Fourier transform

Let $f(\vartheta)$ with $-\pi \leqslant \vartheta \leqslant \pi$ be a periodic function in ϑ with period 2π. In other words.

$$f(\vartheta + 2k\pi) = f(\vartheta) \quad , \forall k \in \{0, \pm 1, \pm 2, \dots\}$$

Then $f(\vartheta)$ can be expanded in a Fourier expansion that has the form:

$$f(\vartheta) = \sum_{k=0}^{+\infty} c_k \exp[2\pi i (k\vartheta)]$$

where c_k are complex numbers, in general.
Like Legendre expansion, this is also an orthogonal expansion. with basis functions:

$$\boxed{\varphi_k(\vartheta) = \exp[2\pi i (k\vartheta)]}$$

The orthogonality relation is that

$$\int_{-\pi}^{\pi} \varphi_k(\vartheta)\varphi_j(\vartheta)\,d\vartheta = \delta_{kj}$$

therefore it follows that the relation between c_k and $f(\vartheta)$ is:

$$c_k = \int_{-\pi}^{\pi} f(\vartheta) \exp[2\pi i (k\vartheta)]\,d\vartheta$$

Fourier expansions can be very useful in expanding the longitude for computations that are not axisymmetric.

Discrete Fourier transform

To discretize the integral for c_k we sample $f(\vartheta)$ on the following points:

$$\vartheta_j = -\pi + 2\pi(j/N) \quad , \ j \in \{0, 1, \dots, N-1\}.$$

Note that the point ϑ_N is redundant be cause it is identical to ϑ_0 through periodicity. The points $\vartheta_0, \vartheta_1, \dots, \vartheta_{N-1}$ are the optimal sampling that we use.
Since $f(\vartheta)$ is known at N points, it take N coefficients c_k to store equivalent information in Fourier space. This means that the discrete Fourier transform can be defined as:

$$\boxed{f_j = \sum_{K=0}^{N-1} \tilde{f}_K \exp\left[+2\pi i \frac{jK}{N}\right]} \quad \boxed{\tilde{f}_K = \frac{1}{N} \sum_{K=0}^{N-1} f_j \exp\left[-2\pi i \frac{jK}{N}\right]}$$

In general f_j and $\tilde{f}_K$ are complex arrays of length N. and this is the complex discrete Fourier transform (Complex DFT).
My package, as an interface to FFTPACK, implements the complex DFT in the above form, using the Fast Fourier Transform algorithm. The FFT can do this computation in $O(N \log(N))$ time instead of $O(N^2)$.

▼ The Real Discrete Fourier Function

The $\tilde{f}_K$ representation is 2N real numbers. If the original f_j are all real, then the spectral representation is redundant by a factor of 2. Now we show how to eliminate the redundancy.
Let $f_j \in \mathbb{R}$ be the real-space representation with $j \in \{0, 1, \ldots, N-1\}$.
Define the spectral representation (and simplify the definition) like this:

$$\tilde{f}_{2K} = \mathrm{Re}\left\{\frac{1}{N} \sum_{j=0}^{N-1} f_j \exp\left[-2\pi i \frac{jK}{N}\right]\right\} =$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} f_j \cos\left(-2\pi \frac{jK}{N}\right) = \frac{1}{N} \sum_{j=0}^{N-1} f_j \cos\left(2\pi \frac{jK}{N}\right)$$

and

$$\tilde{f}_{2K+1} = \mathrm{Im}\left\{\frac{1}{N} \sum_{j=0}^{N-1} f_j \exp\left[-2\pi i \frac{jK}{N}\right]\right\} =$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} f_j \sin\left(-2\pi \frac{jK}{N}\right) = \frac{-1}{N} \sum_{j=0}^{N-1} f_j \sin\left(2\pi \frac{jK}{N}\right)$$

where $K \in \mathbb{Z}$ is an arbitrary integer.
~~Note that~~ $\hat{c}_K = \tilde{f}_{2K} + i f_{2K+1}$ is the Fourier coefficient for k'th term as it appears in the complex notation. ~~This follows from~~

$\cancel{\tilde{c}_K = \tilde{f}_{2K} + i \tilde{f}_{2K+1}}$

$$f_j = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[+2\pi i \frac{jk}{N}\right] \qquad \tilde{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f_j \exp\left[-2\pi i \frac{jk}{N}\right]$$

In general f_j and $\tilde{f}_k$ are complex ~~numbers~~ arrays of length N, and this is called the discrete Fourier transform (complex DFT). My package, as an interface to FFTPACK, implements the complex DFT in the above form using the FFT algorithm

