JOURNAL OF RESEARCH of the National Bureau of Standards — B. Mathematical Sciences
Vol. 76B, Nos. 3 and 4, July—December 1972

"Plural-Series" Approximations of Functions*

L. V. Spencer

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(May 15, 1972)

A method is given for developing approximations to neutron and gamma-ray transport distributions in the form of a superposition of U_n^k polynomial series multiplied by exponentials and characterized by different scale factors. Convergence conditions and error bound expressions are given. Biorthogonality properties are worked out. Examples are given in which these approximations are compared with polynomial approximations.

Key words: Biorthogonal function; gamma-ray transport; moment methods; neutron transport; polynomial representations; radiation penetration.

1. Introduction

In the moment method of calculating space distributions in radiation transport theory, spatial moments defined by

$$M_n = \frac{1}{n!}\int_0^\infty dz z^n F(z), \tag{1}$$

or

$$M_n = \frac{1}{n!}\int_{-\infty}^\infty dz z^n F(z), \tag{1'}$$

are evaluated by numerical integration of a recursive system of Volterra integral equations of the second kind [1, 2].[1] For any of several reasons, one frequently encounters the problem of constructing distributions by use of alternate, rather than consecutive moments [2, 5]. Because spatial trends are basically exponential, this leads to the possibility of representations in a family of biorthonormal systems of polynomials $U_n^k(z)$, with adjoint polynomials $\hat{U}_n^k(z)$, satisfying the condition

$$\int_0^\infty dz z^k e^{-z} \hat{U}_n^k(z) U_m^k(z) = \delta_{nm}, \tag{2}$$

with

$$z^k \hat{U}_n^k(z) = \sum_{i=0}^n (-)^i \binom{n}{i} \frac{z^{k+2i}}{(k+2i)!}. \tag{2'}$$

Many other properties of these functions have been given, in references [1–4], and particularly in reference [4]. Perhaps we should say here that we draw freely on the results and terminology of reference [4] and reference [6] in this paper.

AMS Subject Classification: Primary 4110, Secondary 3036.

*Work supported by the Office of Naval Research and the Defense Civil Preparedness Agency.

[1] Figures in brackets indicate the literature references at the end of this paper.

The application of these polynomials to gamma-ray and neutron distributions leads to questions (a) of convergence in the limit, and (b) of convergence of a truncated series to within known error bounds. In the latter case, the utility of the method depends on the rapidity of convergence, because it is not practical to evaluate more than 6 to 10 of the series coefficients.

The problem of convergence in the limit was treated in reference [4], and a more recent paper [6] developed error bounds for truncated series. In addition, for gamma-ray distributions, the convergence does tend to be rapid. Thus the problem of constructing distributions from moments would appear to be completely solved. The convergence arguments are summarized in appendix B, with additions.

Unfortunately, however, many important problems do not have rapidly converging series. For example, if the radiation source has components of differing energy, their attenuation is a superposition of exponentials, and the more rapidly attenuated components give slowly converging contributions to the coefficients of the polynomial representation.

Another case is that in which the radiation initially travels at an oblique angle to the direction of penetration. A still more important case is that of the neutrons, where very high numbers of collisions with nuclei give spatial distributions which combine exponential with Gaussian features [7].

Existence of these problems led very early to use of nonlinear approximations which were designated "function-fitting" methods, in which the individual terms in an approximating series have the same functional form, with differing weight and differing scale factor [2]. While very useful, and in good agreement with the more basic polynomial representation, these methods have the limitation that it is difficult to assess their accuracy. In fact, it is easy to show that the more obvious error bounds which can be determined for such representations must be broader than error bounds for the polynomial representation. This is highly unsatisfactory, because one turns to these methods mainly when the polynomial representations are poor.

In this paper we develop a type of approximation which we designate a "plural-series" representation or approximation. It is a generalization of the polynomial approach which incorporates the flexibility of the function-fitting methods. But unlike the latter, one can prove convergence in the limit, and can evaluate bounds to truncation errors. Thus it combines the advantages of both methods. Because the polynomial method is a special case, we will refer to it herein as a "single-series" approximation.

We will show that it is possible to use plural-series calculations to evaluate error bounds for at least some function-fitting representations. This makes it possible to evaluate accuracy for previously published calculations.

We have begun to apply the plural-series method to types of distribution for which polynomial approximations converge poorly, and we include an example of this in which the distribution has no physical significance.

2. Plural-Series Representations

The representation which we wish to use in obtaining an approximation to $F(z)$ is

$$F_N(z)=\sum_{j=1}^{J} (A_j/x_j^{k+1})F_N^j(z), \tag{3}$$

where

$$F_N^j(z)=\sum_{n=0}^{N-1} a_n^j U_n^k(z/x_j)e^{-z/x_j}. \tag{3'}$$

The x_j are arbitrarily chosen scale factors and the A_j are arbitrary multipliers. The approximate function $F_N(z)$ is required to have N moments which have values exactly agreeing with known values M_k, M_{k+2}, M_{k+4}, . . . for the corresponding sequence of moments of $F(z)$.

For $J > 1$, there are $J \cdot N$ coefficients a_n^j in (3), a much larger number than the number of moments, N. Hence other requirements must be invoked to determine the coefficients. For this purpose we use a simple variational rule, that the sum S_N defined as follows is to be minimized:

$$S_N = \sum_{j=1}^{J} (A_j/x_j^{k+1}) \sum_{n=0}^{N-1} (c_n a_n^j)^2, \tag{4}$$

where the c_n are arbitrary weighting coefficients. This leads to an elementary Lagrange multiplier calculation for the coefficients a_n^j, with side conditions as follows expressing the requirements of the moments of the representation:

$$M_{k+2n} = \sum_{j=1}^{J} (A_j/x_j^{k+1}) M_{k+2n}^j, \tag{5}$$

where

$$M_{k+2n}^j = \frac{1}{(k+2n)!} \int_0^\infty dz z^{k+2n} F_N^j(z). \tag{5'}$$

Because of the simplicity of (2′), the expression for a_n^j in terms of the moments of the "partial" functions F_N^j is very simple. Since

$$a_n^j = \int_0^\infty d(z/x_j)(z/x_j)^k \hat{U}_n^k(z/x_j) F_N^j(z), \tag{6}$$

insertion of the expression (2′) for $\hat{U}_n^k$ into (6) gives

$$a_n^j = \sum_{i=0}^{n} (-)^i \binom{n}{i} M_{k+2i}^j / x_j^{k+2i+1}. \tag{7}$$

Before proceeding with the further analysis, let us mention restrictions to be observed on the various types of arbitrary coefficients. The x_j must be positive or else the integrals do not converge. In addition, we will limit our considerations to positive values of A_j so that S_N will always be positive. Then S_N turns out to be a squared norm and plays a central role in the discussion of error bounds. In addition, we assign positive values to the weighting coefficients c_n, which play a role here similar to that of the c_n coefficients in reference [6].

