JOURNAL OF COMPUTATIONAL PHYSICS 21, 208–226 (1976)

Approximating with Nonorthogonal Basis Functions

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Received June 30, 1975; revised January 8, 1976

Approximations of functions by nonorthogonal basis functions are examined and criteria for best fits for several types of convergence discussed. In particular, expansions in Gaussian and Breit–Wigner functions are examined and some specific numerical examples with Gaussian functions are given, illustrating how the expansion parameters can be calculated analytically, rather than searching for a best fit in a multidimensional space, as is conventionally done.

1. INTRODUCTION

In many physical problems it is important to be able to approximate functions by sums of other functions that have predetermined desirable properties. For example, wavefunctions of bound state systems often are approximated by sums of Gaussian functions which have convenient integration properties. While the results of this paper are general our motivation for investigating the approximation of functions arises from the need to approximate wavefunctions and scattering amplitudes that appear in atomic, nuclear, and particle physics. The approximations will consist of finite expansions in nonorthogonal functions, with coefficients chosen to give a best fit. This means that it will be necessary to discuss what is meant by "best fit." Section 2 will review two types of convergence often used in numerical analysis and show how these different criteria for a best fit lead to equations for determining the unknown parameters of the expansion.

The equations for the unknown expansion parameters often turn out to be nonlinear equations that are themselves difficult to solve. For this reason one is often forced to search in a multidimensional parameter space and hope that the values for the parameters so obtained correspond to the true minimum. We show in Section 3 how one can expand in Gaussian functions in such a way as to be able to solve analytically for the unknown parameters, as functions of the moments of the function being approximated; some numerical results with simple functions are also given in this section.

Since we are considering expansions in nonorthogonal basis functions it is clear

that the modulus squared of the expansion coefficients will not sum to the norm of the function being expanded. In particular, with the addition of new basis functions intruding partially into the subspaces spanned by the other basis functions, the expansion parameters may vary wildly with the inclusion of just a few new terms. This shows that it is important to be able to solve for the unknown parameters of the expansion in terms of the function being expanded, for only then is it possible to directly connect the number of terms needed in an expansion with the predetermined goodness of fit desired.

While it is not possible to recover all the convenient features associated with orthogonal expansions, it is possible to find functions that are biorthogonal which can be used to find the expansion coefficients. The general features of biorthogonal sets are discussed in Section 2, where it is shown how a weak convergence criterion for best fit leads to sets of biorthogonal functions that can be computed with certain transforms. Specific transforms generating biorthogonal functions are given in Section 3 for Gaussian functions and in Section 4 for Breit–Wigner functions.

2. General Results

The general mathematical problem under consideration in this paper is the expansion of a given function f in a set of functions $f_{\alpha_i} \equiv f_i$ so that

$$f \sim \sum_{i=1}^{N} c_i f_i , \tag{2.1}$$

where "$\sim$" means "approximated by" and the expansion coefficients c_i are chosen to give the best fit. Generally the f_i will depend on some parameters, as for example the Gaussian functions $f_i = e^{-\alpha_i x^2}$. There are two parts to this problem, the first being to establish criteria showing that for a given set of parameters $\{\alpha_i\}_{i=1}^{\infty}$ that f can be approximated as accurately as desired by letting N in Eq. (2.1) become sufficiently large. Once these denseness criteria are established one must deal with the more practical computational problem of finding those c_i and α_i, $i = 1 \cdots N$, that give a best fit to the function f. We will discuss two ways of defining "best fit," involving the notion of convergence in norm (strong convergence) and weak convergence [1]. Both definitions make use of the fact that f and $\{f_i\}$ are elements of some Hilbert space $\mathscr{H}$, although a rigged Hilbert space [2] will also be used when discussing weak convergence.

We begin by discussing norm convergence; in this case it must first be established that, for a given $\{\alpha_i\}_{i=1}^{\infty}$ and $\epsilon > 0$, there exists an N such that

$$\left\| f - \sum_{i=1}^{N} c_i f_i \right\|^2 < \epsilon \tag{2.2}$$

for all $f \in \mathscr{H}$. The type of norm used need not be specified at this point; it includes the chi-squared norm often used in computational analysis [1] as well as the norm defined by $\|f\|^2 = \int_0^\infty \omega(x)\, dx\, |f|^2$. $\omega(x)$ is a weighting function that can be chosen to improve convergence in desired regions; for simplicity $\omega(x)$ is set equal to 1 in Sections 3 and 4. Section 3 will show what sorts of sequences $\{\alpha_i\}_{i=1}^\infty$ guarantee that Eq. (2.2) holds when the f_i are Gaussian functions, while in Section 4 analogous results will be given when the f_i are Breit–Wigner types of functions.

Assuming now that Eq. (2.2) holds, so that the f_i are dense in $\mathscr{H}$ we turn to the problem of computing the $2N$ coefficients c_i and α_i. For simplicity it is assumed that both the c_i and α_i are real, although this condition will be relaxed in Section 4 when dealing with Breit–Wigner functions, where the parameters are complex. It is also to be noted that there is no contradiction between assuming certain properties on the $\{\alpha_i\}_{i=1}^\infty$ to ensure denseness and then attempting to compute the first N of the α_i; it is the behavior of the infinite sequence of α_i that determines denseness, and changing the first N α_i will not change the convergence properties of the infinite set.

