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Spline Approximations to Spherically Symmetric Distributions*

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Summary. We discuss the problem of approximating a function f of the radial distance r in $\mathbb{R}^d$ on $0 \leqq r < \infty$ by a spline function of degree m with n (variable) knots. The spline is to be constructed so as to match the first $2n$ moments of f. We show that if a solution exists, it can be obtained from an n-point Gauss-Christoffel quadrature formula relative to an appropriate moment functional or, if f is suitably restricted, relative to a measure, both depending on f. The moment functional and the measure may or may not be positive definite. Pointwise convergence is discussed as $n \to \infty$. Examples are given including distributions from statistical mechanics.

Subject Classifications: AMS (MOS): 41A15, 65D32; 33A65; CR: G1.2.

1. Introduction

Following earlier work of Laframboise and Stauffer [10] and Calder, Laframboise and Stauffer [1], one of us in [8] considered the problem of approximating a function $f(r)$ of the radial distance $r = \|x\|$, $0 \leqq r < \infty$, in $\mathbb{R}^d$, $d \geqq 1$, by a piecewise constant function of r (and also by a linear combination of Dirac delta functions). The approximation was to preserve as many moments of f as possible. It was found that the problem can be solved by means of Gauss-Christoffel quadrature. Here we extend this work to spline approximation of arbitrary degree. Under suitable assumptions on f it will be shown that the problem has a unique solution if and only if certain Gaussian quadrature rules exist corresponding to a (possibly nonpositive) moment functional or weight distribution depending on f. Existence and uniqueness is assured if f is completely monotonic on $[0, \infty)$. Pointwise convergence of our approximation process depends on a convergence property of the Gauss-Christoffel quadrature rule. A number of examples are presented illustrating the quality of approximation.

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2. Moment-Preserving Approximation by Spline Functions

A spline function of degree $m \geqq 0$ on the interval $0 \leqq r < \infty$, vanishing at $r = \infty$, with $n \geqq 1$ positive knots r_ν, $\nu = 1, 2, \ldots, n$, can be written in the form

$$s_n(r) = \sum_{\nu=1}^{n} a_\nu (r_\nu - r)_+^m, \qquad 0 \leqq r < \infty, \tag{2.1}$$

where a_ν are real numbers and the plus sign on the right is the cutoff symbol, $t_+ = t$ if $t > 0$ and $t_+ = 0$ if $t \leqq 0$. Given a function $f(r)$ on $0 \leqq r < \infty$, we wish to determine $s_n(r)$ such that

$$\int_0^\infty r^j s_n(r)\, dV = \int_0^\infty r^j f(r)\, dV, \qquad j = 0, 1, \ldots, 2n-1, \tag{2.2}$$

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 to faithfully reproduce the first $2n$ spherical moments of f.

A first approach to this problem can be based on the moment functional

$$\mathscr{L} t^j = \mu_j, \qquad \mu_j = \frac{(j+d+m)!}{m!\,(j+d-1)!} \int_0^\infty r^{j+d-1} f(r)\, dr, \qquad j = 0, 1, 2, \ldots. \tag{2.3}$$

The functional $\mathscr{L}$, by virtue of (2.3), and being linear, is well defined for any polynomial, and therefore gives rise to the concept of orthogonality with respect to the functional $\mathscr{L}$: Two polynomials p and q are orthogonal with respect to $\mathscr{L}$ if $\mathscr{L}(p \cdot q) = 0$ (cf. [2, Chapter 1, Sect. 2]).

Theorem 2.1. *Given f with $\int_0^\infty r^{j+d-1} f(r)\, dr$, $j = 0, 1, \ldots, 2n-1$, finite, there exists a unique spline function s_n of the form* (2.1) *with distinct positive knots r_ν and satisfying* (2.2) *if and only if there exists a unique (monic) polynomial $\pi_n(\cdot\,; \mathscr{L})$ of degree n orthogonal with respect to $\mathscr{L}$ to all lower-degree polynomials and having zeros $r_\nu^{(n)}$, $\nu = 1, 2, \ldots, n$, that are all simple and positive. In that event, the knots r_ν and weights a_ν in* (2.1) *are given by*

$$r_\nu = r_\nu^{(n)}, \; a_\nu = r_\nu^{-(m+d)} w_\nu, \qquad \nu = 1, 2, \ldots, n, \tag{2.4}$$

where $\{w_\nu\}$ is the (unique) solution of the Vandermonde system

$$\sum_{\nu=1}^{n} w_\nu r_\nu^j = \mu_j, \qquad j = 0, 1, \ldots, n-1. \tag{2.5}$$

