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S-ORTHOGONALITY AND GENERALIZED TURÁN QUADRATURES: CONSTRUCTION AND APPLICATIONS

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1. Introduction

Solving some problems in computational plasma physics, Calder and Laframboise [1] considered the problem of approximating the Maxwell velocity distribution by a step function, i.e., by "multiple-water-bag distribution" in their terminology, in such a way that as many of the initial moments as possible of the Maxwell distribution are preserved. They used a classical method of reduction to an eigenvalue problem for Hankel matrices, requiring high precision calculations because of numerical instability. A similar problem, involving Dirac's δ-function instead of Heaviside's step function, was treated earlier by Laframboise and Stauffer [23], using the classical Prony's method. A stable procedure for these problems was given by Gautschi [10]. Precisely, he considered the problem of approximating a spherically symmetric function $t \mapsto f(t)$, $t = \|\boldsymbol{x}\|$, $0 \le t < \infty$, in $\mathbb{R}^d$, $d \ge 1$, by a piecewise constant function

$$t \mapsto s_n(t) = \sum_{\nu=1}^{n} a_\nu H(\tau_\nu - t) \qquad (a_\nu \in \mathbb{R},\ 0 < \tau_1 < \cdots < \tau_n < +\infty),$$

where H is the Heaviside step function, and found the close connection of this problem with Gaussian quadrature formulas. Also, he considered an approximation by a linear combination of Dirac delta functions. This work was extended to spline approximation of arbitrary degree by Gautschi and Milovanović [13]. Namely, they considered a spline function of degree $m \ge 0$ on $[0, +\infty)$, vanishing at $t = +\infty$, with $n \ge 1$ positive knots τ_ν, $\nu = 1, \ldots, n$, which can be written in the form

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (\tau_\nu - t)_+^m \qquad (a_\nu \in \mathbb{R},\ 0 \le t < +\infty),$$

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where the plus sign on the right is the cutoff symbol, $u_+ = u$ if $u > 0$ and $u_+ = 0$ if $u \le 0$. Given a function $t \mapsto f(t)$ on $[0, +\infty)$, they determined $s_{n,m}$ such that

$$\int_0^{+\infty} s_{n,m}(t)t^j \, dV = \int_0^{+\infty} f(t)t^j \, dV \qquad (j = 0, 1, \dots, 2n-1),$$

where dV is the volume element depending on the geometry of the problem. (For example, $dV = Ct^{d-1}\,dt$ if $d > 1$, where C is some constant, and $dV = dt$ if $d = 1$ were used in [13]. For some details see Gautschi [11].) In any case, the spline $s_{n,m}$ is such to faithfully reproduce the first $2n$ moments of f. Under suitable assumptions on f, it was shown that the problem has a unique solution if and only if certain Gauss-Christoffel quadratures exist corresponding to a moment functional or weight distribution depending on f. Existence, uniqueness and pointwise convergence of such approximation were analyzed.

Frontini, Gautschi and Milovanović [5] and Frontini and Milovanović [6] considered analogous problems on an arbitrary finite interval, which can be standardized to $[a, b] = [0, 1]$. If the approximations exist, they can be represented in terms of generalized Gauss-Lobatto and Gauss-Radau quadrature formulas relative to appropriate measures depending on f.

At the Singapore Conference on Numerical Mathematics (1988) we presented a moment-preserving approximation on $[0, +\infty)$ by defective splines of degree m, with odd defect (see Milovanović and Kovačević [26]).

A spline function of degree $m \ge 1$ on the interval $0 \le t < +\infty$, vanishing at $t = +\infty$, with the variable positive knots τ_ν, $\nu = 1, \dots, n$, and multiplicity k_ν $(\le m)$, $\nu = 1, \dots, n$ $(n > 1)$, respectively, can be represented in the form

$$S_{n,m}(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{k_\nu - 1} \alpha_{\nu,i}(\tau_\nu - t)_+^{m-i}, \quad 0 \le t < +\infty, \tag{1.1}$$

where $\alpha_{\nu,i}$ are real numbers.

Using the following conditions

$$\int_0^{+\infty} t^{j+d-1} S_{n,m}(t)\,dt = \int_0^{+\infty} t^{j+d-1} f(t)\,dt, \quad j = 0, 1, \dots, 2(s+1)n - 1, \tag{1.2}$$

we [26] considered the problem of approximating a function $f(t)$ of the radial distance $t = \|x\|$, $0 \le t < +\infty$ in $\mathbb{R}^d$, $d \ge 1$, by the spline function (1.1), where $k_\nu = 2s + 1$, $\nu = 1, \dots, n$, $s \in \mathbb{N}_0$. Under suitable assumptions on f, we showed that the problem has a unique solution if and only if certain generalized Turán quadratures exist corresponding to a measure depending on f. A more general case with variable defects was considered by Gori and Santi [17] and Kovačević and Milovanović [22]. In that case, approximation problems reduce to Gauss-Turán-Stancu type of quadratures and σ-orthogonal polynomials (cf. Gautschi [8], Gori, Lo Cascio and Milovanović [18]).

Further extensions of the moment-preserving spline approximation on $[0, 1]$ are given by Micchelli [24]. He relates this approximation to the theory of the monosplines. A similar problem by defective spline functions on the finite interval $[0, 1]$ has been studied by Gori and Santi [16] and solved by means of monosplines.

In Section 2 we give a survey on generalized Gauss-Turán quadrature formulas and s-orthogonal polynomials. A stable method for numerically constructing s-orthogonal polynomials and their zeros is presented in Section 3, and calculation of the corresponding coefficients (i.e., Cotes numbers of higher order) is given in Section 4. Some alternative methods for coefficients were proposed by Stroud and Stancu [36] (see also [33]) and Milovanović and Spalević [28]. A few numerical examples and some applications in moment-preseving spline approximation are presented in Setions 5 and 6, respectively.