What the minimizing condition on S_N does is to select a particular biorthogonal system for the approximation. Our task is largely that of familiarizing ourselves with properties of this system, which turn out to be attractive as well as useful.

3. Evaluation of Coefficients

Equation (7) expresses a linear system whose formal solution makes it easier to express the main calculation to be performed. In matrix form, (7) is seen to be simply

$$x_j^{k+1} \begin{pmatrix} a_0^j \\ a_1^j \\ a_2^j \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot \\ 1 & -1 & 0 & \cdot & \cdot & \cdot \\ 1 & -2 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & x_j^{-2} & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & x_j^{-4} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} M_k^j \\ M_{k+2}^j \\ M_{k+4}^j \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

Since the binomial matrix is its own inverse, we can immediately write

$$\begin{pmatrix} M^j_k \\ M^j_{k+2} \\ M^j_{k+4} \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = x_j^{k+1} \begin{pmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & x_j^2 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & x_j^4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot \\ 1 & -1 & 0 & \cdot & \cdot & \cdot \\ 1 & -2 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} a^j_0 \\ a^j_1 \\ a^j_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}. \tag{8}$$

Designating the matrix elements of the product of the first two matrices on the right by γ^j_{in}, we have the desired result,

$$M^j_{k+2i} = x_j^{k+1} \sum_{n=0}^{N-1} \gamma^j_{in} a^j_n \,. \tag{9}$$

Let us note in passing that the γ^j_{in} are the coefficients which, according to (2′), change a series of $\hat{U}^k_n$ polynomials into a power series,

$$\frac{z^{2i}}{(k+2i)!} = \sum_{n=0}^{N-1} \gamma^j_{in} \hat{U}^k_n(z/x_j). \tag{10}$$

To obtain the form of the side conditions which we wish to use, we insert (9) into (5), with the result

$$M_{k+2i} = \sum_{j=1}^{J} A_j \sum_{n=0}^{N-1} \gamma^j_{in} a^j_n. \tag{11}$$

Then, designating the N Lagrange multipliers as $\lambda_1, \lambda_2, \ldots \lambda_N$, we write out the quantity to be minimized,

$$S_N = \sum_{j=1}^{J} (A_j/x_j^{k+1}) \left\{ \sum_{n=0}^{N-1} (c_n a^j_n)^2 \right\} + 2 \sum_{i=0}^{N-1} \lambda_i \left\{ M_{k+2i} - \sum_{j=1}^{J} A_j \sum_{n=0}^{N-1} \gamma^j_{in} a^j_n \right\}. \tag{12}$$

Vanishing of linear variations of S_N with respect to the λ_i gives back equations (11). The conditions $\{\partial S_N/\partial a^j_n = 0\}$ yield the following additional $J \cdot N$ equations:

$$a^j_n = x_j^{k+1} \sum_{i=0}^{N-1} \lambda_i \gamma^j_{in}/c_n^2. \tag{13}$$

Formal solution of the linear system of $J \cdot (N+1)$ equations requires only a straightforward matrix inversion. We insert (13) into (11) to obtain

$$M_{k+2i} = \sum_{i'=0}^{N-1} u_{ii'} \lambda_{i'}, \tag{14}$$

where

$$u_{ii'} = \sum_{j=1}^{J} A_j x_j^{k+1} \sum_{n=0}^{N-1} \gamma^j_{in} \gamma^j_{i'n}/c_n^2. \tag{15}$$

The matrix whose elements are $u_{ii'}$ is symmetric and readily evaluated. Writing $v_{nn'}$ for the elements of the inverse matrix, the equations (14) become

$$\lambda_n = \sum_{n'=0}^{N-1} v_{nn'} M_{k+2n'}, \tag{16}$$

and values of the a_n^j follow from (13).

4. Norm Convergence for $N \to \infty$

Let us assume that $J=1$, that x_1 and c_n values have been selected, and that for this case $\lim_{N\to\infty} S_N$ is finite. Then it follows that for $J>1$, for the same set of c_n values, and for a set of x_j values which include the same x_1, the sequence of S_N values must again have a finite limit. In addition, the sequence of S_N values is monotone increasing.

To demonstrate that these assertions hold true we first note that F_{N+1} is an approximation which fits the same moments as does F_N (plus one more). If, in the expression for F_{N+1}, one arbitrarily changes the a_N^j values to zero, for all j, the first N moments are unaffected due to biorthogonality. Call such a modified approximation F'_{N+1}, and calculate the corresponding quantity S'_{N+1}. Then

$$S_{N+1} \geqslant S'_{N+1} \geqslant S_N, \qquad J \geqslant 1. \tag{17}$$

The first of the inequalities holds because the a_N^j would not usually be zero, while the second holds because S_N was calculated to have the smallest value possible for a set of approximations which includes S'_{N+1}. Thus the S_N sequence is monotone increasing, as well as positive.

That the S_N sequence for $J>1$ is bounded follows if the $J=1$ sequence converges, and if any one of the x_j has the same value in the plural series case as the x_1 of the single-series case, as we have assumed. After all, for each value of N, the single-series approximation is only one in which $a_n^j=0$ for all j except that corresponding to the single-series x_1. It is therefore an element in the set of approximations among which the plural-series S_N is smallest. Hence the value of S_N, $J>1$, is always bounded above by the single-series limit and therefore the limit, $N\to\infty$, exists and is less than or equal to the single-series limit.

This argument makes no requirement on the values of x_j, $J>1$, other than convergence of a single-series sequence in which one of the x_j values is used as scale factor. Therefore, plural-series approximations can include components with exponential trends inappropriate for use in single-series representations.

5. Transformation Properties

The transformation properties of plural-series approximations follow from the fact that adjoint to $F_N(z)$ is a function which we designate $\hat{F}_N$,

$$\hat{F}_N(z) = \sum_{i=0}^{N-1} \lambda_i \frac{z^{2i}}{(k+2i)!}\,. \tag{18}$$

We establish this by an argument in terms of "transformation kernels", and for this purpose we first observe that

$$\{c_n^{-1} U_n^k(z) e^{-z}\} = \int_0^\infty dy y^k e^{-(z+y)} T^k(z,y) \{c_n \hat{U}_n^k(y)\}, \tag{19}$$

where

$$T^k(z,y) = \sum_{n=0}^{\infty} \{c_n^{-1}U_n^k(z)\}\{c_n^{-1}U_n^k(y)\}. \tag{19'}$$

The series (19′) is assumed either to converge for all y, z or else to diverge at $z=0$, $y=0$ in such a way that the integration (19) still leads to convergent results. For $c_n=1$, T^k is a combination of modified Bessel functions, with a divergence at $y=z=0$ [4]. Because of the factor y^k, this divergence is harmless in the integration.

