Quadrature on the half line and two-point Padé approximants to Stieltjes functions. Part I: Algebraic aspects*

A. Bultheel† P. González-Vera‡ R. Orive‡

Abstract

Let $f(z)$ be a Stieltjes function with asymptotic expansions L_0 and L_∞ at $z = 0$ and $z = \infty$ respectively. Let $[k/n]$ denote the two-point Padé approximant of type (m, n) which matches k of the coefficients of the series L_0 and which takes its remaining interpolation conditions from L_∞. We discuss in this paper the algebraic aspects of this problem. We shall emphasize the relation between quadrature formulas and two-point Padé approximants and derive expressions for the error. In a subsequent paper we shall consider the convergence aspects of these approximants. For example, the positivity of the error, which is obtained here, will result in the monotonic convergence of certain sequences of two-point Padé approximants, a property which is well known in the case of classical Padé approximants.

Keywords: two-point Padé approximation, Stieltjes function, orthogonal Laurent polynomials, quadrature formula.
AMS Classification: 41A21, 30E05, 34E05, 41A55, 42C05.

1 Introduction

In this paper we are concerned with the approximation of Stieltjes functions. That are functions of the form

$$f(z) = \int_0^\infty \frac{d\alpha(x)}{1 - xz} \tag{1.1}$$

where α is a distribution function (non decreasing, bounded and with infinitely many points of increase). Suppose

$$I_n\{g\} = \sum_{j=1}^{n} A_j g(x_j)$$

is a quadrature formula which approximates the integral

$$I_\alpha\{g\} = \int_0^\infty g(x) d\alpha(x).$$

*This research was performed as part of the European project ROLLS under contract CHRX-CT93-0416.
†Department of Computer Science, K.U.Leuven, Belgium
‡Department Análisis Math., Univ. La Laguna, Tenerife, Spain

Then we get an approximant for $f(z)$ in (1.1) if we replace the integral by the quadrature. This approximant is a rational Stieltjes function of the form

$$f_n(z) = \sum_{j=1}^{n} \frac{A_j}{1 - x_j z} = \int_0^\infty \frac{d\alpha_n(x)}{1 - xz}.$$

If the quadrature is exact for all Laurent polynomials in $\Lambda_{-p,q} = \text{span}\{x^k, k = -p, \ldots, q\}$, then the moments

$$c_k = \int_0^\infty x^k d\alpha(x) \quad \text{and} \quad c_k^{(n)} = \int_0^\infty x^k d\alpha_n(x)$$

are the same for $k = -p, \ldots, q$. This means that $f_n(z)$ is a two-point Padé approximant (2PA) for $f(z)$ since it matches the appropriate number of the initial terms in the asymptotic expansions of $f(z)$ at 0 and at ∞.

In section 2, we shall recall the well known definition of two-point Padé approximants.

In section 3, we derive quadrature formulas in two different ways. In the Gaussian approach, the nodes are chosen as the zeros of orthogonal polynomials, leading to quadrature formulas with a maximum domain of validity. In the orthogonal approach, we take the nodes to be the zeros of the nth orthogonal Laurent polynomial from a sequence of nested spaces $\mathcal{R}_n = \Lambda_{-p(n),q(n)}$ with $p(n) + q(n) = n$. In general, this will not lead to a maximal domain of validity, except when

$$p(n) + p(n-1) = p(2n-1) \tag{1.2}$$

in which case we get the same formulas as with the Gaussian approach. This gives rise to new quadrature formulas which generalize several results from the literature.

Section 4 uses the technique explained before to generate 2PAs for Stieltjes functions. This approach is new. Moreover, we easily obtain expressions for the approximation error. For different choices of $p(n)$, we obtain rows, columns or diagonals in the table of 2PAs. Explicit expressions for these errors are particularly interesting because they reveal certain monotonicity properties of the 2PAs for Stieltjes functions. Such properties were known for some of these paths, but we are now able to recognize any possible monotonicity in a more general situation.

Some of the error formulas could be derived from a general Hermite formula which has been published before. However, such formula usually holds for measures with compact support. (Here α has a non-compact support $[0, \infty)$.) Moreover we need the explicit forms for the different situations considered to get the monotonicity properties. Therefore, deriving the error formulas from a known general formula would not be easy and we prefer our simple and direct approach.

A subsequent paper shall be devoted to more qualitative and quantitative convergence properties of these 2PAs.

2 Two-point Padé approximants

Two-point Padé approximants are a particular case of multipoint Padé approximants. They arise as a natural generalization of the classical (one-point) Padé approximants when the function to be approximated is known (in terms of coefficients of Taylor series or asymptotic expansions) around more than one point. When expansions around the origin and infinity are considered, 2PAs appear. They were first introduced in the context of different physical

problems [3] and of continued fractions [20, 24, 15]. To make the paper self-contained, we start from the definition of these approximants as given in [9] (compare with [20]) which is inspired essentially by [21, 23].

Given two formal power series

$$L_0 = \sum_{j=0}^{\infty} c_j z^j; \quad z \to 0; \quad L_\infty = \sum_{j=1}^{\infty} c^*_{-j} z^{-j}; \quad z \to \infty; \tag{2.1}$$

and two nonnegative integers k and n ($0 \le k \le 2n$), two polynomials $Q_{kn}(x)$ and $P_{kn}(x)$ of degrees n and $n-1$ respectively are to be found such that the following holds:

$$\begin{cases} L_0 Q_{kn}(z) - P_{kn}(z) = \alpha_k z^k + \alpha_{k+1} z^{k+1} + \cdots = O(z^k) \\ L_\infty Q_{kn}(z) - P_{kn}(z) = \alpha^*_{k-n-1} z^{k-n-1} + \alpha^*_{k-n-2} z^{k-n-2} + \cdots = O\Big((z^{-1})^{n-k+1}\Big) \end{cases} \tag{2.2}$$

Clearly, when Q_{kn} has exact degree n and $Q_{kn}(0) \neq 0$, then (2.2) implies

$$\begin{cases} L_0 - P_{kn}(z)/Q_{kn}(z) = O(z^k) \\ L_\infty - P_{kn}(z)/Q_{kn}(z) = \beta^*_{2n-k+1} z^{-(2n-k+1)} + \cdots = O((z^{-1})^{2n-k+1}) \end{cases} \tag{2.3}$$

The rational function P_{kn}/Q_{kn} satisfying (2.2) is said to be a $[k/n]$ 2PA to the pair (L_0, L_∞) in the weak sense, while if conditions (2.3) are satisfied, it is a 2PA in the strong sense. We denote it for both cases as $[k/n]_{(L_0,L_\infty)}$ and call it 2PA. Note that the approximants are always of type $(n-1, n)$ and that the parameter k denotes the number of coefficients that are matched in the series L_0.

