Discrete Fourier Transforms

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Abstract

Here we give details on Green's functions and fourier transforms used in the in the Mathematica package MultipleScattering2D. One unusually feature in the package is that we use do a discrete Fourier transforms without including the zero frequency $\omega = 0$. The reason for avoiding $\omega = 0$ is for functions, like Hankel functions, which have a singularity at $\omega = 0$. The notebook `DiscreteFourierOffset.nb`, in the same directory, shows how to implement these methods and compares them with known analytic results.

Keywords: Discrete Fourier, Discrete offset Fourier, Greens functions

1 Incident wave

We look to solve the 3D wave equation

$$\mathcal{L}\{\varphi\}(\boldsymbol{x}, t) = \frac{1}{c^2}\frac{\partial^2 \varphi}{\partial t^2}(\boldsymbol{x}, t) - \nabla^2 \varphi(\boldsymbol{x}, t) = \frac{1}{c^2} B(\boldsymbol{x}, t), \tag{1}$$

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with the conditions

$$\varphi(\boldsymbol{x}, 0^-) = 0, \quad \dot{\varphi}(\boldsymbol{x}, 0^-) = 0 \quad \text{and} \quad \lim_{\|\boldsymbol{x}\| \to 0} \varphi(\boldsymbol{x}, t) = 0, \tag{2}$$

where B is the body force*. To solve this we use the Delta Dirac $\delta(\boldsymbol{x}) = \delta(x)\delta(y)\delta(z) = \delta(r)/(4\pi r^2)$ if r is the radius of a spherical coordinate system, and first solve the wave equation in spherical coordinates

$$\frac{1}{c^2}\frac{\partial^2 g}{\partial t^2} - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial g}{\partial r}\right) = \frac{\delta(r)}{4\pi r^2}\delta(t) \tag{3}$$

with $g(r,t) = 0$ for $t < 0$. This is not trivially solved, as when differentiating r^{-1} a distribution appears on the origin. The solution can be found in p. 92 Achenbach (1973)†

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$$g(r,t) = \frac{1}{4\pi r}\delta(t - r/c). \tag{4}$$

If we let $B(\boldsymbol{x}, t) = \delta(\boldsymbol{x})b(t)$, then the solution to Eq. (1) without a scatterer, i.e. for the incident wave, becomes

$$\varphi^I(\boldsymbol{x}, t) = \int g(\boldsymbol{x} - \boldsymbol{\xi}, t - \tau)\frac{1}{c^2}B(\boldsymbol{\xi}, \tau)d\boldsymbol{\xi}d\tau = \\ \int g(\boldsymbol{x} - \boldsymbol{\xi}, t - \tau)\frac{1}{c^2}\delta(\boldsymbol{\xi})b(\tau)d\boldsymbol{\xi}d\tau = \int \delta(t - \tau - r/c)\frac{b(\tau)}{4c^2\pi r}d\tau = \frac{b(t - r/c)}{4c^2\pi r}. \tag{5}$$

which is the solution to Eq. (1) because

$$\mathcal{L}\{\varphi^I\}(\boldsymbol{x}, t) = \int \mathcal{L}\{g\}(\boldsymbol{x} - \boldsymbol{\xi}, t - \tau)\frac{1}{c^2}B(\boldsymbol{\xi}, \tau)d\xi d\tau = \int \delta(\boldsymbol{x} - \boldsymbol{\xi}, t - \tau)\frac{1}{c^2}B(\boldsymbol{\xi}, \tau)d\xi d\tau = \frac{1}{c^2}B(\boldsymbol{x}, t).$$

*This B is technically only a body force for an elastic SH-wave. The interpretation of B depends on the physical interpretation of φ.

†There he changes to spherical coordinates, substitutes $\varphi(r,t) = \Phi(r,t)/r$, and with witchcraft solves the resulting scalar wave equation, picking only the outgoing wave

Let us adopt the Fourier transform convention:

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{f}(\omega)\mathrm{e}^{-\mathrm{i}\omega t}d\omega \quad \text{and} \quad \hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)\mathrm{e}^{\mathrm{i}\omega t}dt.$$

If we took one frequency $g(r,t) = \hat{g}(r,\omega)\mathrm{e}^{-\mathrm{i}\omega t}$ and solved for $\hat{g}$ with $B = c^2\mathrm{e}^{-\mathrm{i}\omega t}\delta(\boldsymbol{x})$, one frequency of $c^2\delta(\boldsymbol{x})\delta(t)$, the solution using only outgoing waves would be

$$\hat{g}(r,\omega) = \frac{\mathrm{e}^{\mathrm{i}kr}}{4\pi r}, \tag{6}$$

with $k = \omega/c$, which after a Fourier transform would give the causal 3D Greens function (4) as expected.