Thus, the criterion for a best fit in norm comes from minimizing the norm of the difference $f - \sum c_i f_i$:

$$\left\| f - \sum_{i=1}^{N} c_i f_i \right\|^2 = \text{minimum}, \tag{2.3}$$

which is equivalent to

$$\begin{aligned} &\partial/\partial c_k \left\| f - \textstyle\sum c_i f_i \right\|^2 = 0, \\ &\qquad\qquad\qquad\qquad k = 1 \cdots N \\ &\partial/\partial \alpha_k \left\| f - \textstyle\sum c_i f_i \right\|^2 = 0. \end{aligned} \tag{2.4}$$

These equations define an extremum of the norm and it is necessary to check whether a local minimum has been obtained. This can be done either by computing the appropriate second derivatives or by comparing the approximate expansion with the function. In any event, working out the inner products gives

$$(f_k, f) = \sum_{i=1}^{N} (f_k, f_i)\, c_i \tag{2.5a}$$

$$(\partial f_k/\partial \alpha_k, f) = \sum_{i=1}^{N} (\partial f_k/\partial \alpha_k, f_i)\, c_i\,. \tag{2.5b}$$

Defining the $N \times N$ matrix $M_{ij}(\alpha) = (f_i, f_j)$, which is dependent on α_i and nonsingular when the α_i are distinct, gives

$$c_i = \sum_{k=1}^{N} M_{ik}^{-1}(\alpha)(f_k, f). \tag{2.6}$$

It is to be noted that M^{-1} can be computed explicitly with the help of the Gram–Schmidt orthogonalization process. Thus, let the functions f_i be ordered so that $\hat{e}_1 = \beta_{11} f_1$, $\hat{e}_2 = \beta_{12} f_1 + \beta_{22} f_2, \ldots, \hat{e}_N = \sum_{i=1}^{N} \beta_{iN} f_i$, where the β_{ij} are chosen to make $(\hat{e}_i, \hat{e}_j) = \delta_{ij}$. That is

$$\hat{e}_k = \sum_{i=1}^{k} \beta_{ik} f_i, \qquad \beta_{ik} = 0, i > k, \quad k = 1 \cdots N. \tag{2.7}$$

It then follows that

$$(\hat{e}_i, \hat{e}_j) = \sum_{k1} (\beta_{ki} f_k, \beta_{\ell j} f_\ell) = \sum_{k1} \beta_{ki} M_{k\ell} \beta_{\ell j} = \delta_{ij} \tag{2.8}$$

or in matrix notation $\beta^T M \beta = I$. Since both β and M are nonsingular because the f_i are all linearly independent, it follows that

$$M^{-1} = \beta \beta^T, \tag{2.9}$$

which means that M^{-1} always can be computed analytically if the entries M_{ij} are known.

Substituting Eq. (2.6) into (2.5b) then results in a set of N equations for the $\{\alpha_i\}_{i=1}^{N}$;

$$\left(\frac{\partial f_k}{\partial \alpha_k}, f\right) = \sum_{i,\ell} \left(\frac{\partial f_k}{\partial \alpha_k}, f_i\right) M_{i\ell}^{-1}(f_\ell, f) = \left(P(\alpha) \frac{\partial f_k}{\partial \alpha_k}, f\right) \tag{2.10a}$$

or

$$\left(Q(\alpha) \frac{\partial f_k}{\partial \alpha_k}, f\right) = 0, \qquad k = 1 \cdots N, \tag{2.10b}$$

where $P(\alpha)$ is the projection operator into the finite-dimensional subspace spanned by the f_i, while $Q(\alpha)$ is the projection operator into the orthogonal complement so that $P(\alpha) + Q(\alpha) = I$; as indicated by the notation both operators depend on α_i. The result (2.10b) has an interesting geometrical interpretation. The best choice of $\{\alpha_i\}_{i=1}^{N}$ minimizing the norm Eq. (2.3) is obtained by varying the finite-dimensional

subspace spanned by the f_i in the Hilbert space so that the component of the vector $\partial f_k/\partial \alpha_k$ orthogonal to the span of f_i is orthogonal to f. That is, if

$$\partial f_k/\partial \alpha_k = \sum_{j=1}^{N} d_{kj} f_j + f_k^{\perp}, \tag{2.11}$$

then $f_k^{\perp}$ $(= Q\partial f_k/\partial \alpha_k)$ should be orthogonal to f for all $k = 1 \cdots N$. For a given set f_i it is of course possible to compute $f_k^{\perp}$ and thus arrive at a set of equations for the α_i. But this set will usually be nonlinear in the α_i and thus difficult to solve.

For that reason we turn to the second type of convergence, weak convergence, for which denseness means that an N can be found such that

$$\left|\left(f - \sum_{i=1}^{N} c_i f_i , g_\ell\right)\right|^2 < \epsilon, \tag{2.12}$$

where again $\epsilon > 0$ and $\{\alpha_i\}_{i=1}^{\infty}$ are given. In this case, however, another set of functions $\{g_\ell\}$ must also be specified. If the g_ℓ are elements of $\mathscr{H}$, then denseness in norm implies denseness in the weak convergence sense. We will also be interested in functions g_ℓ that are not elements of $\mathscr{H}$, but rather in the rigging of $\mathscr{H}$. For example in Section 3 g_ℓ will be chosen of the form x^ℓ and these function are not elements of $\mathscr{H}$. In that case the question of denseness in the weak convergence sense is much more delicate.