We can define 2PAs for more general power series (see [8]). Let

$$L = \sum_{j=\nu}^{\infty} c_j z^j, \quad |z| \to 0; \qquad L^* = \sum_{j=-\infty}^{\mu} c^*_j z^j, \quad |z| \to \infty; \quad \nu, \mu \in \mathbb{Z}, \tag{2.4}$$

be two formal series. A 2PA $[k/n]_{(L,L^*)}$ for this pair will again be a rational function which matches k of the initial terms of L and takes its remaining conditions from the series L^*. The degree structure of the approximant however depends on the form of the series L and L^*. In fact, the 2PA for the pair (L, L^*) can be given via the 2PA for derived series L_l and L^*_l which have the standard form of L_0 and L_∞. For the series (L, L^*) as above, let k and n be nonnegative integers such that $\nu - \mu - 1 \le k \le 2n$. Set $r = \max\{0, -\nu\}$ and suppose l satisfies $\min\{\nu, \mu + 1\} \le l \le \mu + 1$. Then we can associate with the series (2.4), two series of standard type (2.1)

$$L_l = \sum_{j=0}^{\infty} (c_{j+l} - c^*_{j+l}) z^j, \quad |z| \to 0; \qquad L^*_l = \sum_{j=-\infty}^{-1} (c^*_{j+l} - c_{j+l}) z^j, \quad |z| \to \infty, \tag{2.5}$$

where $c^*_j = 0$ for $j > \mu$ and $c_j = 0$ for $j < \nu$. We define (see also [8, p. 259], [9, p. 443])

Definition 2.1 *Let $[k/n]_{(L_l,L^*_l)}$ be a 2PA for the standard series (L_l, L^*_l) of (2.5), then 2PAs for the series (2.4) are defined by*

$$F_{kn}(z) = [k + l + r/n + r]_{(L,L^*)}(z) = \sum_{j=\nu}^{l-1} c_j z^j + \sum_{j=l}^{\mu} c^*_j z^j + z^l [k/n]_{(L_l,L^*_l)}(z),$$

where $\sum_n^m = 0$ for $m < n$.

Thus the 2PA problem for series (2.4) reduces to the 2PA problem for series (2.1). Later on we shall be interested in the specific situation where $\mu = \nu = 0$. Taking $r = l = 0$, one gets $F_{kn}(z) = c_0^* + [k/n]_{(L_0, L_0^*)}(z)$ with $L_0 = (c_0 - c_0^*) + \sum_{j\geq 1} c_j z^j$ and $L_0^* = \sum_{j\geq 1} c_{-j}^* z^{-j}$.

Just like in the case of one-point approximants, we may fix (part of) the denominator and use the remaining coefficients as parameters to be determined by interpolation conditions. Such approximants were introduced by Brezinski [5] for the one-point case and coined Padé-type approximants. Draux [8] discusses two-point Padé-type approximants (2PTA) in the context of a noncommutative algebra. They are defined as follows: Let n and k be positive integers ($0 \leq k \leq n$) and $Q_{kn}(z)$ a given polynomial of degree n ($Q_{kn}(0) \neq 0$), then the rational function $P_{kn}(z)/Q_{kn}(z)$ with $P_{kn}(z)$ a polynomial is said to be a (k/n) 2PTA for the pair (L_0, L_∞) and denoted as $(k/n)_{(L_0, L_\infty)}$ if $P_{kn}(z)$ is of degree $n-1$ with coefficients deduced from (2.3) where $O\Big((z^{-1})^{2n-k+1}\Big)$ is replaced by $O\Big((z^{-1})^{n-k+1}\Big)$. For further details about 2PTA see [7, 10, 11, 13].

3 Laurent polynomials: Orthogonality and quadrature

Let α be a distribution function on $[0, \infty)$ such that the moments $c_k = \int_0^\infty x^k d\alpha(x)$ exist for $k \in \mathbb{Z}$. Our main concern in this section is to estimate the integral

$$I_\alpha\{f\} = \int_0^\infty f(x) d\alpha(x) \tag{3.1}$$

by a quadrature formula. In the next section, we shall use these to construct 2PAs (and 2PTAs) for the Stieltjes function $\int_0^\infty (1 - xz)^{-1} d\alpha(x)$. Moreover, we shall easily find expressions for the error, which is of course important to prove convergence of the approximants later on.

Let Λ denote the space of all Laurent (or L-) polynomials and let $\Lambda_{p,q}$ ($p \leq q$, both integers) be the subspace of all L-polynomials of the form $\sum_{j=p}^q a_j z^j$. For ordinary polynomials, we set $\Pi_n = \Lambda_{0,n}$ and Π is the space of all polynomials.

We consider n-point quadrature formulas for the integral (3.1) which are of the form

$$I_n\{f\} = \sum_{j=1}^n A_j f(x_j). \tag{3.2}$$

If the weights $\{A_j\}$ and nodes $\{x_j\}$ are chosen such that $I_\alpha\{f\} = I_n\{f\}$ for all $f \in \Lambda_{p,q}$, then we call $\Lambda_{p,q}$ a domain of validity. If $q - p = n - 1$, then $\Lambda_{p,q}$ has dimension n, so that given n distinct, nonzero nodes $\{x_j\}$, the n weights $\{A_j\}$ are uniquely defined to make $\Lambda_{p,q}$ a domain of validity for $I_n\{f\}$. If $R_{p,q} \in \Lambda_{p,q}$ interpolates f in the nodes $\{x_j\}$, thus

$$R_{p,q}(x) = \sum_{j=1}^n L_j^p(x) f(x_j), \quad L_j^p(x) = \frac{V_n^p(x)}{(x - x_j)(V_n^p)'(x_j)} \in \Lambda_{p,q}, \quad V_n^p(x) = x^p \prod_{j=1}^n (x - x_j),$$

then

$$\int_0^\infty R_{p,q}(x) d\alpha(x) = \sum_{j=1}^n \left[\int_0^\infty L_j^p(x) d\alpha(x)\right] f(x_j) = \sum_{j=1}^n A_j^p f(x_j) \tag{3.3}$$

is called an interpolatory quadrature formula in $\Lambda_{p,q}$. It is well known that the quadrature formula $I_n\{f\}$ has domain of validity $\Lambda_{p,q}$, $p \le q$, $q - p = n - 1$ if and only if it is of interpolatory type in $\Lambda_{p,q}$.

In the sequel, we consider a sequence of subspaces $\{\mathcal{R}_n\}$ with $\dim \mathcal{R}_n = n+1$, $n = 0, 1, \ldots$. Setting $\mathcal{R}_n = \Lambda_{-p(n),q(n)}$, with $p(n)$ and $q(n)$ nonnegative then, since $\dim \mathcal{R}_n = n + 1$, one obviously has $p(n) + q(n) = n$. We shall construct quadrature formulas whose domain of validity is some $\mathcal{R}_N$ with $N \ge n$. There are two strategies to do this: the Gaussian approach and the orthogonal approach.

Gaussian approach: In this case, we want to make N as large as possible. It turns out that $\mathcal{R}_{2n-1}$ is a maximal domain of validity. Indeed, define the distribution function $\tilde{\alpha}$ by $d\tilde{\alpha}(x) = x^{-p(2n-1)} d\alpha(x)$. Let $\tilde{Q}_n$ denote the n-th orthogonal polynomial for $d\tilde{\alpha}$ and let $x_1, \ldots, x_n$ be its zeros. These zeros are all simple and positive. It is also well known that then positive weights $\tilde{A}_j$ exist (the Christoffel numbers) so that $\int_0^\infty P(x) d\tilde{\alpha}(x) = \sum_{j=1}^n \tilde{A}_j P(x_j)$ for all $P \in \Pi_{2n-1}$ and this is the maximal domain of validity. Since any $F \in \mathcal{R}_{2n-1}$ can be written as $x^{-p(2n-1)} P(x)$ with $P \in \Pi_{2n-1}$, it follows easily that all $F \in \mathcal{R}_{2n-1}$ will be integrated exactly by a quadrature formula (3.2) if we set $A_j = x_j^{p(2n-1)} \tilde{A}_j > 0$, $1 \le j \le n$. Indeed,

$$\int_0^\infty F(x) d\alpha(x) = \int_0^\infty P(x) \frac{d\alpha(x)}{x^{p(2n-1)}} = \sum_{j=1}^n \tilde{A}_j P(x_j) = \sum_{j=1}^n A_j F(x_j) = I_n\{F\}.$$

We shall call this the n-th L-Gaussian formula for $d\alpha$, corresponding to the sequence $\{p(n)\}$ (or equivalently, corresponding to the sequence $\{\mathcal{R}_n\}$).

