10.0 Overview of Fourier Transforms and Spectral Analysis

A. Introduction

The subroutines in this chapter compute discrete Fourier transforms, using the fast Fourier transform (FFT). Discrete Fourier transforms can be used in turn to approximate Fourier coefficients or evaluate truncated Fourier series, to approximate power spectra, to compute convolutions and lagged products (as might be required in computing correlations and in filtering), and in several other applications where the speed of the FFT has been found of value, see, *e.g.*, [1].

The purpose of this introductory section is to outline what is available, to help the reader in the selection of the appropriate subroutine, to outline how the discrete transform can be used for the computation of convolutions and lagged products, to examine the errors introduced in using the discrete transform as an approximation to other transforms, and to suggest a computational procedure to those with doubts on how to proceed.

Lower case English letters are used for functions of t, the independent variable, and Greek letters for Fourier transform functions, that are functions of ω, with units of radians/(units of t).

B. Subroutines Available

The one dimensional discrete transform pairs available are indicated below. In "SRFT1/DRFT1" (for example) SRFT1 is the name for the single precision version and DRFT1 is the name for the double precision version. In all cases $\mathrm{N} = 2^M$ where M is a nonnegative integer and $\mathrm{W} = e^{2\pi i/N} = \cos 2\pi/N + i\ \sin 2\pi/N$.

SRFT1/DRFT1 One dimensional real transform

$$x_j = \sum_{k=0}^{N-1} \xi_k W^{jk}, \quad j = 0, 1, ..., N-1 \tag{1}$$

$$\xi_k = \frac{1}{N} \sum_{j=0}^{N-1} x_j W^{-jk}, \quad k = 0, 1..., N-1 \tag{2}$$

STCST/DTCST Trigonometric transform

$$y_j = \frac{1}{2}\alpha_0 + \sum_{k=1}^{(N/2)-1} \left[\alpha_k \cos\frac{2\pi jk}{N} + \beta_k \sin\frac{2\pi jk}{N}\right] + \frac{1}{2}\alpha_{N/2}(-1)^j, \quad j = 0, 1, ..., N-1 \tag{3}$$

$$\begin{aligned} \alpha_k &= \frac{2}{N}\sum_{j=0}^{N-1} y_j \cos\frac{2\pi jk}{N}, \quad k = 0, 1, ..., \frac{N}{2} \\ \beta_k &= \frac{2}{N}\sum_{j=1}^{N-1} y_j \sin\frac{2\pi jk}{N}, \quad k = 1, 2, ..., \frac{N}{2}-1 \end{aligned} \tag{4}$$

STCST/DTCST Cosine transform

$$y_j = \frac{1}{2}\alpha_0 + \sum_{k=1}^{N-1} \alpha_k \cos\frac{\pi jk}{N} + \frac{1}{2}\alpha_N(-1)^j, \quad j = 0, 1, ..., N \tag{5}$$

$$\alpha_k = \frac{2}{N}\left[\frac{1}{2}y_0 + \sum_{j=1}^{N-1} y_j \cos\frac{\pi jk}{N} + \frac{1}{2}y_N(-1)^k\right] \quad k = 0, 1, ..., N \tag{6}$$

STCST/DTCST Sine transform

$$y_j = \sum_{k=1}^{N-1} \beta_k \sin\frac{\pi jk}{N}, \quad j = 1, 2, ..., N-1 \tag{7}$$

$$\beta_k = \frac{2}{N}\sum_{j=1}^{N-1} y_j \sin\frac{\pi jk}{N}, \quad k = 1, 2, ..., N-1 \tag{8}$$

SCFT/DCFT Complex transform

$$z_j = \sum_{k=0}^{N-1} \zeta_k W^{jk}, \quad j = 0, 1, ..., N-1 \tag{9}$$

$$\zeta_k = \frac{1}{N}\sum_{j=0}^{N-1} z_j W^{-jk}, \quad k = 0, 1, ..., N-1 \tag{10}$$

All variables in the above equations are real, except W, ξ, z, and ζ which are complex. For each of the transform pairs given, either equation can be derived from the other – there are no approximations involved.

Taking real and imaginary parts of Eq. (2) and making comparisons with Eq. (4), it is clear that if $x_j = y_j$, then $2\ \Re\xi_k = \alpha_k$ and $2\ \Im\xi_k = -\beta_k$. Thus the trigonometric transform and the real transform are closely related. Since SRFT1 is slightly more efficient and shorter than STCST, it is recommended unless one has a distinct preference for the trigonometric form. If one has data that are even (or odd) then one can save a factor of two in both storage and computation by using the cosine (or sine) transform in STCST. One could use SCFT for real data by setting $\Im z_j = 0$, but since this requires twice the storage and twice the work as SRFT1, SCFT is recommended only for complex data.