2. Generalized Gauss-Turán quadratures and s-orthogonality

Let $\mathcal{P}_m$ be the set of all algebraic polynomials of degree at most m. In 1950, P. Turán [37] studied numerical quadratures of the form

$$\int_{-1}^{1} f(t)\,dt = \sum_{i=0}^{k-1}\sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R_{n,k}(f), \tag{2.1}$$

where

$$A_{i,\nu} = \int_{-1}^{1} \ell_{\nu,i}(t)\,dt \qquad (\nu = 1,\dots,n;\ i = 0,1,\dots,k-1)$$

and $\ell_{\nu,i}(t)$ are the fundamental functions of Hermite interpolation. The coefficients $A_{i,\nu}$ are Cotes numbers of higher order. Evidently, the formula (2.1) is exact if $f \in \mathcal{P}_{kn-1}$ and the points $-1 \le \tau_1 \le \cdots \le \tau_n \le 1$ are arbitrary.

For $k = 1$ the formula (2.1), i.e.,

$$\int_{-1}^{1} f(t)\,dt = \sum_{\nu=1}^{n} A_{0,\nu} f(\tau_\nu) + R_{n,1}(f),$$

can be exact for all polynomials of degree at most $2n-1$ if the nodes τ_ν are the zeros of the Legendre polynomial P_n, and it is the well-known Gauss-Legendre quadrature rule.

Because of Gauss's result it is natural to ask whether knots τ_ν can be chosen so that the quadrature formula (2.1) will be exact for algebraic polynomials of degree not exceeding $(k+1)n-1$. Turán [37] showed that the answer is negative for $k = 2$, and for $k = 3$ it is positive. He proved that the knots τ_ν should be chosen as the zeros of the monic polynomial $\pi_n^*(t) = t^n + \cdots$ which minimizes the integral

$$\int_{-1}^{1} [\pi_n(t)]^4 dt,$$

where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \cdots + a_1 t + a_0$.

More generally, the answer is negative for even, and positive for odd k, and then τ_ν are the zeros of the polynomial minimizing

$$\int_{-1}^{1} [\pi_n(t)]^{k+1} dt.$$

When $k = 1$, then π_n is the monic Legendre polynomial $\hat{P}_n$.

Because of the above, we put $k = 2s+1$. It is also interesting to consider, instead of (2.1), more general *Gauss-Turán type* quadrature formulae

$$\int_{\mathbb{R}} f(t)\, d\lambda(t) = \sum_{i=0}^{2s} \sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R_{n,2s}(f), \tag{2.2}$$

where $d\lambda(t)$ is a nonnegative measure on the real line $\mathbb{R}$, with compact or infinite support, for which all moments

$$\mu_k = \int_{\mathbb{R}} t^k d\lambda(t), \quad k = 0, 1, \ \ldots\ ,$$

exist and are finite, and $\mu_0 > 0$. It is known that formula (2.2) is exact for all polynomials of degree at most $2(s+1)n - 1$, i.e.,

$$R_{n,2s}(f) = 0 \qquad \text{for} \quad f \in \mathcal{P}_{2(s+1)n-1}.$$

The knots τ_ν $(\nu = 1, \ldots, n)$ in (2.2) are the zeros of the monic polynomial $\pi_n^s(t)$, which minimizes the integral

$$F(a_0, a_1, \ldots, a_{n-1}) = \int_{\mathbb{R}} [\pi_n(t)]^{2s+2}\, d\lambda(t),$$

where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \cdots + a_1 t + a_0$. This minimization leads to the conditions

$$\int_{\mathbb{R}} [\pi_n(t)]^{2s+1} t^k\, d\lambda(t) = 0 \qquad (k = 0, 1, \ldots, n-1). \tag{2.3}$$

Usually, instead of $\pi_n^s(t)$ we write $P_{s,n}(t)$.

The case $d\lambda(t) = w(t)\, dt$ on $[a, b]$ has been investigated by the Italian mathematicians Ossicini [29], Ghizzetti and Ossicini [15], Guerra [19–20]. It is known that there exists a unique $P_{s,n}(t) = \prod_{\nu=1}^{n} (t - \tau_\nu)$, whose zeros τ_ν are real, distinct and located in the interior of the interval $[a, b]$. These polynomials are known as *s-orthogonal* (or s-self associated) *polynomials* in the interval $[a, b]$ with respect to the weight function w (for more details see [8], [29–31]). For $s = 0$ we have the standard case of orthogonal polynomials, and (2.2) then becomes the well-known Gauss-Christoffel formula.

A generalization of the formula (2.1) to rules having nodes with arbitrary multiplicities was given, independently, by Chakalov [2–3] and Popoviciu [32]. In that case the nodes are zeros of so-called σ-orthogonal polynomials. A deep theoretical progress in this subject was made by Stancu [33–35]. An algorithm for constructing σ-orthogonal polynomials was given in [18].

3. Construction of S-Orthogonal Polynomials

An iterative process for computing the coefficients of s-orthogonal polynomials in a special case, when the interval $[a, b]$ is symmetric with respect to the origin and the weight function w is an even function, was proposed by Vincenti [38]. He applied his process to the Legendre case. When n and s increase, the process becomes numerically unstable.

We presented now a stable method for numerically constructing s-orthogonal polynomials and their zeros (see [25] and [14]). It uses an iterative method with quadratic convergence based on a discretized Stieltjes procedure and the Newton-Kantorovič method.

The basic idea for our method to numerically construct s-orthogonal polynomials with respect to the measure $d\lambda(t)$ on the real line $\mathbb{R}$ is a reinterpretation of the *"orthogonality conditions"* (2.3). For given n and s, we put $d\mu(t) = d\mu^{s,n}(t) = (\pi_n(t))^{2s} d\lambda(t)$. The conditions can then be written as

$$\int_{\mathbb{R}} \pi_k^{s,n}(t) t^\nu d\mu(t) = 0 \qquad (\nu = 0, 1, \ldots, k-1),$$

where $\{\pi_k^{s,n}\}$ is a sequence of monic orthogonal polynomials with respect to the new measure $d\mu(t)$. Of course, $P_{s,n}(\,\cdot\,) = \pi_n^{s,n}(\,\cdot\,)$. As we can see, the polynomials $\pi_k^{s,n}$ $(k = 0, 1, \ldots)$ are implicitly defined, because the measure $d\mu(t)$ depends of $\pi_n^{s,n}(t)$. A general class of such polynomials was introduced and studied by Engels (cf. [4, pp. 214–226]).

