On Interpolation and Evaluation of Derivatives from a Finite Number of Equally-Spaced Data Points

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ABSTRACT

Analytic fields, with several spectral variance power laws, are prescribed and evaluated at a finite number of equally-spaced points. For a given accuracy of interpolation, an unaliased truncated Fourier series is found to require less degrees of freedom than both cubic spline and two-point interpolation. With the input truncation chosen here, cubic spline is superior to linear interpolation, except for the roughest field. Very similar results hold for the accuracy of the first derivatives implied by these interpolation schemes.

When the errors in the first derivatives are examined only at the data points, however, the derivative of the aliased series is more accurate than that of the cubic spline. An even more accurate series of the same length can be obtained by analyzing the cubic spline passed through the points. The two finite-difference schemes tested have the largest errors.

1. Introduction

Over the last five years, the distinction between grid-point and spectral numerical models of the atmosphere has become increasingly blurred. It has been found that traditional spectral models (e.g., Silberman, 1954), in which all operations are performed on the time-dependent coefficients of the space basis functions, are too costly, in terms of both computer time and storage, for integrations with realistic resolution. This has led modern spectral modelers to employ the more efficient transform method (e.g., Machenhauer and Rasmussen, 1972) wherein products are actually evaluated on a grid and then analyzed in terms of the spectral basis functions.

On the other hand, some grid-point modelers have become unhappy about the errors involved in the finite-difference approximation to derivatives and have taken to fitting functions to the grid-point values, and then differentiating these functions at the grid points. Among such methods may be numbered the pseudo-spectral method (e.g., Orszag, 1972) and the cubic spline method (e.g., Price and MacPherson, 1973). The continuous functions chosen in these methods are truncated Fourier series and cubic splines, respectively.

It is the purpose of this paper to examine an aspect of the relative accuracy of linear, cubic spline and truncated Fourier series interpolation and also of the first derivatives implied by them.

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2. Atmospheric spectra

In the experiments to be described in the next sections, the "real" distribution of a variable will be given as a Fourier series with a large number of terms. Given this function evaluated at a finite number of grid points, the errors in various methods of interpolation and evaluating derivatives will be calculated using the "true" values. For the experiments to have meteorological interest, the spectrum of the continuous field should be chosen to agree with the global structure of real variables.

There have been many theoretical and observational studies of the power spectra of temperature and kinetic energy on a global scale. Charney (1971) has shown that a quasi-geostrophic theory of three-dimensional flow implies that, for high wavenumbers, the variance spectrum of temperature and the spectrum of kinetic energy behave as wavenumber raised to the power -3. In a numerical study with a two-level, quasi-geostrophic model, Steinberg (1973) has obtained power laws for the kinetic energy, varying from -1.7 to -3.4, depending on the intensity of heating and dissipation.

Kao (1970) has shown from observations that the spectral slope of the temperature variance spectrum is -3 and Kao and Wendell (1970) have deduced a similar law for the spectrum of kinetic energy. Julian *et al.* (1970) have concluded from their observations that, for wavelengths less than 4000 km, the exponent in the kinetic energy power law lies between -2.7 and -3 while Wiin-Nielsen (1967) has set it between -1.9 and -3.1, depending on the height at which the observations were taken. Recently Yang and Shapiro (1973) have suggested that these estimates may have to be modified slightly as the interpolation procedures used to obtain equally-spaced data alter the spectrum of the field being considered.

In view of the range of estimates of the slope of the spectral profile of these two atmospheric quantities, the experiments will be performed with a number of different power laws, which include most of the above laws.