If we insert (10) into (18), and then make use of (13), we obtain the expression

$$\hat{F}_N(z) = x_j^{-(k+1)} \sum_{n=0}^{N-1} a_n^j c_n^2 \hat{U}_n^k(z/x_j). \tag{20}$$

From (19) it then follows that

$$F_N^j(z) = \int_0^\infty dy y^k e^{-(z+y)/x_j} T^k(z/x_j, y/x_j)\hat{F}_N(z), \tag{21}$$

so that

$$F_N(z) = \int_0^\infty dy y^k \left\{\sum_{j=1}^{J} (A_j/x_j^{k+1}) e^{-(z+y)/x_j} T^k(z/x_j, y/x_j)\right\} \hat{F}_N(y). \tag{22}$$

Thus, the transformation appropriate to the plural-series representation has a kernel which is a simple linear combination of the kernels for the component series taken separately.

To conclude this argument, we note that multiplication of (13) by $(c_n)^2 a_n^j$, followed by summation over n, yields

$$\sum_{n=0}^{N-1} (c_n a_n^j)^2 = \sum_{i=0}^{N-1} \lambda_i M_{k+2i}^j = \int_0^\infty dz z^k \hat{F}_N(z) F_N^j(z), \tag{23}$$

so that

$$S_N = \int_0^\infty dz z^k \hat{F}_N(z) F_N(z). \tag{24}$$

6. Biorthogonality Properties of Plural-Series Systems

The discussion of error bounds is perhaps simplest in terms of the biorthogonal functions appropriate to plural-series cases. Let us therefore derive expressions for the two sets of biorthogonal functions, which we designate $P_N(z)$ and $\hat{P}_N(z)$.

We consider first the sequence of moments $M_k=1$, and $M_{k+2n}=0$, for $n>0$. The "function" which has these moments is irrelevant, though it must basically be a Dirac delta function located at $z=0$. In any case, when this "function" is represented in any orthogonal or biorthogonal system, we expect all the terms to appear. The sequence of approximate representations corresponding to this moment system will be designated $G_N(z)$; and a corresponding sequence of adjoint functions, $\hat{G}_N(z)$, can be constructed by use of (18).

Two sequences of difference functions give the biorthogonal functions which we seek. For $N \geq 1$,

$$P_N(z) = \{G_{N+1} - G_N\}/d_N, \tag{25}$$

and

$$\hat{P}_N(z) = \{\hat{G}_{N+1} - \hat{G}_N\}/d_N, \tag{26}$$

where d_N is a normalizing constant still to be specified.

Since G_{N+1} and G_N have identical moments M_{k+2n}, for $n=0, 2, \ldots 2(N-1)$, it is clear that P_N is orthogonal to $\hat{P}_n$ for $n < N$, the latter being a linear combination of even powers:

$$\int_0^\infty dzz^k \hat{P}_n(z) P_N(z) = 0,\ n < N. \tag{27}$$

To prove that $\hat{P}_N(z)$ is also orthogonal to P_n, for $n < N$, we write

$$\int_0^\infty dzz^k \hat{P}_N P_n = \int_0^\infty dzz^k \int_0^\infty dyy^k \left\{ \sum_{j=1}^{J} (A_j/x_j^{k+1}) T^k(z/x_j, y/x_j) e^{-(y+z)/x_j} \right\} \hat{P}_N(z) \hat{P}_n(y)$$

$$= \int_0^\infty dyy^k \hat{P}_n(y) P_N(y) = 0. \tag{27'}$$

Therefore (25) and (26) describe a biorthogonal system which obeys the transformation (22). To complete the system we add the terms

$$P_0(z) = G_1(z)/d_0, \tag{28}$$

$$\hat{P}_0(z) = \hat{G}_1(z)/d_0. \tag{28'}$$

The normalizing condition for this system is

$$\int_0^\infty dzz^k \hat{P}_N(z) P_N(z) = 1, \tag{29}$$

which may be written by means of (24) and (4) in the form

$$d_N^2 = \sum_{j=1}^{J} (A_j/x_j^{k+1}) \sum_{n=0}^{N} c_n^2 \{(a_n^j)_{N+1} - (a_n^j)_N\}^2, \tag{30}$$

$$d_0^2 = \sum_{j=1}^{J} (A_j/x_j^{k+1}) c_0^2 (a_0^j)_1^2, \tag{30'}$$

where $(a_n^j)_N$ is the coefficient a_n^j, determined for the construction G_N, and $(a_N^j)_N$ is always zero.

This completes the specification of the plural series biorthonormal system. In the special single-series case, there is cancellation between the quantities in braces in (30); and the usual normalization is recovered if we choose $c_n = 1$, and $A_1 = x_1^{k+1}$.

7. Convergence of Plural-Series Approximations

Norm convergence of plural-series approximations was earlier shown to hold if there is norm convergence of any of the single-series approximations which can be formed using the plural-series scale factors x_j. But this does not guarantee pointwise convergence of these approximations. To examine the latter, let us first note that (3) may be rewritten in the form of a P_N series,

$$F_N = \sum_{n=0}^{N-1} f_n P_n(z), \tag{31}$$

with

$$\|F_N\|^2 = \sum_{n=0}^{N-1} f_n^2 = S_N. \tag{32}$$

The form (31) follows from (22); one must recall that $\hat{F}_N$ is a polynomial and can therefore be written as a linear combination of the polynomials $\hat{P}_n$. Equation (32) follows from the normalization (29),

$$\|P_N\|^2 = 1. \tag{33}$$

We proceed by designating the kernel function of the transformation (22) as $\mathscr{T}^k(z, y)$, with the following extension of the notation to the N'th finite sum:

$$\overline{\mathscr{T}}_N^k(z, y) = \sum_{j=1}^{J} (A_j/x_j^{k+1}) \sum_{n=0}^{N-1} c_n^{-2} U_n^k(z/x_j) U_n^k(y/x_j) e^{-(y+z)/x_j}. \tag{34}$$

Next, applying (22) to $\hat{P}_n$, but noting that $U_{n'}^k(z/x_j)$ is orthogonal to the polynomial $\hat{P}_n(z)$ for all j and all $n' \geqslant N > n$, we observe that

$$P_n(y) = \int_0^\infty dz z^k \mathscr{T}^k(z, y) \hat{P}_n(z) = \int_0^\infty dz z^k \overline{\mathscr{T}}_N^k(z, y) \hat{P}_n(z). \tag{35}$$

The second equality holds for $n < N$, and due to biorthonormality, $\overline{\mathscr{T}}_N^k(z, y)$ must have the form

$$\overline{\mathscr{T}}^k(z, y) = \sum_{n=0}^{N-1} P_n(y) P_n(z) + \sum_{n=N}^{\infty} r_n(y) P_n(z), \tag{36}$$

where we do not have to concern ourselves with values for the coefficients $r_n(y)$ of the remainder term. From (36) and (32) it follows that for fixed y,

$$\sum_{n=0}^{N-1} [P_n(y)]^2 \leqslant \| \overline{\mathscr{T}}_N^k \|^2 < \mathscr{T}^k(y, y), \tag{37}$$

since $\mathscr{T}^k(y, y)$ is identical with $\| \mathscr{T}^k \|$.

