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MOMENT-PRESERVING SPLINE APPROXIMATION AND TURÁN QUADRATURES

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Abstract. We consider the problem of approximating a function f of the radial distance r in $\mathbb{R}^d$ on $0 \le r < \infty$ by a spline function of degree m and defect k, with n (variable) knots, matching as many of the initial moments of f as possible. We analyse the case when the defect k is an odd integer, especially when $k = 3$. We show that, if the approximation exists, it can be represented in terms of generalized Turán quadrature relative to a measure depending on f. The knots of the spline are the zeros of the corresponding s-orthogonal polynomials ($s \ge 1$). Numerical example is included.

1. INTRODUCTION

In previous papers [3] and [4], Gautschi and Gautschi and Milovanović have considered the problem of approximating a function f(r) of the radial distance $r = \|x\|$, $0 \le r < \infty$, in $\mathbb{R}^d$, $d \ge 1$, by a spline function of fixed degree (with variable knots). The approximation was to preserve as many moments of f as possible. 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. Later Frontini, Gautschi and Milovanović [1] have considered the analogous problem on an arbitrary finite interval. If the approximations exists, they can be represented in terms of generalized Gauss-Lobatto and Gauss-Radau quadrature formulas relative to appropriate moment functionals or measures depending on f.

In this paper we discuss the problem of approximating a spherically symmetric function $f(r)$, $r = \|x\|$, $0 \le r < \infty$, in $\mathbb{R}^d$, $d \ge 1$, by a spline function of degree $m \ge 2$ and defect k $(1 \le k \le m)$, with n knots. Under suitable assumptions on f and $k = 2s+1$ we will show that our problem has a unique solution if and only if certain generalized Turán quadratures exist corresponding to a measure depending of f. Existence and uniqueness is assured if f is completely monotonic on $[0,\infty)$. One simple numerical example is included.

2. MOMENT-PRESERVING SPLINE APPROXIMATION AND GENERALIZED TURÁN QUADRATURE FORMULAE

A spline function of degree $m \ge 2$ and defect k on the interval $0 \le r < \infty$, vanishing at $r = \infty$, with $n \ge 1$ positive knots $r_1, r_2, \dots, r_n$ can be written in the form

$$s_{n,m}(r) = \sum_{\nu=1}^{n} \sum_{i=m-k+1}^{m} a_{i,\nu}(r_\nu - r)_+^i , \tag{2.1}$$

where $a_{i,\nu}$ are real numbers. The plus sign on the right side of (2.1) is the cutoff symbol, $t_+ = t$ if $t > 0$ and $t_+ = 0$ if $t \le 0$. For a given function $r \to f(r)$ on $[0,\infty)$, we wish to determine $s_{n,m}(r)$ such that

$$\int_0^\infty r^j s_{n,m}(r)dV = \int_0^\infty r^j f(r)dV, \quad j = 0,1,\dots,2(s+1)n-1, \tag{2.2}$$

where $dV = (2\pi^{d/2}/\Gamma(d/2))r^{d-1}dr$ is the volume element of the spherical shell in $\mathbb{R}^d$ if $d > 1$, and $dV = dr$ if $d = 1$. In other words, we want $s_{n,m}$ to faithfully reproduce the first $2(s+1)n$ spherical moments of f.

In this paper we will reduce our problem to the power-orthogonality (s-orthogonality) and generalized Gauss-Turán quadratures ([2],[5],[7-12]), by restricting the class of functions f. Then we can use recently developed stable procedure of constructing s-orthogonal polynomials ([6]).

The generalized Gauss-Turán quadratures with a given nonnegative measure $d\lambda(r)$ on the real line $\mathbb{R}$ (with compact or infinite support for which all moments $\mu_k = \int_{\mathbb{R}} r^k d\lambda(r)$, $k = 0,1,\dots$, exist and are finite, and $\mu_0 > 0$),

$$\int_{\mathbb{R}} g(r)d\lambda(r) = \sum_{\nu=1}^{n} \sum_{i=0}^{k-1} A_{i,\nu}\, g^{(i)}(r_\nu) + R_n(g;d\lambda),$$

is exact for all polynomials of degree at most $(k+1)n-1$, if k is odd, i.e. $k = 2s+1$. The nodes r_ν, $\nu = 1,\dots,n$, are the zeros of the (monic) polynomial π minimizing

$$\int_{\mathbb{R}} \pi_n(r)^{2s+2}\, d\lambda(r). \tag{2.3}$$

Such polynomials are known as power-orthogonal (s-orthogonal or s-self associated) polynomials with respect to the measure $d\lambda(r)$. For a given n and s, the minimization of the integral (2.3) leads to the "orthogonality conditions"

