

An International Journal computers & mathematics with applications

PERGAMON Computers and Mathematics with Applications 45 (2003) 1829-1840

www.elsevier.com/locate/camwa

Symmetric Quadrature Rules on a Triangle

S. Wandzura[†] **HRL** Laboratories 3011 Malibu Canyon Road Malibu, CA 90265, U.S.A.

H. XIAO[‡]

Department of Computer Science, Yale University New Haven, CT 06520, U.S.A.

(Received and accepted May 2002)

Abstract—We present a class of quadrature rules on triangles in \mathbb{R}^2 which, somewhat similar to Gaussian rules on intervals in \mathbb{R}^1 , have rapid convergence, positive weights, and symmetry. By a scheme combining simple group theory and numerical optimization, we obtain quadrature rules of this kind up to the order 30 on triangles. This scheme, essentially a formalization and generalization of the approach used by Lyness and Jespersen over 25 years ago, can be easily extended to other regions in \mathbb{R}^2 and surfaces in higher dimensions, such as squares, spheres. We present example formulae and relevant numerical results. © 2003 Elsevier Science Ltd. All rights reserved.

Keywords—Symmetric quadrature, Triangle, Gaussian quadrature.

1. INTRODUCTION

Gaussian quadratures are a classical tool of numerical integration, and possess several desirable features such as positivity of weights, and an optimal number of nodes: an n-point Gaussian rule is exact for all polynomials of orders up to 2n-1, and no n-point rule is exact for all polynomials of order 2n. In one dimension, since each quadrature node contributes two parameters (one as the coordinate, and the other as the weight), it is expected that an n-point quadrature rule can integrate exactly 2n functions (not necessarily polynomials). Indeed, for many classes of functions including smooth functions and functions with end-point singularities, such quadratures exist (see, for example, [1,2]); when the functions to be integrated are polynomials, such integration rules are referred to as Gaussian quadratures.

Naturally, one would attempt to generalize the above theory to two-dimensional cases, and expect that an n-point quadrature in 2-d integrates 3n functions exactly. Obviously, an excellent upper bound for the number of quadrature nodes that is required to integrate exactly all

The authors thank Professor V. Rokhlin for his encouragement, advice, and support.

†The work of this author was supported in part by the Defense Advanced Research Projects Agency (DARPA) of the U.S. Department of Defense under Air Force Office of Scientific Research Contract No. F49620-91-C-0064, and in part by DARPA Contract No. MDA972-95-C-0021.

†The work of this author was supported by DARPA/AFOSR under Grant F49620-97-1-0011.

polynomials up to order n is given by tensor product rules; a lower bound is given by Stroud in [3] for triangles and other simplexes in \mathbb{R}^n . However, no general theory regarding the optimal number of quadrature nodes in two dimensions is known to the authors. In fact, the situation in two dimensions seems to be considerably more complex. While the interval is the only connected compact subset of \mathbb{R}^1 , regions of \mathbb{R}^2 come in an infinite variety of shapes, each with its own topological features. It seems likely that each shape should require a different set of quadrature formulae, and should have its own theories.

Since triangles are a standard tool for describing regions and surfaces in higher dimensions, and are one of the simplest forms in \mathbb{R}^2 , quadratures for triangles have been studied in some detail. In particular, Lyness and Jespersen published a class of quadratures of moderate degree (up to order 12) on triangles over 25 years ago [4]. Their quadratures have many desirable properties of Gaussian quadratures in one dimension, such as rapid convergence, symmetry (or equivalently, invariance under a preselected finite group of linear transformations of the plane), and positivity of weights. Since then, several new quadratures of this type have been constructed (see [5]).

In this paper, we formalize the approach used in [4] by combining simple facts of group theory and straightforward numerical optimization, and develop a scheme for the construction of quadratures of relatively high orders. Since this scheme does not directly depend upon detailed geometry of the integration regions (rather, the geometric information is encapsulated in the corresponding symmetry groups as formulated below), it is easily extendable to other regions in \mathbb{R}^2 , and to regions in higher dimensions.

The paper is organized as follows. In Section 2, we summarize elementary mathematical and numerical facts to be used in this paper. In Section 3, we develop the analytical apparatus for the numerical construction of quadratures on triangles. We summarize our numerical scheme in Section 4, and present results in Section 5. The last section contains discussions and conclusions.

2. MATHEMATICAL AND NUMERICAL PRELIMINARIES

In this section, we collect the mathematical and numerical tools to be used in the construction of the quadratures of this paper.

2.1. Symmetry Group of Equilateral Triangles

We start with summarizing several elementary facts of the symmetry group of equilateral triangles in \mathbb{R}^2 .

As is well known, the symmetry group of an equilateral triangle—the group of all orthogonal linear transformations of the plane under which the equilateral triangle is invariant—is a reflection group often referred to as D_3 (see [6]). D_3 has six elements, and has a two-dimensional matrix representation shown below (see Table 1). Clearly, seen as orthogonal transformations of the plane, matrices A, B, and C correspond to rotations by π about the corresponding three medians of the equilateral triangle (see Figure 1), and matrices D and F correspond to clockwise rotations about the center by $2\pi/3$ and $4\pi/3$, respectively.

