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OPTIMAL AVERAGED PADÉ-TYPE APPROXIMANTS*

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Abstract. Padé-type approximants are rational functions that approximate a given formal power series. Boutry [Numer. Algorithms, 33 (2003), pp 113–122] constructed Padé-type approximants that correspond to the averaged Gauss quadrature rules introduced by Laurie [Math. Comp., 65 (1996), pp. 739–747]. More recently, Spalević [Math. Comp., 76 (2007), pp. 1483–1492] proposed optimal averaged Gauss quadrature rules, that have higher degree of precision than the corresponding averaged Gauss rules, with the same number of nodes. This paper defines Padé-type approximants associated with optimal averaged Gauss rules. Numerical examples illustrate their performance.

Key words. Gauss quadrature, averaged Gauss quadrature, optimal averaged Gauss quadrature, Padé-type approximant

AMS subject classifications. 65D30, 65D32

1. Introduction.

Consider a formal power series

$$f(t) = \sum_{i=0}^{\infty} c_i t^i \tag{1.1}$$

with real coefficients. If the series diverges for some $t \in \mathbb{C}$, then $f(t)$ represents the corresponding analytic continuation, which is assumed to exist. The power series (1.1) is associated with the linear functional $\mathfrak{c}$, whose moments are the coefficients c_i, i.e.,

$$\mathfrak{c}(x^i) = c_i \quad \text{for} \quad i = 0, 1, \dots,$$

where we for notational simplicity assume that $c_0 = 1$. The functional $\mathfrak{c}$ is defined on polynomials and extended by continuity to all power series in the variable x with a positive radius of convergence. Then,

$$f(t) = c_0 + c_1 t + c_2 t^2 + \cdots = \mathfrak{c}(1 + xt + x^2 t^2 + \cdots) = \mathfrak{c}\Big(\frac{1}{1 - xt}\Big);$$

see Brezinski [2] for details.

For an arbitrary polynomial $P(x)$ of degree n, we define

$$\widetilde{P}(x) = x^n P(x^{-1}) \quad \text{and} \quad P^*(t) = \mathfrak{c}\Big(\frac{P(x) - P(t)}{x - t}\Big). \tag{1.2}$$

The polynomial P^* is of degree $n-1$ and is said to be *pseudo-associated* to the polynomial P. We will write $\widetilde{P}^*$ for the polynomial $(P^*)\widetilde{\ }$, which is in general not the same as $(\widetilde{P})^*$. We have

$$\begin{aligned} \frac{\widetilde{P}^*(t)}{\widetilde{P}(t)} &= \frac{P^*(t^{-1})}{tP(t^{-1})} = \mathfrak{c}\Big(\frac{1 - P(x)/P(t^{-1})}{1 - xt}\Big) = f(t) - \frac{1}{P(t^{-1})}\mathfrak{c}\Big(\frac{P(x)}{1 - xt}\Big) \\ &= f(t) - \frac{t^n}{\widetilde{P}(t)} \sum_{i=0}^{\infty} \mathfrak{c}(x^i P(x)) t^i = f(t) + o(t^{n-1}), \end{aligned} \tag{1.3}$$

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as $t \to 0$. Thus, $f(t)$ can be approximated accurately by the rational function $\widetilde{P}^*(t)/\widetilde{P}(t)$ when t is close to zero.

The quotient $\widetilde{P}^*/\widetilde{P}$ is called a *Padé-type approximant of f generated by the polynomial* P, and its poles are the reciprocals of the zeros of P; see Brezinski [2]. The Maclaurin expansion of this approximant matches that of $f(t)$ at least up to the t^{n-1}-term. As can be seen from (1.3), a match of further terms, say up to the t^{n+k-1}-term, can be achieved if

$$\mathfrak{c}(x^i P(x)) = 0 \quad \text{for} \quad i = 0, 1, \dots, k-1,$$

i.e., if $P(x)$ is *orthogonal* with respect to $\mathfrak{c}$ to all polynomials of degree less than k.

A sequence of monic polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is said to be a *formal orthogonal polynomial sequence* with respect to a linear functional $\mathfrak{c}$ if

- $\mathfrak{c}(P_n(x)P_k(x)) = 0$ for $k \neq n$,
- $\mathfrak{c}(P_n(x)^2) \neq 0$ for all n.

Necessary and sufficient conditions for the existence of a sequence of monic orthogonal polynomials with respect to the linear functional $\mathfrak{c}$ are that the *Hankel determinants* are nonvanishing:

$$\Delta_n = \begin{vmatrix} c_0 & c_1 & \cdots & c_{n-1} \\ c_1 & c_2 & \cdots & c_n \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1} & c_n & \cdots & c_{2n-2} \end{vmatrix} \neq 0 \quad \text{for} \quad n = 1, 2, \dots,$$

where $c_i = \mathfrak{c}(x^i)$ are the moments of the functional $\mathfrak{c}$; see Brezinski [2] or Chihara [5] for details. In this case the functional $\mathfrak{c}$ is said to be *quasi-definite*. Then, the monic orthogonal polynomials $P_k(x)$ satisfy a three-term recurrence relation of the form

$$P_{k+1}(x) = (x - \alpha_k)P_k(x) - \beta_k P_{k-1}(x) \quad \text{for} \quad k = 0, 1, \dots, \tag{1.4}$$

with $P_{-1}(x) \equiv 0$ and $P_0(x) \equiv 1$. We will henceforth assume the functional $\mathfrak{c}$ to be quasi-definite.

