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Gradimir V. Milovanović, Tomislav Igić, and Novica Tončev

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Quadrature Formulae for Problems in Mechanics

Gradimir V. Milovanović*, Tomislav Igić† and Novica Tončev†

*Mathematical Institute of the Serbian Academy of Sciences and Arts, Knez Mihailova 36, P.O. Box 367, 11001 Beograd, Serbia
†Faculty of Civil Engineering and Architecture, University of Niš, A. Medvedeva 14, 18000 Niš, Serbia

Abstract. The fast progress in recent years in symbolic computation and variable-precision arithmetic provide a possibility for generating the recursion coefficients in the three-term recurrence relation for orthogonal polynomials with respect to several nonclassical weight functions, as well as the construction of the corresponding quadrature rules of Gaussian type. Such quadratures are very important in many applications in engineering (fracture mechanics, damage mechanics, etc.), as well as in other computational and applied sciences. The boundary element method (BEM), finite element method (FEM), methods for solving integral equations, etc. very often require the numerical evaluation of one dimensional or multiple integrals with singular or near singular integrands with a high precision. In this paper we give some improvements of quadrature rules of Gaussian type with logarithmic and/or algebraic singularities. A numerical examples is included.

Keywords: quadrature formula; weight function; integral equation; orthogonality; nodes; weight coefficients.
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INTRODUCTION

In 1972 Hajdin and Krajčinović [7] presented an integration method for the solution of boundary value problems (BVP) for ordinary differential equations. The method involves construction of only simple polynomial Green's functions and gives a very good accuracy. In general, numerical integration is a more accurate process than numerical differentiation that is implicitly present in the finite difference methods (for an error analysis see [2]). Hajdin and Krajčinović considered the completely inhomogeneous system (BVP) $Lu = f(x)$, $a \le x \le b$, with boundary conditions at $x = a$ and $x = b$ given by $B_1(u) = \alpha$ and $B_2(u) = \beta$ $(\alpha, \beta \in \mathbb{R})$, where L is a linear difference operator of nth order, $f(x)$ is an arbitrary piecewise function of x, and B_1 and B_2 are some linear combinations of the function $u(x)$ and its derivatives up to order $n-1$. Constructing Green's function $G(x,y)$ they reduced the given BVP differential problem to the Fredholm integral equation of the second kind

$$u(x) + \int_a^b G(x,y)u(y)\mathrm{d}y = g(x), \quad a < x < b, \tag{1}$$

where g(x) is a known function, and then they use two ways for solving (1):

– a quadrature rule and some selected colocation points to reduce (1) to a system of linear algebraic equations;

– an approximation of $u(x)$ by a spline function of a given order.

Although most of the problems treated in [7] related to structural mechanics, the method itself is naturally much more general. Today, integral equations appear in many fields including continuum and quantum mechanics, optimization and optimal control systems, kinetic theory of gases, communication theory, geophysics, electricity and magnetism, potential theory, biology and population genetics, mathematical economics, queueing theory, etc.

In general, the Fredholm integral equations of the second kind (FK2) are given by

$$u(x) + \mu \int_A K(x,y)u(y)w(y)\dot{\mathrm{y}} = g(x), \quad x \in A \subset \mathbb{R}, \tag{2}$$

where $K(x,y)$ is the kernel, w is a given weight function, g is a known function, $\mu \in \mathbb{R}$ is a parameter, and u is a unknown function. Today, there are many numerical methods for solving integral equations (cf. [1], [9]). Sometimes, they are developed for specific type of kernels. Numerical methods for this kind of integral equations (FK2) lead to systems of linear algebraic equations and sometimes these systems are ill-conditioned. The solution of an integral equation can be done in a polynomial form, spline function, as a piecewise polynomial, etc. For some recent very efficient methods see [4], [11], [12].

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Several methods for reducing (2) to a system of linear equations need good quadrature rules for approximating the weighted integral in (2). In addition, we mention also that the boundary element method (BEM), as well as the finite element method (FEM), which are very popular in computational applications in engineering (fracture mechanics, damage mechanics, electromagnetic diffraction, etc.), very often need accurate numerical evaluation of one dimensional or multiple integrals with singular kernels and/or singular basis functions.

