On Gauss-type quadrature formulas with prescribed nodes anywhere on the real line

Adhemar Bultheel, Ruymán Cruz-Barroso
Marc Van Barel

Report TW 530, September 2008

Katholieke Universiteit Leuven
Department of Computer Science
Celestijnenlaan 200A – B-3001 Heverlee (Belgium)

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Adhemar Bultheel [*,1], Ruymán Cruz-Barroso [1], Marc Van Barel [1,2]

Department of Computer Science, K.U.Leuven, Celestijnenlaan 200 A, B-3001 Heverlee (Leuven), Belgium.

Abstract

In this paper, quadrature formulas on the real line with the highest degree of accuracy, with positive weights, and with one or two prescribed nodes anywhere on the interval of integration are characterized. As an application, the same kind of rules but with one or both (finite) endpoints being fixed nodes and one or two more prescribed nodes inside the interval of integration are derived. An efficient computation of such quadrature formulas is analyzed by considering certain modified Jacobi matrices. Some numerical experiments are finally presented.

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* Corresponding author.
Email address: Adhemar.Bultheel@cs.kuleuven.be (Adhemar Bultheel).

[1] This work is partially supported by the Fund of Scientific Research (FWO), project "RAM: Rational modelling: optimal conditioning and stable algorithms", grant ♯G.0423.05 and the Belgian Network DYSCO (Dynamical Systems, Control, and Optimization), funded by the Interuniversity Attraction Poles Programme, initiated by the Belgian State, Science Policy Office. The scientific responsibility rests with the authors.
[2] The work of this author is also supported by the Research Council K.U.Leuven, project OT/05/40 (Large rank structured matrix computations), CoE EF/05/006 Optimization in Engineering (OPTEC).

Preprint 23 September 2008

1 Introduction

By Gauss-type quadrature formulas we mean the set of Gaussian, Gauss-Radau and Gauss-Lobatto rules and their generalizations. The classical n-point Gauss quadrature formulas are of interpolatory type, which means that they are obtained by integrating an interpolating polynomial of degree n. An interpolatory quadrature formula will obviously have degree of accuracy at least equal to n, i.e., they integrate exactly any polynomial of degree n or lower. By an appropriate choice of nodes of interpolation (which are also the nodes of the quadrature formula), it is possible to increase the degree of accuracy. For an n-point formula, the maximal possible degree of accuracy is $2n-1$ which is obtained by the Gauss quadrature formulas whose nodes are the zeros of the orthogonal polynomial of degree n. They are particularly interesting because it is guaranteed that all these nodes are in the support of the measure (we suppose here that this is a finite or infinite interval of the real line) and also that the weights of the quadrature formula are positive. These properties are important for practical, numerical and theoretical reasons.

For some applications though, it may be interesting to fix some of the nodes in advance. For example because these points correspond to points where some particular property should hold, or because we know some special values of the integrand in those nodes. Most often these are one or both of the endpoints if the integral is over a finite interval. For each node that is fixed in advance, the maximal degree of accuracy will decrease by one. For example, fixing one or two endpoints corresponds to the classical Gauss-Radau and Gauss-Lobatto formulas having a maximal degree of accuracy equal to $2n-2$ and $2n-3$ respectively. These Gauss-type formulas have been discussed over and over in the literature and can be found in almost any textbook dealing with numerical quadrature. See for example [10] to mention a recent one.

The situation where one or two prefixed nodes are endpoints is rather simple because the remaining nodes can be obtained by constructing a classical Gauss-type formula with fewer points for a modified measure. If μ is the original measure on the interval $[a,b]$ and for example a is a (finite) prefixed node, then the remaining $n-1$ nodes are the zeros of the $(n-1)$th orthogonal polynomial for the measure $\tilde{\mu}(x) = (x-a)\mu(x)$. This measure is positive. Any other prefixed node less than a would also give a positive measure, but will obviously be outside the interval. Similarly if both (finite) endpoints are prefixed, then the remaining $n-2$ nodes are the zeros of the $(n-2)$th orthogonal polynomial for the measure $\tilde{\mu}(x) = (x-a)(b-x)\mu(x)$. However, when a prefixed node is inside the interval, things are not so simple. The quadrature formula may not exist or may have non-positive weights or nodes may drift outside the interval. The subject of this paper is precisely to discuss for which choices of the prefixed nodes we shall have "good" quadrature formulas with

positive weights, nodes inside the interval and maximal degree of accuracy. This will be analysed in detail for one or two points. For more points, the analysis becomes intractable, unless in some special cases. The computation can always be done, and we shall also discuss this aspect, and show with several numerical experiments with the classical orthogonal polynomials where the "good" formulas can be found.

Fixing more than two nodes, and/or fixing nodes inside the interval can also have applications. For example in [18], a quadrature formula is discussed for the Lebesgue measure on the interval $[0, 1]$, with positive weights, maximal degree of accuracy, and with three fixed nodes, two of them being the endpoints of the interval and the third one in $(0, 1)$. This is used in the context of constructing implicit Runge-Kutta methods for the numerical solution of stiff problems and algebraic differential equations.

Note that the quadrature formulas discussed here are quite different from Gauss-Kronrod formulas where several nodes are added to the classical Gauss nodes. Also the situation is much more complicated than the corresponding Szegő-type formulas for integration over the unit circle of the complex plane $\mathbb{T} := \{z \in \mathbb{C} : |z| = 1\}$. Recall that Szegő quadrature formulas on the unit circle were introduced and characterized in [16], and they represent the analogue on the unit circle of the Gaussian rules for intervals of the real axis. However, two big differences must be remarked: the nodes are not the zeros of the nth orthogonal polynomial with respect to the considered measure on $\mathbb{T}$ and an n-point Szegö quadrature formula has maximal domain of accuracy in a subspace of Laurent polynomials whose dimension is $2n-1$ instead of $2n$; see also [2], [5], [4], [12], [14] and references therein. The counterpart of the deficiency in the dimension of the maximal domain of exactness is that the nodes of such formulas are the zeros of a nth para-orthogonal polynomial with respect to the measure on $\mathbb{T}$, also introduced and characterized in [16]. Such para-orthogonal polynomials are shown to depend on one parameter of unit magnitude, and thus a one-parameter family of Szegő quadrature formulas arises. It is trivial to choose this free parameter in an appropriate way in order to fix one node in the rule and so, Szegő-Radau quadrature formulas arises trivially. Recently, in [15] Szegő-Lobatto quadrature formulas have been deduced, proving their existence without restrictions on the two distinct nodes on the unit circle to be prescribed; for an alternative approach, see [3]. In the results presented in this paper we will prove that Gauss-type quadrature formulas with prescribed nodes anywhere on the real line exists only under certain conditions on the nodes to be fixed.

In Section 2 we shall first recall some general background and known results about Gauss-type quadrature formulas. Then we give a detailed analysis of the Radau and of the Logatto case and give some remarks about special cases and some generalizations. For example the quadrature formula of [18] will be

derived. In Section 3, we discuss some computational aspects, generalizing the classical approach for Radau and Lobatto formulas, but we also give an alternative giving a simpler algorithmic linear algebra approach. Finally, in Section 4 several numerical examples are presented.

2 Gauss-type quadrature formulas

We start this section by recalling briefly some well known results on orthogonal polynomials and Gauss-type quadrature formulas on intervals of the real line that will be necessary in the rest of the paper. We shall first recall some general results in section 2.1 and consider in section 2.2 the Radau and 2.3 the Lobatto cases where one or two nodes are prefixed. In section 2.4 we briefly note some simple generalisations when besides the internal prefixed nodes also one or two nodes are prefixed at the endpoints of the interval.

2.1 General considerations

Let μ be a positive Borel measure on a finite or infinite interval $[a, b]$ of the real line and such that all the moments

$$m_n = \int_a^b x^n d\mu(x) \quad n = 1, 2, \ldots$$

are finite and that the support of μ

$$\text{supp}(\mu) = \{x \in [a, b] : \mu(x - \epsilon, x + \epsilon) > 0 \text{ for every } \epsilon > 0\}$$

contains infinitely many points. Orthogonalizing the linear space of polynomials, we obtain a system of orthonormal polynomials on $[a, b]$ which will be denoted for all $n \geq 0$ by $p_n(x)$, and so

$$\langle p_n(x), p_m(x)\rangle = \int_a^b p_n(x)p_m(x)d\mu(x) = \delta_{n,m}, \quad ; \; m, n \geq 0,$$

with $\delta_{n,m}$ the Kronecker delta symbol. This system is unique if we impose the leading coefficients to be positive:

$$p_n(x) = \gamma_n x^n + \delta_n x^{n-1} + \cdots, \quad \gamma_n > 0.$$

As usual, for $f \in L_2^\mu([a, b])$, we define the norm $\|f(x)\| = \sqrt{\langle f(x), f(x)\rangle}$. It is very well known that the family $\{p_n(x)\}_{n=0}^\infty$ satisfies for all $n \geq 0$ the

three-term recurrence relation

$$xp_n(x) = u_{n+1}p_{n+1}(x) + v_n p_n(x) + u_n p_{n-1}(x), \tag{1}$$

with initial conditions $p_{-1}(x) \equiv 0$, $p_0(x) \equiv 1/\sqrt{m_0}$ and

$$u_n = \int_a^b xp_{n-1}(x)p_n(x)d\mu(x) = \frac{\gamma_{n-1}}{\gamma_n} > 0\ , \quad v_n = \int_a^b xp_n^2(x)d\mu(x) = \frac{\delta_n}{\gamma_n} - \frac{\delta_{n+1}}{\gamma_{n+1}}.$$

From this recurrence relation it is easy to deduce that

$$\sum_{k=0}^{n-1} p_k(x)p_k(y) = u_n \frac{p_n(x)p_{n-1}(y) - p_{n-1}(x)p_n(y)}{x-y}.$$

This formula is known as the *Christoffel-Darboux* identity and when y tends to x we obtain its confluent form

$$\sum_{k=0}^{n-1} p_k^2(x) = u_n \left[p_n'(x)p_{n-1}(x) - p_{n-1}'(x)p_n(x)\right]. \tag{2}$$

The recurrence (1) can be alternatively written in a matrix form as

$$J_n P_n(x) = xP_n(x) - u_n p_n(x)e_n, \tag{3}$$

with

$$J_n = \begin{bmatrix} v_0 & u_1 & 0 & 0 & \cdots & 0 \\ u_1 & v_1 & u_2 & 0 & \cdots & 0 \\ 0 & u_2 & v_2 & u_3 & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & & u_{n-2} & v_{n-2} & u_{n-1} \\ 0 & 0 & \cdots & 0 & u_{n-1} & v_{n-1} \end{bmatrix}, \quad P_n(x) = \begin{bmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \\ p_{n-2}(x) \\ p_{n-1}(x) \end{bmatrix}, \quad e_n = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \tag{4}$$

The matrix J_n is tridiagonal and symmetric and it is known as the (finite) *Jacobi matrix*. From (3)-(4) it is observed that if we take $x_{j,n}$ so that $p_n(x_{j,n}) = 0$ for all $j = 1, \ldots, n$ then $x_{j,n}$ turns out to be an eigenvalue of J_n with eigenvector

$$[p_0(x_{j,n}), p_1(x_{j,n}), \cdots, p_{n-2}(x_{j,n}), p_{n-1}(x_{j,n})]^T. \tag{5}$$

The zeros of orthogonal polynomials on the real line have the following crucial property

Theorem 2.1 *(1) The zeros of $p_n(x)$ are all simple and located in (a,b).*
(2) Suppose $x_{1,n} < x_{2,n} < \cdots < x_{n,n}$ are the zeros of $p_n(x)$, then they interlace with those of $p_{n-1}(x)$, that is $x_{j,n} < x_{j,n-1} < x_{j+1,n}$.

