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Generalised Gauss-Laguerre Quadrature Formulae

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Abstract : Gauss-Laguerre formulae for the computation of integrals of functions of a given class are widely used in modern computer programmes. These formulae are restricted to the single weight function exp(—*ax*). However, in calculations involving vibrations of many modes in transients, as well as in atomic and molecular physics, several exponential functions, eg. exp(—*ax*), exp(—bx), etc., are needed to economically describe the spectrum of characteristic functions of the physical system. The standard Gauss-Laguerre approach, based on the theory of orthogonal polynomials cannot be easily generalised to yield a theory of quadrature for the multi-exponent case. Using a more direct approach to the problem, this study presents a general method for obtaining quadrature formulae for multi-exponential systems. Numerical results are given for a number of cases.

1. Introduction

The well known quadrature formulae[1,3] of Gauss, Hermite, Legendre and Laguerre treat the case

$$\int_a^b p(x) f(x)\, dr \quad \sim \quad \sum_{k=1}^{n} A_k f(x_k) \qquad (1)$$

where (a,b) is any finite or infinite segment of the real line, and f(x) is an arbitrary function of a certain class. The weight function p(x) is fixed, measurable on (a,b) and is not the identically zero function. Further, p(x) f(x) is summable on (a,b). The r.h.s. of equation (1) contains 2n+1 parameters, viz., the n nodes x_k, the n coefficients (weights) A_k and the number ' n '. Let us assume that f(x) belongs to the class of functions F, for which ϕ_m (x), m = 1,2,... form a basis set. Then, for any linear form L_n,

$$L_n(x) = \sum_{k=1}^{n} a_k \phi_k(x)$$

we define

$$\rho(f, L_n) = \int_a^b | p(x) (f - L_n) | dx.$$

Then, for each fϵF and any $\varepsilon > 0$, there exists an L_n such that

$$\rho(f, L_n) < \varepsilon.$$

$$\text{Since } \left| \int_a^b p f\,dx - \int_a^b p L_n dx \right| \leqslant \int_a^b | p\,(f - L_n) |\,dx = \rho\,(f, L_n),$$

it is clear that $\int_a^b p f\,dx$ can be calculated to as high a degree of accuracy as desired if f(x) is replaced by the appropriate linear combination.

If the nodes x_k and the coefficients A_k in equation (1) give good precision in integrating functions of the basis set, then the formulae must also give good precision for all $f \in F$. The formula (1) is said to have a degree of precision m with respect to the set ϕ_k if it is exact when $f(x) = \phi_k(x)$ for $k = 1,2...,m$. Formulae of the highest precision for a given n, and for the case $p(x) = 1$ were first given by Gauss. The n nodes are found to be the roots of the Legendre polynomial of degree n, viz., the roots of the equation :

$$P_n(x) = 0 \qquad (2)$$

where P_n is the orthogonal Legendre polynomial of degree n. The Hermite and Laguerre polynomials give the integration formulae for the weight functions $\exp(-x^2)$ and $\exp(-x)$, in the ranges $-\infty$ to $+\infty$ and 0 to ∞ respectively.

Numerical integration of atomic and molecular wave-functions usually involve linear combinations of S,P,D, and higher functions which involve different Slater exponents.[6] Similarly, even in classical systems, vibrational processes involving a number of modes, or processes involving several different transients would require several exponential functions for their adequate description. Attempts to interpolate such functions with a set of Laguerre functions (polynomials multiplied by a single exponential function) become computationally uneconomical owing to the large number of basis functions needed to achieve good accuracy. An economical basis set will always consist of a number of exponential functions. If a set of integration points and weights suitable for multi-exponential basis could be found, numerical integration of atomic and molecular wavefunctions could be carried out to good accuracy with a single integration grid. This avoids the messy change-overs of the integration grid for different regions, etc. during the process of integration, and adds to the accuracy as well as to the efficiency and tidiness of the computer programme.

However, a formula for a multi-exponent basis set cannot be directly formulated in terms of the usual Gauss-Legendre approach via orthogonal polynomials. We shall follow an alternative procedure.

