Fourier Conventions

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1 Continuous case

In the continuum, the density contrast $\delta(\mathbf{x})$ and its Fourier transform $\delta(\mathbf{k})$ are related through

$$\delta(\mathbf{x}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\delta(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}},$$
$$\delta(\mathbf{k}) = \int \mathrm{d}^3x \; \delta(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

Reality of $\delta(\mathbf{x})$ ensures that $\delta(\mathbf{k}) = \delta(-\mathbf{k})^*$. The power spectrum $P(k)$ satisfies

$$\langle\delta(\mathbf{k})\delta(\mathbf{k}')^*\rangle = (2\pi)^3\delta^{(3)}(\mathbf{k}+\mathbf{k}')P(k).$$

and the related quantity $\Delta^2(k)$ is defined by[1]

$$\Delta^2(k) = \frac{k^3}{2\pi^2}P(k).$$

There is also σ_8, which is given by

$$\sigma_8^2 = \int \frac{\mathrm{d}^3k}{(2\pi)^3}P(k)|W(kR)|^2 = \int \frac{k^2\mathrm{d}k}{2\pi^2}P(k)|W(kR)|^2 = \int \frac{\mathrm{d}k}{k}\Delta^2(k)|W(kR)|^2,$$

where $R = 8$ Mpc/h is the filtering radius and $W(k)$ is the Fourier transform of the spherical top-hat filter

$$W(k) = W^{\mathrm{TH}}(k) = \frac{3}{k^3}\left[\sin(k) - k\cos(k)\right].$$

We may also want to use the cloud-in-cell window function, whose Fourier transform is given by

$$W^{\mathrm{CIC}}(\mathbf{k}) = \mathrm{sinc}^2\left(\frac{k_x}{2}\frac{L}{N}\right)\mathrm{sinc}^2\left(\frac{k_y}{2}\frac{L}{N}\right)\mathrm{sinc}^2\left(\frac{k_z}{2}\frac{L}{N}\right).$$

[1] This is such that $\langle\delta^2\rangle = \int \mathrm{d}\log k \; \Delta^2(k)$.

2 Discrete case

Now we restrict $\delta(\mathbf{x})$ to a cube with physical dimensions $L^3 = V$ and periodic boundary conditions. We introduce a grid of N^3 real triplets $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ whose (i, j, k) entry is given by

$$\mathbf{x}(i, j, k) = \frac{L}{N}(i, j, k), \qquad i, j, k = 0, \cdots, N-1.$$

The Fourier transform $\delta(\mathbf{k})$ is similarly realized on a grid of N^3 complex triplets[2] $\mathbf{k} = (k_x, k_y, k_z) \in \mathbb{C}^3$ given by

$$\mathbf{k}(i, j, k) = (f(i), f(j), f(k)), \qquad i, j, k = 0, \cdots, N-1,$$
$$f(i) = \begin{cases} 2\pi L^{-1} i & \text{if } i < \lfloor \frac{1}{2} N \rfloor, \\ 2\pi L^{-1}(i - N) & \text{if } i \geq \lfloor \frac{1}{2} N \rfloor. \end{cases}$$

For example, for constant i, j and $L = 1$ and even N, the k_x entries read $0, 2\pi, 4\pi, \cdots, (N-2)\pi, -N\pi, -(N-2)\pi, \cdots, -2\pi$.

Having set this up, the discrete Fourier transform relations are

$$\delta(\mathbf{x}) = \sum_{i,j,k} \frac{\delta(\mathbf{k})}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \Delta k_x \Delta k_y \Delta k_z = \left(\frac{1}{2\pi}\frac{2\pi}{L}\right)^3 \sum_{i,j,k} \delta(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} = \frac{1}{L^3} \sum_{i,j,k} \delta(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}},$$
$$\delta(\mathbf{k}) = \sum_{i,j,k} \delta(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \Delta x \Delta y \Delta z = \left(\frac{L}{N}\right)^3 \sum_{i,j,k} \delta(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}}.$$

To get the power spectrum, we also have to discretize the Dirac delta function into Kronecker delta functions:

$$\delta^{(3)}(\mathbf{k} + \mathbf{k}') = \left(\frac{L}{2\pi}\right)^3 \delta_{ii'} \delta_{jj'} \delta_{kk'},$$

where we used $\nabla \cdot \mathbf{k} = (2\pi L^{-1}, 2\pi L^{-1}, 2\pi L^{-1})$ and

$$\delta(f(x)) = \sum_{x_i:\, f(x_i)=0} \frac{1}{|f'(x_i)|} \delta(x - x_i).$$

We thus obtain

$$\langle \delta(\mathbf{k}) \delta(\mathbf{k}')^* \rangle = V \delta_{ii'} \delta_{jj'} \delta_{kk'} P(k).$$

This relation can be inverted to show how to generate a Gaussian random field

$$\delta(\mathbf{k}) = \sqrt{\frac{VP(k)}{2}}(a + bi),$$

[2] However, one can save memory by exploiting the $\delta(\mathbf{k}) = \delta(-\mathbf{k})^*$ relation like FFTW does.

where $a, b \sim \mathcal{N}(0,1)$.

To calculate the power spectrum from a grid of $\delta(\mathbf{k})$, we need to choose a certain number of momentum bins. Let k_b be a representative value for bin b and let N_b be the number of observations in that bin. Then a simple estimate for the power spectrum is

$$P(k_b) = \frac{1}{V}\frac{1}{N_b}\sum_{\mathbf{k}\in b}\delta(\mathbf{k})\delta(\mathbf{k})^*.$$

If the original density contrast $\delta(\mathbf{x})$ was obtained using cloud-in-cell interpolation, then it is appropriate to deconvolve the CIC window function by setting

$$\delta(\mathbf{k})^{\mathrm{real}} = \delta(\mathbf{k}) \cdot \frac{1}{W(k)}.$$

So our estimate for the power spectrum becomes

$$P(k_b) = \frac{1}{V}\frac{1}{N_b}\frac{1}{W(k)^2}\sum_{\mathbf{k}\in b}\delta(\mathbf{k})\delta(\mathbf{k})^*.$$

3 FFTW implementation

Finally, some remarks on how this can be handled with FFTW. FFTW computes unnormalized discrete Fourier transforms. That is,

$$\mathrm{FT}^{\mathrm{FFTW}}[\delta(\mathbf{x})] = \sum_{i,j,k}\delta(\mathbf{x})e^{i\mathbf{x}\cdot\mathbf{k}}$$
$$\mathrm{BFT}^{\mathrm{FFTW}}[\delta(\mathbf{k})] = \sum_{i,j,k}\delta(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}},$$

where BFT stands for Backward Fourier Transform. This means that if one computes a Fourier transform followed by a backward Fourier transform, one picks up a factor N^3. If one uses the r2c and c2r methods, then FFTW expects the complex array to be $N \times N \times (\lfloor N/2 \rfloor + 1)$, because $\delta(\mathbf{k}) = \delta(-\mathbf{k})^*$. If one uses the complex-to-complex methods, the full N^3 grid is needed.