We will write simply $\pi_k(\,\cdot\,)$ instead of $\pi_k^{s,n}(\,\cdot\,)$. These polynomials satisfy a three-term recurrence relation

$$\begin{aligned} &\pi_{\nu+1}(t) = (t - \alpha_\nu)\pi_\nu(t) - \beta_\nu \pi_{\nu-1}(t), \quad \nu = 0, 1, \ldots, \\ &\pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \end{aligned} \tag{3.1}$$

where, because of orthogonality,

$$\begin{aligned} \alpha_\nu &= \alpha_\nu(s,n) = \frac{(t\pi_\nu, \pi_\nu)}{(\pi_\nu, \pi_\nu)} = \frac{\int_{\mathbb{R}} t\pi_\nu^2(t)\, d\mu(t)}{\int_{\mathbb{R}} \pi_\nu^2(t)\, d\mu(t)}, \\ \beta_\nu &= \beta_\nu(s,n) = \frac{(\pi_\nu, \pi_\nu)}{(\pi_{\nu-1}, \pi_{\nu-1})} = \frac{\int_{\mathbb{R}} \pi_\nu^2(t)\, d\mu(t)}{\int_{\mathbb{R}} \pi_{\nu-1}^2(t)\, d\mu(t)}, \end{aligned} \tag{3.2}$$

and, by convention, $\beta_0 = \int_{\mathbb{R}} d\mu(t)$.

The coefficients α_ν and β_ν are the fundamental quantities in the constructive theory of orthogonal polynomials. They provide a compact way of representing orthogonal polynomials, requiring only a linear array of parameters. The coefficients of orthogonal polynomials, or their zeros, in contrast need two-dimensional arrays.

Knowing the coefficients α_ν, β_ν $(\nu = 0, 1, \ldots, n-1)$ gives us access to the first $n+1$ orthogonal polynomials π_0, π_1, $\ldots$, π_n. Of course, for a given n, we are interested only in the last of them, i.e., $\pi_n \equiv \pi_n^{s,n}$. Thus, for $n = 0, 1, \ldots$, the diagonal (boxed) elements in Table 3.1 are our s-orthogonal polynomials $\pi_n^{s,n}$.

Table 3.1

n	$d\mu^{s,n}(t)$	Orthogonal Polynomials			
0	$(\pi_0^{s,0}(t))^{2s}\,d\lambda(t)$	$\boxed{\pi_0^{s,0}}$			
1	$(\pi_1^{s,1}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,1}$	$\boxed{\pi_1^{s,1}}$		
2	$(\pi_2^{s,2}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,2}$	$\pi_1^{s,2}$	$\boxed{\pi_2^{s,2}}$	
3	$(\pi_3^{s,3}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,3}$	$\pi_1^{s,3}$	$\pi_2^{s,3}$	$\boxed{\pi_3^{s,3}}$
$\vdots$					

A stable procedure for finding the coefficients α_ν, β_ν is the discretized Stieltjes procedure, especially for infinite intervals of orthogonality (see [7–9] and [12]). Unfortunately, in our case this procedure cannot be applied directly, because the measure $d\mu(t)$ involves an unknown polynomial $\pi_n^{s,n}$. Consequently, we consider the system of nonlinear equations

$$\begin{aligned} f_0 &\equiv \beta_0 - \int_{\mathbb{R}} \pi_n^{2s}(t)\,d\lambda(t) = 0, \\ f_{2\nu+1} &\equiv \int_{\mathbb{R}} (\alpha_\nu - t)\pi_\nu^2(t)\pi_n^{2s}(t)\,d\lambda(t) = 0 \quad (\nu = 0, 1, \ldots, n-1), \\ f_{2\nu} &\equiv \int_{\mathbb{R}} (\beta_\nu \pi_{\nu-1}^2(t) - \pi_\nu^2(t))\pi_n^{2s}(t)\,d\lambda(t) = 0 \quad (\nu = 1, \ldots, n-1), \end{aligned} \tag{3.3}$$

which follows from (3.2).

Let $\boldsymbol{x}$ be a $(2n)$-dimensional column vector with components α_0, β_0, $\ldots$, α_{n-1}, β_{n-1} and $\boldsymbol{f}(\boldsymbol{x})$ a $(2n)$-dimensional vector with components f_0, f_1, $\ldots$, f_{2n-1}, given by (3.3), in which π_0, π_1, $\ldots$, π_n are thought of as being expressed in terms of the α's and β's via (3.1). If $W = W(\boldsymbol{x})$ is the corresponding Jacobian of $\boldsymbol{f}(\boldsymbol{x})$, then we can apply Newton-Kantorovič's method

$$\boldsymbol{x}^{[k+1]} = \boldsymbol{x}^{[k]} - W^{-1}(\boldsymbol{x}^{[k]})\boldsymbol{f}(\boldsymbol{x}^{[k]}) \qquad (k = 0, 1, \ldots) \tag{3.4}$$

for determining the coefficients of the recurrence relation (3.1). If a sufficiently good approximation $\boldsymbol{x}^{[0]}$ is chosen, the convergence of the method (3.4) is quadratic.

Notice that the elements of the Jacobian can be easily computed in the following manner.