It is possible to define Gauss-type quadrature rules with respect to this functional; see [2, 5, 8, 14, 17, 18] for discussions. However, the orthogonal polynomials may have zeros of multiplicity larger than one; see [2, p. 57] for an illustration. We will assume, for simplicity, that the zeros of the required orthogonal polynomials P_k are simple. This is the generic situation. Then, the n-node Gauss quadrature rule associated with the functional $\mathfrak{c}$ can be expressed as

$$\mathcal{G}_n(g) = \sum_{k=1}^{n} g(t_k^{(n)})\omega_k^{(n)}, \tag{1.5}$$

and satisfies $\mathcal{G}_n(x^i) = c_i$, for $i = 0, 1, \dots, 2n-1$; see [2, 5, 8, 14, 17, 18].

In the special case when the functional $\mathfrak{c}$ is *positive definite*, i.e., when

$$\mathfrak{c}(P_n(x)^2) > 0 \quad \text{for all} \quad n = 0, 1, 2, \dots,$$

there is a nonnegative measure $\mathrm{d}\omega$ with infinitely many points of support such that

$$c_i = \int t^i \mathrm{d}\omega(t), \qquad i = 0, 1, 2, \dots;$$

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see, e.g., [2, p. 42]. The n-node Gauss rule (1.5) is then a quadrature rule for approximating the integral

$$\mathcal{I}(g) = \int g(t)\,\mathrm{d}\omega(t),$$

for suitable integrands g. In particular, $\mathcal{G}_n$ has degree of precision $2n-1$, i.e., $\mathcal{G}_n(p) = \mathcal{I}(p)$ for all polynomials p of degree at most $2n-1$; see, e.g., [5, 14, 17] for properties of orthogonal polynomials associated with a quasi-definite functional $\mathfrak{c}$.

Since $\mathfrak{c}$ is assumed to be quasi-definite, we have $\mathfrak{c}(x^i P(x)) = 0$, for $i = 0, 1, \ldots, n-1$, if and only if P is the n-th orthogonal polynomial P_n with respect to $\mathfrak{c}$. By (1.3), this choice of P yields a Padé-type approximant which agrees with the Maclaurin expansion of f at least up to the t^{2n-1}-term (inclusive). This approximant, called a *Padé approximant* of f, is precisely the n-node Gauss quadrature rule associated with the functional $\mathfrak{c}$, i.e.,

$$R_n[f](t) = \mathcal{G}_n\Big(\frac{1}{1-xt}\Big) = \frac{t}{P_n(t^{-1})} \cdot \mathfrak{c}\left(\frac{P_n(t^{-1}) - P_n(x)}{1-xt}\right) = \frac{\widetilde{P}_n^*(t)}{\widetilde{P}_n(t)}, \tag{1.6}$$

with the same notation as in (1.2). We refer the reader to Brezinski and Van Iseghem [3], as well as to Gragg [12], for discussions on Padé approximants. By (1.3), the remainder term can be written as

$$f(t) - R_n[f](t) = \frac{1}{P_n(t^{-1})}\mathfrak{c}\Big(\frac{P_n(x)}{1-xt}\Big) = o(t^{2n-1}).$$

It is important to be able to estimate the quadrature error $\mathcal{I}(g) - \mathcal{G}_n(g)$ for a given integrand. When the measure $\mathrm{d}\omega$ is nonnegative and has infinitely many points of support on the real axis, a classical method for estimating this error is to evaluate the $(2n+1)$-node Gauss-Kronrod rule $\mathcal{K}_{2n+1}$ associated with the Gauss rule (1.5) and estimate the quadrature error by $\mathcal{K}_{2n+1}(g) - \mathcal{G}_n(g)$. However, the rule $\mathcal{K}_{2n+1}$ is not guaranteed to exist for every measure $\mathrm{d}\omega$ and number of nodes n; see Notaris [16] for a fairly recent discussion on Gauss-Kronrod quadrature.

This shortcoming of Gauss-Kronrod rules led Laurie [13] to introduce anti-Gauss rules and averaged Gauss rules for nonnegative real measures $\mathrm{d}\omega$. These rules also exist when Gauss-Kronrod rules do not, and they can be used to estimate the quadrature error. Subsequently, Ehrich [9] defined *optimal averaged rules* for Gauss-Laguerre and Gauss-Hermite measures. Spalević [22] derived a new representation of these rules and introduced optimal averaged rules for more general nonnegative real measures. For properties and applications of optimal averaged Gauss rules associated with nonnegative real measures; see [6, 7, 15, 20, 23] and references therein.

Anti-Gauss, averaged Gauss, and optimal averaged Gauss rules can be defined for quasi-definite functionals $\mathfrak{c}$; see [4, 21]. These references define these quadrature rules by using recursion coefficients of two sets of biorthogonal polynomials. Here we will define these rules with the recursion coefficients (1.4).

Boutry [1] introduced Padé-type approximants determined by averaged Gauss quadrature rules associated with the quasi-definite functional $\mathfrak{c}$. It is the purpose of the present paper to define Padé-type approximants that are determined by optimal averaged Gauss rules associated with $\mathfrak{c}$.

This paper is organized as follows. Section 2 is concerned with averaged and optimal averaged Gauss rules associated with the quasi-definite functional $\mathfrak{c}$, and Section 3 discusses

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orthogonal polynomials related to the generalized averaged Gauss rule. The main results are in Section 4, where optimal averaged Padé-type approximants are introduced and proved to correspond to optimal averaged Gauss rules. A few computed examples are presented in Section 5. Section 6 contains concluding remarks.

2. Averaged and optimal averaged Gauss rules. This section describes averaged and optimal averaged Gauss rules associated with a quasi-definite functional $\mathfrak{c}$. We start with the former and first note that the recursion coefficients β_k in (1.4) are real and nonzero.