Proof. Substituting (2.1) in (2.2) yields, since $r_\nu > 0$,

$$\sum_{\nu=1}^{n} a_\nu \int_0^{r_\nu} r^{j+d-1} (r_\nu - r)^m\, dr = \int_0^\infty r^{j+d-1} f(r)\, dr, \qquad j = 0, 1, \ldots, 2n-1. \tag{2.6}$$

Introducing on the left the new variable of integration t through $r = tr_\nu$ gives

$$\sum_{\nu=1}^{n} a_\nu r_\nu^{j+d+m} \int_0^1 t^{j+d-1}(1-t)^m\,dt = \int_0^\infty r^{j+d-1} f(r)\,dr.$$

The integral on the left is the well-known beta integral which can be expressed in terms of factorials. There results

$$\sum_{\nu=1}^{n} w_\nu r_\nu^j = \mu_j, \qquad j = 0, 1, \ldots, 2n-1, \tag{2.7}$$

where

$$w_\nu = a_\nu r_\nu^{d+m}, \qquad \nu = 1, 2, \ldots, n, \tag{2.8}$$

and μ_j is given by (2.3). By virtue of the first relation in (2.3), the system of nonlinear equations (2.7) can be written in the form

$$\sum_{\nu=1}^{n} w_\nu p(r_\nu) = \mathscr{L} p, \qquad \text{all } p \in \mathbb{P}_{2n-1}, \tag{2.9}$$

which identifies r_ν and w_ν as the nodes and weights of the "Gaussian quadrature formula" for the functional $\mathscr{L}$. It is well known (see, e.g., [6, § 1.3]) that (2.9) is equivalent to the following two conditions:

(i) The formula (2.9) is interpolatory, i.e., valid for every $p \in \mathbb{P}_{n-1}$;

(ii) The node polynomial $\omega(r) = \prod_{\nu=1}^{n} (r - r_\nu)$ is orthogonal with respect to $\mathscr{L}$ to all polynomials of degree $< n$.

The second condition identifies ω as $\omega(\cdot) = \pi_n(\cdot\,; \mathscr{L})$ and the knots r_ν as the zeros of $\pi_n(\cdot\,; \mathscr{L})$. The first condition is equivalent to (2.5). □

It is well known that $\pi_n(\cdot\,; \mathscr{L})$ exists uniquely if and only if

$$\det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{bmatrix} \tag{2.10}$$

While Theorem 2.1 is of some theoretical interest, it does not lend itself to constructive purposes because of the well-known ill-conditioning associated with power moments.

By further restricting the class of functions f, it is possible, however, to relate our problem to Gauss-Christoffel quadrature relative to an absolutely continuous measure supported on $[0, \infty]$ (and depending of f). Therefore, recently developed stable methods of constructing orthogonal polynomials (see, e.g., [7]) can be brought to bear upon the problem.

Theorem 2.2. *Let f be such that the integrals $\int_0^\infty r^{j+d-1} f(r)\,dr$, $j = 0, 1, \ldots, 2n-1$, converge and, in addition, that*

$$f \in C^{m+1}[0, \infty], \qquad \lim_{r\to\infty} r^{2n-1+d+\mu} f^{(\mu)}(r) = 0, \qquad \mu = 0, 1, \ldots, m. \tag{2.11}$$

Then a spline function s_n *of the form* (2.1) *with positive knots* r_ν, *that satisfies* (2.2), *exists and is unique if and only if the measure*

$$d\lambda(r)=\frac{(-1)^{m+1}}{m!}\, r^{m+d} f^{(m+1)}(r)\,dr \quad on \quad [0,\infty) \tag{2.12}$$

admits an n-point Gauss-Christoffel quadrature formula

$$\int_0^\infty p(r)\,d\lambda(r)=\sum_{\nu=1}^{n} \lambda_\nu^{(n)} p(r_\nu^{(n)}), \qquad p\in \mathbb{P}_{2n-1}, \tag{2.13}$$

with distinct positive nodes $r_\nu^{(n)}$. *In that event, the knots* r_ν *and weights* a_ν *in* (2.1) *are given by*

$$r_\nu=r_\nu^{(n)},\ a_\nu=r_\nu^{-(m+d)}\lambda_\nu^{(n)}, \qquad \nu=1,2,\dots,n. \tag{2.14}$$

Remark. The case $m=0$ of Theorem 2.2 has been obtained in [8].