Example 2.2 Set $[a,b] = [-1,1]$ and consider for $l \in \{1,2\}$ the absolutely continuous measures given by $d\mu_l(x) = \omega_l(x)dx$, with weight functions $\omega_1(x) = \frac{1}{\sqrt{1-x^2}}$ and $\omega_2(x) = \sqrt{1-x^2}$. The corresponding orthogonal polynomials are the well known Chebyshev polynomials of first and second kind, defined by $T_n(\cos\theta) = \cos(n\theta)$ and $U_n(\cos\theta) = \frac{\sin((n+1)\theta)}{\sin\theta}$ respectively, where $x = \cos\theta$ for $\theta \in [0,\pi]$. They satisfy the same three term recurrence relation $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$ and $U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x)$, but with different initial values: $T_0(x) = U_0(x) \equiv 1$ and $T_1(x) = x$, $U_1(x) = 2x$. Thus, the entries of the associated Jacobi matrices are given by $v_n = 0$ for all $n \geq 0$ (observe that both measures are symmetric on $[-1,1]$), $u_m = 1/2$ for all $m \geq 2$ and $u_1 = \sqrt{2}/2$ and $u_1 = 1/2$ for the polynomials of the first and second kind respectively. The definition given for such polynomials give rise to an explicit expression for their zeros:

$$x_{j,n}^{(1)} = \cos\left(\frac{\pi}{2}\frac{2j-1}{n}\right) \ , \ \ x_{j,n}^{(2)} = \cos\left(\frac{j}{n+1}\pi\right) \ ; \ \ j = 1,\ldots,n.$$

$\diamond$

Numerical quadrature consists of approximating the integral of a function f

$$I_\mu(f) = \int_a^b f(x)d\mu(x) \tag{6}$$

by a finite sum which uses only n function evaluations

$$I_n(f) = \sum_{k=1}^{n} A_{k,n} f(x_{k,n}). \tag{7}$$

Here f belongs to a class of functions for which $I_\mu(f)$ and $I_n(f)$ exist. The n nodes $x_{k,n}$ and the n weights (quadrature coefficients) $A_{k,n}$ for $1 \leq k \leq n$ have to be chosen properly so that the quadrature formula is correct for as many functions f as possible. Since the Weierstrass approximation theorem states that any continuous function on a closed and bounded interval can be uniformly approximated on that interval by polynomials to any degree of accuracy, it is usual to determine the nodes and the weights in the quadrature rule imposing it to be exact in the space of polynomials of degree as high as possible. We say that the *degree of accuracy* of the quadrature rule is s when all polynomials of degree s are integrated correctly but there is a polynomial of degree $s+1$ which is not integrated correctly.

It is very well known that if we fix n distinct points in $[a,b]$, then n weights can be determined so that the corresponding quadrature rule has degree of

accuracy at least $n-1$. Such quadrature formulas are called *of interpolatory type* and the weights are explicitly given by

$$A_{k,n} = \int_a^b l_{k,n}(x) d\mu(x),$$

where the fundamental polynomials of Lagrange interpolation are given by

$$l_{k,n}(x) = \frac{\pi_n(x)}{\pi_n'(x_{k,n})(x - x_{k,n})}, \quad \pi_n(x) = \prod_{j=1}^{n}(x - x_{j,n}).$$

The following triviality shows that the degree of accuracy of an n-point quadrature formula is strictly less than $2n$:

$$I_n(\pi_n^2(x)) = \sum_{k=1}^{n} A_{k,n}\pi_n^2(x_{k,n}) = 0 \ \text{ and } \ I_\mu(\pi_n^2(x)) > 0.$$

The next result proves that the nodes of the quadrature formula can be appropriately chosen to get the highest degree of accuracy, that is $2n-1$, leading to the well known *Gaussian quadrature formulas*.

Theorem 2.3 (Gauss) *The quadrature formula $I_n(f)$ given by (7) for $I_\mu(f)$ given by (6) has degree of accuracy $2n-1$, if and only if, it is of interpolatory type and the nodes are the zeros of the nth orthogonal polynomial $p_n(x)$ with respect to μ. Moreover, the weights are positive and are given by*

$$A_{k,n} = \frac{1}{u_n p_{n-1}(x_{k,n}) p_n'(x_{k,n})} = \frac{-1}{u_{n+1} p_{n+1}(x_{k,n}) p_n'(x_{k,n})}$$

or equivalently by

$$A_{k,n} = \left(\sum_{j=0}^{n-1} p_j^2(x_{k,n}) \right)^{-1} = \left(\sum_{j=0}^{n} p_j^2(x_{k,n}) \right)^{-1}. \tag{8}$$

Thus, from Theorem 2.3 and (5) it is deduced that the nodes and weights of the quadrature formula $I_n(f)$ for $I_\mu(f)$ can be computed as the eigenvalues and the first component of the normalized eigenvectors of J_n given by (4), respectively. Moreover, it is also a well known fact (see e.g. [17, pp. 264-265]) that the positive character of the weights in an interpolatory type quadrature formula guarantees its convergence.

Quadrature formulas with a or/and b being one or two prescribed nodes and maximal domain of validity have also been considered in the literature. In this respect, we recall that a polynomial R_n of exact degree $n \geq r$ is called *quasi-orthogonal of order r* on $[a, b]$ with respect to μ if it satisfies the orthogonality

conditions

$$\int_a^b x^k R_n(x) d\mu(x) \begin{cases} = 0 \text{ for } k = 0, \ldots, n-1-r, \\ \neq 0 \text{ for } k = n-r. \end{cases}$$

It is not difficult to prove (see e.g. [1, Theorem 1]) that if $R_n(x)$ is a polynomial of degree n, then it is quasi-orthogonal of order r on $[a, b]$ with respect to μ, if and only if,

$$R_n(x) = c_0 p_n(x) + c_1 p_{n-1}(x) + \cdots + c_r p_{n-r}(x), \tag{9}$$

where $\{p_n(x)\}_{n=0}^{\infty}$ is a sequence of orthogonal polynomials on $[a, b]$ with respect to μ and $c_i = c_i(n)$ are numbers for all $i = 0, \ldots, r$ such that $c_0 c_r \neq 0$. The following result states the role played by quasi-orthogonality in the construction of quadrature rules with degree of accuracy $n + k$, with $0 \leq k \leq n - 1$. Thus, by taking $k = 0$ and $k = n - 1$ we recover the interpolatory type and Gaussian formulas respectively (see e.g. [17, pp. 101-102], [6, pp. 109-112] and [19]).

Theorem 2.4 *The quadrature formula $I_n(f) = \sum_{j=1}^{n} A_{j,n} f(x_{j,n})$ for $I_\mu(f) = \int_a^b f(x) d\mu(x)$ has degree of accuracy $n + k$, if and only if, it is of interpolatory type and the nodal polynomial $\pi_n(x) = \prod_{j=1}^{n}(x - x_{j,n})$ is quasi-orthogonal of order $n - k - 1$ in $[a, b]$ with respect to $d\mu$.*

When one endpoint is assumed to be fixed, the corresponding rule is called *Gauss-Radau quadrature formula*. When both endpoints are fixed, then the corresponding rule is called a *Gauss-Lobatto quadrature formula*. Two direct consequences of Theorem 2.4 are the following charaterization results (see e.g. [6, pp. 102-105]).

Theorem 2.5 (Gauss-Radau) *Let $[a, b]$ be a finite interval on the real line. The quadrature formula $I_n(f) = A_\alpha f(\alpha) + \sum_{k=1}^{n-1} A_{k,n} f(x_{k,n})$ with $\alpha \in \{a, b\}$, approximating the integral $I_\mu(f)$ given by (6), has the highest degree of accuracy, that is $2n - 2$, if and only if, it is of interpolatory type and the nodes $\{x_{k,n}\}_{k=1}^{n-1}$ are the zeros of the $(n-1)$th orthogonal polynomial with respect to $\tilde{\mu}(x) = (x - a)\mu(x)$ if $\alpha = a$ or with respect to $\tilde{\mu}(x) = (b - x)\mu(x)$ if $\alpha = b$. Moreover, the weights are positive.*

Theorem 2.6 (Gauss-Lobatto) *Let $[a, b]$ be a finite interval on the real line. The quadrature formula $I_n(f) = A_a f(a) + A_b f(b) + \sum_{k=1}^{n-2} A_{k,n} f(x_{k,a})$, approximating the integral $I_\mu(f)$ given by (6), has the highest degree of accuracy, that is $2n - 3$, if and only if, it is of interpolatory type and the nodes are the zeros of the $(n-2)$th orthogonal polynomial with respect to $\tilde{\mu}(x) = (x - a)(b - x)\mu(x)$. Moreover, the weights are positive.*

Example 2.7 From Example 2.2 and Theorem 2.6 it follows that the $(n+2)$-

point Gauss-Lobatto quadrature formula for the Chebyshev weight function of the first kind $d\mu_1(x)$ has as fixed nodes $\{\pm 1\}$ and the remainder nodes in $(-1,1)$ are the nodes of the n-point Gauss quadrature formula for the Chebyshev weight funcion of the second kind $d\mu_2(x)$. $\diamond$

The set of Gauss, Gauss-Radau and Gauss-Lobatto rules are known in the literature as Gauss-type quadrature formulas (see e.g. [7]).

In this paper we shall be concerned in the characterization and the effective computation of quadrature formulas with positive weights and with one or two fixed nodes but not necessarily being the endpoints of the interval of integration. For this purpose and from Theorem 2.4 we also need the following crucial result proved in [19].

Theorem 2.8 *If $R_n(x)$ is quasi-orthogonal of order r on $[a,b]$ with respect to μ, then at least $(n-r)$ distinct zeros of $R_n(x)$ lie in the interval (a,b).*

2.2 Gauss-Radau with an arbitrary prefixed node

We start by considering an n-point quadrature formula for $I_\mu(f)$ given by (6) with one fixed point $\alpha \in [a,b]$, positive weights, and with the highest degree of accuracy, that is $2n-2$, namely

$$I_n(f) = A_\alpha f(\alpha) + \sum_{k=1}^{n-1} A_{k,n} f(x_{k,n}). \tag{10}$$

It is an evidence that if $p_n(\alpha) = 0$, then the Gauss-Radau rule is actually a Gaussian quadrature formula, characterized in Theorem 2.3. We will suppose from now on that $p_n(\alpha) \neq 0$. If $\alpha \in \{a,b\}$, then the Gauss-Radau rule has been already characterized by Theorem 2.5. Suppose first that $p_{n-1}(\alpha) \neq 0$. From Theorem 2.4, the nodes of such rule will be the zeros of

$$R_n(x) = p_n(x) + a_n p_{n-1}(x), \tag{11}$$

where a_n is an appropriate nonzero constant to ensure that $R_n(\alpha) = 0$, that is

$$a_n = -\frac{p_n(\alpha)}{p_{n-1}(\alpha)}. \tag{12}$$

The positive character of the weights is assured in this case since, setting $\alpha = x_{n,n}$ and $A_\alpha = A_{n,n}$, then

$$0 < \int_a^b l_{k,n}^2(x) d\mu(x) = \sum_{j=1}^{n} A_{j,n} l_{k,n}^2(x_{j,n}) = A_{k,n}, \quad k = 1, \ldots, n.$$

So, we distinguish two situations. If $p_{n-1}(\alpha) = 0$ it follows from Theorem 2.1 that $R_n(\alpha) \neq 0$ and hence there does not exist a Gauss-Radau quadrature formula with the highest degree of accuracy and with α as the prescribed node; see further. If $p_{n-1}(\alpha) \neq 0$ then by taking a_n as given by (12) it follows in this case that there exists a Gauss-Radau quadrature formula with degree of accuracy equal to $2n-2$, with positive weights and with α as a fixed node. However, from Theorem 2.8 it follows that at least $(n-1)$ distinct zeros of $R_n(x)$ given by (11) lie in the interval (a, b). Our interest now will be to analyze which choices of the parameter α assure us to have the n nodes of the desired rule distinct and on $[a, b]$.

Thus, for $n > 0$ consider the function $f_n(x) = p_n(x)/p_{n-1}(x)$. The following sharper result on the localization of the zeros of $R_n(x)$ given by (11) is stated in [1, Theorem 3].