2. Alternative formulation

Let $\psi(x)$ be a function of the sort encountered in atomic and molecular wave-function calculations. $\psi(x)$ can thus be regarded as being most economically expandable in terms of Slater functions.[6] We may consider, as an example, the set $\phi_k(x)$, given by

$$\begin{array}{l} \exp(-x),\quad x.\exp(-x),\quad x^2.\exp(-x),\ldots \\ \exp(-ax),\ x.\exp(-ax),\ x^2.\exp(-ax),\ldots \\ \exp(-bx),\ x.\exp(-bx),\ x^2.\exp(-bx),\ldots \end{array} \qquad (3\,a)$$

to form a multi-exponential generalisation of the Laguerre set. Indeed, such a set has a characteristic of being over-complete but this is of no practical consequence as only finite sets of functions are considered. In the following we shall, for simplicity, limit ourselves to the bi-exponential case $(1, \alpha)$ where the exponential parameters are 1 and α. We are interested in a p point integration formula in E_1, such that the members of the set $(1, \alpha)$ with a total of n functions is exactly intergrated, n being equal to 2p.

3. The method of localised functions

Let $\phi_k(x)$ be a set of basis functions which span the space of functions to be intergrated. We define linear combinations $g_i(x)$, $\bar{g}_i(x)$ such that[2]

$$g_i(x) = \sum_{j=1}^{2p} a_{ij}\,\phi_j(x),\ i = 1, 2, \ldots p;$$

$$\bar{g}_i(x) = \sum_{j=1}^{2p} \bar{a}_{ij}\,\phi_j(x) \qquad (3\,b)$$

and

$$g_i(x_s) = \delta_{is}\ ;\ g'_i(x_s) = 0 \qquad (4)$$

$$\bar{g}_i(x_s) = 0\ ;\ \bar{g}'_i(x_s) = \delta_{is} \qquad (5)$$

where x_s is a given set of points in (a,b). In equations (4) and (5) the derivative with respect to x is indicated by a prime on g. A discrete set of points x_s, $s = 1,2 \ldots p$ is used to define the properties of the g and $\bar{g}$ functions indicated in equations (4) and (5). This discrete set will play the role of the trial set of integration points once the theory is developed. From equations (4) and (5), it is seen that g_k is zero at all x_s except at x_k where it is unity. Further, g_k is stationary at all x_s. The set $\bar{g}_k$ is zero at every point x_s but the gradient becomes unity at x_k, whilst remaining zero at all other points in the set x_s.

The functions $g_i(x)$, $\bar{g}_i(x)$ exist only if the determinants associated with the solution of the sets of equations (4) and (5) given above do not become identically zero. Using the standard theory of orthogonal polynomials and re-expanding $g_i(x)$ and $\bar{g}_i(x)$, it can be shown that a_{ij} and $\bar{a}_{ij}$ exist for the one dimensional case as long as no two points coincide. In higher dimensions, no general results on existence are known. However, the case of two points in two dimensions can be trivially shown to lead to a determinant which is identically zero. Some other singular cases involving higher numbers of points in two-dimensions are discussed by Salzar.[4] In this publication we shall be concerned with the one-dimensional case only ; in this case the equations are non-singular and a_{ij}, $\bar{a}_{ij}$ can be obtained by standard matrix inversion methods used for the solution of simultaneous linear equations.[1]

Any function f expandable in the set ϕ_k can also be expanded in terms of the set g. Thus,

$$f(x) = \sum_{i=1}^{\rho} (b_i g_i + \bar{b}_i \bar{g}_i), \quad \textit{and} \tag{6}$$

using equations (4) and (5),

$$f(x_s) = b_s, \; f'(x_s) = \bar{b}_s .$$

Hence,

$$f(x) = \sum \left\{ f(x_i) g_i + f'(x_i) \bar{g}_i \right\}$$

and

$$\int_a^b f(x)\, dx = \sum_{i=1}^{p} \left\{ f(x_i) \int_a^b g_i\, dx + f'(x_i) \int_a^b \bar{g}_i\, dx \right\}.$$

Let

$$I = \int_a^b f(x)\, dx; \; h_i = \int_a^b g_i\, dx, \; \bar{h}_i = \int_a^b \bar{g}_i\, dx. \tag{7}$$