Orthogonal approach: Now we suppose that the spaces $\{\mathcal{R}_n\}$ are nested, i.e., $\mathcal{R}_{n-1} \subset \mathcal{R}_n$, which implies that $0 \le p(n) - p(n-1) \le 1$. In general, by the orthogonal approach, we do not get a maximal domain of validity. Normally, we only obtain $N = n$ but by a special choice for the nesting, we get much better results as we shall see. Consider the inner product $(f, g) = \int_0^\infty f(x) g(x) d\alpha(x)$ and construct by orthogonalization $L_n \in \mathcal{R}_n$ orthogonal to $\mathcal{R}_{n-1}$. If we set $L_n(x) = x^{-p(n)} Q_n(x)$ with $Q_n \in \Pi_n$, then with $d\hat{\alpha}(x) = x^{-p(n)-p(n-1)} d\alpha(x)$ and $-p(n-1) \le j \le q(n-1)$

$$0 = \int_0^\infty L_n(x) x^j d\alpha(x) = \int_0^\infty \frac{Q_n(x)}{x^{p(n)+p(n-1)}} x^{j+p(n-1)} d\alpha(x) = \int_0^\infty Q_n(x) x^J d\hat{\alpha}(x)$$

where $J = j + p(n-1)$. Since $p(n-1) + q(n-1) = n - 1$ we have $0 \le J \le n - 1$. In other words, Q_n is the n-th orthogonal polynomial w.r.t. $d\hat{\alpha}$, and thus has n simple positive zeros t_j. We can then find positive weights B_j such that $I_\alpha\{F\} = \sum_{j=1}^n B_j F(t_j)$ for all $F \in \mathcal{R}_n$. These B_j are given by $B_j = t_j^{p(n)+p(n-1)} \hat{B}_j > 0$, where $\hat{B}_j$ are the (positive) weights for the n-point Gaussian formula for the distribution $d\hat{\alpha}$. Indeed, the latter is exact in Π_{2n-1} and because $x^K \in \Pi_{2n-1}$ if $x^k \in \mathcal{R}_n$ when $K = k + p(n) + p(n-1)$ (recall $0 \le p(n) \le n$), we have

$$\int_0^\infty x^k d\alpha(x) = \int_0^\infty x^K d\hat{\alpha}(x) = \sum_{j=1}^n \hat{B}_j t_j^K = \sum_{j=1}^n B_j t_j^k.$$

In fact, this is valid for any k satisfying $-p(n) - p(n-1) \le k \le q(n) + q(n-1)$. Thus it follows immediately that if the sequence $\{p(n)\}$ satisfies

$$p(n) + p(n-1) = p(2n-1) \tag{3.4}$$

then the Gaussian and the orthogonal approach result in the same formula. For further discussion on this topic, especially about quadrature formulas based on more general Chebyshev systems of rational functions with prescribed poles, see [27] and the references cited there.

Note that in the polynomial situation, i.e. $\mathcal{R}_n = \Pi_n$, we orthogonalize the basis $\{1, x, x^2, \ldots\}$ and thus $p(n) = 0$ and $q(n) = n$ for all n, so that (3.4) is trivially satisfied. Also for $q(n) = 0$ and thus $p(n) = n$, we satisfy (3.4) and the orthogonal L-polynomials are orthogonal polynomials in the variable x^{-1} obtained by orthogonalization of the basis $\{1, x^{-1}, x^{-2}, \ldots\}$. This situation is of course the symmetric image of the usual polynomial situation. If we use $E[x]$ to denote the integer part of x, then setting $p(n) = E[\frac{n+1}{2}]$ also results in a sequence satisfying (3.4). In this case $\{\mathcal{R}_n\}$ is a sequence of L-polynomial spaces studied by Jones, Thron and Njåstad [16, 14]. Also, $p(n) = E[\frac{n}{2}]$ satisfies (3.4). The latter two choices correspond to the orthogonalization of the bases $\{1, x^{-1}, x, x^{-2}, \ldots\}$ or $\{1, x, x^{-1}, x^2, x^{-2}, \ldots\}$. See [4]. More generally, any sequence $p(n) = E[\frac{n+1}{L}]$ or $p(n) = E[\frac{n}{L}]$ with L a positive integer satisfies (3.4).

The following characterizes L-Gaussian formulas for a sequence $\{p(n)\}$ and generalizes a well known result for polynomials.

Theorem 3.1 *If the integer sequence $\{p(n)\}$ satisfies $0 \le p(n) \le n$ and (3.4), then $I_n\{f\}$ of (3.1) is the n-th L-Gaussian formula iff (a) $I_n\{f\}$ is exact in any n-dimensional subspace of $\mathcal{R}_{2n-1}$ and (b) $x_1, \ldots, x_n$ are the zeros of the n-th orthogonal L-polynomial Q_n for the nesting $\mathcal{R}_n$ (i.e. for the sequence $\{p(n)\}$).*

Proof. "$\Rightarrow$": (a) is trivial. For (b), set $\pi_n(x) = \prod_{j=1}^n (x - x_j)$ and $Q_n(x) = x^{-p(n)}\pi_n(x) \in \mathcal{R}_n$. For any $Q \in \mathcal{R}_{n-1}$ we have $QQ_n \in \mathcal{R}_{2n-1}$ and thus $(Q, Q_n) = \sum_{j=1}^n A_j Q(x_j) Q_n(x_j) = 0$, or $Q_n \perp \mathcal{R}_{n-1}$.
"$\Leftarrow$": Let Q_n be the n-th orthogonal L-polynomial, then we know that the quadrature formula with nodes in the n simple positive zeros of Q_n and with weights as in (3.3) with $p = -p(n-1)$ will be valid in $\mathcal{R}_n$. Since (3.4) is satisfied, the Gaussian and the orthogonal approach coincide and thus this formula will also be valid in the larger space $\mathcal{R}_{2n-1}$. To complete the proof we should show that these weights A_j^p of (3.3) obtained for $p = -p(n-1)$ are independent of this particular choice p. I.e. the n-dimensional subspace of $\mathcal{R}_{2n-1}$ we choose need not be $\mathcal{R}_{n-1}$ but can be any subspace $\Lambda_{p,q}$ with $q - p = n$. We use arguments similar to those used in [6, Theorem 6] for the unit circle. We use the notation A_j^p of (3.3) for general p and the short hand A_j for $A_j^{-p(n-1)}$. Then, with $\pi_n(x) = \prod_{j=1}^n (x - x_j)$,

$$\begin{aligned} A_j - A_j^p &= \frac{1}{\pi_n'(x_j)} \int_0^\infty \frac{\pi_n(x)}{x - x_j} \left[\frac{x_j^{p(n-1)}}{x^{p(n-1)}} - \frac{x_j^{-p}}{x^{-p}} \right] d\alpha(x) \\ &= \frac{1}{\pi_n'(x_j)} \int_0^\infty \pi_n(x) \left[\frac{x_j^{p(n-1)} x^{-p} - x_j^{-p} x^{p(n-1)}}{x - x_j} x^{p(n)+p} \right] d\hat{\alpha}(x) \end{aligned}$$

with $d\hat{\alpha}(x) = x^{-p(2n-1)} d\alpha(x)$. If $-p(n-1) \ge p$ then, we find between the brackets a polynomial from $\Pi_{p(n)-1} \subset \Pi_{n-1}$. If $-p(n-1) \le p$, then the brackets represent a polynomial from $\Pi_{p(2n-1)+p-1}$. This is also a subset of Π_{n-1} because it is easily checked that $p + p(2n-1) \le n$. Noting that $\pi_n(x)$ is the n-th monic orthogonal polynomial for $d\hat{\alpha}$, we find that the integral is zero and thus $A_j^p = A_j$, $1 \le j \le n$. □

Remark 1 A similar argument holds for a general sequence $\{p(n)\}$ if we replace (b) by (b') $x_1, \ldots, x_n$ are the zeros of the n-th orthogonal polynomial for the distribution $d\tilde{\alpha}(x) = x^{-p(n)-p(n-1)}d\alpha(x)$.