Table 1. Two-dimensional matrix representation of $D_3 = \{E, A, B, C, D, F\}$.

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \cos \frac{2\pi}{3} & \sin \frac{2\pi}{3} \\ -\sin \frac{2\pi}{3} & \cos \frac{2\pi}{3} \end{pmatrix} & \begin{pmatrix} \cos \frac{4\pi}{3} & \sin \frac{4\pi}{3} \\ -\sin \frac{4\pi}{3} & \cos \frac{4\pi}{3} \end{pmatrix} \\ E & A & B \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \begin{pmatrix} \cos \frac{2\pi}{3} & -\sin \frac{2\pi}{3} \\ -\sin \frac{2\pi}{3} & -\cos \frac{2\pi}{3} \end{pmatrix} & \begin{pmatrix} \cos \frac{4\pi}{3} & -\sin \frac{4\pi}{3} \\ -\sin \frac{4\pi}{3} & -\cos \frac{4\pi}{3} \end{pmatrix} \\ C & D & F \end{pmatrix}$$

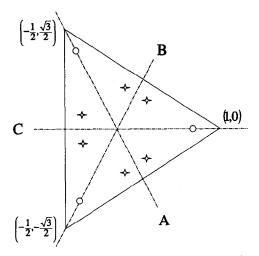


Figure 1. An equilateral triangle with the vertices $(-1/2, \sqrt{3}/2)$, $(-1/2, -\sqrt{3}/2)$, (1,0), and orbits.

The action of D_3 separates points of the equilateral triangle into disjoint subsets. In particular, denoting the equilateral triangle by T, and defining the orbit $S_{(x,y)}$ of an arbitrary point (x,y) in T by the formula

$$S_{(x,y)} = \{ g(x,y) \mid g \in D_3 \}, \tag{1}$$

we have

$$S_{(x,y)} \cap S_{(u,v)} = \emptyset, \qquad \text{if } (x,y) \notin S_{(u,v)}, \tag{2}$$

and

$$T = \bigcup_{(x,y) \in T} S_{(x,y)}. \tag{3}$$

A quick inspection of the group D_3 shows that each orbit of T assumes one of the three forms: the class one orbit which consists of one point (which, inevitably, is the center of the triangle); the class two orbit which consists of three points, one from each median; and the class three orbit which consists of six points, none of which can be on a median. In Figure 1, we show an equilateral triangle and two of its orbits. The points depicted by small circles are points from a class two orbit, and the points depicted by diamonds are points from a class three orbit.

2.2. Invariant Polynomials of Equilateral Triangles

Let p be any polynomial defined on an equilateral triangle and g an arbitrary element in D_3 . We define the polynomial gp (the image of p under the action of g) by the following formula:

$$(g p)(x,y) = p \left(g^{-1}(x,y)\right). \tag{4}$$

Then, we say that p is an invariant polynomial with respect to D_3 (or equivalently, p is D_3 invariant) if for all $g \in D_3$,

$$(g p)(x,y) = p(x,y).$$

$$(5)$$

Let us refer to the set of all D_3 invariant polynomials as I. Clearly, I is nonempty, since polynomials $1, x^2 + y^2, x^3 - 3xy^2$ are elements of I. The structure of I is well known in invariant theory (see, for example, [7,8]); we summarize relevant results in the following theorem.

THEOREM 2.1. The set I is a finitely generated ring. Furthermore, $\{x^2 + y^2, x^3 - 3xy^2\}$ is a set of fundamental invariants that generate I.

2.3. Newton's Method

Newton's method is a classical iterative technique used in solving equations of the form

$$F(\mathbf{x}) = \mathbf{0},\tag{6}$$

where $F: \mathbb{R}^n \to \mathbb{R}^n$ is of the form

$$F(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_n(\mathbf{x}) \end{bmatrix}. \tag{7}$$

Newton's method has quadratic convergence when the initial approximation is sufficiently close to the solution, as summarized below in Theorem 2.2; when the initial point is not sufficiently close to the solution, the iteration may diverge.

DEFINITION 2.1. The Jacobian **DF**: $\mathbb{R}^n \to \mathbb{R}^n$ of the function **F** (see (7)) is defined by

$$\mathbf{DF}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}. \tag{8}$$

THEOREM 2.2. Suppose that $\mathbf{F}: \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable in a neighborhood $n_b(\xi)$ of ξ , where

$$\mathbf{F}(\xi) = \mathbf{0} \tag{9}$$

and

$$|\mathbf{DF}(\mathbf{x})| \neq 0,\tag{10}$$

for all $\mathbf{x} \in n_b(\xi)$. Suppose further that $\mathbf{x}_0, \mathbf{x}_1, \ldots$, is a sequence of points in $n_b(\xi)$ such that

$$\mathbf{x_{k+1}} = \mathbf{x_k} - DF(\mathbf{x_k})^{-1}F(\mathbf{x_k}),\tag{11}$$

for all $k \geq 0$. Then, there exist $\epsilon > 0$, $\delta > 0$, and integer $N_{\epsilon,\delta} \geq 0$, such that if

$$\|\mathbf{x}_0 - \boldsymbol{\xi}\| < \epsilon, \tag{12}$$

then

$$\|\mathbf{x}_{k+1} - \xi\| < \delta \|\mathbf{x}_k - \xi\|^2,$$
 (13)

for all $k \geq N_{\epsilon,\delta}$.

