Variational derivation and extensions of distributed approximating functionals

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Extensions of the "Distributed Approximating Functional" (DAF) approach to approximating functions and their derivatives are given. The method, although inherently approximate, can be made arbitrarily accurate, numerically stable, and computationally efficient by appropriate choice of parameters. It also provides approximate representations of quantum operators which are analytic and which can be made arbitrarily accurate. Differences between the DAFs and more standard basis set approaches are discussed in order to clarify the properties of the DAFs. Some illustrative examples are given.

1. Introduction

Recently, Distributed Approximating Functionals (DAFs) [1–10] have been introduced as a means of fitting or approximating a continuous function from values known only on a discrete set of points, and also with obtaining approximate linear transformations of the (continuous) function, particularly its derivatives to

various orders. An especially useful realization of the DAF approach is that for which there are no "special points" in the approximation, i.e., the order of accuracy of the fit to the function is the same on or between the grid points. Fitting and approximating functions and their linear transformations are old and important topics in numerical analysis which have been approached from many points of view. The history of the subject is far too long to treat here and we refer the reader to some the relevant literature [11–20]. However, it may be helpful to point out a few distinctions between DAFs and some of the more recent computational techniques employed in the literature. For example, a particularly popular approach among quantum scattering theorists is the "Discrete Variable Representation" (DVR) approach first developed by Lill et al. [16]. This is essentially a basis set method founded upon Gaussian quadrature. The wavefunction in the DVR approach is related to the wavefunction in the relevant orthogonal basis by a unitary transformation. The DVR satisfies what is essentially an interpolation formula. The DAF approximation, by contrast, is not exact on the grid points, and the DAF approximation to the wavefunction is not a projection onto a subspace. Another group of popular approaches are those based on collocation techniques [19]. In these, a function satisfying a differential equation is expanded in a basis set. Equations for the expansion coefficients are obtained by projecting the differential operator, applied to the truncated basis expansion of the function, with Dirac delta functions centered on selected discrete points (the number of which equals the number of basis functions employed). This yields a system of linear algebraic equations for the expansion coefficients, which must be solved. DAFs can be employed without necessitating the solution of systems of algebraic equations. A third group of approaches is based on dividing the ranges of the independent variables (in a judicious manner) and introducing polynomials on the various intervals [17]. By contrast, the DAF approach associates a distinct basis set with every point on the axis. Similarly, differences exist between DAFs and a host of other numerical approaches (e.g., wavelets, splines, finite differences, finite boundaries, etc.).

Up to the present time, except for studies that examined DAFs associated with non-Cartesian coordinate systems [6], we have concentrated on DAFs constructed as finite sums of Hermite functions (Hermite polynomials times their generating function [1,2]). In addition, the DAFs have been derived either as solutions of linear algebraic equations determining approximations to a function [1] (for discrete DAFs) in terms of known values on a grid, or (for continuous DAFs) by taking the continuum limit of the discrete DAF [2]. Equivalently, for the continuous DAF case, one can truncate the completeness expansions of the Dirac δ-function [3].

In general, however, it is desirable to obtain more powerful approaches to defining DAFs. In particular, in the case of standard basis set approximations to functions, it is well known that one can derive them by variationally minimizing the absolute square deviation between the exact and basis set expansion functions. This paper derives a more general form of DAF approximation by minimizing a variational functional. The result shows that the linear algebraic equations solved earlier

for Hermite-function based DAFs are, in fact, variationally accurate. Another consequence of this is that standard basis set expansions can be viewed as a special case of DAFs. However, the DAFs are more general, and we explore some of their more useful possibilities. In particular, we obtain a procedure for constructing DAFs based on polynomials orthogonal under summation over a discrete grid. Having obtained a generalized family of DAFs, we then proceed to explore a number of their salient properties. We also explore in more detail the property of approximating functions in a manner which avoids special grid points. This property of the DAFs is referred to as the "well-tempered" property.

This paper is organized as follows: the next section presents the general variational principle satisfied by the DAF representation of a function. Section 3 explores the important special case of an equally spaced grid, and section 4 contains the a formal analysis of the "well tempered" approximation property of those DAFs for which the grid points are not special [10]. Essentially, this analysis shows that such DAF approximations to a function yield equivalent order accuracy for the function both on the grid and also between the grid points. This is a highly desirable property in that it reflects a faithful reproduction of the function and its derivatives. By way on contrast, interpolation formulae give *exact* results for the function on the grid points, but often at the expense of giving poor results between grid points. Also, standard basis set expansions tend to oscillate about the function being expanded. It is easy to see that in both of these cases the representation of the derivatives (and other linear transforms) of the function will not be nearly as accurate as the representation of the function itself. Section 5 explores more general realizations of DAFs, and section 6 discusses the use of DAFs to obtain derivatives and linear transformations of functions. The demonstration of the "well-tempered" property in section 2 for the DAF representation of the function is shown to hold as well for DAF representations of its derivatives. In section 7, we demonstrate the fact that DAFs can be used to construct a sequence of representations that converge asymptotically to the function. In section 8, we obtain a closed form expression for the DAFs created from orthogonal polynomials by two distinct methods. Finally, we summarize our findings in section 9.

2. The DAF variational principle

Consider a function $g(x)$ defined for $-\infty < x < \infty$. (Generalizations to functions defined on line segments and functions in higher dimensions can be carried out readily.) We assume that the values of the function on a discrete set of grid points are known. Our objective is to construct an approximation to the function of the form

$$g_{app}(x) = \sum_{k=-\infty}^{\infty} I(x, x_k) g(x_k) \,, \tag{1}$$

where $g(x_k)$ is the known value of the function on the kth grid point and in general, g_{app} is only approximately equal to $g(x)$, even on the grid points. The quantity $I(x, x_k)$ is an example of an "Approximate Identity Kernel" (AIK). Eq. (1) is a mapping of the vector, whose component elements are the known values on the grid, onto a point x. For each point x, there is one such mapping, specified by a "row" of the AIK. Note that x can assume any value in the interval $(-\infty, \infty)$, so that eq. (1) generates a representation of the continuous function from a discrete set of values. In the most general case, we can construct each row of the AIK $I(x, x_k)$ in any manner we wish, provided that the approximation of eq. (1) is satisfied to sufficient accuracy for whatever particular application is under consideration. That is, a different functional dependence in $I(x, x_k)$ on x_k can be chosen for each value of x.

We wish to construct an approximation $g_x(x')$ to $g(x')$ which, in the neighborhood of x, is a sufficiently good approximation for the purpose at hand. (What is meant by "sufficiently good" will depend on the application.) We proceed by expressing $g_x(x')$ in a conventional basis set expansion using the functions $\{\xi_j\}$ centered on the point x (we therefore write the "point-of-origin", x, as a subscript index rather than as a variable). That is,

$$g_x(x') = \sum_j a_j(x) \xi_j(x' - x) .\qquad(2)$$

In general, we do not require that the set of functions $\{\xi_j\}$ be complete; if the set is not complete, $g_x(x')$ will provide only an approximation to $g(x')$.

