Interpolating distributed approximating functionals

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In this paper, we present a class of distributed approximating functionals (DAF's) for solving various problems in the sciences and engineering. Previous DAF's were specifically constructed to avoid interpolation in order to achieve the ''well-tempered'' limit, in which the same order error is made both on and off the grid points. These DAF's are constructed by combining the DAF concept with various interpolation schemes. The approach then becomes the same as the ''moving least squares'' method, but the specific ''interpolating DAF's'' obtained are new, to our knowledge. These interpolating DAF's are illustrated using Lagrange interpolation (the ''LDAF'') and a Gaussian weight function. Four numerical tests are used to illustrate the LDAF's: differentiation on and off a grid, fitting a function off a grid, time-dependent quantum dynamical evolution, and solving nonlinear Burgers' equation. [S1063-651X(98)10204-0]

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I. INTRODUCTION

Recently we have conducted a series of investigations exploring the use of distributed approximation functionals (DAF's) for solving partial differential equations (PDE's). In the course of these studies we developed a class of DAF's which are of comparable effectiveness to other DAF's in solving PDE's, but that have interesting features. These DAF's also establish a connection with the ''moving least squares'' approach to interpolation [1–3]. The purpose of this paper is to discuss the theoretical underpinnings of these DAF's, and to demonstrate their efficacy.

The present work is motivated by our investigations of solution methods for partial differential equations describing the time behavior of various systems. The study of such equations (which arise in almost all areas of science and engineering) is one of the most important research fields in applied mathematics. There are two major classes of solution methods, namely, global approaches (such as spectral and pseudospectral methods) and local methods (finite elements, finite volumes, and finite differences). For linear equations with relatively simple boundary conditions, such as the Schrödinger equation in typical applications to quantum dynamics, various spectral and pseudospectral methods [4–19] are highly accurate, and can be implemented with a relatively small number of basis functions, thus achieving computational efficiency. Most spectral and pseudospectral methods use standard basis functions constructed from well-known polynomials (e.g., Jacobi, Laguerre, Legendre, Hermite, Chebyshev, etc.). The expansion coefficients are usually determined by the τ method, the Galerkin method, or by a collocation method. Shizgal and co-worker's method [8,9] utilizes nonstandard weight functions that are especially adapted to the problem under study, and thus may reduce the number of grid points needed for a particular application. This method becomes equivalent to the discrete variable representation (DVR) method [7,10–12], which is widely used in quantum-chemical dynamics, if one uses classical weight functions. For nonlinear systems the superposition principle is no longer valid, and complicated boundary conditions and geometries can significantly affect the relative usefulness of spectral methods. Local methods, such as finite element methods [20,21,22,61] and finite difference methods [23–27], are much easier to employ in these instances, and are the ones most commonly used. The fundamental difference between global methods and local methods is that the former approximate the values of a function and its derivatives at a given grid point using all grid values of the function on the entire domain, whereas the latter do this using only the values of the function on a compact set of grid points containing the given grid point as an interior point. In general, if applicable, global, spectral, or pseudospectral methods are more accurate than local methods. It is desirable to have a method that possesses spectral method accuracy and local method flexibility for both linear and nonlinear systems. Distributed approximating functional methods are of this type [28–42].

A variety of realizations of DAF's have been proposed, depending on the nature of the application of interest [30–34]. In particular, these DAF's have been successfully applied to the solution of a variety of partial differential equations, including those arising in quantum dynamics [35–37], linear and nonlinear Fokker-Planck equations [38–40], and the nonlinear Burgers' equation with moderate and high Reynolds numbers [41,42]. The ability of the DAF's to provide an analytical representation of a function and its derivatives in terms of a discrete set of values of the function is central to its successful use in various computational applications.

In this work we introduce a new class of DAF's which we refer to as *interpolating* DAF's (and, by contrast, we refer to earlier DAF's as *noninterpolating*). One such DAF (the so called Lagrange or LDAF) has already been applied successfully to the solution of the linear bound-state Schrödinger equation and a linear Fokker-Planck equation. In this paper,

we discuss how our DAF's can be obtained from the previous DAF formalism [34].

Interpolating DAF's are constructed by combining interpolation formulas with decreasing weight functions. They systematically generate distributed localized basis functions that are easily applied to nonlinear PDE's (as are finite element and finite difference methods); but they are extremely accurate for time-dependent quantum dynamical problems, for fitting functions off the input grid, and for approximating derivatives of functions.

This paper is organized as follows: The formalism of the interpolating DAF's is introduced in Sec. II. The numerical application of the particular LDAF to fitting functions and their derivatives is presented in Sec. III. Section IV illustrates the time-dependent quantum dynamical application. The utility and accuracy of our LDAF are further demonstrated using the nonlinear Burgers' equation with a moderate Reynolds number. Section V contains our conclusions.