Theorem 2.9 *(1) The zeros $y_1 < \cdots < y_n$ of $R_n(x)$ are real and distinct and at most one of them lies outside (a, b).*
(2) (a) If $a_n < 0$, then $x_{i,n} < y_i < x_{i,n-1}$ for $i = 1, \ldots, n-1$ and $x_{n,n} < y_n$.
(b) If $a_n > 0$, then $y_1 < x_{1,n}$ and $x_{i-1,n-1} < y_i < x_{i,n}$ for $i = 2, \ldots, n$.
(3) If $-a_n < f_n(a) < 0$, then $y_1 < a$.
(4) If $-a_n > f_n(b) > 0$, then $b < y_n$.
(5) If $f_n(a) < -a_n < f_n(b)$, then $R_n(x)$ has all its zeros in (a, b).

Now, we notice some elementary properties of the function $f_n(x)$. From Theorem 2.1 we have that $f_n(x)$ has n zeros at $\{x_{j,n}\}_{j=1}^{n}$ and $(n-1)$ interlaced poles in between these zeros at $\{x_{j,n-1}\}_{j=1}^{n-1}$. Since we are assuming that the leading coefficients of the family of orthogonal polynomials are all positive, $f_n(x) < 0$ for $x < x_{1,n}$ and $f_n(x) > 0$ for $x > x_{n,n}$. Moreover, from (2) it is clear that $f_n'(x) > 0$, so it increases from $-\infty$ to ∞ in the intervals $x_{\nu,n-1} < x < x_{\nu+1,n-1}$ for $\nu = 0, 1, \ldots, n-1$, where $x_{0,n-1} = -\infty$ and $x_{n,n-1} = +\infty$. In our situation, we have from (12) that $a_n = -f_n(\alpha)$.

Consider $\alpha \in (a, x_{1,n})$. Then, $f_n(\alpha) < 0$, implying $a_n > 0$ and from Theorem 2.9-(2b) it can occur that $\alpha = y_1 < x_{1,n}$. But $f_n(x)$ increases in $(-\infty, x_{1,n})$, so we have that $-a_n = f_n(\alpha) > f_n(a)$ and from Theorem 2.9-(3) it follows that $y_1 > a$. Thus, the n zeros of $R_n(x)$ are distinct and located in (a, b). A similar argument yields the same result when $\alpha \in (x_{n,n}, b)$.

Consider now simultaneously the cases $\alpha \in I_i := (x_{i,n}, x_{i,n-1})$ and $\alpha \in J_i := (x_{i,n-1}, x_{i+1,n})$ for a fixed $i \in \{1, \ldots, n-1\}$. Here, $f_n(x) > 0$ for $x \in I_i$, $f_n(x) < 0$ for $x \in J_i$ and $f_n(x)$ increases in $I_i \cup J_i$. Moreover, we know that $f_n(a) < 0$ and $f_n(b) > 0$, so there exist a unique $\zeta_i \in I_i$ and a unique $\xi_i \in J_i$ such that $f_n(\zeta_i) = f_n(b)$ and $f_n(\xi_i) = f_n(a)$. Thus, denoting by $\{y_j\}_{j=1}^{n}$ the zeros of $R_n(x)$, we can conclude from Theorem 2.9 that the following situations are possible:

(1) If $\alpha \in (x_{i,n}, \zeta_i) \subset I_i$, then $R_n(x)$ has all its distinct zeros on (a,b) and $x_{n,n} < y_n$.
(2) If $\alpha = \zeta_i \in I_i$, then the $(n-1)$ first distinct zeros of $R_n(x)$ are located in (a,b) and $y_n = b$.
(3) If $\alpha \in (\zeta_i, x_{i,n-1}) \subset I_i$, then $R_n(x)$ has exactly $n-1$ distinct zeros in (a,b) and $y_n > b$.
(4) If $\alpha \in (x_{i,n-1}, \xi_i) \subset J_i$, then $R_n(x)$ has exactly $n-1$ distinct zeros in (a,b) and $y_1 < a$.
(5) If $\alpha = \xi_i \in J_i$, then $y_1 = a$ and the remaining $n-1$ distinct zeros of $R_n(x)$ are in (a,b).
(6) If $\alpha \in (\xi_i, x_{i+1,n}) \subset J_i$, then $R_n(x)$ has all its distinct zeros on (a,b) and $y_1 < x_{1,n}$.

Note that with only slight modifications, the previous discussion also holds for $a = -\infty$ and/or $b = +\infty$ if we set $f_n(-\infty) = -\infty$ and $f_n(+\infty) = +\infty$. A consequence is that ζ_i will coincide with $x_{i,n-1}$ if $b = +\infty$, i.e., $f_n(b) = +\infty$, and $\xi_i = x_{i,n-1}$ if $a = -\infty$, i.e., $f_n(a) = -\infty$.

With these considerations, we have proved the following (see Figure 1)

Theorem 2.10 (Gauss-Radau) *Let μ be a positive Borel measure on a finite or infinite interval $[a,b]$ of the real line and let $\{p_n(x)\}_{n=0}^{\infty}$ be the sequence of orthonormal polynomials with respect to μ in $[a,b]$ normalized to have positive leading coefficients. Set $f_n(x) = \frac{p_n(x)}{p_{n-1}(x)}$ for all $n \geq 1$ and $\alpha \in [a,b]$ a fixed point such that $p_{n-1}(\alpha) \neq 0$. Let $I_n(f)$ be a n-point quadrature formula for $I_\mu(f)$ given by (6) of the form (10) with fixed node α. Then, $I_n(f)$ has the highest degree of accuracy, that is $2n-2$, if and only if, it is of interpolatory type and the nodes are the zeros of $R_n(x) = p_n(x) - f_n(\alpha)p_{n-1}(x)$. The weights of the quadrature are positive. Moreover, all the nodes of the quadrature lie in (a,b), if and only if,*

$$\alpha \in (a,b) \setminus \bigcup_{i=1}^{n-1} [\zeta_i, \xi_i], \tag{13}$$

where for all $i = 1, \ldots, n-1$, $\zeta_i \in (x_{i,n}, x_{i,n-1})$ and $\xi_i \in (x_{i,n-1}, x_{i+1,n})$. If b is finite, then ζ_i is the unique solution of $f_n(\zeta_i) = f_n(b)$, while $\zeta_i = x_{i,n-1}$ if $b = \infty$. If a is finite, then ξ_i is the unique solution of $f_n(\xi_i) = f_n(a)$, while $\xi_i = x_{i,n-1}$ if $a = -\infty$. The endpoint a is one of the nodes of $I_n(f)$, if and only if, $\alpha \in \{a, \xi_1, \ldots, \xi_{n-1}\}$ while the endpoint b is one of the nodes of $I_n(f)$ if and only if $\alpha \in \{\zeta_1, \ldots, \zeta_{n-1}, b\}$.

Remark 2.11 From Theorem 2.10 it follows that if $p_{n-1}(\alpha) = 0$, then there does not exist a Gauss-Radau quadrature formula for $I_\mu(f)$ with α as the prescribed node and with the highest degree of accuracy, that is $2n-2$. In what follows we will prove that even a Gauss-Lobatto quadrature rule with degree of accuracy equal to $2n-3$ and a zero of $p_{n-1}(x)$ as one prescribed node can not be constructed in general.

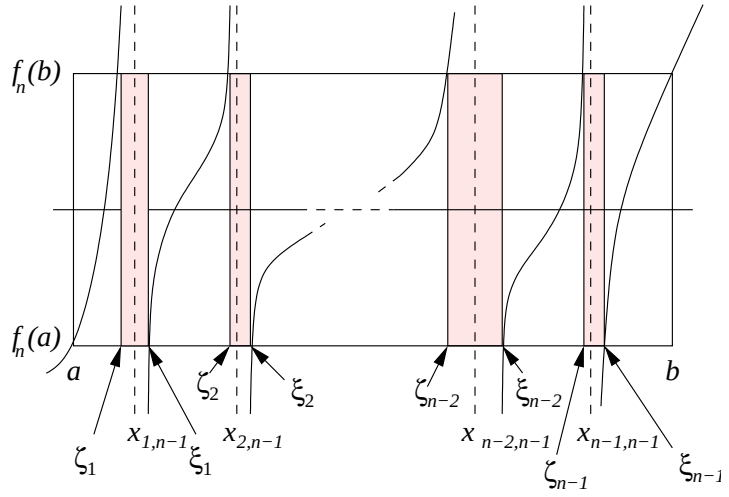

Fig. 1. The plot shows the function $y = f_n(x)$ in $[a, b]$. The set of points $\{\zeta_i\}_{i=1}^{n-1}$ and $\{\xi_i\}_{i=1}^{n-1}$ are the abcissas of the intersection of this function with $y = f_n(b)$ and $y = f_n(a)$, respectively. Thus, for all $i = 1, \ldots, n-1$, if $\alpha = \zeta_i$, then b is a node of the rule and if α moves from ζ_i to $\to x_{i,n-1}^-$, then this node moves from b to ∞; if $\alpha = \xi_i$, then a is a node of the rule and if α moves from ξ_i to $\to x_{i,n-1}^+$, then this node moves from a to $-\infty$. When α satisfies (13), then all the nodes of the Gauss-Radau quadrature formula are in (a, b).

Remark 2.12 If $\{p_n(x)\}_{n=0}^{\infty}$ is a sequence of orthogonal polynomials with respect to μ on a finite interval $[a, b]$, then it is clear that $Q_{n-1}(x, a) := \frac{1}{x-a}\left[p_n(x) - f_n(a)p_{n-1}(x)\right]$ and $Q_{n-1}(x, b) := \frac{1}{b-x}\left[p_n(x) - f_n(b)p_{n-1}(x)\right]$ are $(n-1)$th orthogonal polynomials with respect to $\tilde{\mu}(x) = (x-a)\mu(x)$ and $\tilde{\mu}(x) = (b-x)\mu(x)$, respectively. Thus, by taking $\alpha \in \{a, b\}$ in Theorem 2.10, then Theorem 2.5 is recovered.

Example 2.13 Consider the weight functions $\omega_l(x)$ given in Example 2.2 for a fixed $l \in \{1, 2\}$. Set $\alpha \in [-1, 1]$ with $\alpha \neq \cos\left(\frac{[2(i-1)+l]\pi}{2(n-2+l)}\right)$ for all $i = 1, \ldots, n-1$ and $f_n(x) = 2n - 1/f_{n-1}(x)$ for all $n \geq 2$ with $f_1(x) = lx$. Then, the nodes of a n-point Gauss-Radau quadrature formula for $I_{\omega_l}(f)$ of the form (10) are for all $j = 1, \ldots, n$ of the form $y_j = \cos\gamma_j$ with γ_j the solutions of $\cos(n\theta) = f_n(\alpha)\cos((n-1)\theta)$ for $l = 1$ and $\sin((n+1)\theta) = f_n(\alpha)\sin(n\theta)$ for $l = 2$ with $\theta \in [0, \pi]$. Moreover, the set $\{\zeta_i, \xi_i\}_{i=1}^{n-1}$ defined in Theorem 2.10 can be computed as follows: setting $\zeta_i = \cos\omega_i$ and $\xi_i = \cos\nu_i$ for all $i = 1, \ldots, n-1$, and

$$\tilde{I}_i := \left(\frac{2(i-1)+l}{2(n-1+l)}\pi, \frac{2(i-1)+l}{2(n-2+l)}\pi\right), \ \tilde{J}_i := \left(\frac{2(i-1)+l}{2(n-2+l)}\pi, \frac{2i+l}{2(n-1+l)}\pi\right),$$

then $\omega_i \in \tilde{I}_i$ and $\nu_i \in \tilde{J}_i$ are respectively the unique solutions of $\cos n\theta = \cos(n-1)\theta$ and $\cos n\theta = -\cos(n-1)\theta$ for $l = 1$ and $\sin((n+1)\theta) = \frac{n+1}{n}\sin(n\theta)$ and $\sin((n+1)\theta) = -\frac{n+1}{n}\sin(n\theta)$ for $l = 2$. $\diamond$

2.3 Gauss-Lobatto with two arbitrary prefixed nodes

Our next step will be to consider an n-point quadrature formula for $I_\mu(f)$ given by (6) with two distinct fixed points $\alpha, \beta \in [a, b]$, positive weights and with the highest degree of accuracy, that is $2n-3$, namely

$$I_n(f) = A_\alpha f(\alpha) + A_\beta f(\beta) + \sum_{k=1}^{n-2} A_{k,n} f(x_{k,n}). \tag{14}$$

By Theorem 2.4, the nodes of such a rule will be the zeros of

$$R_n(x) = p_n(x) + a_n p_{n-1}(x) + b_n p_{n-2}(x), \tag{15}$$

where a_n and b_n are appropriate constants to ensure that $R_n(\alpha) = R_n(\beta) = 0$. The following result follows from [19].