The n-node Gauss quadrature rule (1.5) with respect to $\mathfrak{c}$ can be represented as

$$\mathcal{G}_n(g) = e_1^T g(J_n) e_1, \tag{2.1}$$

where J_n is the symmetric $n \times n$ tridiagonal matrix

$$J_n = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{n-2}} & \alpha_{n-2} & \sqrt{\beta_{n-1}} \\ \mathbf{0} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}$$

determined by recursion coefficients (1.4) for the polynomials P_k; see [17]. Here $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n$ stands for the first axis vector, and the superscript ^{T} denotes transposition. The Gauss quadrature rule (2.1) has degree of precision $2n-1$; see [5].

The $(n+1)$-node *anti-Gauss* rule $\breve{\mathcal{G}}_{n+1}$ associated with the quasi-definite functional $\mathfrak{c}$ is determined by the requirement

$$(\breve{\mathcal{G}}_{n+1} - \mathfrak{c})(x^k) = -(\mathcal{G}_n - \mathfrak{c})(x^k), \qquad k = 0, 1, \ldots, 2n+1.$$

It can be represented as

$$\breve{\mathcal{G}}_{n+1}(g) = e_1^T g(\breve{J}_{n+1}) e_1,$$

where $\breve{J}_{n+1}$ is the $(n+1) \times (n+1)$ tridiagonal matrix obtained from J_{n+1} by replacing the two occurrences of $\sqrt{\beta_n}$ by $\sqrt{2\beta_n}$. Then, the averaged Gauss rule associated with the n-node Gauss rule (2.1) for the functional $\mathfrak{c}$ is defined as

$$\mathcal{G}^L_{2n+1}(g) = \frac{1}{2}\big(\mathcal{G}_n(g) + \breve{\mathcal{G}}_{n+1}(g)\big).$$

It has degree of precision at least $2n+1$; see [4, 13] for related results.

The *optimal averaged Gauss rule* for the functional $\mathfrak{c}$ associated with the n-node Gauss rule (2.1) can be written as

$$\mathcal{G}^S_{2n+1}(g) = e_1^T g(J^S_{2n+1}) e_1, \tag{2.2}$$

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where J^S_{2n+1} is the (possibly complex) symmetric matrix

$$J^S_{2n+1} = \left[\begin{array}{cccccc:cccc}
\alpha_0 & \sqrt{\beta_1} & & & & & & & & \\
\sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & & & & & \\
 & \ddots & \ddots & \ddots & & & & & & \\
 & & \sqrt{\beta_{n-2}} & \alpha_{n-2} & \sqrt{\beta_{n-1}} & & & & & \\
 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} & \sqrt{\beta_n} & & & & \\
 & & & & \sqrt{\beta_n} & \alpha_n & \sqrt{\beta_{n+1}} & & & \\
\hdashline
 & & & & & \sqrt{\beta_{n+1}} & \alpha_{n-1} & \sqrt{\beta_{n-1}} & & \\
 & & & & & & \ddots & \ddots & \ddots & \\
 & & & & & & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\
 & & & & & & & & \sqrt{\beta_1} & \alpha_0
\end{array}\right]. \tag{2.3}$$

3. Some properties of polynomials related to generalized averaged Gaussian rules. Let n be fixed and let $\mathcal{G}_n$ denote the n-node Gauss rule with respect to a linear functional $\mathfrak{c}$. For an arbitrary constant $\theta \neq -1$, we introduce the functional $\acute{\mathfrak{c}}$ as

$$\acute{\mathfrak{c}} = \mathfrak{c} + \theta\big(\mathfrak{c} - \mathcal{G}_n\big)$$

and define a quadrature rule $\acute{\mathcal{G}}_{n+1}$ as the Gauss rule with respect to the functional $\acute{\mathfrak{c}}$. The $n+1$ nodes of the rule $\acute{\mathcal{G}}_{n+1}$ are the zeros of the $(n+1)$-th orthogonal polynomial $\acute{P}_{n+1}$ with respect to $\acute{\mathfrak{c}}$. A *generalized averaged quadrature rule* $\mathcal{G}^{\theta}_{2n+1}$ is then defined as

$$\mathcal{G}^{\theta}_{2n+1}(g) = \frac{\theta \cdot \mathcal{G}_n(g) + \acute{\mathcal{G}}_{n+1}(g)}{\theta + 1}. \tag{3.1}$$

It is shown in [19] that, under the assumption that the functional $\mathfrak{c}$ is positive definite, the choice

$$\theta = \frac{\beta_{n+1}}{\beta_n}$$

yields a quadrature rule (3.1) of highest possible algebraic degree of precision, which in this case is $2n+2$. For this particular choice of θ, when $\mathfrak{c}$ is positive definite, the quadrature rule (3.1) coincides with the optimal averaged quadrature rule $\mathcal{G}^S_{2n+1}$ from (2.2). In this case,

$$\mathcal{G}^S_{2n+1}(g) = \frac{\beta_{n+1}\mathcal{G}_n(g) + \beta_n\acute{\mathcal{G}}_{n+1}(g)}{\beta_n + \beta_{n+1}}, \tag{3.2}$$

and the $n+1$ nodes of the rule $\acute{\mathcal{G}}_{n+1}$ are the zeros of the polynomial

$$Q_{n+1} = P_{n+1} - \beta_{n+1}P_{n-1}. \tag{3.3}$$

More generally, since $\acute{\mathfrak{c}}(P) = \mathfrak{c}(P)$ for all polynomials P of degree up to $2n-1$, the monic orthogonal polynomials $\acute{P}_k$ with respect to $\acute{\mathfrak{c}}$ coincide with the monic orthogonal polynomials P_k with respect to $\mathfrak{c}$ for $k \leqslant n$. In fact,

$$\acute{P}_k = P_k \ \text{ for } \ k = 0, 1, \ldots, n, \quad \text{and} \quad \acute{P}_{n+1} = P_{n+1} - \theta\beta_n P_{n-1}.$$

