs) and inverse fast Fourier transforms (iFFTs). Advanced users can achieve scalability and promising practical performance by exploiting various other forms of sparsity. Further, the library also supports the partial inverse Fourier transforms which utilizes the smoothness properties of functions by maintaining only the first few Fourier coefficients. Out of the box, $S_n$FFT currently offers two non-trivial operations for functions defined on $S_n$, namely convolution and correlation. While the potential applicability of $S_n$FFT is fairly broad, as an example, we show how it can be used for clustering ranked data, where each ranking is modeled as a distribution on $S_n$.

Keywords: permutations, Fourier analysis, fast Fourier transform, Julia

1. Introduction

Over the last few years, there has been a growing interest in the analysis of data given (or expressed) as a probability distribution over permutations. The set of all possible permutations of $n$ elements constitutes a group called the symmetric group, denoted $S_n$. Several recent solutions to ranking problems, hard combinatorial problems, multi-target tracking and feature point matching tasks (in computer vision) have used harmonic analysis on $S_n$ to derive more efficient algorithms (Huang et al., 2009; Kondor, 2010; Pachauri et al., 2012). While the idea of generalizing the Fourier transform to non-commutative groups is well established in the Mathematics literature, an easy to use and accessible software library will facilitate the adoption of such concepts within machine learning. In this paper, we describe a Julia based open source library which implements the Fourier transform (and associated functionality) for harmonic analysis of functions defined on $S_n$. ©2015 Gregory Plumb, Deepti Pachauri, Risi Kondor and Vikas Singh.
The implementation can use a multi-core cluster (when available) without any need for low-level message passing interface (MPI) programming.

Harmonic analysis on $S_n$ is defined via the notion of representations. A matrix valued function $\rho: S_n \rightarrow \mathbb{C}^{d_\rho \times d_\rho}$ is said to be a $d_\rho$ dimensional representation of the symmetric group if $\rho(\sigma_2)\rho(\sigma_1) = \rho(\sigma_2\sigma_1)$ for any pair of permutations $\sigma_1, \sigma_2 \in S_n$. A representation $\rho$ is said to be reducible if there exists a unitary basis transformation which simultaneously block diagonalizes each $\rho(\sigma)$ matrix into a direct sum of lower dimensional representations. If $\rho$ is not reducible, then it is said to be irreducible. Irreducible representations or irreps are the elementary building blocks of all of $S_n$'s representations. A complete set of inequivalent irreducible representations are denoted by $\mathcal{R}$. The Fourier transform of a function $f: S_n \rightarrow \mathbb{C}$ is then defined as the sequence of matrices

$$\hat{f}(\rho) = \sum_{\sigma \in S_n} f(\sigma)\rho(\sigma) \quad \rho \in \mathcal{R}.$$  

The inverse transform is

$$f(\sigma) = \frac{1}{n!} \sum_{\rho \in \mathcal{R}} d_\rho \text{tr}[\hat{f}(\rho)\rho(\sigma)^{-1}] \quad \sigma \in S_n.$$  

Much of the practical interest in Fourier transform can be attributed to various interesting properties of irreps, such as conjugacy and unitarity.

1.1 The Irreducible Representation of $S_n$

There are several ways to construct irreducible representation of $S_n$ (Sagan, 2001). One such representation is called Young’s orthogonal representation (YOR). The YOR matrices are real and unitary and therefore orthogonal. To benefit from the computational advantages of orthogonal matrices, $S_n$ FFT uses YOR internally. In the online documentation, we provide a short review of the technical background relevant for constructing YORs.

2. $S_n$ FFT Toolkit

$S_n$ FFT is implemented in a high-level programming language called Julia (provided under a MIT license). The most important features of the toolkit are accessibility, extensibility, and performance. The toolkit and the required documentation is available at: https://github.com/GDPlumb/SnFFT.jl/.

Accessibility. We placed a great deal of emphasis on the ease of use of the toolkit. This will allow a non-specialist (in harmonic analysis) to utilize the functionality of this library within standard machine learning algorithms, when analyzing data on $S_n$. In particular, the full functionality of $S_n$ FFT is available simply by loading the package “SnFFT” through Julia’s built in package manager. The $S_n$ FFT user manual provides many examples demonstrating the syntax for accessing the various features of $S_n$ FFT and gives a high level overview of the key properties of YOR matrices and the Fourier transform. The minimalist design and coding consistency makes $S_n$ FFT easy to use and modify.
Extensibility. Interoperability is a key component of Julia — it allows easy access to various pre-existing high quality and mature libraries written in many other languages with minimal additional overhead. Therefore, various machine learning libraries can be easily incorporated into $S_n$FFT projects. For example, C and Fortran functions can be called directly from $S_n$FFT projects without any “glue” code.

$S_n$FFT allows access to external libraries written in languages such as Python, Java, and R, by easily passing the data to these libraries.

Finally, Julia code can be called directly from C/C++. As a result, $S_n$FFT can be used seamlessly within existing machine learning tools as needed.