For the frequency decomposition of the 2D Greens function $\hat{g}_2$, we imagine that all functions will be independent of the z coordinate. So to use $\hat{g}$ in a convolution we need to first integrate over z:

$$\hat{g}_2 = \int_{-\infty}^{\infty} \hat{g}(r,\omega)dz = \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}k\sqrt{r^2+z^2}}}{4\pi\sqrt{r^2+z^2}}dz = \frac{\mathrm{i}}{4}H_0^{(1)}(kr), \tag{7}$$

where $r^2 = x^2 + y^2$ and $\hat{g}_2$ is an outgoing wave solution to

$$k^2\hat{g}_2 + \nabla_2^2\hat{g}_2 = -\delta(x)\delta(y), \tag{8}$$

where $\hat{B}(\boldsymbol{x},\omega) = c^2\delta(\boldsymbol{x})$ and ∇_2 is the gradient in x and y. Note that Graf's and Gegenbauer's addition formulas are very useful to rewrite any bessel or hankel function.

To calculate g_2 we can take the 3D Greens (4) substitute $r \to \sqrt{r^2+z^2}$ and integrate in z to get

$$g_2 = \int_{-\infty}^{\infty} \frac{\delta(ct - \sqrt{r^2+z^2})}{4\pi\sqrt{r^2+z^2}}c dz = \frac{c}{2\pi}\frac{H_s(t-|r|/c)}{\sqrt{c^2t^2-r^2}}, \tag{9}$$

where H_s is the Heavside step function, so that $H_s(t-|r|/c)$ is zero for $r > ct$.

We can now calculate the 2D incident wave for $B(\boldsymbol{x},t) = \delta(\boldsymbol{x})b(t)$ by using the procedure (5) for g_2 to find

$$\varphi^I(\boldsymbol{x},t) = \int_{-\infty}^{\infty} g_2(r,t-\tau)\frac{b(\tau)}{c^2}d\tau = \int_{|r|/c}^{\max\{t,\frac{|r|}{c}\}} \frac{1}{2\pi c}\frac{b(t-\tau)}{\sqrt{c^2\tau^2-r^2}}d\tau, \tag{10}$$

where we changed variables $\tau \leftarrow t-\tau$ so that we can differentiate the above expression in t more easily (specially numerically) and assumed that $b(-t)=0$ for $t>0$. Alternatively, Eq. (10) can also be written in terms of the Fourier transforms $\hat{g}_2(r,\omega)$ and $\hat{b}(\omega)$ as

$$\varphi^I(\boldsymbol{x},t) = \frac{1}{c^2}\int_{-\infty}^{\infty} g_2(r,\tau)b(t-\tau)d\tau = \frac{1}{2\pi c^2}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\hat{g}_2(r,\omega)\hat{b}(\omega)d\omega. \tag{11}$$

Assuming that $b(t)=0$ for $t \notin [0,T]$, then we turn into a numerical method by approximating $b(t)$ with its truncated Fourier series.

$$\varphi^I(\boldsymbol{x},t) \approx \frac{1}{Tc^2}\sum_{n=-N}^{N} \mathrm{e}^{-\mathrm{i}\frac{2\pi n}{T}t}\hat{g}_2(r,2\pi n/T)\hat{b}_N^n. \tag{12}$$

One issue is that $\hat{g}_2$ has a singularity at $\omega=0$. More generally, every Hankel function of the first type has a singularity at $\omega=0$, which we will deal with carefully in the next section.

1.1 The offset Discrete Fourier Transform

Approximating an impulse $b(t)$ with its truncated Fourier series $b_N(t)$ means that

$$b_N(t) = \frac{1}{T}\sum_{n=-N}^{N}\hat{b}_N^n\mathrm{e}^{-\mathrm{i}t\frac{2\pi n}{T}}, \quad \text{where } \hat{b}_N^n := \hat{b}_N\left(\frac{2\pi n}{T}\right) = \int_0^T b(t)\mathrm{e}^{\mathrm{i}\frac{2\pi nt}{T}}dt, \tag{13}$$

Alternatively we can fix $\omega_n = n\delta\omega$, so that $T = 2\pi/\delta\omega$ and $N = \Omega/\delta\omega$.

