

AN ITERATIVE METHOD FOR NUMERICAL INTEGRATION OF RATIONAL FUNCTIONS

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ABSTRACT. We describe a new method for numerical integration of rational functions on the real line. Given a rational integrand, we provide a new rational function preserving its integral on the line. The coefficients of the new function are explicit polynomials in the original ones. These transformations depend on the degree of the input and the desired order of the method. Both parameters are arbitrary. The formulas can be precomputed. Iteration yields an approximation of the desired integral, with m -th order convergence. Examples illustrating the automatic generation of these formulas and a comparison with standard numerical schemes are also presented.

1. INTRODUCTION

The problem of numerical integration of a function over the real line is described in Numerical Analysis texts such as [4, 11]. The standard algorithms for the numerical integration of

$$(1.1) \quad I := \int_{-\infty}^{\infty} F(x) dx$$

start by dealing with the unboundedness of the domain of integration. This is usually resolved in two ways: the first one considers the problem on a finite interval

$$(1.2) \quad I_L := \int_{-L}^L F(x) dx$$

followed by a convergence study as $L \rightarrow \infty$. The alternative is to transform the real line to a bounded interval. For example, the map $t = x/(1+x)$ maps $[0, \infty)$ to $[0, 1]$ and then

$$(1.3) \quad \begin{aligned} \int_{-\infty}^{\infty} F(x) dx &= \int_0^{\infty} (F(x) + F(-x)) dx \\ &= \int_0^1 \left[F\left(\frac{t}{1-t}\right) + F\left(\frac{t}{t-1}\right) \right] \frac{dt}{(1-t)^2}. \end{aligned}$$

The unboundedness of the original interval of integration is now reflected in the (possible) singularity of the new integrand at the boundary $t = 1$. Observe that if the original integrand is a rational function, then so is the new one in (1.3).

In this paper we present a new numerical method for the integration of rational functions on \mathbb{R} . It is different in spirit to the standard ones: the numerical approximation to the integral is obtained from a *recurrence* acting on the coefficients of

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the integrand. In particular, the integrand is never evaluated. We illustrate the comparison with the standard methods; a more systematic study will be presented elsewhere.

The method presented here is based on a transformation of the coefficients of a rational function, that preserves its integral. This is the so-called *rational Landen transformation*. The original problem discussed by Landen, Gauss, Legendre and others deals with the elliptic integral

$$(1.4) \quad G(a, b) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2 \cos^2 \theta + b^2 \sin^2 \theta}}.$$

Gauss [5] made the *numerical observation* that the function $G(a, b)$ was invariant under the transformation

$$(1.5) \quad (a, b) \mapsto \left(\frac{a+b}{2}, \sqrt{ab} \right).$$

The iteration of (1.5) leads to a numerical evaluation of the elliptic integral, or, as it has been explained by J. and P. Borwein in [3], to efficient methods for the numerical evaluation of π . The rational analogue of this transformation was developed in [2, 10] and here we show how to use it as a numerical method to evaluate rational integrals. The reader will find in [9] a survey of the diverse aspects related to these transformations.

Section 2 discusses the basic structure of the algorithm. Section 3 introduces a family of polynomials that play an important role in the development of the formulas given in Section 4. Finally, Section 5 contains some examples. The first illustrates the steps for a method of order 2 acting on a rational function of degree 6. The next two examples illustrate the accuracy of the method and its comparison to the trapezoidal rule. A systematic study of the cost involved in this algorithm will be presented elsewhere.

2. THE LANDEN TRANSFORMATION AND ALGORITHM

We present a general description of an iterative algorithm for the evaluation of

$$(2.1) \quad I := \int_{-\infty}^{\infty} F(x) dx.$$

Here F is a rational function given as

$$(2.2) \quad F(x) = \frac{B(x)}{A(x)},$$

with

$$(2.3) \quad A(x) = \sum_{k=0}^p a_k x^{p-k} \text{ and } B(x) = \sum_{k=0}^{p-2} b_k x^{p-2-k},$$

where $a_p \neq 0$. The general construction treats the coefficients a_i and b_j as indeterminates. Naturally, for specific integrands the parameters a_i and b_j are real numbers and the maps described in this section are defined on parts of \mathbb{R}^{2p} where the integrals are convergent.

The set

$$\mathcal{R}^{2p} : \{(a_0, a_1, \dots, a_p, b_0, \dots, b_{p-2}) : \text{such that } F \text{ in (2.2) has finite integral}\},$$

will be used to represent the rational function F in terms of its coefficients. It will be referred as the *coefficient space*.