Subroutines STCST, SCFT, and SRFT (similar to SRFT1) can be used for data in more than one dimension. As above, there is a connection between the real transform and the trigonometric transform, but the relations connecting the two are not as simple. Indexing of the coefficients in SRFT is more complicated, and thus we recommend STCST for multi-dimensional real data unless one prefers the form of the solution provided by SRFT.

C. Discrete Convolutions and Correlations

Here we consider computing sums of the form

$$c_n = \sum_{j=0}^{N-1} a_j b_{n \pm j}, \quad n = 0, 1, ..., N-1 \tag{11}$$

Initially it is assumed that a_j and b_j are periodic with period N. (That is, if j is not in the range $0 \leq j \leq N-1$, it is replaced by its value mod N.) Thus α_k and β_k can be defined by

$$a_j = \sum_{k=0}^{N-1} \alpha_k W^{jk}, \quad \text{and} \quad b_j = \sum_{k=0}^{N-1} \beta_k W^{jk}.$$

Substitution in Eq. (11) yields

$$\begin{aligned} c_n &= \sum_{j=0}^{N-1} \left[\sum_{k'=0}^{N-1} \alpha_{k'} W^{jk'} \right] \left[\sum_{k=0}^{N-1} \beta_k W^{(n \pm j)k} \right] \\ &= \sum_{k'=0}^{N-1} \sum_{k=0}^{N-1} \alpha_{k'} \beta_k W^{nk} \sum_{j=0}^{N-1} W^{j(k' \pm k)}. \end{aligned} \tag{12}$$

From the easily verified fact that

$$\sum_{j=0}^{N-1} W^{j(k' \pm k)} = \begin{cases} N & \text{if } k' \equiv \mp k \bmod N \\ 0 & \text{if } k' \not\equiv \mp k \bmod N \end{cases} \tag{13}$$

and since α_k is periodic with period N there follows from Eq. (12)

$$\begin{aligned} c_n &= N \sum_{k=0}^{N-1} \alpha_{\mp k} \beta_k W^{nk}, \quad n = 0, 1, ..., N-1 \\ &= N \sum_{k=0}^{N-1} \gamma_k W^{nk}, \qquad \text{where } \gamma_k = \alpha_{\mp k} \beta_k. \end{aligned} \tag{14}$$

The c_n can be computed most efficiently by the indirect route of using the FFT to compute the α's and β's from the a's and $b's$, then computing γ_k as defined in Eq. (14), and finally using the FFT to compute the c's from the $\gamma's$. For real data, SRFT1 is recommended for computing the transforms. Note that with SRFT1 α_k, β_k, and γ_k are only computed for $k = 0, 1, ..., N/2$; for $k = (N/2)+1, ..., N-1$, one must use the fact that for real data $\alpha_{N-k} = \overline{\alpha}_k$ ($\overline{z}$ = conjugate of z).

Ordinarily one has a_j and b_j defined for $j = 0, 1, ..., J-1$, assumed to be 0 for other values of j, and desires c_n for $n = 0, 1, ..., L-1$, where $L \leq J$. The above procedure can be used to get the first L values of c_n if one sets N = smallest power of $2 > J + L$ and sets a_j and $b_j = 0$ for $j = J, J+1, ..., N-1$. (If $J + L$ is equal to or just slightly greater than a power of 2, it pays to reduce L so that $J + L$ is one less than a power of 2, and to compute c_n directly from Eq. (11) for values of $n = new\ L, ...,$ desired $L - 1$.) Direct computation of the c_n for $n = 0, 1, ..., L-1$ from Eq. (11) requires $L(2J - L + 1)/2$ multiplies and adds. Using SRFT1 and the procedure above requires approximately $(9/4)N \log_2 N$ multiplies, $(33/8)N(\log_2 N+1)$ adds, and a little additional overhead. If $a_j = b_j$ then the counts using SRFT1 can be multiplied by 2/3. The fastest procedure clearly depends on the values of J, L, and N. For $J < 64$, or for values of L small relative to J, the direct method is fastest, see [1].

Note that no assumption need be made about a_j and b_j; the only errors introduced in the calculation of c_n using SRFT1 are round-off errors.

D. Estimating Power Spectra

To within a constant factor (different normalizations are used), an estimate of the power at the k^{th} frequency (defined in E below) is given by $|\xi_k|^2 = (\Re \xi_k)^2 + (\Im \xi_k)^2$, where the ξ_k are obtained from SRFT1, Eq. (2) above. This estimate suffers from the same type of errors discussed below for the case of computing Fourier integrals.

E. Replacement of Continuous Transforms with Discrete Ones

To simplify the material that follows we consider only the case of complex functions. Results for real data follow immediately by considering real and imaginary parts of the variables and equations below. Proofs for the transform pairs are given in many books on Fourier transforms, although different scalings for φ and ω are used. We have used definitions that maximize symmetry while matching up with the form of the discrete transform provided by the FFT.

For continuous data we have the following transform pairs.