2.4. Simulated Annealing

In this section, we give a brief summary of the technique of simulated annealing; for more detailed discussions on this topic, see, for example, [9–11].

As is well known, simulated annealing is a Monte Carlo approach for minimizing certain multivariate functions (see, for example, [9,10]); it simulates the physical process of repeatedly heating and slowly cooling, which is often used to lower a physical system's energy level.

Suppose we would like to minimize a nonnegative scalar function $J(\mathbf{S})$ where the variables \mathbf{S} of J have to satisfy certain constraints. Clearly, we may regard J as the energy of a physical system at the state \mathbf{S} , where each allowable assignment to \mathbf{S} is a valid state of the system. We may also associate each state \mathbf{S} by a parameter T (denoting the temperature) so that as T decreases, the energy J of the physical system also decreases. Thus, the problem of minimizing J is equivalent to finding the minimum energy state \mathbf{S}_{\min} of the physical system at a low temperature. In simulated

annealing, the global minimum state S_{min} is searched systematically in the space of allowable states through a randomized state modification algorithm (or, randomized update) applied at a sequence of gradually lowered temperatures.

The most distinct feature of the simulated annealing process is the randomized state modification algorithm, which ensures that any allowable state of the system is reachable. More specifically, suppose that the current state of the system is \mathbf{S}_i with energy $J(\mathbf{S}_i)$. \mathbf{S}_i is then tentatively altered to a random state $\tilde{\mathbf{S}}_i$, with the resulting change ΔJ of energy computed by the formula

$$\Delta J = J\left(\tilde{\mathbf{S}}_{i}\right) - J(\mathbf{S}_{i}). \tag{14}$$

If $\Delta J \leq 0$, this update is accepted, and the system evolves to the new state $\mathbf{S}_{i+1} = \tilde{\mathbf{S}}_i$; if $\Delta J > 0$, the update is accepted with the probability

$$P(\Delta J) = \exp\left(-\frac{\Delta J}{kT}\right) \tag{15}$$

(k, T > 0 are constants), and rejected with the probability $1 - P(\Delta J)$. If the proposed update is rejected, another random state $\tilde{\mathbf{S}}_i$ is proposed, and the decision process above is repeated.

Obviously, when the temperature T approaches zero, only states with minimum energy have a nonzero probability of occurrence. This, combined with the condition that T is lowered in a sufficiently slow manner so that the system achieves thermal equilibrium at each temperature, shows that a global minimum energy state at the low final temperature can be achieved (see [12]). Much work of the implementation of the simulated annealing process involves the development of an annealing (or cooling) schedule which includes the initial temperature setting, the scheduling of the decrease of T, and the final temperature setting.

3. ANALYTICAL APPARATUS

In this section, we develop analytical tools to be used in Section 4. Theorem 3.1 shows that the integral of any function on the equilateral triangle can be calculated by integrating its average over D_3 ; this result is an immediate consequence of the fact that all elements in D_3 have unit determinants. The simple fact that the average of any function over D_3 is D_3 invariant is shown in Theorem 3.2.

THEOREM 3.1. Suppose that p is an arbitrary function defined on an equilateral triangle R in \mathbb{R}^2 . Suppose further that function \bar{p} is defined by the formula

$$\bar{p}(x,y) = \frac{1}{|D_3|} \sum_{g \in D_3} (g \, p)(x,y). \tag{16}$$

Then,

$$\int_{R} p(x,y) dx dy = \int_{R} \bar{p}(x,y) dx dy. \tag{17}$$

THEOREM 3.2. Suppose that p is an arbitrary function defined on an equilateral triangle R in \mathbb{R}^2 . Then, the function \bar{p} defined by formula (16) is D_3 invariant.

As is seen in Section 2.2, all polynomials that are D_3 invariant on the equilateral triangle can be generated from the two fundamental polynomials $p_1 = x^2 + y^2$ and $p_2 = x^3 - 2xy^2$. More specifically, all invariant polynomials over the equilateral triangle can be written as linear combinations of terms of the form $p_1^m \cdot p_2^n$, where m, n are nonnegative integers. Since p_1 , p_2 are algebraically independent, the set $B = \{p_1^m \cdot p_2^n, m, n \geq 0\}$ constitutes a basis of I (see Section 2.2). Thus, an orthogonal basis \tilde{B} of I is easily constructed from B via a Gram-Schmidt process.