Using this result together with the Schwarz inequality, for $z \neq 0$, we see that if the set of coefficients f_n in (31) and (32) has the property $S_N \leqslant S_\infty < \infty$, then

$$\left| \sum_{n=M}^{N} f_n P_n(z) \right|^2 \leqslant \left\{ \sum_{n=M}^{N} [P_n(z)]^2 \right\} \sum_{n=M}^{N} f_n^2 \leqslant \mathscr{T}^k(z, z) \sum_{n=M}^{N} f_n^2. \tag{38}$$

The term on the right goes to zero as $M, N \to \infty$; hence the Cauchy criterion is satisfied, and $\Sigma f_n P_n$ converges. Thus, pointwise convergence of a plural-series approximation follows if there is norm convergence of any of the single-series representations based on the plural-series scale factors x_j.

There remains the question as to whether the limit of a plural-series sequence of approximations agrees with that of the single-series approximations. To establish this we refer to the form (3), (3′), obtainable for any representation (31). We first note that if x_J is the largest of the plural-series scale factors, then the functions

$$F^j(z) = \sum_{n=0}^{\infty} a_n^j U_n^k(z/x_j) e^{-z/x_j}, j = 1, 2, \ldots, J, \tag{39}$$

in any convergent representation of the type (3), (3′), can also be represented by a convergent series using $U_n^k(z/x_J)$ only. One has, therefore, a convergent single-series representation for

$$\sum_{j=1}^{J} (A_j/x_j^{k+1}) F^j(z), \tag{39'}$$

if one exists for $F(z)$. The coefficients of the single-series representation of this function must be exactly those of the corresponding single-series representation for $F(z)$, because both are given by the same linear combinations of the moments of $F(z)$ if the same series representation (based on x_J) is used for both. Hence (39′) is equivalent to a single-series representation of $F(z)$ in the limit.[2]

8. Bounds to Truncation Errors

To calculate bounds to truncation errors we require norm convergence (37), which follows from norm convergence of a single-series representation based on one of the x_j, as already stated.

As a result of (35), the kernel of the transformation (22) must be representable in a form analogous to (19′),

$$\mathscr{T}^k(z, y) = \sum_{j=1}^{J} (A_j/x_j^{k+1}) e^{-(z+y)/x_j} T^k(z/x_j, y/x_j) = \sum_{n=0}^{\infty} P_n(z) P_n(y). \tag{40}$$

This follows from biorthogonality, plus the fact that, considered as a function of z, say, for fixed y, this function can be represented as a series of $U_n^k(z/x_J)$ functions with finite norm, where x_J is the largest scale factor. (See appendix B.)

Following the notation of reference [6], we put $y = z$ and make the designation

$$[D_0^k(z)]^2 = \sum_{j=1}^{J} (A_j/x_j^{k+1}) e^{-2z/x_j} T^k(z/x_j, z/x_j) = \sum_{n=0}^{\infty} [P_n(z)]^2. \tag{41}$$

For approximations correct to N terms, one can accurately use the following truncated kernel function:

$$\sum_{n=0}^{N-1} P_n(z) P_n(y). \tag{42}$$

If we now apply the Schwartz inequality to the quantity $(F - F_n)$ as in (19′) of reference [6], we obtain

$$|F - F_N|^2 \leq \left\{ \sum_{n=0}^{\infty} (f_n)^2 \right\} \sum_{n=N}^{\infty} \{P_n(z)\}^2 \leq S_\infty \left\{ [D_0^k(z)]^2 - \sum_{n=0}^{N-1} [P_n(z)]^2 \right\}, \tag{43}$$

or

$$|F - F_N| \leq \sqrt{S_\infty}\, D_N^k(z), \tag{43'}$$

where we employ the notation of reference [6] except that exponentials now appear both in the function being approximated and in the definition of $D_N^k(z)$,

$$[D_N^k(z)]^2 = [D_0^k(z)]^2 - \sum_{n=0}^{N-1} [P_n(z)]^2. \tag{44}$$

We can follow reference [6] farther by defining an "error build-up" function $Eb(z)$,

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[2] See Appendix B for a discussion of the automatic exclusion of functions having all moments zero.

$$Eb(z) = \sqrt{S_\infty}\, D_0^k(z)/F(z), \tag{45}$$

so that the (fractional) bounds to the truncation error are given by

$$\frac{|F - F_N|}{F} = Eb(z) \left\{\frac{D_N^k(z)}{D_0^k(z)}\right\}. \tag{46}$$

Both factors on the right of (46) reduce in the single-series case to the results of reference [6] because the extra exponential factor cancels out.

EXAMPLES: In transport problems, different energy components, characterized by exponentials which decrease at different rates, are commonly superposed. We choose a very simple case of this type as an example, namely

$$g(z) = 0.75e^{-z/0.2} + 0.25e^{-z}. \tag{47}$$

Table 1 gives the function $e^z g(z)$, together with five approximations, of which (a) is a single-series case, while (b) is a 3-term plural-series case. The exponential coefficients x_j are listed below the table of values.[3] The plural-series approximation (b) has a component with one scale factor very near unity and another which is about 0.33, and therefore much closer to the value 0.2 in (47). All calculations were performed with the computer program sketched in appendix A.

Below the scale factors in table 1 and norms S_N are listed for 5 through 8 terms in the approxi-

[3] See Appendix A for the rules used in selecting both x_j and A_j values.