▼ The Real Discrete Fourier transform

The $\tilde{f}_k$ representation is equivalent to $2N$ real numbers. If the original $f_j \in \mathbb{R}$ are all real, then the spectral representantion is redundant by a factor of 2. Now we show how to eliminate the redundancy.
Let $f_j \in \mathbb{R}$ be the representation in real space with $j \in \{0, 1, \dots, N-1\}$. Define $\tilde{c}_k$ like this:

$$\tilde{c}_{2k} = \mathrm{Re}\left[\tilde{f}_k\right] \qquad \tilde{c}_{2k+1} = \mathrm{Im}\left[\tilde{f}_k\right]$$

Substituting $\tilde{f}_k$ and taking into account that $f_j \in \mathbb{R}$, we obtain:

$$\tilde{c}_{2k} = \mathrm{Re}\left[\tilde{f}_k\right] = \mathrm{Re}\left[\frac{1}{N}\sum_{k=0}^{N-1} f_j \exp\left[-2\pi i \frac{jk}{N}\right]\right] = \quad f_j \in \mathbb{R}.$$

$$= \frac{1}{N}\sum_{k=0}^{N-1} f_j \,\mathrm{Re}\left[\exp\left(-2\pi i \frac{jk}{N}\right)\right] =$$

$$= \frac{1}{N}\sum_{k=0}^{N-1} f_j \cos\left(-2\pi \frac{jk}{N}\right) = \frac{1}{N}\sum_{k=0}^{N-1} f_j \cos\left(2\pi \frac{jk}{N}\right).$$

and

$$\tilde{c}_{2k+1} = \mathrm{Im}\left[\tilde{f}_k\right] = \mathrm{Im}\left[\frac{1}{N}\sum_{k=0}^{N-1} f_j \exp\left(-2\pi i \frac{jk}{N}\right)\right] =$$

$$= \frac{1}{N}\sum_{k=0}^{N-1} f_j \,\mathrm{Im}\left[\exp\left(-2\pi i \frac{jk}{N}\right)\right] =$$

$$= \frac{1}{N}\sum_{k=0}^{N-1} f_j \sin\left(-2\pi \frac{jk}{N}\right) = -\frac{1}{N}\sum_{k=0}^{N-1} f_j \sin\left(2\pi \frac{jk}{N}\right).$$

From all this we also obtain the following relation for $\tilde{f}_k$:

$$\tilde{f}_K = \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left(2\pi \frac{jK}{N}\right) - \frac{i}{N}\sum_{K=0}^{N-1} f_j \sin\left(2\pi\frac{jK}{N}\right)$$

From this relation we can derive a relation between $\tilde{f}_K$ and $\tilde{f}_{N-K}$.
Begin with:

$$\tilde{c}_{2(N-K)} = \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left[2\pi \frac{j(N-K)}{N}\right] =$$

$$= \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left[2\pi j - 2\pi\frac{jK}{N}\right] =$$

$$= \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left(-2\pi\frac{jK}{N}\right) = \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left(2\pi\frac{jK}{N}\right) = \tilde{c}_{2K}.$$

$$\tilde{c}_{2(N-K)+1} = \frac{-1}{N}\sum_{K=0}^{N-1} f_j \sin\left[2\pi\frac{j(N-K)}{N}\right] =$$

$$= -\frac{1}{N}\sum_{K=0}^{N-1} f_j \sin\left(2\pi j - 2\pi\frac{jK}{N}\right) =$$

$$= \frac{1}{N}\sum_{K=0}^{N-1} f_j \sin\left(2\pi\frac{jK}{N}\right) = -\tilde{c}_{2K+1}$$

It follows that

$$\tilde{f}_{N-K} = \tilde{c}_{2(N-K)} + i\,\tilde{c}_{2(N-K)+1} = \tilde{c}_{2K} - i\,\tilde{c}_{2K+1} = \tilde{f}_K^*$$

In other words $\tilde{f}_{N-K}$ and $\tilde{f}_K^*$ are complex conjugate, therefore it is not necessary to know the entire sequence

$$\tilde{f}_0, \tilde{f}_1, \ldots, \tilde{f}_{N-1}.$$

We will show now how the entire spectral representation $\tilde{f}_K$ can be encoded with N real numbers.
Consider the following cases:

a) <u>Case 1</u>: N is even.
Then only the following complex numbers are required:

$$\underline{\tilde{f}_0, \tilde{f}_1, \ldots, \tilde{f}_{N/2}}$$

This is a total of ~~N real numbers~~. $N+2$ real numbers.
For example if $N=6$: $\tilde{f}_0, \tilde{f}_1, \tilde{f}_2, \tilde{f}_3, \tilde{f}_4, \tilde{f}_5$

b) Case 2: N is odd.