Assuming that Eq. (2.12) holds for all $f \in \mathscr{H}$ we again wish to find the coefficients c_i and α_i that minimize $|(f - \sum c_i f_i , g_\ell)|^2$. However, in this case both sets of partial derivatives used in Eq. (2.4) lead to equations of the form

$$\begin{aligned} \left(f - \sum_{i=1}^{N} c_i f_i , g_\ell\right) &= 0, \\ (g_\ell , f) &= \sum_{i=1}^{N} (g_\ell , f_i)\, c_i , \end{aligned} \tag{2.13}$$

which again define only an extremum. Since there is only one equation for both the c_i and α_i coefficients, it is clear that ℓ will have to range over $2N$ different values in order to uniquely determine the $2N$ unknown coefficients. The big advantage of Eq. (2.13) over the analogous Eqs. (2.6) and (2.10) is that (g_ℓ , f) may not depend on the α_i. That is, the g_ℓ may be chosen so that (g_ℓ , f) gives a set of $2N$ numbers that are fixed and do not change with new choices of α_i. Section 3 will show how both the α_i and c_i can be computed when $f_i = e^{-\alpha_i x^2}$ and $g_\ell = x^\ell$.

A second advantage of Eq. (2.13) is that the g_ℓ can be chosen orthogonal to the f_i, so that $\{f_i , g_k\}$ form a biorthogonal set satisfying $(f_i , g_k) = 0$, $i \neq k$. In this

case the c_i can be computed immediately; however, (g_ℓ, f) may then depend on the α_i.

It should be emphasized that the inner product used in Eq. (2.13) may contain a weight factor necessary to improve convergence in desired regions; also different sets $\{g_\ell\}$ will emphasize different regions. In Section 3 where the weighting factor is unity and the $\{g_\ell\}$ of the form x^ℓ, better fits for larger values of x are obtained. If it is important to fit small values of x accurately, a weighting factor of the form $e^{-\lambda x^2}$ would be appropriate.

To conclude this section we discuss a method for generating classes of biorthogonal functions that can be used as the g_ℓ functions of Eq. (2.13). The method given generalizes a result of [3] and makes use of the assumption that there exists a transform $\mathscr{T}$ carrying functions from $\mathscr{H}$ to the the complex plane, the kernel of which includes the function f_i. For the Gaussian functions to be discussed in Section 3 the transform is the Laplace transform, while for Breit–Wigner functions it is the Stieltjes transform. Thus, we wish to find functions φ_k such that $(\varphi_i, f_j) = 0$, $i \neq j$ by writing

$$F_i(z) = \mathscr{T}_z \varphi_i, \tag{2.14}$$

where $\mathscr{T}$ is the appropriate transform. If functions $F_i(z)$ can be found with zeroes at $z = \alpha_1, \alpha_2, \ldots$, so that $F_i(\alpha_k) = 0$, $i \neq k$, then the transform inverse to Eq. (2.14) will generate a set $\{\varphi_i\}_{i=1}^N$ that satisfies the required conditions. However, in the examples we have computed the φ_i are not elements of $\mathscr{H}$, but of the rigging of $\mathscr{H}$. Thus we turn briefly to how the Hilbert space structure used thus far is generalized to include functions not in $\mathscr{H}$. Let $\mathscr{S}$ denote a dense subspace of $\mathscr{H}$ spanned by the f_i for a given $\{\alpha_i\}_{i=1}^\infty$. Then $\mathscr{S} \subset \mathscr{H}$ and $\mathscr{H}^* \subset \mathscr{S}^*$, where "*" means dual. But $\mathscr{H}$ is its own dual so that $\mathscr{S} \subset \mathscr{H} \subset \mathscr{S}^*$. This triplet of spaces is called a rigged Hilbert space [2] and makes use of the fact that for $f \in \mathscr{S}$ and $g \in \mathscr{S}^*$, (f, g) is well defined. But this is exactly what is needed in Eq. (2.13), for $f_i \in \mathscr{S}$, $g_\ell \in \mathscr{S}^*$ and for most applications $f \in \mathscr{S}$, so that the inner products in (2.13) are well defined. Thus, as will be shown in Sections 3 and 4, Eq. (2.13) leads to well defined equations even when g_ℓ is in $\mathscr{S}^*$.

It is to be noted that some very delicate mathematical problems arise when the biorthogonal set $\{\varphi_i, f_i\}$ is an infinite set. Since the functions φ_i are highly nonunique, denseness in the norm sense does not always lead to denseness in the weak convergence sense. For assume that two sets of functions $\{\varphi_i\}, \{\varphi_i'\}$ both satisfy $(\varphi_i, f_j) = (\varphi_i', f_j) = \delta_{ij}$, with $\varphi_i, \varphi_i' \in \mathscr{S}^*$ obtained by some choices of the $F_i(z)$ in Eq. (2.14). Then $(\varphi_i - \varphi_i', f_j) = 0$, which means that $\varphi_i - \varphi_i'$ are orthogonal to the f_j, contradicting the denseness assumption. A similar sort of problem arises when considering biorthogonal sets in the norm type of convergence. It would seem that biorthogonal functions φ_i could be defined as $\varphi_i = M_{ik}^{-1}(\alpha) f_k$, for then Eq. (2.6) would read $c_i = (\varphi_i \cdot f)$. But the problem in the infinite dimensional

case is that $M^{-1} = \beta\beta^T$ may not be defined because β is an unbounded operator. Since we are concerned with finite subspaces these technical mathematical problems will not be pursued further here; rather we discuss two examples in the next sections showing how the general results of this section lead to easy computational results for fitting functions.