II. FORMALISM

A. General variational approach and well-tempered DAF's

The general features of the theory of DAF's have been extensively discussed in a number of articles [28–42]. Here we outline only the basic ideas. The ultimate goal is to construct an approximate analytic representation of a function $f(\underline{x})$, and its derivatives from the values of the function on a set of grid points in the $\underline{x}$ domain. In the DAF method one first writes an approximation to the function at the point $\underline{x}'$,

$$f_{\rm app}(\underline{x}'|\underline{x})=\sum_i a_i(\underline{x})\phi_i(\underline{x}'-\underline{x}), \tag{1}$$

using a basis set of functions centered on $\underline{x}$, and then uses the approximation only for $\underline{x}'=\underline{x}$ (i.e., replaces $\underline{x}'$ by $\underline{x}$) to obtain

$$f_{\rm DAF}(\underline{x})=f_{\rm app}(\underline{x}|\underline{x})=\sum_i a_i(\underline{x})\phi_i(0). \tag{2}$$

In other words, each point $\underline{x}$ has its own truncated basis set with expansion coefficients, that in the general case are themselves functions of $\underline{x}$. To obtain the DAF-approximated function at $\underline{x}$, one evaluates the expansion for the point $\underline{x}$ at the origin. Although we have not explicitly so indicated, the basis functions can also depend implicitly on the point $\underline{x}$. This is a point crucial for our present considerations, and one which we will discuss in some detail later. Equation (2) should be contrasted with a standard basis set expansion

$$f(\underline{x})=\sum_i a_i\phi_i(\underline{x}). \tag{3}$$

This simple approach, as represented by Eq. (2), speaks more to a very general conceptual framework rather than an operational procedure. It is so general that virtually *all* fitting techniques, viewed in the right way, can be considered as special cases. To be useful one must specify exactly how the local approximation is to be made.

In nearly all of our work to date, we have used a pointwise, weighted least-squares variational principle to determine the coefficients, $a_i(\underline{x})$ in Eq. (2), for all points $\underline{x}$ (although by no means is one limited to such an approach and preliminary calculations suggest some interesting modifications [43]). The resulting DAF coefficients $a_i(\underline{x})$ are then linear functionals of the set of all input data points. The pointwise variational function is of the form [34]

$$\lambda(\underline{x})=\sum_i w_i(\underline{x})|f(\underline{x}_i)-f(\underline{x}_i|\underline{x})|^2, \tag{4}$$

where the sum is over all grid points and $w_i(\underline{x})$ is the (nonnegative) weight of the ith grid point for origin $\underline{x}$. The weight which has been investigated most extensively is

$$w_i(\underline{x})=\exp\left[\frac{-(\underline{x}_i-\underline{x})^2}{2\sigma^2}\right]. \tag{5}$$

Substitution of Eq. (1) into Eq. (4), followed by requiring that $\lambda(\underline{x})$ be minimized with respect to the expansion coefficients, leads to linear algebraic equations for the expansion coefficients $a_i(\underline{x})$. The general form of the solution, at each $\underline{x}$, is

$$a_i(\underline{x})=\sum_{k,n} w_k(\underline{x})\phi_n^*(\underline{x}_k-\underline{x})[\mathbf{C}^{-1}(\underline{x})]_{i,n}f(\underline{x}_k), \tag{6}$$

where the ''overlap matrix'' $\mathbf{C}$ is defined by

$$[\mathbf{C}(\underline{x})]_{j,n}=\sum_k w_k(\underline{x})\phi_j^*(\underline{x}_k-\underline{x})\phi_n(\underline{x}_k-\underline{x}). \tag{7}$$

If $\phi_j^*(\underline{x}_k-\underline{x})$ also happens to be the biorthogonal complement [under summation over the grid, subject to the weight, $w_k(\underline{x})$] of ϕ_j, then

$$[\mathbf{C}(\underline{x})]_{j,n}=\delta_{jn}, \tag{8}$$

and the matrix element of the inverse, $[\mathbf{C}^{-1}(\underline{x})]_{\rm in}$, is trivially also $\delta_{\rm in}$.

The variational function $\lambda(\underline{x})$ of Eq. (4) therefore leads to the DAF approximation [34]

$$f_{\rm DAF}(\underline{x})=\sum_i I(\underline{x},\underline{x}_i)f(\underline{x}_i), \tag{9}$$

where

$$I=(\underline{x},\underline{x}_i)=\sum_j w_i(\underline{x})\phi_j(0)\xi_j^*(\underline{x}_i-\underline{x}), \tag{10}$$

and

$$\xi_j^*=\sum_n [\mathbf{C}^{-1}]_{\rm in}\phi_n^* \tag{11}$$

is the biorthogonal complement of ϕ_j under summation for the weight $w_i(\underline{x})$. It should be noted that such a variational functional is also the starting point for the moving least-squares and reproducing kernel, methods [1–3]. As noted previously, the approach in general leads to noninterpolative approximations to the function of interest. However, the focus of these earlier efforts has been on interpolative versions.

In contrast, earlier DAF studies focused on taking advantage of the absence of interpolation to achieve the ''well-tempered DAF's''.