Order	Polynomial
0	1
2	$\sqrt{\frac{5}{3}} \left(4x^2 + 4y^2 - 1 \right)$ $\left(\frac{2}{3} \right)^{5/2} \left(4 - 30x^2 + 35x^3 - 30y^2 - 105xy^2 \right)$
3	$\left(\frac{2}{3}\right)^{5/2} \left(4 - 30x^2 + 35x^3 - 30y^2 - 105xy^2\right)$
4	$5\sqrt{\frac{7}{243}}\left[1-12\left(x^2+y^2\right)+36\left(x^2+y^2\right)^2+16x\left(-x^2+3y^2\right)\right]$
5	$\frac{4}{9\sqrt{3}} \left[8 - 140\left(x^2 + y^2\right) + 420\left(x^2 + y^2\right)^2 + 70x\left(x^2 - 3y^2\right) - 385x\left(x^2 + y^2\right)\left(x^2 - 3y^2\right) \right]$
6	$\frac{7\sqrt{5}}{9\sqrt{11863}} \left[\frac{9 - 2960x(x^2 - 3y^2) + 10560x(x^2 - 3y^2)(x^2 + y^2)}{-216(x^2 + y^2) + 3300(x^2 + y^2)^2 - 11440(x^2 + y^2)^3} \right]$
6	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$
7	$\frac{8\sqrt{2}}{243} \begin{bmatrix} 40 - 1260(x^2 + y^2) + 9240(x^2 + y^2)^2 \\ +15015x(x^2 - 3y^2)(x^2 + y^2)^2 - 770x(x^2 - 3y^2) \\ -2002(11x^6 + 15x^4y^2 + 45x^2y^4 + 9y^6) \end{bmatrix}$

Table 2. Invariant polynomials in \tilde{B} up to order seven. Each polynomial is normalized such that its L^2 norm on the triangle in Figure 1 is $\sqrt{27}/4$.

In Table 2, we list polynomials in \tilde{B} of orders up to seven. These polynomials are normalized so that their L^2 norms on the equilateral triangle specified by vertices $(-1/2, \sqrt{3}/2), (-1/2, -\sqrt{3}/2), (1,0)$ are $\sqrt{27}/4$.

4. SYMMETRIC QUADRATURES FOR THE TRIANGLE

In this paper, we construct quadrature rules of the form

$$\sum_{i=1}^{n} w_i \cdot f(x_i, y_i), \tag{18}$$

which serves to approximate the integral

$$\int_{R} dx \, dy \, f(x, y),\tag{19}$$

where R is chosen arbitrarily to be the equilateral triangle shown in Figure 1. Throughout this paper, we focus our attention to the class of quadratures whose nodes, (x_i, y_i) , lie entirely within the boundaries of the triangle, and whose weights, w_i , assume positive values.

Additionally, we construct quadratures that are symmetric with respect to D_3 on the given equilateral triangle; in other words, the quantity defined by (18) should stay invariant if we subject the nodes and weights to the group action of D_3 . The following definition characterizes more explicitly the nature of symmetric quadratures of triangles.

DEFINITION 4.1. Given an equilateral triangle R in \mathbb{R}^2 . We say that a quadrature of form (18) is symmetric with respect to D_3 if the set of quadrature nodes $V = \{(x_1, y_1), (x_1, y_1), \dots, (x_n, y_n)\}$ is of the form

$$V = \bigcup_{i=1}^{A} S_{(x_{k_i}, y_{k_i})}$$
 (20)

 $(S_{(x_{k_i},y_{k_i})})$ is the orbit of (x_{k_i},y_{k_i}) ; see Section 2.1), and that

$$w_i = w_j, \tag{21}$$

for all i, j such that (x_i, y_i) and (x_j, y_j) belong to the same orbit. The parameter A in (20) is the total number of orbits contained in V, and the sequence $\{k_i\}$ is a subsequence of $\{1, 2, \ldots, n\}$.

REMARK 4.1. Requirements (20) and (21) for the quadrature formula (18) greatly reduce the number of free parameters in a formula. More specifically, a node at the center of the triangle (or equivalently, a class one orbit) provides just one parameter (the weight) instead of three, and the six nodes in a class three orbit provide three parameters (two for coordinates and one for weight) instead of 18.

We parameterize the coordinates of each orbit by a set of parameters $\{\lambda_i\} = \lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,\mu_i}$ and an integer m_i (the multiplicity). For the equilateral triangle, m_i equals 1, 3, and 6 for orbits of class one, two, and three, respectively; correspondingly, μ_i equals 0, 1, and 2, respectively. The nodes and weights could then be found by solving the set of nonlinear equations

$$\sum_{i=1}^{A} w_{i} m_{i} f_{n} \left[x \left(\lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,\mu_{i}} \right) \right] = \int_{R} f_{n}, \tag{22}$$

for n ranging over all invariant polynomials for which the quadrature rule will be exact.

REMARK 4.2. Due to Theorems 3.1 and 3.2, in order for the quadrature to integrate exactly all polynomials on the triangle up to a predetermined order, only those polynomials that are invariant need to be considered in (22); all other polynomials (up to the same order) will be integrated exactly by the resulting quadrature formula through averaging.

The combination of the reduction of the number of equations in (22) (see Remark 4.2), and the reduction of the number of free parameters in the quadrature formula (see Remark 4.1) greatly lowers the rank of the system that we are required to solve; this formulation is essentially a generalization of the approach used by Lyness and Jespersen in [4].