3. Approximating with Gaussians

The use of Gaussian functions as a nonorthogonal basis set arises in a number of physical problems [4]. One advantage of Gaussian functions is their easy integrability over the whole real line. Expanding functions in a Gaussian basis set can often reduce a manydimensional integral to a sum of simpler terms. This feature is particularly useful in the calculation of many-body matrix elements where it is necessary to transform between different classes of center of mass variables. The accuracy of this technique is dependent on the goodness of the appropriate expansion.

In this section we consider only Gaussian functions $G_i = f_i$ of the form

$$G_i(x) \equiv e^{-\alpha_i x^2} \tag{3.1}$$

as elements of the Hilbert space $f \in \mathscr{H}$

$$\|f\|^2 = \int_0^\infty dx\, |f|^2 < \infty. \tag{3.2}$$

For these functions the matrix $M(\alpha_i)$ can be computed analytically, and is of the form

$$M_{ij} = (G_i, G_j) = \frac{\pi^{1/2}}{2(\alpha_i + \alpha_j)^{1/2}}. \tag{3.3}$$

Given M_{ij} one can easily compute its inverse using Eq. (2.9). According to the Müntz–Satz Theorem [5] the Gaussian functions are dense whenever $\sum_{i=1}^{\infty} 1/\alpha_i$ diverges. A particular case is when $\alpha_i = i$ or when $\alpha_i = i\alpha_0$. Any finite set of N Gaussian functions can be considered a subset of a complete set since one can always add on the set $\alpha_{N+i} = k + i$, where k is an integer larger than α_N, and $i = 1, 2, \ldots, \infty$.

For a given function $f \in \mathscr{H}$ which is to be approximated by N Gaussian functions, N fixed and finite, using the norm convergence criterion for goodness of fit,

Eq. (2.5), the parameters $\{\alpha_i\}_{i=1}^N$ can be found from Eqs. (2.10) and (2.11). For the Gaussian functions this becomes

$$(x^2 G_k, f) = \sum_\ell \mathscr{M}_{k\ell}(\alpha)(G_\ell, f), \tag{3.4}$$

where

$$\mathscr{M}_{k\ell}(\alpha) = \sum_i (x^2 G_k, G_i) M_{i\ell}^{-1}.$$

This is a nonlinear equation whose solutions are usually difficult to obtain numerically. Not only is $\mathscr{M}_{k\ell}(\alpha)$ a complicated function of the α_i, but also the inner products $(x^2 G_k, f)$ and (G_ℓ, f) depend on the α_i. If the α_i could be found, it would of course be a straightforward problem to solve for the c_i. This difficulty in solving Eq. (3.4) for the α_i is a serious practical limitation on the method. We now show that the equations following from weak convergence lead to a much simpler procedure for finding the α_i.

Using Eq. (2.13) with $g_\ell = x^\ell$, the expansion parameters are found by solving the equations

$$(x^\ell, f) = \sum_{i=1}^N c_i (x^\ell, G_i), \qquad \ell = 0, 1, 2, \ldots, 2N-1 \tag{3.5}$$

for both the c_i and the α_i. The advantage of Eq. (3.5) over Eq. (3.4) is that (f, x^ℓ), the moment of f with respect to x^ℓ, is independent of the expansion parameters; consequently, the $2N$ moments of the function to be approximated need to be calculated only once. Other functions besides x^ℓ could be used for g_ℓ, but we will now show that with the choice x^ℓ there is an explicit method for solving for the c_i and α_i. It should be noted that the inner product (f, x^ℓ) may not always be defined for $f \in \mathscr{H}$. Rather f must be an element of a dense subspace of $\mathscr{H}$, for x^ℓ is an element of the rigging. In practice this condition is usually met, since in most physical problems the functions have an asymptotic behavior of the form e^{-kx}, so that the inner product is well defined.

We make use of a variation of Proney's method [6] to solve for the α_i. The moments of the Gaussian functions are of the form

$$(x^\ell, G_i) = \frac{\Gamma((\ell+1)/2)}{2\alpha_i^{1/2(\ell+1)}} = \frac{\Gamma((\ell+1)/2)}{2} a_i^{\ell+1}, \tag{3.6}$$

where $a_i = \alpha_i^{-1/2}$. Now let

$$(x^\ell, f) = \frac{\Gamma((\ell+1)/2)}{2} f_\ell. \tag{3.7}$$

Equation (3.5) then becomes

$$f_\ell = \sum_{i=1}^{N} c_i a_i^{\ell+1}, \qquad \ell = 0, 1, \ldots, 2N - 1. \tag{3.8}$$

Define $\{\lambda_j\}$ by

$$\prod_{i=1}^{N} (a - a_i) = \sum_{j=0}^{N} \lambda_j a^j, \qquad \lambda_N \equiv 1; \tag{3.9}$$

this is a polynomial of degree N whose roots are the desired a_i. To find the λ_j we use (3.8) and (3.9) to obtain

$$\begin{aligned} \sum_{j=0}^{N} f_{k+j}\lambda_j &= \sum_{j=0}^{N} \left\{ \sum_{i=1}^{N} c_i a_i^{k+j+1} \right\} \lambda_j \\ &= \sum_{i=1}^{N} c_i a_i^{k+1} \left\{ \sum_{j=0}^{N} \lambda_j a_i^j \right\} = 0. \end{aligned} \tag{3.10}$$