This point can best be illustrated by an example, which will be important in our later discussions. Consider a one-dimensional grid, with the weight function of Eq. (5), and the basis functions $(x_i-x)^j$, $j=0$ to M. Then

$$I(x,x_i)\equiv\Delta\,\delta_M(x-x_i|\sigma), \tag{12}$$

where Δ is the grid spacing (assumed to be uniform) and

$$\delta_M(x-x_i|\sigma)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left[\frac{-(x-x')^2}{2\sigma^2}\right]\times\sum_{n=0}^{M/2}\left(-\frac{1}{4}\right)^n\frac{1}{n!}H_{2n}\left(\frac{x-x'}{\sqrt{2}\sigma}\right), \tag{13}$$

is the so-called Hermite DAF. The functions H_{2n} are *not*, strictly speaking, Hermite polynomials (as the notation might suggest), or for that matter polynomials at all. In fact, they are quite complicated functions (i.e., no simple expression for them exists), and, although it is not so indicated, they depend implicitly on the placement of x between its two neighboring grid points (i.e., the value of x modulo the grid). However, as $\Delta\to0$, H_{2n} becomes the $2n$th Hermite polynomial.

An interesting and important fact is that these functions approach the Hermite polynomial limit very sharply, and for values of Δ that are still large enough to be extremely useful for practical fitting applications. In the regime where Eq. (13) can be effectively expressed in terms of Hermite polynomials, we say that the approximation is ''well tempered.'' (This is a fundamental feature of our earlier DAF analysis and, so far as we have been able to determine, distinguishes that work from the interpolative versions of the moving least-squares method.) The DAF approximation being well tempered is tantamount to being able to write

$$f_{\mathrm{DAF}}(x)=\int dx'\,\delta_M(x-x'|\sigma)f(x') \tag{14}$$

(the so-called ''continuous DAF'' case [30,31,34]), from which it is clear that the grid points have in a sense lost their special identity and that the well-tempered DAF fit is as good off the grid as it is on. [Note that the well-tempered Hermite DAF can be obtained in a heuristic way by discretizing Eq. (14), although at first blush discretizing a δ-function integral—even if the δ function is only approximate—might seem risky. Further note that in the limit $\sigma\to0$ or $M\to\infty$ the Hermite DAF goes exactly to the Dirac delta function.]

Saying that ''the fit is as good off the grid as on'' implies that there is a unique, underlying function being approximated. What this means is that for *any* regular grid with spacing Δ, there is a unique set of functional values on the grid that would give rise to exactly the same analysis, and, therefore, from the functional values on any one grid, one is able to deduce the entire function. (This function is, of course, the one that can be constructed from the grid data by Fourier transform theory using continuous wave numbers in the range $-\pi/\Delta\leqslant k\leqslant\pi/\Delta$.)

An important property of a well-tempered approximation is that it yields very accurate derivatives. In fact, it can be shown that the derivative of the DAF approximation is the DAF approximation of the derivative for a well-tempered fit. This property of yielding highly accurate derivatives is extremely important for solving differential equations. The well-tempered ''differentiating Hermite DAF'' has the very simple form

$$\frac{d^l}{dx^l}\,\delta_M(x-x'|\sigma)=\frac{1}{\sqrt{2\pi}2^{l/2}\sigma^{l+1}}\exp\left[-\frac{(x-x')^2}{2\sigma^2}\right]\times\sum_{n=0}^{M/2}\left(-\frac{1}{4}\right)^n(-1)^l\frac{1}{n!}H_{2n+l}\left(\frac{x-x'}{\sqrt{2}\sigma}\right), \tag{15}$$

which is easily established from the generating function of the Hermite polynomials.

Outside the well-tempered limit (which, for example, occurs for the Hermite DAF if σ is too small or M is too large for fixed Δ) the fit becomes increasingly interpolative (more nearly exact on the grid points) but inaccurate off the grid. This leads to increasingly inaccurate derivatives.

It should be pointed out that a well-tempered DAF is *not* a projection operator on the grid (i.e., $I^2\neq I$). In fact, in the limit that the grid spacing goes to zero, the Hermite DAF of Eq. (13) has a continuously indexed spectrum with an eigenvalue of unity only at a single point (all other eigenvalues are less than unity). Despite this the Hermite DAF in the limit $\Delta\to0$ is an identity for all polynomials of degree $\leqslant M+1$. This might at first seem to be a contradictory result, but it is in fact possible because polynomials do not belong to the Hilbert space. Because well-tempered DAF's are not projection operators, their repeated application will degrade the fit of a Hilbert space function. One might think that this would present difficulties in applications, but in fact the degradation of the fit is predictable, and controllable due to its near linearity. In addition to yielding highly accurate derivatives, the well-tempered property makes DAF's extremely useful for data fitting and smoothing (including eliminating experimental noise), data padding, predicting, and similar data manipulations that are applicable in a wide variety of fields [44–46].