In this paper we propose a method for constructing the weighted Gaussian quadrature rules for integrals with algebraic and/or logarithmic singularities. In general, quadratures of Gaussian type are very appropriate in methods for solving integral equations of type (2), as well as in numerical implementation of the BEM (see [8, Chapters 4 & 5]). They play a very important role, especially for higher order elements, for calculating integrals of the corresponding influence coefficients (for off-diagonal elements and diagonal elements), etc. For sufficiently smooth functions on a finite interval $[a,b]$ a linear transformation to the standard interval $[-1,1]$ can be used and then an application of Gauss-Legendre quadrature formula provides numerical integration with a satisfactory accuracy. However, for integrals with a logarithmic singularity and/or some kind of algebraic singularities, the convergence of the corresponding quadrature process is very slow, so that certain weighted quadratures are recommended. In such cases, the weight functions of the corresponding weighted Gaussian quadratures include these "difficult parts (with singularities)" of the integrand. In the next section, we consider two cases of such quadratures on the standard interval $[0,1]$.

GAUSSIAN QUADRATURES WITH LOGARITHMIC WEIGHTS FUNCTIONS

Let $\mathcal{P}_m$ be a set of all algebraic polynomials of degree at most m. We consider the weighted n-point quadrature formula

$$\int_0^1 f(x)w(x)\,\mathrm{d}x = \sum_{k=1}^{n} A_k f(x_k) + R_n(f), \tag{3}$$

with respect to the weight function $w(x) = (1-x)^\alpha x^\beta \log(1/x)$, with parameters $\alpha,\beta > -1$. Piessens and Branders [14] considered cases when $\alpha = 0$ and $\beta = 0, \pm 1/2, \pm 1/3, -1/4, -1/5$ (cf. Gautschi [5]). In the case $\alpha = \beta = 0$, the parameters of quadrature rules for $n \leq 8$ can be found in the book Katsikadelis [8, pp. 297–298].

In a general Gaussian quadrature formula the nodes x_k and the weights A_k in (3) must be selected so that $R_n(f) = 0$ for each $f \in \mathcal{P}_{2n-1}$. In that case, the nodes x_k are zeros of the monic orthogonal polynomial $\pi_n(w;x)$ and the corresponding weights A_k (Christoffel numbers) can be expressed by the so-called Christoffel function $\lambda_n(w;x)$ (cf. [10, Chapters 2 & 5]) in the form $A_k = \lambda_n(w;x_k) > 0$, $k = 1,\ldots,n$.

As we know [10, Chapters 2], the (monic) polynomials $\pi_n(w;x)$ orthogonal with respect to the weight function $w(x)$ on $[a,b]$ satisfy the three-term recurrence equation

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k(t)\pi_{k-1}(t), \quad k = 0,1,2,\ldots, \quad \pi_0(t) = 0, \;\; \pi_{-1}(t) = 0, \tag{4}$$

where $(\alpha_k) = (\alpha_k(w))$ and $(\beta_k) = (\beta_k(w))$ are sequences of recursion coefficients. The coefficient β_0 which is multiplied by $\pi_{-1}(x) = 0$ in (4) may be arbitrary, but it is convenient to define it by $\beta_0 = \mu_0 = \int_a^b w(x)\,\mathrm{d}x$.

The characterization of the Gaussian quadratures via an eigenvalue problem for the Jacobi matrix

$$J_n(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathrm{O} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ \mathrm{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix} \tag{5}$$

has become the basis of current methods for generating these quadratures. The most popular of them is one due to Golub and Welsch [6]. The nodes x_k in the Gaussian rule (3), with respect to the weight function $w(x)$ on $[a,b]$, are the eigenvalues of the n-th order Jacobi matrix (5), and the corresponding weights A_k are given by $A_k = \beta_0 v_{k,1}^2$, $k = 1,\ldots,n$, where $\beta_0 = \mu_0 = \int_a^b w(x)\,\mathrm{d}x$ and $v_{k,1}$ is the first component of the normalized eigenvector $\mathbf{v}_k$ corresponding to the eigenvalue x_k, $J_n(w)\mathbf{v}_k = x_k\mathbf{v}_k$, $\mathbf{v}_k^{\mathrm{T}}\mathbf{v}_k = 1$, $k = 1,\ldots,n$. Simplifying QR algorithm so that only the first components of the eigenvectors are computed, Golub and Welsch [6] gave a very efficient algorithm, which is implemented in our package `OrthogonalPolynomials` realized in `Mathematica` [3].