Fourier Integral $\left(\int_{-\infty}^{\infty} |f(t)|\, dt \quad \text{exists} \right)$

$$f(t) = \int_{-\infty}^{\infty} \varphi(\omega) e^{2\pi i \omega t} d\omega \tag{15}$$

$$\varphi(\omega) = \int_{-\infty}^{\infty} f(t) e^{-2\pi i \omega t} dt \tag{16}$$

Fourier Series ($s(t) = s(t+T)$)

$$s(t) = \sum_{k=-\infty}^{\infty} \sigma_k e^{2\pi ikt/T} \tag{17}$$

$$\sigma_k = \frac{1}{T}\int_{-T/2}^{T/2} s(t) e^{-2\pi ikt/T} dt \tag{18}$$

The discrete transform Eq. (10) can be used to approximate Eq. (16) if the infinite limits are replaced by finite limits and f is sampled at equally spaced points between the two limits. As an example let the infinite limits be replaced by $-T/2$ and T/2, and let

$$z_j = \begin{cases} f(-\frac{T}{2} + j\Delta t), & j = 1, 2, ..., N-1 \\ \frac{1}{2}\left[f(-\frac{T}{2}) + f(\frac{T}{2})\right], & j = 0, \end{cases} \tag{19}$$

$$\Delta t = \frac{T}{N}. \tag{20}$$

This value of z_0 gives significantly better results than simply setting $z_0 = f(-T/2)$. With the assumption that the contribution to the integral in Eq. (16) is negligible for $|t| > T/2$, the trapezoidal rule gives

$$\begin{aligned} \varphi(\omega) &\approx \Delta t \sum_{j=0}^{N-1} z_j e^{-\pi i\omega(-T+2j\Delta t)} \\ &\approx \frac{T}{N} e^{\pi i\omega T} \sum_{j=0}^{N-1} z_j e^{-2\pi ij\omega T/N}. \end{aligned} \tag{21}$$

In order that Eq. (21) have the form of Eq. (10), the solution is obtained for $\omega = \omega_k$, where

$$\omega_k = \frac{k}{T}, \quad k = 0, 1, ...N-1. \tag{22}$$

Then

$$\varphi(\omega_k) \approx \frac{T}{N} e^{\pi ik} \sum_{j=0}^{N-1} z_j W^{-jk} \quad (W = e^{2\pi i/N}). \tag{23}$$

Thus $\varphi(\omega_k) \approx Te^{\pi ik}\zeta_k$, ζ_k defined as in (10). The factor $e^{\pi ik} (= (-1)^k)$ is due to shifting the lower limit of $-T/2$ on the integral to a lower limit of 0 on the summation.

Note that the k^{th} frequency, $2\pi\omega_k$, depends only on T, the length of the interval over which f is sampled. Thus, from Eq. (22), $2\pi\omega_k$ radians/(units of t) $= k/T$ cycles/(units of t). From Eqs. (20) and Eq. (21) it follows that the largest frequency for which a result is obtained is $\omega_{N-1} = (N-1)/(N\Delta T)$ cycles. For real data, our approximation is such that $\varphi(\omega_{N-k})$ is the conjugate of $\varphi(\omega_{-k})$, and thus in this case the largest effective frequency is

$$\omega_{N/2} = \frac{1}{2\Delta t} \text{ cycles/(units of } t). \tag{24}$$

This frequency is commonly called the *Nyquist frequency.* Note that this frequency depends only on the sampling interval Δt.

All that has been said above for Eq. (16) applies almost word for word to Eq. (18), except that Eq. (18) does not require replacing infinite limits by finite ones. Because of the factor $1/T$ appearing in Eq. (18), in place of $\varphi(\omega_k) \approx Te^{\pi ik}\zeta_k$, we have $\sigma_k \approx e^{\pi ik}\zeta_k$.

F. Errors Introduced by Using the Discrete Transform

The discrete Fourier transform when used as above is a crude approximation to a continuous transform. Its primary virtue is the speed with which it can be computed using the FFT (**F**ast **F**ourier **T**ransform). Many procedures have been suggested for computing continuous transforms and power spectra, some of which permit the use of the FFT and some which do not. References in Section H below give a sampling of what has been suggested.

Any computational procedure involves making assumptions about either $f(t)$ or $\varphi(\omega)$ (or both), and any assumption about one implies something about the other. Answers to questions such as the following help one in understanding the implications of a computational procedure.

(Q1) How are the true and computed transform related?

(Q2) What is the error in the computed transform?

(Q3) What assumptions (if any) are made or implied concerning the transform?

(Q4) What assumptions are made about the function at points where its value is not used?

(Q5) At the points where the value of the function is used, how is the function related to a function that would give the true transform at selected values of ω?

These questions are considered below for the case of the discrete transform. We begin by giving some results required in the analysis, then consider the effect of limiting the sampling of f to a finite range, the effect of discrete sampling, a combination of the two, and finally the effect on the discrete transform of filling in with zeros.