Next define $\lambda(\{a_j\}; x)$ to be the weighted absolute square deviation of $g_x(x_k)$ from $g(x_k)$; i.e.,

$$\lambda(\{a_j\}; x) = \sum_k w(x_k - x) \left| g(x_k) - \sum_j a_j(x) \xi_j(x_k - x) \right|^2 ,\qquad(3)$$

where $w(x_k - x)$ is a non-negative weight function centered on the point x. It is convenient to include a volume element in the weight so that

$$\sum_k \rightarrow \int dx_k\qquad(4)$$

in the limit that the grid spacing becomes infinitesimal. For a grid of equally spaced points, the volume element is constant, and for unequally spaced grids it is a function of x. The limit is thus well defined irrespective of whether the grids used to construct the limiting sequence have equal spacing.

To obtain the values of the expansion coefficients, $a_j(x)$, we invoke the variational principle that $\lambda(\{a_j\}; x)$ be a minimum with respect to variation of the a_j coefficients for each value of x. Minimization of $\lambda(\{a_j\}; x)$ by variation of the expansion coefficients leads to the set of linear equations

$$\sum_k w(x_k - x)\xi_j^*(x_k - x)g(x_k) = \sum_n C_{jn}a_n(x)\,, \tag{5}$$

where C_{jn} is the *jn* element of the "overlap matrix" **C** defined by

$$C_{jn}(x) = \sum_k w(x_k - x)\xi_j^*(x_k - x)\xi_n(x_k - x)\,. \tag{6}$$

Eq. (5) is a variational generalization of the algebraic equations developed in the first paper introducing the discretized DAFs [1]. The formal solution of eq. (5) leads to a set of *x*-dependent expansion coefficients. Substituting these coefficients into eq. (2) yields

$$g_x(x') = \sum_k w(x_k - x)\sum_{j,n} C_{jn}^{-1}(x)\xi_n^*(x_k - x)\xi_j(x' - x)g(x_k)\,, \tag{7}$$

where $\mathbf{C}^{-1}$ is the inverse of the "overlap matrix" defined in eq. (6). Eq. (7) is valid provided that $\mathbf{C}^{-1}$ exists, and when compared with eq. (2), yields

$$a_j(x) = \sum_{k,n} w(x_k - x)\xi_n^*(x_k - x)C_{jn}^{-1}(x)g(x_k)\,. \tag{8}$$

Equivalently, comparison with eq. (1) shows that for a basis set expansion the AIK is given by

$$I_x(x', x_k) = \sum_{j,n} w(x_k - x)\xi_n^*(x_k - x)C_{jn}^{-1}(x)\xi_j(x' - x)\,, \tag{9}$$

where the parametric dependence on *x*, the "origin" of the basis functions, has been explicitly noted.

The functional $\lambda(\{a_j\}; x)$ provides a least squares measure of the error in representing $g(x)$ for a given set of a_j coefficients. For any *x*, use of the $a_j(x)$ given by eq. (8) minimizes $\lambda(x)$. Our analysis thus far has yielded a basis set expansion of the function *g* with *x* as the origin. If the basis functions were taken to be independent of *x*, i.e., relative to a single origin, then the standard basis set expansion results. By contrast, the variational principle yields the DAF by supplying a separate basis set for each *x*.

For weight function $w(x_k - x)$, peaked about *x*, the representation supplied by eq. (9) will be most accurate in a region about *x*. Therefore, we define the distributed approximating functional representation, $\tilde{g}$, of the function *g* to be

$$\tilde{g}(x) \equiv g_x(x) = \sum_k I(x, x_k)g(x_k)\,, \tag{10}$$

where

$$\begin{aligned} I(x, x_k) &\equiv \sum_{j,n} w(x_k - x)\xi_j(0)C_{jn}^{-1}(x)\xi_n^*(x_k - x) \\ &= \sum_n b_n(x)w(x_k - x)\xi_n^*(x_k - x)\,. \end{aligned} \tag{11}$$

Here

$$b_n(x) = \sum_j \xi_j(0) C_{jn}^{-1}(x) . \qquad (12)$$

It should be noted that eq. (7) provides an approximation for the original function that is valid only locally in a neighborhood around the origin (the point x in our development). The size of the neighborhood is determined by the width of the weight function. Thus, although eq. (7) yields an approximate value for any x' in the neighborhood of x, only the single value when $x' = x$ is used in the DAF approximation. This completes the construction of the kernel of the DAF approximate identity based on the variational principle. Although the arguments have been developed assuming a discrete grid, they immediately generalize to the case of a continuous grid (i.e., the continuous DAF) by replacing sums by integrals where appropriate. Also, although for clarity of the presentation we have restricted our attention to the one dimensional domain $-\infty < x < \infty$, it is straightforward to generalize the results to other domains or to higher dimensions. Eq. (10) then provides an approximation that is valid everywhere on the line, since the weight function is always centered at the point of approximation.

In the foregoing, the DAF approximation to the function has been motivated qualitatively by a desire to give a "best fit" to a function g, where all points are treated equivalently. Computational difficulty or efficiency were not considerations. At first glance it would seem that constructing the DAF is computationally extremely intensive, since from eq. (11) the overlap matrix **C** must be calculated and inverted for each point x at which the approximate function is evaluated. In fact, a suitable (and straightforward) choice of parameters eliminates the need to deal with the overlap matrix. We now discuss some important particular realizations of the DAFs and their properties.

3. The special case of an equally spaced grid

The DAF representation, with appropriate parameters, provides a "best fit" mapping (in the sense determined by the variational principle at each x point) from a function known only on a discrete set of points to one known to the same level of accuracy at any point on a continuous interval. In the important special case that the grid points have equal spacing, Δ, and the weight function and basis set are functions of $x - x_k$, with the form of the weight and basis functions being the same for each x, the structure of the DAF simplifies significantly and the DAF approximation can be applied in an extremely efficient manner. Specifically, in this case, the overlap matrix of eq. (6) and the b_n-coefficients of eq. (12) are functions only of η, the value of x modulo the grid (i.e., η is the smallest non-negative value of $x - n\Delta$, for integer n). That is,

$$C_{jn}(x) = C_{jn}(\eta) \tag{13}$$

and

$$b_n(x) = b_n(\eta) \,. \tag{14}$$

Thus the AIK is invariant to translations of the x, x_k pair over an integral number of grid spacings. This implies that

$$I(x, x_k) = I(x - x_k) \,, \tag{15}$$

which in turn means that the AIK is a Toeplitz operator. The Toeplitz condition proves very convenient numerically since eq. (10) becomes a convolution. As is well known, the frequency space representation of an operator that is Toeplitz in the coordinate representation will be diagonal. Thus, the DAF is simply a multiplicative factor in frequency space. In addition, it turns out that the frequency space DAF, though analytic, is effectively one over a range of frequency and zero elsewhere. Consequently, such DAFs can be used as window functions and frequency filters and allow "fast transform" [8,22] methods for computing the action of the DAF on a function. In addition, for a proper choice of parameters the need to calculate and invert $\mathbf{C}(\eta)$ can be eliminated, providing even more numerical efficiency.