Theorem 2.14 *Consider the polynomial $R_n(x)$ given by (15) with $b_n < 0$. Then, all the zeros are real, distinct and at most $n-2$ of them lie in (a, b). In that case, the weights of the n-point quadrature formula with nodes the zeros of $R_n(x)$ and degree of accuracy equal to $2n-3$ are positive. If $b_n > 0$, then double zeros may appear.*

Observe from (15) that if $p_{n-1}(\lambda) \neq 0$, then $R_n(\lambda) = 0$, if and only if, $f_n(\lambda) = -a_n - b_n/f_{n-1}(\lambda)$ where $f_k = p_k/p_{k-1}$. From this, the following sharper result on the localization of the zeros of $R_n(x)$ can be proved (see [1, Theorem 5]):

Theorem 2.15 *If $b_n < 0$, then the zeros $\{y_i\}_{i=1}^n$ of $R_n(x)$ given by (15) are such that $y_1 < x_{1,n-1}$, $x_{i-1,n-1} < y_i < x_{i,n-1}$ for $i = 2, \ldots, n-1$, and $x_{n-1,n-1} < y_n$. The $\{x_{j,n-1}\}_{j=1}^{n-1}$ are the zeros of p_{n-1}. Moreover, setting $T(x) = -a_n - b_n/f_{n-1}(x)$, with $f_n(x) = p_n(x)/p_{n-1}(x)$, then*

(1) $y_n < b \Leftrightarrow T(b) < f_n(b)$ and $y_n = b \Leftrightarrow T(b) = f_n(b)$,
(2) $y_1 > a \Leftrightarrow T(a) > f_n(a)$ and $y_1 = a \Leftrightarrow T(a) = f_n(a)$.

Consider $\alpha, \beta \in [a, b]$, $\alpha \neq \beta$ and such that $R_n(\alpha) = R_n(\beta) = 0$. This yields the system

$$\Delta \begin{bmatrix} a_n \\ b_n \end{bmatrix} = - \begin{bmatrix} p_n(\alpha) \\ p_n(\beta) \end{bmatrix}, \quad \Delta = \begin{bmatrix} p_{n-1}(\alpha) & p_{n-2}(\alpha) \\ p_{n-1}(\beta) & p_{n-2}(\beta) \end{bmatrix},$$

which has a unique solution, if and only if,

$$\det\Delta = p_{n-1}(\alpha)p_{n-2}(\beta) - p_{n-2}(\alpha)p_{n-1}(\beta) \neq 0. \tag{16}$$

In case $\det\Delta \neq 0$, the unique solutions are given by

$$a_n = \frac{p_n(\beta)p_{n-2}(\alpha) - p_n(\alpha)p_{n-2}(\beta)}{\det\Delta}, \quad b_n = \frac{p_n(\alpha)p_{n-1}(\beta) - p_n(\beta)p_{n-1}(\alpha)}{\det\Delta}. \tag{17}$$

If $\det\Delta = 0$, then the desired Gauss-Lobatto quadrature formula (14) does not exist. For $\det\Delta \neq 0$ and depending on α and β, the following situations may occur:

GL1. If $b_n = 0$, then the problem is reduced to Theorem 2.10. The Gauss-Radau quadrature formula with fixed node α or β is actually a Gauss-Lobatto rule with prescribed nodes α and β, and hence the degree of accuracy is now $2n-2$. The nodes are the zeros of $R_n(x)$ given by (11) with $a_n = -f_n(\alpha) = -f_n(\beta)$ and the weights are positive.

GL2. If $b_n > 0$, then the Gauss-Lobatto quadrature formula (14) exists, if and only if, the nodes are the zeros of $R_n(x)$ given by (15) and all are distinct. However, even if this last condition holds, one node may be on $(-\infty, a)$ whereas another one in (b, ∞). If the rule exists, the degree of accuracy is $2n-3$ and the weights are positive.

GL3. If $b_n < 0$, then the existence of the Gauss-Lobatto quadrature formula (14), with α and β prescribed nodes, degree of accuracy $2n-3$ and positive weights is guaranteed. The nodes are the zeros of $R_n(x)$ given by (15) and with $f_n(x)$ and $T(x)$ defined as in Theorem 2.15, the following also may occur:

GL3a. If $T(b) > f_n(b)$, then the largest node of the Gauss-Lobatto quadrature formula lies in (b, ∞).

GL3b. If $T(a) < f_n(a)$, then the smallest node of the Gauss-Lobatto quadrature formula lies in $(-\infty, a)$.

GL3c. If $T(b) \leq f_n(b)$ and $T(a) \geq f_n(a)$, then all the nodes of the Gauss-Lobatto rule are in $[a, b]$.

Note that in the previous enumeration and in the discussion that follows, the statements also hold if we interpret $f_n(\pm\infty) = \pm\infty$ while $T(\pm\infty) = -a_n$.

Before analyzing a general situation, and making use of Theorems 2.1-(2) and 2.15, we consider first two particular cases.

Suppose that $p_{n-1}(\alpha) = 0$. Then, $\det\Delta = -p_{n-2}(\alpha)p_{n-1}(\beta)$ and $\det\Delta = 0 \Leftrightarrow p_{n-1}(\beta) = 0$. So, when $p_{n-1}(\alpha) = 0$ and $p_{n-1}(\beta) \neq 0$, then (17) becomes

$$a_n = \frac{f_n(\alpha)f_{n-1}(\alpha)}{f_{n-1}(\beta)} - f_{n-1}(\beta), \quad b_n = -f_n(\alpha)f_{n-1}(\alpha) \neq 0. \tag{18}$$

But it follows in this case that $b_n = -\frac{p_n(\alpha)}{p_{n-2}(\alpha)} > 0$, yielding the case GL2. This explains Remark 2.11.

Suppose now that $p_{n-2}(\alpha) = 0$ (and $p_{n-1}(\beta) \neq 0$; so, this case is not reduced to the previous one). Then, $\det\Delta = p_{n-1}(\alpha)p_{n-2}(\beta)$ and $\det\Delta = 0 \Leftrightarrow p_{n-2}(\beta) = 0$. So, when $p_{n-2}(\alpha) = 0$ and $p_{n-2}(\beta) \neq 0$, then (17) becomes

$$a_n = -f_n(\alpha), \quad b_n = f_{n-1}(\beta)\left[f_n(\alpha) - f_n(\beta)\right]. \tag{19}$$

Here, the condition $f_n(\alpha) = f_n(\beta)$ implies the case GL1. Clearly, the case GL3 is obtained, if and only if, $f_{n-1}(\beta) > 0$ when $f_n(\alpha) < f_n(\beta)$ or if $f_{n-1}(\beta) < 0$ when $f_n(\alpha) > f_n(\beta)$. If $[a, b]$ is finite, the conditions $T(b) \leq f_n(b)$ and $T(a) \geq f_n(a)$ are equivalent to $b_n \geq f_{n-1}(b)\left[f_n(\alpha) - f_n(b)\right]$ and $b_n \geq f_{n-1}(a)\left[f_n(\alpha) - f_n(a)\right]$, respectively. Thus, setting

$$C_1 := f_{n-1}(b)\frac{f_n(\alpha) - f_n(b)}{f_n(\alpha) - f_n(\beta)}, \;\; C_2 := f_{n-1}(a)\frac{f_n(\alpha) - f_n(a)}{f_n(\alpha) - f_n(\beta)}, \tag{20}$$

it is obtained the case GL3c, if and only if, $0 < f_{n-1}(\beta) \leq \min\{C_1, C_2\}$ when $f_n(\alpha) < f_n(\beta)$ or $\max\{C_1, C_2\} \leq f_{n-1}(\beta) < 0$ when $f_n(\alpha) > f_n(\beta)$. Clearly, GL3a and GL3b never occur if $b = \infty$ and $a = -\infty$, respectively.

In a more general situation, suppose that α, β are not in the set of zeros of $p_{n-1}(x)$ and $p_{n-2}(x)$. Then, $\det\Delta = 0 \Leftrightarrow f_{n-1}(\alpha) = f_{n-1}(\beta)$. When $\det\Delta \neq 0$, then (17) becomes

$$\begin{aligned} a_n &= \tfrac{f_n(\beta)f_{n-1}(\beta) - f_n(\alpha)f_{n-1}(\alpha)}{f_{n-1}(\alpha) - f_{n-1}(\beta)}, \\ b_n &= f_{n-1}(\alpha)f_{n-1}(\beta)\tfrac{f_n(\alpha) - f_n(\beta)}{f_{n-1}(\alpha) - f_{n-1}(\beta)}. \end{aligned} \tag{21}$$

Again, the condition $f_n(\alpha) = f_n(\beta)$ implies the case GL1. When $f_n(\alpha) \neq f_n(\beta)$, cases GL2 and GL3 depends on $\mathrm{sgn}(b_n)$. Moreover, if $[a, b]$ is finite, setting

$$C_1 := -f_{n-1}(b)\left[a_n + f_n(b)\right] \;, \;\; C_2 := -f_{n-1}(a)\left[a_n + f_n(a)\right], \tag{22}$$

then the case GL3c is obtained, if and only if, $\min\{C_1, C_2\} \leq b_n < 0$, whereas GL3a and GL3b never occur when $b = \infty$ and $a = -\infty$, respectively.

With these considerations, we have proved the following

Theorem 2.16 (Gauss-Lobatto) *Let μ be a positive Borel measure on a finite or infinite interval $[a, b]$ of the real line and let $\{p_n(x)\}_{n=0}^{\infty}$ be the sequence of orthonormal polynomials with respect to μ in $[a, b]$ with positive leading coefficients. Set $f_n(x) = \frac{p_n(x)}{p_{n-1}(x)}$ for all $n \geq 1$, $R_n(x)$ given by (15) and $\alpha, \beta \in [a, b]$ two distinct finite fixed points. Let $I_n(f)$ be a n-point Gauss-Lobatto quadrature formula for $I_\mu(f)$ given by (6) and of the form (14), with prescribed nodes α and β and degree of accuracy $2n - 3$. Then, we distinguish the following situations depending on α and β:*

(1) Suppose that $p_{n-1}(\alpha) = 0$.
  (a) If $p_{n-1}(\beta) = 0$, *then does not exist such* $I_n(f)$.
  (b) If $p_{n-1}(\beta) \neq 0$, *then case GL2 holds, with* a_n *and* b_n *given by (18).*

(2) Suppose that $p_{n-2}(\alpha) = 0$.
  (a) If $p_{n-2}(\beta) = 0$, *then does not exist such* $I_n(f)$.
  (b) If $p_{n-2}(\beta) \neq 0$ *and* $f_n(\alpha) = f_n(\beta)$, *then the case GL1 is obtained.*
  (c) If $p_{n-2}(\beta) \neq 0$ *and* $f_n(\alpha) \neq f_n(\beta)$, *let* a_n *and* b_n *be given by (19). Then, the case GL2 occurs, if and only if,* $\operatorname{sgn}(f_{n-1}(\beta)) = \operatorname{sgn}(f_n(\alpha) - f_n(\beta))$. *Otherwise, the case GL3 is obtained. Moreover, if* $[a, b]$ *is finite, the case GL3c holds, if and only if,* $0 < f_{n-1}(\beta) \leq \min\{C_1, C_2\}$ *when* $f_n(\alpha) < f_n(\beta)$ *or* $\max\{C_1, C_2\} \leq f_{n-1}(\beta) < 0$ *when* $f_n(\alpha) > f_n(\beta)$, *where* C_1 *and* C_2 *are given by (20). In particular, the cases GL3a and GL3b occur if* $f_n(\alpha) \geq f_n(b)$ *and* $f_n(\alpha) \leq f_n(a)$, *respectively, and they never occur if* $b = \infty$ *and* $a = -\infty$, *respectively.*

(3) Suppose that α *and* β *are not in the set of zeros of* $p_{n-1}(x)$ *and* $p_{n-2}(x)$.
  (a) If $f_{n-1}(\alpha) = f_{n-1}(\beta)$, *then does not exist such* $I_n(f)$.
  (b) If $f_{n-1}(\alpha) \neq f_{n-1}(\beta)$ *and* $f_n(\alpha) = f_n(\beta)$, *then case GL1 occurs.*
  (c) If $f_{n-1}(\alpha) \neq f_{n-1}(\beta)$ *and* $f_n(\alpha) \neq f_n(\beta)$, *then let* a_n *and* b_n *be given by (21). Cases GL2 and GL3 depend on* $\operatorname{sgn}(b_n)$. *If* $[a, b]$ *is finite, the case GL3c occur, if and only if* $\min\{C_1, C_2\} \leq b_n < 0$, *where* C_1 *and* C_2 *are given by (22). In particular, if* $b_n < 0$, *then GL3a and GL3b occur if* $a_n < -f_n(b)$ *and* $a_n \geq -f_n(a)$, *respectively, and never occur if* $b = \infty$ *and* $a = -\infty$, *respectively.*

In all the cases where the Gauss-Lobatto quadrature rule exist, it must to be of interpolatory-type and the positivity of the weights is guaranteed.