First, we have to determine the partial derivatives $a_{\nu,i} = \dfrac{\partial \pi_\nu}{\partial \alpha_i}$ and $b_{\nu,i} = \dfrac{\partial \pi_\nu}{\partial \beta_i}$. Differentiating the recurrence relation (3.1) with respect to α_i and β_i, we obtain

$$a_{\nu+1,i} = (t - \alpha_\nu)a_{\nu,i} - \beta_\nu a_{\nu-1,i}, \qquad b_{\nu+1,i} = (t - \alpha_\nu)b_{\nu,i} - \beta_\nu b_{\nu-1,i},$$

where

$$\begin{aligned} a_{\nu,i} &= 0, \quad b_{\nu,i} = 0 \quad (\nu \le i), \\ a_{i+1,i} &= -\pi_i(t), \quad b_{i+1,i} = -\pi_{i-1}(t). \end{aligned}$$

These relations are the same as those for π_ν, but with other (delayed) initial values. The elements of the Jacobian are

$$
\begin{aligned}
\frac{\partial f_{2\nu+1}}{\partial \alpha_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)\left[(\alpha_\nu - t)p_{\nu,i}(t) + \tfrac{1}{2}\delta_{\nu,i}\pi_\nu^2(t)\pi_n(t)\right] d\lambda(t),\\
\frac{\partial f_{2\nu+1}}{\partial \beta_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)(\alpha_\nu - t)q_{\nu,i}(t)\, d\lambda(t),\\
\frac{\partial f_{2\nu}}{\partial \alpha_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)(\beta_\nu p_{\nu-1,i}(t) - p_{\nu,i}(t))\, d\lambda(t),\\
\frac{\partial f_{2\nu}}{\partial \beta_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)\left[(\beta_\nu q_{\nu-1,i}(t) - q_{\nu,i}(t)) + \tfrac{1}{2}\delta_{\nu,i}\pi_{\nu-1}^2(t)\pi_n(t)\right] d\lambda(t),
\end{aligned}
\tag{3.5}
$$

where

$$
p_{\nu,i}(t) = \pi_\nu(t)(a_{\nu,i}\pi_n(t) + s a_{n,i}\pi_\nu(t)), \quad q_{\nu,i}(t) = \pi_\nu(t)(b_{\nu,i}\pi_n(t) + s b_{n,i}\pi_\nu(t)),
$$

and $\delta_{\nu,i}$ is Kronecker's delta.

All of the above integrals in (3.3) and (3.5) can be computed exactly, except for rounding errors, by using a Gauss-Christoffel quadrature formula with respect to the measure $d\lambda(t)$,

$$
\int_{\mathbb{R}} g(t)\, d\lambda(t) = \sum_{\nu=1}^{N} A_\nu^{(N)} g(\tau_\nu^{(N)}) + R_N(g), \tag{3.6}
$$

taking $N = (s+1)n$ knots. This formula is exact for all polynomials of degree at most $2N - 1 = 2(s+1)n - 1 = 2(n-1) + 2ns + 1$.

Thus, for all calculations we use only the fundamental three-term recurrence relation (3.1) for the orthogonal polynomials $\pi_k(\,\cdot\,; d\lambda)$ and the Gauss-Christoffel quadrature (3.6). As intial values $\alpha_\nu^{[0]} = \alpha_\nu^{[0]}(s,n)$ and $\beta_\nu^{[0]} = \beta_\nu^{[0]}(s,n)$ we take the values obtained for $n-1$, i.e., $\alpha_\nu^{[0]} = \alpha_\nu(s, n-1)$, $\beta_\nu^{[0]} = \beta_\nu(s, n-1)$, $\nu \le n-2$. For $\alpha_{n-1}^{[0]}$ and $\beta_{n-1}^{[0]}$ we use corresponding extrapolated values.

In the case $n = 1$ we solve the equation

$$
\phi(\alpha_0) = \phi(\alpha_0(s,1)) = \int_{\mathbb{R}} (t - \alpha_0)^{2s+1}\, d\lambda(t) = 0,
$$

and then determine

$$
\beta_0 = \beta_0(s,1) = \int_{\mathbb{R}} (t - \alpha_0)^{2s}\, d\lambda(t).
$$

The zeros $\tau_\nu = \tau_\nu(s,n)$ $(\nu = 1, \ldots, n)$ of $\pi_n^{s,n}$, i.e., the nodes of the Gauss-Turán type quadrature formula (2.2), we obtain very easily as eigenvalues of a (symmetric tridiagonal) Jacobi matrix J_n using the QR algorithm, namely

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

where $\alpha_\nu = \alpha_\nu(s,n)$, $\beta_\nu = \beta_\nu(s,n)$ $(\nu = 0, 1, \ldots, n-1)$.

4. Calculation of Cotes Coefficients

Let $\tau_\nu = \tau_\nu(s,n)$, $\nu = 1,\ldots,n$, be the zeros of the s-orthogonal (monic) polynomial $\pi_n(t)\,(\equiv \pi_n^{s,n}(t))$. In order to find the coefficients $A_{i,\nu}$ in the Gauss-Turán type quadrature formula

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \sum_{i=0}^{2s}\sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f), \tag{4.1}$$

we define

$$\Omega_\nu(t) = \left(\frac{\pi_n(t)}{t-\tau_\nu}\right)^{2s+1} = \prod_{i\neq\nu}(t-\tau_i)^{2s+1} \qquad (\nu = 1,\ldots,n). \tag{4.2}$$

Then the coefficients $A_{i,\nu}$ can be expressed in the form (see Stancu [35])

$$A_{i,\nu} = \frac{1}{i!(2s-i)!}\left[D^{2s-i}\frac{1}{\Omega_\nu(t)}\int_{\mathbb{R}}\frac{\pi_n(x)^{2s+1}-\pi_n(t)^{2s+1}}{x-t}\,d\lambda(x)\right]_{t=\tau_\nu},$$

where D is the differentiation operator. In particular, for $i = 2s$, we have

$$A_{2s,\nu} = \frac{1}{(2s)!(\pi_n{}'(\tau_\nu))^{2s+1}}\int_{\mathbb{R}}\frac{\pi_n(x)^{2s+1}}{x-\tau_\nu}\,d\lambda(x),$$

i.e.,

$$A_{2s,\nu} = \frac{B_\nu{}^{(s)}}{(2s)!(\pi_n'(\tau_\nu))^{2s}} \qquad (\nu = 1,\ldots,n),$$

where $B_\nu^{(s)}$ are the Christoffel numbers of the following Gaussian quadrature (with respect to the measure $d\mu(t) = \pi_n^{2s}(t)d\lambda(t)$),

$$\int_{\mathbb{R}} g(t)\,d\mu(t) = \sum_{\nu=1}^{n} B_\nu^{(s)} g(\tau_\nu) + R_n(g), \qquad R_n(\mathcal{P}_{2n-1}) = 0. \tag{4.3}$$