To illustrate these considerations, consider the case of an equally spaced grid, a Gaussian weight function, and a basis set in eq. (2) consisting of polynomials of degree less than or equal to M. (Because the basis functions corresponding to a Gaussian weight are Hermite polynomials we refer to this case as the Hermite DAF [1–3].) Specifically,

$$w(x) = \exp\left[\frac{-x^2}{2\sigma^2}\right] \,, \tag{16}$$

where σ is a parameter that fixes the Gaussian width. To motivate our discussion of the next section, we remark that such a DAF can be chosen to deliver an approximation with the same level of accuracy that the function can be represented by using a polynomial of degree $M + 1$, under the Gaussian weight.

Because Hermite polynomials are orthogonal under integration for this weight function, it is convenient to define

$$\xi_n(x) = H_n\left(\frac{x}{\sqrt{2}\sigma}\right) \tag{17}$$

in eq. (2), in which case

$$C_{jn}(x) \equiv C_{jn}(\eta) = \sum_k e^{-(x-x_k)^2/2\sigma^2} H_j\left(\frac{x - x_k}{\sqrt{2}\sigma}\right) H_n\left(\frac{x - x_k}{\sqrt{2}\sigma}\right) \frac{\Delta}{\sqrt{2\pi\sigma^2}} \,. \tag{18}$$

This coefficient, $C_{jn}(\eta)$, can be computed, using the Euler–MacLaurin approximation [11], as the overlap integral

$$S_{jn} = \int e^{-(x-x')^2/2\sigma^2} H_j\left(\frac{x-x'}{\sqrt{2}\sigma}\right) H_n\left(\frac{x-'}{\sqrt{2}\sigma}\right) \frac{dx'}{\sqrt{2\pi\sigma^2}} \tag{19}$$

$$= A_j \delta_{jn}, \tag{20}$$

where for the Hermite polynomials

$$A_j = \sqrt{\pi} 2^j j! . \tag{21}$$

For suitable values of j, n and σ/Δ, for which the Euler–MacLaurin approximation is sufficiently accurate, the discrete sum in eq. (18) is essentially diagonal and the $b_n(x)$ coefficients will be constants independent of x. Fig. 1 shows the behavior of an even and an odd b-coefficient (b_0 and b_1 respectively) as a function of x. The plot illustrates that the $b_n(x)$, $n = 0, 1$ are periodic and hence $b_n(x) = b_n(\eta)$ (i.e., the plot between $x = 0$ and $x = 1$ can be considered the graph of $b_n(\eta)$). A particularly useful
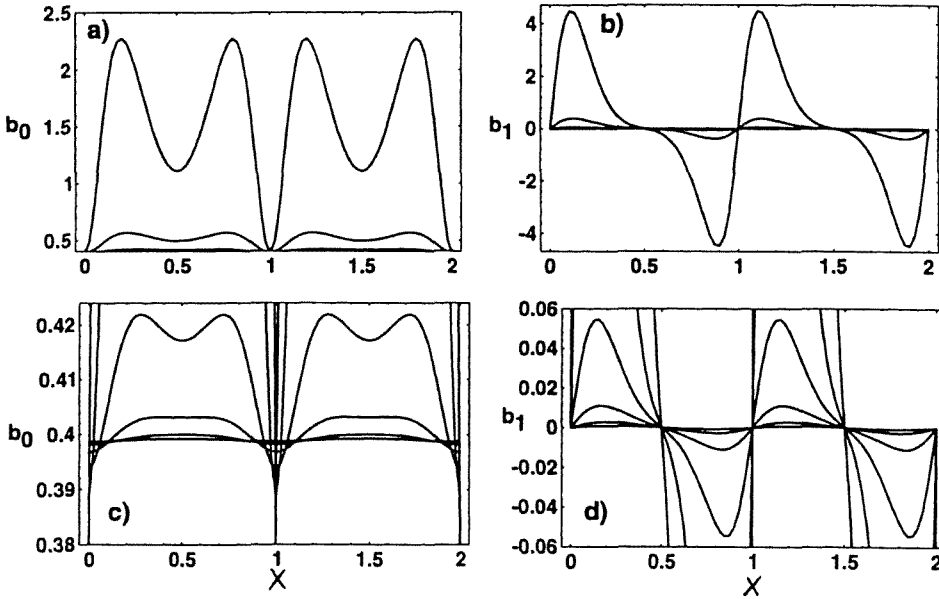

Fig. 1. Demonstration of periodicity and convergence of $b_n(x)$ (plotted in units of σ, see eq. (22)) for the distributed approximating functional based on Hermite polynomials. Fig. 1(a) shows $b_0(x)$ for several values of σ/Δ, while (b) shows $b_1(x)$ for the same values of σ/Δ. Fig. 1(c) is a "blow-up" of (a) demonstrating that as σ/Δ increases b_0 becomes essentially constant and converges to the value $(2\pi)^{-1/2} \approx 0.398$. Similarly, Fig. 1(d) is a blow-up of Fig. 1(b) and shows b_1 becoming independent of x and converging to 0. All plots are for two periods of x, explicitly demonstrating the periodicity of the $b_n(x)$. For this case a value of $M = 6$ was used, with $\sigma/\Delta = 0.55, 0.6, 0.65, 0.7, 0.75$ and 0.8. The larger σ/Δ the closer b_0 comes to convergence.

form of DAF is that for which the $b_n(x)$ is independent of the point x (the origin of the basis $\{\xi_n^*(x_k - x)\}$). The figure shows the onset of this behavior as the value of σ/Δ is increased (see especially the blow-ups in panels c and d). Note that the constant value limit of b_1 (and for any odd n-index) is zero.

In Fig. 2 the behavior of the b-coefficients as a function of σ/Δ is shown for a set of b_n with fixed M. As σ/Δ approaches a certain (M dependent) value from below, the b_n become essentially constant, with the odd coefficients vanishing (due to the symmetry of the weight function) and the even coefficients are given by

$$b_n = \frac{1}{\sqrt{2\pi\sigma^2}} \left(-\frac{1}{4}\right)^n \frac{1}{n!} \,. \tag{22}$$

The onset of this limiting behavior occurs when it is a valid approximation to replace the sum by an integral in eq. (6). As noted above, in the Euler–MacLaurin approximation the overlap matrix and its inverse are diagonal as a consequence of the orthogonality of the Hermite polynomials on integration under the Gaussian weight. The applicability of this approximation is determined by M, a measure of the highest degree of the polynomials, and σ/Δ, the ratio of the width of the Gaussian to the grid spacing. The conditions under which the approximation is valid have been explored previously and will not be repeated here [10]. Suffice it to say that this approximation holds under such general conditions that it is extremely useful for numerical applications.