Remark 2 Taking $p = p(n)$ in (3.3), then it follows that the the L-polynomial $V_n(x)$ is equal to the n-th orthogonal L-polynomial $Q_n(x)$ (w.r.t. α and for indices $\{p(n)\}$).

To stress the positivity of the weights we formulate

Proposition 3.2 *For given $\{p(n)\}$, satisfying (3.4), set $\lambda_n = p(n) - p(n-1) \in \{0, 1\}$. Then*

$$A_j = \frac{1}{x_j^{\lambda_n}} \int_0^\infty x^{\lambda_n} S_j(x) d\alpha(x), \quad S_j(x) = \left[\frac{Q_n(x)}{(x - x_j)Q_n'(x_j)}\right]^2, \quad 1 \leq j \leq n \tag{3.5}$$

where Q_n is the n-th orthogonal L-polynomial for the sequence $\{p(n)\}$ w.r.t. α whose zeros are $x_1, \ldots, x_n$.

Proof. Since $Q_n \in \mathcal{R}_n$, it follows from (3.4) that $x^{\lambda_n} S_j(x) \in \mathcal{R}_{2n-1}$. Because the quadrature formula is exact in $\mathcal{R}_{2n-1}$ and because $S_j(x_i) = \delta_{ij}$, the expression for the weights follows. □

Remark 3 If we take the sequence $p(n) = E[\frac{n+1}{2}]$, then $\lambda_n = 0$ for n even and $\lambda_n = 1$ for n odd. We obtain the sequence of orthogonal L-polynomials studied in [16]. The previous proposition then gives a more complete representation of the weights for the corresponding L-Gaussian quadrature formula discussed in [14]. We get indeed

Corollary 3.3 *Let $\{Q_n(x)\}$ be the sequence of orthogonal L-polynomials for the sequence $\{p(n)\}$ with $p(n) = E[\frac{n+1}{2}]$. Then the nodes of the n-th L-Gaussian formula are the zeros of Q_n and the weights are given by*

$$A_j = x_j^{-\lambda_n} \int_0^\infty x^{\lambda_n} S_j(x) d\alpha(x), \quad S_j(x) = \left[\frac{Q_n(x)}{(x - x_j)Q_n'(x_j)}\right]^2$$

with $\lambda_n = 0$ for n even and $\lambda_n = 1$ for n odd.

For 2PAs on paths parallel to the "main horizontal" in the 2PA table (see Section 3), we need to consider the choice $p(2n-1) = n - M$ where $n \geq |M|$. In this case, (3.4) is not satisfied. However the next considerations show that the weights of the corresponding L-Gaussian quadrature can be derived from the weights for the choice $p'(n) = E[\frac{n+1}{2}]$, i.e. $p'(2n-1) = n$. Indeed, we know that the nodes of this formula, exact in $\mathcal{R}_{2n-1}$, are the zeros of $\pi_n^M \in \Pi_n$ which is orthogonal to Π_{n-1} w.r.t. the distribution $x^{-p(n-1)}d\alpha(x) = x^{-n}d\beta(x)$ with $d\beta(x) = x^M d\alpha(x)$. Set $q'(n) = n - p'(n)$, then $R_n^M(x) = x^{-p'(n)}\pi_n^M(x) \in \Lambda_{-p'(n),q'(n)} = \mathcal{R}_n'$, and $R_n^M \perp \mathcal{R}_{n-1}'$ since the $p'(n)$ satisfy (3.4). Let x_j be the zeros of R_n^M (or π_n^M) and A_j^M the weights of the L-Gaussian formula valid in $\mathcal{R}_{2n-1}' = \Lambda_{-n,n-1}$ w.r.t. the distribution $d\beta(x)$, then

$$\int_0^\infty F(x) d\beta(x) = \sum_{j=1}^n A_j^M F(x_j), \quad \forall F \in \mathcal{R}_{2n-1}'.$$

Substituting in this formula $G(x) = x^M F(x) \in \mathcal{R}_{2n-1}$, it then follows that x_j are the nodes and $A_j = x_j^{-M} A_j^M$ are the weights for the n-th L-Gaussian formula exact in $\mathcal{R}_{2n-1}$. Thus

Corollary 3.4 *If $p'(n) = E[\frac{n+1}{2}]$ and $p(2n-1) = n - M$, and if $\{R_n^M\}$ is the sequence of orthogonal L-polynomials for $\{p'(n)\}$ w.r.t. the distribution $d\beta(x) = x^M d\alpha(x)$, then the n-th L-Gaussian formula for the sequence $\{p(n)\}$ and w.r.t. α has nodes which are the zeros of R_n^M and the weights are given by*

$$A_j = x_j^{-M-\lambda_n} \int_0^\infty \left[\frac{R_n^M(x)}{(x-x_j)(R_n^M)'(x_j)} \right]^2 x^{M+\lambda_n} d\alpha(x), \tag{3.6}$$

with $\lambda_n = 0$ for n even and $\lambda_n = 1$ for n odd.

To end this section on quadrature, we want to generalize the well known expression for the weights in the polynomial case: $A_j = 1/\sum_{i=0}^{n-1}[P_i(x_j)]^2$ if P_i are the orthonormal polynomials.

We first take the simple case $p(n) = K$. The x_j are the zeros of P_n^K which is the n-th orthonormal polynomial w.r.t. $d\hat{\alpha}(x) = x^{-K} d\alpha(x)$. Hence, by our previous results, the weights are given by $A_j = x_j^K / \sum_{i=0}^{n-1}[P_i^K(x_j)]^2$.

Next we consider the case $p(n) = E[\frac{n+1}{2}]$. Let $R_i(x)$ be the orthonormal sequence for these indices. Suppose u_{2i}, u_{2i+1} and v_{2i}, v_{2i+1} are defined through

$$R_{2i}(x) = v_{2i}x^{-i} + \cdots + u_{2i}x^i, \quad R_{2i+1}(x) = v_{2i+1}x^{-i-1} + \cdots + u_{2i+1}x^i, \quad u_{2i}, u_{2i+1} > 0.$$

Then the following Christoffel-Darboux formula holds [22] where $d(n) = (-1)^n$

$$\sum_{i=0}^{n} R_i(x)R_i(y) = \frac{d(n)v_n}{u_{n+1}} \left[(xy)^{1/2} \frac{(x/y)^{d(n)} R_{n+1}(x)R_n(y) - (y/x)^{d(n)} R_n(x)R_{n+1}(y)}{x-y} \right].$$

Set $x = x_j$ and suppose that n is even, then

$$\sum_{i=0}^{n-1} R_i(x_j)R_i(y) = -\frac{v_n}{u_{n+1}} \frac{x_j R_{n+1}(x_j)R_n(y)}{y - x_j}. \tag{3.7}$$

Since $\int_0^\infty R_k^2(x)d\alpha(x) = 1$, we get

$$1 = -\frac{v_n}{u_{n+1}} x_j R_{n+1}(x_j) \int_0^\infty \frac{R_n(x)}{x - x_j} d\alpha(x).$$

Thus

$$A_j = \frac{1}{R_n'(x_j)} \int_0^\infty \frac{R_n(x)d\alpha(x)}{x - x_j} = -\frac{u_{n+1}}{v_n} \frac{1}{x_j R_{n+1}(x_j) R_n'(x_j)}.$$

Comparing this with (3.7) where we let tend y to x_j, we have proved the following theorem for n even. For n odd, similar arguments hold.