However, the general theory of DAF's that we have outlined allows the possibility of a kind of DAF quite different from well-tempered DAF's such as our Hermite DAF example. These are interpolative and hence projection operators. Nevertheless, they still deliver highly accurate derivatives, and consequently can be used to solve PDE's as effectively as well-tempered DAF's (as we shall presently demonstrate). Their repeated application does not degrade functions, preserving all the information in the data set. Therefore, they cannot be used for data smoothing and predicting. However, since they preserve all information in the data set, they are useful for quite different types of applications. In Sec. II B we develop these ''interpolative DAF's'' more fully.

B. Basis set choice for interpolating DAF's

The procedure outlined in Sec. II A is very general. In particular, every x point has its own basis set for application of the DAF variational principle. For most applications of DAF's, we have used a polynomial basis under a Gaussian weight. The only two parameters of the fit then are the width (variance), σ, of the Gaussian, and the degree M of the Hermite polynomial, which is, of course, an integer. (Actually there is a generalized form of the DAF that, in effect, varies the ''order'' continuously [47].) In practice we have most often taken both parameters to be constant over the entire x domain. Under these circumstances one can either choose the basis set to have the same form for each point relative to its local origin [i.e., $(x'-x)^j$, $j=0$, to M, where M equals the highest degree polynomial] or the same form for each point relative to an absolute origin [i.e., $(x)^j$, $j=0$, to M], since these are equivalent. (This same equivalence exists for $e^{ikx'}$ or any other basis set that is also a basis for the translation group.) Once the basis set and weight function have been chosen, then the procedure for generating the DAF approximation is completely prescriptive.

Let us now consider the situation where the weight is constant (which, for example, can be thought of as the limit where the width of the Gaussian weight becomes infinite). Although there is no difficulty in principle in constructing the DAF, as outlined in Sec. II A, we can no longer use a polynomial basis (or any similar basis set that cannot be normalized on the grid). Stated equivalently, the overlap matrix $\mathbf{C}(x)$ is not well defined. To carry out the procedure for constructing the DAF, it is necessary to have a basis set for which $\mathbf{C}(x)$ can be computed. Any basis set $\{\phi_j\}$, indexed on the grid, for which

$$\phi_j(x_k)=\delta_{jk}, \tag{16}$$

and which satisfies translational invariance

$$\phi_j(x)=\phi_k(x+x_k-x_j), \tag{17}$$

satisfies the DAF procedure requirements. Conversely, by symmetric orthogonalization on the grid, any normalizable basis is equivalent to such a basis. It is obvious that not every set of basis functions that satisfies Eqs. (16) and (17) is acceptable for constructing a satisfactory approximation. Hence the case where one satisfies the above two conditions *cannot* be made prescriptive with respect to off-grid predictions, and is fundamentally different from where the weight is local.

Since not all basis sets that satisfy Eqs. (16) and (17) are acceptable, it is necessary to impose an additional condition on the $\phi_j(x)$ in order to generate an acceptable approximation. *The condition we adopt is that every grid point contributes equivalently to the approximation.* For a uniform grid, this means that

$$\int dx'\,\phi_j(x')=\Delta, \tag{18}$$

where Δ is the grid spacing. (For a nonuniform grid the integral is equal to the *average* of the spacings to the left and to the right of grid point x_j.) The resulting DAF from the variational principle is $\delta(x,x_j)=\phi_j(x)$. This quantity can be viewed as a ''Kronecker delta function'' (discrete on one index and continuous on the other, as opposed to either the Kronecker delta or the Dirac delta function). Equations (16) and (18) then respectively assure the twin conditions

$$\sum_k \delta(x_j,x_k)=1 \tag{19}$$

and

$$\int dx'\,\delta(x',x_j)=\Delta \tag{20}$$

for any point x_j on the grid. Through these conditions the nature of the interpolating DAF as a Kronecker delta function (''halfway'' between a Kronecker delta and a Dirac delta function) is made manifest.

For the case where the weight function is local and the DAF procedure is prescriptive, neither conditions (19) or (20) is precisely obeyed, but, by appropriate choice of DAF parameters, they can be made to be satisfied to any desired accuracy (up to the well-tempered limit). Obviously, for the constant weight case where Eq. (16) is satisfied, the DAF approximation is strictly an interpolation (i.e., exact on the grid); hence such a DAF approximation can never be well tempered (i.e., of comparable accuracy on and off the grid). However, it should be emphasized that being well tempered does not necessarily equate to being accurate.

The Gaussian Lagrange DAF (GLDAF) [48]

$$\delta_M(x,x_k|\sigma)=e^{(x-x_k)^2/2\sigma^2}\prod_{j\neq k}^{M}\frac{(x-x_j)}{(x_k-x_j)} \tag{21}$$

satisfies Eq. (19), but does not satisfy Eq. (20) exactly, but it can be made to so to arbitrary accuracy by choosing M sufficiently large for fixed σ and Δ. Thus it generates an acceptable DAF approximation for the constant weight case. Note that Eq. (21) is only posited, and is in no sense derived. However, its form is implied by the fact that the well-tempered Hermite DAF for very large M has almost evenly spaced zeros that lie very near to the grid points (for those zeros closest to the center). Equation (1) provides a good approximation long before the large M limit is ever realized [49,50].