TABLE 1. *Values of $g(z)e^z$ and five approximations.*

Scale factors x_j are listed below the values of the function. At the bottom of the table are the last four values of S_N together with an extrapolated value for S_∞.

z	Exact	(a) $k=0$, $J=1$	(b) $k=0$, $J=3$	(c) $k=2$, $J=3$	(d) $k=6$, $J=3$	(e) $k=6$, $J=3$
0	1.0000	0.680	0.799	1.000	1.000	1.000
0.05	0.8641	.650	.737	0.864	0.863	0.864
0.10	.7527	.622	.682	.753	.748	.753
0.2	.5870	.569	.588	.587	.574	.589
0.4	.4014	.478	.452	.402	.377	.406
0.6	.3180	.406	.366	.318	.292	.323
0.8	.2806	.349	.312	.280	.252	.284
1.0	.2637	.305	.278	.263	.246	.265
1.5	.2519	.241	.242	.252	.243	.249
2.0	.2503	.220	.237	.251	.248	.251
3.	.2500	.238	.248	.250	.254	.249
5.	.2500	.271	.256	.251	.248	.250
7.	.2500	.232	.243	.250	.251	.250
10.	.2500	.255	.254	.251	.250	.250
13.	.2500	.324	.267	.253	.249	.250
16.	.2500	.0835	.199	.241	.254	.250
20.	.2500	.0717	.241	.264	.243	.249
24.	.2500	3.505	1.08	.297	.251	.252
28.	.2500			.722	.297	.254
34.	.2500			−1.06	.077	.226
	x_1	1.000	0.991	0.801	0.850	0.771
	x_2		.572	.462	.491	.474
	x_3		.330	.267	.283	.280
	S_N, $N=5$	0.234	0.2761	0.7506	0.7606	0.01013
	6	.249	.2789	.7514	.7611	.01014
	7	.262	.2821	.7521	.7611	.01023
	8	.275	.2856	.7524	.7613	.01023
	S_∞, extrapolated:	(0.446)	(0.324)	(0.759)	(0.763)	(0.0108)

mation. The final value in parentheses represents a very rough (linear) extrapolation to S_∞ using $N^{-1/2}$ as variable; while arbitrary, it tends to be quite conservative:

$$S_\infty \approx S_{N+1} - \frac{1}{\sqrt{N+1}} \left\{ \frac{S_{N+1} - S_{N-1}}{\dfrac{1}{\sqrt{N+1}} - \dfrac{1}{\sqrt{N-1}}} \right\} \tag{48}$$

The difference between the 8th norm and the extrapolation is an indicator of the degree of convergence, although the extrapolated value cannot be taken very seriously, particularly when, as in case (b), successive differences are still increasing. It turned out that with increasing N, these extrapolations first increased, and then in high-quality approximations decreased to meet the (rising) norm values.

Both the approximation values and the data on norms indicate that the plural-series approximation is better, the single-series approximation being generally unacceptable.

The remaining three columns represent an attempt to improve the approximations through use of information about the value and the first derivative of $g(z)$ at $z=0$. This information makes possible the approximation of a modified function, selected to be

$$g'(z) = g(z) - e^{-z/0.25} \tag{49}$$

which has a trend near $z=0$ which is proportional to z^2, and which can thus be represented with plural-series approximations involving U_n^k polynomials with $k \leq 2$. Three-term plural-series approximations are used in all cases (*c*)–(*e*). The cases (*d*) and (*e*) ignore the first four even moments and use U_n^6 polynomials [9]. In addition, for case (*e*) the x_j values were scaled down according to the rule

$$x_j' = \frac{x_j}{\sqrt{1+ax_j^2}}, \quad a=0.3. \tag{50}$$

This form is suggested by a condition that a single adjoint function of the form $\cos(az)$ be transformed by the appropriate kernel functions $T(z/x_j', y/x_j')$, as in (21), to the exponentials e^{-z/x_j}.

Some of the sharp behavior for z near zero is subtracted out by the additional term in (49), so that one expects improvement in the convergence, in the values for large z, and especially for small z which is now given correctly in the limit. But because there is sharp behavior remaining, one does not expect the improvement to be as dramatic as shown.

We should note that reducing the scale factor would also improve (*a*) and (*b*); the advantages in rising build-up factors which were discussed in references [6] and [8] apply here also.

Dropping the lower moments tends to degrade the approximation (*d*) relative to the approximation (*c*) for small z values, while introducing an improvement for large z values. Reducing the x_j values, on the other hand, improves the quality at all z. Recall that at least one of the x_j must always give a converging single-series approximation. That is the case for all approximations here shown.

Table 2 compares errors with estimated error bounds.[4] In all cases shown, we have used S_8 rather than the extrapolated approximation to S_∞ as multiplier in estimating error bounds. As a result, in (*a*) at $z=0.4$ the estimated error bound falls slightly below the error. This shows the problem of "estimating" an error bound in a poorly convergent case. Perhaps the extrapolated S_∞ would be a better multiplier to use generally, though there is not much difference when convergence is at all satisfactory.

Elsewhere the estimated error bounds are reasonable, even excessive. Some use of the option $c_n \neq 1$ was made, with the following prescription [6]:

$$c_n = (n+1)^{m/4}, \tag{51}$$

[4] See appendix A for details on the calculations. They made use of (44) to (46), with data on D_0^2 obtained using (19′) with $y=z$.

TABLE 2. *Comparisons between the fractional error,* $(F-F_N)/F$, *designated "Err," and an estimated fractional error bound, designated "EB."*

Read "A−B" as $A\times10^{-B}$.

z	(a) $k=0$ $J=1$ Err	(a) EB	(b) $k=0$ $J=3$ Err	(b) EB	(c) $k=2$ $J=3$ Err	(c) EB	(d) $k=6$ $J=3$ Err	(d) EB	(e) $k=6$ $J=3$ Err	(e) EB
0.	−0.32	0.50	−0.20	1.0	0.	0.	0.	0.	0.	0.
.05	−.25	.38	−.15	0.54	.2−4	.019	−0.0016	9.9	.25−3	1.2
.10	−.17	.27	−.094	.32	.8−4	.051	−.0061	28.	.99−3	3.6
.20	−.031	.11	0.001	.24	.3−3	.10	−.022	55.	.38−2	7.7
.40	0.19	.18	.13	.35	.6−3	.13	−.061	43.	.012	9.1
.6	.28	.29	.15	.39	−0.2−3	.16	−.083	25.	.016	7.7
.8	.24	.31	.11	.34	−.14−2	.25	−.082	16.	.012	5.5
1.0	.16	.28	.053	.25	−.21−2	.30	−.068	9.8	.44−2	3.4
1.5	−0.043	.17	−.041	.16	0.3−3	.22	−.034	3.3	−0.010	0.89
2.0	−.12	.23	−.054	.20	.3−2	.19	−.009	1.8	−.77−2	.68
3.0	−.049	.22	−.006	.12	−0.17−2	.23	0.016	0.84	0.52−2	.21
5.	0.083	.23	0.023	.15	0.28−2	.26	−.009	.36	−0.30−2	.087
7.	−0.071	.22	−.027	.14	−0.47−3	.26	0.003	.21	.13−2	.059
10.	0.019	.44	0.017	.22	0.6−4	.37	−.002	.20	−0.12−2	.044
13.	.30	1.2	.067	.73	.011	.88	0.004	.31	0.35−3	.037
16.	−0.67	7.7	−0.21	1.8	−0.037	2.4	.014	.64	.19−2	.052
20.							−0.027	1.2	−0.48−2	.12
24.							0.005	2.9	0.68−2	.21
28.							.19	11.6	.014	.45
34.									−0.096	2.5

with $m=0$ for cases (a) and (b), and $m=2, 3, 6$ for cases (c), (d), and (e), respectively. Large values of m can lead to poor convergence of the norms, but for the functions $g(z)$ and $g'(z)$ approximated here, choice of m does not affect ultimate convergence. The evidence of table 1 is that the choices were reasonable.