Remark 2.17 Let $\{p_n(x)\}_{n=0}^{\infty}$ be a sequence of orthogonal polynomials with respect to μ on a finite interval $[a, b]$ and set

$$Q_{n-2}(x, a, b) := \frac{1}{(x-a)(b-x)} \left[p_n(x) + a_n p_{n-1}(x) + b_n p_{n-2}(x) \right],$$

with a_n and b_n given by (17) taking $\alpha = a$ and $\beta = b$ (here, $b_n \neq 0$). Then, it is clear that $Q_{n-2}(x, a, b)$ is a $(n-2)$th orthogonal polynomial with respect to $\tilde{\mu}(x) = (x-a)(b-x)\mu(x)$, and thus by taking $\alpha = a$ and $\beta = b$ in Theorem 2.16, then Theorem 2.6 is recovered.

2.4 Particular cases and generalisations

A particular case of Theorem 2.16 is to consider one of the two prescribed nodes to be an endpoint of the interval of integration. In this case, an alternative approach to this problem trivially follows from Theorems 2.5 and 2.10. The Lobatto formula with one point in an endpoint of the interval is actually

a Radau formula for a modified measure (modified to fix the endpoint) with one other prefixed node that can be anywhere.

Corollary 2.18 *Let μ be a positive Borel measure on a finite or half-infinite interval $[a,b] \subsetneq \mathbb{R}$ of the real line and consider the following n-point quadrature formula for $I_\mu(f)$ given by (6):*

$$I_n(f) = A_\lambda f(\lambda) + A_\alpha f(\alpha) + \sum_{k=1}^{n-2} A_{k,n} f(x_{k,n}), \tag{23}$$

with $\alpha \in [a,b]\backslash\{\lambda\}$ and $\lambda = a$ or b if $[a,b]$ is finite, or λ equal to the finite endpoint if the interval is half-infinite. Consider the positive Borel measure $\tilde{\mu}(x) = (x-a)\mu(x)$ ($\tilde{\mu}(x) = (b-x)\mu(x)$, respectively) on $[a,b]$ if it is finite, $\tilde{\mu}(x) = (x-a)\mu(x)$ if $b = \infty$ and $\tilde{\mu}(x) = (b-x)\mu(x)$ if $a = -\infty$. Let $\{\tilde{p}_n(x)\}_{n=0}^{\infty}$ be the sequence of orthonormal polynomials with respect to $\tilde{\mu}$ in $[a,b]$ and normalized to have positive leading coefficients and set $\tilde{f}_n(x) = \frac{\tilde{p}_n(x)}{\tilde{p}_{n-1}(x)}$ for all $n \geq 1$. Let $\tilde{x}_{i,n}$ denote the ith root of $\tilde{p}_n(x)$ and for all $i = 1, \ldots, n-2$, let $\tilde{\zeta}_i \in (\tilde{x}_{i,n-1}, \tilde{x}_{i,n-2})$ and $\tilde{\xi}_i \in (\tilde{x}_{i,n-2}, \tilde{x}_{i+1,n-1})$ be the unique solutions of $\tilde{f}_{n-1}(\tilde{\zeta}_i) = \tilde{f}_{n-1}(b)$ and $\tilde{f}_{n-1}(\tilde{\xi}_i) = \tilde{f}_{n-1}(a)$, respectively when $[a,b]$ is finite, $\tilde{\zeta}_i = \tilde{x}_{i,n-2}$ if $b = \infty$ and $\tilde{\xi}_i = \tilde{x}_{i,n-2}$ if $a = -\infty$. Suppose that $\tilde{p}_{n-2}(\alpha) \neq 0$ and that $\alpha \notin \{\tilde{\xi}_1, \ldots, \tilde{\xi}_{n-2}\}$ when $\lambda = a$ or $\alpha \notin \{\tilde{\zeta}_1, \ldots, \tilde{\zeta}_{n-2}\}$ when $\lambda = b$. Then, $I_n(f)$ has the highest degree of accuracy, that is $2n-3$, if and only if, it is of interpolatory type and the $(n-1)$ nodes except λ are the zeros of $\tilde{R}_{n-1}(x) = \tilde{p}_{n-1}(x) - \tilde{f}_{n-1}(\alpha)\tilde{p}_{n-2}(x)$. The weights of the quadrature are positive. Moreover, all the nodes of the quadrature, except λ lie in (a,b), if and only if,

$$\alpha \in (a,b) \setminus \bigcup_{i=1}^{n-2} [\tilde{\zeta}_i, \tilde{\xi}_i],$$

and when $[a,b]$ is finite, the endpoint b (a, respectively) is one of the nodes of $I_n(f)$, if and only if, $\alpha \in \{\tilde{\zeta}_1, \ldots, \tilde{\zeta}_{n-2}, b\}$ ($\alpha \in \{a, \tilde{\xi}_1, \ldots, \tilde{\xi}_{n-2}\}$, respectively).

In a similar way, the combination of Theorems 2.5, 2.6, 2.10 and 2.16 allows us to characterize the following n-point quadrature formulas with positive weights and the highest degree of accuracy. It boils down to saying that prefixing three nodes, two of them being at the endpoints of a finite interval is equivalent to considering a Radau formula for a modified measure (modified to prefix the two endpoints) with one other prefixed node. Prefixing four nodes, two of which are the endpoints of a finite interval is equivalent with considering a Lobatto formula with two free points prefixed, but for a measure modified in such a way that the two endpoints are prefixed nodes. And so on. We omit the details.

$$I_n(f) = A_a f(a) + A_b f(b) + A_\alpha f(\alpha) + \sum_{k=1}^{n-3} A_{k,n} f(x_{k,n});$$
$$\alpha \in (a,b), \quad -\infty < a < b < \infty,$$
$$I_n(f) = A_\lambda f(\lambda) + A_\alpha f(\alpha) + A_\beta f(\beta) + \sum_{k=1}^{n-3} A_{k,n} f(x_{k,n});$$
$$\alpha, \beta \in (a,b), \quad \alpha \neq \beta; \quad \lambda \in \{a,b\},$$
$$-\infty < a < b \leq \infty \text{ if } \lambda = a,$$
$$-\infty \leq a < b < \infty \text{ if } \lambda = b,$$
$$I_n(f) = A_a f(a) + A_b f(b) + A_\alpha f(\alpha) + A_\beta f(\beta) + \sum_{k=1}^{n-4} A_{k,n} f(x_{k,n});$$
$$\alpha, \beta \in (a,b), \quad \alpha \neq \beta, \quad -\infty < a < b < \infty.$$

Example 2.19 As an application of the latter approach, we will show how to derive the quadrature formula recently deduced in [18] in the context of the numerical solution of stiff problems and algebraic differential equations. It is proved there that a quadrature formula exists for the Lebesgue measure $d\mu(x) \equiv dx$ in $[0,1]$ with the following properties. It has positive weights, and both endpoints are prescribed; it has one arbitrary parameter which can be used to fix another node, and it has the highest possible degree of precision, that is $2n-4$. The nodes of that quadrature formula are the zeros of the polynomial

$$R_n(x) = p_n^*(x) - p_{n-2}^* + \beta\sqrt{2n-1}\left(p_{n-1}^*(x) - p_{n-3}^*\right),$$

where $p_n^*(x)$ denotes the nth Legendre polynomial shifted into $[0,1]$ and β is the free parameter. Setting $\gamma_n = \sqrt{2n-1}/(2n-3)$, then for $|\beta| < \gamma_n$, all the nodes belong to $[0,1]$ and for $|\beta| > \gamma_n$, one node is outside the interval, whereas in the case $|\beta| = \gamma_n$ there does not exist such rule.

So, let us check that this quadrature formula can be recovered from our results. Explicit expressions for the polynomials $p_n^*(x)$ are known. What we need is the fact that $p_n^*(0) = (-1)^n$ and $p_n^*(1) = 1$, and that the derivative at $x = 0$ equals $(-1)^{n+1} n(n+1)$. Since the quadrature formula has degree of accuracy $2n-4$, it follows from Theorem 2.4 that the nodes of the quadrature are the zeros of a quasi-orthogonal polynomial of order three, that is of a polynomial of the form

$$R_n(x) = p_n^*(x) + \tilde{a}_n p_{n-1}^*(x) + \tilde{b}_n p_{n-2}^*(x) + \tilde{c}_n p_{n-3}^*(x).$$

The conditions $R_n(0) = R_n(1) = 0$ imply that $R_n(x)$ can be rewritten as

$$R_n(x) = p_n^*(x) - p_{n-2}^*(x) + a\left[p_{n-1}^*(x) - p_{n-3}^*(x)\right], \tag{24}$$

where a is an arbitrary constant. Observe that with the choice $a = 0$ we recover the Gauss-Lobatto rule characterized in Theorem 2.6.

Since we are dealing with three prefixed nodes, two of them at the endpoints of $[0,1]$ and one at $\alpha \in (0,1)$, we should consider the Radau case for the modified weight $x(1-x)$. Therefore recall the definition of the Jacobi$^{(a,b)}$ weight functions defined in $[-1,1]$ by $\omega(x) = (1-x)^a(1+x)^b$ for $a, b > -1$. Observe that if we denote by $q_n(x)$ the nth Jacobi$^{(1,1)}$ polynomial and we shift it to $[0,1]$ we obtain a polynomial $\tilde{p}_n(x) = 2q_n(2x-1)$ which is the nth orthogonal polynomial in $[0,1]$ with respect to the weight function $\omega(x) = x(1-x)$. From the well known explicit expression for the polynomial $q_n(x)$, it follows that

$$\tilde{p}_n(x) = 2\frac{n+1}{n+2}\sum_{m=0}^{n}\binom{n}{m}\binom{n+m+2}{m+1}(x-1)^m, \tag{25}$$

and so $\tilde{p}_n(0) = 2(-1)^n(n+1)$ and $\tilde{p}_n(1) = 2(n+1)$. This implies that $\tilde{f}_{n-2} = \tilde{p}_{n-2}/\tilde{p}_{n-3}$ takes values $\tilde{f}_{n-2}(1) = -\tilde{f}_{n-2}(0) = \frac{n-1}{n-2}$. The "good" node α should satisfy

$$-\frac{n-1}{n-2} = \tilde{f}_{n-2}(0) < A = \tilde{f}_{n-2}(\alpha) < \tilde{f}_{n-2}(1) = \frac{n-1}{n-2} \quad \text{or} \quad |A| < \frac{n-1}{n-2}.$$