In Section 4 we describe the construction, for each integer $m \geq 2$, of a rational function $F_{1,m}$ that satisfies

$$(2.4) \quad \int_{-\infty}^{\infty} F_{1,m}(x) dx = \int_{-\infty}^{\infty} F(x) dx.$$

The function $F_{1,m}(x)$ has the same degree as the original F and the new coefficients are *polynomials* in the old coefficients $a_0, \dots, a_p, b_0, \dots, b_{p-2}$. Naturally, this produces a map on \mathcal{R}^{2p} that we denote by $\mathfrak{L}_{m,p} : \mathcal{R}^{2p} \rightarrow \mathcal{R}^{2p}$, called the *rational Landen transformation of order m and degree p* . We denote by $\mathfrak{L}_{m,p}^n$ its n -fold composition. Now introduce a new operator by $\phi : \mathcal{R}^{2p} \rightarrow \mathbb{R}$ as the map which takes a vector of length $2p$ corresponding to a rational function in \mathcal{R} of degree p and returns the value of the rational function at $x = 0$. In terms of the vector of coefficients, this is the ratio of the last entry over its $(p+1)$ -th one. The composition $\phi \circ \mathfrak{L}_{m,p}^n$ will be denoted by $\phi_{m,p}^n$. The motivation behind ϕ is the following: if

$$(2.5) \quad F(x) = \frac{b_0 + b_1x + \dots + b_{p-2}x^{p-2}}{a_0 + a_1x + \dots + a_px^p},$$

then the function obtained by iterating the map $\mathfrak{L}_{m,p}$ n times is written as

$$(2.6) \quad F_{n,m}(x) = \frac{b_{0,n} + b_{1,n}x + \dots + b_{p-2,n}x^{p-2}}{a_{0,n} + a_{1,n}x + \dots + a_{p,n}x^p}.$$

The value of $F_{n,m}$ at $x = 0$ gives a sequence of real numbers that converges to $1/\pi$ times the integral of F in (2.5); see [10] for details. The update on this sequence comes from the coefficients of $F_{n,m}$. These are obtained by applying $\mathfrak{L}_{m,p}$ to those of $F_{n-1,m}$. Finally, define $\vec{\alpha} := (a_0, \dots, a_p, b_0, \dots, b_{p-2})$.

The main result of [10] is that the Landen transformation satisfies

$$(2.7) \quad \phi_{m,p}^n(\vec{\alpha}) \rightarrow \frac{I}{\pi}$$

as $n \rightarrow \infty$ if $I < \infty$. Furthermore, the convergence is of *order m* , that is,

$$(2.8) \quad \left| \phi_{m,p}^{n+1}(\vec{\alpha}) - \frac{I}{\pi} \right| \leq C \left| \phi_{m,p}^n(\vec{\alpha}) - \frac{I}{\pi} \right|^m.$$

This convergence result appears in [6] for the case $m = 2$ and the general case can be established along the same lines. See [8] for details.

Adapting the rational Landen transformations into a numerical method for calculating I involves a process with two parts. The first one is a symbolic calculation of the explicit algebraic formulae for the rational Landen transformation. The steps in this calculation are described in detail in Section 4. The second one is the iteration of these formulas.

Algorithm 1

Input:

- 1) An integer p : the degree of the denominator A .
- 2) An integer $m \geq 2$: the order of the transformation.

Output:

The explicit formula for the transformation $\mathfrak{L}_{m,p} : \mathcal{R}^{2p} \rightarrow \mathcal{R}^{2p}$, as polynomials in the a_i and b_j .

Note 2.1. Observe that, given m and p , the map $\mathfrak{L}_{m,p}$ can be *precomputed* and the result can be stored for its use in the second algorithm. Therefore, the first algorithm carries a *one-time cost* and is not figured into the time of the method. This precomputation will be assumed in the discussion of the second algorithm.

Algorithm 2

Input:

- 1) A vector $\vec{\alpha}$ representing the coefficients of the rational integrand F .
- 2) An integer $m \geq 2$: the order of convergence.
- 3) An integer $n \in \mathbb{N}$: the number of iterations of the Landen map.

Output: The expression $\phi_{m,p}^n(\vec{\alpha})$ that approximates I/π .

3. THE EVALUATION OF THE POLYNOMIALS P_m AND Q_m

The algorithm described in Section 4 employs the polynomials

$$(3.1) \quad P_m(x) := \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j \binom{m}{2j} x^{m-2j}$$

and

$$(3.2) \quad Q_m(x) := \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} (-1)^j \binom{m}{2j+1} x^{m-(2j+1)}.$$

The integration algorithm discussed here is based on the fact that the rational function

$$(3.3) \quad R_m(x) := \frac{P_m(x)}{Q_m(x)}$$

satisfies

$$(3.4) \quad \cot(m\theta) = R_m(\cot \theta).$$

For instance, for $m = 2$, we have

$$(3.5) \quad P_2(x) = x^2 - 1, \text{ and } Q_2(x) = 2x.$$

Note 3.1. This trigonometric property is instrumental in the proof that the integral of F is the same as that of F_1 . See [10] for details.