Thus, we need the recursion coefficients α_k and β_k, $k \le N-1$, for the monic polynomials $\pi_\nu(w;\cdot)$, in order to construct the n-point Gauss-Christofell quadrature formula, with respect to the weighte $w(x)$, for each $n \le N$. These coefficients are known explicitly for the classical orthogonal polynomials (see [10, Chapters 2]). Usually, in other cases, we need an additional numerical construction of recursion coefficients, using the Chebyshev method of moments or the so-called discretized Stieltjes procedure (see [10, § 2.4.8]).

The fast progress in recent years in symbolic computation and variable-precision arithmetic provide a possibility for generating the coefficients α_k and β_k in the three-term recurrence relation (4) directly using only Chebyshev method of moments. Using such symbolic/variable-precision software for orthogonal polynomials [13] we can construct Gaussian quadratures with the logarithmic weight $w(x) = (1-x)^\alpha x^\beta \log(1/x)$ on $(0,1)$. Thus, all that is required is a procedure for (symbolic) calculation of the moments in variable-precision arithmetic in order to overcome the numerical instability, which is always present in the method of moments.

Using symbolic integration we find the moments $\mu_k = \mu_k(\alpha,\beta)$ in terms of the gamma function and harmonic numbers,

$$\mu_k(\alpha,\beta) = \int_0^1 x^k w(x)\,\mathrm{d}x = \int_0^1 (1-x)^\alpha x^{k+\beta} \log\frac{1}{x}\,\mathrm{d}x = \frac{\Gamma(\alpha+1)\Gamma(\beta+k+1)}{\Gamma(\alpha+\beta+k+2)}\left[H(\alpha+\beta+k+1) - H(\beta+k)\right]. \quad (6)$$

For example, for $\alpha = \beta = 0$ it reduces to $\mu_k(0,0) = 1/(k+1)^2$, $k \ge 0$. The standard meaning of the k-th harmonic number H_k is the sum of the reciprocals of the first k natural numbers, i.e.,

$$H_k = H(k) = \sum_{\nu=1}^{k} \frac{1}{\nu} = \int_0^1 \frac{1-t^k}{1-t}\,\mathrm{d}t = \sum_{\nu=1}^{k} (-1)^{\nu-1} \frac{1}{\nu}\binom{k}{\nu}.$$

Taking a fractional argument x between 0 and 1, the harmonic number $H(x)$ is defined by the previous integral, where k is simply replaced by x. Then it can be generated by $H(x) = H(x-1) + x^{-1}$ or $H(1-x) - H(x) = \pi\cot(\pi x) - \frac{1}{x} + \frac{1}{1-x}$. More generally, for every $x > 0$ (integer or not), the harmonic number is determined by

$$H(x) = x\sum_{k=1}^{+\infty} \frac{1}{k(x+k)} = \psi(x+1) + \gamma, \quad \psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}, \quad \gamma = 0.577215664901532\ldots\,.$$

In order to overcome the severe ill-conditioning in obtaining the recursion coefficients with a satisfactory accuracy, a multi-precision arithmetic can be used. For example, in the simplest case $\alpha = \beta = 0$, taking 55-decimal-digit arithmetic we get the first $N = 50$ recursion coefficients to about 20 decimal digits. The following code in the `Mathematica` package `OrthogonalPolynomials` [3] generates recursion coefficients for $k \le 2N-1 = 99$ and quadrature parameters (nodes and weights) to 20 decimal digits for $n = 10(10)50$:

```
<<orthogonalPolynomials`
w[t_,a_,b_]:=(1-t)^1 t^b Log[1/t]
mom=Integrate[t^k w[0,0],{t,0,1}]; moments=Table[mom,{k,0,99}];
{alpha,beta}= aChebyshevAlgorithm[moments, WorkingPrecision->55];
param=Table[aGaussianNodesWeights[n,alpha,beta,Precision->20,
            WorkingPrecision->20,{n,10,50,10}];
```

