Lagrange Distributed Approximating Functionals

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Lagrange distributed approximating functionals (LDAFs) are proposed as the basis for a new, collocation-type method for accurately approximating functions and their derivatives both on and off discrete grids. Example applications are presented to illustrate the use of LDAFs for solving the Schrödinger equation and Fokker-Planck equation. LDAFs are constructed by combining the DAF concept with the Lagrange interpolation scheme. [S0031-9007(97)03702-2]

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Since analytical solutions to most ordinary and partial differential equations in theoretical physics are available only for a few simple cases, there is great interest in developing new methods for accurately and efficiently solving such equations. There are two major approaches available for generating numerical solutions, namely, global methods and local methods. For a linear system with relatively simple boundary conditions (e.g., the Schrödinger equation describing quantum dynamics), global methods, such as spectral and pseudospectral methods [1–9], are powerful both in terms of accuracy and in minimizing the number of grid points required in order to achieve computational efficiency. For nonlinear systems, such as arise in statistical mechanics and fluid dynamics, spectral methods are not as useful. Here local methods, such as various finite element [10–12] and finite difference methods [13–19], are typically more robust and are the ones commonly used. In general, however, global methods, if applicable, are more accurate than local methods. It is highly desirable to have a method that possesses global method accuracy and local method flexibility for *both* linear and nonlinear systems. Distributed approximating functionals (DAFs) [20] provide the basis for such approaches. Although robust, existing DAFs achieve their highest accuracy within a fairly tight functional relationship among the DAF parameters (which fortunately do not depend sensi-

tively on the function being fit, however). In this Letter we present a new DAF that achieves comparable accuracy for a wider range of DAF parameters.

DAFs have been introduced [20] as generalized delta sequences, for approximating functions of polynomial growth in the domain of definition, accurate to a specified tolerance. In this context, DAFs are able to approximate the identity acting on *any* physically realizable state. As approximations to the identity operator, one can also view DAFs as linear *functionals*. The approximate identity operator role of DAFs underlies their use to approximate a function. As members of generalized delta sequences, DAFs tend to the Dirac delta function in the appropriate limits of the DAF parameters [21]. However, in contrast to the Dirac delta function and Gaussian test functions, which do not have much numerical utility, DAFs are very powerful tools for numerical applications.

In this Letter we propose a new class of DAFs (the Lagrange DAF or LDAF), which is constructed by combining Lagrange interpolation type formulas with rapidly decreasing weight functions. The relationship to earlier DAFs will be examined in more detail in a subsequent paper [22]. As for previous DAFs, the LDAF can be chosen to generate extremely accurate solutions both for time-dependent quantum dynamical problems and for eigenvalue problems of the linear Schödinger

equation. However, our numerical experience [22] has been that the LDAF is less sensitive to parameters and is accurate for a wider range of parameters than previous DAFs. When used to solve differential equations with the LDAF, we use a collocation strategy.

On the domain of R^1, the LDAF, defined relative to the point x_k on a fundamental, finite, or infinite grid, can be expressed in the form

$$\delta_{M,\sigma_k}(x \mid x_k) = C_k P_{M,k}(x) w_{\sigma_k}(x - x_k), \qquad (1)$$

where C_k is determined from

$$\int dx\, \delta_{M,\sigma_k}(x \mid x_k) = 1, \qquad (2)$$

and $P_{M,k}(x)$ and $w_{\sigma_k}(x - x_k)$ are defined below. The (non-negative) weight $w_{\sigma_k}(x - x_k)$ can be chosen for computational convenience. A common weight function used in many DAF applications (including this work) is the Gaussian function

$$w_{\sigma_k}(x - x_k) = e^{-(x-x_k)^2/2\sigma_k^2}, \qquad (3)$$

where σ_k is a width parameter. However, it should be noted that we are not restricted to standard functions in our choice of weights. Nonstandard weight functions arise naturally in various practical problems (e.g., non-Gaussian distributions in statistical mechanics) and can also be considered. In Eq. (1), the quantity $P_{M,k}(x)$ is the (unnormalized) Lagrange polyomial defined by