Thus we find

$$\sum_{j=0}^{N-1} f_{k+j}\lambda_j = -f_{k+N}, \qquad k = 0, 1, \ldots, N - 1. \tag{3.11}$$

This set of N linear equations can be solved for the λ_j if the matrix f_{k+j} is nonsingular. However, for a given N the moments f_ℓ may result in a singular f_{k+j} matrix. In such a case N must be made larger until the new f_{k+j} matrix is no longer singular. Then, given the a_i, and consequently the α_i, the first N equations in (3.8) can then be used to solve for the c_i; that is, one must solve the equations

$$f_\ell = \sum_{i=1}^{N} c_i a_i^{\ell+1}, \qquad \ell = 0, 1, \ldots, N - 1. \tag{3.12}$$

The solutions of this equation can be expressed in terms of the λ_j and a_i. Define $\{A_{j\ell}\}$ by

$$\sum_{\ell=0}^{N-1} A_{j\ell} a^{\ell+1} = K_j a \prod_{\substack{n=1 \\ n \neq j}}^{N} (a - a_n), \tag{3.13}$$

where K_j is chosen such that

$$K_j a_j \prod_{\substack{n=1 \\ n \neq j}}^{N} (a_i - a_n) = 1; \tag{3.14}$$

that is,

$$K_j = \left[a_j \prod_{\substack{n=1 \\ n \neq j}}^{N} (a_j - a_n) \right]^{-1}. \tag{3.15}$$

Given the $A_{j\ell}$, c_i is given by

$$\begin{aligned} \sum_{\ell=0}^{N-1} A_{j\ell} f_\ell &= \sum_{\ell=0}^{N-1} A_{j\ell} \sum_{i=1}^{N} c_i a_i^{\ell+1} = \sum_{i=1}^{N} c_i \left\{ \sum_{\ell=0}^{N-1} A_{j\ell} a_i^{\ell+1} \right\} \\ &= \sum c_i \delta_{ij} = c_j . \end{aligned} \tag{3.16}$$

Thus

$$c_j = \sum_{\ell=0}^{N-1} A_{j\ell} f_\ell . \tag{3.17}$$

To find $A_{j\ell}$ we use (3.13) and (3.9) to write

$$(a - a_j) \sum_{\ell=0}^{N-1} A_{j\ell} a^{\ell+1} = K_j a \prod_{n=1}^{N} (a - a_n) = K_j a \sum_{\ell=0}^{N} \lambda_\ell a^\ell. \tag{3.18}$$

This can be rewritten in the form

$$\sum_{\ell=1}^{N} A_{j\ell-1} a^{\ell+1} - \sum_{\ell=0}^{N-1} a_j A_{j\ell} a^{\ell+1} = K_j \sum_{\ell=0}^{N} \lambda_\ell a^{\ell+1}. \tag{3.19}$$

From (3.19) one obtains the relations

$$\begin{aligned} A_{jN-1} &= \lambda_N K_j = K_j , \\ A_{j\ell-1} - a_j A_{j\ell} &= K_j \lambda_\ell , \qquad \ell < N. \end{aligned} \tag{3.20}$$

This gives the recursion relation

$$A_{j\ell} = a_j A_{j\ell+1} + K_j \lambda_{\ell+1} , \qquad \ell = 0, 1, 2, \ldots, N - 2.$$

One can interpret the $A_{j\ell}$ as defining a polynomial that projects out G_j from the N-dimensional subspace. That is, they define biorthogonal functions $\varphi_j(x)$:

$$\varphi_j(x) = \sum_{\ell=0}^{N-1} A_{j\ell} \left[\frac{2}{(\Gamma(\ell + 1)/2)} \right] x^\ell; \tag{3.21}$$

then

$$[\varphi_j(x), G_i] = \sum_{\ell=0}^{N-1} A_{j\ell} \left[\frac{2}{\Gamma((\ell+1)/2)}\right] \int_0^\infty x^\ell e^{-\alpha_i x^2}\, dx$$

$$= \sum_{\ell=0}^{N-1} \frac{A_{j\ell}}{\alpha_i^{((\ell+1)/2)}} = \sum A_{j\ell} a_i^{\ell+1} = \delta_{ij}\,. \tag{3.22}$$

We now consider a specific example to illustrate the utility of this method. Since it has been demonstrated [4] that Gaussian functions can approximate complicated oscillating bounded functions, we choose for simplicity the function $f = e^{-\beta x}$, which is smooth and has the "wrong" behavior at the origin. Using Eq. (3.7) we find

$$f_\ell = \frac{(2/\beta)^{\ell+1}\, \Gamma((\ell+2)/2)}{\pi^{1/2}}\,.$$

In Table I we list the α_i for $N = 5, 10, 15$ as well as ϵ, the norm of the difference