Proof of Theorem 2.2. The left-hand side in (2.6), through m integrations by parts, can be seen to be equal to

$$\begin{aligned} &m![(j+d)(j+d+1)\cdots(j+d+m-1)]^{-1}\sum_{\nu=1}^{n} a_\nu \int_0^{r_\nu} r^{j+d+m-1}\,dr \\ &=m![(j+d)(j+d+1)\cdots(j+d+m)]^{-1}\sum_{\nu=1}^{n} a_\nu r_\nu^{j+d+m}. \end{aligned} \tag{2.15}$$

The integral on the right of (2.6) is transformed similarly by $m+1$ integrations by parts. We carry out the first of these in detail to exhibit the reasonings involved. We have, for any $b>0$,

$$\int_0^b r^{j+d-1} f(r)\,dr=(j+d)^{-1} r^{j+d} f(r)\,|_0^b-(j+d)^{-1}\int_0^b r^{j+d} f'(r)\,dr.$$

The integrated term clearly vanishes at $r=0$ and tends to zero as $r=b\to\infty$ by the second assumption in (2.11) with $\mu=0$. Since $j\leqq 2n-1$ and the integral on the left converges by assumption, we conclude the convergence of the integral on the right as $b\to\infty$. Therefore,

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

Continuing in this manner, using the second assumption in (2.11) to show convergence to zero of the integrated term at the upper limit (its value at $r=0$ always being zero) and the existence of $\int_0^\infty r^{j+d-1+\mu} f^{(\mu)}(r)\,dr$ already established to infer the existence of $\int_0^\infty r^{j+d+\mu} f^{(\mu+1)}(r)\,dr$, $\mu=1,2,\dots,m$, we arrive at

$$\int_0^\infty r^{j+d-1} f(r)\,dr=(-1)^{m+1}[(j+d)(j+d+1)\cdots(j+d+m)]^{-1}\int_0^\infty r^{j+d+m} f^{(m+1)}(r)\,dr. \tag{2.16}$$

Comparing (2.16) with (2.15), we see that Eqs. (2.6), and hence Eqs. (2.2), are equivalent to

$$\sum_{\nu=1}^{n} (a_\nu r_\nu^{m+d}) r_\nu^j = \int_0^\infty \left[\frac{(-1)^{m+1}}{m!} r^{m+d} f^{(m+1)}(r)\right] r^j\, dr, \qquad j=0, 1, \ldots, 2n-1.$$

These are precisely the conditions for r_ν to be the nodes of the Gauss-Christoffel formula (2.12), (2.13) and $a_\nu r_\nu^{m+d}$ their weights.

The nodes $r_\nu^{(n)}$, being the zeros of the orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ (if it exists), are uniquely determined, hence also the weights $\lambda_\nu^{(n)}$. $\square$

If f is completely monotonic on $[0, \infty)$ (see, e.g., Widder [12, p. 145 ff.]) then $d\lambda(r)$ in (2.12) is a positive measure for every m. Moreover, the first $2n$ moments exist by virtue of the assumptions made on f in Theorem 2.2. The Gauss-Christoffel quadrature rule (2.13) therefore exists uniquely, all nodes $r_\nu^{(n)}$ being distinct and positive and all weights $\lambda_\nu^{(n)}$ positive. The latter implies $a_\nu > 0$, $\nu = 1, 2, \ldots, n$, in (2.1).

