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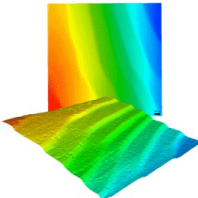
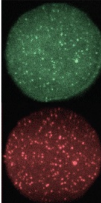
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Improved method for the discrete fast Fourier transform^{a)}

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A new algorithm is proposed here for the discrete fast Fourier transform with greatly reduced aliasing which is known to be inherent in the conventional algorithm of Cooley and Tukey, unless the function is band limited and the sampling frequency satisfies the Nyquist condition. Like the algorithm recently proposed by Schütte and extended by Mäkinen in this journal, this is also based on the polynomial expansion of the function to be transformed but more general in formulation and less restrictive than theirs. Its power is demonstrated with a few non-band-limited functions that can be exactly transformed with chosen limits as usually met in different experimental situations. In all cases tried, this yields, in general, much improved accuracy in comparison to others at little or no corresponding increase of computation time.

INTRODUCTION

The Fourier transform (FT) as a technique is finding increasing applications in different scientific disciplines such as physics, chemistry, engineering, etc. The simple relation of FT for transforming one function to the other is very attractive both from experimental and theoretical viewpoints. From the former, which is our interest here, it offers the possibility of measuring a function of a certain parameter most amenable to an experimental situation while its FT is most desired from other considerations. This is why this technique is finding increasing applications in different fields of spectroscopy. The two functions $x(t)$ and $X(f)$ in the time and frequency domains are related by the FT defined as

$$X(f) = \int_0^{\infty} x(t) \exp(-2\pi if t) dt, \quad (1)$$

where $x(t)$ for different times t are measured but $X(f)$ for different f 's are required to understand the results. As can be noticed from Eq. (1), one cannot expect to get $x(t)$ to the limits of integration since any measurement would be of finite duration. Hence, there will be some unavoidable but in most cases acceptable error in $X(f)$ for this finite duration of $x(t)$. Similar error in $X(f)$, known as the cutoff error, is also inherent in any method of numerical integration. Fortunately, an estimation of such errors can be made, at least in principle, with different choices of the limits. In all practical situations, this integral is to be evaluated with a finite upper limit and preferably with an estimation of error for the cutoff. The finer the divisions, the more accurately the integral is evaluated. The finer the divisions, on the other hand, the longer is the time of integration; this time increases almost in a power law and becomes prohibitive for any practical purpose. In order to reduce this time, Cooley and Tukey¹ introduced an algorithm, known as the fast Fourier transform (FFT), which is quite convenient for a computer. But, as regards to the accuracy, their method is restricted to the situation where $X(f)$ is band limited, i.e., $X(f) = 0$ for $f > f_c$, and the maximum sampling interval τ_c must satisfy $2f_c \tau_c = 1$, known as the Nyquist condition.² Rigorously, the

Nyquist condition can be realized only for band-limited $X(f)$. The transformed function departs from its exact value when the above conditions are not satisfied. This error, which increases with increasing frequency, is known to be due to aliasing and is very common in experiments. This is the reason to seek a FT sufficiently fast and at the same time giving errors due to aliasing within acceptable limits. Accurate $X(f)$ is very important for the spectral line shape and for the time-dependent spectral phenomena, where the Nyquist condition is very stringent to meet, as Schütte³ has already pointed out. He has also proposed a method which has been extended by Mäkinen⁴ to the next higher order to reduce this error on $X(f)$ without correspondingly enhancing the time for evaluating the integral. Various window functions⁵ have been proposed to reduce the aliasing but at the expense of the spectral shape. From such considerations, methods of Schütte and of Mäkinen offer some distinct advantages. Unfortunately, both these methods are restricted to limited types of $x(t)$ and are not sufficiently general to meet different experimental situations. Furthermore, none of these methods, although based on polynomial expansion of first and second order, respectively, offers the possibility of improving the accuracy except by increasing the number of points as in FT. As we shall see later, such improvements are not very significant. The purpose of the present communication is to propose a method for the Fourier transform free of these limitations. Like the methods of Schütte and of Mäkinen, ours is also based on the polynomial expansion of $x(t)$ involving different sampled points, but avoids their limitations using a well-known property of FT. This is shown here to the second order with some functions that can be exactly evaluated with the integration limits. Prior to these demonstrations, a brief description of the theoretical background is given.