TABLE I

Gaussian Parameters α_i for the expansion of $e^{-\beta x}$ for $\beta = 2.0$

N / i	5 $\epsilon = 2.13 \times 10^{-4}$	10 $\epsilon = 1.69 \times 10^{-5}$	15 $\epsilon = 3.99 \times 10^{-6}$
1	0.1230144183	0.0519875157	0.0301361296
2	0.2568384320	0.0771273312	0.0411820185
3	0.6318974855	0.1148207757	0.0546169159
4	2.2739798430	0.1771734293	0.0688349233
5	21.1332263357	0.2908079533	0.0915737882
6		0.5246383739	0.1245532619
7		1.0940882812	0.1747226532
8		2.8832857586	0.2554718373
9		11.5722926611	0.3948329579
10		121.0983765153	0.6578809088
11			1.2174405445
12			2.6252286703
13			7.1884093365
14			29.9710506086
15			323.3605768853

between the true and the approximate function. From the values of ϵ one can see that the expansion is converging as N increases. In practice one usually increases N until ϵ is less than some desired value; this is one reason why it is necessary to have a fast and efficient method for determining the α_i.

To illustrate the pointwise convergence of the expansion we plot in Figs. 1 and 2 the absolute value of the fractional difference between the true and the approximate function,

$$\Delta \equiv \frac{|f - \sum_{i=1}^{N} c_i e^{-\alpha_i x^2}|}{|f|}.$$

Since this difference varies over several orders of magnitude we have plotted it on a logarithmic scale. From Figs. 1 and 2 one can see the Gaussian expansion oscillates about the true function and the period of this oscillation is smallest near the origin. As N is increased the magnitude of the error as well as its period decreases. The convergence is slower near the origin which is not surprising since the Gaussian functions have a zero slope at the origin while the exponential has a nonzero slope. Faster convergence at the origin could be obtained by a different choice of the weight function; as mentioned in Section 2 we have chosen $\omega(x) = 1$. If a weight function that emphasized the region near the origin were used then the expansion

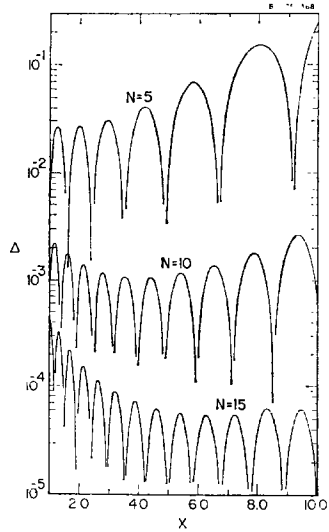

FIG. 1. $\Delta = (|\, e^{-2x} - \sum_{i=1}^{N} c_i e^{-\alpha_i x^2}\,|)/|\, e^{-2x}\,|$ plotted for x between 1 and 10.

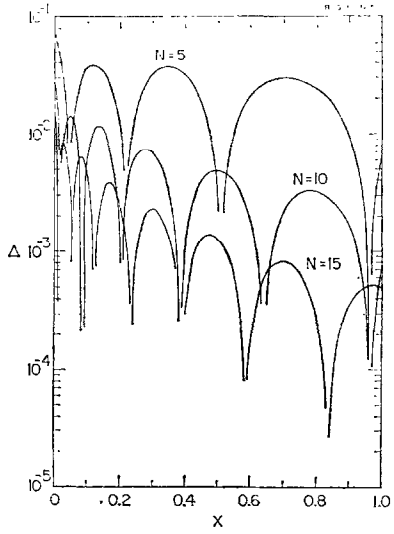

FIG. 2. $\Delta = (|\, e^{-2x} - \sum_{i=1}^{N} c_i e^{-\alpha_i x^2} \,|)/|\, e^{-2x} \,|$ plotted for x between 0 and 1.

would converge more slowly for large values of x. The proper choice of the weight function will be determined by the particular problem for which the expansion is to be used.

To demonstrate the convergence of the expansion for a slightly more complicated function we also apply the method to the expansion of

$$f = (1.0 - 0.5x)\, e^{-2x}$$

for $N = 10$. The c_i and α_i for this expansion are listed in Table II.

One important difference between using orthogonal and nonorthogonal functions is that when using nonorthogonal functions Parseval's equation is not satisfied; consequently, one cannot use the c_i as an indication of the convergence of the expansion. This means that as N is changed all of the c_i will in general change.

In Figs. 3 and 4 we plot the absolute value of f and the absolute value of the difference between f and the Gaussian expansion. (Note that this difference has been multiplied by 10^2 in order to plot it on the same graph.) Once again the expanded function oscillates about f with a period increasing as x increases. The relative errors are largest at the origin and at $x = 2$, where f changes sign. Nevertheless, the pointwise convergence is good, and again by increasing N the error will decrease.

To conclude this section we discuss other possible biorthogonal functions for

the Gaussian functions. When the weak convergence criterion is used the biothogonal functions are not unique. There are many functions both in the Hilbert space itself and in the rigged Hilbert space that are biorthogonal to the Gaussian functions. We now show how one can use the Laplace transform to find some of these

TABLE II

Expansion Parameters for $(1.0-0.5x)\,e^{-2x}$

i	c_i	α_i
1	$-0.7282206917 \times 10^{-8}$	0.0476780509
2	$-0.2490166040 \times 10^{-5}$	0.0692151582
3	$-0.1203542040 \times 10^{-3}$	0.1004217601
4	$-0.1630506231 \times 10^{-2}$	0.1499618316
5	$-0.7059997756 \times 10^{-2}$	0.2356322424
6	$0.7473219467 \times 10^{-1}$	0.7627205554
7	0.2207613552	1.7440743614
8	0.3177433884	5.4255833881
9	0.2747537302	31.0985293429
10	0.1344389778	1206.1456524617

