User Manual for FFTLog and Beyond

Xiao Fang

1 Problem Description

The integral we are solving is

$$F(y) = \int_0^\infty \frac{dx}{x} f(x) j_\ell^{(n)}(xy) , \qquad (1)$$

where f(x) is an input of array, j_{ℓ} is the order- ℓ spherical Bessel function of the first kind, the superscript ⁽ⁿ⁾ denotes the order of derivative. This type of integrals are numerically challenging due to the rapidly oscillitory nature of the spherical Bessel functions, especially when the input f(x) data array correspond to sampling array x over a large range (*i.e.*, over several orders of magnitude).

2 Efficient Computation with FFTLog-and-Beyond

The essential idea is to expand f(x) into a series of power-laws and solve each component integral analytically. We require a logarithmic sampling of x with linear spacing in $\ln(x)$ equal to $\Delta_{\ln x}$, i.e., $x_q = x_0 \exp(q\Delta_{\ln x})$ with x_0 being the smallest value in the x array. The power-law decomposition then means

$$f(x_q) = \frac{1}{N} \sum_{m=-N/2}^{N/2} c_m x_0^{\nu} \left(\frac{x_q}{x_0}\right)^{\nu + i\eta_m} , \qquad (2)$$

where N is the sample size of the input function, $\eta_m = 2\pi m/(N\Delta_{\ln x})$, and ν is the bias index. The Fourier coefficients satisfy $c_m^* = c_{-m}$ since function f(x) is real, and are computed by discrete Fourier transforming the "biased" input function $f(x)/x^{\nu}$ as

$$c_m = W_m \sum_{q=0}^{N-1} \frac{f(x_q)}{x_q^{\nu}} e^{-2\pi i mq/N} , \qquad (3)$$

where W_m is a window function which smooths the edges of the c_m array and takes the form of Eq. (C.1) in McEwen et al (2016, arXiv: 1603.04826). This filtering is found to reduce the ringing effects.

Each term is now analytically solvable. For n = 0, *i.e.* no derivative,

$$F(y) = \frac{1}{Ny^{\nu}} \sum_{m=-N/2}^{N/2} c_m x_0^{-i\eta_m} y^{-i\eta_m} \int_0^{\infty} \frac{dx}{x} x^{\nu+i\eta_m} j_{\ell}(x)$$

$$= \frac{\sqrt{\pi}}{4Ny^{\nu}} \sum_{m=-N/2}^{N/2} c_m x_0^{-i\eta_m} y^{-i\eta_m} g_{\ell}(\nu+i\eta_m) , \qquad (4)$$

where the first equality uses change of variable $xy \to x$. Function $q_{\ell}(z)$ is given by

$$g_{\ell}(z) = 2^{z} \frac{\Gamma\left(\frac{\ell+z}{2}\right)}{\Gamma\left(\frac{3+\ell-z}{2}\right)} , \quad -\ell < \Re(z) < 2 , \tag{5}$$

giving the range of bias index $-\ell < \nu < 2$.

Finally, assuming that y is logarithmically sampled with the same linear spacing $\Delta_{\ln y} = \Delta_{\ln x}$ in $\ln y$, we can write the last summation in Eq. (4) as

$$F(y_p) = \frac{\sqrt{\pi}}{4y_p^{\nu}} \text{IFFT} \left[c_m^*(x_0 y_0)^{i\eta_m} g_{\ell}(\nu - i\eta_m) \right] , \qquad (6)$$

where y_p $(p = 0, 1, \dots, N - 1)$ is the p-th element in the y array. IFFT stands for the Inverse Fast Fourier Transform. In summary, this method performs two FFT operations, one in computing c_m , one in the final summation over m. Thus, the total time complexity is $\mathcal{O}(N \log N)$. So far we have described the principle of the FFTLog algorithm.