$$P_{M,k}(x) = \prod_{i \neq k}^{M} (x - y_i^{(k)}), \qquad (4)$$

which vanishes for $x = y_i^{(k)}$. The index i labels the set of "nodal points" and $\{M\}_k$ is the set of such nodal points used in the construction of the polynomial $P_{M,k}(x)$. The nodal points are taken to be positioned relative to grid point x_k and we require that $y_i^{(k)} \neq x_k$. As an example, for a uniform and infinite grid, we usually employ $M/2$ nodal points, $y_i^{(k)}$, on either side of the grid point, x_k. Every point on the fundamental grid serves as a reference point for constructing an associated DAF. In practice, of course, one always uses a finite grid of N points. If x_k is close to the boundary of the grid, some of the nodal points used to form the LDAF $\delta_{M,\sigma_k}(x \mid x_k)$ will be located outside the domain of the fundamental grid; see Ref. [22] for details. We emphasize that the LDAF need not be limited to a uniform grid, and, as should be clear, the LDAF is defined by choosing the sets of nodal points $\{M\}_k$. Another obvious generalization is to replace $P_{M,k}(x)$ by a general function whose nodal points are the $y_i^{(k)}$. We have studied several choices of the $P_{M,k}(x)$, but have not systematically explored all possibilities. Clearly, there are constraints on the allowed form of the $P_{M,k}(x)$.

Suitable functions can be approximated by the LDAFs through the expression

$$f(x) \approx \sum_k \Delta_k \delta_{M,\sigma_k}(x \mid x_k) f(x_k), \qquad (5)$$

where Δ_k arises from approximating the normalization expression, Eq. (2), by quadrature, and the summation index k runs over all fundamental grid points. In particular, $\Delta_k = \Delta$ for a uniform grid. In practice, due to the rapid fall off of the Gaussian weight, only $2W$ grid points x_k, which are the "near neighbor" grid points to x, need be included in the sum. Thus, for x equal to a grid point, $x_{k'}$, we need include only W grid points on either side of $x_{k'}$ in the sum in Eq. (5). Because of the decay of the Gaussian, the LDAF is a banded matrix with bandwidth $2W + 1$ and the Gaussian decay is typically such that $2W$ can be taken to be less than or equal to M.

The qth derivative of the LDAF is analytically expressed as

$$\begin{aligned} \delta^{(q)}_{M,\sigma_k}(x \mid x_k) = C_k \sum_{t=0}^{q} \frac{q!}{t!\,(q-t)!} P^{(t)}_{M,k}(x) \\ \times\, w^{(q-t)}_{\sigma_k}(x - x_k), \end{aligned} \qquad (6)$$

which gives rise to the equation

$$f^{(q)}(x) \approx \sum_k \Delta_k \delta^{(q)}_{M,\sigma_k}(x \mid x_k) f(x_k) \qquad (7)$$

as the appropriate expression for the qth DAF derivative of the function. In the case of a uniform spacing of nodal points (coinciding with the grid spacing), $\prod_{i \neq k}^{M}(x - y_i^{(k)})$ can be rewritten as

$$\prod_{i \neq k}^{M} (x - y_i^{(k)}) = \prod_{i=1}^{M/2} (x - x_k + i\Delta)(x - x_k - i\Delta). \qquad (8)$$

When combined with a Gaussian weight this leads to the Gaussian Lagrange DAF (or GLDAF)

$$\begin{aligned} \delta_{M,\sigma}(x - x_k) = C \prod_{i=1}^{M/2} (x - x_k + i\Delta)(x - x_k - i\Delta) \\ \times\, e^{-(x-x_k)^2/2\sigma^2}, \end{aligned} \qquad (9)$$

which explicitly has a Toeplitz structure. Because it is simple and highly accurate, we restrict our consideration in this Letter to the uniform GLDAF of Eq. (9). This form has important potential applications for the complex geometry boundary value problems often encountered in science and engineering.

For simplicity, the discussion in this Letter has been restricted to the one-dimensional case; however, the extension of the GLDAFs to multidimensions is immediate and straightforward. The simplest procedure for doing so is to construct a product of one-dimensional GLDAFs. Although nonproduct multidimensional DAFs are of great interest, we shall leave further consideration of them to the future. In the remainder of this Letter we demonstrate the utility, and test the accuracy, of the

GLDAF (9) by solving an eigenvalue problem described by the Schrödinger equation and by evolving an Ornstein-Uhlenbeck process in time. These problems illustrate the accuracy and efficiency of the GLDAF for solving a variety of differential equations.