$$\int_{\mathbb{R}} \pi_n^{2s+1}(r) r^i\, d\lambda(r) = 0, \quad i = 0,1,\dots,n-1.$$

which can be interpreted as (see [6])

$$\int_{\mathbb{R}} \pi_\nu^{s,n}(r) r^i d\mu(r) = 0, \quad i = 0,1,\dots,\nu-1,$$

where $(\pi_\nu^{s,n})$ is a sequence of monic orthogonal polynomials with respect to the new measure $d\mu(r) = d\mu^{s,n}(r) = (\pi_n^{s,n}(r))^{2s} d\lambda(r)$. As we can see, the polynomials $\pi_\nu^{s,n}$, $\nu = 0,1,\dots,$ are implicitly defined because the measure $d\mu(r)$ depends on $\pi_n^{s,n}(r) (\equiv \pi_n(r))$. Of course, we are interested only in $\pi_n^{s,n}(r)$. A stable procedure of constructing such polynomials (s-orthogonal) is given in [6].

In order to reduce our problem (2.2) to the power-orthogonality, we have to put $k = 2s+1$, i.e. the defect of the spline function (2.1) should be odd.

Using (2.1) and observing that $r_\nu > 0$, we have

$$\int_0^\infty r^{j+d-1} s_{n,m}(r)dr = \sum_{\nu=1}^{n} \sum_{i=m-2s}^{m} a_{i,\nu} \int_0^{r_\nu} r^{j+d-1}(r_\nu - r)^i dr.$$

Changing variables, $r = tr_\nu$, in the integral on the right, we obtain the well-known beta integral which can be expressed in terms of factorials. So we find

$$\int_0^\infty r^{j+d-1} s_{n,m}(r)dr = \frac{(j+d-1)!m!}{(j+d+m)!} \sum_{\nu=1}^{n} \sum_{i=m-2s}^{m} \frac{i!(j+d+m)!}{m!(j+d+i)!} a_{i,\nu} r_\nu^{j+d+i}.$$

Let

$$\mu_j = \frac{(j+d+m)!}{m!(j+d-1)!} \int_0^\infty r^{j+d-1} f(r)dr, \quad j = 0,1,\dots 2(s+1)n-1, \tag{2.4}$$

where the moments of f on the right are assumed to exist. Then, the conditions (2.2) can be represented in the form

$$\sum_{\nu=1}^{n} \sum_{i=m-2s}^{m} \frac{i!}{m!} a_{i,\nu} [D^{m-i} r^{j+d+m}]_{r=r_\nu} = \mu_j, \quad j = 0,1,\ldots,2(s+1)n-1,$$

where D is the standard differentiation operator.

Changing indices $(k = m-i)$, the second sum on the left becomes

$$\sum_{k=0}^{2s} \frac{(m-k)!}{m!} a_{m-k,\nu} [D^k (r^{d+m} r^j)]_{r=r_\nu} ,$$

or, after the application of Leibnitz formula to k-th derivative,

$$\sum_{i=0}^{2s} A_{i,\nu}^{(n)} [D^i r^j]_{r=r_\nu} ,$$

where

$$A_{i,\nu}^{(n)} = \sum_{k=i}^{2s} \frac{(m-k)!}{m!} \binom{k}{i} [D^{k-i} r^{d+m}]_{r=r_\nu} a_{m-k,\nu} , \quad i = 0,1,\ldots,2s. \tag{2.5}$$

Hence,

$$\sum_{\nu=1}^{n} \sum_{i=0}^{2s} A_{i,\nu}^{(n)} [D^i r^j]_{r=r_\nu} = \mu_j , \quad j = 0,1,\ldots,2(s+1)n-1. \tag{2.6}$$

Now, we state the main result :

<u>**THEOREM 2.1.**</u> Let $f \in C^{m+1}[0,\infty]$ and

$$\int_0^\infty r^{2(s+1)n+d+m} |f^{(m+1)}(r)| dr < \infty. \tag{2.7}$$

Then a spline function $s_{n,m}$ of the form

$$s_{n,m}(r) = \sum_{\nu=1}^{n} \sum_{i=m-2s}^{m} a_{i,\nu} (r_\nu - r)_+^i , \tag{2.8}$$

with positive knots r_ν, that satisfies (2.2), exists and is unique if and only if the measure

$$d\lambda(r) = \frac{(-1)^{m+1}}{m!} r^{m+d} f^{(m+1)}(r) dr \text{ on } [0,\infty) \tag{2.9}$$

admits a generalized Gauss-Turán quadrature

$$\int_0^\infty p(r) d\lambda(r) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s} A_{i,\nu}^{(n)} p^{(i)}(r_\nu^{(n)}), \quad p \in \mathbb{P}_{2(s+1)n-1} , \tag{2.10}$$

with distinct positive nodes $r_\nu^{(n)}$. The knots r_ν in (2.8) are given by $r_\nu = r_\nu^{(n)}$, and coefficients $a_{i,\nu}$ by the triangular system (2.5).