Theorem 2.3. *Given f as in Theorem 2.2, assume that the measure $d\lambda$ in (2.12) admits an n-point Gauss-Christoffel quadrature formula (2.13) with distinct positive nodes $r_\nu = r_\nu^{(n)}$. Define*

$$\sigma_r(t) = t^{-(m+d)}(t-r)_+^m. \tag{2.17}$$

Then, for any $r > 0$, we have for the error of the approximation (2.1), (2.2),

$$f(r) - s_n(r) = R_n(\sigma_r; d\lambda), \tag{2.18}$$

where $R_n(g; d\lambda)$ is the remainder term in the Gauss-Christoffel quadrature formula (2.12), (2.13),

$$\int_0^\infty g(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} g(r_\nu^{(n)}) + R_n(g; d\lambda). \tag{2.19}$$

Proof. By Taylor's formula, one has for any $b > 0$,

$$f(r) = f(b) + f'(b)(r-b) + \cdots + \frac{f^{(m)}(b)}{m!}(r-b)^m + \frac{1}{m!}\int_b^r (r-t)^m f^{(m+1)}(t)\, dt. \tag{2.20}$$

Since by (2.11), $\lim_{t\to\infty} t^\mu f^{(\mu)}(t) = 0$ for $\mu = 0, 1, \ldots, m$, we obtain from (2.20), letting $b \to \infty$,

$$f(r) = \frac{(-1)^{m+1}}{m!}\int_r^\infty (t-r)^m f^{(m+1)}(t)\, dt = \frac{(-1)^{m+1}}{m!}\int_0^\infty (t-r)_+^m f^{(m+1)}(t)\, dt,$$

hence, by (2.12) and (2.17),

$$f(r) = \int_0^\infty \sigma_r(t)\, d\lambda(t). \tag{2.21}$$

On the other hand, by (2.1) and (2.14),

$$s_n(r)=\sum_{\nu=1}^{n}\lambda_\nu r_\nu^{-(m+d)}(r_\nu-r)_+^m=\sum_{\nu=1}^{n}\lambda_\nu\sigma_r(r_\nu). \tag{2.22}$$

Subtracting (2.22) from (2.21) yields (2.18). □

To discuss convergence as $n\to\infty$ (for fixed m), we assume f to satisfy the assumptions of Theorem 2.2 for all $n=1,2,3,\ldots$. Then, by Theorem 2.3, our approximation process converges pointwise (at r), as $n\to\infty$, if and only if the Gauss-Christoffel quadrature formula (2.19) converges when applied to the special function $g(t)=\sigma_r(t)$ in (2.17). Since σ_r is uniformly bounded on $\mathbb{R}$, this is true, for example, if $d\lambda$ is a positive measure and the moment problem for $d\lambda$ on $[-\infty,\infty]$ (with $d\lambda(t)=0$ for $t<0$) is determined (cf. [4, Chapter 3, Theorem 1.1]).

3. Examples

We begin with, perhaps, the simplest example – the exponential distribution in $\mathbb{R}^d$. All computations reported in this section were done on the CDC 6500 computer in single precision (machine precision $\approx 3.55\times 10^{-15}$), except for Table 2, which was computed in double precision.

Example 3.1. $f(r)=c_d e^{-r}$ on $[0,\infty)$, where $c_1=1$, $c_d=\Gamma(d/2)/(2\Gamma(d)\pi^{d/2})$ if $d>1$.

For this distribution the measure (2.12) becomes the generalized Laguerre measure

$$d\lambda(r)=\frac{c_d}{m!}r^{m+d}e^{-r}dr,\qquad 0\leqq r<\infty. \tag{3.1}$$

The knots r_ν, therefore, are the zeros of the generalized Laguerre polynomial $L_n^{(\alpha)}$ with parameter $\alpha=m+d$, and the weights a_ν follow readily from (2.14) in terms of the corresponding Christoffel numbers $\lambda_\nu^{(n)}$. It is a straightforward matter to calculate the desired spline (2.1) for any value of m, d and n.

Table 1 shows approximate values of the resulting maximum absolute errors $\max_{0\leqq r\leqq r_n}|s_n(r)-f(r)|$, for $m=1,2,3$; $d=1,2,3$; and $n=5,10,20,40$. (Numbers in parentheses indicate decimal exponents.) Clearly, $|s_n(r)-f(r)|=f(r)$ for $r\geqq r_n$. Since the moment problem for the measure $d\lambda$ in (3.1) is determined (see, e.g., [4, Chapter 2, Theorem 5.2]), it follows from the remark at the end of Sect. 2 that $s_n(r)\to f(r)$ as $n\to\infty$, for any fixed $r>0$.