Unlike the single-series case, the value of m affects the approximation as well as the error bound functions.

Error bounds generally tend to become large as one approaches large values of z at which convergence breaks down. But one also finds extremely large error bounds for small values of z in cases (d) and (e). These are due to the insensitivity of large moments to the details of the distribution at small z. That these bounds are realistic was demonstrated in some calculations not shown, in which for some m values, with calculations otherwise like (d) and (e), the errors in the small z region were very large indeed. In this region, for large k, the approximations were either very good or very bad. Use of large k approximations should evidently be accompanied by supplementary studies at small z.

9. Additional Comments

It was mentioned earlier that the plural-series approach can be used to gauge the accuracy of representations of the function-fitting type which make use of sums of exponentials, as in eq (A4) of appendix A. This requires that the x_j be assigned the values of the specified representation, and that the plural-series solution have $a_n^j=0$ for $n>0$. The latter requirement may or may not be satisfied, depending on the norm of the function-fitting representation in the plural-series system. Other plural-series representations can have smaller norms, particularly when some of the A_j have opposite signs and are large.

When all the constant factors in expressions such as (A4), in appendix A, have the same sign, the simple sum of exponentials tends to be the plural-series solution for all N less than or equal to the number of moments given correctly by the approximation. Very likely, with properly stated conditions one could prove a theorem to this effect. But when this simple property does not hold, one can still modify norm values by adjusting the shape of the error function D_o^k through choice of the A_j values. Further, one can modify the moments of the unknown function by addition of moments of known terms, with final subtraction of these functions from the plural-series construction. A simple case of this would be transferral of some of the negative terms in a function-fitting representation to the other side, with corresponding changes in the moments of the function to be constructed. But such a simple prescription cannot be recommended as a general procedure because it removes exponential components somewhat indiscriminately from the plural-series approximating system.

Selection of A_j values for the examples of the preceding section was based on the assumption that the error function D_0^k should have terms corresponding to an elementary function-fitting rule, as discussed in appendix A. Cases with peculiar features, such as large terms which nearly cancel, probably require more care in specification of the A_j values. But the quality of the approximations usually appears to be surprisingly independent of such assignments.

10. Appendix A. A Plural-Series Computer Program

A general-purpose computer program which we have called FFPOL was constructed to perform calculations such as those described as examples. The following operations are performed by the main constituent components:

(1) *Specification of exponential scale factors* x_j, by subroutines designated BCOF and SCALE.

(2) *Solution of the basic Lagrange multiplier problem*, using a routine called SEP.

(3) *Computation of the error estimate functions* D_N^k and D_0^k, with a routine ESEP, which makes use of SEP.

(4) *Evaluation of both approximation and error bound data*, with a subroutine designated UNESEP.

More specifically, the following are the computations performed by the main subroutines just mentioned:

The scale factors x_j are evaluated as a product

$$x_j = \xi_j / s, \tag{A1}$$

where the ξ_j are pre-specified according to the rule

$$\xi_j^2 = \beta^{j-1}, j = 1,2, \ldots, J, \tag{A2}$$

$$\xi_J = J^{-1}, \tag{A3}$$

which ensures that these values cover the unit interval in steps which are basically geometric, but with roughly uniform coverage. BCOF evaluated the ξ_j. The overall scale factor s is evaluated by SCALE so that an expression of the type

$$\sum_{j=1}^{J} (f_j / x_j^{k+1}) e^{-z/xj} \tag{A4}$$

can correctly fit $(J+1)$ moments. This calculation also determines the A_j of (3) and (4), by an arbitrary rule such as $A_j = |f_j|$.[5]

The procedure followed by SEP in evaluating both the λ_i values and the a_n^j coefficients is a straightforward evaluation first of the γ_{in}^j matrix elements and then the $u_{ii'}$ matrix elements.

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[5] The effect of this selection on the quality of the representation is not clear, and not as strong as one might expect. According to (41), specification of large A_j values for small x_j components would appear to emphasize the small z region in the D^k functions, for example. The data of tables 1 and 2 were obtained with the function-fitting parameters, as in (A4), in the combination $|f_j / x_j^{k+1}|$. Perhaps a more logical choice for the A_j of (3), (4) might be the combination f_j^2 / x_j^{k+1}, which tends to give $D^k \propto |f_j| / x_j^{k+1}$, at least for the dominant terms.

The inversion of the latter matrix, followed by the matrix multiplications (16) and (13) completes the calculation.

The error estimate function D_0^k is evaluated by ESEP with (25), using (19′). The sums are carried to 30–40 terms ordinarily, with evaluation of the $U_n^k(z)$ mostly by recursion. The recursion formula,

$$4(n+1)(n+2)[U_{n+2}^k - U_{n+1}^k] = z^2 U_n^k + 2(n+1)(4n+2k+1)[U_{n+1}^k - U_n^k] - (2n+k)(2n+k-1)[U_n^k - U_{n-1}^k], \tag{A5}$$

was derived from the differential equation, using eq (17.16′), both given on p. 744 of reference [2]. The recursion approach eventually breaks down, particularly for large values of k; but with suitable restrictions, and depending somewhat on the size of the argument z, 30–40 terms gives accurate results. ESEP evaluates D_N^k by subtracting from $(D_0^k)^2$ terms of the type $P_n(z)^2$, as shown in (44).

Evaluation of the approximation data by UNESEP utilizes (3). The (estimated) error bound data is calculated using D_N^k data from ESEP, with S_N taken to be an adequate approximation to S_∞.

Finally, the master routine, FFPOL, first calls BCOF and SCALE. This is followed by an optional provision to modify the x_j values just determined to obtain a related set which does *not* have the property of fitting $(J+1)$ moments, through use of (50). Lastly, UNESEP is called to give both approximation and (estimated) error bound data. All calculations have used double precision (60 bits).

11. Appendix B. Convergence of U_n^k Polynomial Representations

We summarize and complete here the arguments of reference [4] relating to convergence of the U_n^k series representations.

(1) First, let us note two properties of these biorthogonal functions:

$$U_n^k(z) = O(n^{-1/2}), \text{ for } z \neq 0, \tag{B1}$$

and, also for $z \neq 0$,[6]

$$\left(\frac{z}{|z|}\right)^k \left(\frac{1}{\sqrt{1-u}}\right)^{k+1} e^{-\frac{|z|}{\sqrt{1-u}}} = \sum_{n=0}^{\infty} u^n U_n^k(z) e^{-|z|}. \tag{B2}$$

Note that (B1) does not usually hold at $z=0$, where $U_n^k(0) = O(n^{(k-1)/2})$. The U_n^k functions could be (but have not been) defined as coefficients of the different powers of u in the expansion (B2). This expansion converges uniformly for $z \neq 0$ on the unit circle $|u| \leq 1$, except that, given $\epsilon > 0$, we must have $|u-1| \geq \epsilon$.