I. THEORY

For finite duration of $x(t)$, $X(f)$ given by Eq. (1) can be written as⁶

$$X(\omega) = \frac{1}{T} \int_0^T x(t) \exp(-i\omega t) dt, \quad (2)$$

where $\omega = 2\pi f$, and where the contribution to the integral for $t > T$ is neglected. The existence of FT with this form assumes that $x(t)$ is a periodic function with period T .

Using the time translation property of FT,⁶ Eq. (2) can be written in the following form:

$$X(\omega) = \frac{1}{T} \int_{-\tau/2}^{T-\tau/2} x(t) \exp(-i\omega t) dt, \quad (3)$$

where τ is any arbitrary time. We choose this τ as the sampling interval so that $N\tau = T$ with N the number of sampling points. Equation (3) can be written as

$$X(\omega) = \frac{1}{T} \sum_{k=0}^{N-1} \int_{(k-1/2)\tau}^{(k+1/2)\tau} x(t) \exp(-i\omega t) dt. \quad (4)$$

The standard FFT takes

$$x(t) \exp(-i\omega t) = x(k\tau) \exp(-i\omega k\tau)$$

as a constant inside the integration limits and, hence, arise the aliasing in $X(\omega)$ when it is not band limited. In principle, $x(t)$ about any point can be expanded in an infinite power series as

$$x(t) = \sum_{p=0}^{\infty} a_{kp}(t - k\tau)^p. \quad (5)$$

With this expansion of $x(t)$, Eq. (4) becomes

$$X(\omega) = \frac{1}{T} \sum_{p=0}^{\infty} (\tau/2)^{p+1} I_p(u) \sum_{k=0}^{N-1} a_{kp} \exp(-2iku), \quad (6)$$

where $u = \omega\tau/2$ and $I_p(u) = i^p d^p I_0/du^p$, with $I_0(u) = 2 \sin u/u$. The constants $a_{kp} = (d^p x/dt^p)_{t=k\tau}/p!$.

Using Eq. (6), $X(\omega)$ can be calculated to any order of accuracy by choosing the proper value of p . Here we shall

TABLE I. (A) Percent errors defined in the text of the real part of the Fourier transform of the function $\exp(-t)$ obtained by different algorithms with different number of sampling points N . The total time T has been chosen with the condition $\exp(-T) = 10^{-3}$. The last two numbers of each error given are the exponents of ten and only negative signs are shown explicitly. The following notations for different algorithms have been used: FFT for Cooley and Tukey (Ref. 1), POLFFT for Schütte (Ref. 3), POL2FFT for Mäkinen (Ref. 4), and POL2*FFT for the present one. (B) Imaginary part of $\exp(-t)$, otherwise similar to A.