It is likely that convergence also takes place if n is fixed and $m\to\infty$. When $n=1$, for example,

$$s_1(r)=c_d\frac{(m+1)\cdots(m+d)}{(m+d+1)^d}\left(1-\frac{r}{m+d+1}\right)_+^m, \tag{3.2}$$

which implies $s_1(r)=c_d e^{-r}+O(m^{-1})$ as $m\to\infty$. For other values of n, and selected values of r (with $d=1$), the convergence behavior as $m\to\infty$ is illustrated in Table 2, which shows the respective absolute errors.

Our next example is the Bose-Einstein distribution; for simplicity we do not normalize it to have unit integral over space.

Example 3.2. $f(r)=(\alpha e^r-1)^{-1}$, $\alpha>1$ if $d=1$ and $\alpha\geqq 1$ if $d\geqq 2$.

Table 1. Accuracy of the spline approximation for Example 3.1

n	$d=1$			$d=2$			$d=3$		
	$m=1$	$m=2$	$m=3$	$m=1$	$m=2$	$m=3$	$m=1$	$m=2$	$m=3$
5	5.9 (-2)	1.8 (-2)	7.9 (-3)	2.4 (-2)	1.1 (-2)	5.9 (-3)	1.2 (-2)	6.5 (-3)	3.9 (-3)
10	1.8 (-2)	3.5 (-3)	1.0 (-3)	8.9 (-3)	2.7 (-3)	9.4 (-4)	5.0 (-3)	1.9 (-3)	7.6 (-4)
20	1.5 (-2)	1.2 (-3)	1.9 (-4)	2.8 (-3)	4.9 (-4)	1.0 (-4)	1.7 (-3)	3.9 (-4)	9.8 (-5)
40	7.5 (-3)	4.2 (-4)	4.7 (-5)	1.2 (-3)	7.6 (-5)	8.8 (-6)	5.1 (-4)	6.5 (-5)	9.2 (-6)

Table 2. Convergence behavior as $m \to \infty$ of the spline approximation for Example 3.1

m	$r=5$			$r=1.0$			$r=5.0$		
	$n=5$	$n=10$	$n=20$	$n=5$	$n=10$	$n=20$	$n=5$	$n=10$	$n=20$
5	7.3 (-4)	3.2 (-5)	3.3 (-7)	5.1 (-4)	1.6 (-5)	3.5 (-6)	1.2 (-4)	2.5 (-5)	1.3 (-6)
10	6.7 (-5)	6.3 (-7)	7.3 (-10)	4.4 (-5)	2.1 (-7)	3.3 (-9)	8.3 (-7)	1.8 (-8)	1.3 (-9)
20	4.0 (-6)	4.6 (-9)	2.4 (-13)	2.6 (-6)	1.5 (-9)	6.3 (-13)	2.1 (-7)	7.0 (-10)	4.6 (-13)
40	1.8 (-7)	1.5 (-11)	1.1 (-17)	1.2 (-7)	4.9 (-12)	2.2 (-17)	9.9 (-9)	1.8 (-12)	6.1 (-18)
80	7.0 (-9)	3.0 (-14)	1.0 (-22)	4.6 (-9)	9.5 (-15)	1.8 (-22)	3.7 (-10)	2.8 (-15)	2.8 (-23)

It can be shown by induction that

$$f^{(m+1)}(r) = (-1)^{m+1} f(r) \sum_{k=0}^{m+1} q_{m+1,k} [f(r)]^k,$$

where

$$\left.\begin{aligned} q_{1,0} &= q_{1,1} = 1, \\ q_{\mu+1,0} &= q_{\mu,0}, \\ q_{\mu+1,\kappa} &= \kappa q_{\mu,\kappa-1} + (\kappa+1) q_{\mu,\kappa}, \qquad \kappa = 1, \ldots, \mu \\ q_{\mu+1,\mu+1} &= (\mu+1) q_{\mu,\mu} \end{aligned}\right\} \mu = 1, \ldots, m.$$

The measure (2.12) thus becomes

$$d\lambda(r) = \frac{r^{m+d}}{m!} f(r) \sum_{k=0}^{m+1} q_{m+1,k} [f(r)]^k \, dr, \qquad 0 \leqq r < \infty, \tag{3.3}$$

and is clearly positive. All moments of $d\lambda$ exist, if $\alpha > 1$, for arbitrary $m \geqq 0$ and $d \geqq 1$. The same is true for $\alpha = 1$, if $d \geqq 2$, since $d\lambda(r) \sim (m+1) r^{d-2} [r/(e^r - 1)]^{m+2}$ as $r \to 0$. In these cases, the moment problem for $d\lambda$ is determined, since $d\lambda(r) \sim (\alpha m!)^{-1} r^{m+d} e^{-r} dr$ as $r \to \infty$ (cf. [4, Chapter 2, Theorem 5.2]), and therefore $s_n(r) \to f(r)$ as $n \to \infty$.