Proof. Let $j \le 2(s+1)n-1$. Because of (2.7), the integral $\int_0^\infty r^{j+d+m+1} f^{(m+1)}(r)dr$ exists and $\lim_{r\to\infty} r^{j+d+m+1} f^{(m+1)}(r) = 0$. Then, L'Hospital's rule implies

$$\lim_{r\to\infty} r^{j+d+m}\, f^{(m)}(r) = 0.$$

Continuing in this manner, we find that

$$\lim_{r\to\infty} r^{j+d+\mu}\, f^{(\mu)}(r) = 0, \quad \mu = m,m-1,\dots,0.$$

Under these conditions we can prove that (see [4])

$$\int_0^\infty r^{j+d-1}\, f(r)dr = (-1)^{m+1}[(j+d)(j+d+1)\dots(j+d+m)]^{-1} \int_0^\infty r^{j+d+m} f^{(m+1)}(r)dr.$$

Therefore, the moments μ_j, defined by (2.4), exist and

$$\mu_j = \int_0^\infty r^j d\lambda(r), \quad j = 0,1,\dots,2(s+1)n-1,$$

where $d\lambda(r)$ is given by (2.9). Hence, we conclude that Eqs. (2.2) are equivalent to Eqs. (2.6). These are precisely the conditions for r_ν to be the nodes of the generalized Gauss-Turán quadrature formula (2.10) and $A_{i,\nu}^{(n)}$, determined by (2.6), their coefficients.

The nodes $r_\nu^{(n)}$, being the zeros of the s-orthogonal polynomial $\pi_n^{s,n}$ (if exists), are uniquely determined, hence also the coefficients $A_{i,\nu}^{(n)}$. □

REMARK. The case $s = 0$ of Theorem 2.1 has been obtained in [4].

If f is completely monotonic on $[0,\infty)$ then $d\lambda(r)$ in (2.9) is a positive measure for every m. Also, the first $2(s+1)n$ moments exist by virtue of the assumptions in Theorem 2.1. Then, the generalized Gauss-Turán quadrature formula exists uniquely, with n distinct and positive nodes $r_\nu^{(n)}$.

In the special case when $s = 1$, the coefficients of the spline function (2.8) are

$$a_{m-2,\nu} = m(m-1)A_{2,\nu}^{(n)} r_\nu^{-(d+m)},$$

$$a_{m-1,\nu} = m\left[A_{1,\nu}^{(n)} r_\nu - 2(d+m)A_{2,\nu}^{(n)}\right] r_\nu^{-(d+m+1)},$$

$$a_{m,\nu} = \left[(d+m)(d+m+1)A_{2,\nu}^{(n)} - (d+m)A_{1,\nu}^{(n)} r_\nu + A_{0,\nu}^{(n)} r_\nu^2\right] r_\nu^{-(d+m+2)}.$$

Similarly as in [4] we can prove the following statement :

THEOREM 2.2. Given f as in Theorem 2.1, assume that the measure $d\lambda$ in (2.9) admits a generalized Gauss-Turán quadrature formula (2.10) with distinct positive nodes $r_\nu = r_\nu^{(n)}$. Define

$$\sigma_r(t) = t^{-(m+d)}(t-r)_+^m .$$

Then the error of the spline approximation (2.1), (2.2),

$$f(r) - s_{n,m}(r) = R_{n,s}(\sigma_r; d\lambda), \quad r > 0, \tag{2.11}$$

where $R_{n,s}(g;d\lambda)$ is the remainder term in the formula

$$\int_0^\infty g(r)d\lambda(r) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s} A_{i,\nu}^{(n)} g^{(i)}(r_\nu^{(n)}) + R_{n,s}(g;d\lambda). \tag{2.12}$$