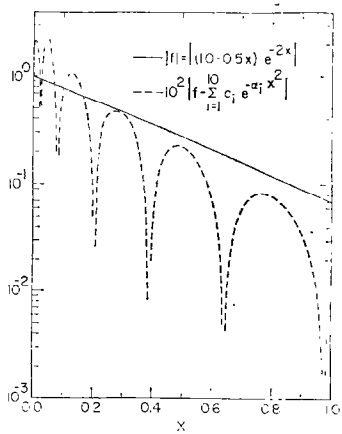

FIG. 3. $|f|$ and $10^2\left|f-\sum_{i=1}^{10} c_i e^{-\alpha_i x^2}\right|$ plotted for x between 0 and 1.

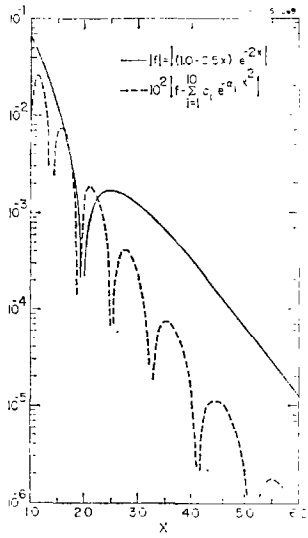

FIG. 4. $|f|$ and $\left|f-\sum_{i=1}^{10} c_i e^{-\alpha_i x^2}\right|$ plotted for x between 1 and 6.

functions, and we give two specific examples. The method consists of finding functions $F_j(z)$ satisfying $F_j(\alpha_i) = 0$, $i \neq j$, where $F_j(z)$ is the Laplace transform:

$$\begin{aligned} F_j(z) &= \int_0^\infty dx\, \omega(x)\, \varphi_j(x)\, e^{-zx^2} \\ &= \int_0^\infty dt\, \frac{\omega(t)^{1/2}}{2t^{1/2}}\, \varphi_j(t)^{1/2}\, e^{-zt} \\ &= \int_0^\infty dt\, \tilde{\varphi}_j(t)\, e^{-zt}, \end{aligned} \tag{3.23}$$

where

$$\tilde{\varphi}_j(t) = \frac{\omega(t^{1/2})\, \varphi_j(t^{1/2})}{2t^{1/2}}, \tag{3.24}$$

and $\omega(x)$ is a weight function that is chosen to be unity in our examples.

The simplest choice for $F_j(z)$ is the ratio of two polynomials, i.e., let

$$F_j(z) = \frac{N_j P_j(z)}{Q(z)}, \tag{3.25}$$

where N_j is a normalization constant and

$$P_j(z) = \prod_{\substack{n=1 \\ n \neq j}}^{N} (z - \alpha_n) = \sum_{m=0}^{N-1} D_{jm} z^m \tag{3.26}$$

is a polynomial of degree $N - 1$. Different choices of the polynomial $Q(z)$ lead to different biorthogonal functions.

If one chooses $Q(z) = z^N$ then

$$F_j(z) = N_j \sum_{m=0}^{N-1} D_{jm} z^{m-N} = \sum_{k=1}^{N} A_{jk}/z^k. \tag{3.27}$$

For this case

$$\tilde{\varphi}_j(t) = \sum_{k=1}^{N} A_{jk}(t^{k-1}/(k-1)! \tag{3.28}$$

and

$$\varphi_j(x) = 2 \sum_{k=1}^{N} A_{jk}(x^{2k-1}/(k-1)!). \tag{3.29}$$

This is similar to the function in Eq. (3.21) except now only odd powers of x are used.

A second example is obtained by choosing

$$Q(z) = \prod_{n=1}^{N} (z + \alpha_n). \tag{3.30}$$

Then

$$F_j(z) = N_j \frac{\prod_{n \neq j} (z - \alpha_n)}{\prod_n (z + \alpha_n)} = \sum_{k=1}^{N} \frac{A_{jk}}{z + \alpha_k}. \tag{3.31}$$

From this one finds

$$\tilde{\varphi}_j(t) = \sum A_{jk} e^{-\alpha_k t} \tag{3.32}$$

or

$$\varphi_j(x) = 2 \sum A_{jk} x e^{-\alpha_k x^2}.$$

Clearly there are many more possible biorthogonal functions which can be obtained from the Laplace transform. Depending on their application they can be used in Eq. (2.5) to compute the α_i and c_i coefficients.

4. Expansions using Breit–Wigner Functions

In the last section Gaussian functions of the form $e^{-\lambda_i x^2}$ were used as non-orthogonal basis functions; in this section we will consider expansions in Breit–Wigner functions. Functions of the type $B(\lambda) = (x + \lambda)^{-1}$ arise in scattering amplitudes, and describe unstable systems with the complex parameter λ equal to the (dimensionless) energy $+ i$ width. Thus, by the general results of Section 2, for a given finite N the function $f \in \mathscr{H}$ is best approximated with the sum $\sum_{i=1}^{N} c_i B(\lambda_i)$ by writing $c_i = \sum_j M_{ij}^{-1}(B_j, f)$, where

$$M_{ij} = (B_i, B_j) = \int_0^\infty \frac{dx}{(x + \lambda_i^*)(x + \lambda_j)} = \frac{1}{\lambda_i^* - \lambda_j} \ln \frac{\lambda_i^*}{\lambda_j}. \tag{4.1}$$

This problem is discussed at some length in [3], where in particular the quantum mechanical meaning of the c_i coefficients is discussed. However the sense in which the c_i give a "best fit" was not pursued in this reference and the goal of this section is to elaborate somewhat more on this point.