4. THE ALGORITHM

In this section we describe each of the steps in the first algorithm. This algorithm has been implemented in Mathematica 6.0.

Step 1. Construct the polynomial

$$(4.1) \quad H(x) = \sum_{i=0}^p h_i x^{p-i}$$

defined by

$$(4.2) \quad H(x) := \text{Res}_z (A(z), P_m(z) - xQ_m(z)),$$

where Res_z denotes the *resultant* in the variable z . The degrees of the polynomials involved in (4.2) are $p = \deg A$ and $m = \deg(P_m(z) - xQ_m(z))$, respectively.

The resultant. Given two polynomials $\alpha(t)$ and $\beta(t)$, the resultant of α and β is defined by

$$(4.3) \quad \text{Res}(\alpha, \beta) := \prod_{i=1}^r \prod_{j=1}^s (y_j - x_i),$$

where x_i are the roots of $\alpha(t) = 0$ and y_j are the roots of $\beta(t) = 0$.

The resultant of two polynomials can be computed as the determinant of the *Sylvester matrix* formed by their coefficients; see [7]. For instance, if

$$\alpha(t) = a_0 + a_1t + a_2t^2 + a_3t^3 \text{ and } \beta(t) = b_0 + b_1t + b_2t^2,$$

then the Sylvester matrix is defined by

$$(4.4) \quad S_{3,2} := \begin{pmatrix} a_3 & a_2 & a_1 & a_0 & 0 & 0 \\ 0 & a_3 & a_2 & a_1 & a_0 & 0 \\ 0 & 0 & a_3 & a_2 & a_1 & a_0 \\ b_2 & b_1 & b_0 & 0 & 0 & 0 \\ 0 & b_2 & b_1 & b_0 & 0 & 0 \\ 0 & 0 & b_2 & b_1 & b_0 & 0 \\ 0 & 0 & 0 & b_2 & b_1 & b_0 \end{pmatrix}$$

and it is a square matrix of size $\deg(\alpha) + \deg(\beta) + 2 = 7$. The resultant of $\alpha(t)$ and $\beta(t)$ in (4.4) is

$$\begin{aligned} \text{Res}(\alpha, \beta) &= a_3^2b_0^3 - a_2a_3b_0^2b_1 + a_1a_3b_0b_1^2 - a_0a_3b_1^3 + a_2^2b_0^2b_2 \\ &\quad - 2a_1a_3b_0^2b_2 - a_1a_2b_0b_1b_2 + 3a_0a_3b_0b_1b_2 + a_0a_2b_1^2b_2 \\ &\quad + a_1^2b_0b_2^2 - 2a_0a_2b_0b_2^2 - a_0a_1b_1b_2^2 + a_0^2b_2^3. \end{aligned}$$

In general, the resultant of two polynomials is a polynomial in their coefficients.

Note 4.1. The polynomial H has the same degree as A , the denominator of the integrand $R(x)$. It will become the denominator of the new rational function. Its coefficients h_i are polynomials in those of A . The calculation of H can be obtained by evaluating the determinant of a square matrix of dimension $\deg(A) + \deg(P_m) + 2 = p + m + 2$. For instance, for $m = 2$ and

$$(4.5) \quad A(x) = a_0x^4 + a_1x^3 + a_2x^2 + a_1x + a_4,$$

we obtain

$$\begin{aligned} H(x) &= 16a_0a_4x^4 + 8(a_1a_4 - a_0a_3)x^3 + 4(a_0a_2 - a_1a_3 + 4a_0a_4 + a_2a_4)x^2 \\ &\quad + 2(-a_0a_1 + a_1a_2 - 3a_0a_3 - a_2a_3 + 3a_1a_4 + a_3a_4)x \\ &\quad + (a_0 - a_1 + a_2 - a_3 + a_4)(a_0 + a_1 + a_2 + a_3 + a_4). \end{aligned}$$

Step 2. Form the polynomial

$$(4.6) \quad E(x) = \sum_{i=0}^p h_i (P_m(x))^{p-i} (Q_m(x))^i.$$

Step 3. The polynomial $E(x)$ formed in Step 2 is a multiple of the denominator $A(x)$. Compute the quotient

$$(4.7) \quad Z(x) = \frac{E(x)}{A(x)}$$

and write it as

$$(4.8) \quad Z(x) = \sum_{k=0}^r z_k x^{r-k}, \text{ with } r = p(m-1).$$

Step 4. Compute the product

$$(4.9) \quad C(x) = B(x)Z(x)$$

and write it as

$$(4.10) \quad C(x) = \sum_{k=0}^s c_k x^{s-k}, \text{ with } s = mp - 2.$$

Step 5. Form the expression

$$(4.11) \quad T_x(a, b) := \sum_{j=0}^x (-1)^{a-x+j} \binom{a}{x-j} \binom{b}{j},$$

for $a, b, x \in \mathbb{N}$.