Then only the following complex numbers are required:

$$\tilde{f}_0, \tilde{f}_1, \dots, \tilde{f}_{(N-1)/2}$$

This is appearently a total of $2[(N-1)/2+1] = N-1+2 = N+1$ real numbers.

This however is not the complete story. Take note of the following crucial observations:

a) For $k=0$: $\tilde{c}_0 = \frac{1}{N}\sum_{j=0}^{N-1} f_j \cos 0 = \frac{1}{N}\sum_{j=0}^{N-1} f_j$

$$\tilde{c}_1 = \frac{1}{N}\sum_{j=0}^{N-1} f_j \sin 0 = 0$$

We see that $\tilde{c}_0$ is just the average of f_j for all $j \in \{0,1,\dots,N-1\}$. More importantly we see that $\tilde{c}_1$ is always 0. This means that $\tilde{c}_1$ carries no information at all!

- This observation resolves Case 2 above. Even though appearently we require N+1 real numbers, one of ~~theese~~ these numbers is $\tilde{c}_1$ so the information content of that representation is only N real numbers as we would expect.
- We may also resolve Case 1 above as follows. First of all note that the result that $\tilde{c}_1 = 0$ reduces the count from N+2 real numbers to N+1. Also consider this observation:

b) If N = even then for $k = N/2$:

$$\tilde{c}_N = \tilde{c}_{2(N/2)} = \frac{1}{N}\sum_{j=0}^{N-1} f_j \cos\left(2\pi \frac{j(N/2)}{N}\right) =$$

$$= \frac{1}{N}\sum_{j=0}^{N-1} f_j \cos(\pi j) = \frac{1}{N}\sum_{j=0}^{N-1} (-1)^j f_j$$

$$\tilde{c}_{N+1} = \tilde{c}_{2(N/2)+1} = \frac{-1}{N}\sum_{j=0}^{N-1} f_j \sin\left(2\pi \frac{j(N/2)}{N}\right) =$$

$$= \frac{-1}{N}\sum_{j=0}^{N-1} f_j \sin(\pi j) = 0$$

Recall that $\tilde{f}_{N/2} = \tilde{c}_N + i\tilde{c}_{N+1}$, which is the last complex number that appears in the sequence at Case 1. $\tilde{c}_{N+1} = 0$ is the second redundancy that brings down the size of the

spectral representation down to N.
To summarize, the representation of f_j in spectral space can be ~~to~~ fully encoded by the following N real numbers:

$$\boxed{\tilde{c}_0,\ \tilde{c}_2,\ \tilde{c}_3,\ \dots,\ \tilde{c}_N}$$

where $\tilde{c}_n$ are given by the following relations:

$$\tilde{c}_0 = \frac{1}{N}\sum_{j=0}^{N-1} f_j$$

$$\tilde{c}_{2K} = \frac{1}{N}\sum_{K=0}^{N-1} f_j \cos\left(2\pi\frac{jK}{N}\right) \qquad \tilde{c}_{2K+1} = -\frac{1}{N}\sum_{K=0}^{N-1} f_j \sin\left(2\pi\frac{jK}{N}\right)$$

For $N=$ even: $\tilde{c}_N = \frac{1}{N}\sum_{j=0}^{N-1}(-1)^j f_j$

These relations and the representation above is how FFTPACK performs the forward real DFT.
Now, given this representation, we show how to compute the inverse.

$$f_j = \sum_{K=0}^{N-1}\tilde{f}_K \exp\left[2\pi i\frac{jK}{N}\right] = \tilde{c}_0 + \sum_{K=1}^{N-1}\tilde{f}_K \exp\left[2\pi i\frac{jK}{N}\right] =$$

$$= \tilde{c}_0 + \sum_{K=1}^{N-1}\left(\tilde{c}_{2K} + i c_{2K+1}\right)\left[\cos\left(2\pi\frac{jK}{N}\right) + i\sin\left(2\pi\frac{jK}{N}\right)\right] =$$

$$= \tilde{c}_0 + \sum_{K=1}^{N-1}\tilde{c}_{2K}\cos\left(2\pi\frac{jK}{N}\right) - \sum_{K=1}^{N-1}\tilde{c}_{2K+1}\sin\left(2\pi\frac{jK}{N}\right)$$

since we know well in advance that $f_j \in \mathbb{R}$.
To simplify this expression further, we need to substitute the relation that

$$\tilde{c}_{2(N-K)} = \tilde{c}_{2K} \quad \text{and} \quad \tilde{c}_{2(N-K)+1} = -\tilde{c}_{2K+1}$$