3. Interpolation experiments

A one-dimensional scalar field $f(x)$ is defined

$$f(x)=\sum_{k=0}^{K}(a_k \cos kx+b_k \sin kx). \tag{1}$$

This function will be considered for four spectral variance power laws n, $n=-2, \ldots, -5$. The variance spectra of atmospheric fields may have their maxima at some non-zero wavenumber k_0. In keeping with these considerations, the spectrum of $f(x)$ is constructed as

$$\left.\begin{matrix} a \\ b \end{matrix}\right\}_k=\begin{cases} k^{n/2} & \\ \lambda k \exp(-\mu k^2) & \end{cases} \cdot \left.\begin{matrix}\cos\\ \sin\end{matrix}\right\}[2\pi r(k)] \quad \begin{matrix} , & k\geqslant k_0 \\ , & k<k_0 \end{matrix}$$

where

$$\mu=\frac{1}{2k_0^2},$$

$$\lambda=k_0^{[(n/2)-1)]}\exp(\mu k_0^2).$$

The quantities $r(k)$ have values between 0.0 and 1.0 and set the phases of the waves.

Suppose $\tilde{f}(x)$ is a continuous approximation to $f(x)$. The mean square error in $\tilde{f}(x)$ is

$$\sigma_I^2=\frac{1}{2\pi}\int_0^{2\pi}[f(x)-\tilde{f}(x)]^2 dx. \tag{2}$$

If the approximation may be represented as

$$\tilde{f}(x)=\sum_{l=0}^{L}(\tilde{a}_l \cos lx+\tilde{b}_l \sin lx), \tag{3}$$

Eq. (2) may be shown to reduce to

$$\sigma_I^2=(a_0-\tilde{a}_0)^2+\tfrac{1}{2}\sum_{m=1}^{M}[(a_m-\tilde{a}_m)^2+(b_m-\tilde{b}_m)^2], \tag{4}$$

where $M\equiv\max(K,L)$ and a finite series is considered to be an infinite series, whose coefficients are zero past the truncation.

Consider the function (1) evaluated at the N equally-spaced points

$$x_i=(i-1)\frac{2\pi}{N}, \quad i=1,\ldots,N.$$

Two methods of interpolation will be considered. The linear form of $\tilde{f}(x)$ consists of straight lines between neighboring grid points while the cubic spline form imposes cubics between each pair of grid points. The coefficients of these cubics are obtained by requiring the spline pass through each of the data points and that its first and second derivatives be continuous everywhere. The details of the technique may be found, for example, in Ahlberg *et al.* (1967). To calculate the error (4), the Fourier coefficients of the approximation are expressed in terms of those of the input function. The cosine coefficient for wavenumber $k(\neq 0)$ is given by

$$\tilde{a}_k=\frac{1}{\pi}\int_0^{2\pi}\tilde{f}(x)\cos kx dx. \tag{5}$$

In the case of spline interpolation, integration of (5) by parts gives

$$\tilde{a}_k=\frac{1}{\pi k^4 \Delta x}\sum_{i=1}^{N}(\tilde{f}''_{i-1}-2\tilde{f}''_i+\tilde{f}''_{i+1})\cos kx_i, \tag{6}$$

where

$$\tilde{f}''_i=\left[\frac{d^2}{dx^2}[\tilde{f}(x)]\right]_{x=x_i}, \quad \Delta x=2\pi/N.$$

From theory (e.g., Ahlberg *et al.*, 1967), these second derivatives at the data points are given by the tri-diagonal system

$$\frac{\tilde{f}''_{i-1}}{4}+\tilde{f}''_i+\frac{\tilde{f}''_{i+1}}{4}=\frac{3}{2\Delta x^2}(f_{i-1}-2f_i+f_{i+1}). \tag{7}$$

As the data points are equally spaced, the right-hand side of (7) is

$$\frac{3}{\Delta x^2}\sum_{k=0}^{K}(\cos k\Delta x-1)(a_k \cos kx_i+b_k \sin kx_i).$$