Step 6. Define the expressions

$$\begin{aligned} M_1(j, \alpha, \beta, \gamma, m, p) &:= (-1)^{j+\alpha-\beta} c_{2j} \frac{2^{2(\alpha-\beta)} \alpha}{2\alpha-\beta} \binom{2\alpha-\beta}{\beta} \binom{\nu-\alpha-1+\beta}{\gamma} \times \\ &\times [T_{\lambda+\alpha m}(2j, s-2j) + T_{\lambda-\alpha m}(2j, s-2j)], \end{aligned}$$

and

$$\begin{aligned} M_2(j, \alpha, \beta, \gamma, m, p) &:= (-1)^{j+\beta} c_{2j+1} 2^{2\beta+1} \binom{\alpha+\beta}{2\beta+1} \binom{\nu-2-\beta}{\gamma} \times \\ &\times [T_{\lambda+\alpha m}(2j+1, s-2j-1) - T_{\lambda-\alpha m}(2j+1, s-2j-1)], \end{aligned}$$

with $\nu := p/2$ and $\lambda := (mp-2)/2$.

Step 7. Define

$$\begin{aligned}
 J(x) &:= \frac{1}{2^s} \sum_{\gamma=0}^{\nu-1} \left(\binom{\nu-1}{\gamma} \sum_{j=0}^{\lambda} (-1)^j c_{2j} T_{\lambda}(2j, s-2j) \right) x^{2\gamma} + \\
 &+ \frac{1}{2^s} \sum_{\gamma=0}^{\nu-2} \left(\sum_{j=0}^{\lambda} \sum_{\alpha=1}^{\nu-1-\gamma} \sum_{\beta=0}^{\alpha} M_1(j, \alpha, \beta, \gamma, m, p) \right) x^{2\gamma} \\
 &+ \frac{1}{2^s} \sum_{\gamma=1}^{\nu-1} \left(\sum_{j=0}^{\lambda} \sum_{\alpha=\nu-\gamma}^{\nu-1} \sum_{\beta=\alpha-\nu+\gamma+1}^{\alpha} M_1(j, \alpha, \beta, \gamma, m, p) \right) x^{2\gamma} \\
 &+ \frac{1}{2^s} \sum_{\gamma=0}^{\nu-2} \left(\sum_{j=0}^{\lambda-1} \sum_{\alpha=1}^{\nu-1-\gamma} \sum_{\beta=0}^{\alpha-1} M_2(j, \alpha, \beta, \gamma, m, p) \right) x^{2\gamma+1} \\
 &+ \frac{1}{2^s} \sum_{\gamma=1}^{\nu-2} \left(\sum_{j=0}^{\lambda-1} \sum_{\alpha=\nu-\gamma}^{\nu-1} \sum_{\beta=0}^{\alpha-1} M_2(j, \alpha, \beta, \gamma, m, p) \right) x^{2\gamma+1}.
 \end{aligned}$$

Step 8. The new rational function is defined by

$$(4.12) \quad F_{1,m}(x) := \frac{J(x)}{H(x)}.$$

It satisfies (2.4).

The reader is referred to [10] for the proofs of the formulas describing this algorithm.

5. EXAMPLES

In this section we give examples that illustrate the rational Landen transformations.

Example 5.1. We provide a step by step construction of the rational Landen transformation of order $m = 2$ for the function

$$(5.1) \quad F(x) = \frac{b_0x^4 + b_1x^3 + b_2x^2 + b_3x + b_4}{a_0x^6 + a_1x^5 + a_2x^4 + a_3x^3 + a_4x^2 + a_5x + a_6}.$$

The goal is to produce a function $F_{1,6}(x)$ with the same integral as $F(x)$.

Note 5.1. The special case $b_1 = b_3 = a_1 = a_3 = a_5 = 0$ was the first example of this new type of transformation. It appears in [1].

Note 5.2. The choice of $m = 2$ requires the evaluation of the polynomials $P_2(x) = x^2 - 1$ and $Q_2(x) = 2x$. These are computed directly from (3.1) and (3.2).