To do that, we need to consider two cases seperately.

a) <u>Case 1</u>: Suppose that N is even.
Then the correlation between $\tilde{f}_K$ is as follows:

$$\boxed{\tilde{f}_0},\ \tilde{f}_1,\ \tilde{f}_2,\ \dots,\ \tilde{f}_{N/2-1},\ \boxed{\tilde{f}_{N/2}},\ \tilde{f}_{N/2+1},\ \dots,\ \tilde{f}_{N-2},\ \tilde{f}_{N-1}$$

The $\tilde{f}_0$ and $\tilde{f}_{N/2}$ terms are stray terms. All the other terms are pairwise complex conjugate. Therefore,

$$\sum_{K=1}^{N-1} \tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right) = \tilde{c}_N \cos(\pi j) + \sum_{K=1}^{N/2-1}\left[\tilde{c}_{2K}\cos\left(2\pi\frac{jK}{N}\right) + \tilde{c}_{2(N-K)} \cos\left(2\pi \frac{j(N-K)}{N}\right)\right.$$

$$= \tilde{c}_N (-1)^j + \sum_{K=1}^{N/2-1} \left(\tilde{c}_{2K} + \tilde{c}_{2(N-K)}\right) \cos\left(2\pi \frac{jK}{N}\right) =$$

$$= \tilde{c}_N (-1)^j + \sum_{K=1}^{N/2} 2\tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right)$$

and

$$\sum_{K=1}^{N-1} \tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right) =$$

$$= \tilde{c}_N \sin(\pi j) + \sum_{K=1}^{N/2-1}\left[\tilde{c}_{2K+1} \sin\left(2\pi\frac{jK}{N}\right) + \tilde{c}_{2(N-K)+1} \sin\left(2\pi\frac{j(N-K)}{N}\right)\right] =$$

$$= \sum_{K=1}^{N/2-1} \left(\tilde{c}_{2K+1} - \tilde{c}_{2(N-K)+1}\right) \sin\left(2\pi \frac{jK}{N}\right) =$$

$$= \sum_{K=1}^{N/2-1} 2\tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right)$$

Putting it all-together:

$$\boxed{f_j = \tilde{c}_0 + (-1)^j \tilde{c}_N + \sum_{K=1}^{N/2-1} 2\left[\tilde{c}_{2K} \cos\left(2\pi\frac{jK}{N}\right) - \tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right)\right]}$$

A direct implementation of this equation, computes the <u>backward</u> real DFT in $O(N^2)$ and can be used to verify FFTPACK.

b) <u>Case 2</u>: Suppose that N is odd.

Then the correlation between $\tilde{f}_K$ is as follows:

$$\boxed{\tilde{f}_0}, \tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_{(N-1)/2}, \tilde{f}_{(N+1)/2}, \ldots, \tilde{f}_{N-2}, \tilde{f}_{N-1}$$

In this case only $\tilde{f}_0$ is a stray term and all the other terms are pairwise complex conjugates of one another.

Therefore, the two sums are now decomposed differently.

$$\sum_{K=1}^{N-1} \tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right) = \sum_{K=1}^{(N-1)/2} \left[\tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right) + \tilde{c}_{2(N-K)} \cos\left(2\pi \frac{j(N-K)}{N}\right)\right] =$$

$$= \sum_{K=1}^{(N-1)/2} \left(\tilde{c}_{2K} + \tilde{c}_{2(N-K)}\right) \cos\left(2\pi \frac{jK}{N}\right) =$$

$$= \sum_{K=1}^{(N-1)/2} 2\tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right).$$

and

$$\sum_{K=1}^{N-1} \tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right) =$$

$$= \sum_{K=1}^{(N-1)/2} \left[\tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right) + \tilde{c}_{2(N-K)+1} \sin\left(2\pi \frac{j(N-K)}{N}\right)\right] =$$

$$= \sum_{K=1}^{(N-1)/2} \left(\tilde{c}_{2K+1} - \tilde{c}_{2(N-K)+1}\right) \sin\left(2\pi \frac{jK}{N}\right)$$

$$= \sum_{K=1}^{(N-1)/2} 2\tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right)$$