F.1 Convolution Theorems

For Fourier integrals we have

$$\varphi(\omega) = \varphi_1(\omega)\varphi_2(\omega) \qquad \text{if and only if} \tag{25}$$

$$f(t) = \int_{-\infty}^{\infty} f_1(\tau) f_2(t-\tau)\, d\tau. \tag{26}$$

This result can be derived from Eqs. (15) and (16), and is also true if φ and f are interchanged throughout Eqs. (25) and (26).

In the case of Fourier series there are two convolution theorems. We work with the three transform pairs (a, α), (b, β), and (c, γ). If $c(t) = a(t)b(t)$, then

$$\gamma_n = \frac{1}{T} \int_{-T/2}^{T/2} \sum_{k=-\infty}^{\infty} \sum_{k'=-\infty}^{\infty} \alpha_k \beta_{k'} e^{2\pi i t(k+k'-n)/T} dt. \tag{27}$$

Interchanging integration and summation, the integral is 0 if $k' \neq n-k$, and is T if $k' = n-k$. Thus

$$\gamma_n = \sum_{k=-\infty}^{\infty} \alpha_k \beta_{n-k}. \tag{28}$$

The second convolution theorem starts with

$$c(t) = \frac{1}{T} \int_{-T/2}^{T/2} a(\frac{1+\tau}{2}) b(\frac{1-\tau}{2})\, d\tau$$
$$= \frac{1}{T} \int_{-T/2}^{T/2} \sum_{k=-\infty}^{\infty} \sum_{k'=-\infty}^{\infty} \alpha_k \beta_{k'} e^{2\pi i [t(k+k')+\tau(k-k')]/2T} d\tau. \tag{29}$$

Moving the integral inside the summations, we get a nonzero result only for $k' = k$ in which case the integral is $\exp(2\pi i t k/T)$. Thus

$$c(t) = \sum_{k=-\infty}^{\infty} \alpha_k \beta_k e^{2\pi i t k/T}, \quad \text{and so}$$

$$\gamma_k = \alpha_k \beta_k. \tag{30}$$

The convolution theorem for the discrete Fourier transform has already been given in Eqs. (11) and (14).

F.2 Fourier Transform of a Step Function

For Fourier integrals, let

$$r_T(t) = \begin{cases} 1 & -\frac{T}{2} < t < \frac{T}{2} \\ 0 & |t| > \frac{T}{2} \end{cases} \tag{31}$$

$$\begin{aligned} \rho_T(\omega) &= \int_{-\infty}^{\infty} r_T(t) e^{-2\pi i \omega t} dt \\ &= \int_{-T/2}^{T/2} e^{-2\pi i \omega t} dt = \frac{\sin \pi \omega T}{\pi \omega}. \end{aligned} \tag{32}$$

Similarly, one has the transform pair $(\frac{1}{\pi t} \sin \pi t \Omega,\ r_\Omega(\omega))$. For Fourier series, we are interested in the case

$$\hat{\rho}_k^{(K)} = \begin{cases} 1 & -K \leq k < K \\ 0 & k \geq K \text{ or } k < -K \end{cases} \tag{33}$$

$$\begin{aligned} \hat{r}^{(K)} &= \sum_{k=-\infty}^{\infty} \hat{\rho}_k^{(K)} e^{2\pi i t k/T} = \sum_{k=-K}^{K-1} e^{2\pi i t k/T} \\ &= \frac{2i(\sin 2\pi K t/T)}{e^{2\pi i t/T} - 1} \\ &= \frac{(1 + e^{-2\pi i t/T})(\sin 2\pi K t/T)}{\sin 2\pi t/T}. \end{aligned} \tag{34}$$

For the discrete Fourier transform, consider

$$\tilde{r}_{j+kN}^{(J)} = \begin{cases} 1 & 0 \leq j \leq J-1 \\ 0 & J \leq j \leq N-1 \end{cases} \quad k = 0, \pm 1, \pm 2, ... \tag{35}$$

$$\tilde{\rho}_k^{(J)} = \frac{1}{N} \sum_{j=0}^{N-1} \tilde{r}_j^{(J)} W^{-jk} = \frac{1}{N} \sum_{j=0}^{J-1} W^{-jk}$$

$$\tilde{\rho}_k^{(J)} = \begin{cases} J/N & k = 0, \pm N, \pm 2N, ... \\ \dfrac{1 - W^{-Jk}}{N(1 - W^{-k})} & \text{otherwise.} \end{cases} \tag{36}$$

F.3 Errors Due to a Finite Range

Consider approximating $\varphi(\omega)$ in Eq. (16) with

$$\hat{\varphi}(\omega) = \int_{-T/2}^{T/2} f(t) e^{-2\pi i \omega t} dt. \tag{37}$$

This is equivalent to answering (Q4) with $f(t) = 0$ for $|t| > T/2$.