Proof. As in [4] we have

$$f(r) = \int_0^\infty \sigma_r(t)d\lambda(t). \tag{2.13}$$

On the other hand, we consider the sum

$$F_\nu(r) = \sum_{i=0}^{2s} A_{i,\nu}^{(n)} [D^i\sigma_r(t)]_{t=r_\nu} ,$$

where $A_{i,\nu}^{(n)}$ are the coefficients of the generalized Gauss-Turán quadrature (2.12). By (2.5) and Leibnitz formula, we obtain

$$\begin{aligned}
F_\nu(r) &= \sum_{i=0}^{2s} [D^i\sigma_r(t)]_{t=r_\nu}\left[\sum_{k=i}^{2s} \frac{(m-k)!}{m!} \binom{k}{i} [D^{k-i}t^{d+m}]_{t=r_\nu} a_{m-k,\nu}\right] \\
&= \sum_{k=0}^{2s} a_{m-k,\nu} \frac{(m-k)!}{m!} \sum_{i=0}^{k} \binom{k}{i} [(D^{k-i}t^{d+m})(D^i\sigma_r(t))]_{t=r_\nu} \\
&= \sum_{k=0}^{2s} a_{m-k,\nu} \frac{(m-k)!}{m!} [D^k(t^{d+m}\sigma_r(t))]_{t=r_\nu} \\
&= \sum_{k=0}^{2s} a_{m-k,\nu} (r_\nu - r)_+^{m-k} .
\end{aligned}$$

Finally, changing indices (m-k=i) we find

$$F_\nu(r) = \sum_{i=m-2s}^{m} a_{i,\nu}(r_\nu - r)_+^i ,$$

i.e.

$$\sum_{\nu=1}^{n} F_\nu(r) = s_{n,m}(r). \tag{2.14}$$

Now, using (2.13) and (2.14), we obtain (2.11). □

The error estimation and convergence of generalized Gauss-Turán quadrature were given in [8-9].

3. NUMERICAL EXAMPLE.

In this section we give a simple example - the exponential distribution in $\mathbb{R}^d$. All computations were done on the ZENITH PC/XT in the double precision (machine precision ≅ 8.88×10^{-16}).

EXAMPLE 3.1. $f(r) = c_d e^{-r}$ on $[0,\infty)$, where $c_d = \Gamma(d/2)/(2\Gamma(d)\pi^{d/2})$ if $d > 1$, and $c_1 = 1$. This example was considered in [4] for $s = 0$.

For this exponential distribution the measure (2.9) becomes the generalized Laguerre measure

$$d\lambda(r) = \frac{c_d}{m!} r^{d+m} e^{-r} dr, \quad 0 \le r < \infty.$$

Firstly, for a given (n,s,m,d), we determine the zeros of the polynomial $\pi_n^{s,n}$ and weight coefficients of the Turán quadrature (2.12). Then, using the triangular system of equations (2.5), we find the coefficients of the spline function (2.8). For example, for $n = m = 3$, $s = 1$, and $d = 2$, the parameters of (2.8) are presented in Table 3.1 (to 10 decimals only, to save space). Numbers in parenthesis indicate decimal exponents.

Table 3.1

The coefficients of spline function for $n = 3$, $m = 3$, $s = 1$, $d = 2$

ν	r_ν	$a_{1,\nu}$	$a_{2,\nu}$	$a_{3,\nu}$
1	3.358776981(0)	5.259487383(-3)	-9.525138685(-3)	1.200758965(-2)
2	9.274670326(0)	4.144453254(-5)	-1.511837278(-4)	1.685532824(-4)
3	1.948478101(1)	6.273730625(-9)	-3.272516603(-8)	3.550824554(-8)

Table 3.2 shows approximate values of the resulting maximum absolute errors $e_{n,m} = \max_{0 \le r \le r_n} |s_{n,m}(r) - f(r)|$, for $n = 2, 3, 4, 5$; $m = 2, 3, 4$; $s = 1$; $d = 1, 2, 3$. Clearly, for $r \ge r_n$, the absolute error is equal to $f(r)$.

Table 3.2

Accuracy of the spline approximation for $s = 1$

n	d=1			d=2			d=3		
	m=2	m=3	m=4	m=2	m=3	m=4	m=2	m=3	m=4
2	1.2(-1)	2.1(-2)	1.2(-2)	2.2(-2)	1.3(-2)	8.3(-3)	1.1(-2)	7.6(-3)	5.2(-3
3	8.4(-2)	1.1(-2)	3.3(-3)	1.2(-2)	5.3(-3)	2.8(-3)	6.3(-3)	3.5(-3)	2.1(-3)
4	5.9(-2)	7.9(-3)	1.3(-3)	9.2(-3)	2.5(-3)	1.2(-3)	3.8(-3)	1.9(-3)	9.5(-4)
5	4.1(-2)	5.6(-3)	7.7(-4)	7.1(-3)	1.4(-3)	5.4(-4)	2.5(-3)	1.1(-3)	4.8(-4)

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