The solution of the system (7) is then

$$\tilde{f}''_i=\frac{6}{\Delta x^2}\sum_{k=0}^{K}\frac{(\cos k\Delta x-1)}{2+\cos k\Delta x}(a_k \cos kx_i+b_k \sin kx_i), \tag{8}$$

which may be verified by substitution in (7). Making use of the identities

$$\sum_{i=1}^{N}\cos lx_i=\begin{cases}0, & l\neq \nu N\\ N, & l=\nu N\end{cases},$$

$$\sum_{i=1}^{N}\sin lx_i=0 \qquad ,$$

substitution of (8) into (6) shows that

$$\tilde{a}_k=R_k\sum_{\nu=-\infty}^{\infty}(a_{\nu N+k}+a_{\nu N-k}), \tag{9}$$

where

$$R_k = \frac{6N}{\pi k^4 \Delta x^3} \frac{(1-\cos k\Delta x)^2}{(2+\cos k\Delta x)}, \tag{10}$$

ν takes on all integer values, and a quantity with a negative subscript is regarded as zero. The corresponding expression for the sine coefficients may easily be shown to be

$$\tilde{b}_k = R_k \sum_{\nu=-\infty}^{\infty} (b_{\nu N+k} - b_{\nu N-k}).$$

By proceeding in a similar fashion, one can show that the response function for linear interpolation is

$$R_k = \frac{N}{\pi k^2 \Delta x}(1-\cos k\Delta x). \tag{11}$$

The expressions (9) obviously depend on the input phases and hence so does the error (4). To avoid having to consider the error for many different choices of phase, it is possible to integrate (4) over all phases and obtain the average, or most likely, error. This may be shown

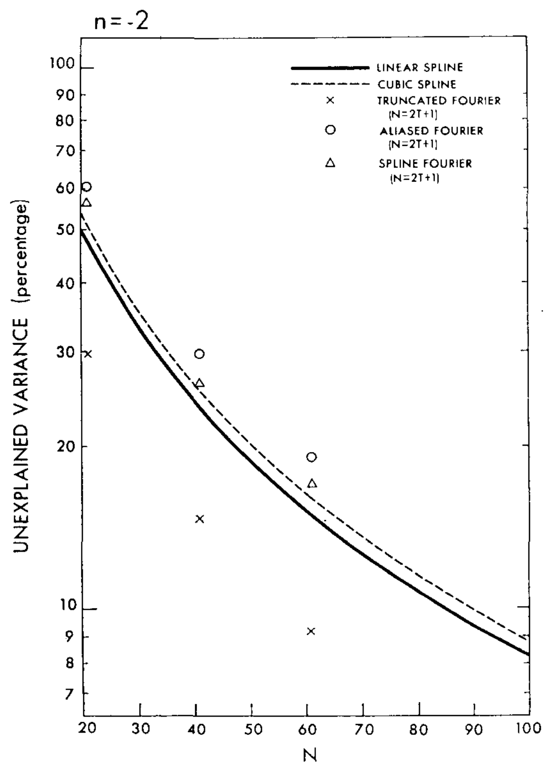

FIG. 1. The average percentage of variance unexplained by linear and cubic spline interpolation applied to N equally-spaced points. The input function has a spectral variance power law of $n=-2$. The error levels denoted by $\times$'s, O's and Δ's are the average percentage of variance unexplained by approximating with the first T Fourier waves, obtained from the input series directly, an aliased calculation from $2T+1$ equally-spaced points, and from Fourier analyzing the cubic spline fitted through the $2T+1$ points, respectively.