To answer (Q1), rewrite the above equation as follows

$$\hat{\varphi}(\omega) = \int_{-\infty}^{\infty} r_T(t) f(t) e^{-2\pi i \omega t} dt, \tag{38}$$

and using Eqs. (25) and (26) (with f and φ interchanged)

$$\hat{\varphi}(\omega) = \int_{-\infty}^{\infty} \varphi(\omega) \frac{\sin \pi T(\omega - w)}{\pi(\omega - w)}\, dw. \tag{39}$$

Thus the effect of a finite range is a loss of resolution due to the smearing as indicated in Eq. (39).

One answer to (Q2) is to subtract both sides of Eq. (39) from $\varphi(\omega)$. A more useful result is obtained by subtracting Eq. (37) from Eq. (16).

$$\varphi(\omega) - \hat{\varphi}(\omega) = \int_{T/2}^{\infty} \left[f(t) e^{-2\pi i \omega t} + f(-t) e^{2\pi i \omega t} \right] dt. \tag{40}$$

Thus a bound on the error is given by

$$|\varphi(\omega) - \hat{\varphi}(\omega)| \leq \int_{T/2}^{\infty} [|f(t)| + |f(-t)|] \, dt. \tag{41}$$

If $\int_{-\infty}^{\infty} |f^{(j)}(t)| \, dt$ exists for $j = 0, 1, ..., J+1$, integration by parts of the two terms in the integral of Eq. (40) yields (k an integer)

$$\varphi(k/T) - \hat{\varphi}(k/T) = \\ (-1)^k \sum_{j=0}^{J} \left[\frac{-iT}{2\pi k}\right]^{(j+1)} \left[f^{(j)}(T/2) - f^{(j)}(-T/2)\right] + R, \tag{42}$$

where R is a remainder term that goes to 0 as $k \to \infty$. Except for the form of the remainder, the same result is obtained in the same way from the negative of the right side of Eq. (37), where $\hat{\varphi}$ is defined. Thus for large ω, $\hat{\varphi}(\omega)$ is mainly error unless derivatives of f at $-T/2$ are very nearly equal to those at T/2. If the j^{th} derivatives of f at the endpoints are not equal, then $\hat{\varphi}(\omega)$ decreases no faster than $\omega^{-(j+1)}$ for large ω. We find below that nearly equal derivatives at the ends of the interval are also important when estimating $\hat{\varphi}$ using the FFT.

To answer (Q5) consider

$$\begin{aligned} \varphi(k/T) &= \int_{-\infty}^{\infty} f(t) e^{-2\pi ikt/T} dt \\ &= \sum_{j=-\infty}^{\infty} \int_{-T/2+jT}^{T/2+jT} f(t) e^{-2\pi ikt/T} dt \\ &= \int_{-T/2}^{T/2} \sum_{j=-\infty}^{\infty} f(t+jT) e^{-2\pi ik(t+jT)/T} dt. \end{aligned}$$

And since $e^{-2\pi ijk} = 1$, we have

$$\begin{aligned} \varphi(k/T) &= \int_{-T/2}^{T/2} \hat{f}(t) e^{-2\pi ikt/T} dt, \quad \text{where} \\ \hat{f}(t) &= \sum_{j=-\infty}^{\infty} f(t+jT) \end{aligned} \tag{43}$$

If $f(t)$ is replaced by $\hat{f}(t)$ as defined above, then $\hat{\varphi}(k/T) = \varphi(k/T)$.

F.4 Errors Due to Discrete Sampling

Given $f(j\Delta t)$, $j = 0, \pm1, \pm2, ...$, we have (proceeding much as was done in obtaining Eq. (42))

$$\begin{aligned} f(j\Delta t) &= \int_{-\infty}^{\infty} \varphi(\omega) e^{2\pi i\omega j\Delta t} d\omega \\ &= \sum_{k=-\infty}^{\infty} \int_{(k-1/2)/\Delta t}^{(k+1/2)/\Delta t} \varphi(\omega) e^{2\pi i\omega j\Delta t} d\omega \end{aligned}$$

$$\begin{aligned} f(j\Delta t) &= \int_{-1/2\Delta t}^{1/2\Delta t} \tilde{\varphi}(\omega) e^{2\pi i\omega j\Delta t} d\omega, \quad \text{where} \\ \tilde{\varphi}(\omega) &= \sum_{k=-\infty}^{\infty} \varphi(\omega + \frac{k}{\Delta t}). \end{aligned} \tag{44}$$

Clearly $\tilde{\varphi}(\omega)$ is periodic with period $1/\Delta t$, thus from Eqs. (18) and (17)

$$\tilde{\varphi}(\omega) = \Delta t \sum_{j=-\infty}^{\infty} f(j\Delta t) e^{-2\pi i\omega j\Delta t}. \tag{45}$$

If no assumptions are made about f or φ, then given just $f(j\Delta t)$, $j = 0, \pm1, ...$ values of φ for frequencies that differ by a multiple of $1/\Delta t$ cycles are irrevocably mixed. This phenomenon is commonly called *aliasing*.