III. GAUSSIAN LAGRANGE DAF FITTING AND DIFFERENTIATION

The quality of any computational method can be evaluated by how well the method approximates a function off the input grid points, and the derivatives of the function both on and off the grid points. The ability of approximating a function from a discrete set of data points is important for a wide range of applications, such as potential fitting [51–54]. Accurately approximating various derivatives is crucial for solving ordinary and partial differential equations. In this section we examine the accuracy of the Gaussian Lagrange DAF for differentiation on or off a grid and for fitting a function off the grid.

For the application of spectral methods, like that of Shizgal [8], to the solution of partial differential equations, a polynomial basis set is typically chosen. The degree of the

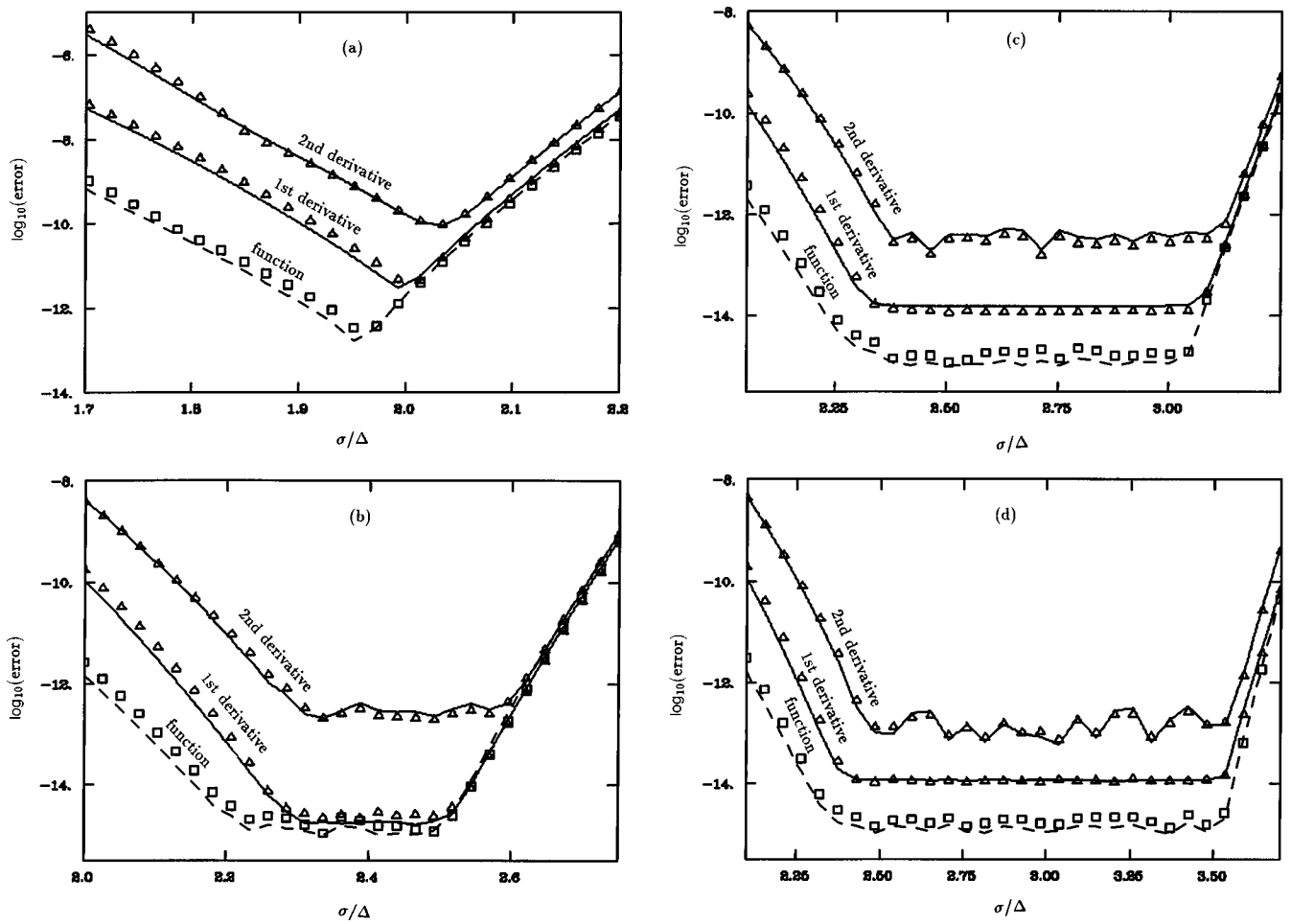

FIG. 1. Errors of the Gaussian Lagrange DAF differentiation and fitting for $f(x)=e^{-\sin(x)}\cos(2x)+\sin(x)$. Solid and dashed lines denote the L_∞ errors. Triangles and squares denote the L_2 errors. Solid lines and triangles denote the errors in the first two derivatives evaluated on the grid. Dashed lines and squares denote the errors for fitting the function off the grid. (a) $M=40$. (b) $M=60$. (c) $M=80$. (d) $M=100$.