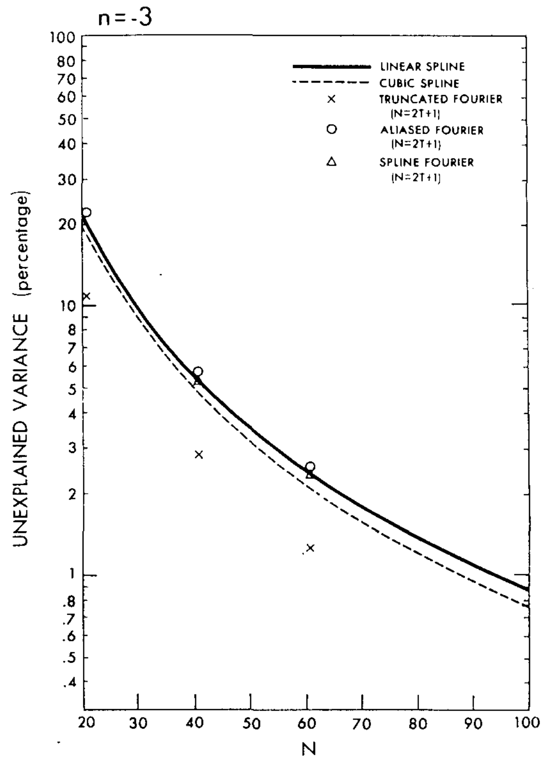

FIG. 2. As in Fig. 1 except for $n=-3$.

to be

$$\sigma_I^2 = \tfrac{1}{2}\Big\{\sum_{\nu=1}^{\infty} A_{\nu N}^2 + \sum_{m=1}^{M} \Big[(1-R_m^2)A_m^2 + R_m^2 \sum_{\substack{\nu=-\infty \\ \nu\neq 0}}^{\infty} (A_{\nu N+m}^2 + A_{\nu N-m}^2)\Big]\Big\}, \tag{12}$$

where

$$A_m^2 = a_m^2 + b_m^2.$$

The two response functions (10) and (11) were used in (12) to obtain the average errors for all values of N from 20 to 100. The length of the input series (K) was chosen to be 200 and the length of the interpolation Fourier series (L) taken as 500. (Some runs were repeated with $L=1000$, with virtually no difference in the results, indicating $L=500$ is an adequate choice.) The value of k_0 was set to 5. The mean square errors for each value of N were then expressed as a percentage of the variance of the original field. These results are presented in Figs. 1–4, for the power laws $-2, \ldots, -5$, respectively.

It is desirable to compare these errors with three Fourier approximations. If an approximation to $f(x)$ is obtained by taking the first T waves of (1), then the error is

$$\sigma_{I,F}^2 = \tfrac{1}{2} \sum_{k=T+1}^{K} A_k^2, \tag{13}$$

which is independent of phases. If the input function is evaluated at $2T+1$ points, then an aliased Fourier analysis performed to obtain T waves of an approximation, the average error is

$$\sigma^2_{I,AF}=\sigma^2_{I,F}+\tfrac{1}{2}\Big\{\sum_{\nu=1}^{\infty}\Big[A^2_{\nu(2T+1)}+\sum_{k=1}^{T}\left(A^2_{\nu(2T+1)+k}+A^2_{\nu(2T+1)-k}\right)\Big]\Big\}. \quad (14)$$

Finally, use as an approximation the first T Fourier waves obtained from the analysis of a cubic spline passed through the $2T+1$ points. It can be shown with an analysis similar to that previously, that the average error is given by

$$\sigma^2_{I,SF}=\sigma^2_{I,F}+\tfrac{1}{2}\Big\{\sum_{\nu=1}^{\infty}A^2_{\nu(2T+1)}+\sum_{k=1}^{T}\Big[(1-R_k)^2A_k^2+R_k^2\sum_{\nu=1}^{\infty}\left(A^2_{\nu(2T+1)+k}+A^2_{\nu(2T+1)-k}\right)\Big]\Big\}, \quad (15)$$

where R_k is given by (10). These three errors are expressed as a percentage of the variance of the input field and are shown in each of Figs. 1–4 for the cases $T=10$, 20 and 30.