We can turn this into the discrete Fourier transform by using only the points

$$b_N^m := b_N\left(\frac{mT}{2N+1}\right) = \frac{1}{T}\sum_{n=-N}^{N}\hat{b}_N^n\mathrm{e}^{-2\pi\mathrm{i}\frac{mn}{2N+1}}, \tag{14}$$

for $m = 0, 1, \ldots, 2N$. We can now apply some linear algebra to extract the coefficients $T^{-1}\hat{b}_N^n$ of the vectors

$$(\boldsymbol{v}_n)^m := \mathrm{e}^{-2\pi\mathrm{i}\frac{mn}{2N+1}} \quad \text{for } n = 0, 1, \ldots 2N, \tag{15}$$

where $\boldsymbol{v}_n \cdot \bar{\boldsymbol{v}}_j = (2N+1)\delta_{nj}$, to reach that

$$\hat{b}_N^n = \frac{T}{(2N+1)} \sum_{m=0}^{2N} b_N^m \mathrm{e}^{2\pi\mathrm{i}\frac{mn}{2N+1}}, \tag{16}$$

which is the definition of the discrete Fourier transform.

For wave problems there is often a singularity at $\omega = 0$, a frequency which we used above. The easiest way to deal with this is just to take $\hat{b}_N^0 = 0$ which results in the wrong constant being added to the whole time signal. This wrong constant can be corrected by attempting to make the signal casual, which works well if we know the time signal is a pulse. Failing that, the whole frequency range can be offset by constant.

Suppose we wish to approximate $b(t)$ by

$$b(t) \approx \frac{1}{T} \sum_{n=-N}^{N} \hat{\beta}_N^n \mathrm{e}^{-\mathrm{i}t(2\pi n/T+\delta)}, \tag{17}$$

then we see that by multiplying by $\mathrm{e}^{\mathrm{i}t(2\pi m/T+\delta)}$, for $m = -N, \ldots, N$, on both sides‡ and integrating we get

$$\hat{\beta}_N^n = \int_0^T b(t)\mathrm{e}^{\mathrm{i}t(2\pi n/T+\delta)} dt = \hat{b}\left(\frac{2\pi n}{T} + \delta\right), \tag{18}$$

which looks like the Discrete Fourier transform of $\beta(t) = b(t)\mathrm{e}^{\mathrm{i}t\delta}$. In fact substituting $b(t)$ for $\beta(t)$ we get

$$\beta(t) \approx \frac{1}{T} \sum_{n=-N}^{N} \hat{\beta}_N^n \mathrm{e}^{-\mathrm{i}2\pi nt/T}, \tag{19}$$

‡Check the proof of converges of the Fourier series and see if it can be adapted to this case.

from which we know that by taking $\beta_N^m = \beta(mT/(2N+1))$ we have that

$$\beta_N^m = \frac{1}{T}\sum_{n=-N}^{N} \hat{\beta}_N^n \mathrm{e}^{-2\pi\mathrm{i}\frac{nm}{2N+1}} \quad \text{and} \quad \hat{\beta}_N^n = \frac{T}{2N+1}\sum_{m=0}^{2N} \beta_N^m \mathrm{e}^{2\pi\mathrm{i}\frac{nm}{2N+1}}. \tag{20}$$

The above translated back to $b(t)$ gives us

$$b\left(\frac{mT}{2N+1}\right) \approx \mathrm{e}^{-\mathrm{i}\delta\frac{mT}{2N+1}} \frac{1}{T}\sum_{n=-N}^{N} \hat{b}\left(\frac{2\pi n}{T}+\delta\right)\mathrm{e}^{-2\pi\mathrm{i}\frac{nm}{2N+1}} \quad \text{and} \tag{21}$$

$$\hat{b}\left(\frac{2\pi n}{T}+\delta\right) \approx \frac{T}{2N+1}\sum_{m=0}^{2N} \mathrm{e}^{\mathrm{i}\delta\frac{mT}{2N+1}} b\left(\frac{mT}{2N+1}\right)\mathrm{e}^{2\pi\mathrm{i}\frac{nm}{2N+1}}, \tag{22}$$

where $m = 0, \ldots, 2N$ for $t \in [0, T]$, and $n = -N, \ldots, N$ for $\omega \in [\delta - 2\pi N/T, \delta + 2\pi N/T]$. In our methods the more important parameter is the maximum frequency $\Omega \approx 2\pi N/T$, followed by N, so that $T = 2\pi N/\Omega$, which should be bigger than the period of $b(t)$.