Moreover, the validity of this approximation is not limited to Hermite DAFs but, in our experience, holds quite generally (under appropriate conditions such as the scale of the DAF relative to the grid size) for any underlying basis set. We call
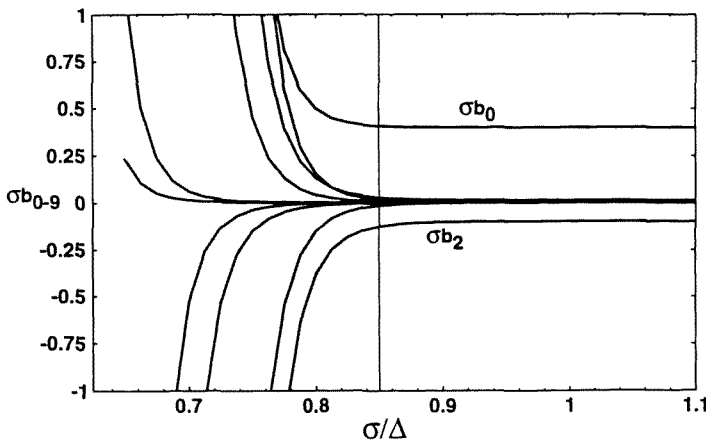

Fig. 2. Onset of constancy in the b_n (in units of σ) as a function of σ/Δ. Shown are b_{0-9} at $\eta = 0.625$ and $M = 10$ for the Hermite Polynomial DAFs for a range of σ/Δ. All of the coefficients become essentially constant at $\sigma/\Delta = 0.85$ (vertical line) with the odd coefficients going to zero and the even ones to values given by eq. (22).

such DAFs "well-tempered". Well-tempered DAFs have the interesting feature that the approximation they generate is of the same order of accuracy on and off the grid points. In an appropriate limit (see below), DAFs based on various systems of orthogonal polynomials are qualitatively similar. This is illustrated in Fig. 3 for DAFs based on the Hermite, Legendre, and one particular Jacobi polynomial. In particular, all such DAFs are sharply peaked at the origin, with decaying oscillations (in the coordinate representation). The weight function for the Hermite DAF and all its derivatives are everywhere continuous on the infinite interval
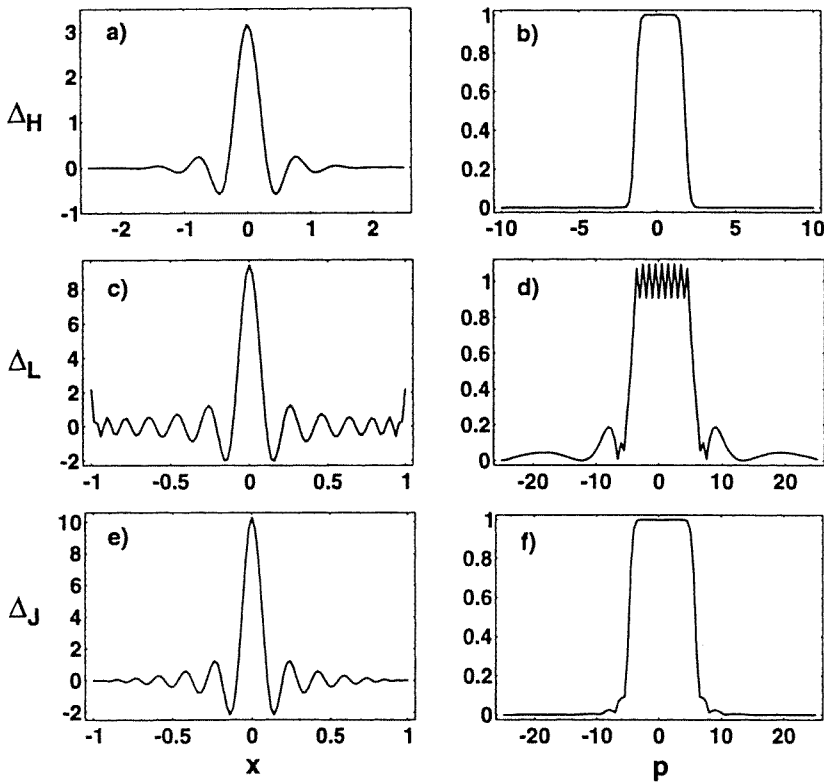

Fig. 3. Comparison of distributed approximating functionals based on various sets of orthogonal polynomials in both coordinate and momentum space. Figs. 3(a), (c) and (e) show the coordinate space representation of DAFs based on sets of Hermite Polynomials, Δ_H, Legendre Polynomials, Δ_L, and Jacobi polynomials, Δ_J. For the Hermite polynomial DAF (Figs. 3(a) and (c)) $\sigma = 0.3$, while for the Legendre polynomial DAF and the Jacobi polynomial DAF $\sigma = 1$. The Jacobi polynomials used are the $J(x, 3, 3)$, meaning the weight function is $w(x) = (1 - x)^3(1 + x)^3$. In all three cases the odd polynomials vanish, and even polynomials to degree 14 (i.e., $M = 28$) were used in calculating the DAF. For both the Legendre and Jacobi polynomial systems the DAF has compact support on the interval $[-1, 1]$, and in addition the Jacobi polynomial DAF (and its first two derivatives) vanish on the boundary.

$(-\infty < x < \infty)$. However, only the Jacobi DAF weight function and its first two derivatives are everywhere continuous on the infinite interval. In the Legendre case, even the Legendre weight function is not everywhere continuous on the infinite interval. This accounts for the differences in the structures of these DAFs in the momentum representation, and for the particular utility of the Hermite DAF.

4. The "well-tempered" approximation

For a set of orthogonal basis functions, normalized under a weight w, the standard basis set expansion can be written as

$$g(x) = \sum_{n=0}^{M} \int dx' \, w(x')\xi_n(x')g(x')\xi_n(x) . \tag{23}$$

The residual, or error, for this formula is a vector that lies in the subspace spanned by the ξ_n for $n = M + 1$ to ∞. That is, it lies in the space complementary to the subspace spanned by the basis functions ξ_n, $n = 0$ to M. For example, if g is a polynomial of degree $M + 1$ then the residual is proportional to $\xi_{M+1}(x)$; if g is a polynomial of order $M + 2$ then the residual is a linear combination of $\xi_{M+1}(x)$ and $\xi_{M+2}(x)$, etc. Typically, such expressions yield an approximation which tends to oscillate about the exact function.

Comparing the above to the continuous DAF representation (using the same orthogonal polynomials) we find that when $C_{jn}^{-1} \approx \delta_{jn}$ holds, eq. (9) reduces to

$$I_M(x, x') = \sum_{j=0}^{M} w(x' - x)\xi_j(0)\xi_j^*(x' - x) , \tag{24}$$

where the subscript M indicates the highest degree polynomial in the basis set. Straightforward calculation demonstrates that the continuous DAF approximation

$$\tilde{g}(x) \equiv \int dx' I_M(x, x')g(x') \tag{25}$$

is exact for a polynomial of degree M. If the construction is done with the origin placed on a zero of ξ_{M+1}, then from eq. (23)

$$I_M(x, x') = I_{M+1}(x, x') \tag{26}$$

and eq. (25) is exact for a polynomial of degree $M + 1$. In general, if g is a polynomial of degree $N \geqslant M + 2$ it can be written in the form

$$g(x') = \sum_{k=0}^{N} d_{N-k}(x)\xi_k(x' - x) = \sum_{j=0}^{N} d_j(x)\xi_{N-j}(x - x') , \tag{27}$$

where $d_j(x)$ is a polynomial of degree j. It then follows that

$$g(x) = \tilde{g}(x) + \sum_{j=0}^{N-M-2} d_j(x)\xi_{N-j}(0). \qquad (28)$$

Thus, if g is a polynomial of order $M + 2$, the residual is constant; if g is a polynomial of order $M + 3$ the residual is linear, etc. Note further that the residual is not constrained to lie in the complementary subspace (which in this case consists of polynomials of degree $N \geqslant M + 2$). The low polynomic degree of the residual allows the DAF approximation to follow the original function with fewer oscillations about the exact value than is generally the case for a basis set expansion. In fact, qualitatively the residual of a function often tends to look roughly like the function itself, although depending on the level of accuracy characterizing the DAF-class of functions, it is orders of magnitude smaller. This behavior is illustrated for some example functions in Fig. 4.