(2) Next, let us consider an *even* function $F(z)$, $-\infty < z < \infty$, whose Fourier transform has singularities *only* to the right and far left of the equilateral hyperbola shown in figure B1, a pair of regions which we refer to as "I". The Fourier transform of $F(z)$, which we designate $\Phi(\eta)$, will be an even function of η and will actually have twin singularities symmetrically located about the imaginary axis. The Fourier inversion integral is

$$F(z) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\eta e^{-\eta|z|} \Phi(\eta). \tag{B3}$$

[6] In physical problems, singular behavior at $z=0$ will be known and usually treated by a special calculation. The remainder at $z=0$ will often, though not always, vanish. Thus, treatment of this point as a special case does not lead to any practical difficulties. Incidentally, eq (40) of reference [4] which is the starting point for the arguments leading to this statement on convergence, can be derived by induction without reference to other expressions for U_n^k which include singular components at $z=0$. This development makes use of (38) of reference [4], and the commutator of the two operators s and $(\partial/\partial s)^k$ in the integrand of (40) of reference [4].

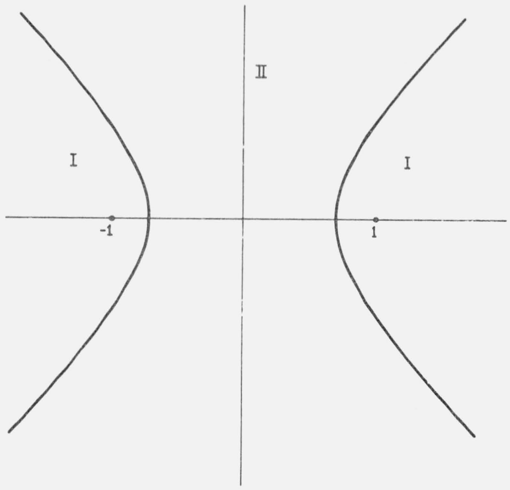

FIGURE B1. *The equilateral hyperbola satisfying* $|\eta^2-1|=|\eta^2|$, *which intersects the real axis at* $\pm 1/\sqrt{2}$.
The Roman numerals identify Regions I and II.

Because of the location of the singularities, we can move the path of integration to a curve C completely to the right of the right-hand branch of the hyperbola.

To apply (B2) to this Fourier integral, we make a change of variables $u=(1-\eta^{-2})$, and note that the path of integration C can then be divided into a part C_1 located in the region of uniform convergence and a part C_2 corresponding to $|1-u|<\epsilon$. In the case of C_2, our change of variables gives

$$|\eta|>1/\sqrt{\epsilon}.$$

The two curve segments give two integrals; and for C_1 it is appropriate to use the series represenation:

$$F(z)=\frac{1}{2\pi i}\int_{C_1}\frac{d\eta}{\eta}\,\Phi(\eta)\sum_{n=0}^{\infty}\left(\frac{\eta^2-1}{\eta^2}\right)^n U_n^0(z)e^{-|z|}+\frac{1}{2\pi i}\int_{C_2}\frac{d\eta}{\eta}\,e^{-\eta|z|}\,\Phi(\eta). \tag{B4}$$

The exponential factor in the integrand of the last term on the right has a magnitude determined by the real part of the exponent, and therefore at least as small as

$$\exp\left\{-\frac{|z|}{\sqrt{2\epsilon}}\right\}.$$

For $z\neq 0$, this factor can be made as small as one pleases; and we choose it so that the second term on the right of (B4) can be neglected altogether.

Because of uniform convergence, the integration and summation can be interchanged in the first term on the right of (B4), with the result

$$F(z)=\sum_{n=0}^{\infty}F_nU_n^0(z)e^{-|z|}, \tag{B5}$$

where

$$F_n=\frac{1}{2\pi i}\int_C\frac{d\eta}{\eta}\left(\frac{\eta^2-1}{\eta^2}\right)^n\Phi(\eta). \tag{B6}$$

We thus find that $F(z)$ has pointwise convergent representations of the type (B5). Also, by writing $\Phi(\eta)$ as a transform over $F(z)$, in (B6), we readily change to the more familiar form

$$F_n=\int_0^{\infty}dz\hat{U}_n^0(z)F(z). \tag{B6$'$}$$

(3) A parallel argument, also making use of the region of uniform convergence of (B2), but with a transformation $-u=\eta^2/(1-\eta^2)$ and an inversion integral confined to Region II, leads to the series form for the transformation kernels of the U_n^k systems: For y, $z>0$,

$$\left\{\frac{\partial^2}{\partial y \partial z}\right\}^k \frac{2}{\pi} K_0(\sqrt{y^2+z^2})=\sum_{n=0}^{\infty}\{U_n^k(y)e^{-y}\}\{U_n^k(z)e^{-z}\}, \tag{B7}$$

where K_0 is the modified Bessel function. For the arguments which follow, the important feature of this expression is the fact that for $y=z>0$, the sum on the right converges to a finite value.

(4) Let some of the singularities of a function $\Phi(\eta)$ be located in Region II. Then it *may* be possible to choose a scale factor β such that the singularities of $\Phi(\eta/\beta)$ all lie in Regions I. If so, since

$$F(z)=\frac{\beta^{-1}}{2\pi i}\int_{-i\infty}^{i\infty} d\eta e^{-\eta|z|/\beta}\Phi(\eta/\beta), \tag{B8}$$

it is clear that a representation of the type

$$F(z)=\sum_{n=0}^{\infty} F'_n U_n^0(z/\beta)e^{-|z|/\beta} \tag{B9}$$

exists. But this will *not* be the case if any singularities of $\Phi(\eta)$ lie *on* the imaginary axis or if any point of the imaginary axis is a limit point for singularities of $\Phi(\eta)$.