polynomial is determined by the number of grid points used in the problem. In contrast, in the DAF methods, the degree of the polynomials is more or less independent of the number of grid points. Therefore an appropriate polynomial degree M must be chosen for a given problem. A sufficiently large M value is important for accuracy (which explains why the Gaussian test functions used in the mathematical theory of distributions are not practical for numerical applications). The σ value determines the range of data contributing to the prediction at any off-grid point x. The value of the Gaussian is sufficiently small as to be approximated by zero at about a distance of 15 σ. Therefore, further increases in M will not improve the accuracy due to the cutoff provided by the Gaussian factor for given σ and grid spacing Δ. In uniform grid cases, for a sufficiently large M value, say $M=80$, the ratio of σ/Δ is the only parameter that must be appropriately chosen. The illustrative function $f(x)$ used for the present study is

$$f(x)=e^{-\sin(\alpha x)}\cos(\beta x)+\sin(\alpha x), \tag{22}$$

where we take $\alpha=1$ and $\beta=2$, and 40 grid points ($N=40$) are used inside the interval of $[0,\pi]$. Both the L_∞ and L_2 errors for differentiations are calculated for four different M values

$$M=40,\ 60,\ 80,\ 100.$$

As shown in Fig. 1, the present Gaussian Lagrange DAF is extremely accurate for differentiation and is not sensitive to the ratio σ/Δ over a wide range of values. When M ranges from 80 to 100, there is a large interval of σ/Δ ratios that delivers extremely high accuracy for the test function $f(x)$ and its first and second derivatives. It is noted that the stable ranges of the ratios for the function and its derivatives in this test problem are also the ranges of ratios for which the Gaussian Lagrange method provides accurate solutions to the time-dependent Fokker-Planck equations and nonlinear Burgers' equation [48]. This means that it is relatively easy to choose the parameters of the Gaussian Lagrange DAF for dynamical calculations. More details in this regard are given in Sec. IV.

The ability of the Gaussian Lagrange DAF to fit a function is demonstrated by predicting values of the function off the grid. We take the same function as defined in Eq. (22) as our test function, and still use as input values of the function at 40 grid points ($N=40$) inside the interval $[0,\pi]$. We predict the function at 60 evenly spaced grid points within the same interval (thus focussing on off-grid fitting). Only the L_∞ errors are recorded for fitting off the grid (the squares in Fig. 1.). The Lagrange DAF is able to provide 14-significant-figure accuracy in fitting this function off the grid.

TABLE I. Errors for solving the Ornstein-Uhlenbeck Fokker-Planck equation. Numbers in brackets denote powers of 10.

	$N=50,\ \Delta t=0.05$		$N=100,\ \Delta t=0.01$			
	$[-5,5]$		$[-5.5,5.5]$		$[-11.5,11.5]$	
Time	L_2	L_∞	L_2	L_∞	L_2	L_∞
0.1	1.61[−02]	2.07[−02]	1.50[−04]	2.17[−04]	6.40(−0.2)	8.04[−02]
0.2	1.32[−03]	1.64[−03]	1.79[−06]	2.90[−06]	4.98[−03]	4.94[−03]
0.3	3.14[−04]	4.47[−04]	2.97[−07]	5.08[−07]	5.99[−04]	5.49[−03]
0.6	1.21[−05]	1.77[−05]	1.43[−08]	2.10[−08]	9.07[−06]	8.49[−06]
1.0	1.17[−06]	1.54[−06]	1.54[−09]	2.04[−09]	1.48[−07]	1.37[−07]
2.0	5.23[−08]	5.99[−08]	7.52[−11]	8.70[−11]	4.35[−10]	2.60[−10]
4.0	2.71[−09]	2.29[−09]	3.56[−12]	3.67[−12]	2.83[−10]	2.60[−10]
6.0	8.41[−10]	6.63[−10]	5.75[−13]	5.67[−13]	2.78[−10]	2.49[−10]
8.0	6.18[−10]	5.94[−10]	2.35[−13]	2.06[−13]	2.75[−10]	2.46[−10]
10.0	4.92[−10]	4.70[−10]	2.96[−13]	1.58[−13]	2.74[−10]	2.44[−10]

IV. GAUSSIAN LAGRANGE DAF SOLUTION TO QUANTUM AND CLASSICAL DYNAMICAL PROBLEMS

Another important test for the present Gaussian Lagrange DAF is its accuracy for solving various quantum and classical (nonlinear) dynamical time evolutions. Since analytical solutions to real physical problems are limited to a few simple cases, there is great interest in developing methods for accurately and efficiently solving ordinary and partial differential equations, which are important to a wide range of scientific problems.