It may be seen from Fig. 1 that linear is more accurate than cubic spline interpolation when the slope of the variance spectrum is -2. However, the other figures show that the latter is more accurate at -3 and is progressively more so at steeper slopes. The reason for this behavior is intuitively clear from (12). For all values of wavenumber k up to and including $N/2$ the expression (10) is greater than (11), except for $k=0$ when both equal unity. Hence for a given spectrum, the first term inside the summation over m in (12) is greater for linear than for cubic interpolation, provided the response functions are considered only in the wavenumber range above. The reverse is obviously true for the second term inside the summation. This second term represents the effect of all the spectral folding into the wavenumber of interest and obviously becomes important for rough fields (i.e., those which have variance spectra which decay only slowly with respect to wavenumber). Thus the second term is expected to dominate the first for rough fields and linear interpolation should be better than cubic spline in these cases. Since the contributions to these terms for wavenumbers $>N/2$ are small, the above argument should hold for any length of summation. It is clear from Fig. 1 that for an input with spectral slope -2 the amount of variance unexplained is only reduced to 10% by taking $N=85$–90 for the schemes. However, for a -5 power law this unexplained variance is reduced to 1% by taking $N=27$ and 36 for cubic spline and linear interpolation, respectively.

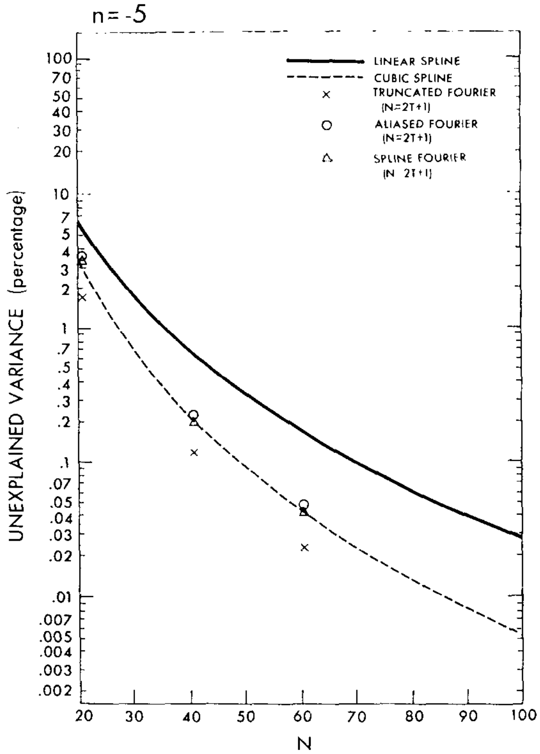

FIG. 4. As in Fig. 1 except for $n=-5$.

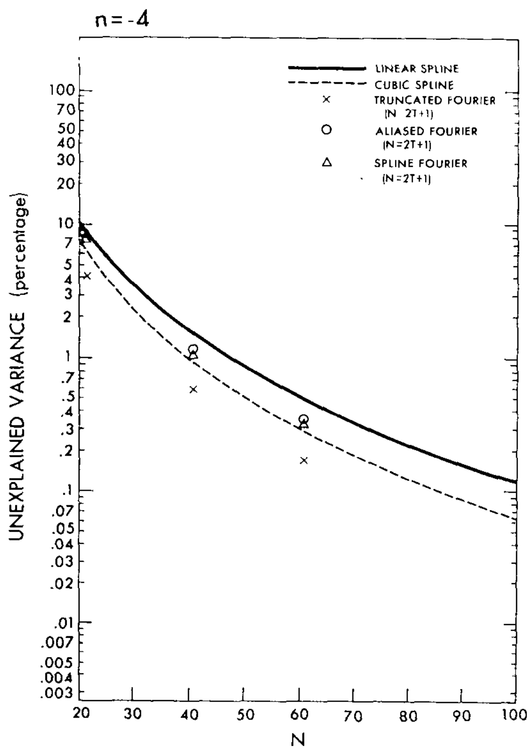

FIG. 3. As in Fig. 1 except for $n=-4$.

All the figures show that for a prescribed number of degrees of freedom to represent a function, a truncated unaliased Fourier series is the most accurate. However, if only a given number of data points are known it is not possible to calculate these coefficients. It may be seen that T Fourier waves give a better approximation if obtained by analyzing the cubic spline through $2T+1$ points, rather than performing an aliased calculation from these points directly. This is a result of the type of smoothing inherent in the spline.