Theorem 3.5 *Let R_n be the n-th orthonormal L-polynomials for sequence $\{p(n) = E[\frac{n+1}{2}]\}$ w.r.t. $d\alpha$ with zeros $x_1, \ldots, x_n$. Define the Christoffel function $C_n(x) = 1/\sum_{i=0}^{n} R_i^2(x)$. Then the weights of the n-th L-Gaussian formula are given by $A_j = C_n(x_j)$, $j = 1, \ldots, n$.*

By Theorem 3.5 and Corollary 3.4, we get

Corollary 3.6 *Let R_n^M be the n-th orthonormal L-polynomial for the sequence $\{p(n) = E[\frac{n+1}{2}] - M\}$ w.r.t. $d\beta(x) = x^M d\alpha(x)$. Define the Christoffel function $C_n(x) = 1/\sum_{i=0}^{n}[R_i^M(x)]^2$. Then the weights of the n-th L-Gaussian formula are given by $A_j = x_j^{-M} C_n(x_j)$.*

4 Stieltjes functions and 2PA

For a given distribution function α on $[0,\infty)$, a Stieltjes function f and its moments c_k are defined as

$$f(z) = \int_0^\infty \frac{d\alpha(x)}{1-xz}, \qquad c_k = \int_0^\infty x^k d\alpha(x), \quad k \in \mathbb{Z}. \tag{4.1}$$

In the literature, one can find alternative definitions for Stieltjes (or Markov) functions like

$$\int_0^\infty \frac{d\alpha(x)}{1+xz}, \quad z\int_0^\infty \frac{d\alpha(x)}{z+x}, \quad \int_0^\infty \frac{d\alpha(x)}{z+x}, \quad \int_0^\infty \frac{d\alpha(x)}{z-x}.$$

See [1] for a survey. The last one has been used by Russian mathematicians. It is the Cauchy transform of the distribution α. We assume that the moments exist for all $k \in \mathbb{Z}$. It is well known that the Stieltjes function (4.1) is holomorphic in the cut plane $\mathbb{C} - \mathbb{R}_+$ ($\mathbb{R}_+ = \{z \in \mathbb{R} : z \geq 0\}$) and that the series

$$L_0 = \sum_{k=0}^{\infty} c_k z^k, \qquad L_\infty = -\sum_{k=1}^{\infty} c_{-k} z^{-k} \tag{4.2}$$

are asymptotic expansions of $f(z)$ respectively at $z = 0$ and $z = \infty$ w.r.t. the sectors $R_\gamma = \{z \in \mathbb{C} : |\mathrm{Arg} z| > \gamma\}$, $0 < \gamma < \pi$. See e.g. [17]. The purpose of this section is to construct 2PAs for the pair (4.2), i.e., for the Stieltjes function $f(z)$, using the results about L-Gaussian formulas.

From (4.2), it is clear that, in order to mimic the asymptotic behavior of f at ∞, we must consider approximants of type $(n-1,n)$. However, Tokarzewski et al. [25, 26] has recently considered a Stieltjes function for which the distribution α had the form

$$\alpha(x) = 0.02H(x) + \frac{1}{\ln 1000}\begin{cases} 0, & 0 \leq x \leq 1 \\ x-1, & 1 < x < 1000 \\ 999, & x \geq 1000 \end{cases}$$

$H(x)$ is the Heaviside (step) function at $x = 0$. This arises in the computation of the effective transport coefficients of heterogeneous materials. Obviously, the asymptotic expansions for f are now of the form (2.4) with $\mu = \nu = 0$ and 2PAs of type (n,n) should be used. But as mentioned in Section 1, this reduces basically to the study of 2PAs for the pair (4.2), so that the latter will be our main concern. It is worth mentioning that the physical example of Tokarzewski is related to the so called Markov type meromorphic functions studied by Gonchar and López (see [18] and the references there). In our terminology, such functions can be written as $F(z) = r(z) + \int_0^\infty (1-xz)^{-1} d\alpha(x)$ where $r(z)$ is a rational function of type (n,n) whose poles belong to $\mathbb{C} - \mathbb{R}_+$. Setting

$$r(z) = A_0 + \sum_{j=1}^{n} \frac{A_j}{1-x_j z},$$

where $x_j \notin \mathbb{R}_+$ turns F into a Markov type meromorphic function. If the $x_j \in \mathbb{R}_+$, then we get an ordinary Stieltjes function since $F(z)$ can be expressed as $F(z) = \int_0^\infty (1-xz)^{-1} d\beta(x)$ with $\beta(x) = \alpha(x) + \sum_{j=0}^{n} A_j \delta_{x_j}(x)$ where $x_0 = 0$.

For simplicity of notation, we shall denote the 2PAs for the series (4.2) for f as $[k/n]$ or $[k/n]_f$ but drop the indication of the two series. This notation is also used for ordinary Padé

approximants, but confusion is not likely in this paper. We shall arrange the 2PAs for the series (4.2) in a triangular array (the 2PA table)

$$\begin{array}{ccccc} & & & [0/3] & \cdots \\ & & [0/2] & [1/3] & \cdots \\ & [0/1] & [1/2] & [2/3] & \cdots \\ [0/0] & [1/1] & [2/2] & [3/3] & \cdots \\ & [2/1] & [3/2] & [4/3] & \cdots \\ & & [4/2] & [5/3] & \cdots \\ & & & [6/3] & \cdots \end{array}$$

The sequence $[n/n], n = 0, 1, \ldots$ is called the main row. Parallel to these you find the 2PAs $[n + k/n], n \geq |k|$ on the k-th row. In part two of this paper, we shall consider for k fixed and $n \to \infty$, the convergence of $[n + k/n]$ (along row) and of $[k/n]$ and $[2n - k/n]$ (along diagonals).

To link the quadrature formulas of Section 2 with the 2PAs of Section 1, we observe

Lemma 4.1 *Consider the quadrature formula $I_n\{f\} = \sum_{j=1}^{n} A_j f(x_j)$ with distinct nonzero nodes $x = x_j$, valid in $\Delta_{-p,q}$ $(p, q \geq 0)$. Then $f_n(z) = I_n\{(1 - xz)^{-1}\}$ represents a rational function of type $(n - 1, n)$ with poles x_j^{-1}, $j = 1, \ldots, n$ and such that*

$$L_0(z) - f_n(z) = O(z^{q+1}), \qquad L_\infty(z) - f_n(z) = O\Big((z^{-1})^{p+1}\Big) \tag{4.3}$$

Remark 4 (a) If $p + q = n - 1$, then $f_n(z)$ represents a 2PTA for the pair (L_0, L_∞) or equivalently for the Stieltjes function f. I.e., $f_n = (q + 1/n)_{(L_0, L_\infty)} = (q + 1/n)_f$.
(b) If $p + q = 2n - 1$, then f_n is a 2PA for the pair (L_0, L_∞), or equivalently, for the Stieltjes function f, thus $f_n = [q + 1/n]_f$.