n	N = 256				N = 128			
	FFT	POLFFT	POL2FFT	POL2*FFT	FFT	POLFFT	POL2 FFT	POL2*FFT
A.								
0	-1.36 00			2.00 -06	-2.72 00			3.10 -05
1	-2.48 00	-2.30 -01	-2.22 -01	3.26 -06	-4.98 00	-2.51 -01	-2.22 -01	5.05 -05
9	-9.22 01	-1.09 -01	-1.02 -01	1.06 -04	-1.85 02	-1.28 -01	-1.02 -01	1.75 -03
17	-3.25 02	-1.08 -01	-1.01 -01	3.90 -04	-6.54 02	-1.27 -01	-1.01 -01	7.22 -03
25	-7.02 02	-1.08 -01	-1.00 -01	9.11 -04	-1.41 03	-1.25 -01	-1.01 -01	1.91 -02
33	-1.22 03	-1.07 -01	-1.00 -01	1.78 -03	-2.46 03	-1.24 -01	-1.01 -01	4.06 -02
41	-1.89 03	-1.07 -01	-1.00 -01	2.95 -03	-3.80 03	-1.21 -01	-1.01 -01	7.43 -02
49	-2.69 03	-1.07 -01	-1.00 -01	4.68 -03	-5.43 03	-1.18 -01	-1.01 -01	1.21 -01
57	-3.65 03	-1.07 -01	-1.00 -01	7.01 -03	-7.36 03	-1.14 -01	-1.01 -01	1.79 -01
65	-4.74 03	-1.07 -01	-1.00 -01	1.00 -02				
73	-5.98 03	-1.06 -01	-1.00 -01	1.39 -02				
81	-7.37 03	-1.06 -01	-1.00 -01	1.85 -02				
89	-8.89 03	-1.06 -01	-1.00 -01	2.40 -02				
97	-1.06 04	-1.05 -01	-1.00 -01	3.04 -02				
105	-1.24 04	-1.05 -01	-1.00 -01	3.74 -02				
112	-1.44 04	-1.04 -01	-1.00 -01	4.51 -02				
121	-1.65 04	-1.04 -01	-1.00 -01	5.32 -02				
B.								
0	0			0	0			0
1	4.11 -02	-2.27 -01	-2.22 -01	4.10 -07	4.43 -02	-2.45 -01	-2.22 -01	5.85 -06
9	4.13 -01	-1.07 -01	-1.02 -01	-1.49 -06	1.66 00	-1.26 -01	-1.02 -01	-5.20 -05
17	1.46 00	-1.07 -01	-1.01 -01	-6.30 -06	5.90 00	-1.25 -01	-1.01 -01	-1.83 -04
25	3.16 00	-1.06 -01	-1.00 -01	-1.36 -05	1.29 01	-1.25 -01	-1.01 -01	-3.41 -04
33	5.58 00	-1.06 -01	-1.00 -01	-2.27 -05	2.29 01	-1.26 -01	-1.01 -01	-4.56 -04
41	8.59 00	-1.06 -01	-1.00 -01	-3.20 -05	3.63 01	-1.26 -01	-1.01 -01	-4.57 -04
49	1.24 01	-1.06 -01	-1.00 -01	-4.29 -05	5.36 01	-1.27 -01	-1.01 -01	-2.74 -04
57	1.69 01	-1.06 -01	-1.00 -01	-5.18 -05	7.57 01	-1.28 -01	-1.01 -01	1.40 -04
65	2.22 01	-1.06 -01	-1.00 -01	-5.83 -05				
73	2.83 01	-1.07 -01	-1.00 -01	-6.18 -05				
81	3.53 01	-1.07 -01	-1.00 -01	-5.95 -05				
89	4.33 01	-1.07 -01	-1.00 -01	-5.19 -05				
97	5.24 01	-1.07 -01	-1.00 -01	-3.76 -05				
105	6.26 01	-1.07 -01	-1.00 -01	-1.59 -05				
112	7.42 01	-1.07 -01	-1.00 -01	-1.36 -05				
121	8.72 01	-1.07 -01	-1.00 -01	6.12 -05				

TABLE II. (A) Real part of $\exp(-t) \cos(7\pi t/T)$, otherwise similar to Table I A. (B) Imaginary part of $\exp(-t) \cos(7\pi t/T)$, otherwise similar to Table I A.

n	N = 256				N = 128			
	FFT	POLFFT	POL2FFT	POL2*FFT	FFT	POLFFT	POL2FFT	POL2*FFT
A.								
0	-1.51 01			-6.96 -04	-3.03 01			-1.14 -02
1	-1.24 01	9.16 -01	9.72 -01	-5.76 -04	-2.49 01	6.51 -01	6.74 -01	-9.41 -03
17	-2.87 02	2.43 -01	7.47 -02	-1.08 -02	-5.76 02	7.12 -01	5.29 -02	-2.12 -01
33	-1.18 03	2.54 -01	8.28 -02	-5.31 -02	-2.88 03	6.71 -01	7.90 -02	-1.31 00
49	-2.65 03	2.49 -01	8.53 -02	-1.46 -01	-5.35 03	5.18 -01	1.33 -01	-3.97 00
57	-3.61 03	2.45 -01	8.68 -02	-2.29 -01	-7.28 03	3.88 -01	1.76 -01	-5.88 00
73	-5.94 03	2.32 -01	9.08 -02	-4.36 -01				
89	-8.85 03	2.13 -01	9.69 -02	-7.55 -01				
105	-1.23 04	1.86 -01	1.06 -01	-1.18 00				
121	-1.64 04	1.47 -01	1.19 -01	-1.67 00				
B.								
0	0			0	0			0
1	-8.00 -02	-1.51 00	-1.59 00	-5.03 -05	-3.21 -01	-1.25 00	-1.58 00	-7.03 -04
17	1.40 00	4.80 -02	4.05 -03	8.20 -04	5.66 00	2.14 -01	1.39 -02	6.23 -03
33	5.47 00	1.55 -01	1.01 -01	7.80 -04	2.27 01	3.30 -01	1.20 -01	1.51 -02
49	1.28 01	1.56 -01	1.02 -01	1.36 -03	5.35 01	3.45 -01	1.22 -01	9.11 -03
57	1.68 01	1.57 -01	1.02 -01	1.68 -03	7.56 01	3.56 -01	1.23 -01	4.46 -03
73	2.83 01	1.58 -01	1.02 -01	1.83 -03				
89	4.33 01	1.60 -01	1.03 -01	1.63 -03				
105	6.26 01	1.62 -01	1.03 -01	5.05 -04				
121	8.72 01	1.66 -01	1.03 -01	1.59 -03				

restrict ourselves to the second order, i.e., $p = 2$. Correct to this order, we have

$$X(\omega) = \frac{1}{T} \sum_{p=0}^2 (\tau/2)^{p+1} I_p(u) \sum_{k=0}^{N-1} a_{kp} \exp(-2iku). \quad (7)$$