Putting it all together:

$$\boxed{f_j = \tilde{c}_0 + \sum_{K=1}^{(N-1)/2} 2\left[\tilde{c}_{2K} \cos\left(2\pi \frac{jK}{N}\right) - \tilde{c}_{2K+1} \sin\left(2\pi \frac{jK}{N}\right)\right]}$$

These two equation encapsulate what the backward real DFT is. Both these and the forward transform equations can be implemented directly. Such an implementation would execute in $O(N^2)$ time. FFTPACK implements a recursive method known as the "fast Fourier transform" algorithm which implements this in $O(N \log N)$. To derive an FFT algorithm for the special case of real DFT we need to use these equations as a starting point. that we derived here.

The implementation of real DFT is nonstandard among different packages which is why we had to go through all this development to explain how FFTPACK deals with the representation of f in spectral space.

▼ Spectral differentiation

Let $f(\vartheta)$ with $\vartheta \in [-\pi, \pi]$ be a function such that
$f(\cancel{\vartheta}) = f(-\pi) = f(\pi)$.
Then f has a Fourier expansion:

$$f(\vartheta) = \sum_{k=0}^{+\infty} c_k \exp[2\pi i (k\vartheta)]$$

Suppose that the derivative of f also has the same property:

$$f'(-\pi) = f'(\pi) \Rightarrow \exists\, d_k \in \mathbb{C} : f'(\vartheta) = \sum_{k=0}^{+\infty} d_k \exp[2\pi i (k\vartheta)]$$

Then d_k can be computed from c_k algebraicly:

$$f'(\vartheta) = \frac{d}{d\vartheta} \sum_{k=0}^{+\infty} c_k \exp[2\pi i (k\vartheta)] = \sum_{k=0}^{+\infty} c_k \frac{d}{d\vartheta} \exp[2\pi i (k\vartheta)] =$$
$$= \sum_{k=0}^{+\infty} [2\pi i c_k k] \exp[2\pi i (k\vartheta)] \Rightarrow \boxed{d_k = 2\pi i c_k}$$

Now we will show how to exploit this property numerically.

● Differentiation with complex DFT

As a discrete operation, the complex DFT says:

$$f_j = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[+2\pi i \frac{jk}{N}\right] \quad \text{and} \quad \tilde{f}_k = \frac{1}{N} \sum_{k=0}^{N-1} f_j \exp\left[-2\pi i \frac{jk}{N}\right]$$

f_j is meant to approximate f by giving the value of f at specific points. In particular:

$$f_j = f(\vartheta_j) \quad \text{for} \quad \vartheta_j = -\pi + 2\pi (j/N) \quad , j \in \{0, 1, \dots, N-1\}$$

It follows that $2\pi (j/N) = \vartheta_j + \pi$, therefore:

$$f_j = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[+2\pi i \frac{jk}{N}\right] = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[ik(\vartheta_j + \pi)\right]$$

Assume that $f(\vartheta)$ can be approximated by:

$$f(\vartheta) = \sum_{k=0}^{+\infty} \tilde{f}_k \exp[ik(\vartheta_j + \pi)] \Rightarrow$$

$$\Rightarrow f'(\vartheta) = \frac{d}{d\vartheta} \sum_{k=0}^{+\infty} \tilde{f}_k \exp[ik(\vartheta_j + \pi)] =$$

$$= \sum_{k=0}^{+\infty} \tilde{f}_k \frac{d}{d\vartheta} \exp[ik(\vartheta + \pi)] = \sum_{k=0}^{+\infty} ik\tilde{f}_k \exp[ik(\vartheta+\pi)] \Rightarrow$$

$$\Rightarrow f'_j = f'(\vartheta_j) = \sum_{k=0}^{+\infty} ik\tilde{f}_k \exp[ik(\vartheta_j + \pi)] =$$

$$= \sum_{k=0}^{+\infty} ik\tilde{f}_k \exp\left[2\pi i \frac{jk}{N}\right] = \sum_{k=0}^{+\infty} \tilde{f}'_k \exp\left[2\pi i \frac{jk}{N}\right] \Rightarrow$$

$$\Rightarrow \boxed{\tilde{f}'_k = ik\tilde{f}_k}$$

More generally, the function $f(\vartheta)$ will be defined on the interval $[a,b]$ instead of $[-\pi,\pi]$ such that

$$f(a) = f(b) \quad \text{and} \quad f'(a) = f'(b).$$

Then the points at which f_j samples f will be:

$$\vartheta_j = -a + (b-a)(j/N)$$

It follows that:

$$2\pi \frac{j}{N} = \frac{2\pi}{b-a}(b-a)(j/N) = \frac{2\pi(\vartheta_j + a)}{b-a} \Rightarrow$$

$$\Rightarrow f_j = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[+2\pi i \frac{jk}{N}\right] = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[\frac{2\pi i k(\vartheta_j + a)}{b-a}\right]$$

therefore

$$f(\vartheta) = \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[\frac{2\pi i k(\vartheta + a)}{b-a}\right] \Rightarrow$$

$$\Rightarrow f'(\vartheta) = \frac{d}{d\vartheta} \sum_{k=0}^{N-1} \tilde{f}_k \exp\left[\frac{2\pi i k(\vartheta+a)}{b-a}\right] =$$

$$= \sum_{k=0}^{N-1} \tilde{f}_k \frac{d}{d\vartheta} \exp\left[\frac{2\pi i k(\vartheta+a)}{b-a}\right] =$$

$$= \sum_{k=0}^{N-1} \frac{2\pi i k}{b-a} \tilde{f}_k \exp\left[\frac{2\pi i k(\vartheta+a)}{b-a}\right] \cancel{= \sum_{k=0}^{N-1} \tilde{f}'_k \exp[2}$$

$$\Rightarrow f_j' = f'(\vartheta_j) = \sum_{k=0}^{N-1} \frac{2\pi i k}{b-a} \tilde{f}_k \exp\left[\frac{2\pi i k(\vartheta_j + a)}{b-a}\right] =$$

$$= \sum_{k=0}^{N-1} \frac{2\pi i k}{b-a} \tilde{f}_k \exp\left[2\pi i \frac{jk}{N}\right] \Rightarrow$$

$$\Rightarrow \tilde{f}_k' = \frac{2\pi i k}{b-a} \tilde{f}_k$$

For the special case $a=-\pi$ and $b=\pi$ this reduces to the result we derived earlier.

• Differentiation with real DFT

Recall that in general f_j is given by $\tilde{c}_{2k}, \tilde{c}_{2k+1}$ by:

$$f_j = \tilde{c}_0 + \sum_{k=1}^{N-1} \tilde{c}_{2k} \cos\left(2\pi \frac{jk}{N}\right) - \sum_{k=1}^{N} \tilde{c}_{2k+1} \sin\left(2\pi \frac{jk}{N}\right).$$

We can argue using this form like we did with the complex DFT. Recall that,

$$2\pi \frac{j}{N} = \frac{2\pi(\vartheta_j + a)}{b-a}$$

therefore:

$$f(\vartheta) = \tilde{c}_0 + \sum_{k=1}^{N-1} \tilde{c}_{2k} \cos\left[\frac{2\pi(\vartheta+a)k}{b-a}\right] - \sum_{k=1}^{N-1} \tilde{c}_{2k+1} \sin\left[\frac{2\pi(\vartheta+a)k}{b-a}\right] \Rightarrow$$

$$\Rightarrow f'(\vartheta) = \sum_{k=1}^{N-1} \frac{-2\pi k}{b-a} \tilde{c}_{2k} \sin\left[\frac{2\pi(\vartheta+a)}{b-a} k\right] - \sum_{k=1}^{N-1} \frac{2\pi k}{b-a} \tilde{c}_{2k+1} \cos\left[\frac{2\pi(\vartheta+a)k}{b-a}\right] \Rightarrow$$

$$\Rightarrow f_j' = f'(\vartheta_j) = \sum_{k=1}^{N-1} \frac{-2\pi k}{b-a} \tilde{c}_{2k} \sin\left(2\pi \frac{jk}{N}\right) - \sum_{k=1}^{N-1} \frac{2\pi k}{b-a} \tilde{c}_{2k+1} \cos\left[2\pi \frac{jk}{N}\right] =$$

$$= 0 + \sum_{k=1}^{N-1} \frac{2\pi k}{b-a} (-c_{2k+1}) \cos\left[2\pi \frac{jk}{N}\right] - \sum_{k=1}^{N-1} \frac{2\pi k}{b-a} \tilde{c}_{2k} \sin\left(2\pi \frac{jk}{N}\right) \Rightarrow$$

$$\Rightarrow \quad \tilde{c}_0' = 0$$

$$\tilde{c}_{2k}' = -\frac{2\pi k}{b-a} \tilde{c}_{2k+1}$$

$$\tilde{c}_{2k+1}' = \frac{2\pi k}{b-a} \tilde{c}_{2k}$$

which is a tricky operation because we only store:

$$\tilde{c}_0, \tilde{c}_2, \tilde{c}_3, \ldots, \tilde{c}_N$$

There are two cases:

a) If $N = \text{even}$ then:

$$f_j = \tilde{c}_0 + (-1)^j \tilde{c}_N + \sum_{k=1}^{N/2-1} \left[2\tilde{c}_{2k} \cos\left(2\pi \frac{jk}{N}\right) - 2\tilde{c}_{2k+1} \sin\left(2\pi \frac{jk}{N}\right)\right]$$

therefore:

$$\tilde{c}_0' = 0$$
$$\tilde{c}_{2k}' = -\frac{2\pi k}{b-a}\tilde{c}_{2k+1}, \quad \tilde{c}_{2k+1}' = \frac{2\pi k}{b-a}\tilde{c}_{2k}, \quad \forall k \in \{1, 2, \dots, N/2-1\}$$

The term $\tilde{c}_N'$ needs special treatment. Recall that for real functions $\tilde{c}_{N+1} = 0$, therefore:

$$\tilde{c}_N' = \frac{-2\pi(N/2)}{b-a}\tilde{c}_{N+1} = 0$$

so we just set $\tilde{c}_N' = 0$

b) If $N = \text{odd}$ then:

$$f_j = \tilde{c}_0 + \sum_{k=1}^{(N-1)/2} \left[2\tilde{c}_{2k} \cos\left(2\pi \frac{jk}{N}\right) - 2\tilde{c}_{2k+1} \sin\left(2\pi \frac{jk}{N}\right)\right]$$

therefore:

$$\tilde{c}_0' = 0$$
$$c_{2k}' = -\frac{2\pi k}{b-a}\tilde{c}_{2k+1}, \quad \tilde{c}_{2k+1}' = \frac{2\pi k}{b-a}\tilde{c}_{2k}, \quad \forall k \in \{1, 2, \dots, (N-1)/2\}$$

No terms need any special treatment.

- ~~Remark about higher-order derivatives.~~

~~With complex DFT, repeating the spectral differentiation numerous times, allows us to compute higher order derivatives.~~
~~This is not necessarily true for the case of real DFT because we ~~then~~~~

Spectral differentiation as a linear operator

The spectral differentiation operation is a linear transformation that can be represented by matrix multiplication. In particular:

a) For the case of Complex DFT:

$$\tilde{f}_K' = D_C(N)\, f_K$$

where $D_C(N)$ is a diagonal matrix.

b) For the case of real DFT, we define $\hat{f}_K$ in terms of $\tilde{c}_K$ by:

$$\hat{f}_K = (\tilde{c}_0, \tilde{c}_2, \tilde{c}_3, \ldots, \tilde{c}_N)$$

which is the spectral representation of f_j using N real numbers instead of 2N. To indicate the use of this special representation we use ^ instead of ~. In terms of $\hat{f}_K$:

$$\hat{f}_K' = D_R(N)\, \hat{f}_K$$

Note that to compute $\hat{f}_K'$ we permute $\tilde{c}_{2K}, \tilde{c}_{2K+1}$ and then multiply both by the same factor. It follows that $D_R(N)$ can be decomposed as:

$$D_R(N) = D_R'(N)\, P(N)$$

where $D_R'(N)$ = a diagonal matrix

$P(N)$ = a permutation matrix. (also responsible for sign changes).

Using similar arguments as before, we can generalize these results to n^{th}-order differentiation. In particular, we define the following notation:

$D_C^{(n)}(N)$ = complex DFT n^{th}-order spectral differentiation

$D_R^{(n)}(N)$ = real DFT n^{th}-order spectral differentiation.

Higher order differentiation

Now we show how $D_C^{(n)}(N)$ and $D_R^{(n)}(N)$ can be expressed in terms of $D_C(N)$, $D_R'(N)$, $P(N)$.

For the case of complex DFT: $\tilde{f}_K^{(n)} = \left[\frac{2\pi i K}{b-a}\right]^{n} \tilde{f}_K$

It follows that $\boxed{D_C^{(n)}(N) = [D_C(N)]^n}$

Unfortunately, this is not generally true for $D_R(N)$.