We first consider a Morse oscillator, which is a commonly used model potential for diatomic molecules. This is one of the few model systems in quantum mechanics for which the eigenfunctions are known analytically [23]. They are the generalized Laguerre polynomials [23]

$$\Phi_n = N_n z^{\frac{p}{2}} e^{-\frac{z}{2}} L_n^P(z), \tag{10}$$

where $z = \beta e^{-\alpha x}$, $p = \beta - 2n - 1$, $\beta = 156.047\,612\,535$, and the normalization constant, obtained using the generating function of the generalized Laguerre polynomials [23], is

$$N_n = \left[\frac{\Gamma(p)}{\alpha} \sum_{\gamma=0}^{n} (-1)^\gamma \binom{-p}{\gamma} \right]^{-\frac{1}{2}}. \tag{11}$$

The exact expression for the eigenvalues is

$$E_n = \kappa \left[n + \frac{1}{2} - \frac{1}{\beta}\left(n + \frac{1}{2} \right)^2 \right], \tag{12}$$

where $\kappa = 5.741\,837\,286 \times 10^{-4}$ a.u. We specifically consider the I_2 molecule to test the accuracy of the GLDAF method. The Morse potential for this molecule is given by

$$V(x) = D[e^{-2\alpha x} - 2e^{-\alpha x}] + D, \tag{13}$$

where $D = 0.0224$ a.u., $\alpha = 0.9374$ a.u. The reduced mass for this system is $\mu = 119\,406$ a.u. This system has recently been studied computationally by Braun $et\ al.$ [8] using an efficient Chebyshev-Lanczos method and a grid of 128 points to achieve an accuracy ranging from seven to nine digits. Our calculation makes use of the direct diagonalization of the GLDAF-Hamiltonian matrix. The GLDAF parameters are $M = 80$ and $\sigma/\Delta = 3.173$ for this example. We use N (the total number of fundamental grid points) equal to 100 and 80 (for a convergence comparison) on the interval of $[-0.8, 2.0]$ in our present

computations and the bandwidth of the GLDAF is 71, so $W = 35$. The uniform step size Δ is computed as $(x_N - x_1)/(N - 1)$, where x_1 is the first grid point and x_N is the last. Note that this means that to generate the approximate Φ_n at the gth grid point $x = x_g$, we include 35 points x_ks on either side of x_g in Eq. (5). If x_g is closer than 35 grid points to either end of the grid, the values of $\Phi(x_k)$ outside the fundamental grid are determined by boundary conditions. For bound states, $\Phi(x_k)$ is zero for $x \leq x_1$ and $x \geq x_N$. Other situations may require other conditions (e.g., periodic boundary conditions, etc.). In fact, the result of either requiring the $\Phi(x_k)$ to vanish beyond the boundary or to be periodic results in Eqs. (5) and (7) involving only contributions from $1 \leq k \leq N$. The results of our study and those of Braun $et\ al.$ are listed in Table I. As seen from the error, our $N = 100$ grid point results are 100 to 1000 times more accurate than those of Braun $et\ al.$, although we employ significantly fewer grid points. It is to be noted that our $N = 80$ grid point results are still about 1000 times better than those of Braun $et\ al.$ for the low eigenvalues and are 30 times better for the highest ones in the Table I. Of course, even higher accuracy could be easily achieved by increasing the density of grid points. It should be emphasized that the DAF method is inherently local (i.e., the DAF has a $finite$ bandwidth of $2W + 1$), and hence an increase in the number of fundamental grid points N does not automatically lead to an increase either in the degree M of the DAF polynomial or the bandwidth of the DAF. Consequently, the computation time does not increase as rapidly with total grid size N as in some commonly used spectral methods or pseudospectral methods.

We next consider the (stationary and Markovian) Ornstein-Uhlenbeck process [24,25], describing a linear drift-diffusion system. It has been used for various physical applications, such as to describe a laser field far below (or above) its threshold [25], a linear overdamped oscillator in the presence of colored Gaussian noise [26], and the velocity relaxation of a Rayleigh gas [27]. The process provides an important benchmark problem for testing

TABLE I. Results for the 1D I_2 Morse oscillator.

k	Analytical [23]	Difference[a]	Difference[b]	Difference[c]
0	0.852 996 623 626 694 2E-03	−0.10E-10	−0.14E-13	−0.14E-13
1	0.141 246 218 462 970 6E-02	−0.30E-10	−0.43E-13	−0.43E-13
2	0.196 456 866 183 422 4E-02	−0.50E-10	−0.70E-13	−0.70E-13
3	0.250 931 605 524 024 7E-02	−0.70E-10	−0.98E-13	−0.98E-13
4	0.304 670 436 484 777 7E-02	−0.89E-10	−0.13E-12	−0.13E-12
5	0.357 673 359 065 681 3E-02	−0.11E-09	−0.15E-12	−0.15E-12
10	0.611 649 346 272 457 9E-02	−0.20E-09	−0.28E-12	−0.28E-12
15	0.847 227 623 982 999 3E-02	−0.28E-09	−0.25E-12	−0.40E-12
20	0.106 440 819 219 730 6E-01	−0.36E-09	0.96E-11	−0.30E-12