On evaluating the sums (see the Appendix), Eq. (7) can be written as

$$X(\omega) = E(u)X_{\text{FFT}}(\omega) + [aY(u) - ibZ(u)] \exp(iu)/N, \quad (8)$$

TABLE III. (A) Real part of $\exp(-t) \sin(2\pi t/T)$, otherwise similar to Table I A. (B) Imaginary part of $\exp(-t) \sin(2\pi t/T)$, otherwise similar to Table I A.

n	N = 256				N = 128			
	FFT	POLFFT	POL2FFT	POL2*FFT	FFT	POLFFT	POL2FFT	POL2*FFT
A.								
0	1.11 -02			-8.06 -06	4.40 -02			-1.28 -04
1	2.61 -02	6.75 -01	5.38 -01	-1.64 -05	1.05 -01	6.75 -01	5.55 -01	-2.69 -04
17	-1.48 00	-1.17 -01	-1.04 -01	8.75 -04	-6.07 00	-1.58 -01	-1.08 -01	1.65 -02
33	-5.66 00	-1.16 -01	-1.03 -01	3.86 -03	-2.51 01	-1.51 -01	-1.10 -01	9.21 -02
49	-1.30 01	-1.15 -01	-1.04 -01	1.04 -02	-6.62 01	-1.39 -01	-1.14 -01	2.74 -01
57	-1.81 01	-1.15 -01	-1.04 -01	1.56 -02	-1.02 02	-1.29 -01	-1.15 -01	4.05 -01
73	-3.17 01	-1.14 -01	-1.05 -01	3.08 -02				
89	-5.14 01	-1.12 -01	-1.05 -01	5.33 -02				
105	-8.00 01	-1.10 -01	-1.05 -01	8.31 -02				
121	-1.22 02	-1.07 -01	-1.06 -01	1.18 -01				
B.								
0	0			0	0			0
1	9.39 -07	5.09 -03	-3.17 -04	-1.80 -06	1.52 -05	2.02 -02	1.56 -03	-2.28 -05
17	1.28 -02	1.46 00	2.13 -02	1.74 -03	2.14 -01	5.87 00	1.70 -01	5.04 -02
33	1.89 -01	5.53 00	7.92 -02	2.29 -02	3.56 00	2.29 01	6.48 -01	4.66 -01
49	9.80 -01	1.24 01	1.73 -01	9.48 -02	2.29 01	5.36 01	1.47 00	6.16 -01
57	1.87 00	1.69 01	2.32 -01	1.55 -01	5.11 01	7.57 01	2.06 00	-4.21 -01
73	5.60 00	2.83 01	3.79 -01	3.00 -01				
89	1.42 01	4.33 01	5.65 -01	3.78 -01				
105	3.27 01	6.26 01	7.99 -01	1.62 -01				
121	7.16 01	8.72 01	1.10 00	-6.86 -01				

where $X_{\text{FFT}}(\omega)$ is the standard FFT of $x(t)$ with $\omega = 2\pi n/T$ and the other terms are defined below:

$$E(u) = (1 + u^2/2) (\sin u/u)^3,$$

$$Y(u) = 1/u^2 - E(u) \cos u/\sin^2 u,$$

$$Z(u) = 1/u - E(u)/\sin u,$$

$$a = (2x_0 - 3x_1 + x_2 + x_{N-3} - 3x_{N-2} + 2x_{N-1})/4,$$

$$b = (4x_0 - 3x_1 + x_2 - x_{N-3} + 3x_{N-2} - 4x_{N-1})/4,$$

with $x_k = x(k\tau)$. Similar expressions can be obtained for $p > 2$, if needed, using Eq. (6). The functions $E(u)$, $Y(u)$, $Z(u)$, and $\exp(iu)$ are all universal and depend only on the choices of N and n . Hence, the required values of these functions can be stored in a computer memory prior to the actual computation of $X(\omega)$. The same can be done for a and b for known functions of the experimental data to be transformed. $X_{\text{FFT}}(\omega)$ is the standard FFT of $x(t)$ obtained by the conventional algorithm of Cooley and Tukey. Hence, $X(\omega)$ can be obtained with a little extra time than that required for $X_{\text{FFT}}(\omega)$ but with greatly enhanced accuracy as demonstrated below. It may be pointed out that like the other FFT algorithms^{1,3,4} the maximum number of independent frequency points or the maximum of n is $N/2$; the other $N/2$ of the total N points are related to these as in the standard FFT². Thus, the maximum frequency retained in the FFT for a given T is determined by the number of sampling points. On the other hand, the frequency resolution is determined by T . The choices of these two parameters in any experimental situation are dictated by the necessary requirements.

II. RESULTS AND DISCUSSIONS

In order to demonstrate the power of the present algorithm, we report below FFT of three different functions: (i) $\exp(-\alpha t)$, (ii) $\exp(-\alpha t)\cos(7\pi t/T)$, and (iii) $\exp(-\alpha t)\sin(2\pi t/T)$, where T is the upper limit of t . The choices of these functions have been made on the following basis: (i) None of the functions are band limited and all the integrals like Eq. (2) can be exactly evaluated. (ii) The first two functions are nonzero at $t = T$. (iii) The third function goes exactly to zero as t approaches T . The FT of these functions have been calculated to orders up to $p = 2$ for $N = 64, 128$, and 256 . Some of these results, in the form of % error for different choices of N , are shown in Tables I A–III B under the column heading POL2*FFT. The real and imaginary parts of $X(\omega)$ are shown, respectively, in A and B. The % error P has been defined in the following way:

$$P = [X_{\text{ex}}(n) - X_{\text{cal}}(n)] 100/X_{\text{ex}}(n),$$

where the suffixes ex and cal denote, respectively, the exact and calculated values with $\omega = 2\pi n/T$ as noted earlier; the former is obtained by Eq. (2) and the latter by Eq. (8). Similar results obtained by other algorithms are also included for comparison in the tables under the column headings FFT, POLFFT, and POL2FFT, respectively, for Cooley and Tukey, for Schütte and for Mäkinen. For all the above functions, we have chosen $\exp(-\alpha T) = 10^{-3}$ and used dimensionless units for computational convenience. It can be noticed that all the algorithms based on the polynomial ex-

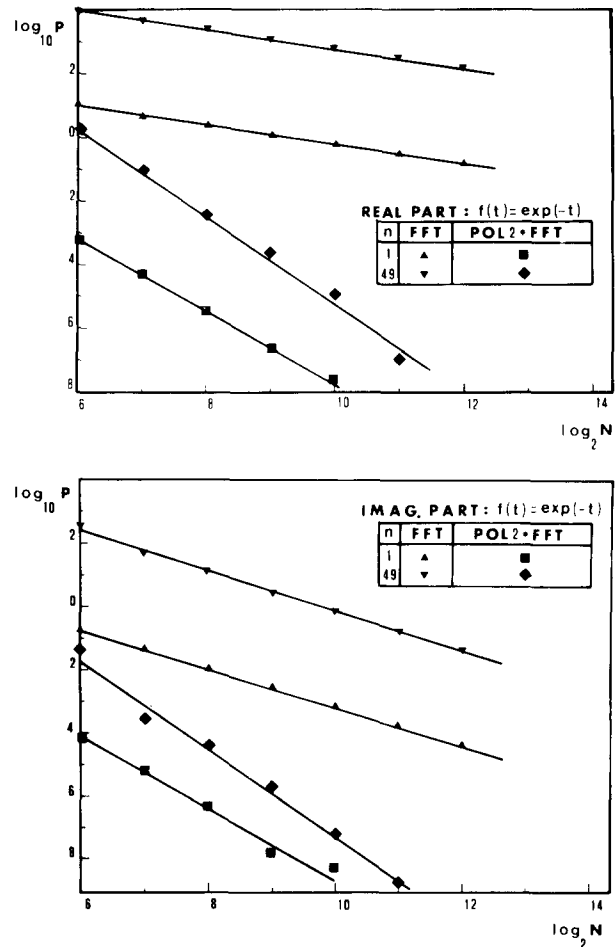


FIG. 1. (a) Log-log plots of P , the percentage errors in the real part of FT of the function $\exp(-t)$, obtained by FFT and POL2*FFT for two frequency points $n = 1$ and 49 are shown with the variation of N . The total time T has been chosen with the condition $\exp(-T) = 10^{-3}$. The straight lines show the least-squares fits. (b) The same as (a) for the imaginary part.