The function $f(r)$, however, is unbounded near the origin, when $\alpha = 1$, which renders approximation by low-degree splines difficult. In the range where f is significant, and not too close to $r = 0$, the accuracy attainable is typically about 1–10 percent.

Table 3. Relative accuracy of the spline approximation for Example 3.2

n	$m=1$			$m=2$			$m=3$		
	ν	r_ν	rel. err.	ν	r_ν	rel. err.	ν	r_ν	rel. err.
5	1	1.272		1	1.468		1	1.646	
	2	3.771	5.5(-1)	2	4.333	2.7(-1)	2	4.885	1.4(-1)
	3	7.152	7.5(-1)	3	7.992	4.8(-1)	3	8.821	2.9(-1)
10	1	0.597		1	0.664		1	0.724	
	2	1.910	3.6(-1)	2	2.142	1.7(-1)	2	2.350	6.6(-2)
	3	3.757	3.2(-1)	3	4.199	1.0(-1)	3	4.625	3.9(-2)
	4	6.057	4.3(-1)	4	6.677	1.6(-1)	4	7.286	6.4(-2)
20	1	0.271		1	0.293		1	0.313	
	2	0.895	3.1(-1)	2	0.971	1.4(-1)	2	1.037	5.5(-2)
	3	1.837	1.7(-1)	3	2.002	4.1(-2)	3	2.146	1.4(-2)
	4	3.049	1.6(-1)	4	3.328	3.2(-2)	4	3.584	9.1(-3)
	5	4.500	1.9(-1)	5	4.890	4.1(-2)	5	5.264	1.1(-2)
	6	6.187	2.4(-1)	6	6.675	5.8(-2)	6	7.151	1.6(-2)
40	1	0.123		1	0.131		1	0.137	
	2	0.412	2.9(-1)	2	0.436	1.3(-1)	2	0.458	5.1(-2)
	3	0.859	1.3(-1)	3	0.912	3.2(-2)	3	0.958	9.6(-3)
	4	1.458	8.8(-2)	4	1.551	1.2(-2)	4	1.631	4.4(-3)
	5	2.197	7.3(-2)	5	2.343	1.0(-2)	5	2.469	2.7(-3)
	6	3.065	8.0(-2)	6	3.271	1.0(-2)	6	3.456	2.2(-3)
	7	4.055	9.3(-2)	7	4.321	1.2(-2)	7	4.569	2.3(-3)
	8	5.164	1.1(-1)	8	5.487	1.6(-2)	8	5.796	3.0(-3)
	9	6.393	1.3(-1)	9	6.770	2.0(-2)	9	7.134	4.1(-3)

Maximum relative errors in some of the early intervals $[r_\nu, r_{\nu+1}]$, $\nu=1,2,3,\ldots$, are shown in Table 3 for $\alpha=1$, $d=3$, $1\leqq m\leqq 3$, and $n=5$, 10, 20, 40. The Gauss-Christoffel quadrature formula for the measure (3.3) was obtained by first computing the recursion coefficients of the respective orthogonal polynomials by a discretized Stieltjes procedure, similarly as in [8, Example 3.2], and then using well-known methods to compute the Gauss-Christoffel formula in terms of the eigensystem of the associated Jacobi matrix; see, e.g., [5, 9].

Our last example deals with the Maxwell velocity distribution treated previously in [8] for $m=0$.

Example 3.3. $f(r)=\pi^{-d/2}e^{-r^2}$ on $[0,\infty]$.