When sampling at discrete points the usual assumption made is that f is band-limited. That is, $\varphi(\omega) = 0$ for $|\omega| > 1/(2\Delta t)$. Thus the computed transform is equal to $\hat{\varphi}$ as given in Eq. (45), and questions (Q1) and (Q2) are answered by the expression for $\hat{\varphi}$ as given in Eq. (44).

To answer (Q4) and (Q5), note that if $\tilde{f}$ is a function whose true transform is 0 for $|\omega| > 1/(2\Delta t)$ and is $\varphi(\omega)$ otherwise, then

$$\tilde{f}(t) = \int_{-\infty}^{\infty} r_{1/\Delta t}(\omega) \varphi(\omega) e^{2\pi i\omega t} d\omega, \tag{46}$$

and using Eqs. (25), (26), (31), and (32)

$$\tilde{f}(t) = \int_{-\infty}^{\infty} f(\tau) \frac{\sin(\pi(t-\tau)/\Delta t)}{\pi(t-\tau)} \, d\tau. \tag{47}$$

Note the symmetries between f and φ in Eqs. (38) and (46); (39) and (47); and (43) and (44). Relations symmetric to Eqs. (40) – (42) are easily obtained, but we do not bother to do so here.

F.5 Errors Due to Discrete Sampling on a Finite Interval

Here we consider errors that result from evaluating the integral in Eq. (18) using the discrete Fourier transform. The results also apply to the integral in Eq. (37), and thus errors examined here combined with those due to a finite range give the total error due to replacing a Fourier integral with a discrete Fourier transform.

The aliasing problem is revealed much as it was obtained in Eq. (44). Let $\Delta t = T/N$, and from Eq. (17)

$$\begin{aligned} s(j\Delta t) &= \sum_{k=-\infty}^{\infty} \sigma_k e^{2\pi ijk/N} = \sum_{m=-\infty}^{\infty} \sum_{k=mN}^{(m+1)N-1} \sigma_k W^{jk} \\ &= \sum_{k=0}^{N-1} \sum_{m=-\infty}^{\infty} \sigma_{k+mN} W^{jk}, \end{aligned}$$

$$s(j\Delta t) = \sum_{k=0}^{N-1} \tilde{\sigma}_k W^{jk}, \text{ where } \tilde{\sigma}_k = \sum_{m=-\infty}^{\infty} \sigma_{k+mN}. \quad (48)$$

And, as for Eq. (45), there results from Eqs. (9) and (10)

$$\tilde{\sigma}_k = \frac{1}{N} \sum_{j=0}^{N-1} s(j\Delta t) W^{-jk}. \quad (49)$$

Since $\tilde{\sigma}_{k-N} = \tilde{\sigma}_k$, and $W^{j(k-N)} = W^{jk}$, Eq. (48) can be rewritten to make more apparent the assumption that s is band-limited. Subtracting N from all indices $k \geq N/2$, there results

$$s(j\Delta t) = \sum_{k=-N/2}^{(N/2)-1} \tilde{\sigma}_k W^{jk}. \quad (50)$$

As before, if we assume that $s(t)$ is band-limited, questions (Q1) and (Q2) are answered by the expression for $\tilde{\sigma}$ given in Eq. (48).

To answer (Q4) and (Q5) as in Eq. (47) we use Eqs. (29), (30), (33), and (34) to obtain from

$$\tilde{s}(t) = \sum_{k=-\infty}^{\infty} \sigma_k \hat{\rho}_k^{(N/2)} e^{2\pi ikt/T}, \quad (51)$$

$$\tilde{s}(t) = \frac{1}{T} \int_{-T/2}^{T/2} \left[s(\frac{t+\tau}{2}) \left(1 + e^{-\pi i(t-\tau)/T}\right) \times \frac{\sin(\pi N(t-\tau)/2T)}{\sin(\pi(t-\tau)/T)} \right] d\tau. \quad (52)$$

Another answer to (Q2) can be obtained using the Euler-Maclaurin formula. Let $S_k(t) = s(t)e^{-2\pi ikt/T}$, define $S_{k,j}^{(\mu)}$ to be the μ^{th} derivative of S_k evaluated at $t = -\frac{T}{2} + j\,\Delta t$, and $S_{k,j} = S_{k,j}^{(0)}$. Then the Euler-Maclaurin formula applied to Eq. (18) gives

$$\sigma_k = \frac{\Delta t}{T} \left\{ \frac{1}{2}\left[S_{k,N} + S_{k,0}\right)] + \sum_{j=1}^{N-1} S_{k,j} + C_k^{(r)} \right\} + R_k^{(r)}, \quad (53)$$

where

$$C_k^{(r)} = \sum_{\nu=1}^{r} \frac{B_{2\nu}(\Delta t)^{2\nu-1}}{2\nu!} \left[S_{k,N}^{(2\nu-1)} - S_{k,0}^{(2\nu-1)}\right],$$