pansion give much more improved accuracy than those obtained by FFT. The errors, in general, increase with increasing frequency (n) and decrease with increasing N . This behavior is regular although not uniform for FFT and POL2*FFT but not for POLFFT and POL2FFT, particularly, note Table I A where errors decrease with increasing n . It can be noticed that errors for both POLFFT and POL2FFT are, in general, comparable and their decrease with increasing N is fairly slow, even in comparison to FFT. On the other hand, POL2*FFT yields improved results in comparison to FFT with increasing N , as can be noted in Figs. 1(a) and 1(b). Almost identical results, not shown here, are also obtained for other functions. Such graphs can be obtained for known functions even with a hand-held calculator. Note also in the tables is the improved accuracy obtained by POL2*FFT over others in almost all cases, except in a few for large n . These unfavorable results with respect to POLFFT and POL2FFT are not surprising, as discussed more fully below, since POL2*FFT reduces inherent errors in FFT to a certain order. Higher accuracy with the same N , if needed, can be obtained by the present algorithm by using higher order terms given by Eq. (6) choosing $p > 2$, without enhancing corresponding time for computation.

The principal aspect of the present method is to reduce errors inherent in FFT by two ways: (i) by the choice of the order of polynomial expansion p and (ii) by the choice of N . Here only the results for $p = 2$ have been presented. The errors decrease with increasing p for any fixed N , although not uniformly; but the general behavior is improved accuracy with increasing p . Furthermore, this improvement is faster with increasing N . For example, the errors in FT for the different functions with N reported here decrease by factors of 10 to 10^3 over all frequencies in changing $p = 1$ to 2. A similar, if not more, decrease in errors can be expected in changing $p = 2$ to 3. Such calculations to different orders of accuracy cannot be achieved with POLFFT or POL2FFT, as we have noted already. A further advantage of the present algorithm over POLFFT and POL2FFT is the rapid increase of accuracy with increasing N as can be noted in the Tables and in the figures. Hence, it gives two choices for improving results at any given situation. It is not possible to predict the exact error to be present in any FT as is true for any other methods, but the error can be easily estimated by the proper choices since the computation time can be reduced appreciably.

APPENDIX

Equation (7) can be written as

$$X(\omega) = \frac{1}{T} \left[\frac{\tau}{2} I_0 \sum_{k=0}^{N-1} a_{k0} \exp(-2iku) + \frac{\tau^2}{4} I_1 \sum_{k=0}^{N-1} a_{k1} \exp(-2iku) + \frac{\tau^3}{8} I_2 \sum_{k=0}^{N-1} a_{k2} \exp(-2iku) \right]. \quad (\text{A1})$$

To evaluate the sums, we need to know a_{k0} , a_{k1} , and a_{k2} for $0 \leq k \leq (N-1)$. This can be achieved from the knowledge of $x(k\tau)$, written hereafter as x_k , by the use of Eq. (5). We then obtain

$$a_{k0} = x_k, \quad a_{k1} = (x_{k+1} - x_{k-1})/2\tau,$$

and

$$a_{k2} = (x_{k+1} - 2x_k + x_{k-1})/2\tau^2 \quad (\text{A2})$$

for all k except $k = 0$ and $N-1$. For $k = 0$ and $N-1$, we have

$$a_{00} = x_0, \quad a_{01} = (4x_1 - x_2 - 3x_0)/2\tau,$$

and

$$a_{02} = (x_0 - 2x_1 + x_2)/2\tau^2, \quad (\text{A3})$$

$$a_{N-1,0} = x_{N-1},$$

$$a_{N-1,1} = (3x_{N-1} - 4x_{N-2} + x_{N-3})/2\tau,$$

and

$$a_{N-1,2} = (x_{N-3} - 2x_{N-2} + x_{N-1})/2\tau^2. \quad (\text{A4})$$

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It should be pointed out that three adjacent points have been chosen for determining the three constants a_{k0} , a_{k1} , and a_{k2} . These three points are symmetrical for $1 \leq k \leq N-2$, and are asymmetrical for $k = 0$ and $N-1$ for obvious reasons.

Using Eqs. (A2) – (A4), Eq. (A1) can be evaluated to yield Eq. (8) of the text.

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