The measure (2.12) here becomes

$$d\lambda(r)=\frac{\pi^{-d/2}}{m!}r^{m+d}H_{m+1}(r)e^{-r^2}dr,\qquad 0\leqq r<\infty, \tag{3.4}$$

where H_{m+1} is the Hermite polynomial of degree $m+1$. If $m>0$, as we assume, H_{m+1} changes sign at least once on $(0,\infty)$, so that $d\lambda$ is no longer a positive measure. The existence of the Gauss-Christoffel quadrature formula (2.13) is therefore in doubt, and even if it exits, we cannot be sure that its nodes are all simple and positive as in the previous examples. The matter depends on whether the nth degree orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ relative to $d\lambda$ exists, and in addition whether its zeros – the nodes $r_\nu^{(n)}$ in (2.13) – are distinct and positive. If so, the solution of our approximation problem is given by (2.14), where the $\lambda_\nu^{(n)}$ are uniquely determined by the nodes $r_\nu^{(n)}$; if not, the problem has no solution.

To resolve these issues computationally, we try to generate the recurrence relation (i.e., the coefficients α_k, β_k) for the (monic) orthogonal polynomials $\pi_k(\cdot)=\pi_k(\cdot\,; d\lambda)$,

$$\begin{aligned} &\pi_{k+1}(r)=(r-\alpha_k)\,\pi_k(r)-\beta_k\,\pi_{k-1}(r), \qquad k=0,1,\dots,n-1,\\ &\pi_{-1}(r)=0, \qquad \pi_0(r)=1, \end{aligned} \tag{3.5}$$

by a discretized Stieltjes procedure; cf. [7, Example 4.6]. If the procedure does not break down, that is, $\beta_k \neq 0$ for $k=0,1,\dots,n-1$, then $\pi_n(\;\cdot\,; d\lambda)$ exists uniquely. Its zeros $r_\nu^{(n)}$ are the eigenvalues of the (nonsymmetric) Jacobi matrix

$$J_n(d\lambda)=\begin{bmatrix} \alpha_0 & 1 & & & 0\\ \beta_1 & \alpha_1 & 1 & & \\ & \beta_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & 1\\ 0 & & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix}. \tag{3.6}$$

Since some of the β's are expected to be negative, we are not attempting to symmetrize the matrix J_n, as is customary, and possible, in the classical case of positive measures. From (3.5) it follows easily that the columns of the matrix

$$P_n(d\lambda)=[\pi_{\mu-1}(r_\nu^{(n)}; d\lambda)]_{\mu,\nu=1}^{n} \tag{3.7}$$

are the eigenvectors of $J_n(d\lambda)$, normalized to have the first component equal to 1. Putting in turn $p(r)=\pi_{\mu-1}(r; d\lambda)$, $\mu=1,2,\dots,n$, in (2.13), and observing that $\int_0^\infty \pi_{\mu-1}(r)\,d\lambda(r)=\mu_0\,\delta_{\mu,1}$, where $\mu_0=\int_0^\infty d\lambda(r)$ and $\delta_{\mu,1}$ is the Kronecker delta, one obtains for the vector $\lambda^T=[\lambda_1^{(n)}, \lambda_2^{(n)}, \dots, \lambda_n^{(n)}]$ the system of linear algebraic equations

$$P_n(d\lambda)\,\lambda=\mu_0\,e_1, \qquad e_1^T=[1,0,\dots,0]. \tag{3.8}$$

We have carried out the computation for the cases $m=1,2,3$; $d=1,2,3$; and $n=1(1)20$. All coefficients β_k were found to be different from zero, but quite a few of them negative; see Table 4. Interestingly, the negative β's seem to occur in pairs of two.

With the α's and β's at hand, we used the EISPACK routine HQR2 [11, p. 248] to compute the eigenvalues and eigenvectors of $J_n(d\lambda)$ and, if all eigenvalues are positive, the LINPACK routines SGECO, SGESL [3, Chapter 1] to solve the system (3.8). A summary of the results is presented in Table 5. A dash indicates the presence of a negative eigenvalue and an asterisk the presence of a pair of conjugate complex eigenvalues. In all cases computed, there were never more than one negative eigenvalue or more than one pair of complex

