QUARTERLY OF APPLIED MATHEMATICS
VOLUME XLVII, NUMBER 2
JUNE 1989, PAGES 309-311

COMMENTS UPON "DIFFERENTIATION BY FOURIER TRANSFORMATION AND ITS CONNECTION WITH DIFFERENTIATION BY FINITE DIFFERENCING"*

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Introduction. In their interesting paper the authors put forward the proposal that the conventional rule for differentiation by discrete Fourier transformation, namely, multiplication by the factor $i2\pi\nu/N$ and subsequent inverse Fourier transformation, is a first-order approximation to more complete rules. They give a revised formula based upon the multiplicative factor $i\sin(2\pi\nu/N)$ and claim that this gives the exact finite difference result. From the examples they quote it is clear that the revised factor can produce superior results when considering gradients of fields with high frequency content. They are, however, implying certain underlying assumptions which they do not make explicit and which demand more careful investigation. In particular, the claim that either one rule or the other is superior in all cases must be questioned.

Discussion. With the numbering system used in the paper, Eq. (4) gives the central difference approximation for the derivative of the general function $f(x)$,

$$\frac{df}{dx} = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}. \tag{4}$$

If F denotes the discrete Fourier transform, the authors show that the corresponding formula is

$$\frac{df}{dx} = \frac{1}{\Delta x} F^{-1}\{i\sin(2\pi\nu/N)\cdot F[f(x)]\}, \tag{7}$$

whereas the standard rule is

$$\frac{df}{dx} = \frac{1}{\Delta x} F^{-1}\{i(2\pi\nu/N) F[f(x)]\}. \tag{10}$$

They suggest that Eq. (10) is just a first approximation to Eq. (7), because $2\pi\nu/N$ is the first term in the expansion of $\sin(2\pi\nu/N)$.

The first point that should be noted is that Eq. (4) is itself a first approximation to $f'(x)$ of accuracy $O((\Delta x)^2)$. If one includes higher terms in the central difference approximation to $f'(x)$ then Eq. (7) ceases to be valid. The next approximation, with error $O((\Delta x)^4)$ is

$$\frac{df}{dx} = \frac{1}{\Delta x}\left(\mu\delta - \frac{1}{6}\mu\delta^3\right) f$$

*Received May 11, 1988.

giving

$$\frac{df}{dx} = \frac{1}{12\Delta x}[f(x-2\Delta x) - 8f(x-\Delta x) + 8f(x+\Delta x) - f(x+2\Delta x)].$$

The expression corresponding to Eq. (7) is then

$$\frac{df}{dx} = \frac{1}{\Delta x}F^{-1}\left\{i\left(\frac{4}{3}\sin\frac{2\pi\nu}{N} - \frac{1}{6}\sin\frac{4\pi\nu}{N}\right)F[f(x)]\right\}.$$

When expanded in powers of $2\pi\nu/N$ the multiplicative factor becomes $i2\pi\nu/N + O((2\pi\nu/N)^5)$. Further higher-order approximations to $f'(x)$ give multiplicative factors which tend to $i2\pi\nu/N$ in the limit. So, in this sense, Eq. (7) is an approximation to Eq. (10) rather than the other way around.

Nevertheless, the use of Eq. (7) for the derivative of a discretized delta function can be effective as is demonstrated in Fig. 1 in the paper. It produces an accurate discretized doublet whereas the normal rule, Eq. (10), produces a function with a high frequency component. Following up the question as to which is the more correct, the answer clearly depends upon the assumptions being made regarding the underlying signal from which the discrete data sequence arises. If the data is regarded as corresponding to a band-limited signal then the normal rule applies. It effectively depends upon reconstruction of the signal followed by differentiation and sampling to get the final derivative ordinates. When applied to the discretized delta function having substantial high frequency content it is to be expected that a strong oscillatory feature will be observed.

On the other hand, if the assumption is made that the correct derivative of a discretized delta function should be a discretized doublet then that is implying something extra about the *shape* of the function concerned, i.e., information is being implied at a higher frequency than is present in the actual samples.