We solve system (22) iteratively via Newton's method (see Section 2.3), with the parameters of the system $X \in \mathbb{R}^{A+\sum_{i=1}^{A} \mu_i}$ defined by

$$X = (w_1, \lambda_{1,1}, \dots, \lambda_{1,\mu_1}, w_2, \lambda_{2,1}, \dots, w_A, \lambda_{A,1}, \dots, \lambda_{A,\mu_A})^{\mathsf{T}},$$
(23)

and the function $F: \mathbb{R}^{A+\sum_{i=1}^{A}\mu_i} \to \mathbb{R}^n$ defined by

$$F(X) = \begin{bmatrix} \sum_{i=1}^{A} w_i \, m_i \, f_1 \left[x(\lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,\mu_i}) \right] - \int_R f_1 \\ \vdots \\ \sum_{i=1}^{A} w_i \, m_i \, f_n \left[x(\lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,\mu_i}) \right] - \int_R f_n \end{bmatrix}$$
(24)

REMARK 4.3. In practice, the number of unknowns $A + \sum_{i}^{A} \mu_{i}$ may be greater than the number n of equations. In such cases, we use a pseudoinverse in Newton's method.

Table 3. Seven-point symmetric quadrature on triangles for polynomials up to order 5.

m	x y		w	
1	0.000000000000000E+00	0.000000000000000E+00	0.225000000000000E+00	
3	-0.4104261923153453E+00	0.000000000000000E+00	0.1323941527885062E+00	
3	0.6961404780296310E+00	0.0000000000000000E+00	0.1259391805448271E+00	

Table 4. 25-point symmetric quadrature on triangles for polynomials up to order 10.

m	\boldsymbol{x}	x y	
1	0.000000000000000E+00	0.000000000000000E+00	0.8352339980519638E-01
3	-0.4935962988634245E+00	0.000000000000000E+00	0.7229850592056743E-02
3	-0.2840373491871686E+00	0.000000000000000E+00	0.7449217792098051E-01
3	0.4457307617703263E+00	0.00000000000000E+00	0.7864647340310853E-01
3	0.9385563442849673E+00	0.000000000000000E+00	0.6928323087107504E-02
6	-0.4474955151540920E+00	-0.5991595522781586E+00	0.2951832033477940E-01
6	-0.4436763946123360E+00	-0.2571781329392130E+00	0.3957936719606124E01

Table 5. 54-point symmetric quadrature on triangles for polynomials up to order 15.

m	\boldsymbol{x}	у	`w
3	-0.3748423891073751E+00	0.0000000000000000E+00	0.3266181884880529E-01
3	-0.2108313937373917E+00	0.00000000000000000E+00	0.2741281803136436E-01
3	0.1204084962609239E+00	0.00000000000000E+00	0.2651003659870330E-01
3	0.5605966391716812E+00	0.000000000000000E+00	0.2921596213648611E-01
3	0.8309113970031897E+00	0.00000000000000E+00	0.1058460806624399E-01
3	0.9502746194248890E+00	0.000000000000000E+00	0.3614643064092035E02
6	-0.4851316950361628E+00	-0.4425551659467111E+00	0.8527748101709436E-02
6	-0.4762943440546580E+00	-0.1510682717598242E+00	0.1391617651669193E-01
6	-0.4922845867745440E+00	-0.6970224211436132E+00	0.4291932940734835E-02
6	-0.4266165113705168E+00	-0.5642774363966393E+00	0.1623532928177489E-01
6	-0.3968468770512212E+00	-0.3095105740458471E+00	0.2560734092126239E-01
6	-0.2473933728129512E+00	-0.2320292030461791E+00	0.3308819553164567E-01

Table 6. 85-point symmetric quadrature on triangles for polynomials up to order 20.

m	\boldsymbol{x}	у	w		
1	0.000000000000000E+00	0.00000000000000000E+00	0.2761042699769952E-01		
3	-0.4977490260133565E+00	0.00000000000000E+00	0.1779029547326740E-02		
3	-0.3587903720915737E+00	0.00000000000000E+00	0.2011239811396117E-01		
3	-0.1932918138657104E+00	0.000000000000000E+00	0.2681784725933157E-01		
3	0.2064993924016380E+00	0.000000000000000E+00	0.2452313380150201E-01		
3	0.3669431077237697E+00	0.000000000000000E+00	0.1639457841069539E-01		
3	0.6767931784861860E+00	0.000000000000000E+00	0.1479590 7 39864960E-01		
3	0.8827927364865920E+00	0.0000000000000000E $+00$	0.4579282277704251E-02		
3	0.9664768608120111E+00	0.000000000000000E+00	0.1651826515576217E-02		
6	-0.4919755727189941E+00	-0.7513212483763635E+00	0.2349170908575584E-02		
6	-0.4880677744007016E+00	-0.5870191642967427E+00	0.4465925754181793E-02		
6	-0.4843664025781043E+00	-0.1717270984114328E+00	0.6099566807907972E-02		
6	-0.4835533778058150E+00	-0.3833898305784408E+00	0.6891081327188203E-02		
6	-0.4421499318718065E+00	-0.6563281974461070E+00	0.7997475072478163E-02		
6	-0.4466292382741727E+00	-0.6157647932662624E-01	0.7386134285336024E-02		
6	-0.4254937754558538E+00	-0.4783124082660027E+00	0.1279933187864826E-01		
6	-0.4122204123735024E+00	-0.2537089901614676E+00	0.1725807117569655E-01		
6	-0.3177533194934086E+00	-0.3996183176834929E+00	0.1867294590293547E-01		
6	-0.2889337325840919E+00	-0.1844183967233982E+00	0.2281822405839526E-01		