Table 4. The sign of the coefficients β_k in (3.5) for Example 3.3

d	m	$\beta_k<0$ for $k=$
1	1	2-3, 6-7, 10-11, 15-16
	2	1-2, 4-5, 7-8, 11-12, 14-15, 18-19
	3	1-2, 4-5, 9-10, 16-17
2	1	3-4, 7-8, 12-13, 17-18
	2	2-3, 5-6, 8-9, 12-13, 15-16, 19
	3	1-2, 4-5, 10-11, 16-17
3	1	4-5, 8-9, 13-14, 18-19
	2	2-3, 6-7, 9-10, 13-14, 17-18
	3	2-3, 5-6, 10-11, 17-18

Table 5. Existence and accuracy of the spline approximation for Example 3.3

n	$d=1$			$d=2$			$d=3$		
	$m=1$	$m=2$	$m=3$	$m=1$	$m=2$	$m=3$	$m=1$	$m=2$	$m=3$
1	3.9 (-2)	1.0 (-1)	1.4 (-1)	3.8 (-2)	7.1 (-2)	1.3 (-1)	4.4 (-2)	2.8 (-2)	8.2 (-2)
2	4.6 (-2)	–	1.3 (-1)	3.5 (-2)	8.2 (-2)	–	1.4 (-2)	5.7 (-2)	8.8 (-2)
3	–	6.2 (-3)	1.4 (-3)	3.8 (-2)	1.3 (-1)	5.9 (-3)	2.5 (-2)	–	4.0 (-2)
4	2.1 (-2)	3.8 (-3)	1.2 (-3)	–	4.5 (-3)	9.6 (-4)	2.5 (-2)	8.3 (-3)	1.4 (-3)
5	1.5 (-2)	–	8.8 (-4)	8.9 (-3)	5.9 (-3)	–	–	5.9 (-3)	1.8 (-3)
6	1.4 (-2)	1.8 (-3)	*	6.4 (-3)	–	8.6 (-4)	7.3 (-3)	6.0 (-3)	3.2 (-3)
7	–	1.3 (-3)	*	6.9 (-3)	7.2 (-4)	6.8 (-4)	5.3 (-3)	4.9 (-2)	6.5 (-4)
8	9.1 (-3)	–	2.0 (-4)	–	8.1 (-4)	*	6.1 (-3)	7.7 (-4)	5.7 (-4)
9	7.2 (-3)	9.5 (-4)	1.5 (-4)	3.9 (-2)	–	8.1 (-5)	–	1.0 (-3)	*
10	6.8 (-3)	6.4 (-4)	–	3.7 (-3)	4.2 (-4)	1.4 (-4)	–	–	2.3 (-1)
11	–	6.3 (-4)	6.4 (-5)	3.4 (-3)	2.9 (-4)	*	1.9 (-3)	1.9 (-4)	–
12	–	–	*	3.4 (-3)	2.9 (-4)	5.0 (-5)	2.0 (-3)	2.3 (-4)	*
13	5.4 (-3)	3.8 (-4)	*	–	–	4.3 (-5)	2.1 (-3)	2.3 (-4)	5.9 (-5)
14	4.8 (-3)	3.5 (-4)	4.9 (-5)	2.8 (-3)	1.9 (-4)	*	–	–	5.0 (-5)
15	4.8 (-3)	–	4.5 (-5)	2.5 (-3)	1.7 (-4)	2.5 (-5)	–	9.4 (-5)	*
16	–	3.0 (-4)	4.5 (-5)	2.3 (-3)	–	2.5 (-5)	1.3 (-3)	8.2 (-5)	–
17	–	2.2 (-4)	2.4 (-5)	2.3 (-3)	–	–	1.1 (-3)	8.2 (-5)	–
18	3.6 (-3)	2.2 (-4)	*	–	1.1 (-4)	1.5 (-5)	1.1 (-3)	–	*
19	3.3 (-3)	–	*	1.9 (-3)	1.1 (-4)	1.2 (-5)	–	5.8 (-5)	1.2 (-5)
20	3.2 (-3)	1.8 (-4)	*	1.7 (-3)	–	*	–	5.4 (-5)	8.5 (-6)

eigenvalues. The numbers shown in Table 5 represent (approximately) the maximum absolute errors, $\max\limits_{0\leqq r\leqq r_n} |s_n(r)-f(r)|$; they are usually (but not always) attained at one of the early knots r_ν of the spline.

Unlike in the previous examples, the weights α_ν in (2.1) are no longer necessarily positive, the solution of (3.8) having components of either sign, in general.

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