Since $B_\nu^{(s)} > 0$, we conclude that $A_{2s,\nu} > 0$. The expressions for the other coefficients ($i < 2s$) become very complicated. For numerical calculation we could use a triangular system of linear equations obtained from the formula (4.1) by replacing f with the Newton polynomials: 1, $t-\tau_1$, $\ldots$, $(t-\tau_1)^{2s+1}$, $(t-\tau_1)^{2s+1}(t-\tau_2)$, $\ldots$, $(t-\tau_1)^{2s+1}(t-\tau_2)^{2s+1}\cdots(t-\tau_n)^{2s}$ (cf. [8, §2.2.4]).

In this paper we take instead the polynomials

$$f_{k,\nu}(t) = (t-\tau_\nu)^k\Omega_\nu(t) = (t-\tau_\nu)^k\prod_{i\neq\nu}(t-\tau_i)^{2s+1}, \tag{4.4}$$

where $0 \le k \le 2s$, $1 \le \nu \le n$.

Since the quadrature (4.1) is exact for all polynomials of degree at most $2(s+1)n-1$ and

$$\deg f_{k,\nu} = (n-1)(2s+1)+k \le (2s+1)n-1,$$

we see that (4.1) is exact for the polynomials (4.4), i.e.,

$$R(f_{k,\nu}) = 0 \qquad (0 \le k \le 2s,\ 1 \le \nu \le n).$$

Thus, we have

$$\sum_{i=0}^{2s} \sum_{j=1}^{n} A_{i,j} f_{k,\nu}^{(i)}(\tau_j) = \int_{\mathbb{R}} f_{k,\nu}(t)\, d\lambda(t),$$

that is,

$$\sum_{i=0}^{2s} A_{i,\nu} f_{k,\nu}^{(i)}(\tau_\nu) = \mu_{k,\nu}, \tag{4.5}$$

because for every $j \ne \nu$ we have $f_{k,\nu}^{(i)}(\tau_j) = 0$ when $0 \le i \le 2s$. Here, we have put

$$\mu_{k,\nu} = \int_{\mathbb{R}} f_{k,\nu}(t)\, d\lambda(t) = \int_{\mathbb{R}} (t-\tau_\nu)^k \prod_{i \ne \nu} (t-\tau_i)^{2s+1} d\lambda(t).$$

For each ν, we have in (4.5) a system of $2s+1$ linear equations in the same number of unknowns, $A_{i,\nu}$, $i = 0, 1, \ldots, 2s$.

Using Leibniz's formula of differentiation, we can prove that for polynomials $f_{k,\nu}$ given by (4.4), the following differentiation formula

$$f_{k,\nu}^{(i)}(\tau_\nu) = \begin{cases} 0, & i < k, \\ i^{(k)} \Omega_\nu^{(i-k)}(\tau_\nu), & i \ge k, \end{cases}$$

holds, where $i^{(k)} = i(i-1)\cdots(i-k+1)$ [with $0^{(0)} = 1$] and Ω_ν is defined in (4.1).

This shows that each system of linear equations (4.5) is upper triangular. Thus, once all zeros of the s-orthogonal polynomial π_n, i.e., the nodes of the quadrature formula (4.1), are known, the determination of its weights $A_{i,\nu}$ is reduced to solving the n linear systems of $(2s+1)$ equations

$$\begin{bmatrix} f_{0,\nu}(\tau_\nu) & f'_{0,\nu}(\tau_\nu) & \ldots & f_{0,\nu}^{(2s)}(\tau_\nu) \\ & f'_{1,\nu}(\tau_\nu) & \ldots & f_{1,\nu}^{(2s)}(\tau_\nu) \\ & & \ddots & \\ & & & f_{2s,\nu}^{(2s)}(\tau_\nu) \end{bmatrix} \begin{bmatrix} A_{0,\nu} \\ A_{1,\nu} \\ \vdots \\ A_{2s,\nu} \end{bmatrix} = \begin{bmatrix} \mu_{0,\nu} \\ \mu_{1,\nu} \\ \vdots \\ \mu_{2s,\nu} \end{bmatrix}.$$

Put $a_{k,k+j} = f_{k-1,\nu}^{(k-1+j)}(\tau_\nu)$, so that the matrix of the system has elements $a_{\ell,j}$ $(1 \le \ell, j \le 2s+1)$, with $a_{\ell,j} = 0$ for $j < \ell$. Then, we have

$$a_{\ell,j} = (j-1)^{(\ell-1)} \Omega_\nu^{(j-\ell)}(\tau_\nu) \qquad (j \ge \ell;\ 1 \le \ell, j \le 2s+1). \tag{4.6}$$

Also we can prove (see Gautschi and Milovanović [14]) that for the elements $a_{\ell,j}$, defined by (4.6). the following relations hold:

$$a_{k,k} = (k-1)!a_{1,1} \qquad (1 \le k \le 2s+1),$$

$$a_{k,k+j} = -(2s+1)(k+j-1)^{(k-1)} \sum_{\ell=1}^{j} u_\ell a_{\ell,j} \qquad \begin{pmatrix} 1 \le k \le 2s-j+1 \\ j = 1, \ldots, 2s \end{pmatrix},$$

where

$$a_{1,1} = \Omega_\nu(\tau_\nu) = [\pi_n'(\tau_\nu)]^{2s+1},$$
$$u_\ell = \sum_{i\neq\nu}(\tau_i - \tau_\nu)^{-\ell} \qquad (l = 1, \dots, 2s) \tag{4.7}$$

and $\tau_1, \dots, \tau_n$ are the zeros of the s-orthogonal polynomial π_n.