$B_{2\nu}$ is the $2\nu^{th}$ Bernoulli number, and $R_k^{(r)}$ is a remainder term. The terms in Eq. (53) that contain S are what one would use following the procedure given in Section E above. The terms involving a $(2\nu-1)^{st}$ derivative of S are correction terms, which if not used, give an indication (which can be misleading) of the error. To examine the errors as they depend on the derivatives of s, we write

$$S_k^{(\mu)}(t) = \sum_{j=1}^{\mu} \binom{\mu}{j} s^{(j)}(t) \left[\frac{-2\pi ik}{T}\right]^{\mu-j} e^{-2\pi ikt/T}, \quad (54)$$

$$S_k^{(\mu)}(\pm T/2) = \sum_{j=1}^{\mu} \binom{\mu}{j} \left[\frac{-2\pi ik}{T}\right]^{\mu-j} (-1)^k s^{(j)}(\pm T/2). \quad (55)$$

Substitution into $C_k^{(r)}$ and a little algebraic manipulation gives the following result.

$$\frac{\Delta t}{T} C_k^{(r)} = \frac{(-1)^k}{N} \sum_{j=0}^{2r-1} b_j^{(r)} \left[\frac{iT}{2\pi k}\right]^j \left[s^{(j)}(\frac{T}{2}) - s^{(j)}(-\frac{T}{2})\right], \quad (56)$$

where

$$b_j^{(r)} = \sum_{\nu=\lfloor j/2\rfloor+1}^{r} \binom{2\nu-1}{j} \frac{B_{2\nu}(-2\pi ik/N)^{2\nu-1}}{(2\nu)!}, \quad (57)$$

and $\lfloor j/2 \rfloor$ is the integer part of $j/2$. Note the similarities between Eqs. (42) and (56). The degree of continuity in the periodic extension of the function sampled on $[-T/2, T/2]$ is extremely important in determining how well the discrete Fourier transform will approximate either of the other Fourier transforms.

F.6 Filling in with Zeros

The requirement that N be a power of 2 imposed by the FFT routines in this chapter may be inconvenient. It is sometimes suggested that if one has N' function values, that the remaining $N - N'$ values be set to 0, where N is the first power of $2 \geq N'$. Let z_j denote the true values of the function for $j = 0, 1, ..., N-1$, and let ζ_k and $\hat{\zeta}_k$ denote the true and computed coefficients for the discrete Fourier transform of z. Then clearly

$$\zeta_k - \hat{\zeta}_k = \frac{1}{N} \sum_{j=N'}^{N-1} z_j W^{-jk}. \quad (58)$$

And, using Eqs. (11), (14), (35), and (36)

$$\hat{\zeta}_k = \sum_{\nu=0}^{N-1} \zeta_\nu \frac{1 - W^{-N'(k-\nu)}}{N(1 - W^{-(k-\nu)})} \quad (59)$$

where for $\nu = k$ the multiplier of ζ_ν is N'/N.

It is perhaps more instructive to consider the connection between $\hat{\zeta}_k$ and $\tilde{\zeta}_k$, where

$$\tilde{\zeta}_k = \frac{1}{N'} \sum_{j=0}^{N'-1} z_j e^{-2\pi ijk/N'}. \tag{60}$$

By extending the definitions of $\hat{\zeta}_k$, and $\tilde{\zeta}_k$ to noninteger k in the obvious way, one obtains

$$\begin{aligned} \hat{\zeta}_{kN/N'} &= \frac{1}{N} \sum_{j=0}^{N'-1} z_j e^{-2\pi ijk/N'} = \frac{N'}{N}\tilde{\zeta}_k, \quad \text{and} \\ \tilde{\zeta}_{kN'/N} &= \frac{1}{N'} \sum_{j=0}^{N'-1} z_j e^{-2\pi ijk/N} = \frac{N}{N'}\hat{\zeta}_k \end{aligned} \tag{61}$$

Thus $\frac{N}{N'}\hat{\zeta}_k$ can be thought of as a way of computing $\tilde{\zeta}$ with a smaller than usual $\Delta\omega$. In particular, if $N = 2N'$, $\hat{\zeta}_{2k} = \tilde{\zeta}_k/2$. It is sometimes suggested that N' extra zeros be added even when N' is a power of 2. By doing this one can use the FFT to get the autocorrelation from Eqs. (11) and (14), and the power spectrum, which can be defined as the Fourier transform of the autocorrelation function, is obtained automatically. An alternative method for those who like this approach is to compute $\tilde{\zeta}_k/2$ (N' a power of 2) to get $\hat{\zeta}_{2k}$, and obtain $\hat{\zeta}_{2k+1}$ by setting it equal to the k^{th}discrete Fourier coefficient of z' where $z'_j = z_j e^{\pi ij/N'}$, $j = 0, 1, ..., N' - 1$.