As Newton's method is guaranteed of convergence only when the starting point is sufficiently close to the solution (see Section 2.3), we use a second method to obtain the initial approximations. In particular, we consider the problem of minimizing the scalar function J defined by the

\overline{m}	x	y	w
3	-0.4580802753902387E+00	0.000000000000000000E+00	0.8005581880020417E-02
3	-0.3032320980085228E+00	0.000000000000000E+00	0.1594707683239050E-01
3	-0.1696674057318916E+00	0.0000000000000000E+00	0.1310914123079553E-01
3	0.1046702979405866E+00	0.000000000000000000E+00	0.1958300096563562E01
3	0.2978674829878846E+00	0.00000000000000000E+00	0.1647088544153727E-01
3	0.5455949961729473E+00	0.000000000000000000E+00	0.8547279074092100E-02
3	0.6617983193620190E+00	0.000000000000000E+00	0.8161885857226492E-02
3	0.7668529237254211E+00	0.00000000000000E+00	0.6121146539983779E-02
3	0.8953207191571090E+00	0.000000000000000000E+00	0.2908498264936665E-02
3	0.9782254461372029E+00	0.000000000000000E+00	0.6922752456619963E-03
6	-0.4980614709433367E+00	-0.4713592181681879+00	0.1248289199277397E-02
6	-0.4919004480918257E+00	-0.1078887424748246+00	0.3404752908803022E-02
6	-0.4904239954490375E+00	-0.3057041948876942+00	0.3359654326064051E-02
6	-0.4924576827470104E+00	-0.7027546250883238+00	0.1716156539496754E-02
6	-0.4897598620673272E+00	-0.7942765584469995+00	0.1480856316715606E-02
6	-0.4849757005401057E+00	-0.5846826436376921+00	0.3511312610728685E-02
6	-0.4613632802399150E+00	-0.4282174042835178+00	0.7393550149706484E-02
6	-0.4546581528201263E+00	-0.2129434060653430+00	0.7983087477376558E-02
6	-0.4542425148392569E+00	-0.6948910659636692+00	0.4355962613158041E-02
6	-0.4310651789561460E+00	-0.5691146659505208+00	0.7365056701417832E-02
6	-0.3988357991895837E+00	-0.3161666335733065+00	0.1096357284641955E-01
6	-0.3949323628761341E+00	-0.1005941839340892+00	0.1174996174354112E-01
6	-0.3741327130398251E+00	-0.4571406037889341+00	0.1001560071379857E-01
6	-0.3194366964842710E+00	-0.2003599744104858+00	$0.1330964078762868E{-01}$
6	-0.2778996512639500E+00	-0.3406754571040736+00	0.1415444650522614E-01
6	-0.2123422011990124E+00	-0.1359589640107579+00	0.1488137956116801E-01

Table 7. 126-point symmetric quadrature on triangles for polynomials up to order 25.

formula

$$J = \sum_{k=1}^{n} \omega_k \left[\int_R f_k - \sum_i w_i \, m_i \, f_k(\lambda_i) \right]^2, \tag{25}$$

where $f_k(\lambda_i)$ stands for $f_k[x(\lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,\mu_i})]$, and ω_k is expirically chosen to be $1/d_k$ with d_k the degree of f_k .

Clearly, any solution to the nonlinear system (22) is a global minimum of J. However, for high order quadrature rules, J may have many local minima. We construct solutions to the minimization problem (25) via the technique of simulated annealing, as is discussed in Section 2.4.

5. NUMERICAL RESULTS

We have implemented the scheme of Section 4 in Mathematica, and obtained symmetric quadrature rules of orders up to 30. In this section, we present examples of quadrature formulae, and relevant numerical results.

In Tables 3-8, we present several symmetric quadratures for the equilateral triangle in Figure 1. These formulae are exact for integrating polynomials up to orders 5, 10, 15, 20, 25, and 30, respectively. In each table, the coordinates x and y of the nodes are listed in columns two and three, respectively, and the weights w are listed in column four. Due to the symmetry of the quadrature rules, only one node (represented by the four-tuple (m, x, y, w)) is listed per orbit; the coordinates of the remainder nodes of the orbit are calculated by the formula

$$g(x,y), (26)$$

Table 8. 175-point symmetric quadrature on triangles for polynomials up to order 30.