Using the normalization

$$\hat{a}_{k,j} = \frac{a_{k,j}}{(j-1)!a_{1,1}} \qquad (1 \le k, j \le 2s+1),$$

and putting

$$b_k = (k-1)A_{k-1,\nu} \qquad (1 \le k \le 2s+1),$$
$$\hat{\mu}_{k,\nu} = \frac{\mu_{k,\nu}}{(\pi_n'(\tau_\nu))^{2s+1}} = \int_{\mathbb{R}} (t-\tau_\nu)^k \left(\prod_{i\neq\nu} \frac{t-\tau_i}{\tau_\nu - \tau_i}\right)^{2s+1} d\lambda(t), \tag{4.8}$$

we have the following result:

Theorem 4.1. *For fixed ν $(1 \le \nu \le n)$, the coefficients $A_{i,\nu}$ in the generalized Gauss-Turán type quadrature formula* (4.1) *are given by*

$$b_{2s+1} = (2s)!A_{2s,\nu} = \hat{\mu}_{2s,\nu},$$
$$b_k = (k-1)!A_{k-1,\nu} = \hat{\mu}_{k-1,\nu} - \sum_{j=k+1}^{2s+1} \hat{a}_{k,j} b_j \qquad (k = 2s, \dots, 1),$$

where $\hat{\mu}_{k,\nu}$ are given by (4.8)*, and*

$$\hat{a}_{k,k} = 1, \quad \hat{a}_{k,k+j} = -\frac{2s+1}{j} \sum_{\ell=1}^{j} u_\ell \hat{a}_{\ell,j} \qquad (k = 1, \dots, 2s;\ j = 1, \dots, 2s-k+1),$$

the u_ℓ being defined by (4.7).

The coefficients b_k $(1 \le k \le 2s+1)$ are obtained from the corresponding upper triangular system of equations $\hat{A}\boldsymbol{b} = \boldsymbol{c}$, where

$$\hat{A} = [\hat{a}_{ij}], \quad \boldsymbol{b} = \begin{bmatrix} b_1, & \dots, & b_{2s+1} \end{bmatrix}^T, \quad \boldsymbol{c} = \begin{bmatrix} \hat{\mu}_{0,\nu}, & \dots, & \hat{\mu}_{2s,\nu} \end{bmatrix}^T.$$

The normalized moments $\hat{\mu}_{k,\nu}$ can be computed exactly, except for rounding errors, by using the same Gauss-Christoffel formula as in the construction of s-orthogonal polynomials, i.e., (3.6) with $N = (s+1)n$ knots.

5. Numerical Examples

Using the procedures for constructing s-orthogonal polynomials and calculating the coefficients in the generalized Gauss-Turán type quadrature formulae, we prepared corresponding software with the following types of polynomials $\pi_n(\,\cdot\,; d\lambda)$ (identified by the integer `ipoly`):

```
c  ipoly - integer identifying the kind of polynomials:
c
c    0 = Nonclassical polynomials with given coefficients
c        in the three-term recurrence relation
c    1 = Legendre polynomials on [-1,1]
c    2 = Legendre polynomials on [0,1]
c    3 = Chebyshev polynomials of the first kind
c    4 = Chebyshev polynomials of the second kind
c    5 = Jacobi polynomials with parameters al=.5, be=-.5
c    6 = Jacobi polynomials with parameters al,be
c    7 = generalized Laguerre polynomials with parameter al
c    8 = Hermite polynomials
c    9 = generalized Gegenbauer polynomials with parameters al,be
c   10 = polynomials for the logistic weight
c        w(t)=e^{-t}/(1+e^{-t})^2  on the real line
c
c  al,be - parameters for Jacobi, generalized Laguerre
c          and generalized Gegenbauer polynomials
c  For ipoly=9, the weight function is given by
c          w(x)=|x|^mu(1-x^2)^al, where be=(mu-1)/2.
```

All computations were done on the MICROVAX 3400 computer using VAX FORTRAN Ver. 5.3 in D- and Q-arithmetic, with machine precision $\approx 2.76 \times 10^{-17}$ and $\approx 1.93 \times 10^{-34}$, respectively.

For example, taking the simplest case $d\lambda(t) = dt$ on $(-1, 1)$ (Legendre case) for $s = 3$ and $n = 6$ we obtain the following results in D-arithmetic:

```
--------------------------------------------------------------
EXAMPLE:  Legendre case  (s=3,  n= 6)
--------------------------------------------------------------
k              alpha(k)                         beta(k)
--------------------------------------------------------------
--------------------------------------------------------------
0        .000000000000000E+00           .421734239962151E-09
1        .000000000000000E+00           .440736117396359E+00
2        .000000000000000E+00           .261370723991856E+00
3        .000000000000000E+00           .254308492588985E+00
4        .000000000000000E+00           .252419703332403E+00
5        .000000000000000E+00           .251673508288773E+00
--------------------------------------------------------------
zero(4)= .253024354005831E+00   zero(5)= .693971226426183E+00
--------------------------------------------------------------
A(0,4)=  .490428415587130E+00   A(0,5)=  .364261355363419E+00
A(1,4)= -.337436711843437E-02   A(1,5)= -.687117834633461E-02
A(2,4)=  .410826884080729E-02   A(2,5)=  .172546325400200E-02
A(3,4)= -.199019633412152E-04   A(3,5)= -.224545089649575E-04
A(4,4)=  .731050299239644E-05   A(4,5)=  .172499364044568E-05
A(5,4)= -.187335372501814E-07   A(5,5)= -.116086450996926E-07
A(6,4)=  .328312605939431E-08   A(6,5)=  .409342595779103E-09
--------------------------------------------------------------
zero(6)= .956499429571622E+00
--------------------------------------------------------------
A(0,6)=  .145310229049452E+00
A(1,6)= -.373106603607300E-02
A(2,6)=  .140016792703096E-03
A(3,6)= -.203140295590650E-05
A(4,6)=  .256664306399549E-07
A(5,6)= -.157872874923525E-09
```

```
A(6,6)=  .644174120159092E-12
-------------------------------------------------------------
```