Recall that in terms of $\tilde{c}_k$, the real DFT expansion for f_j is:

$$f_j = \tilde{c}_0 + \sum_{k=1}^{N-1} \tilde{c}_{2k} \cos\left(2\pi \frac{jk}{N}\right) - \sum_{k=1}^{N-1} \tilde{c}_{2k+1} \sin\left(2\pi \frac{jk}{N}\right)$$

and $2\pi \frac{j}{N} = \frac{2\pi(\vartheta_j + a)}{b-a}$

Assuming: $f(\vartheta) = \tilde{c}_0 + \sum_{k=1}^{N-1} \tilde{c}_{2k} \cos\left(2\pi k \frac{\vartheta + a}{b-a}\right) - \sum_{k=1}^{N-1} \tilde{c}_{2k+1} \sin\left(2\pi k \frac{\vartheta + a}{b-a}\right)$

Now compute the $2n$ order derivative:

$$\frac{d^{2n}}{d\vartheta^{2n}} \cos\left(2\pi k \frac{\vartheta + a}{b-a}\right) = (-1)^n \left(\frac{2\pi k}{b-a}\right)^{2n} \cos\left(2\pi k \frac{\vartheta + a}{b-a}\right)$$

$$\frac{d^{2n}}{d\vartheta^{2n}} \sin\left(2\pi k \frac{\vartheta + a}{b-a}\right) = (-1)^n \left(\frac{2\pi k}{b-a}\right)^{2n} \sin\left(2\pi k \frac{\vartheta + a}{b-a}\right)$$

From this it follows that

$$\tilde{c}_0^{(2n)} = 0, \quad \tilde{c}_{2k}^{(2n)} = (-1)^n \left(\frac{2\pi k}{b-a}\right)^{2n} \tilde{c}_{2k}, \quad \tilde{c}_{2k+1}^{(2n)} = (-1)^n \left(\frac{2\pi k}{b-a}\right)^{2n} \tilde{c}_{2k+1}$$

which leads ~~th~~to the following results:

a) The $2n$-order operators are multiplicative: $\boxed{D_R^{(2n)}(N) = \left[D_R^{(2)}(N)\right]^n}$

b) The $D_R^{(2)}(N)$ matrix is diagonal, therefore, unlike $D_R(N)$, it contains no permutations.

The second result has an important consequence.
Recall that if N = even, then

$$\tilde{c}'_N = -\frac{2\pi(N/2)}{b-a} \tilde{c}_{N+1} = 0$$

However, for the 2nd-order derivative:

$$\tilde{c}''_N = +\left[\frac{2\pi(N/2)}{b-a}\right]^2 \tilde{c}_N = +\left(\frac{\pi N}{b-a}\right)^2 \tilde{c}_N \neq 0.$$

This means that if we were to apply $D_R(N)$ to $\hat{f}_k$ twice we would get the wrong result: that $\tilde{c}''_N = 0$.
So in general, it is not true that $D_R^{(2)}(N)$ is equal to $D_R(N) D_R(N)$.
Instead, to obtain results for $D_R^{(2)}(N)$ we must consider the two cases seperately.

a) If the size of the vectors is odd, then we do not have this problem with $\tilde{c}_N$. In this case:

$$\boxed{D_R^{(2)}(2N+1) = D_R(2N+1)\, D_R(2N+1).}$$

b) If the size of the vectors is even, then:

$$\boxed{D_R^{(2)}(2N) \neq D_R(2N)\, D_R(2N).}$$

However, we can correct this if we simply set

$$\tilde{c}_N'' = -\left(\frac{\pi N}{b-a}\right)^2 \tilde{c}_N .$$

Let $A(N)$ be a matrix which ~~is~~ leave all else unchanged but applies the above to $\tilde{c}_N$ (or f_{N-1}). Then:

$$\boxed{D_R^{(2)}(2N) = D_R(2N)\, D_R(2N) + A(N).}$$

In practical terms we implement all this as follows:

a) For the $2N+1$ case simply invoke 1st-order differentiation multiply times.

b) For the $2N$ case

i) If n = odd simply invoke 1st-order multiplication multiple times.

ii) If n = even invoke 2nd-order differentiation $n/2$ times

c) Provide seperate implementations for 1st-order and 2nd-order differentiation, even ~~thow thow~~ though it is possible to merge them into one routine.

Note that in the $2N$, n=odd case $\tilde{c}_N^{(n)} = 0$ therefore

$$\boxed{D_R^{(2n+1)}(N) = \left[D_R(N)\right]^{2n+1}}$$

<u>Remark</u>: This observation is only important when solving ~~non~~-linear problems. With non-linear problems we filter out all high wavenumbers for anti-aliasing, making this a moot issue. However a correct implementation must take this into account and do the right thing!