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Thus the polynomials $\acute{P}_k$ satisfy $\acute{P}_{-1}(x) \equiv 0$, $\acute{P}_0(x) \equiv 1$, and

$$\acute{P}_{k+1}(x) = (x - \acute{\alpha}_k)\acute{P}_k(x) - \acute{\beta}_k \acute{P}_{k-1}(x) \quad \text{for} \quad k = 0, 1, 2, \ldots,$$

where $\acute{\alpha}_k = \alpha_k$ for $k = 0, 1, \ldots, n$, $\acute{\beta}_k = \beta_k$ for $k = 0, 1, \ldots, n-1$, and

$$\acute{\beta}_n = (\theta + 1)\beta_n.$$

Recalling that $\alpha_k = \acute{\mathfrak{c}}(x\acute{P}_k^2)/\acute{\mathfrak{c}}(\acute{P}_k^2)$ and $\acute{\beta}_k = \acute{\mathfrak{c}}(\acute{P}_k^2)/\acute{\mathfrak{c}}(\acute{P}_{k-1}^2)$, it is easy to derive the following properties of the functional $\mathfrak{c}$.

THEOREM 3.1. *We have* $\mathfrak{c}(x^k \acute{P}_{n+1}) = 0$ *for* $k = 0, 1, \ldots, n-2$. *Moreover,*

$$\begin{aligned} \mathfrak{c}(x^{n-1}\acute{P}_{n+1}) &= -\theta\beta_n \mathfrak{c}(P_{n-1}^2) = -\tfrac{\mathfrak{c}(P_{n+1}^2)}{\mathfrak{c}(P_n^2)}\mathfrak{c}(P_{n-1}^2), \\ \mathfrak{c}(x^{n}\acute{P}_{n+1}) &= -\theta\beta_n \mathfrak{c}(x^n P_{n-1}) = -\tfrac{\mathfrak{c}(P_{n+1}^2)}{\mathfrak{c}(P_n^2)}\mathfrak{c}(x^n P_{n-1}). \end{aligned}$$

3.1. Pseudo-associated polynomials. Since the polynomials $\acute{P}_k$ are orthogonal with respect to the functional $\acute{\mathfrak{c}}$, the pseudo-associated polynomials

$$\acute{P}^*_{k+1}(t) = \mathfrak{c}\left(\frac{\acute{P}_{k+1}(x) - \acute{P}_{k+1}(t)}{x - t}\right),$$

for $k \leqslant n$, satisfy the same recurrence relation as the polynomials $\acute{P}_k$, but with $\acute{P}^*_{-1}(x) \equiv -1$ and $\acute{P}^*_0(x) \equiv 0$.

THEOREM 3.2. *It holds that*

$$\acute{P}_n(x)\acute{P}^*_{n+1}(x) - \acute{P}^*_n(x)\acute{P}_{n+1}(x) = (\theta + 1)\beta_n \mathfrak{c}(\acute{P}^2_{n-1}).$$

Proof. From the recurrence relations $\acute{P}_k(x)\acute{P}^*_{k+1}(x) = (x - \acute{\alpha}_k)\acute{P}^*_k(x) - \acute{\beta}_k \acute{P}^*_{k-1}(x)$ and $\acute{P}_{k+1}(x) = (x - \alpha_k)\acute{P}_k(x) - \acute{\beta}_k \acute{P}_{k-1}(x)\acute{P}^*_k(x)$, it follows that

$$\acute{P}_k(x)\acute{P}^*_{k+1}(x) - \acute{P}^*_k(x)\acute{P}_{k+1}(x) = \acute{\beta}_k\big(\acute{P}_{k-1}(x)\acute{P}^*_k(x) - \acute{P}_k(x)\acute{P}^*_{k-1}(x)\big),$$

for $k = 0, 1, \ldots, n$. Multiplying the above equality over all k yields

$$\begin{aligned} \acute{P}_n(x)\acute{P}^*_{n+1}(x) - \acute{P}^*_n(x)\acute{P}_{n+1}(x) &= \acute{\beta}_n \cdot \acute{\beta}_{n-1} \cdots \acute{\beta}_1 \big(\acute{P}_0(x)\acute{P}^*_1(x) - \acute{P}^*_0(x)\acute{P}_1(x)\big) \\ &= (\theta + 1)\beta_n \cdot \frac{\acute{\mathfrak{c}}(\acute{P}^2_{n-1})}{\acute{\mathfrak{c}}(\acute{P}^2_{n-2})} \cdots \frac{\acute{\mathfrak{c}}(\acute{P}^2_1)}{\acute{\mathfrak{c}}(\acute{P}^2_0)} \cdot 1, \end{aligned}$$

which reduces to what we claimed. ∎

The following result is an immediate consequence of Theorem 3.2.

THEOREM 3.3. *If* $\mathfrak{c}$ *is positive definite, then for all* k

- $\acute{P}^*_k$ *and* $\acute{P}^*_{k+1}$ *have no common zeros,*
- $\acute{P}_k$ *and* $\acute{P}^*_k$ *have no common zeros.*

We recall a general fact about orthogonal polynomials that can be applied to the polynomials $\acute{P}^*_k$.

