Construction and application of fully symmetric quadrature rules on the simplexes

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Abstract. A method for constructing fully symmetric quadrature rules of Gaussian type with positive weights, and with nodes lying inside the simplex and their applications are discussed.

Introduction

Substantial part of mathematical models in nuclear physics are formulated initially as the multidimensional elliptic boundary-value problems, for example, the consistent quadrupole-octupole vibration collective nuclear model [1]. To study such models a significant computer resource is needed because for its reduction, where the potential energy and components of the metric tensor are given by an order of 2×10^6 tabular values, to an algebraic problem the Monte-Carlo calculations of multidimensional integrals where conventionally applied. Some win can be achieved by application of the new economical computational schemes of the finite element method (FEM) [2].

The key problem in the implementation of the FEM schemes is the calculation of multidimensional integrals. It is well known [3] that as a result of applying the p-th order FEM to the solution of the discrete spectrum problem for the elliptic (Schrödinger) equation, the eigenfunction and the eigenvalue are determined with an accuracy of the order $p+1$ and $2p$, respectively, provided that all intermediate quantities are calculated with a sufficient accuracy. It follows that for the realization of the FEM of the order p, the corresponding integrals must be computed at least with an accuracy of the order $2p$. The most economical way of calculating of such integrals is the application of the quadratures of the Gaussian type.

In this talk, we restrict ourselves to constructing a system of nonlinear algebraic equations and numerical methods for solving it. The detailed description of construction of the fully symmetric quadrature rules with positive weights and with nodes lying in the simplex is given in [4].

1. Fully symmetric quadrature rules for the d-simplex

Let us construct the d-dimensional p-ordered quadrature rule

$$\int_{\Delta_d} V(x)dx=\frac{1}{d!}\sum_{j=1}^{N_{dp}} w_j V(x_{j1},\ldots,x_{jd}), \quad x=(x_1,\ldots,x_d), \quad dx=dx_1\cdots dx_d, \quad (1)$$

for integration over the d-dimensional standard unit simplex Δ_d with vertices $\hat{x}_j=(\hat{x}_{j1},\ldots,\hat{x}_{jd})$, $\hat{x}_{jk}=\delta_{jk}$, $j=0,\ldots,d$, $k=1,\ldots,d$, which is exact for all polynomials of the variables $x_1,\ldots,x_d$ of degree not exceeding p. In Eq. (1) N_{dp} is the number of nodes, w_j are the weights, and $(x_{j1},\ldots,x_{jd})$ are the nodes.

We consider fully symmetric quadrature rules with positive weights and with nodes lying in the simplex (so-called PI-type) and for this will use the symmetric combinations of barycentric coordinates (BC) $(y_1,\ldots,y_{d+1})$ that called orbits [4]. The orbit $S_{[i]}\equiv S_{m_1\ldots m_{r_{di}}}$ contains the BC

$$(y_1,\ldots,y_{d+1})=(\overbrace{\lambda_1,\ldots,\lambda_1}^{m_1\text{ times}},\ldots,\overbrace{\lambda_{m_{r_{di}}},\ldots,\lambda_{m_{r_{di}}}}^{m_{r_{di}}\text{ times}}),$$
$$\sum_{j=1}^{r_{di}} m_j=d+1, \quad \sum_{j=1}^{r_{di}} m_j\lambda_j=1, \quad m_1\geq\cdots\geq m_{r_{di}}.$$

Substituting symmetric polynomials of degree p in (1) instead of $V(x)$, we obtain a system of nonlinear algebraic equations w.r.t unknowns $W_{i,j}$ and $\lambda_{i,jl}$:

$$\int_{\Delta_d} s_2^{l_2}s_3^{l_3}\times\cdots\times s_{d+1}^{l_{d+1}}dx=\frac{1}{d!}\sum_{i=0}^{M_d}P_{di}\sum_{j=1}^{K_{di}}W_{i,j}s_{i,j2}^{l_2}s_{i,j3}^{l_3}\times\cdots\times s_{i,jd+1}^{l_{d+1}}, \quad (2)$$
$$s_k=\sum_{l=1}^{d+1}x_l^k, \quad s_{i,jk}=\sum_{l=1}^{r_{di}}m_l\lambda_{i,jl}^k \quad 2l_2+3l_3+\cdots+(d+1)l_{d+1}\leq p,$$

where P_{di} is the number of different permutations of the BC corresponded to the orbit $S_{[i]}$. The number of independent equations for fully symmetric p-order quadrature rules is presented in Table 1.

$d\backslash p$	4	6	8	10	12	14	16	18	20
2	4	7	10	14	19	24	30	37	44
3	5	9	15	23	34	47	64	84	108
4	5	10	18	30	47	70	101	141	192
5	5	11	20	35	58	90	136	199	282
6	5	11	21	38	65	105	164	248	364

TABLE 1. The numbers E_{dp} of independent equations for fully symmetric p-order quadrature rules.

2. Numerical technique

We have chosen a modified Levenberg-Marquardt method [5, 6] to solve a system of nonlinear equations with convex constraints, that is more robust to the initial guess than Newton-type methods, and can be more stable than Newton-type method in the cases when the inverse problem becomes ill-posed.

Consider the problem of solving the constrained system of nonlinear equations

$$f_i(\mathbf{x}) = 0, \quad i = 1, \dots, m, \quad \mathbf{x} = (x_1, \dots, x_n) \in \mathbf{X}, \tag{3}$$

and the corresponding minimization problem

$$\min_{\mathbf{x}\in\mathbf{X}} \|\mathbf{F}(\mathbf{x})\|^2, \quad \mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_m(\mathbf{x}))^T, \tag{4}$$

where $\mathbf{X} \subseteq R^n$ is a nonempty, closed and convex set. LM-type algorithm is an iterate method which, basically, solves at each iteration a linearization subproblem with the form

$$\min_{\mathbf{x}^k+\mathbf{h}\in\mathbf{X}} G_k(\mathbf{h}), \quad G_k(\mathbf{h}) = \frac{1}{2}\|\mathbf{F}(\mathbf{x}^k) + \mathbf{J}_k\mathbf{h}\|^2 + \frac{1}{2}\mu_k(\mathbf{h}, \mathbf{D}_k\mathbf{h}), \tag{5}$$

where $\mathbf{x}^k$ is the current iterate, $\mathbf{J}_k \in R^{m\times n}$ is a Jacobian of $\mathbf{F}(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^k$, $\mathbf{D}_k \in R^{n\times n}$ is a positive diagonal matrix and in most cases $\mathbf{D}_k = \mathrm{diag}(\mathbf{J}_k^T\mathbf{J}_k)$ or a unit matrix, and μ_k is a positive parameter. Note that $G_k(\mathbf{h})$ is a strictly convex quadratic function. Hence the solution $G_k(\mathbf{h})$ of subproblem (5) always exists uniquely, in particular for unconstrained case

$$\mathbf{h}^k = -(\mathbf{J}_k^T\mathbf{J}_k + \mu_k\mathbf{D}_k)^{-1}\mathbf{J}_k^T\mathbf{F}(\mathbf{x}^k). \tag{6}$$

Conclusion

Using the presented technique the quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5- and 6-simplexes are obtained [4]. For the convenience of their use, the INQSIM program for unpacking them in expanded form, and examples of their application are provided in JINRLIB Program Library [7]. The developed method is oriented on solving the six-dimensional elliptic boundary value problem by the finite element method for describing the discrete spectrum of the collective model of the atomic nuclei [1, 2].

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