Typically the discrete Fourier, and its inverse, are implemented so that both n and m run from 0 to $2N$. That is the input to a DFT is $(\hat{\beta}_N^0, \hat{\beta}_N^1, \ldots, \hat{\beta}_N^{2N})$. So we must adjust Eq. (23) so that n runs from 0 to $2N$. Turning to Eq.(22) we see that

$$\hat{b}\left(-\frac{2\pi n}{T}+\delta\right) = \hat{b}_{-n} = \hat{b}_{-n+2N+1},$$

which for $n = 1, 2, \ldots, N$ gives $\hat{b}_{-1} = \hat{b}_{2N}$, $\hat{b}_{-2} = \hat{b}_{2N-1}$, $\ldots$, $\hat{b}_{-N} = \hat{b}_{N+1}$. We use this to rewrite Eq. (23) as

$$b_m \approx \mathrm{e}^{-\mathrm{i}\delta\frac{mT}{2N+1}} \frac{1}{T}\sum_{n=0}^{2N} \hat{b}_n \mathrm{e}^{-2\pi\mathrm{i}\frac{nm}{2N+1}}. \tag{23}$$

To be clear, the input vector for DFT would typically be

$$\hat{\boldsymbol{b}} = (\hat{b}_0, \hat{b}_1, \ldots, \hat{b}_N, \hat{b}_{-N}, \ldots, \hat{b}_{-1}),$$

calculated from $\boldsymbol{\omega} = \delta + (1, 2\pi/T, \ldots, 2N\pi/T, -N\pi/T, \ldots, -\pi/T)$. Below are some examples.

The default Mathematica DFT calculates

$$\hat{\boldsymbol{f}}_n = \text{Fourier}[\boldsymbol{f}]_n = \frac{1}{\sqrt{2N+1}} \sum_{m=0}^{2N} f_m \mathrm{e}^{2\pi \mathrm{i} \frac{nm}{2N+1}}, \tag{24}$$

$$\boldsymbol{f}_m = \text{InverseFourier}[\hat{\boldsymbol{f}}]_m = \frac{1}{\sqrt{2N+1}} \sum_{n=0}^{2N} \hat{f}_n \mathrm{e}^{-2\pi \mathrm{i} \frac{nm}{2N+1}}. \tag{25}$$

So taking $\hat{f}_n = \hat{b}_n \sqrt{2N+1}/T$ leads to $b_m = \mathrm{e}^{-\mathrm{i}\delta \frac{mT}{2N+1}} f_m$.

Julia's fft reverse the role of the forward and back DFT. For Julia's taking $\hat{f}_n = \hat{b}_{-n}(2N+1)/T$ leads to $b_m = \mathrm{e}^{\mathrm{i}\delta \frac{mT}{2N+1}} f_m$.

Note that when we cut out the discontinuity from $\hat{b}$, the Discrete Fourier Transform will approximate $\hat{b}$ for some bell shaped curve (and likewise for the time curve). If δ is to small in comparison to $\delta\omega$ this bell shape will be much too big and rounded to approximate the sharp step from the hankel function. For example, numerically we find that for $\delta = 0.01\delta\omega$ are already significantly off, whereas for $\delta = 0.1\delta\omega$ they results are always decent (within 1% error when reconstructing the time signal).

Convolution formulas such as (11) can also be written in terms of the Offset Discrete Fourier Transform. Let

$$h(t) = \frac{1}{c^2} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t} \hat{g}(\omega) \hat{b}(\omega) d\omega. \tag{26}$$

Assuming Ω an N is given, we can represent the above by the inverse of the Offset Discrete Fourier Transform by using Eq. (23) to get

$$h\left(\frac{m\pi}{\Omega} \frac{2N}{2N+1}\right) \approx \mathrm{e}^{-\mathrm{i}\delta \frac{m\pi}{\Omega} \frac{2N}{2N+1}} \frac{\Omega}{2\pi N c^2} \sum_{n=-N}^{N} \mathrm{e}^{-2\pi \mathrm{i} \frac{nm}{2N+1}} \hat{g}\left(\Omega \frac{n}{N} + \delta\right) \hat{b}\left(\Omega \frac{n}{N} + \delta\right). \tag{27}$$

1.2 Scattered wave

The Fourier transform of the outgoing waves from a cylinder can be anything in the form

$$\hat{\varphi}^S(r,\omega) = \sum_{n=-\infty}^{\infty} a_n H_n^{(1)}(\omega r/c)\mathrm{e}^{\mathrm{i}n\theta} \approx \sum_{n=-Na}^{Na} a_n H_n^{(1)}(\omega r/c)\mathrm{e}^{\mathrm{i}n\theta} \tag{28}$$

where we call Na the number of angular modes. To choose $Na = 6$ for the package add `"NAngularModes"->6` to the function call.