It should be noted that M_{ij}^{-1} could not be computed in reference 3 and hence biorthogonal functions were introduced to get around this difficulty. From Eq. (2.9) it is clear that M_{ij}^{-1} can be computed, once the Breit-Wigner functions are formed into orthonormal functions via the Gram–Schmidt process. However, the meaning of the biorthogonal functions in [3], Eq. (3.18), remained obscure, particularly because the choice was not unique. Classes of biorthogonal functions with respect to Breit–Wigner amplitudes can be obtained via the Stieltjes transform, in which

$$F_m(z) = \int_0^\infty (\varphi_m(x)\, dx/(x + z)). \tag{4.2}$$

The functions $F_m(z)$ have a cut in the complex z plane running from 0 to $-\infty$. The inverse to (4.2), assuming certain growth conditions discussed in [3] are met, is given by

$$\varphi_m(x) = \text{Discontinuity } F_m(z). \tag{4.3}$$

Thus, from the general discussion of Section 2, if $F_m(z)$ has prescribed zeroes at $z = \lambda_1, \lambda_2, \ldots$, then

$$F_m(\lambda_n) = \int_0^\infty (\varphi_m(x)\, dx/(x + \lambda_n)) = 0, \qquad m \neq n \tag{4.4}$$

and the φ_m are orthogonal to $B_n = (x + \lambda_n)^{-1}$. The functions φ_n given in [3] are examples of a biorthogonal set that can be used to compute the expansion coefficients c_i of Eq. (1.12). Unlike Section 2, where a procedure was given for also computing the parameter α_i for a best fit to Gaussians, we do not pursue the

analogous question for Breit–Wigner functions. The reason is that Breit–Wigner functions arise as approximations to scattering amplitudes, and data comes in the form of $|f|^2$, rather than f itself, so it is necessary to use new procedures for obtaining the c_i and λ_i from $|f|^2$. This topic will be discussed in more detail in a subsequent paper.

To conclude this section we briefly remark on the denseness of Breit–Wigner functions. It is clear that the Breit–Wigner functions can be made dense in $\mathscr{H}$, simply by choosing the λ_i to have an accumulation point in the complex z plane, say at z_0, not on the cut from 0 to $-\infty$. For assume that f is orthogonal to all the Breit–Wigner functions, so that $(f, B_i) = 0$, $i = 1 \cdots \infty$. Then

$$\begin{aligned} F(z) &= \int_0^\infty (f^*(x)\, dx/(x + z)) \\ F(\lambda_n) &= \int_0^\infty (f^*(x)\, dx/(x + \lambda_n)) = 0. \end{aligned} \tag{4.5}$$

But λ_n accumulates at z_0, so that $F(\lambda_n) = 0$ implies that $F(z) \equiv 0$, which means f is zero. The fact that the B_i are dense in $\mathscr{H}$ when $\lambda_n \to z_0$ is not very useful when trying to find an infinite biorthogonal set, for as discussed in Section 2, the φ_i will not be elements of $\mathscr{H}$ but rather the rigging of $\mathscr{H}$. This is clear from the example worked out in [3]. For approximating functions with a finite number of Breit–Wigner functions, the Stieltjes transform can be used to generate g_ℓ that are orthogonal to the B_i; however, we have not found functions $F_m(z)$ having the property that the inner products (φ_m, f) are independent of λ, as was the case for Gaussians and the moments $g_\ell = x^\ell$ of Section 3.

5. Conclusion

We have shown how the use of the weak convergence criterion for the "best" approximation can lead to new methods of finding biorthogonal functions by the use of appropriate transforms. Specific examples were given for the Gaussian functions using the Laplace transform and for the Breit–Wigner functions using the Stieltjes transform. In addition it was shown how the weak convergence criterion can be used to find techniques for determining expansion parameters. An explicit example was carried out for expansions using Gaussian functions, where the moments of the function to be expanded could be used to obtain the c_i and the α_i. This technique is much more efficient than chi-squared techniques, for in a chi-squared search in the multidimensional space of the α_i it is difficult to determine when the true minimum has been found, while in the technique presented in Section 2 the α_i for the "best" approximation come directly from the solution of a

well-defined set of equations. Therefore, for a fixed value of N our technique gives a unique best approximation. This is a useful computational feature since one usually increases N until a desired goodness of fit is obtained.

Finally, we have shown by the expansion in Gaussian functions of two different functions how well and how quickly convergence is attained. In both examples good fits were obtained with very little computer time; as discussed in Sections 2 and 3, even better fits could be obtained near the origin by including appropriate weighting functions.

It remains to analyze infinite expansions in the weak convergence sense when the g_ℓ are not in $\mathscr{H}$. As discussed in Section 2 some very delicate mathematical problems appear, having to do with unbounded operators and choices of $\{\alpha_i\}_{i=1}^{\infty}$ that allow for the existence of infinite biorthogonal sets. But for finite expansions we have shown how different sets of φ_i can be generated via appropriate transforms, sets that should be useful depending on the desired application.

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