Step 1 computes the polynomial $H(x)$ from (4.2). The Mathematica command *Resultant* yields the expressions

$$\begin{aligned}
h_0 &= 64a_0a_6 \\
h_1 &= -32(a_0a_5 - a_1a_6) \\
h_2 &= 16(a_0a_4 - a_1a_5 + 6a_0a_6 + a_2a_6) \\
h_3 &= -8(a_0a_3 - a_1a_4 + 5a_0a_5 + a_2a_5 - 5a_1a_6 - a_3a_6) \\
h_4 &= 4(a_0a_2 - a_1a_3 + 4a_0a_4 + a_2a_4 - 4a_1a_5 - a_3a_5 + 9a_0a_6 + 4a_2a_6 + a_4a_6) \\
h_5 &= -2(a_0a_1 - a_1a_2 + 3a_0a_3 + a_2a_3 - 3a_1a_4 - a_3a_4 + 5a_0a_5) \\
&\quad -2(3a_2a_5 + a_4a_5 - 5a_1a_6 - 3a_3a_6 - a_5a_6) \\
h_6 &= (a_0 - a_1 + a_2 - a_3 + a_4 - a_5 + a_6)(a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6).
\end{aligned}$$

The polynomial $H(x)$ is the denominator of the new rational function obtained as a product of the Landen transformation.

Step 2 computes the polynomial $E(x)$ from (4.6). In this example, this is a polynomial of degree 12(= mp), that we write as

$$(5.2) \quad E(x) = \sum_{i=0}^{12} e_i x^{12-i}.$$

The symbolic expansion of (4.6) produces

$$\begin{aligned}
e_0 &= e_{12} = 64a_0a_6 \\
e_1 &= -e_{11} = 64(a_0a_5 - a_1a_6) \\
e_2 &= e_{10} = 64(a_0a_4 - a_1a_5 + a_2a_6) \\
e_3 &= -e_9 = 64(a_0a_3 - a_1a_4 + a_2a_5 - a_3a_6) \\
e_4 &= e_8 = 64(a_0a_2 - a_1a_3 + a_2a_4 - a_3a_5 + a_4a_6) \\
e_5 &= -e_7 = 64(a_0a_1 - a_1a_2 + a_2a_3 - a_3a_4 + a_4a_5 - a_5a_6) \\
e_6 &= 64(a_0^2 - a_1^2 + a_2^2 - a_3^2 + a_4^2 - a_5^2 + a_6^2).
\end{aligned}$$

Step 3 computes the quotient of $E(x)$, produced in Step 2, and $A(x)$, the denominator of the original integrand. In the example discussed now we obtain

$$(5.3) \quad Z(x) = 64(a_6x^6 - a_5x^5 + a_4x^4 - a_3x^3 + a_2x^2 - a_1x + a_0).$$

Step 4 simply evaluates the product $C(x) = B(x)Z(x)$, where $B(x)$ is the numerator of the original integrand and $Z(x)$ comes from Step 3. The polynomial $C(x)$ is written as

$$(5.4) \quad C(x) = \sum_{k=0}^{10} c_k x^{10-k},$$

with

$$\begin{aligned}
 c_0 &= 64a_6b_0 \\
 c_1 &= -64(a_5b_0 - a_6b_1) \\
 c_2 &= 64(a_4b_0 - a_5b_1 + a_6b_2) \\
 c_3 &= -64(a_3b_0 - a_4b_1 + a_5b_2 - a_6b_3) \\
 c_4 &= 64(a_2b_0 - a_3b_1 + a_4b_2 - a_5b_3 + a_6b_4) \\
 c_5 &= -64(a_1b_0 - a_2b_1 + a_3b_2 - a_4b_3 + a_5b_4) \\
 c_6 &= 64(a_0b_0 - a_1b_1 + a_2b_2 - a_3b_3 + a_4b_4) \\
 c_7 &= 64(a_0b_1 - a_1b_2 + a_2b_3 - a_3b_4) \\
 c_8 &= 64(a_0b_2 - a_1b_3 + a_2b_4) \\
 c_9 &= 64(a_0b_3 - a_1b_4) \\
 c_{10} &= 64a_0b_4.
 \end{aligned}$$

Step 7 combines the functions defined in Step 5 and 6 to produce the new numerator

$$(5.5) \quad J(x) = \sum_{k=0}^4 d_k x^{4-k},$$

with

$$\begin{aligned}
 d_0 &= 32(a_6b_0 + a_0b_4) \\
 d_1 &= -16(a_5b_0 - a_6b_1 + a_0b_3 - a_1b_4) \\
 d_2 &= 8(a_4b_0 + 3a_6b_0 - a_5b_1 + a_0b_2 + a_6b_2 - a_1b_3 + 3a_0b_4 + a_2b_4) \\
 d_3 &= -4(a_3b_0 + 2a_5b_0 + a_0b_1 - a_4b_1 - 2a_6b_1 - a_1b_2 + a_5b_2) - \\
 &\quad -4(2a_0b_3 + a_2b_3 - a_6b_3 - 2a_1b_4 - a_3b_4) \\
 d_4 &= 2(a_0b_0 + a_2b_0 + a_4b_0 + a_6b_0 - a_1b_1 - a_3b_1 - a_5b_1) + \\
 &\quad +2(a_0b_2 + a_2b_2 + a_4b_2 + a_6b_2 - a_1b_3 - a_3b_3 + a_0b_4 + a_2b_4 + a_4b_4 + a_6b_4).
 \end{aligned}$$