To calculate the scattered wave in time φ^S, we do the same operation on $\hat{\varphi}_S$ that we did on $\hat{g}_2$ in Eq.(12)

$$\begin{aligned}\varphi^S(r,t) &\approx \frac{1}{2\pi c^2}\int_{-2\pi N/T}^{2\pi N/T} \mathrm{e}^{-\mathrm{i}\omega t}\hat{\varphi}^S(r,\omega)\hat{b}_N(\omega)d\omega \\ &= \frac{1}{2\pi c}\sum_{n=-\infty}^{\infty}\int_{-2\pi N/T}^{2\pi N/T} \mathrm{e}^{-\mathrm{i}ckt+\mathrm{i}n\theta} a_n(k)H_n^{(1)}(kr)\hat{b}_N(ck)dk. \end{aligned} \tag{29}$$

The coefficients a_n will be determined by the boundary conditions.

1.2.1 Boundary condition

To compare the incident and scattered wave we use Graf's addition formula § applied to

$$H_0^{(1),(2)}(k\|\boldsymbol{r} - \boldsymbol{r}_I\|) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n(\theta-\theta_1)} J_n(kr) H_n^{(1),(2)}(kr_I) \quad \text{if} \;\; r < r_I, \tag{30}$$

where the body force originates at $\boldsymbol{r}_I = r_I(\cos\theta_I, \sin\theta_I)$ and $\boldsymbol{r} = r(\cos\theta, \sin\theta)$. If $\hat{\varphi}^I = \hat{g}_2(\|\boldsymbol{r} - \boldsymbol{r}_I\|)$ and $\hat{\varphi}^S = a_n H_n^{(1)}(kr)\mathrm{e}^{in\theta}$ then the boundary condition $\hat{\varphi}_I + \hat{\varphi}_S = 0$ on

§ see `http://dlmf.nist.gov/10.23#E7`

$r = r_S < r_I$ implies

$$\frac{\mathrm{i}}{4}\mathrm{e}^{-\mathrm{i}n\theta_I} J_n(kr_S) H_n^{(1)}(kr_I) + a_n H_n^{(1)}(kr_S) = 0 \implies \tag{31}$$

$$a_n = -\frac{\mathrm{i}}{4}\mathrm{e}^{-\mathrm{i}n\theta_I} \frac{J_n(kr_S)}{H_n^{(1)}(kr_S)} H_n^{(1)}(kr_I). \tag{32}$$

while the boundary condition $\partial\hat{\varphi}^I/\partial r + \partial\hat{\varphi}^S/\partial r = 0$ on $r = r_S < r_I$ implies that

$$a_n = -\frac{i}{4}\mathrm{e}^{-\mathrm{i}n\theta_I} \frac{J_n'(kr_S)}{H_n^{'(1)}(kr_S)} H_n^{(1)}(kr_I). \tag{33}$$

1.3 Wave frequency to time response

This module is used for more complicated scattering, such as MST. Any outgoing wave from a scatterer can be expanded as

$$\hat{\psi}^S(\boldsymbol{r}, k) \approx \sum_{n=-Na}^{Na} a_n H_n(kr)\mathrm{e}^{\mathrm{i}n\theta},$$

for a cylindrical coordinate system with origin at the scatterer, where $H_n := H_n^{(1)}$ a Hankel function of the first kind. To recover the wave in time we need to approximate the inverse Fourier transform:

$$\psi^S(\boldsymbol{r}, t) = \frac{c}{2\pi}\int_{-\infty}^{\infty} \hat{\psi}^S(\boldsymbol{r}, k)\mathrm{e}^{-\mathrm{i}ckt} dk \approx \frac{c}{2\pi}\sum_{n=-Na}^{Na} \mathrm{e}^{\mathrm{i}n\theta} \int_{-2\pi N/T}^{2\pi N/T} a_n H_n(kr)\mathrm{e}^{-\mathrm{i}ckt} dk,$$

where T is the period of the incident wave and N is the number of frequency modes.

Assuming that the scatterers are small compared with the wavelength $kr_S << 1$, where r_S is the radius of the scatterer, then the most general form for outgoing waves from the j-th scatterer is

$$\psi^S(\boldsymbol{r}) = aH_0(kr) + (c\cos\theta + s\sin\theta)H_1(kr), \tag{34}$$

which means that $a_0 = a$, $a_1 = (s + c)/4$ and $a_{-1} = (s - c)/4$.