Let us consider a sequence $\{p(n)\}$ of nonnegative integers with $0 \leq p(n) \leq n$ and $0 \leq p(n) - p(n - 1) \leq 1$. Let $I_n\{f\} = \sum_{j=1}^{n} A_j f(x_j)$ be the corresponding L-Gaussian quadrature formula. Then it immediately follows that

$$f_n(z) = [q(2n - 1) + 1/n]_f(z) = \sum_{j=1}^{n} \frac{A_j}{1 - x_j z},$$

where $A_j > 0$ and x_j are the (simple positive) zeros of the n-th orthogonal polynomial w.r.t. $d\hat{\alpha}(x) = x^{-p(n)-p(n-1)} d\alpha(x)$. When $\{p(n)\}$ satisfies (3.4), then the poles x_j^{-1} of the approximant $f_n(z)$ are the inverses of the zeros of the n-th orthogonal L-polynomial $Q_n(x)$ corresponding to $\{\mathcal{R}_n\}$. In the rest of this section we shall derive expressions for the error $E_n(z) = f(z) - f_n(z)$. As said in the introduction, this could probably be found from general formulas in the literature, but we prefer a direct approach, which seems quite natural at this point of the paper.

Lemma 4.2 *Let $R_n^p(x) \in \Delta_{-p,q}$ $(p + q = n - 1)$ be the L-polynomial interpolating the function $g(x, z) = (1 - xz)^{-1}$ at the n distinct nonzero nodes x_j, then (with $q + 1 = k$ and thus $p = n - k$)*

$$R_n^p(x) = \frac{1}{1 - xz}\left[1 - \frac{x^{-p}\pi_n(x)}{z^p \pi_n(z^{-1})}\right], \quad \pi_n(x) = \prod_{j=1}^{n}(x - x_j). \tag{4.4}$$

From Remark 4(a) and (4.4), we get

Corollary 4.3 *Let $(k/n)_f(z) = Q_{n-1}(z)/P_n(z)$ be a 2PTA for f. Suppose $P_n(z) = \prod_{j=1}^n (1 - x_j z)$ with all x_j distinct positive numbers. Then the approximation error is given by*

$$f(z) - (k/n)_f(z) = \frac{1}{z^{n-k}\pi_n(1/z)} \int_0^\infty \frac{x^{-(n-k)}\pi_n(x)}{1 - xz} d\alpha(x) \tag{4.5}$$

where $\pi_n(z) = \prod_{j=1}^n (z - x_j) = z^n P_n(1/z)$.

Taking $n - k = p(n)$ in (4.5), then by Theorem 3.1

$$E_n(z) = f(z) - [q(2n-1) + 1/n]_f(z) = \frac{1}{z^{p(n)}\pi_n(1/z)} \int_0^\infty \frac{x^{-p(n)}\pi_n(x)}{1 - xz} d\alpha(x) \tag{4.6}$$

with $\pi_n(z) = \prod_{j=1}^n (z - x_j)$ and x_j the zeros of the n-th orthogonal L-polynomial in $\mathcal{R}_n$. When the sequence $\{p(n)\}$ satisfies (3.4), then $R_n(z) = \rho_n x^{-p(n)}\pi_n(x) \in \mathcal{R}_n$ (ρ_n is a normalizing factor) is the n-th orthonormal L-polynomial and (4.6) reads

$$E_n(z) = \frac{1}{R_n(1/z)} \int_0^\infty \frac{R_n(x) d\alpha(x)}{1 - xz}, \tag{4.7}$$

hence

$$f_n(z) = \frac{1}{z R_n(1/z)} \int_0^\infty \frac{R_n(1/z) - R_n(x)}{1/z - x} d\alpha(x).$$

Setting $f_n(z) = S_n(z)/\tilde{\pi}_n(z)$ with $\tilde{\pi}_n(z) = \rho_n z^n \pi_n(1/z)$, it follows from the previous integral representation for f_n that the following expression for the numerator can be obtained

$$S_n(z) = z^{q(n)-1} T_n(1/z) \quad \text{with} \quad T_n(z) = \int_0^\infty \frac{R_n(z) - R_n(x)}{z - x} d\alpha(x). \tag{4.8}$$

Observe that by definition $T_n \in \Delta_{-p(n),q(n)-1}$ and therefore $S_n(z) \in \Pi_{n-1}$.

As for the error, we have the following

Theorem 4.4 *Let $\{p(n)\}$ be a sequence of nonnegative integers satisfying (3.4). Define $\lambda_n = p(n) - p(n-1)$. Then for $f_n = [q(2n-1) + 1/n]_f$*

$$E_n(z) = f(z) - f_n(z) = \frac{z^{\lambda_n}}{R_n^2(1/z)} \int_0^\infty \frac{x^{\lambda_n} R_n^2(x) d\alpha(x)}{1 - xz} \tag{4.9}$$

where R_n is the n-th orthonormal L-polynomial for $\{p(n)\}$.
Note that $(-1)^{\lambda_n} E_n(z) > 0$ for $z \in \mathbb{R}_- = \{z \in \mathbb{R} : z < 0\}$.

Proof. Assume $R_n(x) = \gamma_n x^{-p(n)} + \cdots + \gamma_n' x^{q(n)} \in \Delta_{-p(n),q(n)}$ and set

$$S(x) = \frac{R_n(x) - R_n(1/z)}{1 - xz} \in \Delta_{-p(n),q(n)-1} = \Delta_{-p(n-1)-\lambda_n, q(n-1)-\lambda_n}.$$

If $\lambda_n = 0$, then $S(x) \in \mathcal{R}_{n-1}$. Thus $\int_0^\infty S(x) R_n(x) d\alpha(x) = 0$, and thus by (4.7)

$$E_n(z) = \frac{1}{R_n^2(1/z)} \int_0^\infty \frac{R_n^2(x)}{1 - xz} d\alpha(x). \tag{4.10}$$

If $\lambda_n = 1$ then we set $S(x) = \gamma_n x^{-p(n)} + T(x)$ with $T \in \Delta_{-p(n-1),q(n-1)-1} \subset \mathcal{R}_{n-1}$. Hence $\int_0^\infty S(x)R_n(x)d\alpha(x) = \int_0^\infty \gamma_n x^{-p(n)} R_n(x)d\alpha(x) = \int_0^\infty R_n^2(x)d\alpha(x) = 1$. The latter gives together with (4.7) the expression

$$E_n(z) = \frac{1}{R_n^2(1/z)}\left[\int_0^\infty \frac{R_n^2(x)d\alpha(x)}{1-xz} - 1\right] = \frac{z}{R_n^2(1/z)}\int_0^\infty \frac{xR_n^2(x)}{1-xz}d\alpha(x). \tag{4.11}$$

This proves the theorem. □

Remark 5 When we choose $p(n) = E[\frac{n}{2}]$, we see that $f_n = [n/n]_f$ and thus is Theorem 2.1 in [12, p. 99] a special case of the previous theorem. When choosing $p(n) = E[\frac{n+1}{2}]$, we find the error for the 2PAs $[n-1/n]_f$. Below, we shall consider the more general row sequence $[n+M/n]_f$.