If one zeros ζ_k for $k = N'$, $N' + 1$, ..., N, then instead of defining a trigonometric polynomial of degree $N - 1$ that passes through z_j, $j = 0, 1, ..., N - 1$, the $\zeta's$ define a trigonometric polynomial of degree $N' - 1$, that fit the z_j in a least-squares sense. Multiplication by the Lanczos sigma factors, see below, should usually give better smoothing characteristics for nonperiodic data.

G. Recommendations

The FFT gives good results if one is sampling a periodic function over one period. Results are less satisfactory for other cases. What we suggest here should usually give an improvement over the FFT, however, in many cases one can undoubtedly do ever better.

It is assumed that trends in the data (*e.g.*, a linear trend) have been removed, and that appropriate action has been taken for wild points or gaps in the data. By a trend, we mean a smooth function S, so that the (estimated) average value of $|S(t) - z(t)|$ is as small as possible for t outside the sampling interval. In some cases one may want to add the Fourier transform of S to the computed transform of z.

For functions that are not periodic it makes little sense to attempt a representation in terms of a discrete set of frequencies. In Eq. (61) the value of the discrete transform for noninteger values is defined. What we propose here amounts to computing ζ_k, which is an average of the values of the discrete transform for nearby noninteger values of k. Starting from Eq. (21), consider

$$\begin{aligned} \varphi_a(\omega) =& \frac{1}{2a} \int_{\omega-a}^{\omega+a} \varphi(\alpha)\, d\alpha \\ =& \frac{T}{N} \sum_{j=0}^{N-1} z_j \frac{1}{2a} \int_{\omega-a}^{\omega+a} e^{\pi i\alpha T(N-2j)/N} d\alpha \\ =& \frac{T}{N} e^{\pi i\omega T} \sum_{j=0}^{N-1} \left[\frac{\sin[\pi aT(N-2j)/N]}{\pi aT(N-2j)/N}\right] z_j e^{-2\pi ij\omega T/N}. \end{aligned} \tag{62}$$

With $\omega = \omega_k$, Eq. (62) is the same as Eq. (23) except for the multiplier of z_j. The choice $a = 1/T$ is attractive for several reasons: it is the smallest value of a that gives a multiplier of 0 for z_0(and for z_N if it were used), and thus helps to minimize the effect of a discontinuity in the periodic extension of z_j; the value of $\varphi_{1/T}(\omega_k)$ is the average value of φ from ω_{k-1} to ω_{k+1}, so not much resolution is lost; finally, if Eq. (39) is integrated from $\omega - a$ to $\omega + a$ as was done in Eq. (21), one finds that the choice $a = 1/T$ minimizes the effect of $\varphi(\hat{\omega})$ on $\hat{\varphi}_k(\omega)$ for values of $\hat{\omega}$ remote from ω. Thus, we define

$$\sigma_j = \begin{cases} \dfrac{\sin \pi j/N}{\pi j/N} & j \neq 0 \\ 1 & j = 0 \end{cases} \tag{63}$$

and the multiplier of z_j in Eq. (62) is σ_{N-2j}. And since $\sigma_{-N+2j} = \sigma_{N-2j}$, z_{N-j} has the same multiplier.

The σ_j defined in Eq. (63) are the Lanczos sigma factors, see [2] for a different motivation in their derivation, and for instructive examples. If one wants a greater smoothing, rather than increasing a, we recommend averaging the average. Thus if the same procedure is applied to Eq. (62) as was applied to Eq. (21) one finds that σ_{N-2j} is replaced by σ^2_{N-2j}. This process can of course be repeated, depending on how much resolution one is willing to give up. The $\sin \pi j/N$ are readily available from the sine table required by the FFT subroutines as illustrated in the example for SRFT1.

The choice of $a = 1/T$ is not appropriate if one has filled out with zeros because N' values are given and N' is not a power of 2. We assume the given values of z are stored in z_j, $j = N'/2$, ..., $[(N + N')/2]$, and that both ends have been zero filled. Then one should set $a = N/(N'T)$.

The σ factors are also useful for smoothing. Given real data, x, one can replace x_j by the average value of the trigonometric polynomial interpolating the data on the interval $x_{j-1} \leq x \leq x_{j+1}$ using the σ factors. Simply compute the ζ_k using the FFT, multiply ζ_k by σ_{2k}, $k = 1, 2, ..., N/2$, and then compute the inverse transform. This application is illustrated in the example for SRFT.

When the number of data points is not a power of two, one may have an interest in using a mixed radix algorithm such as that in [3], or one could use the codes given here together with the technique described in [4]. Before making the decision to go with something more complicated than padding the data with 0's, (or when padding the data with 0's), one should understand the connections described from Eq. (60) to just below Eq. (61).

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For information on the web, see:
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