THEOREM 3.4. *If* $\mathfrak{c}$ *is positive definite and* $\theta > -1$, *then for all* k

- *the zeros of* $\acute{P}^*_k$ *are real and distinct,*
- *the zeros of* $\acute{P}^*_k$ *and the zeros of* $\acute{P}_k$ *interlace.*

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4. Optimal averaged Padé-type approximants. Boutry [1] introduced the anti-Gauss Padé-type approximants, which can be used to construct *averaged Padé-type approximants*. The latter are also discussed in [1]. The anti-Gauss approximants correspond to anti-Gauss quadrature rules.

A more general construction uses another approximant $\acute{R}_{n+1}$ of the form (1.3), where $P := Q$ is some polynomial of degree $n+1$, and considers a linear combination of the Padé approximant (1.6) and $\acute{R}_{n+1}$:

$$R^{\theta}_{2n+1}[f](t) = \frac{\theta \cdot R_n[f](t) + \acute{R}_{n+1}[f](t)}{\theta+1} = \frac{\theta}{\theta{+}1} \cdot \frac{\widetilde{P}^*_n(t)}{\widetilde{P}_n(t)} + \frac{1}{\theta{+}1} \cdot \frac{\widetilde{Q}^*(t)}{\widetilde{Q}(t)}. \tag{4.1}$$

where $\theta \neq -1$ is a constant.

Our main result shows that there is a unique Padé-type approximant of the form (4.1) that coincides with the power series of f up to the degree $2n+2$. The analogy with the representation (3.2) of the optimal averaged quadrature rule is obvious, so we will call this Padé-type approximant *optimal averaged* and denote it by R^S_{2n+1}.

THEOREM 4.1. *The approximant R^{θ}_{2n+1} given by (4.1) has degree of exactness at least $2n+2$ if and only if $Q = Q_{n+1}$ is given by (3.3) and $\theta = \frac{\beta_{n+1}}{\beta_n}$. Thus,*

$$R^S_{2n+1}[f](t) = \frac{\beta_{n+1} R_n[f](t) + \beta_n \acute{R}_{n+1}[f](t)}{\beta_n + \beta_{n+1}}, \quad \textit{where} \quad \acute{R}_{n+1}[f](t) = \frac{\widetilde{Q}^*_{n+1}(t)}{\widetilde{Q}_{n+1}(t)}, \tag{4.2}$$

and $R_n[f]$ is defined by (1.6). Here we use the same notation as in (1.2).

Proof. We start by noting that the coefficients β_n and β_{n+1} are nonzero by the quasi-definiteness of the functional $\mathfrak{c}$.

In order for the approximant (4.1) to have degree of exactness $2n+2$, the additional approximant $\acute{R}_{n+1}$ must have degree of exactness equal to that of R_n, which is $2n-1$. Moreover, we must have

$$\theta\big(f(t) - R_n\big) + \big(f(t) - \acute{R}_{n+1}\big) = o(t^{2n+2}), \tag{4.3}$$

where, for simplicity of notation, we abbreviate $R_n[f](t)$ and $\acute{R}_{n+1}[f](t)$ by R_n and $\acute{R}_{n+1}$, respectively. By (1.3), $\acute{R}_{n+1}$ has degree of exactness $2n-1$ if and only if Q is orthogonal to all polynomials of degree up to $n-2$. Therefore Q and $\widetilde{Q}$ have the form

$$Q(t) = (t+a)P_n(t) + bP_{n-1}(t) \quad \text{and} \quad \widetilde{Q}(t) = (1+at)\widetilde{P}_n(t) + bt^2\widetilde{P}_{n-1}(t). \tag{4.4}$$

We observe that $\widetilde{P}_n(t) = 1 + o(1)$ and $\widetilde{P}_{n-1}(t) = 1 + o(1)$ when $t \to 0$.

The equality (1.3) gives us expressions for the remainders as

$$\begin{aligned}
\widetilde{P}_n(t)\big(f(t) - R_n\big) &= \mathfrak{c}(x^n P_n)t^{2n} + \mathfrak{c}(x^{n+1}P_n)t^{2n+1} + \mathfrak{c}(x^{n+2}P_n)t^{2n+2} + o(t^{2n+2}),\\
\widetilde{Q}(t)\big(f(t) - \acute{R}_{n+1}\big) &= \mathfrak{c}(x^{n-1}Q)t^{2n} + \mathfrak{c}(x^n Q)t^{2n+1} + \mathfrak{c}(x^{n+1}Q)t^{2n+2} + o(t^{2n+2}),
\end{aligned}$$

when $t \to 0$. We can express all values of $\mathfrak{c}$ in the above equalities in terms of the three quantities

$$g_1 = \mathfrak{c}(x^n P_n), \quad g_2 = \mathfrak{c}(x^{n+1}P_n), \quad g_3 = \mathfrak{c}(x^{n+2}P_n).$$

In particular, we have $\beta_n\mathfrak{c}(x^{n-1}P_{n-1}) = g_1$, $\beta_n\mathfrak{c}(x^nP_{n-1}) = g_2 - \alpha_n g_1$, $\mathfrak{c}(x^{n+1}P_{n+1}) = \beta_{n+1}g_1$, and $\beta_n\mathfrak{c}(x^{n+1}P_{n-1}) = g_3 - \alpha_n g_2 - \beta_{n+1}g_1$, so that

$$\begin{aligned}
\beta_n\mathfrak{c}(x^{n-1}Q) &= (b+\beta_n)g_1,\\
\beta_n\mathfrak{c}(x^{n}Q) &= (b+\beta_n)g_2 + (a\beta_n - b\alpha_n)g_1,\\
\beta_n\mathfrak{c}(x^{n+1}Q) &= (b+\beta_n)g_3 + (a\beta_n - b\alpha_n)g_2 - b\beta_{n+1}g_1.
\end{aligned}$$