For n > 0, following the same procedure of power-law decomposition, we have

$$F_n(y) = \frac{1}{Ny^{\nu}} \sum_{m=-N/2}^{N/2} c_m x_0^{-i\eta_m} y^{-i\eta_m} \int_0^{\infty} \frac{dx}{x} x^{\nu+i\eta_m} j_{\ell}^{(n)}(x) . \tag{7}$$

Again, the integral for each m has an analytic solution, which can be shown with integration by parts. We write the solution in the same form with the FFTLog, i.e.,

$$F_n(y) = \frac{\sqrt{\pi}}{4Ny^{\nu}} \sum_{m=-N/2}^{N/2} c_m x_0^{-i\eta_m} y^{-i\eta_m} \tilde{g}_{\ell}(n, \nu + i\eta_m) , \qquad (8)$$

and its discrete version assuming $\Delta_{\ln y} = \Delta_{\ln x}$,

$$F_n(y_p) = \frac{\sqrt{\pi}}{4y_p^{\nu}} \text{IFFT} \left[c_m^*(x_0 y_0)^{i\eta_m} \tilde{g}_{\ell}(n, \nu - i\eta_m) \right] , \qquad (9)$$

where $\tilde{g}_{\ell}(n,z) = 4\pi^{-1/2} \int_0^\infty dx \, x^{z-1} j_{\ell}^{(n)}(x)$. For n = 0, $\tilde{g}_{\ell}(0,z) = g_{\ell}(z)$, and for n = 1, 2, it is given by

$$\tilde{g}_{\ell}(1,z) = -2^{z-1}(z-1)\frac{\Gamma\left(\frac{\ell+z-1}{2}\right)}{\Gamma\left(\frac{4+\ell-z}{2}\right)} , \quad \begin{pmatrix} 0 < \Re(z) < 2, & \text{for } \ell = 0\\ 1 - \ell < \Re(z) < 2, & \text{for } \ell \ge 1 \end{pmatrix} , \tag{10}$$

$$\tilde{g}_{\ell}(2,z) = 2^{z-2}(z-1)(z-2)\frac{\Gamma\left(\frac{\ell+z-2}{2}\right)}{\Gamma\left(\frac{5+\ell-z}{2}\right)} , \quad \left(\begin{array}{c} -\ell < \Re(z) < 2 , & \text{for } \ell = 0, 1 \\ 2 - \ell < \Re(z) < 2 , & \text{for } \ell \ge 2 \end{array}\right) . \tag{11}$$

We choose $\nu = 1$ for all ℓ 's. With this generalized FFTLog algorithm, the integral containing one derivative of a spherical Bessel function also takes 2 FFT operations to compute.

Most generally, for $n \in \mathcal{N}$,

$$\int_0^\infty dx \, x^{\alpha - 1} j_\ell^{(n)}(x) = (-1)^n \frac{\sqrt{\pi}}{4} 2^{\alpha - n} \frac{\Gamma(\alpha)}{\Gamma(\alpha - n)} \frac{\Gamma(\frac{\ell + \alpha - n}{2})}{\Gamma(\frac{3 + n + \ell - \alpha}{2})} \,, \quad \left(\begin{array}{c} -\ell < \Re(\alpha) < 2 \,, & \text{for } \ell < n \\ n - \ell < \Re(\alpha) < 2 \,, & \text{for } \ell \ge n \end{array} \right). \tag{12}$$

3 Using the Code

This repository contains independent python module and C module for computing Eq. (1).

3.1 Python Version

The main code is all in python/fftlog.py, along with python/test.py which provides an example of calling the module to compute the integrals with f(x) being the power spectrum in Pk_test, and n = 0, 1, 2, respectively. We also have a Hankel function, defined as replacing j_{ℓ} as J_n in Eq. (1). If you find them useful in your research, please cite Fang et al (2019).

3.2 C Version

The code, sitting in cfftlog folder, uses FFTW library. The main code is in cfftlog.c, with auxiliary functions (e.g., extrapolation, window function, g_{ℓ} functions) defined in utils.c and utils_complex.c.

cfftlog.c provides different ways to run the computation. cfftlog provides the simplest usage. cfftlog_ells function enables to compute the same integral with an array of ℓ values. This is more optimal than calling single function cfftlog many times since FFTW plans have to be re-created and destroyed over and over again, and same for the FFTW_COMPLEX arrays used for the FFTs.

cfftlog_ells_increment does the same thing as cfftlog_ells, but increment the results (instead of refreshing). This saves memory for some applications.

test.c and test ells.c show examples of calling those functions.