A. Ornstein-Uhlenbeck process

A useful benchmark problem for testing numerical time propagation methods is the Ornstein-Uhlenbeck process which involves both the first and second derivatives. The Ornstein-Uhlenbeck process is a stationary Markov process, and its corresponding Fokker-Planck equation describing a linear drift-diffusion system is given by

$$\frac{\partial f(x,t)}{\partial t}=\gamma\,\frac{\partial[xf(x,t)]}{\partial x}+D\,\frac{\partial^2 f(x,t)}{\partial x^2}, \tag{23}$$

where γ and D are positive constants. With an initial δ function distribution localized at x_0, the solution of the Ornstein-Uhlenbeck Fokker-Planck equation is given as a Gaussian

$$f(x,t)=\left[\frac{\gamma}{2D\pi\sqrt{(1-e^{-2\gamma(t-t_0)})}}\right]\times\exp\left[-\frac{\gamma(x-x_0e^{-2\gamma(t-t_0)})^2}{2D(1-e^{-2\gamma(t-t_0)})}\right]. \tag{24}$$

The stationary Gaussian distribution results when $\gamma(t-t_0)\gg 1$. The Ornstein-Uhlenbeck process has various physical applications, such as to a laser field far below (or above) its threshold [55], to a linear overdamped oscillator in the presence of colored Gaussian noise [56], and to the velocity relaxation of a Rayleigh gas [57]. The Ornstein-Uhlenbeck Fokker-Planck equation is also computationally important, and has been used for testing various new numerical schemes [9,58]. In the present computations, γ and D are chosen as 0.25 and 0.125, respectively. Two sets of grid points ($N=50$ and 100) are used with corresponding intervals taken as $[-5,5]$ and $[-5.5,5.5]$, respectively, and the initial δ functions are located at -0.6 and -0.55, respectively. The time increments used for $N=50$ and 100 are 0.05 and 0.01, respectively. We have used a fourth order expansion ($R=4$) of a path integral formulation of the Fokker-Planck equation. We refer the reader to Refs. [39–41] for the details of the method. It is found that, for each fixed M value, a wide range of ratios σ/Δ yield accurate results for the present time-dependent problem. This is illustrated in Fig. 1 ($2.4<\sigma/\Delta<3.1$ for $M=80$). The L_2 and L_∞ errors, using the ratio $\sigma/\Delta=2.88$ and $M=80$ for a range of propagation times are listed in Table I. It is evident that using a relatively small number of grid points and reasonably large time increments, the Gaussian Lagrange DAF approach is able to provide accuracy close to the computer roundoff limit for solving a quantum dynamical equation. A basic tendency of the accuracy can be summarized as follows: the more grid points and the later the time, the more accurate the solution is. It is noted that the time-dependent Gaussian Lagrange DAF approach easily provides sufficient accuracy for most practical purposes even if one employs a small number of grid points with very large time step ($\Delta t\approx 0.05$). We expect that an increase in accuracy for the earlier time solutions can be further achieved if the initial δ functions are replaced by numerically smoother functions.

B. Burgers' equation

Burgers' equation [59], in one space dimension, given by

$$\frac{\partial u}{\partial t}+u\,\frac{\partial u}{\partial x}=\frac{1}{\mathrm{Re}}\,\frac{\partial^2 u}{\partial x^2}, \tag{25}$$

where $u(x,t)$ is a velocitylike quantity. There is thus an analogy between Burgers' equation and the Navier-Stokes equation in the roles played by the nonlinear advection and the viscous diffusion terms, and for this reason the analytical solvability of the former makes it an important test problem numerical methods in fluid dynamics. One of the major sources of difficulty for solving both Burgers' equation and

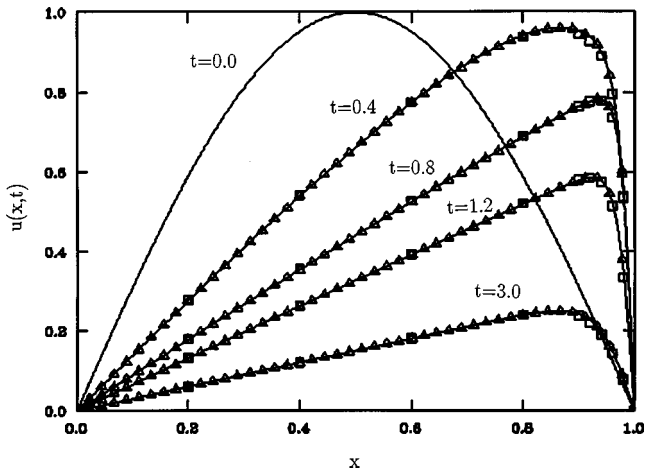

FIG. 2. The exact and numerical solutions of the Burgers' equation (Re=100). Solid line: exact. Triangle: present (45 grid points). Square: Kakuda and Tosaka (100 elements and six iterations).

Navier-Stokes equation is the occurrence of inviscid boundary layers produced by the steepening effect of the nonlinear advection term. It is customary to test new methods in this field by applying them to Burgers' equation.