The same method enables us to include also a logarithmic singularity at $x = 1$, i.e., to take

$$w(x) = w^{(\alpha,\beta)}(x) = (1-x)^\alpha x^\beta \log\frac{1}{x(1-x)}, \quad \alpha,\beta > -1.$$

Similarly as before, we can find the corresponding moments

$$\mu_k(\alpha,\beta) = \int_0^1 (1-x)^\alpha x^{k+\beta} \log\frac{1}{x(1-x)}\,\mathrm{d}x = \frac{\Gamma(\alpha+1)\Gamma(\beta+k+1)}{\Gamma(\alpha+\beta+k+2)}\left[2H(\alpha+\beta+k+1) - H(\beta+k) - H(\alpha)\right].$$

As an example we consider (cf. [5])

$$I = \int_0^1 \frac{(1-x)^{-1/2}x^{-1/2}\log(1/x)}{\sqrt{1+x}}\,\mathrm{d}x = \frac{\sqrt{2\pi}}{8}\Gamma\Big(\frac{1}{4}\Big)^2 = 4.11871837492687201436674\,0\ldots\,. \quad (7)$$

An application of the standard Gauss-Legendre quadrature (transformed to $[0,1]$) gives a very slow convergence. Relative errors $r_n(\mathrm{GL})$ for $n = 10(10)100$ are presented in Table 1. Numbers in parentheses denote decimal exponents. Slightly better results can be obtained by using Gauss-Chebyshev quadratures with relative errors $r_n(\mathrm{GC})$.

However, we can directly apply the quadrature formula (3) to integral (7). Let $Q_n^{(\alpha,\beta)}$ be the corresponding quadrature sum and $r_n^{(\alpha,\beta)} = |(Q_n^{(\alpha,\beta)} - I)/I|$. Taking the quadrature formula with the logarithmic weight $w(x) = \log(1/x)$, the corresponding function in (7) is $f(x) = 1/\sqrt{x(1-x^2)}$. The convergence of this rule is again very slow. Relative errors $r_n^{(0,0)}$ are given in Table 1. But, if we include also algebraic singularities in the weight, i.e., if we take $w(x) = (1-x)^{-1/2}x^{-1/2}\log(1/x)$ $(\alpha = \beta = -1/2)$, the convergence becomes very fast. Gaussian approximations $Q_n^{(-1/2,-1/2)}$ and relative errors are given in the second part of Table 1 for small values of $n \leq 10$. Incorrect decimal digits are underlined. As we can see, 17 exact decimal digits are obtained using Gaussian rule with only $n = 10$ digits.

TABLE 1. Relative errors of quadrature sums for $n = 10(10)100$ and Gaussian approximations with respect to logarithmic weight and the corresponding relative errors for $n = 1(1)10$

n	$r_n(\mathrm{GL})$	$r_n(\mathrm{GC})$	$r_n^{(0,0)}$	n	$Q_n^{(-1/2,-1/2)}$	$r_n^{(-1/2,-1/2)}$
10	1.84(−1)	5.29(−2)	1.42(−1)	1	$4.\underline{0801983843688532}$	9.35(−3)
20	1.08(−1)	2.64(−2)	8.69(−2)	2	$4.11\underline{79039770237825}$	1.98(−4)
30	7.80(−2)	1.76(−2)	6.41(−2)	3	$4.118\underline{6986430715864}$	4.79(−6)
40	6.17(−2)	1.32(−2)	5.14(−2)	4	$4.11871\underline{78694526636}$	1.23(−7)
50	6.17(−2)	1.06(−2)	4.31(−2)	5	$4.1187183\underline{615750484}$	3.24(−9)
60	5.14(−2)	8.81(−3)	3.73(−2)	6	$4.118718374\underline{5672496}$	8.73(−11)
70	4.41(−2)	7.55(−3)	3.30(−2)	7	$4.1187183749\underline{170540}$	2.38(−12)
80	3.88(−2)	6.61(−3)	2.96(−2)	8	$4.1187183749266\underline{013}$	6.57(−14)
90	3.47(−2)	5.87(−3)	2.69(−2)	9	$4.11871837492686\underline{44}$	1.83(−15)
100	2.87(−2)	5.29(−3)	2.47(−2)	10	$4.118718374926871\underline{8}$	5.10(−17)

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