In the -2 power law case, linear interpolation is more accurate than spline interpolation and more accurate than spline-Fourier and aliased Fourier approximation. For the -3 case, linear interpolation is superior to aliased Fourier, but for steeper slopes it is the most inaccurate scheme tested.

The main conclusions concerning the average error are enumerated:

1) For a prescribed number of degrees of freedom, the most accurate interpolation approximaticn is a truncated Fourier series.

2) For all, except one, of the power laws, cubic spline interpolation is more accurate than linear interpolation.

3) Given $2T+1$ points, T Fourier waves are a better approximation to the function if they are obtained from analyzing the cubic spline through the points rather than performing directly an aliased calculation.

4. Evaluation of derivative experiments

In this section experiments are described which are analogous to those in Section 3, except that the verification is performed on the first derivative. The same linear and cubic spline functions are fitted through equally-spaced data points and the derivatives of these used as approximations to the derivative of the input function (1). Hence the mean square errors in these approximations are

$$\sigma_D{}^2=\frac{1}{2\pi}\int_0^{2\pi}\left[\frac{df(x)}{dx}-\frac{d\tilde{f}(x)}{dx}\right]^2dx. \qquad (16)$$

(In the case of two-point interpolation, the data points are omitted from the range of integration.) It is clear that the analysis to determine the average error in the first derivative follows closely that presented in the previous section and the expression analogous to (12) is

$$\sigma_D{}^2=\tfrac{1}{2}\sum_{m=1}^{M} m^2\Big[(1-R_m)^2A_m{}^2 + R_m{}^2\sum_{\substack{\nu=-\infty\\ \nu\neq 0}}^{\infty}(A^2_{\nu N+m}+A^2_{\nu N-m})\Big]. \qquad (17)$$

This expression was evaluated for the response functions R_k corresponding to linear and cubic spline interpolation for the same cases and values of N as used in Section 3, except that only the variance spectrum power laws -4 and -5 were considered. As before, these average errors were expressed as a percentage of the variance of the "true" first derivative field.

Again, it is of interest to compare these errors with Fourier approximations analogous to those in the previous section. Expressions similar to (13), (14) and (15) may be deduced as

$$\sigma^2_{D,F}=\tfrac{1}{2}\sum_{k=T+1}^{K} k^2A_k{}^2, \qquad (18)$$

for the series (1) truncated at T waves, then differentiated,

$$\sigma^2_{D,AF}=\sigma^2_{D,F}+\tfrac{1}{2}\sum_{\nu=1}^{\infty}\sum_{k=1}^{T} k^2[A^2_{\nu(2T+1)+k}+A^2_{\nu(2T+1)-k}], \qquad (19)$$

for T aliased Fourier waves calculated from $2T+1$ points, and

$$\sigma^2_{D,SF}=\sigma^2_{D,F}+\tfrac{1}{2}\sum_{k=1}^{T} k^2\Big[(1-R_k)^2A_k{}^2 + R_k{}^2\sum_{\nu=1}^{\infty}(A^2_{\nu(2T+1)+k}+A^2_{\nu(2T+1)-k})\Big], \qquad (20)$$

for T waves calculated from a cubic spline passed through $2T+1$ points. The errors of the Fourier approximations along with those of the derivatives of linear and cubic spline interpolation are presented in the same manner as before in Figs. 5 and 6 for power laws -4 and -5, respectively.

In both cases, the derivatives of the cubic spline are far more accurate than those calculated from two-point interpolation. For example, in the -4 law case with 50 grid points, 12 and 18% of the variance remains unexplained by these two schemes, respectively. The following conclusions, analogous to those drawn for interpolation, may be extracted from the figures:

4) For a prescribed number of degrees of freedom, the most accurate approximation to the first derivative is the derivative of the truncated original series.

5) For all cases, the derivative of the cubic spline is more accurate than that of linear interpolation.

6) Given $2T+1$ points, the derivative of T Fourier waves is a better approximation to the derivative of a function if the waves are obtained from analyzing the cubic spline through the points, rather than directly performing an aliased calculation.