Note 5.3. Given a rational function of order p and a choice of method of order m , the calculation of H and J illustrated here is done *once*. We have produced a transformation sending

$$(5.6) \quad F(x) = \frac{b_0x^4 + b_1x^3 + b_2x^2 + b_3x + b_4}{a_0x^6 + a_1x^5 + a_2x^4 + a_3x^3 + a_4x^2 + a_5x + a_6}$$

to

$$(5.7) \quad F_{1,6}(x) := \mathfrak{L}_{6,2}F(x) = \frac{d_0x^4 + d_1x^3 + d_2x^2 + d_3x + d_4}{h_0x^6 + h_1x^5 + h_2x^4 + h_3x^3 + h_4x^2 + h_5x + h_6}$$

with the new coefficients given as above. We expect to produce a *precomputed* array of formulas, indexed by (p, m) , to be made available to the community.

In the next series of examples, we will assume that the formulas for the Landen transformations have been precomputed.

Example 5.2. The rational function

$$(5.8) \quad F_0(x) = \frac{1}{x^2 + 4x + 15}$$

satisfies

$$(5.9) \quad I := \int_{-\infty}^{\infty} F_0(x) dx = \frac{\pi}{\sqrt{11}},$$

with numerical value

$$(5.10) \quad I \sim 0.94722582509948293643.$$

We now employ the algorithm, with a method of order 2, to obtain the sequence of rational functions

$$(5.11) \quad F_{n,2}(x) = \frac{c_n}{x^2 + a_n x + b_n},$$

with $F_{0,2}(x) = F_0(x)$, and the property that

$$(5.12) \quad I = \int_{-\infty}^{\infty} F_{n,2}(x) dx = c_n \int_{-\infty}^{\infty} \frac{dx}{x^2 + a_n x + b_n}.$$

The convergence analysis described in [10] shows that $a_n \rightarrow 0$, $b_n \rightarrow 1$, thus

$$(5.13) \quad I = \lim_{n \rightarrow \infty} \pi c_n.$$

Even though the limiting value of the integral depends only upon the terms c_n , the formulas to generate these values also involve a_n and b_n . Therefore one must store the current value of all the parameters. The first few of them are shown in the next table:

| n | c_n | a_n | b_n |
|-----|----------------------|----------------------|-----------------------------|
| 0 | 1 | 4 | 15 |
| 1 | $\frac{8}{15}$ | $\frac{28}{15}$ | 4 |
| 2 | $\frac{1}{3}$ | $\frac{7}{10}$ | $\frac{4841}{3600}$ |
| 3 | $\frac{8441}{29046}$ | $\frac{8687}{96820}$ | $\frac{64900081}{69710400}$ |

TABLE 1. Rational Landen of order 2

Note 5.4. The expression πc_n gives an approximation to the integral of $F_0(x)$. For example, for $n = 6$, we find that

$$c_6 = \frac{3471070386673821384824326347489289738211683509253931254760471}{11512238093504492278949475398059063785494372327433955614454608}$$

and πc_6 agrees with the integral of F_0 up to 13 digits. The coefficients (a_n, b_n, c_n) are rational numbers and their height increases with n . Recall that the *height* of a rational number, written in irreducible form as $x = \frac{u}{v}$, is

$$(5.14) \quad h(x) = \text{Max}\{|u|, |v|\}.$$

For example, at $n = 10$, the heights of a_{10}, b_{10}, c_{10} have approximately 1000 digits. At this stage, the value πc_{10} gives 196 digits of the integral. Naturally, this increases the complexity of the calculations *if we use exact arithmetic*. An interesting way out of this problem is to replace the rational number c_n by the truncation of its continued fraction. For example, the first 20 terms of the continued fraction of c_{10} , a rational number of height *only* 6, differs from c_{10} by less than 10^{-24} . Details will be given in a future publication.