Therefore, the left-hand side of (4.3) multiplied by $\beta_n\widetilde{P}_n(t)\widetilde{Q}(t)$ becomes

$$\begin{aligned}
L &= \theta\beta_n\widetilde{Q}(t)\cdot\tilde{P}_n(t)(f(t)-R_n) + \beta_n\tilde{P}_n(t)\cdot\widetilde{Q}(t)(f(t)-\acute{R}_{n+1})\\
&= \theta\beta_n\big((1{+}at)\widetilde{P}_n(t) + bt^2\widetilde{P}_{n-1}(t)\big)(g_1t^{2n} + g_2t^{2n+1} + g_3t^{2n+2})\\
&\quad + \widetilde{P}_n(t)\big[(b{+}\beta_n)g_1t^{2n} + \big((b{+}\beta_n)g_2 + (a\beta_n{-}b\alpha_n)g_1\big)t^{2n+1}\\
&\qquad + \big((b{+}\beta_n)g_3 + (a\beta_n{-}b\alpha_n)g_2 - b\beta_{n+1}g_1\big)t^{2n+2}\big] + o(t^{2n+2})\\
&= \widetilde{P}_n(t)\big(Ag_1t^{2n} + (Ag_2{+}Bg_1)t^{2n+1} + (Ag_3{+}Bg_2{+}Cg_1)t^{2n+2}\big) + o(t^{2n+2}),
\end{aligned}$$

where

$$A = b{+}(\theta{+}1)\beta_n, \quad B = (\theta{+}1)a\beta_n{-}b\alpha_n, \quad C = b\big(\theta\beta_n\tfrac{\widetilde{P}_{n-1}(t)}{\widetilde{P}_n(t)}{-}\beta_{n+1}\big).$$

In order for the above expression to be $o(t^{2n+2})$ when $t \to 0$, the coefficients A, B, and C must all be zero, which implies that

$$b = -(\theta+1)\beta_n, \quad a = -\alpha_n, \quad \theta = \frac{\beta_{n+1}}{\beta_n}.$$

Now, $Q(x) = (x-\alpha_n)P_n(x) - (\beta_n+\beta_{n+1})P_{n-1}(x) = Q_{n+1}(x)$, which completes the proof. ∎

The optimal averaged Padé approximants can be related to Padé approximants as follows.

THEOREM 4.2. *The following equalities hold:*

$$\begin{aligned}
\acute{R}_{n+1}[f] &= R_{n+1}[f] + \beta_{n+1}t^2\tfrac{\widetilde{P}_{n-1}}{\widetilde{Q}_{n+1}}\left(R_{n+1}[f] - R_{n-1}[f]\right),\\
\acute{R}_{n+1}[f] &= R_{n-1}[f] + \tfrac{\widetilde{P}_{n+1}}{\widetilde{Q}_{n+1}}\left(R_{n+1}[f] - R_{n-1}[f]\right).
\end{aligned}$$

Proof. By Theorem 4.1 and equation (4.4), we have

$$\begin{aligned}
\acute{R}_{n+1} &= \frac{\widetilde{P}^*_{n+1} - \beta_{n+1}t^2\widetilde{P}^*_{n-1}}{\widetilde{P}_{n+1} - \beta_{n+1}t^2\widetilde{P}_{n-1}} = \frac{\widetilde{P}^*_{n+1}}{\widetilde{P}_{n+1}} + \frac{\beta_{n+1}t^2(\widetilde{P}_{n-1}\widetilde{P}^*_{n+1} - \widetilde{P}_{n+1}\widetilde{P}^*_{n-1})}{\widetilde{P}_{n+1}\widetilde{Q}_{n+1}}\\
&= R_{n+1} + \beta_{n+1}t^2\frac{\widetilde{P}_{n-1}}{\widetilde{Q}_{n+1}}\left(\frac{\widetilde{P}^*_{n+1}}{\widetilde{P}_{n+1}} - \frac{\widetilde{P}^*_{n-1}}{\widetilde{P}_{n-1}}\right) \qquad \text{and}\\
\acute{R}_{n+1} &= \frac{\widetilde{P}^*_{n-1}}{\widetilde{P}_{n-1}} + \frac{(\widetilde{P}_{n-1}\widetilde{P}^*_{n+1} - \widetilde{P}_{n+1}\widetilde{P}^*_{n-1})}{\widetilde{P}_{n-1}\widetilde{Q}_{n+1}} = R_{n-1} + \frac{\widetilde{P}_{n+1}}{\widetilde{Q}_{n+1}}\left(\frac{\widetilde{P}^*_{n+1}}{\widetilde{P}_{n+1}} - \frac{\widetilde{P}^*_{n-1}}{\widetilde{P}_{n-1}}\right),
\end{aligned}$$

as claimed. ∎

Finally, we prove that the optimal averaged Padé type approximant is in fact the optimal averaged quadrature rule (2.2) applied to the power series of f.

THEOREM 4.3. *The optimal averaged Padé approximant $R^S_{2n+1}[f]$ (4.2) can be represented as*

$$R^S_{2n+1}[f](t) = \mathcal{G}^S_{2n+1}\Big(\frac{1}{1-xt}\Big) = e_1^T\big(I - tJ^S_{2n+1}\big)^{-1}e_1,$$

where J^S_{2n+1} is given by (2.3).