In a grid-point model, one is not so much concerned with the accuracy of calculating the derivative continuously distributed in space but rather at the grid points. Hence the experiments reported in this section were repeated but defining the mean square errors over the finite number of points rather than the continuum.

That is

$$\sigma_{DP}^2=\frac{1}{N}\sum_{i=1}^{N}\left[\frac{df(x)}{dx}\bigg|_{x=x_i}-\tilde{f}_x(x_i)\right]^2, \tag{21}$$

where $\tilde{f}_x(x_i)$ is an approximation to the derivative at $x=x_i$. Three approximations are considered: derivative of the cubic spline, centered differences

$$\tilde{f}_x(x)=\left(\frac{1}{2\Delta x}\right)[f(x+\Delta x)-f(x-\Delta x)],$$

and the fourth-order scheme

$$\tilde{f}_x(x)=\left(\frac{2}{3\Delta x}\right)[f(x+\Delta x)-f(x-\Delta x)] -\left(\frac{1}{12\Delta x}\right)[f(x+2\Delta x)-f(x-2\Delta x)].$$

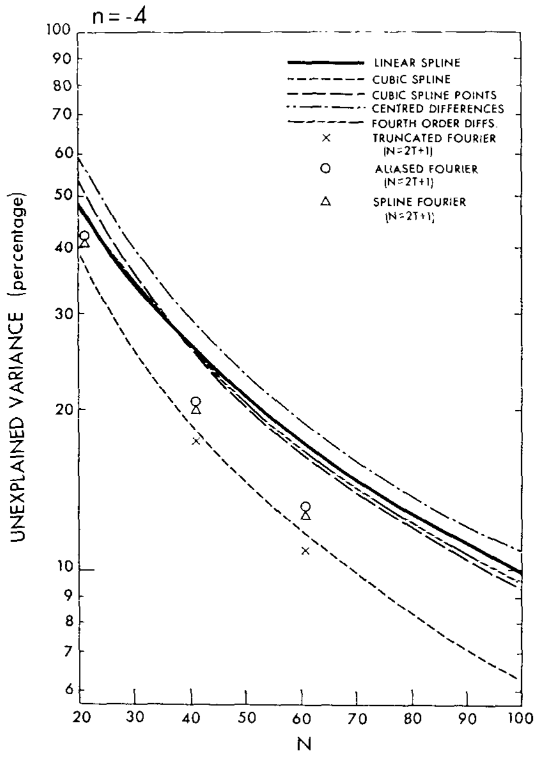

FIG. 5. The linear spline and cubic spline curves give the average percentage of variance unexplained by the first derivative field implied by linear and cubic spline interpolation, respectively, applied to N equally-spaced points. The input function has a spectral variance power law of $n=-4$. The other three curves give the average percentage of variance unexplained of the first derivative at the points using the differentiated cubic spline, centered differences and fourth order differences. The error levels denoted by $\times$'s, O's and Δ's are the average percentage of variance unexplained by approximating the derivative with the derivative of the first T Fourier waves, obtained from the input series directly, an aliased calculation from $2T+1$ equally spaced points, and from Fourier analyzing the cubic spline fitted through the $2T+1$ points respectively.

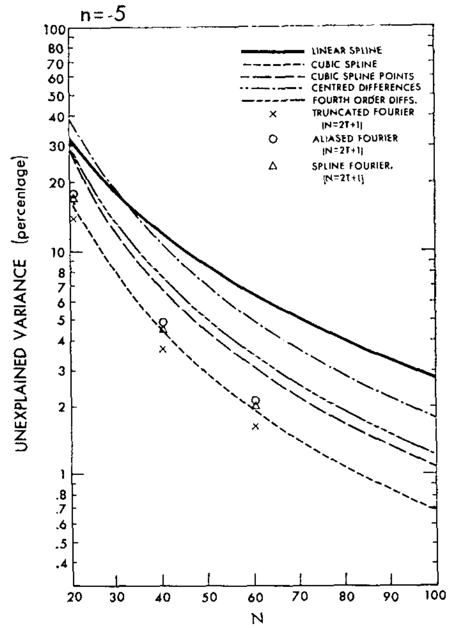

FIG. 6. As in Fig. 5 except for $n=-5$.