Example 5.3. Mathematica 6.0 shows that if

$$(5.15) \quad F(x) = \frac{1}{x^4 + 6x^3 + 16x^2 + 21x + 13}$$

then

$$(5.16) \quad I := \int_{-\infty}^{\infty} F(x) dx = 2\pi \sqrt{\frac{2}{111}(\sqrt{37} - 5)}.$$

We employ the identity (1.3) to map the problem to the interval $[0, 1]$. The new rational function

$$\begin{aligned} g(x) &:= \frac{60x^6 - 288x^5 + 584x^4 - 648x^3 + 422x^2 - 156x + 26}{(3x^4 - 15x^3 + 31x^2 - 31x + 13)(57x^4 - 153x^3 + 157x^2 - 73x + 13)} \\ &= \frac{60x^6 - 288x^5 + 584x^4 - 648x^3 + 422x^2 - 156x + 26}{171x^8 - 1314x^7 + 4533x^6 - 9084x^5 + 11485x^4 - 9314x^3 + 4707x^2 - 1352x + 169} \end{aligned}$$

satisfies

$$(5.17) \quad \int_0^1 g(x) dx = \int_{-\infty}^{\infty} F(x) dx.$$

We now compare the numerical approximation to the integral of g over $[0, 1]$ computed with the methods described here, with a numerical integration using the trapezoidal rule. A more systematic comparison with more sophisticated classical numerical schemes will be described elsewhere.

The trapezoidal rule states that

$$(5.18) \quad \int_a^b g(x) dx = \frac{h}{2}(g(a) + g(b)) - \frac{1}{12}h^3g''(\xi),$$

where $h = b - a$ and $\xi \in [a, b]$. Define

$$(5.19) \quad M := \text{Max}\{|g''(t)| : a \leq t \leq b\}.$$

Then the *error term*, namely the second term in (5.18) is bounded by $Mh^3/12$. To obtain an approximation to the integral I in (5.16), we choose $n \in \mathbb{N}$, partition $[0, 1]$ into n intervals of equal length $h = 1/n$ and apply the trapezoidal rule to each subinterval. This yields the expression

$$(5.20) \quad I_n := \int_0^1 g(x) dx \sim \frac{1}{2n} \left(g_0 + \sum_{i=1}^{n-2} g_i + g_n \right) - \frac{1}{12n^3} \sum_{i=1}^{n-1} g''(\xi_i),$$

where $g_i = g(i/n)$ and $\frac{i-1}{n} \leq \xi_i \leq \frac{i}{n}$. The total error in this approximation is bounded by $M/12n^2$. To compute the approximation I_n to I requires the n values $\{g_i : 0 \leq i \leq n\}$. The relative error $(I - I_n)/I$ for $n = 100$ is 5.29805×10^{-6} . It drops to 3.1505×10^{-8} for $n = 1000$ and to 2.9445×10^{-10} for $n = 10000$.

We now use the method of rational Landen transformations of order m to produce approximations to the integral I of $F(x)$ over \mathbb{R} . Recall that the method yields a family of rational functions $R_{n,m}(x)$ with integral I . For example, the first two functions for a method of order 2 are

$$R_{1,2}(x) = \frac{4(2x^2 + 6x + 15)}{208x^4 + 456x^3 + 600x^2 + 396x + 171},$$

$$R_{2,2}(x) = \frac{8(13848x^2 + 11652x + 11531)}{569088x^4 - 35136x^3 + 756384x^2 - 8616x + 232537}.$$

The approximations to I are then obtained from

$$(5.21) \quad \text{app}_{n,m} := \frac{\text{Constant term in the numerator of } R_{n,m}(x)}{\text{Constant term in the denominator of } R_{n,m}(x)} \times \pi.$$

The next table shows the relative errors

$$(5.22) \quad \text{rel}_{n,m} := \frac{|\text{app}_{n,m} - I|}{|I|}$$

for $2 \leq m \leq 6$ and $2 \leq n \leq 5$.

| n | $m = 2$ | $m = 3$ | $m = 4$ | $m = 5$ | $m = 6$ |
|-----|-------------------------|--------------------------|---------------------------|---------------------------|----------------------------|
| 2 | 0.30314 | 0.022076 | 0.0021170 | 2.2646×10^{-6} | 6.3257×10^{-7} |
| 3 | 0.058475 | 0.000035272 | 5.2932×10^{-12} | 2.9440×10^{-23} | 4.4813×10^{-40} |
| 4 | 0.0021170 | 3.2713×10^{-15} | 2.0616×10^{-47} | 1.9758×10^{-115} | 3.6655×10^{-239} |
| 5 | 3.2700×10^{-6} | 3.6952×10^{-45} | 5.3750×10^{-190} | 3.1671×10^{-577} | 4.0442×10^{-1434} |

TABLE 2. Relative error for the numerical evaluation of I_n .

This table contains clear evidence to support the convergence orders claimed in (2.8).