Eq. (28) is valid also if the polynomials are orthogonal under summation; but in the general case the quantities $\xi_{N-j}(0)$ are also parametrically functions of x and so it is difficult to draw rigorous conclusions about the x-dependence of the residual. However, in the well-tempered approximation, the basis set is nearly independent of any parametric dependence on x and the analysis of the residual carries through as for the continuous DAF case.

The well-tempered nature of the DAF representation of a function can be summarized then, as follows: for a projection operator $\mathbf{P}$ of a P-invariant subspace and its orthogonal complement, $\mathbf{Q} \equiv \mathbf{1} - \mathbf{P}$, we have that $\mathbf{P}^2 = \mathbf{P}$ and $\mathbf{PQ} = 0$. The AIK for an ordinary basis set expansion is such a projection operator. In contrast, if $\mathbf{I}$ is a general AIK for the P-invariant subspace, then we have that $\mathbf{IP} = \mathbf{P}$ but $\mathbf{IQ}$ is unspecified. As a result the residual of a function g, defined to be $(\mathbf{1} - \mathbf{I})g = (\mathbf{Q} - \mathbf{IQ})g$, is not constrained to lie in the Q-invariant subspace. For the example just described, if g is a polynomial of degree N, the residual will be a polynomial of degree $N - M - 2$.

We next consider the well-tempered property of DAFs in the frequency (or Fourier transform) space. It has been established earlier that for the DAF of section 3 (i.e., uniform grid, single set of basis functions) $I(x, x') = I(x - x')$, and such transformations are always diagonal in Fourier space. Thus, in the continuous DAF case

$$\tilde{f}(k) = \mathcal{I}(k)f(k), \qquad (29)$$

where $f(k)$ is the Fourier transform of the exact function $g(x)$, $\tilde{f}(k)$ is the Fourier transform of $\tilde{g}(x)$, the DAF approximation to $g(x)$

$$\tilde{g}(x) = \int dx' \, I(x - x')g(x'), \qquad (30)$$

and $\mathcal{I}(k)$ is the Fourier transform of the continuous DAF kernel, $I(x - x')$. Now,
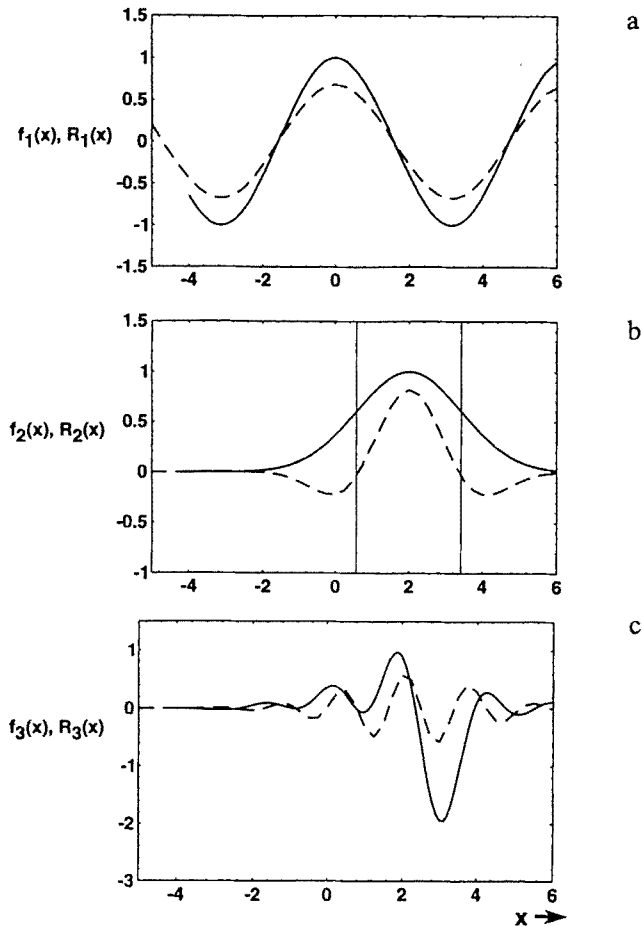
Fig. 4. Demonstration that the "residual" of a DAF fit to a function resembles the function itself for three separate cases. Shown are the original function (solid line) and the residual $R(x) = f(x) - \bar{f}(x)$ (dashed line) for (a) $f_1(x) = \sin(x)$, (b) $f_2(x) = e^{-(x-2)^2/4}$ and (c) $f_3(x) = (0.2x^3 - x^2 + 1)\cos(2x)e^{-(x-2)^2/4}$. A discrete DAF transformation was carried out on each function using Hermite polynomial DAFs with $M = 8$, $\sigma/\Delta = 1.4043$ (this puts the DAF in the "well-tempered" regime) and a grid spacing of $\Delta = 0.25$. For purposes of comparison, the residual has been scaled to have roughly the same range as the original function, with the scale factors used being (a) 3×10^7, (b) 5×10^7 and (c) 2×10^5. Fig. 4(a) demonstrates that for a sinusoidal function the residual is formally proportional to the original function [eq. (36)]. Similarly, in Fig. 4(b) the vertical lines pass through the inflection points of the Gaussian, demonstrating that the residual is indeed nearly zero near an inflection point, as per eq. (35).

if the weight function is symmetric, the kernel has as its natural variable $(x - x')^2$, and its Fourier transform will correspondingly be a function of k^2. We therefore can carry out a Taylor expansion of $\mathcal{I}(k)$ about some particular k_0^2, viz.,

$$\tilde{f}(k) = \left[D(k_0^2) + (k^2 - k_0^2)D'(k_0^2) + \frac{(k^2 - k_0^2)^2}{2!} D''(k_0^2) + \ldots \right] f(k), \qquad (31)$$

where $D(k^2) \equiv \mathcal{I}(k)$. $D'(k_0^2)$ is given by

$$D'(k_0^2) = \left(\frac{d^2 D}{dk^2} \right)_{k^2 = k_0^2} \qquad (32)$$

etc. If we carry out the inverse Fourier transform and note, e.g., that

$$-\frac{d^2 g}{dx^2} = \frac{1}{2\pi} \int dk \, e^{ikx} D(k^2) k^2 f(k), \qquad (33)$$

we conclude that

$$\tilde{g}(x) = D(k_0^2)g(x) - D'(k_0^2)\left[k_0^2 g(x) + \frac{d^2 g}{dx^2} \right] + \ldots . \qquad (34)$$

We are free to choose k_0^2 so as to make the second term small, in which case the residual R is given by

$$R \approx [1 - D(k_0^2)]g(x) \qquad (35)$$

and the error is roughly proportional to the function being approximated. This analysis also suggests that the residual approaches a minimum near an inflection point (see Fig. 4). Of special interest is the case where $g(x)$ is sinusoidal. Then, since all even derivatives of $g(x)$ are proportional to $g(x)$, the Taylor series of eq. (31) can be formally summed to obtain

$$R = \text{constant} \times g(x) \qquad (36)$$

so that the residual is rigorously proportional to the function being fitted. Thus, if $g(x)$ is a polynomial then the residual is a polynomial of lower degree. If the function is sinusoidal the residual is strictly proportional to the function. In either situation, the DAF approximation, $\tilde{g}(x)$, tends to have a much less serpentine behavior than the corresponding basis set expansion and the residual roughly resembles the function. This leads to accurate representations of derivatives (see Fig. 5 and discussion below) as well as the original function on and off the grid, as we later discuss.