$\lceil m \rceil$	· x		w
1	0.00000000000000E+00	y 0.000000000000000000E+00	0.1557996020289920E-01
3	-0.4890048253508517E+00	0.000000000000E+00	0.3177233700534134E-02
3			0.1048342663573077E-01
3	-0.3755064862955532E+00	0.00000000000000E+00	
1	-0.2735285658118844E+00	0.000000000000000000000000000000000000	0.1320945957774363E-01
3	-0.1461412101617502E+00	0.000000000000000000000000000000000000	0.1497500696627150E01
3	0.1570364626117722E+00	0.00000000000000E+00	0.1498790444338419E-01
3	0.3179530724378968E+00	0.00000000000000E+00	0.1333886474102166E-01
3	0.4763226654738105E+00	0.00000000000000E+00	0.1088917111390201E-01
3	0.6302247183956902E+00	0.00000000000000E+00	0.8189440660893461E-02
3	0.7597473133234094E+00	0.0000000000000000E+00	0.5575387588607785E-02
3	0.8566765977763036E+00	0.000000000000000E+00	0.3191216473411976E-02
3	0.9348384559595755E+00	0.000000000000000E+00	0.1296715144327045E-02
3	0.9857059671536891E+00	0.000000000000000E+00	0.2982628261349172E-03
6	-0.4986119432099803E+00	-0.1459114994581331E+00	0.9989056850788964E-03
6	-0.4979211112166541E+00	-0.7588411241269780E+00	0.4628508491732533E-03
6	-0.4944763768161339E+00	-0.5772061085255766E+00	0.1234451336382413E-02
6	-0.4941451648637610E+00	-0.8192831133859931E+00	0.5707198522432062E-03
6	-0.4951501277674842E+00	-0.3331061247123685E+00	0.1126946125877624E-02
6	-0.4902988518316453E+00	-0.6749680757240147E+00	0.1747866949407337E-02
6	-0.4951287867630010E+00	-0.4649148484601980E+00	0.1182818815031657E-02
6	-0.4869873637898693E+00	-0.2747479818680760E+00	0.1990839294675034E-02
6	-0.4766044602990292E+00	-0.7550787344330482E+00	0.1900412795035980E-02
6	-0.4730349181194722E+00	-0.1533908770581512E+00	0.4498365808817451E-02
6	-0.4743136319691660E+00	-0.4291730489015232E+00	0.3478719460274719E-02
6	-0.4656748919801272E+00	-0.5597446281020688E+00	0.4102399036723953E-02
6	-0.4508936040683500E+00	-0.6656779209607333E+00	0.4021761549744162E-02
6	-0.4492684814864886E+00	-0.3024354020045064E+00	$0.6033164660795066E{-02}$
6	-0.4466785783099771E+00	-0.3733933337926417E-01	0.3946290302129598E-02
6	-0.4241903145397002E+00	-0.4432574453491491E+00	$0.6644044537680268 \text{E}{-02}$
6	-0.4144779276264017E+00	-0.1598390022600824E+00	$0.8254305856078458E{-02}$
6	-0.4037707903681949E+00	-0.5628520409756346E+00	0.6496056633406411E-02
6	-0.3792482775685616E+00	-0.3048723680294163E+00	$0.9252778144146602E\!-\!02$
6	-0.3434493977982042E+00	-0.4348816278906578E+00	0.9164920726294280E - 02
6	-0.3292326583568731E+00	-0.1510147586773290E+00	0.1156952462809767E-01
6	-0.2819547684267144E+00	-0.2901177668548256E+00	0.1176111646760917E-01
6	-0.2150815207670319E+00	-0.1439403370753732E+00	0.1382470218216540E-01

with g ranging over all nonidentity elements in D_3 . The weights of remainder nodes are w, and the total number of distinct nodes (or equivalently, the multiplicity) of this orbit is given by m. In these tables, the weights w_i of each quadrature are arbitrarily normalized so that

$$\sum_{i=1}^{n} w_i = \frac{\sqrt{27}}{4}.\tag{27}$$

For the n^{th} -order quadrature, we have tested it on all monomials $x^i \cdot y^j$, where i, j are non-negative integers such that $i+j \leq n$. In Table 9, we present the maximum absolute error over all corresponding monomials for each quadrature of orders between 1 and 30. The columns labeled with O give the orders of the quadratures, the columns labeled with N give the number of quadrature nodes, and the remaining columns give the errors of these quadratures as discussed above.

Table 9. Absolute errors of quadrature rules on triangles, with order N ranging
from 1 to 30. The order of the quadratures is listed in columns with the label O, and
number of nodes is given in columns with the label N .

0	N	Absolute Error	0	N	Absolute Error	0	N	Absolute Error
1	1	0.00000E+00	11	28	4.29344E-16	21	93	7.40621E-16
2	3	0.00000E+00	12	36	4.29344E-16	22	100	7.40621E-16
3	6	1.66533E-16	13	40	6.31439E-16	23	106	1.25601E-15
4	6	2.08166E-16	14	46	5.46437E-16	24	118	1.01394E-15
5	7	2.08166E-16	15	54	6.67705E-16	25	126	1.24250E-15
6	12	2.77555E-16	16	58	7.28583E-16	26	138	7.23678E-16
7	15	2.91433E-16	17	66	8.72105E-16	27	145	1.07031E-15
8	16	6.24500E-16	18	73	5.30825E-16	28	154	1.36241E-15
9	19	2.08166E-16	19	82	8.66526E-16	29	166	1.05724E-15
10	25	4.29344E-16	20	85	1.08149E-15	30	175	1.08730E-15

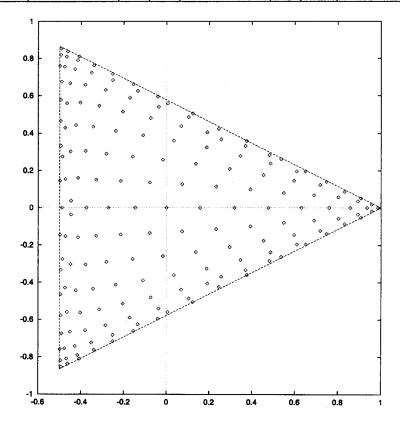


Figure 2. Symmetric quadrature of order 30 on the triangle.