Example 5.4. The rational Landen transformations can be used to evaluate

$$(5.23) \quad \int_{-\infty}^{\infty} \frac{dx}{(x-2)^2 + \epsilon^2} = \frac{\pi}{\epsilon},$$

for $\epsilon > 0$ small. This example illustrates the fact that the proposed method converges, even when the integrand has poles very close to the real axis. A systematic

description of the sensitivity of the iteration with respect to the parameter ϵ , will be presented elsewhere.

For fixed $\epsilon > 0$, we apply a method of order 2 to (5.23). This produces a sequence of rational functions of the form

$$(5.24) \quad R_n(x) = \frac{b_{0,n}}{a_{0,n} + a_{1,n}x + a_{2,n}x^2}$$

that satisfy

$$(5.25) \quad \int_{-\infty}^{\infty} R_n(x) dx = \frac{\pi}{\epsilon}.$$

The explicit Landen transformation of order 2 is given by

$$(5.26) \quad \begin{aligned} a_{0,n+1} &= (a_{0,n} - a_{1,n} + a_{2,n})(a_{0,n} + a_{1,n} + a_{2,n}) \\ a_{1,n+1} &= 2a_{1,n}(a_{0,n} - a_{2,n}) \\ a_{2,n+1} &= 4a_{0,n}a_{2,n} \\ b_{0,n+1} &= 2b_{0,n}(a_{0,n} + a_{2,n}), \end{aligned}$$

with initial conditions

$$(5.27) \quad a_{0,0} = 4 + \epsilon^2, \quad a_{1,0} = -4, \quad a_{2,0} = 1, \quad b_{0,0} = 1.$$

The sequence $R_n(x)$ has coefficients that depend upon the parameter ϵ . For example,

$$R_1(x) = \frac{2(5+\epsilon^2)}{4(4+\epsilon^2)x^2 - 8(3+\epsilon^2)x + (1+\epsilon^2)(9+\epsilon^2)}$$

and

$$R_2(x) = \frac{4(5+\epsilon^2)(25+14\epsilon^2+\epsilon^4)}{(1+6\epsilon^2+\epsilon^4)(49+22\epsilon^2+\epsilon^4) - 16(-1+\epsilon)(1+\epsilon)(3+\epsilon^2)(7+\epsilon^2)x + 16(1+\epsilon^2)(4+\epsilon^2)(9+\epsilon^2)}.$$

The theory described above shows that, for fixed $\epsilon > 0$ and $n \rightarrow \infty$, the sequences

$$(5.28) \quad \frac{a_{0,n}}{b_{0,n}} \rightarrow L, \quad \frac{a_{1,n}}{b_{0,n}} \rightarrow 0, \quad \frac{a_{2,n}}{b_{0,n}} \rightarrow L$$

converge to the stated limits. Moreover, the invariance of (5.23) under the transformations given in (5.26) show that $L = \epsilon$.

Define the error

$$(5.29) \quad \text{err}_n := \left(\left(\frac{a_{0,n}}{b_{0,n}} - \epsilon \right)^2 + \left(\frac{a_{1,n}}{b_{0,n}} \right)^2 + \left(\frac{a_{2,n}}{b_{0,n}} - \epsilon \right)^2 \right)^{1/2}.$$

Then Table 3 shows the ratios $\text{err}_{16}/\text{err}_{15}$ obtained after 15 iterations of (5.26) for methods of order 2 and 3. The calculations are done with 10^6 digit precision.

The data in Table 3 shows the exponential decay of the error. Given a tolerance $\delta > 0$, we have observed that the number of steps required to achieve $\text{err}_n < \delta$ increases as $\epsilon \rightarrow 0$. A quantitative description of this phenomena is in preparation and it will be reported elsewhere.

| ϵ | order 2 | order 3 |
|------------|----------------------------|-------------------------------|
| .1 | 3.58047×10^{-569} | $3.49118 \times 10^{-497802}$ |
| .01 | 1.36862×10^{-57} | $4.24935 \times 10^{-49853}$ |
| .001 | 2.07254×10^{-6} | $4.73905 \times 10^{-4986}$ |
| .0001 | 2.16805×10^{-2} | 3.48094×10^{-499} |
| .00001 | 4.68150×10^{-1} | 1.62880×10^{-50} |

TABLE 3. The quotient $\text{err}_{16}/\text{err}_{15}$ as a function of the parameter ϵ .

6. CONCLUSIONS

We have described the rational Landen transformations and their use in the numerical integration of rational functions. We have exhibited fast convergence of this method and presented an example comparing it to the classical integration schemes.

A systematic comparative analysis of this method with respect to standard numerical algorithms will be discussed elsewhere. An interesting challenging problem is to extend the use of rational Landen transformations to produce fast numerical integrators for arbitrary functions. In particular the method is well suited for the numerical integration of meromorphic function with poles off the real line.

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