5. More general DAFs

There are several ways the results of the previous sections can be generalized. One important case is when the grid spacing is unequal. In this situation, if one wishes the variational expression in eq. (3) to be a quadrature approximation to the integral, it is necessary to include an appropriate volume element in the weight
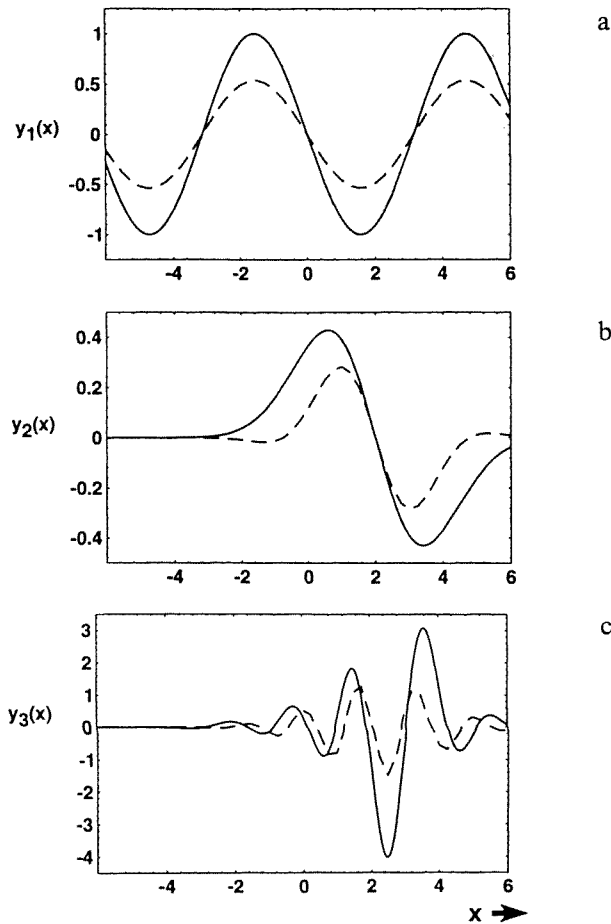
Fig. 5. Generation of derivatives via the DAF transformation: Same as for Fig. 4, but now the DAF representation is used to generate $y_i = f'_i(x)$ for the three functions of Fig. 4 via use of eq. (49) in the well-tempered limit. Shown are the exact derivative (solid line) and the residual of the derivative $R^d_i(x) = y_i(x) - \bar{f}'_i(x)$ (dashed line). Again the residual has been scaled to have roughly the same range as the original function, with the scale factors being (a) 10^6 (b) 10^6 and (c) 2×10^4. All other parameters are as in Fig. 4.

function, thus ensuring that the DAF has a well-defined limiting value no matter how the limit is taken. For example, if there exists a monotonic function $\zeta(x)$ with the property that $\zeta(x_j) = j$, then the ζ-space grid is uniform. In order for the sum of eq. (3) to provide a quadrature approximation the summand must contain the Jacobian $|\partial x / \partial \zeta|$ as a factor. That is, the appropriate weight in the summation is $w(x_j - x) |\partial x / \partial \zeta|_j$, where w is the desired weight function in the continuum limit. Alternatively, eq. (1) can be written in the form

$$g_{app}(x) = \sum_{-\infty}^{\infty} I(x, x_k) \left[\left| \frac{\partial x}{\partial \zeta} \right| g \right]_{x_k}. \tag{37}$$

As a trivial example, in the case of an equal spaced grid $\zeta = x/\Delta$ where Δ is the grid spacing the appropriate weight is thus $w(x_j - x)\Delta$. However, in this special case the Jacobian is constant and its inclusion does not affect the minimization of $\lambda(\{a_j\}; x)$ in eq. (3).

The expression for the DAF transform of eq. (11) is somewhat simplified if the initial basis set is orthogonal under summation; i.e., if the **C** matrix defined by eq. (6) is diagonal. This circumstance makes the inversion of the **C** matrix trivial. In the most general case this requires a different set of orthogonal functions at each x-point; however, the situation is somewhat simpler if the grid is equal spaced, for then one needs only a different set of functions for each η-point (i.e., each x-point modulo the grid).

If the expansion functions are orthogonal polynomials, they can be generated efficiently using the well known fact that orthogonal polynomials obey a three-term recursion relation [11]. To implement the construction we first define the inner product

$$A_{jn}^i(x) = \sum_k w(x_k - x) P_j(x_k - x; x)(x_k - x)^i P_n(x_k - x; x), \tag{38}$$

where $P_j(x_k - x; x)$ is a polynomial of degree j in $x_k - x$ with coefficients that depend parametrically on x. The condition of orthonormality is

$$A_{jn}^0 = \delta_{jn}. \tag{39}$$

To establish the three-term recursion relation, we first note that

$$y P_n(y; x) = \sum_{j=0}^{n+1} A_{jn}^1(x) P_j(y; x), \tag{40}$$

which follows directly from eq. (38). The orthogonality of the polynomials also establishes that A_{jn}^1 is non-zero only if j is $n+1$, or $n-1$, which leads to the recursion relation

$$y P_n(y; x) = A_{n+1,n}^1(x) P_{n+1}(y; x) + A_{nn}^1(x) P_n(y; x) + A_{n-1,n}^1(x) P_{n-1}(y; x). \tag{41}$$

If $P_n(y; x)$ and $P_{n-1}(y; x)$ are known, then $A_{nn}^1(x)$ and $A_{n-1,n}^1(x)$ can be calculated directly from eq. (38). To determine $A_{n+1,n}^1(x)$ we calculate the inner product of each side of eq. (40) with itself to obtain

$$[A_{n+1,n}^1(x)]^2 = A_{nn}^2(x) - [A_{nn}^1(x)]^2 - [A_{n-1,n}^1(x)]^2 \tag{42}$$

from which $A_{n+1,n}^1(x)$ can be obtained to within an arbitrary sign. To begin the recursion we have

$$P_{-1}(y; x) = 0 \tag{43}$$

and

$$P_0(y; x) = \left[\sum_k w(x_k - x) \right]^{-1/2}, \tag{44}$$

which completes the algorithm for the polynomial construction.

As we have stressed, it is not required that every x-point in eq. (2) have the same set of basis functions. To illustrate this, we examine two other ways to construct DAFs. The first is to allow the basis set members in eq. (2), or the weight function (or both) to vary continuously as a function of x. A convenient way to express this is to write in place of eq. (2) the new expression for $g_x(x')$,

$$g_x(x') = \sum_k I_x(x', x_k) g(x_k), \tag{45}$$

where $I_x(x', x_k)$ is the DAF AIK with parameters fixed at the point x. We then define a new DAF approximation $\tilde{g}(x)$ by

$$\tilde{g}(x) \equiv g_x(x) = \sum_k I_x(x, x_k) g(x_k). \tag{46}$$

If $I_x(x', x_k)$ in eq. (10) is derived from a basis set expansion, then eq. (45) can also be so derived. However, the particular form of eq. (45) is convenient for approximating derivatives and other linear transformations of $g(x)$ as is discussed below.