On the other hand, the node α should be a zero of the quasi-orthogonal polynomial $\tilde{R}_{n-2}(x) = \tilde{p}_{n-2}(x) - A\tilde{p}_{n-3}(x)$. To relate this A to the parameter a in (24), we note that $x(1-x)\tilde{R}_{n-2}(x)$ and $R_n(x)$ of (24) should have the same zeros and hence should be the same up to a constant multiple. Comparison of the leading coefficients, which is minus the leading coefficient of $\tilde{p}_{n-2}$ in the first one and the leading coefficient of p_n^* in the second one shows that

$$R_n(x) = -\frac{2n-1}{n-1}x(1-x)\tilde{R}_{n-2}(x).$$

Computing the derivative of both sides in $x = 0$ gives

$$\begin{aligned} 2[(2n-1) - a(2n-3)] &= -\frac{2n-1}{n-1}[\tilde{p}_{n-2}(0) + A\tilde{p}_{n-3}(0)] \\ &= \frac{2n-1}{n-1}2[(n-1) + A(n-2)] \end{aligned}$$

since $(p_k^*)'(0) = (-1)^{k+1}k(k+1)$. Solving this for A results in

$$A = -\frac{(2n-3)(n-1)}{(2n-1)(n-2)}a.$$

Thus $|A| < (n-1)/(n-2)$ is equivalent with $|a| < (2n-1)/(2n-3)$, and if we set $a = \beta\sqrt{2n-1}$, it is equivalent with $|\beta| < \sqrt{2n-1}/(2n-3)$, as was indeed claimed in [18]. $\diamond$

To end this section, let us comment briefly on a drawback of a quadrature formula with the highest degree of accuracy, positive weights and r arbitrary

prescribed nodes, with $r > 2$. A first approach to this problem is given in [19]. In this case, from Theorem 2.4 it follows that the rule has to be of interpolatory type and the nodes are the zeros of the quasi-orthogonal polynomial $R_n(x)$ given by (9). From Theorem 2.8, only $(n - r)$ distinct zeros of $R_n(x)$ are assured to be in the interval (a, b), whereas double zeros may appear in the r remainder ones. It is also proved that if $[a, b]$ is finite and just two zeros lie outside (a, b), then one appears in $(-\infty, a)$ and the other one in (b, ∞); in this case, the weights of the quadrature formula are all positive. However, if more than two zeros lie outside (a, b), then at least two zeros will appear in $(-\infty, a)$ or in (b, ∞), and then it is also proved that the weights of the quadrature formula corresponding to these two nodes alternate sign, being positive the weight corresponding to the node which is nearest to the interval (a, b); the weights corresponding to the interior nodes are still positive. The same behaviour occur if $b = \infty$ ($a = -\infty$, respectively) and two zeros of $R_n(x)$ lie in $(-\infty, a)$ ((b, ∞), respectively). Thus, in the construction of such rules, we need to guarantee that all the zeros of $R_n(x)$ are distinct and that no more than two zeros may appear outside (a, b), in order to assure the convergence of the procedure.

3 Computational aspects

The computation of the quadrature formulas is classical and dates back to work by Golub (e.g., [11]) and Gautschi (e.g., [7–10]). The idea is that the Jacobi matrix is modified in the last elements in such a way that the required nodes become eigenvalues of that modified matrix. The corresponding coefficients in the quadrature formula are given by the first components of the normalized eigenvectors multiplied with the zeroth moment of the measure.

3.1 The classical approach

It will be convenient for the computations to work with the monic orthogonal polynomials $\hat{p}_k$ instead of the normalized ones p_k. This makes no difference since we are only interested in its zeros. The recurrence relation for the monic polynomials is

$$\hat{p}_{n+1}(x) = (x - \hat{v}_n)\hat{p}_n(x) - \hat{u}_n\hat{p}_{n-1}(x), \quad \hat{p}_{-1} \equiv 0, \quad \hat{p}_0 \equiv 1.$$

The $\hat{u}_k = u_k^2$ and $\hat{v}_k = v_k$ where the u_k and v_k are the coefficients appearing in the normalized recurrence. Also $\|\hat{p}_0\|^2$ is needed which is usually stored as $\hat{u}_0$. The advantage of this recursion is that to compute $\hat{p}_{n+1}$ we only need $\{(\hat{v}_k, \hat{u}_k) : k = 0, \ldots, n\}$ and since we do not normalize, $\hat{u}_{n+1}$ is not needed.

The tridiagonal Jacobi matrix

$$\hat{J}_n = \begin{bmatrix} \hat{v}_0 & 1 & 0 & 0 & \cdots & 0 \\ \hat{u}_1 & \hat{v}_1 & 1 & 0 & \cdots & 0 \\ 0 & \hat{u}_2 & \hat{v}_2 & 1 & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & & \hat{u}_{n-2} & \hat{v}_{n-2} & 1 \\ 0 & 0 & \cdots & 0 & \hat{u}_{n-1} & \hat{v}_{n-1} \end{bmatrix}$$

is similar to the symmetric Jacobi matrix J_n and thus it has the same eigenvalues but it is trivial to construct one from the other.

So to obtain for example an n-point *Gauss-Radau* formula with a prefixed node α, given the recursion coefficients $\{\hat{v}_k, \hat{u}_k\}_{k=0}^{n-1}$ for the measure μ under consideration (i.e., the Jacobi matrix of size n), one has to modify the measure μ, to $\tilde{\mu}$ such that its nth orthogonal polynomial $\tilde{p}_n$ has α as one of its zeros, if such a measure exists. This will be obtained by changing $\hat{v}_{n-1}$ into $\tilde{v}_{n-1}$. Thus

$$\tilde{p}_n(x) = (x - \tilde{v}_{n-1})\hat{p}_{n-1}(x) - \hat{u}_{n-1}\hat{p}_{n-2}(x) \tag{26}$$

should vanish for $x = \alpha$. The values $\hat{p}_{n-1}(\alpha)$ and $\hat{p}_{n-2}(\alpha)$ can be computed by the recurrence relation since these recurrence coefficients are not modified: $\{(\hat{u}_k, \hat{v}_k) : k = 0, \ldots, n-2\}$. Only $\hat{v}_{n-1}$ needs to be modified, which can be obtained from (26) by setting it equal to zero for $x = \alpha$:

$$\tilde{v}_{n-1} = \alpha - \hat{u}_{n-1}\hat{p}_{n-2}(\alpha)/\hat{p}_{n-1}(\alpha). \tag{27}$$

We do get orthogonality with respect to the modified measure $\tilde{\mu}$ but by changing $\hat{v}_{n-1}$ we loose one orthogonality condition with respect to the original measure μ. We therefore have only quasi-orthogonality. Since we loose only one orthogonality condition, quasi-orthogonality is only of order 1. This also means that we give in only one degree of accuracy of the quadrature formula. This gives all the elements in the modified Jacobi matrix $\tilde{J}_n$. Whenever the quadrature formula with all the good properties exists, the eigenvalues and eigenvectors of $\tilde{J}_n$ give the nodes and weights just like for ordinary Gauss formulas, which it is, but for a modified measure.

When for a *Gauss-Lobatto* formula, we want to prefix two nodes α and β, then we have that (26) should hold for $x = \alpha$ and for $x = \beta$. This system of two equations can be solved if we allow two parameters. So we modify the last two $\hat{v}_{n-1}$ and $\hat{u}_{n-1}$. Changing both values will cost two orthogonality conditions, and hence we are left with quasi-orthogonality of order 2, giving a degree of accuracy that is 2 less than the usual Gauss quadrature for the original

measure, i.e., it is only $2n-3$. So we require that

$$\tilde{v}_{n-1}\hat{p}_{n-1}(x) + \tilde{u}_{n-1}\hat{p}_{n-2}(x) = x\hat{p}_{n-1}(x), \quad \text{for } \; x \in \{\alpha, \beta\}$$

and solve this system for $\tilde{v}_{n-1}$ and $\tilde{u}_{n-1}$. Together with the original values of $\{(\hat{v}_k, \hat{u}_k) : k = 0, \ldots, n-2\}$, these define the modified Jacobi matrix $\tilde{J}_n$ for which the Gaussian quadrature can be computed. For a bad choice of α and/or β, the $\tilde{u}_{n-1}$ may for instance become negative and lead to complex nodes and weights. In other cases, the nodes may be real but the weights may be negative, etc.

Note that the previous system is related to, but not the same as the system considered in Theorem 2.15.

The previous methods of computing are well known in the literature and nothing is claimed to be original. It may be somewhat less known that a similar kind of method can be used for 3 or more prescribed nodes. Take for example 3 nodes α, β and λ. To make these three points a zero of $\hat{p}_n$ imposes three conditions which will define modifications of the last three recursion parameters $\hat{u}_{n-1}$, $\hat{v}_{n-1}$ and $\hat{v}_{n-2}$. This means 3 fewer orthogonality conditions with respect to μ that can be satisfied, giving quasi-orthogonality of order 3, and a maximal degree of accuracy $2n-4$. Since

$$\tilde{p}_n(x) = (x - \tilde{v}_{n-1})\tilde{p}_{n-1}(x) - \tilde{u}_{n-1}\hat{p}_{n-2}(x)$$

should be zero for $x \in \{\alpha, \beta, \lambda\}$, we have only two parameters. To introduce more parameters we replace $\tilde{p}_{n-1}$ by its recurrence relation $\tilde{p}_{n-1}(x) = (x - \tilde{v}_{n-2})\hat{p}_{n-2}(x) - \hat{u}_{n-2}\hat{p}_{n-3}(x)$ and find that

$$a_n x\hat{p}_{n-2}(x) + b_n\hat{p}_{n-2}(x) + c_n\hat{p}_{n-3}(x) = x^2\hat{p}_{n-2}(x) - \hat{u}_{n-2}x\hat{p}_{n-3}(x), \qquad (28)$$

where

$$a_n = \tilde{v}_{n-1} + \tilde{v}_{n-2}, \quad b_n = \tilde{u}_{n-1} - \tilde{v}_{n-1}\tilde{v}_{n-2}, \quad c_n = -\hat{u}_{n-2}\tilde{v}_{n-1}$$

should hold for $x \in \{\alpha, \beta, \lambda\}$. This gives 3 equations from which the numbers a_n, b_n and c_n can be found. Once these are known, we can solve for the recurrence coefficients, giving

$$\tilde{v}_{n-1} = -c_n/\hat{u}_{n-2}, \quad \tilde{v}_{n-2} = a_n - \tilde{v}_{n-1}, \quad \tilde{u}_{n-1} = b_n + \tilde{v}_{n-1}\tilde{v}_{n-2}.$$

Similarly when we have 4 points prescribed, say $\{\alpha, \beta, \lambda, \gamma\}$ then we have to also modify $\hat{u}_{n-2}$ so that we should rewrite the relation (28) as

$$a_n x\hat{p}_{n-2}(x) + b_n\hat{p}_{n-2}(x) + c_n\hat{p}_{n-3}(x) + d_n x\hat{p}_{n-3}(x) = x^2\hat{p}_{n-2}(x)$$

with a_n, b_n, c_n as before and $d_n = \tilde{u}_{n-2}$. Replacing x by the values $\alpha, \beta, \lambda, \gamma$, delivers 4 equations from which a_n, b_n, c_n, d_n are found. Set $\tilde{u}_{n-2} = d_n$ and proceed as in the previous case to find the modified values of $\tilde{v}_{n-2}, \hat{u}_{n-1}$ and $\tilde{v}_{n-1}$. We omit the details. Similar procedures can be followed for more prescribed nodes. It may however be clear that as the number of prescribed points increases, setting up the right hand side of the linear system such as (28) becomes more involved and, once the linear system is solved, a nonlinear transformation is needed to obtain the modified parameters $\tilde{v}_k$ and $\tilde{u}_k$ from the solution of the linear system.

3.2 An alternative algorithm

There is however a much more systematic approach to this with a simple linear algebra interpretation as we shall explain next. Therefore we need the following lemma.

Lemma 3.1 *Define the matrix*

$$C_n(\hat{\mathbf{w}}) = \hat{J}_n - \mathbf{e}_n \hat{\mathbf{w}}^T$$

where $\hat{J}_n$ is as before and $\hat{\mathbf{w}}^T = (\hat{w}_0, \ldots, \hat{w}_{n-1})$ and $\mathbf{e}_n^T = (0, \ldots, 0, 1)$. Then the characteristic polynomial $\tilde{p}_n(x) = \det(xI_n - C_n(\hat{\mathbf{w}}))$ is given by

$$\tilde{p}_n(x) = \sum_{i=0}^{n-1} \hat{w}_i \hat{p}_i(x) + \hat{p}_n(x) \tag{29}$$

where $\hat{p}_i(x) = \det(xI_i - \hat{J}_i)$, $i = 1, \ldots, n$.