We consider Eq. (25) with the following initial-boundary conditions:

$$u(x,0)=\sin(\pi x),$$
$$u(0,t)=u(1,t)=0. \tag{26}$$

The exact solution [60] for this problem is available as an infinite series for the parameter range Re$\leqslant$100. For the parameter Re=100, the present GLDAF calculations use three sets of grid points (25, 35, and 45 uniformly spaced points for interval [0,1]), with a time increment of $\Delta t=0.01$ and a second order Taylor expansion in time. Both the numerical solution and the exact solution are plotted in Fig. 2. There is no detectable difference between the two solutions. At later times, the solution develops a sharp change at the right boundary which can induce numerical instabilities (Gibbs oscillations). The maximum absolute errors (L_∞) for all sets of grid points at four different times are listed in Table II. It is interesting to compare the present results with the earlier accurate numerical results recently obtained using the generalized boundary element method by Kakuda and Tosaka [61]. These authors used 100 elements, up to six iterations, and the same time increment as ours ($\Delta t=0.01$). While the errors in both methods are very small, the present results range from being ten to a few hundred times more accurate than those of Kakuda and Tosaka [61] (KT), while obtained using fewer grid points.

TABLE II. L_∞ errors of the numerical solutions for Burgers' equation. The numbers in brackets denote powers of 10.

t	KT	Present[a]	Present[b]	Present[c]
0.4	2.6[−2]	1.6[−2]	3.6[−3]	1.1[−3]
0.8	2.9[−2]	2.6[−2]	6.6[−3]	1.4[−3]
1.2	1.8[−2]	8.0[−3]	1.2[−3]	1.9[−4]
3.0	6.9[−3]	4.5[−5]	2.3[−5]	2.2[−5]

[a] $N=25$.
[b] $N=35$.
[c] $N=45$.

V. CONCLUSION

A class of DAF's, called interpolating DAF's, are proposed for a wide range of numerical applications. The approach is illustrated using the Gaussian Lagrange DAF. These DAF's are interpolative solutions of the variational equations generated by a pointwise least squares procedure, and they can be used for approximating any function, or distribution and its derivatives having polynomial growth. The Lagrange DAF's, like many other DAF's, can be viewed as a natural extension to familiar Dirac δ sequences and/or Gaussian test functions, and therefore can be regarded as generalized δ sequences. However, both the usual δ sequences and the Gaussian test functions do not have much numerical utility, whereas the DAF's are powerful numerical computational tools.

The Lagrange DAF's are constructed by combining the DAF concept with the Lagrange interpolation idea. Three types of numerical problems, including differentiation on and off a grid, fitting a function off a grid, time-dependent quantum dynamical evolution, and a standard test problem from fluid dynamics, are used to demonstrate the usefulness, test the accuracy, and explore the limitations of the Gaussian Langrange DAF, a particular realization of the Lagrange DAF's. The parameters in the Gaussian Lagrange DAF are chosen to yield exact results on a grid (the so-called interpolation property). We obtain L_∞ errors of 10^{-14} for the function *off the grid*, and 10^{-13} and 10^{-12}, or better, for first and second order derivatives on the grid respectively for a wide range of parameters. This is illustrated by using an analytically known function with 40 input grid points in the interval of $[0,\pi]$. Because the LDAF's easily generalize to higher dimensions, this is potentially of use in fitting potential energy *ab initio* data to use in molecular dynamics calculations. This test also has a very general significance since, as we discuss below, both the accuracy and the validity range of the parameters are confirmed in an entirely different applications, namely, solving time-dependent partial differential equations of both linear and nonlinear types. The power of the Gaussian Lagrange DAF for solving partial differential equations, and therefore quantum dynamical problems, is demonstrated by treating the Ornstein-Uhlenbeck Fokker-Planck equation which requires evaluation of both the first and second derivatives. A wave packet propagation method is used for this study. It is found that both the L_2 and L_∞ errors for the time-dependent distribution functions are of the order of 10^{-13} at the later times, which is close to the computer roundoff limit. A wide range of σ/Δ ratios, and various choices of polynomial degree M, was found to yield this order of accuracy, as shown in Fig. 1. This demonstrates the robustness of the interpolating DAF approach.

The robustness of the present approach was also confirmed by solving the nonlinear Burgers' equation with a Reynolds number as large as 100. Our results range from being ten to a few hundred times more accurate than those of KT [61], while obtained using fewer grid points. These results indicate strongly that one should not have any difficulty in choosing the Gaussian Lagrange DAF parameters for a

variety of linear and nonlinear PDE's. An interesting and useful study would be to examine the Lagrange DAF's with the nonclassical weights which raise naturally in statistical mechanical problems [8,62]. In the future, we shall test the Lagrange DAF's for fitting multidimensional potentials. We will also examine the accuracy of the Gaussian Lagrange DAF for a wide variety of linear and nonlinear partial differential equations. Finally, other types of interpolating DAF's are under study.

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