Finally, we note that if the weight function and basis set vary in just such a way that

$$w(x'' - x; x) = \bar{w}(x'') \tag{47}$$

and

$$\xi_j(x'' - x; x) = \bar{\xi}_j(x''), \tag{48}$$

where $\bar{w}$ and $\bar{\xi}$ are functions independent of x, then eq. (7) reduces to a simple basis set expansion for all x. From this observation it immediately follows that ordinary basis set expansions can be viewed as a special case of DAFs.

6. The DAF representation of derivatives

Although methods for generating a function everywhere in terms of known values on a discrete grid are of general interest, many applications also require the method to yield accurate linear transformations of functions. The most important of such transformations are derivatives, and their occurrence in the mathematical description of interesting phenomena is ubiquitous. In fact, we have already found

DAFs to be a powerful computational tool for a variety of problems, particularly in the area of quantum dynamics (i.e., solving the Schrödinger equation for systems involving several degrees of freedom). Such problems require accurate representation of the second partial derivatives of the wavefunction (the action of the quantum mechanical kinetic energy operator) [8,22,24] and of the time-evolution propagator, which involves the exponential of the kinetic energy operator [1,2]. Other transformations include integral transforms, such as the Fourier integral. The DAF representation of a function has especially attractive features for dealing with linear transformations of functions, and we discuss these properties in this section.

There are several different ways that we can approximate the derivative of a function, $g(x)$, from its DAF representation. One is to differentiate eq. (8) directly to obtain

$$\frac{dg_x(x)}{dx} = \sum_k \left(\frac{\partial}{\partial x} I(x, x_k) \right) g(x_k) , \tag{49}$$

(assuming, of course, that $I(x, x_k)$ is differentiable, which in the most general construction it need not be). In the special case of the continuous DAF where the AIK is Toeplitz, eq. (49) becomes

$$\frac{dg_x(x)}{dx} = \int \left(\frac{\partial}{\partial x} I(x - x') \right) g(x') dx' \tag{50}$$

$$= \int I(x - x') \frac{dg(x')}{dx'} dx' , \tag{51}$$

where to achieve the final result we have integrated by parts and assumed that the "surface term" vanishes. Thus, for this case, the derivative approximation of eq. (49) satisfies the relation that the derivative of the DAF approximation to a function is equal to the DAF approximation of the derivative.

A different approximation to the derivative is

$$\lim_{x' \to x} \frac{\partial g_x(x')}{\partial x'} = \sum_k w(x_k - x) \sum_{j,n} \xi'_j(0) C_{jn}^{-1} \xi_n^*(x_k - x) . \tag{52}$$

The difference between the approximations of eq. (49) and eq. (52) for the derivative is that in the first instance all of the x dependence of the DAF is differentiated and in the second only part of the x dependence is differentiated. To the extent the two forms are approximately equal it must be true that

$$\lim_{x' \to x} \frac{\partial g_x(x')}{\partial x} = 0 . \tag{53}$$

This will be true if $g_x(x')$ provides a good approximation to $g(x')$ when x' is in the neighborhood of x. Since $\bar{g}(x')$ is an approximation to $g(x')$ everywhere on the line, and $g_x(x')$ is only an approximation in a neighborhood of x, we expect eq. (49), in

general, to deliver a better quality approximation for the derivative than eq. (52). This expectation has been borne out in numerical calculations [23]. Finally, if our approximation for $g(x)$ is obtained from eqs. (45) and (46), we can write

$$\lim_{x' \to x} \frac{\partial g_x(x')}{\partial x'} = \lim_{x' \to x} \frac{\partial}{\partial x'} \sum_k I_x(x', x_k) g(x_k) , \tag{54}$$

which we expect to be a good approximation to the derivative since $g_x(x')$ of eq. (45) provides a well-tempered approximation to $g(x')$ for every x. The advantage of this formula is illustrated by the family of well-tempered DAFs based on Hermite polynomials, all of which have a very simple closed form expression for the first (and higher) derivatives, obtained using eq. (49) [24]. Fig. 5 demonstrates the accuracy of the DAF derivative operator (both on and off the grid points) for some sample functions. In the well-tempered limit the DAF derivative operator is also Toeplitz and can be calculated by fast transform (i.e., an $O(N)$ process). In addition, by taking advantage of eq. (54) it is possible to retain the simple closed form expression for the derivative while arbitrarily varying the particular choice of Hermite DAF for different values of x.

The various methods just presented for obtaining approximations to the first derivative of $g(x)$ can be extended easily to higher derivatives. Again, those approximations based on derivatives of global approximations to the original function are the ones we expect to be most accurate. The methods that we have outlined can also be used to express approximations for other linear transforms of the original function. In general, we can expect the most accurate of these to derive from global approximations to $g(x)$. An important example is the action on an L^2 wavepacket of the quantum "free propagator", $e^{-i\hat{H}_F t/\hbar}$ where $\hat{H}_F = -(1/2)\partial^2/\partial x^2$, which involves derivatives to all orders and can be expressed analytically in closed form for Hermite polynomial DAFs [1,2]. As for integral transforms, the well-tempered DAFs associated with translational invariance result in the possibility of "fast DAF convolution". Essentially the *fast DAF convolution* allows one to take advantage of the "banded" nature of the DAF representation of a function and its derivatives. The result is a convolution algorithm which requires fewer CPU operations (and has lower communication costs) than *fast Fourier transforms*. These details have been discussed elsewhere [7,8,22], and we will not elaborate further on them here.

7. The asymptotic nature of the DAF approximation

For the case of the continuous DAF it is possible to demonstrate that the DAF representation converges uniformly to the exact function. This is true only for continuous DAFs since it is impossible, even in principle, to reconstruct a general function exactly only from its values on a discrete grid. The strategy is to construct an

approximate identity which is exact for some subspace $\mathcal{V}_M$ of the function space, $\mathcal{V}$, of interest. We then consider a sequence of nested subspaces, indexed by M, satisfying the condition

$$\lim_{M \to \infty} \mathcal{V}_M = \mathcal{V}. \tag{55}$$

For any function $g \in \mathcal{V}$ this construction provides a sequence of functions that converges uniformly to g in the limit as $M \to \infty$.

Recall that a basis set expansion of g provides a best fit in a least squares sense for the basis set $\xi_i(x' - x)$. It immediately follows that $g(x)$ is represented exactly if it can be written as a finite linear combination of the basis functions ξ_i. Now suppose that

$$g(x') = \sum_{i=0}^{M} \beta_i \xi_i(x'), \tag{56}$$

where the set of functions ξ_i are a basis for a representation (not necessarily irreducible) of the translation group. Then for any x there exists a set of coefficients $\gamma_{ij}(x)$ satisfying

$$\xi_i(x') = \sum_{j=0}^{M} \gamma_{ij}(x) \xi_j(x' - x), \tag{57}$$

from which it follows that $g(x')$ can be expressed exactly as a linear combination of the $\xi_i(x' - x)$. It further follows that the DAF provides an exact identity transformation for the functions spanned by the ξ_i. By establishing a sequence of such bases $\{\xi_i\}_M$, where in the limit $M \to \infty$ the set of basis functions is complete on $\mathcal{V}$, our objective is obtained.