Parallelism. $S_n$FFT inherits the parallelism offered by the Julia platform. It allows a multi-processing environment to run a code on multiple processes in separate memory domains concurrently. $S_n$FFT uses empirically derived rules to determine the trade-off between synchronization overhead for multithread computation and single thread sequential computation and proceeds with the best option. In our implementation, $S_n$FFT functions are designed to use all worker processes that a user makes available to Julia. This setup allows the user to analyze the data on a single process, on multiple processes on a local machine, or via multiple processes spread across a cluster with essentially no change to the user code beyond initially making the processes available.

Sparsity. For various practical applications, we encounter problems where $n$ is greater than 15. Even storing such data is problematic as $n!$ is $\sim 1$ trillion. Unless one exploits the smoothness/sparsity properties of $f$, computation will be intractable. But notice that often, problems exhibit interesting sparsity patterns (Kueh et al., 1999); for example, the Fourier transform of functions on homogeneous spaces of $S_n$ are usually band-limited in the sense that their Fourier transform is identically zero except for a small set of Fourier matrices. $S_n$FFT is designed to utilize such patterns, making it very efficient. Specifically, the function $\text{snfft.bl()}$ is implemented to offer significant efficiency benefits when the user a priori knows the band-limited form of $f$. For problems with unknown sparsity pattern, the special function $\text{snfft.sp()}$ first determines the sparsity structure of $f$ and then proceeds to the actual FFT calculation. Partial inverse Fourier transform is also supported in $S_n$FFT which is important to induce smoothness in $f$. In particular, function $\text{snifft.p()}$ can be used to approximate $f$ using just first few Fourier coefficients of the full Fourier transform.

2.1 Related Libraries

An existing library, $S_n\text{ob}$ described by (Kondor, 2006), motivated the work presented here and offers some of $S_n$FFT’s functionality but support for band-limited behavior of functions is limited in (Kondor, 2006). Further, our Julia implementation gives seamless access to both single and multiple processes and is easier to modify and extend. We believe that such parallelization features will be useful for scalability and integration within machine learning applications.
3. Example: Fourier Domain Features for Clustering Ranks

Consider a ranking dataset composed of $N$ examples where the $i^{th}$ instance ($i = 1, \cdots, N$), is a permutation $\sigma_i \in S_n$ of $n$ items, listed in order of preference. Given such data, we want to identify groups of examples with similar preferences, which may be helpful for a downstream preference behavior study or rank prediction applications, e.g., (Crammer et al., 2001). Various probabilistic models for ranking are popular in the research community such as Mallows model (Murphy and Martin, 2003), which nicely capture the variability in the observations when the observed rankings are noisy or incomplete (Busse et al., 2007).

Typically, the $i^{th}$ instance is represented as a function $f_i(\sigma) = \frac{e^{-\gamma d(\sigma_i, \sigma)}}{Z_\gamma}$ on $S_n$. Here, $\gamma$ is the spread parameter, $d(\ldots)$ is a valid distance metric on permutations, and $Z_\gamma$ is the normalization constant. The clustering problem seeks to partition the dataset into $K$ clusters to minimize the following objective:

$$\arg \min_{C_1, \ldots, C_K} \sum_{k=1}^K \sum_{1 \leq i, j \leq N: (i,j) \in C_k} \| f_i - f_j \|^2 .$$  \hspace{1cm} (3)

A geometric view of functions defined on $S_n$ as embedded in the space $[0,1]^n$ quickly becomes intractable and hard to interpret. On the other hand, the seminal work of (Diaconis, 1988) explains how the Fourier coefficients precisely encode the structural properties of the distributions on $S_n$. Following ideas described in (Diaconis, 1988), recently, (Clémencçon et al., 2011) introduced a Fourier space formulation equivalent to (3)

$$= \frac{1}{n!} \sum_{\rho \in \mathcal{R}} d_\rho \sum_{k=1}^K \sum_{1 \leq i, j \leq N: (i,j) \in C_k} \| \hat{f}_i(\rho) - \hat{f}_j(\rho) \|_{HS(d_\rho)}^2 .$$  \hspace{1cm} (4)

Further, they used a specialized feature selection procedure for clustering the induced spectral features as in (Witten and Tibshirani, 2010) and showed that frequently one only needs a few spectral features to explain the clustering choices. In $S_n$FFT, only a few lines of code are needed to compute the Fourier transforms, convert them into a data matrix, and pass the data matrix to R’s sparcl library to perform this clustering. The details of the process can be found in the code of `example_clustering()`.

The foregoing example shows that $S_n$FFT is fairly flexible and can be used with advanced machine learning libraries for data analysis on $S_n$. Some example applications which may benefit directly in the short term include multi-object tracking (identity management problem) (Kondor et al., 2007), event based modeling for longitudinal measurements (Huang and Alexander, 2012) and deriving image associations for structure from motion (Pachauri et al., 2014). Some of these applications are described in more detail in the documentation.

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References