First we consider the diagonal sequence $[2n-k/n]_f$, k fixed. Thus we match exactly k coefficients of L_∞, $p(n) = k$ for all $n \geq k$ and $q(2n-1)+1 = 2n-k$. From Theorem 3.1 and (4.6) with $p(n) = k$,

$$E_n(x) = f(z) - [2n-k/n]_f(z) = \frac{1}{z^k\pi_n(1/z)}\int_0^\infty \frac{x^{-k}\pi_n(x)}{1-xz}d\alpha(x) \tag{4.12}$$

where $\pi_n(z) = \rho_n \prod_{j=1}^n (z-x_j)$ is the n-th orthonormal polynomial with respect to $x^{-k}d\alpha(x)$. If on the other hand, we choose $p = 0$ in Theorem 3.1, we shall get the same quadrature formula, hence the same 2PA and thus also the same error, which is now

$$E_n(x) = \frac{1}{\pi_n(1/z)}\int_0^\infty \frac{\pi_n(x)}{1-xz}d\alpha(x). \tag{4.13}$$

Hence

$$\int_0^\infty \frac{\pi_n(x)}{1-xz}d\alpha(x) = \frac{1}{z^k}\int_0^\infty \frac{x^{-k}\pi_n(x)}{1-xz}d\alpha(x). \tag{4.14}$$

Now we define

$$S(x) = \frac{x^{-k}\pi_n(x) - z^k\pi_n(1/z)}{1-xz} = \frac{\pi_n(x) - (xz)^k\pi_n(1/z)}{1-xz}\frac{1}{x^k} = \frac{T(x)}{x^k}, \quad T \in \Pi_{n-1}.$$

Since $\int \pi_n^2(x)x^{-k}d\alpha(x) = 1$, we have $\int_0^\infty S(x)\pi_n(x)d\alpha(x) = \int_0^\infty T(x)\pi_n(x)x^{-k}d\alpha(x) = 0$. Therefore, using (4.14),

$$\int_0^\infty \frac{x^{-k}\pi_n^2(x)}{1-xz}d\alpha(x) = z^k\pi_n(1/z)\int_0^\infty \frac{\pi_n(x)}{1-xz}d\alpha(x) = \pi_n(1/z)\int_0^\infty \frac{x^{-k}\pi_n(x)}{1-xz}d\alpha(x). \tag{4.15}$$

By (4.12) and (4.15) we conclude

$$E_n(z) = f(z) - [2n-k/n]_f(z) = \frac{1}{z^k\pi_n^2(1/z)}\int_0^\infty \frac{\pi_n^2(x)d\alpha(x)}{(1-xz)x^k}, \quad n \geq k. \tag{4.16}$$

Of course similar results can be obtained for the upward sloping diagonal sequence $[k/n]_f$ with k fixed. This basically corresponds to replacing k by $2n-k$ in the previous formulas.

Now, let us also consider the row sequence of 2PAs $f_n = [n+M/n]_f$ for $n \geq |M|$, $M \in \mathbb{Z}$. In this case $q(2n-1) = n+M-1$ and $p(2n-1) = n-M$, or equivalently, with $p'(n) = E[\frac{n+1}{2}]$, $p(n) = p'(n) - M$. Using $p = p(n)$ in Theorem 3.1 we get

$$E_n(z) = f(z) - [n+M/n]_f(z) = \frac{1}{z^{p(n)}\pi_n(1/z)}\int_0^\infty \frac{x^{-p(n)}\pi_n(x)}{1-xz}d\alpha(x),$$

π_n being the n-th orthonormal polynomial w.r.t. $x^{M-n}d\alpha(x) = x^{-p(2n-1)}d\tilde{\alpha}(x)$ where $d\tilde{\alpha}(x) = x^M d\alpha(x)$. We have

$$E_n(z) = \frac{z^M}{z^{p'(n)}\pi_n(1/z)} \int_0^\infty \frac{x^{-p'(n)}\pi_n(x)d\tilde{\alpha}(x)}{1-xz}.$$

By Theorem 4.4, we thus have

$$E_n(z) = [n + M/n]_f(z) = \frac{z^{M+\lambda_n}}{[R_n^M(1/z)]^2} \int_0^\infty \frac{[R_n^M(x)]^2}{1-xz} x^{M+\lambda_n} d\alpha(x) \tag{4.17}$$

with $\lambda_n = 0$ for n even and $\lambda_n = 1$ for n odd, while $\{R_n^M\}$ is the sequence of orthonormal L-polynomials for the sequence $p'(n) = E[\frac{n+1}{2}]$ w.r.t. the distribution $d\tilde{\alpha}(x) = x^M d\alpha(x)$.

After we have specified the result of Theorem 4.4 to the case of a diagonal and a row sequence in formulas (4.16) and (4.17) respectively, we return for a moment to the general case and establish an ordering in the successive approximants $f_n = [q(2n-1) + 1/n]_f$.

Theorem 4.5 *Let f_n be a sequence of 2PAs for a Stieltjes function f, such that the interpolation data for f_n are contained in the interpolation data for f_{n+1} (the spaces $\mathcal{R}_n$ are nested). Let $E_n(z) = f(z) - f_n(z)$ be the approximation error. Then for $z \in \mathbb{R}_-$: $E_n(z) - E_{n+1}(z)$ has the same sign as $E_n(z)$ and $|E_n(z)|$ is monotonically decreasing with n.*

Proof. First note that f_n is by construction a (rational) Stieltjes function. Since the moments of f defining f_n are equal to the corresponding moments of f_{n+1}, because the interpolation conditions are nested, it follows that f_n is not only a 2PA for f, but also a 2PA for f_{n+1}. Thus, for $z \in \mathbb{R}_-$, the sign of $E_n(z) = f(z) - f_n(z)$ will be the same as the sign of $f_{n+1}(z) - f_n(z)$. Because $f_{n+1} - f_n = E_n - E_{n+1}$, the first statement follows. If E_n and E_{n+1} have the same sign, then also the conclusion about $|E_n|$ follows. If E_n and E_{n+1} have opposite sign (e.g. $E_n > 0$ and $E_{n+1} < 0$), then note that $|E_n| - |E_{n+1}| = E_n + E_{n+1} = 2(f - f_n) + (f_n - f_{n+1})$, which is positive because both terms are. □

Remark 6 The nesting of the spaces $\mathcal{R}_n$ actually means a special case of a Newton-Padé table of interpolation data.

Remark 7 The previous theorem says that if for $z \in \mathbb{R}_-$, the errors of the subsequent 2PAs keep their sign (like on diagonals), then the approximants approach f monotonically; if the errors alternate in sign (like on rows), then two successive approximants enclose f and the magniture of the error is monotonically decreasing with n. In column sequences, the errors alternate in sign, but since the interpolation conditions are not nested (they are shifted from L_0 to L_∞), the magnitude of the error is not monotonically decreasing.

For diagonal sequences we have by (4.16) and the previous theorem

Corollary 4.6 *If $z \in \mathbb{R}_-$ then for $n > k$*

$$\begin{aligned} f(z) &< [2n + 2 - k/n + 1]_f(z) < [2n - k/n]_f(z) \qquad \textit{for } k \textit{ even} \\ f(z) &> [2n + 2 - k/n + 1]_f(z) > [2n - k/n]_f(z) \qquad \textit{for } k \textit{ odd.} \end{aligned}$$

Similarly, for the row sequences, we derive from (4.17)

Corollary 4.7 *If $z \in \mathbb{R}_-$ then for $n > |M|$ and $n + M$ even*

$$[n+1+M/n+1]_f(z) > f(z) > [n+2+M/n+2]_f(z) > [n+M/n]_f(z)$$

while for $n + M$ odd

$$[n+1+M/n+1]_f(z) < f(z) < [n+2+M/n+2]_f(z) < [n+M/n]_f(z).$$

Remark 8 When in Corollary 4.6 we set $k = 0$, the 2PAs $[2n/n]_f$ are ordinary Padé approximants of type $(n-1, n)$ for the series L_0, since none of the moments with a negative index are used. Thus we obtain that Padé approximants of type $(n-1, n)$ for a Stieltjes function are monotonically decreasing with n. Of course, one can derive similar results for diagonal paths of 2PAs of the form $[k/n]_f$, in which case setting $k = 0$ would result is a sequence of one-point Padé approximants for L_∞. The monotonic convergence of these approximants is a classical result [2].