PROOF. This follows immediately by computing the Laplace expansion of the determinant along the last row, which results in

$$\tilde{p}_n(x) = \sum_{i=0}^{n-1} \hat{w}_i \hat{p}_i(x) + (x - \hat{v}_{n-1}) \hat{p}_{n-1}(x) + \hat{u}_{n-1} \hat{p}_{n-2}(x)$$

and the recurrence relation shows that the last part is just $\hat{p}_n(x)$. □

If for the Radau case, we require that the quasi-orthogonal polynomial $\tilde{p}_n(x) = \hat{p}_n + \hat{w}_{n-1}\hat{p}_{n-1}(x)$ has a zero for $x = \alpha$, hence $\hat{w}_{n-1} = -\hat{p}_n(\alpha)/\hat{p}_{n-1}(\alpha)$, then, we can use the previous lemma with $\hat{w}_k = 0$ for $k = 0, \ldots, n-2$ and it is clearly seen that then $C_n(\hat{\mathbf{w}})$ becomes $\tilde{J}_n$ by only modifying the last element $\tilde{v}_{n-1} = \hat{v}_{n-1} - \hat{w}_{n-1}$. Thus the following is proved.

Proposition 1 *If $\hat{v}_{n-1}$ is the $(n-1)$th recursion coefficient in the original recursion for the monic orthogonal polynomials $\hat{p}_k$, and $\tilde{v}_{n-1}$ is the modified value needed for the Gauss-Radau formula with prefixed node α, then they are related by*

$$\tilde{v}_{n-1} = \hat{v}_{n-1} + \frac{\hat{p}_n(\alpha)}{\hat{p}_{n-1}(\alpha)}.$$

For the case of Lobatto, two prescribed nodes α and β are imposed on the polynomial

$$\tilde{p}_n(x) = \hat{p}_n(x) + \hat{w}_{n-1}\hat{p}_{n-1}(x) + \hat{w}_{n-2}\hat{p}_{n-2}(x),$$

which results in the system

$$\begin{bmatrix} \hat{p}_{n-2}(\alpha) & \hat{p}_{n-1}(\alpha) \\ \hat{p}_{n-2}(\beta) & \hat{p}_{n-1}(\beta) \end{bmatrix} \begin{bmatrix} \hat{w}_{n-2} \\ \hat{w}_{n-1} \end{bmatrix} = - \begin{bmatrix} \hat{p}_n(\alpha) \\ \hat{p}_n(\beta) \end{bmatrix}.$$

Again, by setting in Lemma 3.1 $\hat{w}_k = 0$ for $k = 0, \ldots, n-3$ and taking $\hat{w}_{n-2}$ and $\hat{w}_{n-1}$ as solutions of the previous system, we see that $C_n(\hat{\mathbf{w}})$ becomes $\tilde{J}_n$ so that the solution of this system is precisely the update needed for the parameters $\hat{v}_{n-1}$ and $\hat{u}_{n-1}$. So the following is proved.

Proposition 2 *If $[\hat{v}_{n-1}, \hat{u}_{n-1}]^T$ are the $(n-1)$th recursion coefficients in the original recursion for the monic orthogonal polynomials $\hat{p}_k$, and $[\tilde{v}_{n-1}, \tilde{u}_{n-1}]^T$ are the modified values needed for the Gauss-Lobatto formula with prefixed nodes α, β, then they are related by*

$$\begin{bmatrix} \tilde{v}_{n-1} \\ \tilde{u}_{n-1} \end{bmatrix} = \begin{bmatrix} \hat{v}_{n-1} \\ \hat{u}_{n-1} \end{bmatrix} + \begin{bmatrix} \hat{p}_{n-1}(\alpha) & \hat{p}_{n-2}(\alpha) \\ \hat{p}_{n-1}(\beta) & \hat{p}_{n-2}(\beta) \end{bmatrix}^{-1} \begin{bmatrix} \hat{p}_{n-1}(\alpha) \\ \hat{p}_{n-1}(\beta) \end{bmatrix}.$$

In general, if $m < n-1$ nodes are prefixed, we set $\hat{w}_k = 0$ for $k = 0, \ldots, n-m-1$ in (29) and determine the remaining $\hat{w}_k$, $k = n-m, \ldots, n-1$ by solving the system of m equations resulting from the conditions $\tilde{p}_n(\alpha_i) = 0$ where α_i, $i = 1, \ldots, m$ are the prefixed nodes. This defines the matrix $C_n(\hat{\mathbf{w}})$ completely, and solving for its eigenvalues will give all the nodes: the prefixed ones and the remaining ones chosen in such a way that they give a maximal domain of validity, whenever such a quadrature formula exists.

Giving explicit expressions of the modified parameters $\tilde{v}_k$, $\tilde{u}_k$ will be as complicated as in the previous approach, but there is a simple algorithm to compute them. Such an algorithm should reduce the matrix $C_n(\hat{\mathbf{w}})$ by similarity transformations to a tridiagonal form like $\hat{J}_n$ is. Since only the trailing elements of $\hat{\mathbf{w}}$ are nonzero, we need the similarity transformations only for the lower right part of $C_n(\hat{\mathbf{w}})$. Thus without loss of generality assume that we have to eliminate by similarity transformations all but the last two elements in the

last row of a matrix with the following structure:

$$\begin{bmatrix} \times & 1 & & & & & \\ \times & \times & 1 & & & & \\ & \times & \times & 1 & & & \\ & & \times & \times & 1 & & \\ & & & \times & \times & 1 & \\ & & & & \times & \times & 1 \\ \times & \times & \times & \times & \times & \times & \times \end{bmatrix}.$$

As long as the subdiagonal elements are nonzero, one may use the following steps.

(1) For $k = 1, \ldots, n-2$
eliminate the elements in column k in the rows $k+2, \ldots, n$ by doing the following:
   (a) for $j = k+2, \ldots, n$: if element (j,k) is nonzero then
   add a multiple of row $k+1$ to row j to eliminate element (j,k) and complete the similarity transform by subtracting the same multiple of column j from column $k+1$.

In the 7×7 example above, eliminating the element (7,1) (by a similarity transform) will result in a nonzero element (6,2). Elimination of the (6,2) element will result in nonzero entries (5,3), (6,3) and (6,4). Elimination of the element (7,2) will not alter the structure. From now on the unwanted elements can be eliminated at each step eliminating one element without introducing new nonzero ones. At all stages of the algorithm, the matrix stays unit lower Hessenberg. Note also that only the last 7 parameters are modified. That are the last 4 elements of the main diagonal and the last 3 on the subdiagonal. The first 3 elements on the main diagonal and the first 3 on the subdiagonal are left unaltered.

If only 3 nodes are prefixed, there is only one similarity transform necessary and this leads to updating formulas

$$\tilde{v}_{n-2} = \hat{v}_{n-2} - A, \quad \tilde{v}_{n-1} = \hat{v}_{n-1} - \hat{w}_{n-1} + A, \quad \tilde{u}_{n-1} = \hat{u}_{n-1} - \hat{w}_{n-2} + A^2,$$

where $A = \hat{w}_{n-3}/\hat{u}_{n-2}$ is the parameter of the tranformation matrix.

When there are several prescribed nodes, the modified Jacobi matrix has several known nodes for its eigenvalues. In that case, it might be interesting to compute the remaining nodes as the zeros of the polynomial q_{n-m} in $\tilde{p}_n(x) = q_{n-m}(x) \prod_{i=1}^{m} (x - \alpha_i)$. This means as the eigenvalues of a deflated ma-

trix. This is easily done by some deflating bulge chasing algorithm [20] applied to the modified Jacobi matrix.

4 Numerical examples

To conclude this section, we present some numerical illustrations of the results presented in the paper for some of the classical weight functions on the real line; so, we are dealing with absolutely continuos measures. The experiments were done with software MATLAB 7.6.

We start by considering the Chebyshev-Radau quadrature formulas with $n = 6$, i.e., one node α is prefixed and the five other nodes are chosen in an optimal way. The results are shown in Figure 2: It is for Chebyshev polynomials of the first kind. For Chebyshev polynomials of the second kind, the figure looks very similar. On the horizontal axis the value of α is seen, ranging from -1.5 on the left to 1.5 on the right. The vertical axis shows the location of the six nodes. The straight diagonal is the location of α. The five vertical asymptotes correspond to $\alpha = x_{k,5}$, the zeros of the Chebyshev polynomial of degree five. For these values, one of the nodes is at infinity. For values of α in the neighborhoods of these asymptotes, one of the nodes is outside the interval $[-1, 1]$, For $\alpha < x_{i,5}$ there is a point ζ_i where the largest node leaves the interval on the right (top of the figure). For $\alpha > x_{i,5}$ there is a point ξ_i where a node enters the interval on the left (bottom of the figure). For $\alpha \in [\zeta_i, \xi_i]$, there is not a Chebyshev-Radau formula with all the nodes in (-1.1). However for all values $\alpha \in [-1, 1] \setminus \cup_{i=1}^{5}[\zeta_i, \xi_i]$, all the nodes are in $(-1, 1)$ and all the weights are positive. In the figure on the right the same plot is given but now the nodes for the "good" intervals of α are plotted with crosses (which are seen as thick lines). Note how the varying node α (corresponding to the straight diagonal line) gradually pushes the nodes to the right in the interval $[-1, 1]$ (upwards in the plot) and eventually outside the interval, while new nodes are coming in from the left at -1 (at the bottom of the plot). This corresponds to Theorem 2.10.

Now we consider the Legendre weight function $\omega(x) = 1/2$ and the Jacobi$^{(a,b)}$ weight functions defined in subsection 2.4, both on the interval $[a, b] = [-1, 1]$. The following examples correspond to the 7-point Gauss-Lobatto quadrature formula (23) for the Legendre weight function with one prefixed point at 0.2 (left) and Jacobi$^{(1,-1/2)}$ with one prefixed point at 0.2 (right). The other point ranges from -1.5 to 1.5 and the crossed nodes correspond to the good situation where all nodes are inside the interval $[-1, 1]$, and all weights are positive. The results are shown in Figure 3. The explanation is like for the previous figure. Note that for the Legendre weight there are only few small intervals for α to the left of $x_{3,5} \approx 0.2$, the third zero of the Legendre polynomial of degree five,

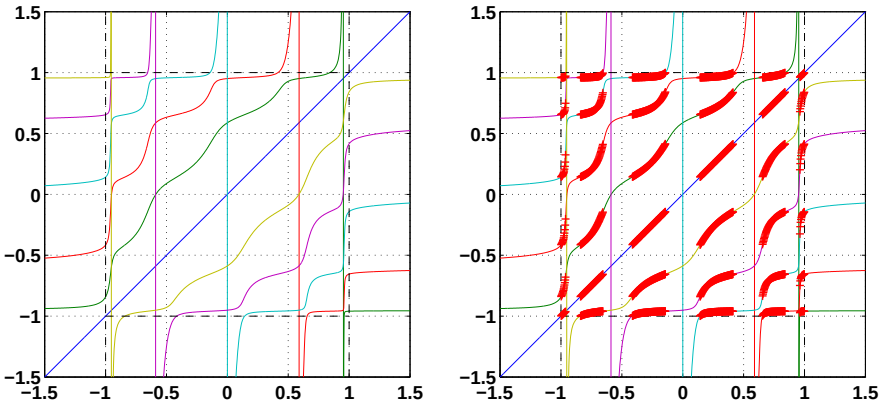

Fig. 2. The location of the nodes in a 6-point Chebyshev-Radau quadrature formula with a prefixed node ranging from -1.5 to 1.5. On the right, the nodes for the "good" formulas are indicated with crosses (thick lines).

where the proper Legendre-Lobatto formula exists. On the other hand, to the right of it, almost all the choices of α are good with only narrow bad intervals near $x_{4,5}$ and $x_{5,5}$.