[a]Braun $et\ al.$ (Ref. [8], $N = 128$).
[b]Present ($N = 80$).
[c]Present ($N = 100$).

numerical time propagation methods and various new numerical schemes [28]. Unlike the Schrödinger equation, it involves both first and second derivatives. The Fokker-Planck equation corresponding to the process is given by

$$\frac{\partial f(x,t)}{\partial t} = \gamma \frac{\partial[xf(x,t)]}{\partial x} + D\frac{\partial^2 f(x,t)}{\partial x^2}, \quad (14)$$

where γ and D are positive constants. With an initial Dirac delta function distribution localized at x_0, the analytical solution of the Ornstein-Uhlenbeck Fokker-Planck equation is known and is given by

$$f(x,t) = \left[\frac{\gamma}{2D\pi\sqrt{(1-e^{-2\gamma(t-t_0)})}}\right]$$
$$\times \exp\left[-\frac{\gamma(x-x_0 e^{-2\gamma(t-t_0)})^2}{2D(1-e^{-2\gamma(t-t_0)})}\right]. \quad (15)$$

A stationary Gaussian distribution results when $\gamma(t-t_0) \gg 1$.

In the present computations, γ and D are chosen to be 0.25 and 0.125, respectively. The GLDAF parameters are taken to be $M = 100$, so a polynomial of degree 100 is employed in Eq. (9), and $\sigma/\Delta = 2.88$. Two sets of fundamental grid points ($N = 51, 101$) are used with corresponding intervals taken as $[-5, 5]$ and $[-5.5, 5.5]$, respectively, and $\Delta = (x_N - x_1)/(N - 1)$. In calculations involving Eqs. (5) and (7), the boundary condition imposed is that the function $f(x_k, t)$ vanishes for $k < 1$ and $k > N$. Various values of W were tested and the results were found to be insensitive to it, provided it was larger than 26; typical calculations were done with W equal to 35. The initial delta functions were located at -0.55 and -0.50, respectively, and the time increments used were 0.05 and 0.01, respectively. We refer the reader to Ref. [29] for more details. The L_2 and L_∞ errors, for a range of propagation times are listed in Table II. It is evident that using a relatively small number of grid points and reasonably large time increments, the time dependent GLDAF approach is able to provide an accuracy close to the computer round off limit in this application.

The most attractive properties of the LDAFs for solving differential equations can be summarized as follows:

TABLE II. Errors for solving the Ornstein-Uhlenbeck Fokker-Planck equation

Time	$N = 50, \Delta t = 0.05$		$N = 100, \Delta t = 0.01$	
	L_2	L_∞	L_2	L_∞
0.1	1.61(−02)	2.07(−02)	1.50(−04)	2.17(−04)
0.2	1.32(−03)	1.64(−03)	1.79(−06)	2.90(−06)
0.3	3.14(−04)	4.47(−04)	2.97(−07)	5.08(−07)
0.6	1.21(−05)	1.77(−05)	1.43(−08)	2.10(−08)
1.0	1.17(−06)	1.54(−06)	1.54(−09)	2.04(−09)
2.0	5.23(−08)	5.99(−08)	7.52(−11)	8.70(−11)
4.0	2.71(−09)	2.29(−09)	3.56(−12)	3.68(−12)
6.0	8.42(−10)	6.63(−10)	5.75(−13)	5.58(−13)
8.0	6.18(−10)	5.94(−10)	2.27(−13)	1.94(−13)
10.0	4.92(−10)	4.70(−10)	2.82(−13)	1.39(−13)

(i) As with most numerical methods, they transform ordinary and partial differentiations to a linear algebraic form, which reduces the calculation to matrix-vector multiplications. (ii) The GLDAF has been shown elsewhere [22] to be a particular realization of the generalized DAFs discussed in Ref. [21], and as such, is a special kind of spectral method which gives rise to a highly banded matrix representation of derivatives. In this regard, DAFs lead to a structure which is similar to finite difference and finite element methods. In the case of the GLDAF, the Gaussian factor produces the banded structure, and this structure is therefore a reflection of the "local" character of the basis functions. Thus, the DAF method for fitting functions possesses the best features of both local and global approaches. (iii) In comparison to spectral methods and finite element methods, the DAF approach is extremely simple and entails low CPU cost due to its slow scaling with problem size. In addition, the banded DAF matrices (on an evenly spaced grid) have a Toeplitz structure (reflecting translational invariance of the basis) and are symmetric. This greatly reduces the storage requirements. (iv) Because the DAF has the form of a convolution, the action of the DAF matrix on a vector can be evaluated by using fast Fourier transforms.

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