Remark 9 Theorem 2.3 given in [12, p. 100] is a special case of Corollary 4.7, obtained when we take $M = 0$.

In view of our restriction $p, q \geq 0$, the one-point Padé approximants appeared rather accidentally. One-point approximants would require p or q to be -1 as can be seen from (4.3). However, by considering the Stieltjes function

$$F(z) = \frac{f(z) - c_0}{z} = \int_0^\infty \frac{x d\alpha(x)}{1 - xz},$$

we see that one-point Padé approximants for f at 0 and of type (n, n) can be obtained as $c_0 + z[2n/n]_F(z)$. The extra factor z explains why the $(n-1, n)$ approximants which were decreasing with n on $\mathbb{R}_-$ will transform in type (n, n) approximants that are increasing with n on $\mathbb{R}_-$.

If we want to consider 2PAs for Stieltjes functions with $c_0^* \neq 0$ in the expansions (2.4) where $\mu = \nu = 0$, then we make use of Definition 2.1 and get approximants of type (n, n) as $c_0^* + [k/n]_F$. Since here no extra factor z appears, the increasing/decreasing nature of the approximant for F is maintained.

5 Conclusion

We have shown how we can construct quadrature formulas which are exact for certain subspaces of Laurent polynomials. Expressions for the weights, generalizing known results for the polynomial situation are given.

It was then shown how these rules give rise to two-point Padé approximants for Stieltjes functions. Expressions for the approximation error were derived. Especially the monotonicity in diagonal and row sequences of the approximants was proved.

In a sequel to this paper, we shall give quantitative and qualitative results about the (monotone) convergence of these 2PAs. Related results are obtained in [19].

References

[1] E. Alden. A survey of weak and strong moment problems with generalizations. Technical report, Dept. Math. Umeå, 1985.

[2] G.A. Baker Jr. *Essentials of Padé Approximants.* Academic Press, New York, 1975.

[3] G.A. Baker Jr., G.S. Rushbrooke, and H.E. Gilbert. High-temperature series expansions for the spin $-1/2$ Heisenberg model by the method of the irreducible representation of the symmetric group. *Phys. Rev.*, 135(5A):1272–1277, 1964.

[4] C.M. Bonan-Hamada, W.B. Jones, W.J. Thron, and A. Magnus. Para-orthogonal Laurent polynomials and associated sequences of rational functions. *Numer. Algorithms*, 3:67–74, 1992.

[5] C. Brezinski. *Padé-type approximants and general orthogonal polynomials*, volume 50 of *Internat. Ser. of Numer. Math.* Birkhäuser Verlag, Basel, 1980.

[6] A. Bultheel, P. González-Vera, E. Hendriksen, and O. Njåstad. Orthogonal rational functions and quadrature on the unit circle. *Numer. Algorithms*, 3:105–116, 1992.

[7] L. Casasús and P. González-Vera. Two-point Padé-type approximants for Stieltjes functions. In C. Brezinski, A. Draux, A.P. Magnus, P. Maroni, and A. Ronveaux, editors, *Proc. Polynômes Orthogoneaux et Applications, Bar-le-Duc, 1984*, volume 1171 of *Lecture Notes in Math.*, pages 408–418. Springer, 1985.

[8] A. Draux. Approximation de type-Padé en deux points. Technical Report ANO-110, Université des Sciences et Techniques de Lille, Lab. d'analyse numérique et d'optimisation, 1983.

[9] A. Draux. *Polynômes orthogonaux formels – applications*, volume 974 of *Lecture Notes in Math.* Springer, Berlin, 1983.

[10] P. González-Vera. On certain applications of the two-point Padé-type approximants with a single pole. *J. Comput. Appl. Math.*, 19:151–160, 1987.

[11] P. González-Vera and M. Jiménez Paiz. Two-point partial Padé approximants. *Appl. Num. Math.*, 11:385–402, 1993.

[12] P. González-Vera and O. Njåstad. Convergence of two-point Padé approximants to series of Stieltjes. *J. Comput. Appl. Math.*, 32:97–105, 1990.

[13] P. González-Vera and R. Orive. Optimization of two-point Padé-type approximants. *J. Comput. Appl. Math.*, 50:325–337, 1994.

[14] W.B. Jones, O. Njåstad, and W.J. Thron. Two-point Padé expansions for a family of analytic functions. *J. Comput. Appl. Math.*, 9:105–124, 1983.

[15] W.B. Jones and W.J. Thron. Two-point Padé tables and T-fractions. *Bull. Amer. Math. Soc.*, 83:388–390, 1977.

[16] W.B. Jones and W.J. Thron. Orthogonal Laurent polynomials and Gaussian quadrature. In K. Gustafson et al., editors, *Quantum mechanics in mathematics, chemistry and physics*, pages 449–455, New York, 1984. Plenum.

[17] W.B. Jones, W.J. Thron, and H. Waadeland. A strong Stieltjes moment problem. *Trans. Amer. Math. Soc.*, 206:503–528, 1980.

[18] G. López-Lagomasino. Survey of multipoint Padé approximation to Markov type meromorphic functions and asymptotic properties of orthogonal polynomials. In C. Brezinski et al., editors, *Polynômes Orthogonaux et Applications*, volume 1171 of *Lecture Notes in Math.*, pages 309–316. Springer, 1985.

[19] G. López-Lagomasino and A.M. Finkelshtein. Rate of convergence of two-point Padé approximants and logarithmic asymptotics of Laurent-type orthogonal polynomials. *Constr. Approx.*, 10, 1995. To appear.

[20] A. Magnus. On the structure of the two-point Padé table. In *Analytic theory of continued fractions*, volume 932 of *Lecture Notes in Math.*, pages 362–372, Berlin, 1982. Springer.

[21] J.H. McCabe. A formal extension of the Padé table to include two-point Padé quotients. *J. Inst. Math. Appl.*, 15:363–372, 1975.

[22] O. Njåstad and W.J. Thron. The theory of sequences of orthogonal L-polynomials. In H. Waadeland and H. Wallin, editors, *Padé Approximants and Continued Fractions*, Det Kongelige Norske Videnskabers Selskab Skrifter, pages 54–91, 1983.

[23] A. Sidi. Some aspects of the two-point Padé approximants. *J. Comput. Appl. Math.*, 6:9–17, 1980.

[24] W.J. Thron. Some properties of continued fractions. *Bull. Amer. Math. Soc.*, 54:206–218, 1948.

[25] S. Tokarzewski. Two-point Padé approximants to Laurent expansions of Stieltjes functions. Preprint, Inst. Fund. Technological Research, Warsaw, 1994.

[26] S. Tokarzewski, J. Bławzdziewicz, and I. Adrianov. Two-point Padé approximants for formal Stieltjes series. *Numer. Algorithms*, 8:313–328, 1994.

[27] W. Van Assche and I. Vanherwegen. Quadrature formulas based on rational interpolation. *Math. Comp.*, 16:765–783, 1993.