In this symmetric case we have

$$\tau_\nu = -\tau_{n-\nu+1}, \quad A_{i,\nu} = (-1)^i A_{i,n-\nu+1} \quad (i = 0, 1, \ldots, 2s;\ \nu = 1, \ldots, [n/2]).$$

In a similar way, taking $d\lambda(t) = e^{-t}\,dt$ on $(0, +\infty)$, for $s = 2$ and $n = 4$ we obtain the following results:

```
-------------------------------------------------------------
EXAMPLE:  Laguerre case  (s=2,  n= 4)
-------------------------------------------------------------
k              alpha(k)                         beta(k)
-------------------------------------------------------------
0        .207388624792579E+01             .303230635818922E+12
1        .822463761482710E+01             .634173445888648E+01
2        .144897291810527E+02             .319077166841049E+02
3        .207314448414547E+02             .777497393014401E+02
-------------------------------------------------------------
zero(1)= .632063951424839E+00   zero(2)= .455606576114603E+01
-------------------------------------------------------------
A(0,1)=  .893868706048056E+00   A(0,2)=  .105965892148938E+00
A(1,1)=  .722539387113141E-01   A(1,2)= -.121748335429446E+00
A(2,1)=  .122430172532510E+00   A(2,2)=  .992761298904123E-01
A(3,1)=  .138636735614257E-01   A(3,2)= -.332242372472303E-01
A(4,1)=  .320971772057328E-02   A(4,2)=  .119138715350092E-01
-------------------------------------------------------------
zero(3)= .127761233967315E+02   zero(4)= .275554447759580E+02
-------------------------------------------------------------
A(0,3)=  .165401159420847E-03   A(0,4)=  .643585948965624E-09
A(1,3)= -.388563922187372E-03   A(1,4)= -.218551256526161E-08
A(2,3)=  .424601031799787E-03   A(2,4)=  .303427339086507E-08
A(3,3)= -.239091931672140E-03   A(3,4)= -.202889024796821E-08
A(4,3)=  .686760628323864E-04   A(4,4)=  .558927293454754E-09
-------------------------------------------------------------
```

Now, we give an example where it is preferable to use a formula of Turán type rather than the standard Gaussian formula,

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n} A_\nu f(t_\nu) + R_n(f), \tag{5.1}$$

for which $R_n(\mathcal{P}_{2n-1}) = 0$. The example is

$$I = \int_{-1}^{1} e^t \sqrt{1-t^2}\,dt = 1.775499689212180946878576537 2\ldots\ .$$

Here we have $f(t) = e^t$ and $d\lambda(t) = \sqrt{1-t^2}\,dt$ on $[-1, 1]$ (the Chebyshev measure of the second kind). Notice that $f^{(i)}(t) = f(t)$ for every $i \geq 0$.

The Gaussian formula (5.1) and the corresponding Gauss-Turán formula (4.1) give

$$I \approx I_n^G = \sum_{\nu=1}^{n} A_\nu e^{t_\nu} \tag{5.2}$$

and

$$I \approx I_{n,s}^T = \sum_{\nu=1}^{n} C_\nu^{(s)} e^{\tau_\nu}, \tag{5.3}$$

respectively, where $C_\nu^{(s)} = \sum_{i=0}^{2s} A_{i,\nu}$.

Table 5.1 shows the relative errors $|(I_{n,s}^T - I)/I_{n,s}^T|$ for $n = 1(1)5$ and $s = 0(1)5$. (Numbers in parentheses indicate decimal exponents and m.p. stands for machine precision.)

TABLE 5.1.
Relative errors in quadrature sums $I_{n,s}^T$

n	$s=0$	$s=1$	$s=2$	$s=3$	$s=4$	$s=5$
1	1.15(−1)	4.71(−3)	9.72(−5)	1.21(−6)	1.01(−8)	5.98(−11)
2	2.38(−3)	2.05(−7)	3.06(−12)	1.36(−17)	2.40(−23)	1.88(−29)
3	1.97(−5)	1.15(−12)	4.02(−21)	9.26(−31)	m.p.	m.p.
4	8.76(−8)	1.71(−18)	4.68(−31)	m.p.	m.p.	m.p.
5	2.43(−10)	9.40(−25)	m.p.	m.p.	m.p.	m.p.

For $s = 0$ the quadrature formula (5.3) reduces to (5.2), i.e., $I_{n,0}^T \equiv I_n^G$. Notice that Turán's formula (5.3) with n nodes has the same degree of exactness as Gaussian formula with $(s+1)n$ nodes, which explains its superior behavior in Table 5.1.

6. An Application in the Moment-Preserving Spline Approximation

In this section we discuss two problems of approximating a function $f(t)$, $0 \le t < +\infty$, by the defective spline function (1.1). Let N denote the sum of the variable knots τ_ν, $\nu = 1, \ldots, n$, of the spline function (1.1), counting multiplicities, i.e., $N = k_1 + \cdots + k_n$.

Problem 1. Determine $S_{n,m}$ in (1.1) such that

$$S_{n,m}^{(k)}(0) = f^{(k)}(0), \quad k = 0, 1, \ldots, N+n-1, \quad m \ge N+n-1. \tag{6.1}$$

Problem 2. Determine $S_{n,m}$ in (1.1) such that

$$S_{n,m}^{(k)}(0) = f^{(k)}(0), \quad k = 0, 1, \ldots, l \quad (l \le m) \tag{6.2}$$

and

$$\int_0^{+\infty} t^j S_{n,m}(t)\, dt = \int_0^{+\infty} t^j f(t)\, dt, \quad j = 0, 1, \ldots, N+n-l-2. \tag{6.3}$$

We first consider the Problem 2.