Proof. Let $J = I - tJ^S_{2n+1}$. Then, $e_1^T J^{-1} e_1$ is the upper-left corner entry of the matrix J^{-1} and equals

$$e_1^T J^{-1} e_1 = \frac{J_{11}}{|J|},$$

where J_{11} denotes the $(1,1)$ minor of the matrix J.

We first compute $|J|$. The characteristic polynomial of the matrix J^S_{2n+1} is $|tI - J^S_{2n+1}| = P_n(t)Q_{n+1}(t)$, where Q_{n+1} is given by (3.3). This can be easily obtained, for example, by expanding $|J^S_{2n+1}|$ along the $(n+1)$-th row. Therefore

$$|J| = t^{2n+1}\big|t^{-1}I - J^S_{2n+1}\big| = \widetilde{P}_n(t)\widetilde{Q}_{n+1}(t).$$

Similarly, an expansion along the n-th row shows that the $(1,1)$ minor of $tI - J^S_{2n+1}$ equals

$$\begin{aligned}
&(t-\alpha_n)P_n(t)P_n^*(t) - \beta_n P_n(t)P^*_{n-1}(t) - \beta_{n+1}P_{n-1}(t)P_n^*(t)\\
&\qquad = \tfrac{\beta_{n+1}}{\beta_n+\beta_{n+1}}P_n^*(t)\big((t-\alpha_n)P_n(t) - (\beta_n+\beta_{n+1})P_{n-1}(t)\big)\\
&\qquad\qquad + \tfrac{\beta_n}{\beta_n+\beta_{n+1}}P_n(t)\big((t-\alpha_n)P_n^*(t) - (\beta_n+\beta_{n+1})P^*_{n-1}(t)\big)\\
&\qquad = \tfrac{\beta_{n+1}}{\beta_n+\beta_{n+1}}P_n^*(t)Q_{n+1}(t) + \tfrac{\beta_n}{\beta_n+\beta_{n+1}}P_n(t)Q^*_{n+1}(t).
\end{aligned}$$

Therefore $J_{11} = \frac{\beta_{n+1}}{\beta_n+\beta_{n+1}}\widetilde{P}_n^*(t)\widetilde{Q}_{n+1}(t) + \frac{\beta_n}{\beta_n+\beta_{n+1}}\widetilde{P}_n(t)\widetilde{Q}^*_{n+1}(t)$ and

$$\frac{J_{11}}{|J|} = \frac{\beta_{n+1}}{\beta_n+\beta_{n+1}}\cdot\frac{\widetilde{P}_n^*(t)}{\widetilde{P}_n(t)} + \frac{\beta_n}{\beta_n+\beta_{n+1}}\cdot\frac{\widetilde{Q}^*_{n+1}(t)}{\widetilde{Q}_{n+1}(t)} = R^S_{2n+1}[f](t),$$

as claimed. □

EXAMPLE 4.4. Consider the function $f(t) = e^t$. Its Padé approximant for $n = 3$ is

$$R_3(t) = \frac{1+\frac{2}{5}t+\frac{1}{20}t^2}{1-\frac{3}{5}t+\frac{3}{20}t^2-\frac{1}{60}t^3} = 1+t+\frac{t^2}{2!}+\frac{t^3}{3!}+\frac{t^4}{4!}+\frac{t^5}{5!}+\frac{11t^6}{7200}+o(t^6)$$

and the corresponding optimal averaged Padé-type approximant R^S_{2n+1} is

$$\begin{aligned}
R_7^S(t) &= \frac{25}{74}\Big(\frac{1+\frac{2}{5}t+\frac{1}{20}t^2}{1-\frac{3}{5}t+\frac{3}{20}t^2-\frac{1}{60}t^3}\Big) + \frac{49}{74}\Big(\frac{1+\frac{3}{7}t+\frac{15}{196}t^2+\frac{19}{2940}t^3}{1-\frac{4}{7}t+\frac{29}{196}t^2-\frac{11}{490}t^3+\frac{1}{490}t^4}\Big)\\
&= 1+t+\frac{t^2}{2!}+\frac{t^3}{3!}+\frac{t^4}{4!}+\frac{t^5}{5!}+\frac{t^6}{6!}+\frac{t^7}{7!}+\frac{t^8}{8!}+\frac{403t^9}{148176000}+o(t^9),
\end{aligned}$$

as $t\to 0$. This approximant agrees with the Maclaurin expansion of the function $f(t)$ up to the t^8-term, but not for the t^9-term. This shows that the degree of precision of the approximant R^S_{2n+1} in general is not larger than $2n+2$.

5. Numerical examples. This section illustrates the behavior of some Padé and Padé-type approximants. We determine these approximants from moments $c_0 = 1, c_1, c_2, \dots$. The evaluation of the approximants requires recursion coefficients $\alpha_0, \beta_1, \alpha_2, \beta_2, \dots$. We evaluate the necessary recursion coefficients with the aid of the Chebyshev algorithm. Gautschi [10, p. 77] presents the modified Chebyshev algorithm, of which the Chebyshev algorithm is a special case, for the case of a positive definite functional $\mathfrak{c}$. The Chebyshev algorithm may be sensitive to errors in the moments and to round-off errors introduced during the computations, and the sensitivity increases with the number of moments used; see [10, Section 2.1] for a discussion. It is therefore important to be able to compute accurate approximations of functions (1.1) by carrying out only a fairly small number of steps of the Chebyshev algorithm. The execution of a large number of steps typically requires the use of high-precision arithmetic, which we will avoid in the present paper.