Then

$$I = \sum_{i=1}^{p} h_i f(x_i) + \bar{h}_i f'(x_i). \tag{8}$$

Equation (8) appearing above can be written as

$$I = \sum h_i [f(x_i) + (\bar{h}_i/h_i) f'(x_i)]$$

and hence, if $\bar{h}_i/h_i$ is small, using the Taylor theorem, we have

$$I = \sum h_i f(x_i + \bar{h}_i/h_i). \qquad (9)$$

Thus if (x_i) is a moderately good integration grid for $f(x)$, then $\{x_i + \bar{h}_i/h_i\}$ is an improved grid to the extent that the correction $\bar{h}_i/h_i$ is small enough for a Taylor expansion of f(x) up to only the linear term being valid. Thus we have an algorithm for determining the nodes x_s and the weights h_s of the p–point quadrature formula of the highest precision in the set ϕ_k. The computational steps involved are as follows :—

1. Choose the set of n expansion functions ϕ_k.
2. Choose an initial set of integration points x_i, i = 1,2,...p, where n = 2 p.
3. Construct the sets g and $\bar{g}$ by solving the sets of linear equations (4) and (5).
4. Evaluate $\bar{h}_i/h_i$ using the analytically known values of the integrals of the basis functions.
5. Calculate $\bar{\bar{h}}_i/h_i$.
6. Hence calculate the new set of points x_i possibly using a scale factor to dampen the adjustments $\bar{h}_i/h_i$.
7. The process is iterated till $\left|\frac{\bar{h}_i}{h_i}\right| < \varepsilon$ where ε is a given refinement criterion.

The above method rapidly converged to the standard Gauss-Laguerre roots when it was used with a single exponential basis set. Similarly, the Gauss-Legendre and Hermite sets could be reproduced very rapidly using the appropriate basis sets. With the multi-exponent case, convergence was slower. Since the integration weights h_i are known to be positive, the use of $\bar{h}_i/|h_i|$ instead of $\bar{h}_i/h_i$, together with a damping factor of about 0.5 led to better convergence. Further, the selection of the trial set of points became an important factor in regard to convergence for formulae with $p \geq 4$. The following method was used to determine a trial set of points to initiate the programme. Let x_i be the Laguerre set of points (p–point formula) in the Gauss-Laguerre formula. We base our formula for the trial set X_i on the previously obtained p–1 point formula whose first and last points are y_1 and y_z.

Let $U = y_1/L_1$ and $V = y_z/L_z$ where L_1 and L_z are the first and last values of the p–1 point Laguerre formula. Then the trial set is taken to be

$$X_i = U x_i + ((V x_p - U x_1)/(x_p - x_i))(x_i - x_1) \qquad (10)$$

Using equation (10) we were able to obtain integration formulae for exponent pairs (1,2), (1,3), (1,4), (1,5) etc., without much difficulty. The resulting integration grids and weights up to a six-point formula are given in Tables 1 to 4; they yield percentage errors of about 10^{-10} in the basis integrals. This error was of the same order of magnitude as the rounding off errors in the computing machine used.

TABLE 1. Exponents (1, 2)

pts	wts
n = 2	
3.92766343569*-1	1.03897236687
2.42705067525	3.38063976925
n = 3	
2.77803885220*-1	7.23353213086*-1
1.56697120948	1.93998244272
4.51515738393	4.32020560176
n = 4	
2.15261994855*-1	5.57160311743*-1
1.17861236353	1.40292149670
3.13847432710	2.61464697291
6.78421272104	5.05193377099
n = 5	
1.75807107797*-1	4.53716182149*-1
9.49590333516*-1	1.110708448147
2.45114720406	1.93338900711
4.94755460834	3.16301081329
9.16563020285	5.65930065613
n = 6	
1.48612567792*-1	3.82907845062*-1
7.96776753329*-1	9.23233266628*-1
2.02475158315	1.55409307082
3.96768950661	2.37688369354
6.91714984147	3.62909694264
1.16248181338*1	6.18448230547
n = 7	
1.28891391018*-1	3.31761250935*-1
6.87950624077*-1	7.92643279769*-1
1.73246219048	1.30911724136
3.34169809601	1.93354102779
5.66762678122	2.76594157498
1.41620456118*-1	6.65672844588

Mean error in basis integrals : 1*-10 per cent.
* at the end of each number indicates a power of ten.