The expression (21) may be rewritten as

$$\sigma_{DP}^2=\frac{1}{N}\sum_{i=1}^{N}\left[\sum_{k=1}^{K}F_k(b_k\cos kx_i+(-a_k)\sin kx_i)\right]^2, \tag{22}$$

where F_k depends upon the scheme being used. By integrating over all phases, the average may be shown to be

$$\sigma_{DP}^2=\tfrac{1}{2}\sum_{k=1}^{K}F_k^2A_k^2. \tag{23}$$

The function F_k takes the form

$$k-\beta, \tag{24}$$

$$k-\beta[1+(1-\cos k\Delta x)/3], \tag{25}$$

$$k-\beta[3/(2+\cos k\Delta x)], \tag{26}$$

for centered differences, fourth-order differences and cubic spline derivatives, respectively. In the above

$$\beta=\frac{\sin k\Delta x}{\Delta x}.$$

The expression (23) was evaluated for the three approximations (24)–(26), again for all values of N between 20 and 100. The resulting curves are drawn in Figs. 5 and 6, and it should be remembered that these errors are calculated at the grid points only, whereas the other two curves in each of the figures are calculated from the continuous errors.

It is clear that the derivatives of the cubic spline at the grid points are more accurate than fourth-order differences and far more so than central differences. This conclusion could also be reached by examining (24)–(26). The averages of the three types of Fourier series are independent of whether they are calculated over the grid points or the continuum. Hence these errors are directly comparable to the grid-point derivatives. The figures show that even a completely aliased Fourier analysis produces more accurate derivatives at the grid points than do any of the three schemes tested. It should be noted that the cubic spline approximation errors are less in the continuous case than at the grid points. In other words, the derivative so approximated from a cubic spline is most accurate midway between the grid points. It may be concluded from the experiments that:

7) For a prescribed number of degrees of freedom, the most accurate approximation to the first derivative is the truncated original series.

8) Given $2T+1$ points, the methods of calculating first derivatives at these points, in order of decreasing accuracy, are as follows:

(i) Fit a cubic spline to the points, calculate the first T waves of it and differentiate.
(ii) Perform an aliased Fourier analysis on the data and differentiate the T waves.
(iii) Differentiate the cubic spline through the points.
(iv) Fourth-order differences.
(v) Centered differences.

In passing, it will be noticed that an equivalent, but more efficient, method of performing (i) is to obtain T waves from an aliased calculation, apply the response functions (10) and differentiate.

5. Conclusion

In these experiments, the "true" value of a one-dimensional function was set in terms of a Fourier series. Several power laws for the variance spectrum of the field were imposed and to avoid doing a large number of cases with different input phases, the errors of various approximations were averaged over all phases.

In the cases chosen for investigation, it has been shown that the series truncated to T waves gives a better fit to the input curve and its derivative a better fit to the input derivative field, both in the continuous case and at $2T+1$ equally-spaced points, than do any of the other approximations based on these points.

In general, of course, data will be known only for a finite number of points and hence it is not possible to calculate these T coefficients exactly. When the function was evaluated at $2T+1$ equally-spaced points, a cubic spline interpolation was more accurate than an aliased Fourier series of length T. Linear interpolation was also found to be more accurate than the aliased series for variance power laws -2 and -3 but the situation was reversed for spectra with steeper decay.

The derivative of the cubic spline was a more accurate approximation to the derivative of the input field than the derivative of the aliased Fourier series. However, when the errors were calculated only at the grid points, this situation was reversed. The most accurate method of calculating derivatives at the points was to take the derivative of the T Fourier waves, obtained from analyzing the cubic spline fitted through the points. Fourth-order differences were slightly inferior to the pure cubic spline method and more accurate than centered differences.

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