Consider the sampled triangular function f illustrated in Fig. 2. Its discrete Fourier transform has coefficients

$$a_\nu = \frac{1}{NN_1}\frac{\sin^2(\pi N_1\nu/N)}{\sin^2(\pi\nu/N)}.$$

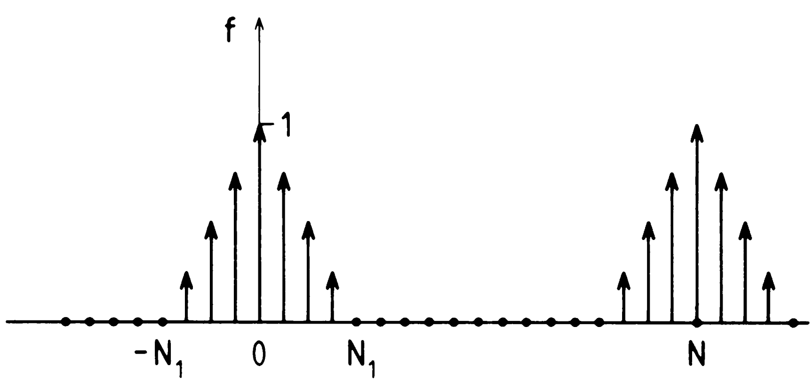

FIGURE 2

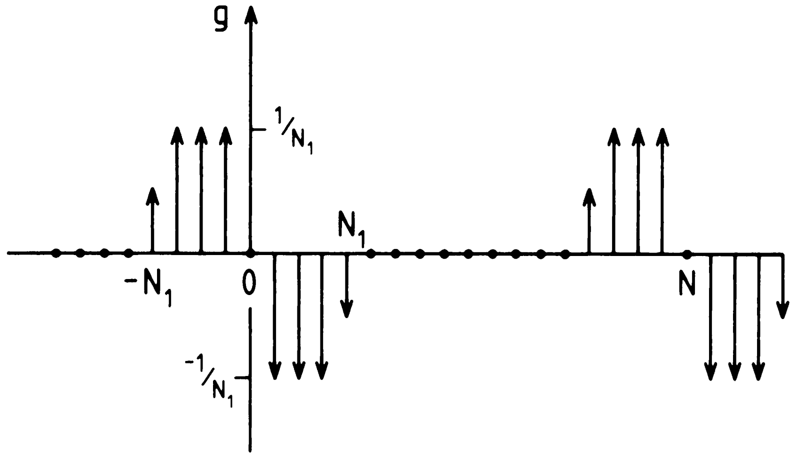

FIGURE 3

Construct a block pulse sequence g, the derivative of f, as illustrated in Fig. 3, by making each ordinate the average of the slopes of $f(x)$ at either side of each node. When $N_1 = 1$, these represent the discretized delta function and doublet, respectively. Then g has the discrete Fourier transform coefficients

$$b_\nu = \frac{2i}{NN_1} \frac{\sin^2(\pi N_1 \nu/N)\cos(\pi\nu/N)}{\sin(\pi\nu/N)}.$$

Clearly

$$b_\nu = (i\sin(2\pi\nu/N))a_\nu,$$

so that Eq. (7) is confirmed as the exact appropriate formula in this case. This example illustrates that the claim that Eq. (4) (or equivalently Eq. (7)) provides an accurate representation of the derivative of the data carries with it the following assumption. That is, that the continuous signal underlying the discrete data is linear between data points and has piecewise constant derivative. The derivative then being evaluated by Eq. (4) is the average of the two gradients at each side of a data point. That explains why the revised formula works well for functions having discontinuities or discontinuities of slope. The usual formula is inapplicable since it is based upon the assumption of the existence of derivatives of all orders.

In general terms it cannot be stated that the usual $i2\pi\nu/N$ rule is simply a first approximation to the "correct" rule. Equally, it cannot be said that the $i\sin(2\pi\nu/N)$ rule is a first approximation to the "correct" $i2\pi\nu/N$ rule. Everything depends upon the most reasonable assumption that can be made regarding the degree of differentiability of the underlying signal. One could construct a "best" formula for each such assumption.

REFERENCE

[1] B. Compani-Tabrizi and R. G. Geyer, *Differentiation by Fourier transformation and its connection with differentiation by finite differencing*, Quart. Appl. Math. XLIV (3), 519–528 (1986)