In our experiments, we find the quantity e given by the formula

$$e = \frac{O(O+1)}{6N} \tag{28}$$

a useful measure of the efficiency of a quadrature, where O denotes the order of the quadrature, and N denotes the total number of nodes. Although no general theory is known regarding the optimal values of e for quadratures in two dimensions, it is expected that e should be close to 1 (may be greater than 1); clearly, e=1 for all Gaussian quadratures on the interval in \mathbb{R}^1 . As can be easily seen from Table 9, e is between 0.84 and 0.94 for the quadratures reported in this paper.

In Figure 2, we show a picture of the nodes (175 in total) of the 30th-order quadrature. Certain resemblance to the Gaussian quadratures in one dimension seems to emerge, in that the nodes are more or less evenly distributed in each direction of the integration region with higher densities in areas away from the center.

REMARK 5.1. The scheme of this paper has been applied to a considerable number of more cases than those reported in this paper. Space limitations prevent us from presenting more examples; a detailed report on quadratures on triangles can be found in [13]. With this scheme, we have also obtained quadratures on integration regions such as squares and spheres; these results will be reported in a separate paper.

6. CONCLUSIONS

We have presented a numerical scheme for the construction of symmetric quadratures on triangles in \mathbb{R}^2 . Our approach is a combination of elementary group theory with straightforward use of optimization; it is essentially a generalization and formalization of the approached used in [4]. With this scheme, we have obtained quadratures of relatively high orders for triangles. These formulae have several desired properties as those of Gaussian quadratures in one dimension, such as rapid convergence, positivity of weights, symmetry, more or less evenly distributed nodes, all nodes are interior to the integration region, etc.

This scheme is easily extendable to other symmetric regions in \mathbb{R}^2 , and integration domains in higher dimensions; with this scheme, we have also obtained quadratures of relatively high orders for integration regions such as squares and spheres.

A principal drawback of this scheme is the significant amount of human intervention involved in the simulated annealing stage. Often, one has to manually adjust the annealing parameters several times, before the process yields a satisfactory initial approximation of w_i s and x_i s that results in a convergence of Newton's method. A more systematic procedure would be desirable.

REFERENCES

- J. Ma, V. Rokhlin and S. Wandzura, Generalized Gaussian quadrature of systems of arbitrary functions, SIAM Journal of Numerical Analysis 33 (3), 971-996, (1996).
- 2. N. Yarvin and V. Rokhlin, Generalized Gaussian quadratures and singular value decompositions of integral operators, SIAM Journal of Scientific Computing 20 (2), 669-718, (1998).
- 3. A.H. Stroud, Approximate Calculation of Multiple Integrals, Prentice-Hall, (1971).
- 4. J.N. Lyness and D. Jespersen, Moderate degree symmetric quadrature rules for the triangle, Journal of the Institute of Mathematics and Its Applications 15, 19-32, (1975).
- 5. J. Berntsen and T.O. Espelid, Degree 13 symmetric quadrature rules for the triangle, In *Reports in Informatics* 44, Dept. of Informatics, University of Bergen, (1990).
- 6. M. Tinkham, Group Theory and Quantum Mechanics, McGraw-Hill, (1964).
- 7. M.D. Neusel and L. Smith, Invariant Theory of Finite Groups, American Mathematical Society, (2001).
- 8. B. Sturmfels, Algorithms in Invariant Theory, Springer-Verlag, Wien, (1993).
- 9. S. Kirkpatrick, C.D. Gelatt and M.P. Vecchi, Optimization by simulated annealing, Science 220, 671, (1983).
- S. Kirkpatrick, Optimization by simulated annealing: Quantitative studies, Journal of Statistical Physics 34, 975, (1984).
- 11. S. Haykin, Neural Networks—A Comprehensive Foundation, Prentice-Hall, (1994).
- 12. N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A. Teller and E. Teller, Equation of state calculations by fast computing machines, *Journal of Chemical Physics* 21, 1087-1092, (1953).
- S. Wandzura and H. Xiao, Quadrature rules on triangles in R², Research Report YALEU/DCS/RR-1168, Department of Computer Science, Yale University, (1998).
- 14. M. Abramowitz, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, National Bureau of Standards, (1972).
- 15. P. Silvester, Symmetric quadrature formulae for simplexes, Mathematics of Computation 24, 95-100, (1970).
- 16. A.H. Stroud and D. Secrest, Gaussian Quadrature Formulas, Prentice-Hall, (1966).