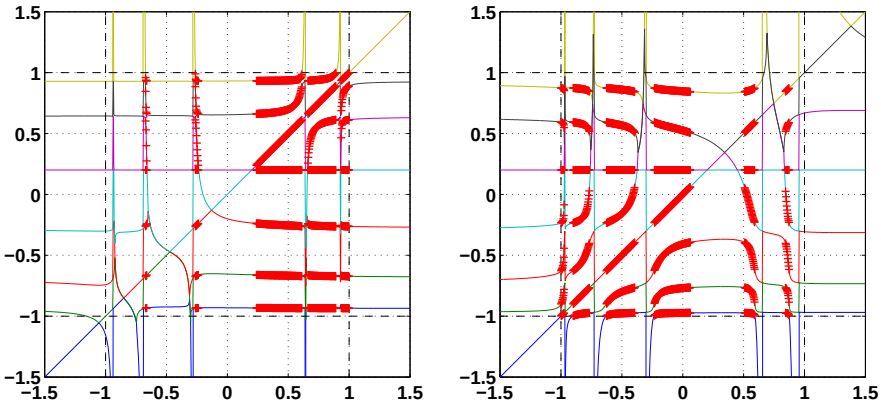

Fig. 3. The location of the nodes in a 7-point Gauss-Lobatto quadrature formula with one prescribed node in 0.2 and the another one ranging from -1.5 to 1.5. The "good" nodes are indicated with crosses. On the left for the Legendre weight, on the right for the Jacobi$^{(1,-1/2)}$ weight.

The next example plotted in Figure 4, corresponds again with a 7-point Gauss-Lobatto quadrature formula (14) for the Chebyshev weight function of the first kind (left) and the Jacobi$^{(1,-1/2)}$ weight (right), but now with the two prescribed nodes varying symmetrically from -1.5 to 1.5: the straight lines from $(-1.5, \pm 1.5)$ to $(1.5, \mp 1.5)$. The location of the nodes are shown in the vertical axis. Note that the left hand side has only four asymptotes. That is because the symmetric nodes hit the symmetric zeros of the Chebyshev polynomial of degree five simultaneously. The fifth asymptote at the origin is not plotted. On the right, the Jacobi weight, and hence also the polynomials are not symmetric, and therefore, ten asymptotes can be seen. There will be

one every time one of the two symmetric varying nodes hit a zero of the Jacobi polynomial of degree five.

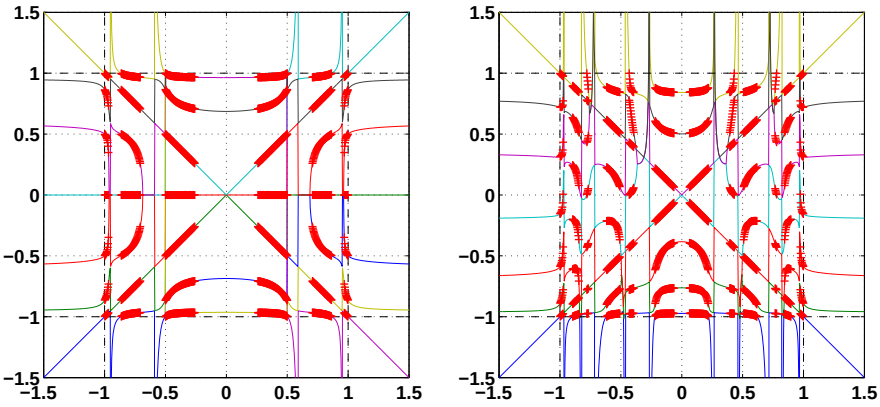

Fig. 4. The location of the nodes in a 7-point Chebyshev-Lobatto quadrature formula (left) and Jacobi$^{(1,-1/2)}$-Lobatto (right) with prescribed nodes varying symmetrically from -1.5 to 1.5.

Our next examples are plotted in Figure 5 and corresponds to the Laguerre$^{(a)}$ and Hermite weight functions defined on $[0,\infty)$ by $\omega(x) = x^a e^{-x}$ for $a > -1$ and on $\mathbb{R}$ by $\omega(x) = e^{-x^2}$, respectively. On the left one can see the 6-point Laguerre$^{(1)}$-Radau nodes are plotted for a prefixed node $\alpha \in [-1, 20]$. The cases of positive nodes and positive weights are indicated by crosses. Note that at the vertical asymptotes, α equals a zero of the Laguerre polynomial of degree $n-1=5$. Since $\xi_k = x_{k,n-1}$, the intervals of "bad" α-values are located on the left of the asymptotes, i.e., in the intervals $[\zeta_k, \xi_k] = [\zeta_k, x_{k,n-1}]$ and all the "good" values are to the right of the asymptotes. On the right, we see the Hermite-Radau nodes for a fixed node $\alpha \in [-5, 5]$. All the values of α are "good" except the ones corresponding to the vertical asymptotes, i.e., the α's equal to one of the zeros of the Hermite polynomial of degree five. Indeed, the "bad" intervals are reduced to just these points because $\zeta_k = \xi_k = x_{k,n-1}$.

In the case of three or more prefixed points, the results look similar.

For example in Figure 6 we plotted the nodes of a Gauss-Legendre formulas with prescribed nodes. On the left we see the nodes of an 8-point formula with prescribed nodes in the endpoints -1 and 1 and a third one $\alpha \in [-1.5, 1.5]$. On the right, a 9-point formula is shown with four prescribed nodes: the two endpoints -1, 1, and the internal point 0.3. The fourth point ranges from -1.5 to 1.5.

Similar cases are plotted in Figure 7 but now for the Gauss-Chebyshev formulas of the first kind where two of the prefixed nodes are varying symmetrically in $[-1.5, 1.5]$ and the other one at -1 for the left plot or -1 and $+0.3$ for the right plot.

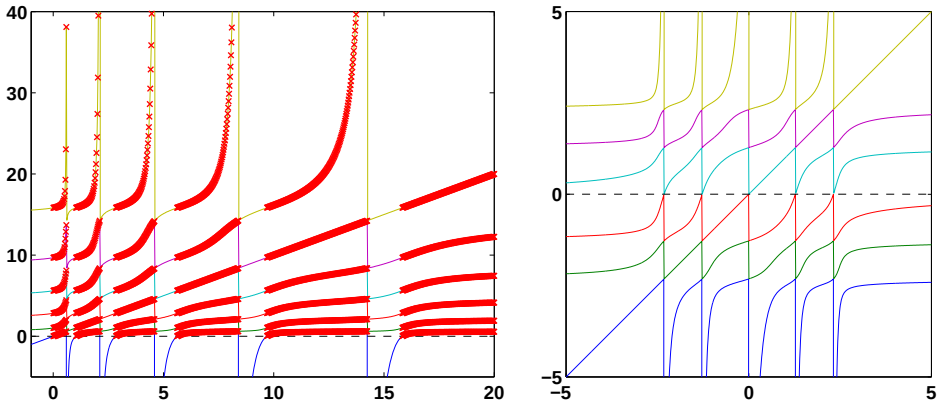

Fig. 5. On the left Laguerre$^{(1)}$-Radau formula with prescribed node ranging from -1 to 20. The good nodes are indicated with crosses. On the right Hermite-Radau formula with prescribed node form -5 to 5.

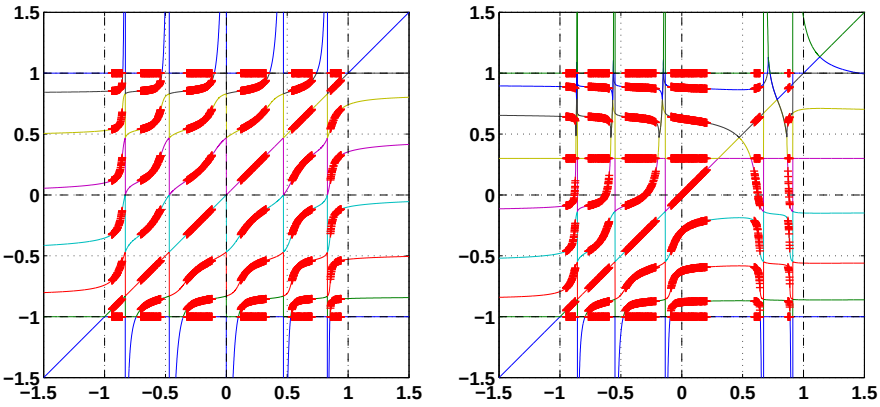

Fig. 6. On the left the nodes of the 8-point Gauss-Legendre formula with three prescribed nodes at the endpoints -1 en 1 and a third node $\alpha \in [-1.5, 1.5]$. The good nodes are again indicated with crosses. On the right a 9-point Gauss-Legendre formula with four prescribed nodes, three of them in the endpoints -1 and 1 and in 0.3, while a fourth ranges form -1.5 to 1.5.

5 Conclusions

Gauss-type quadrature formulas on an interval of the real line have been extensively considered in the literature. Here, none, one or two nodes are prescribed being endpoints of the interval of integration, the remainder nodes are chosen inside this interval in an optimal way and the weights are positive. Some considerations have been given in [19] for quadrature formulas with some nodes outside the interval of integration and highest degree of accuracy; here, the positiveness of the weights is not always guaranteed. When dealing with Szegő-type quadrature formulas on the unit circle, it is well known that one arbitrary

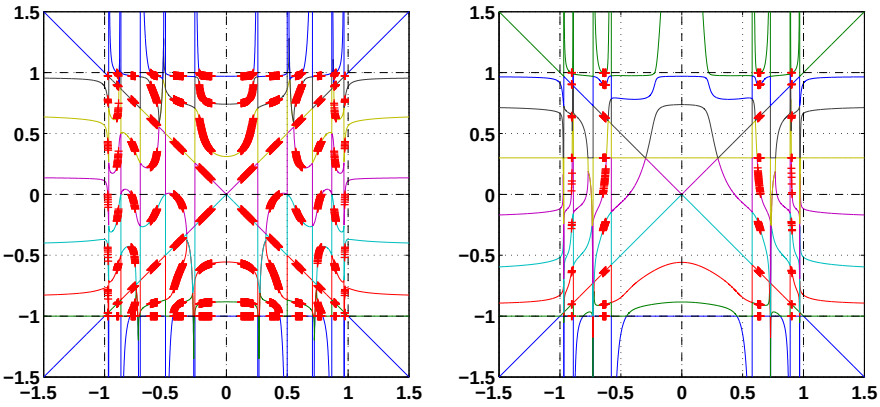

Fig. 7. On the left the nodes of the 8-point Gauss-Chebyshev formula with three prescribed nodes: one at the endpoint -1 and the other nodes are α and $-\alpha$ with $\alpha \in [-1.5, 1.5]$. On the right a 9-point Gauss-Chebyshev formula with four prescribed nodes, two of them in the endpoints -1 and 1 and the other ones are α and $-\alpha$ where α ranges form -1.5 to 1.5.

node on the unit circle can be generically fixed in a trivial way and recently it has been proved in [15] that also two distinct nodes anywhere on the unit circle can be prescribed without restrictions in the quadrature formula. So, Szegő-type quadrature formulas always exists and also have positive weights.

In the results presented in this paper, by using some properties stated in [1] on the location of the zeros of quasi-orthogonal polynomials we have characterized Gauss-type quadrature formulas with at most two prescribed nodes anywhere on the interval of integration, with positive weights and highest degree of accuracy. Such rules do not always exist. Quadrature formulas with one or both (finite) endpoints of the interval of integration fixed, and also one or two more nodes prescribed inside this interval are derived. Such quadratures also have positive weights have special interest as illustrated in [18], in the context of differential equations. In order to guarantee "good" quadrature formulas, i.e., positivity of the weights and nodes inside the interval of integration, in that paper, the degree of accuracy is one less than the maximal one. With the two endpoints prefixed, an n-point formula has maximal degree of accuracy $2n-3$. By imposing only a degree of accuracy that is $2n-4$, the quadrature formulas have one degree of freedom that can be chosen in an appropriate way (which corresponds to fixing a third, internal node). This approach (reducing the degree of accuracy to meet other requirements of the quadrature formula) is another track of investigation that will be faced in a subsequent paper. Concerning the computation of the quadrature formulas considered in the paper, an efficient procedure has been analyzed by considering an eigenvalue-finding problem for modified Jacobi matrices already used in [8] for the computation of the same rules but where the prescribed nodes are the endpoints of the interval of integration. Also an alternative approach based on a simpler linear algebra algorithm is given. We finally present sev-

eral numerical experiments of the introduced quadrature formulas and for the most known families of orthogonal polynomials on the real line.

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