Assume that the moments $c_0, c_1, \dots, c_{2n}$ are known. This allows us to compute the Padé approximant R_n, which requires the moments $c_0, c_1, \dots, c_{2n-1}$. The next Padé approximant R_{n+1} would require also c_{2n+1}, which is assumed not to be available. The evaluaton of the averaged Padé-type approximant R^L_{2n-1} requires the recursion coefficients $\alpha_0, \dots, \alpha_{n-1}$ and $\beta_1, \dots, \beta_{n-1}$, which can be determined from the moments $c_0, c_1, \dots, c_{2n}$ by the Chebyshev algorithm. The evaluation of the optimal averaged Padé-type approximant R^S_{2n-1} demands one more recursion coefficient, β_n, than the evaluation of R^L_{2n-1}. The (modified) Chebyshev algorithm, as presented in [10, p. 77], seemingly also requires the moment c_{2n+1}. However, this additional moment is needed to compute the recursion coefficient α_n, and not β_n. Therefore, with a slight modification of the algorithm, the moments $c_0, c_1, \dots, c_{2n}$ allow us to compute the Padé approximant R_n and the Padé-type approximants R^L_{2n-1} and R^S_{2n-1}.

This section presents a few numerical examples that illustrate the performance of the approximants R_n, R^L_{2n-1}, and R^S_{2n-1}. All computations have been carried out in MATLAB with about 15 significant decimal digits.

EXAMPLE 5.1. Figure 6.1 displays the errors when approximating the function $\Gamma(1+t)$ by the Padé approximant R_4 and the Padé-type approximants R^L_7 and R^S_7. The corresponding errors are presented in a semi-log plot, i.e., with a linear scale on the horizontal t-axis and a base-10 logarithmic scale on the vertical axis.

The figure shows the optimal averaged approximant $R^S_7(t)$ to give a smaller error than both the Padé approximant $R_4(t)$ and the averaged approximant $R^L_7(t)$ described in [1] when t is sufficiently close to zero. Note the "cusps" on the graphs. Downward cusps correspond to points at which the approximant is equal to the function, and upward cusps correspond to the poles of the approximant.

EXAMPLE 5.2. Figure 6.2 depicts the error when approximating the function e^t by the Padé approximant R_4, and the Padé-type approximants R^L_7 and R^S_7. The errors are presented in a semi-log plot. We observe the same behaviour as in the previous example.

6. Conclusion. This paper introduces Padé-type approximants associated with optimal averaged Gauss quadrature rules, and complements results by Boutry [1] on Padé-type approximants associated with averaged Gauss quadrature rules. Computed examples show the former approximants to yields approximations of higher accuracy close to the origin. This can be expected, since the optimal averaged Gauss quadrature rules have higher degree of precision than averaged Gauss quadrature rules with the same number of nodes.

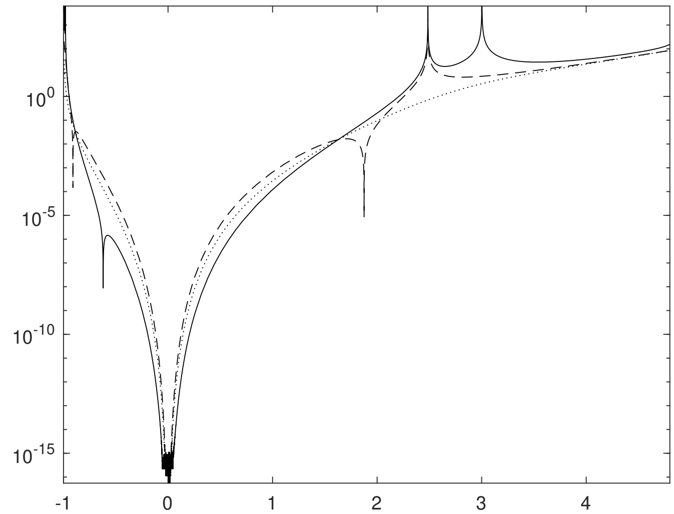

FIG. 6.1. *Comparison of the errors of the Padé approximant $R_4(t)$ (dotted line), the Padé-type approximant $R_7^L(t)$ (dashed line), and the Padé-type approximant $R_7^S(t)$ (continuous line) in log-scale as a function of t.*

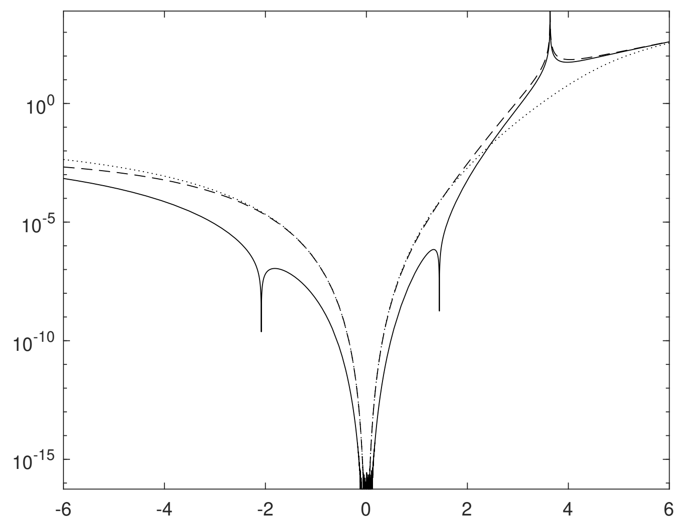

FIG. 6.2. *Comparison of the errors of the Padé approximant $R_4(t)$ (dotted line), the Padé-type approximant $R_7^L(t)$ (dashed line), and the Padé-type approximant $R_7^S(t)$ (continuous line) in log-scale as a function of t.*

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