TABLE 2. Exponents (1, 3)

pts	wts
n = 2	
2.95042873895*–1	7.89685538507*–1
2.00577425563	3.06251041260
n = 3	
2.08422880584*–1	5.45656103877*–1
1.21265818788	1.56989946293
3.78984370062	3.98708422722
n = 4	
1.61370337418*–1	4.18946018487*–1
8.96929464663*–1	1.08918854920
2.48352139537	2.20783787409
5.74610575758	4.71089862717
n = 5	
1.31762781941*–1	3.40713666567*–1
7.18215773264*–1	8.50031331495*–1
1.89289130049	1.54864188033
3.97810828075	2.74659714964
7.81035517600	5.31295574631
n = 6	
1.11372833135*–1	2.87347919245*–1
6.00812593777*–1	7.01653034117*–1
1.54680574887	1.21451578484
3.10471395024	1.95690312426
5.62795699898	5.83252435437

Mean percentage error in basis integrals : 1*–9

TABLE 3. Exponents (1, 4)

pts	wts
n = 2	
2.34727932956*–1	6.32926695504* –1
1.76683343289	2.92316412661
n = 3.	
1.66466463630*–1	4.37598553487*–1
9.96365796716*–1	1.35302815142
3.39053798660	3.85696304910
n = 4.	
1.28858032106*–1	3.35302734366*–1
7.25015489476*–1	8.95708563365*–1
2.09265847320	1.99185741858
5.18385867367	4.58691900163
n = 5.	
1.05233681391*–1	2.72518252288* –1
5.77793482717*–1	6.90518426392*–1
1.55268775060	1.31776819900
3.41178513591	2.54479304440
7.08435976045	5.19305056464
n = 6.	
8.89626835065*–2	2.29767135647*–1
4.82260269270*–1	5.66784354735*–1
1.25574225785	1.00652481779
2.58363625904	1.71772160757
4.88818874215	3.02479590730
9.05956200871	5.71531620205

Mean percentage error in basis integrals: 2*–10

TABLE 4. Exponents (1, 5)

pts	wts
n = 2.	
1.93647537723*–1	5.24303275819*–1
1.61327908973	2.85093607654
n = 3.	
1.38447873728*–1	3.65047814536*–1
8.49532250408*–1	1.21067172441
3.13891919374	3.79529077236
n = 4.	
1.07125716659*–1	2.79211641792*–1
6.08384056716*–1	7.62006957751*–1
1.83136094557	1.86239914247
4.83249728691	4.53118938455
n = 5.	
8.75191314856*–2	2.26891208975*–1
4.83202597639*–1	5.81896003059*–1
1.32110205585 —	1.16164472649
3.03952821284	2.43366000046
6.63364638407	5.14109772282
n = 6.	
7.40060682329*–2	1.91285243538*–1
4.02664850004*–1	4.75559311803*–1
1.05831374211	8.63409358670*–1
2.23122903889	1.56433270651
4.40847609927	2.92825525455
8.50951417896	5.66583153184

Mean percentage error in basis integrals: 2*–10.

4. Discussion

The generalisation of the Gauss-Laguerre quadrature formulae to cases which include multi-exponential basis sets will be found useful in a variety of engineering and scientific calculations. The formulae given, (up to 6 points) would be adequate for accuracies demanded by most problems, though much higher accuracies may be needed in correlation energy calculations of atoms and molecules. However, attempts to go to higher sets of points in widely differing exponentials are bound to be more difficult. In any case, it is very rarely that two widely different exponentials appear with close coupling in a realistic physical problem.

The present method can be used for obtaining generalised Gauss-Hermite quadrature formulae as well and would be of interest in treating multi-Gaussian basis sets which are currently in vogue in nuclear, atomic and molecular calculations[5] as well as in the theory of stochastic processes.

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