(5) Preceding arguments applying only to the U_n^0 system can be generalized to the U_n^k systems, with $k>0$. If $F(z)$ is even and is known to have the following trend for small z values:

$$F(z)=z^k f(z), \tag{B10}$$

then $f(z)$ may be either even or odd. If the singularities of the Fourier transform φ of f lie entirely in Regions I for some scale factor β, the argument already given for the $k=0$ case leads to pointwise convergent series representations of the form

$$f(z)=\sum_{n=0}^{\infty} f_n^k U_n^k(z/\beta)e^{-|z|/\beta}, \tag{B11}$$

with

$$f_n^k=\frac{\beta^{-1}}{2\pi i}\int_C \frac{d\eta}{\eta^{k+1}}\left(\frac{\eta^2-1}{\eta^2}\right)^n \varphi(\eta/\beta)=\int_0^{\infty}\frac{dz}{\beta}(z/\beta)^k \hat{U}_n^k(z/\beta)f(z). \tag{B11$'$}$$

Equation (B11′) makes it clear that $f(z)$ can contain singular terms at $z=0$—Dirac delta functions and their derivatives—which do not contribute to the coefficients f_n^k because they are overriden by the factor z^k.

(6) Consider a function $F(z)$ with Fourier transform having singularities confined to Regions I. This same property will apply also to $f(z)$, if $F(z)$ has the form (B10). If we write expressions for finite approximations to $f(z)$,

$$f_N(z)=\sum_{n=0}^{N-1} f_n^k U_n^k(z)e^{-|z|} \tag{B12}$$

and apply Schwarz's inequality to the difference function $f-f_N$, we obtain the result

$$|f-f_N|^2\leq\left\{\sum_{n=0}^{\infty}(f_n^k)^2\right\}\sum_{n=N}^{\infty}\{U_n^k(z)e^{-|z|}\}^2. \tag{B13}$$

Since the last factor on the right tends to vanish in the limit $N \to \infty$, it is clear that finite norm,

$$\sum_{n=0}^{\infty} (f_n^k)^2 < \infty,$$

implies pointwise convergence, for $z \neq 0$.

(7) Let $F(z)$ be even and representable by a U_n^0 series,

$$F(z) = \sum_{n=0}^{\infty} F_n U_n^0(z) e^{-|z|}. \tag{B15}$$

We further assume that this series has finite norm, and calculate the Fourier transform of both sides of (B15), by a limiting process:

$$\begin{aligned}\Phi(\eta) &= \lim_{\epsilon \to 0} \left\{ \int_{-\infty}^{-\epsilon} dz e^{\eta z} F(z) + \int_{\epsilon}^{\infty} dz e^{\eta z} F(z) \right\} \\ &= \lim_{\epsilon \to 0} \sum_{n=0}^{\infty} F_n \left\{ \int_{-\infty}^{-\epsilon} dz e^{\eta z} U_n^0(z) e^{-|z|} + \int_{\epsilon}^{\infty} dz e^{\eta z} U_n^0(z) e^{-|z|} \right\} \\ &= \sum_{n=0}^{\infty} F_n \frac{2}{1-\eta^2} \left(\frac{\eta^2}{\eta^2 - 1} \right)^n. \end{aligned} \tag{B16}$$

The limit $\epsilon \to 0$ can be taken as above providing $F(z)$ is sufficiently well-behaved near $z = 0$ that the Fourier transform exists.

Now, applying Schwarz's inequality to (B16) we obtain

$$|\Phi(\eta)| \leq \frac{2}{|\eta^2|} \|F\| \left\{ \sum_{n=0}^{\infty} \left| \frac{\eta^2}{\eta^2 - 1} \right|^{2n+2} \right\}^{1/2} \tag{B17}$$

And since $|\eta^2/(\eta^2 - 1)| < 1$, for η in Region II, the right side is finite at all points η in Region II. We conclude that for series representations with finite norm, the Fourier transform can have no divergent singularities in Region II.

(8) Note that for $z \neq 0$, the cases $-\infty < |z| < \infty$ and $0 < z < \infty$ can be considered equivalent, for functions $F(|z|)$ and $F(z)$, respectively. Hence problems in which the functions are defined on the infinite interval, can be analyzed with the use of U_n^k representations defined on the semi-infinite interval.

(9) Although we do not attempt it here, the existence of simple generating functions for the $\hat{U}_n^k$ polynomials makes a similar set of arguments possible, but in connection with even or odd functions whose *Laplace* transforms have singularities confined to Region II of figure B1.

(10) Physical solutions to neutron and gamma ray transport problems are such that the singularities of the Fourier transform lie on the real axis at distances from the origin $|\eta| \geq \mu_{\min}$, where $\mu_{\min}$ is the attenuation coefficient of the most penetrating radiation component and has a known value in any given problem. Thus one always expects convergent representations of the general type (B11) to exist.

One should realize that there exist functions of $|z|$ on the infinite interval whose moments *all* vanish. Such functions cannot be represented by U_n^k expansions; and one infers that these functions have Fourier transforms which are singular on the imaginary axis. This observation is confirmed by the discussion of these functions in reference [10]. Since there is neither physical nor mathematical reason to expect that such functions play any role in transport theory, their automatic exclusion from any representation based on U_n^k functions is appropriate.

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12. References

[1] Spencer, L. V., and Fano, U., Penetration and diffusion of x-rays. Calculation of spatial distributions by polynomial expansion, J. Research NBS 46, 446–456 (June 1951) RP2213.

[2] Fano, U., Spencer, L. V., and Berger, M. J., Penetration and diffusion of x-rays, Handbuch der Physik V. 38 (Springer-Verlag, Berlin, 1959).

[3] Preiser, S., An investigation of biorthogonal polynomials derivable from ordinary differential equations of the third order, J. Math. Anal. Appl. 4, No. 1, 38 (Feb. 1962).

[4] Spencer, L. V., and Flusser, P., Properties of a useful biorthogonal system, J. Res. Nat. Bur. Stand. (U.S.) 71B (Math. and Math. Phys.), No. 4, 197–211 (Oct.–Dec. 1967).

[5] Goldstein, H., and Wilkins, J. E., Jr., Calculation of the Penetration of Gamma Rays, Nucl. Development Associates, Inc. NYO–3075 (1954).

[6] Spencer, L. V., Bounds to Truncation Errors in Biorthogonal Polynomial Approximations, with Illustrative Applications to Gamma Ray Transport Distributions, J. Res. Nat. Bur. Stand. 75B (Math. Sci.), Nos. 1 and 2, 1–16 (Jan.–June 1971).

[7] Soran, P., and Goldstein, H., Reconstruction of neutron spatial distributions from spatial moments, Transactions of the American Nuclear Society 13, No. 1, 405 (1970).

[8] Spencer, L. V., and Simmons, G. L., Improved Moment Method Calculations of Gamma Ray Transport: Application to Point Isotropic Sources in Water, Nucl. Sci. Engr. 50, 20–30 (1973).

[9] Morris, E. E., An Extension of the Polynomial Approximation in Moments Method Calculations to the Deep Penetration of Gamma Radiation, Transactions 11, No. 1, 418–419 (1968).

[10] Shohat, J. A., and Tamarkin, J. D., The Problem of Moments, Mathematical Surveys No. 1, pp. 20, 22, American Mathematical Society (1943).

(Paper 76B3&4–364)