To illustrate, let $\mathcal{V}$ be the space of analytic functions in 1-D and $\mathcal{V}_M$ be the subspace of all polynomials of degree less than or equal to M. Such polynomials form a basis for a representation of the translation group and hence a DAF based on these polynomials provides an exact identity transformation for all polynomials of degree $\leqslant M$. Furthermore, as $M \to \infty$ we have $\mathcal{V}_M \to \mathcal{V}$ and so the DAF approximations to any function form a sequence of functions converging uniformly to the original function.

Another basis for a representation of the translation group is the set of functions obtained by multiplying all polynomials of degree $\leqslant M$ be e^{ikx} for fixed k. This basis also becomes complete as $M \to \infty$. More general bases involving more than one value of k are also possible.

8. A closed form expression for the DAF kernel

For well-tempered DAFs on an equal spaced grid, the b_n can be treated as constants, and we have that

$$I(x, x') = \sum_{n=0}^{M} b_n w(x' - x) \xi_n(x' - x) . \tag{58}$$

This sum can be performed in closed form provided the ξ_n belong to a system of orthogonal polynomials, as we will demonstrate in two ways. First, we define the polynomial $p_M(x' - x)$ by

$$p_M(x' - x) = \sum_{n=0}^{M} b_n \xi_n(x' - x) . \tag{59}$$

If $g(x)$ is also a polynomial of degree M then

$$g(x) = \int dx' w(x' - x) p_M(x' - x) g(x') \tag{60}$$

is exact. However, this equation is also exact for a polynomial of degree $M + 1$ if the weight function is centered so that its origin (which, in absolute terms, is at the point x) is chosen to be a zero of ξ_{M+1} (i.e., $\xi_{M+1}(0) = 0$), because in the expression for $g_x(x)$ that derives from eq. (2) by setting $x' = x$, ξ_{M+1} makes no contribution.

If we take $g(x)$ to be of degree $M + 1$, then the product $p_M(x' - x)g(x')$ is a polynomial of degree $2M + 1$. In this case the integration in eq. (60) can be performed *exactly* by a Gaussian quadrature scheme based on the zeros of ξ_{M+1}. That is [11],

$$g(x) = \rho_0 p_M(0) g(x) + \sum_{k \neq 0}^{M+1} \rho_k p_M(x_k - x) g(x_k) , \tag{61}$$

where the $x_k - x$ are the zeros of ξ_{M+1} (with "0" as the index of the origin) and ρ_k is the corresponding Gaussian quadrature weight. It is seen that there are $M + 1$ values of the function $g(x_k)$ appearing on the right hand side of this equation. These can be chosen arbitrarily since an $M + 1$ degree polynomial can always be found that passes through any such set of points. Since eq. (61) holds exactly for all such polynomials, we conclude that

$$\rho_0 p_M(0) = 1 \tag{62}$$

and

$$p_M(x_k - x) = 0 \tag{63}$$

for all $k \neq 0$. We now have M zeros of the Mth degree polynomial p_M and we also know its value at one other point; this is sufficient to determine it uniquely. Thus, we find

$$p_M(x' - x) = \sum_{n=0}^{M} b_n \xi_n(x' - x) = \frac{1}{\rho_0 \xi'_{M+1}(0)} \frac{\xi_{M+1}(x' - x)}{x' - x} , \tag{64}$$

which provides a closed form expression for the DAF in terms of the original polynomial basis set.

The second method for calculating a closed form expression for the sum is somewhat more general in that it does not require one to be in the well-tempered regime. Making use of eq. (41) we can write

$$(y - z)P_j(y; \eta)P_j(z; \eta) = A^1_{j+1,j}(\eta)[P_{j+1}(y; \eta)P_j(z; \eta) - P_{j+1}(z; \eta)P_j(y; \eta)] \qquad (65)$$

$$+ A^1_{j-1,j}(\eta)[P_{j-1}(y; \eta)P_j(z; \eta) - P_{j-1}(z; \eta)P_j(y; \eta)] . \qquad (66)$$

Summing both sides of this equation over $j = [0, n]$ and cancelling terms on the right hand side we obtain

$$\sum_{j=0}^{n} P_j(y; \eta)P_j(z; \eta) = \left(\frac{1}{y - z}\right) A^1_{n+1,n}(\eta)[P_{n+1}(y; \eta)P_n(z; \eta) - P_{n+1}(z; \eta)P_n(y; \eta)] ,$$

$$(67)$$

which is a form of the well known Christoffel-Darboux identity [25]. Substituting this result into eq. (58) yields

$$I(x, x_k) = w(x_k - x) \sum_{j=0}^{n} P_j(0; \eta)P_j(x_k - x; \eta) \qquad (68)$$

$$= \frac{w(x_k - x)}{x_k - x} A^1_{n+1,n}(\eta)[P_{n+1}(x_k - x; \eta)P_n(0; \eta) - P_{n+1}(0; \eta)P_n(x_k - x; \eta)] .$$

$$(69)$$

The polynomials P_j are easily calculated by recursion, as previously discussed.

9. Summary

This paper has presented a general formulation of the distributed approximating functional technique for numerical analysis. Earlier studies of DAFs focussed, for the most part, on well tempered DAFs and in particular on those constructed as finite superpositions of Hermite functions (products of Hermite polynomials and their generating function). Herein it has been shown (a) that the DAF approximation to a function may be obtained from a variational principle and (b) that DAFs can be constructed as a finite superposition of *any* convenient set of expansion functions (and corresponding weight function) and that the case of orthogonal polynomials can be employed to particular advantage. It was also demonstrated that DAFs contain, as a special case, the standard basis set expansion of a function, but that in its most general form the DAF representation possesses much greater flexibility and robustness.

We discussed the construction of DAF representations of linear transformations

of functions, with particular attention being paid to derivatives. Since ordinary and partial differential equations are the foundations of modern descriptions of a whole host of phenomena (ranging from physical and chemical processes to economics, sociology, etc.), the assurance that DAFs perform well for derivative transformations is extremely important. It was shown that although DAFs inherently deliver *approximations* to functions and their linear transforms, in fact, arbitrary accuracy can be attained. Thus, the formalism is, in principle, sufficiently robust to treat such problems to any level of description.

We also have derived analytical, closed form expressions for DAFs by two summation techniques. These expressions are expected to be quite useful not only in applications, but especially in formal analyses of DAF theory.

Finally, we have carried out a more detailed formal analysis of what is one of the most intriguing and basic of the DAF properties, viz., the well tempered nature of DAF approximations to functions and their linear transforms. Two distinct approaches (appropriate to exact DAF descriptions of either polynomial or sinusoidal functions) were given. The remarkable result is that in contrast to standard basis set methods (which involve projections of the relevant functions onto orthogonal subspaces), the DAF involves an AIK and the residual is such that the error "follows" the function being approximated. This behavior underlies the property that the DAFs provide an accurate description of the function *and* its derivatives, and also reflects the fact that DAFs were developed so that there would be no "special points".

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