Theorem 6.1. *Let $f \in C^{m+1}[0, +\infty)$ and*

$$\int_0^{+\infty} t^{N+n-l+m} \big| f^{(m+1)}(t) \big|\, dt < +\infty.$$

Then a spline function $S_{n,m}$ *of the form* (1.1) *with positive knots* τ_ν *that satisfies* (6.2) *and* (6.3), *exists and is unique if and only if the measure*

$$d\lambda(t) = \frac{(-1)^{m+1}}{m!} t^{m-l} f^{(m+1)}(t)\, dt \tag{6.4}$$

admits a generalized Gauss-Turán quadrature

$$\int_0^{+\infty} g(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \sum_{k=0}^{k_\nu - 1} A_{\nu,k}^{(n)} g^{(k)}(\tau_\nu^{(n)}) + R_n(g; d\lambda), \tag{6.5}$$

with n *distinct positive nodes* $\tau_\nu^{(n)}$, *where* $R_n(g; d\lambda) = 0$ *for all* $g \in \mathcal{P}_{N+n-1}$. *The knots in* (1.1) *are given by* $\tau_\nu = \tau_\nu^{(n)}$, *th coefficients* $\alpha_{\nu,i}$ *by the following triangular system*:

$$A_{\nu,k}^{(n)} = \sum_{i=k}^{k_\nu - i} \frac{(m-i)!}{m!} \binom{i}{k} \left[\mathrm{D}^{\,i-k} t^{m-l}\right]_{t=\tau_\nu} \alpha_{\nu,i} \qquad (k = 0, 1, \ldots, k_\nu - 1), \tag{6.6}$$

where D *is the standard differentiation operator.*

For proof see Kovačević and Milovanović [21–22].

If we let $l = N + n - 1$, Theorem 6.1 gives the solution of Problem 1. The case $k_1 = k_2 = \cdots = k_n = 1$, $l = -1$, of Theorem 2.1 has been obtained by Gautschi and Milovanović [13].

Similarly as in [26–27], we can prove the following result regarding the approximating error (see Kovačević and Milovanović [22]):

Theorem 6.2. *Let* f *be given as in Theorem* 6.1 *and such that the measure* $d\lambda$ *in* (6.4) *admits a generalized Gauss-Turán quadrature formula* (6.5) *with distinct positive nodes* $\tau_\nu = \tau_\nu^{(n)}$. *Define*

$$\sigma_r(x) = x^{-(m-l)} (x - t)_+^m.$$

Then the error of the spline approximation (1.1), (6.1) ($l = N + n - 1$) *or* (1.1), (6.2), (6.3), *is given by*

$$f(t) - S_{n,m}(t) = R(\sigma_r(x); d\lambda(x)), \quad t > 0,$$

where $R(\sigma_r(x); d\lambda(x))$ *is the remainder term in the formula* (6.4) – (6.5)

$$\int_0^{+\infty} g(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \sum_{k=0}^{k_\nu - 1} A_{\nu,k}^{(n)} g^{(k)}(\tau_\nu^{(n)}) + R(g(x); d\lambda(x)).$$

If in the spline function (1.1) we take $k_\nu = 2s + 1$, $\nu = 1, \ldots, n$, $s \in \mathbb{N}_0$, i.e.,

$$S_{n,m}(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s} \alpha_{\nu,i} (\tau_\nu - t)_+^{m-i}, \qquad 0 \le t < +\infty, \tag{6.7}$$

and l is formally replaced by $-d$ in Theorem 6.1, in view of the approximative requirement (1.2), then we get the identical statement as in [26, Theorem 2.1]. Therefore, this fact enables us in this case to use the previously developed software for the problem (1.2). Now, for solving problems (6.1) or (6.2)–(6.3), one can take $d := -l$.

Let $f(t) = e^{-t}$ on $[0, +\infty)$. For this function the measure (6.4) becomes the generalized Laguerre measure

$$d\lambda(t) = \frac{1}{m!} t^{m-l} e^{-t}\, dt, \quad 0 \le t < +\infty.$$

First, for a given (n, s, m, l), we determine τ_ν^n (the zeros of the polynomial $\pi_n^{s,n}$) and the weight coefficients of the Turán quadrature (6.5). Then, the knots in (2.2) are given by $\tau_\nu = \tau_\nu^{(n)}$, $\nu = 1, \ldots, n$, and we find the coefficients of the spline function (6.7) using the triangular system of equations (6.6).

In Tables 6.1 and 6.2 we can see the behavior of approximate values of the resulting maximum absolute errors $e_{n,m}^{(l)} = \max_{0 \le t \le \tau_n} \left|S_{n,m}(t) - f(t)\right|$, for different values of (n, s, m, l). Clearly, for $t \ge \tau_n$, the absolute error is equal to $f(t)$.

Table 6.1.
Accuracy of the spline approximation for $s = 1$

	$l = 0$			$l = 1$			$l = 2$	
n	$m = 2$	$m = 3$	$m = 4$	$m = 2$	$m = 3$	$m = 4$	$m = 3$	$m = 4$
2	1.5(−1)	1.8(−2)	4.9(−3)	1.5(−1)	2.6(−2)	6.4(−3)	3.0(−2)	6.5(−3)
3	8.4(−2)	1.3(−2)	2.5(−3)	6.7(−2)	1.3(−2)	2.3(−3)	1.1(−2)	1.9(−3)
4	5.1(−2)	8.1(−3)	1.2(−3)	4.1(−2)	7.1(−3)	9.2(−4)	4.8(−3)	8.6(−4)
5	3.3(−2)	5.1(−3)	6.2(−4)	3.0(−2)	4.0(−3)	5.2(−4)	4.0(−3)	6.1(−4)

Table 6.2.
Accuracy of the spline approximation for $m = 8$

	$l = 0$		$l = 4$	
n	$s = 1$	$s = 2$	$s = 1$	$s = 2$
6	2.37(−6)	1.24(−6)	2.10(−6)	1.24(−6)
7	1.08(−6)	5.31(−7)	1.00(−6)	6.73(−7)
8	5.62(−7)	2.62(−7)	5.13(−7)	3.59(−7)
9	3.20(−7)	1.88(−7)	2.85(−7)	1.93(−7)
10	2.01(−7)	1.31(−7)	1.80(−7)	1.07(−7)

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