On Rational Function Techniques and Padé Approximants

An Overview

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Abstract.

Continued fractions, rational interpolants, and Padé approximants are mathematical tools that are very appropriate for analyzing nonlinear problems. These technics and concepts are found in many numerical algorithms (equation solving, integration, differential equations, convergence acceleration, sequence transformations, and extrapolation methods in general) and in the applied sciences. In this contribution, a brief introductory review into the field of rational function techniques which may hopefully motivate the reader to apply the methods to his own problems is given.

1. Introduction

1.1. Motivation

This review on Padé approximants and the analytic and numerical techniques based on rational functions was inspirated by a paper (Contopoulos and Seimenis, 1975) on the application of the Prendergast method (Prendergast, 1982) to a logarithmic potential $V(x,y) = \ln(x^2 + y^2/U^2 + C^2)$. In that paper equations of motion are derived, and a rational expansion of x and y is coupled with a Fourier series ansatz in order to represent the solution. This approach leads to a set of nonlinear coupled equations. However the solutions derived by the authors did not fulfill all the equations. It is difficult to see why some equations are considered and others are neglected. A consistent approach to this problem is to treat it as an approximation problem (see Subsection 5.3). In this framework, a given function (here, the solution of the equations of motion) or a set of data is fitted by an ansatz function (here, a rational trigonometric function) with some degrees of freedom. Usually, the ansatz function cannot exactly represent the given function or data set since it leads to an overdetermined system. In this case, the degrees of freedom in the ansatz function are chosen in such a way that a given function, e.g., a least squares function, is minimized.

The rational function approximation problem is closely related to continued fractions, rational interpolants, and Padé approximants. These techniques and concepts are found in many numerical algorithms (equation solving, integration, differential equations, convergence acceleration, approxima-

tion of special functions, the z-transform) and in the applied sciences, e.g., physics, chemistry, mechanics, fluid dynamic, or circuit theory. They form an important class of methods to investigate nonlinear problems, e.g., in the analysis of diverging series.

A Padé approximant is the ratio of two polynomials constructed from the coefficients of the Taylor series expansion of a function. Since it provides an approximation to the function throughout the whole complex plane the study of Padé approximants is simultaneously a topic in mathematical approximation theory and analytic function theory. It has wide applicability to those areas of knowledge that involve analytic techniques. The theory involved connects classical topics in mathematics as continued fraction, one of the oldest subjects in mathematics at all, with very modern concepts as formal orthogonal polynomials (Brezinski, 1983). Padé approximants are the base of many nonlinear methods, and they have close connections with the famous ε-algorithm (Wynn, 1956), continued fractions, and orthogonal polynomials. Padé approximants are the nonlinear counter part to the first order Taylor series expansions which are used in linear methods.

There are many methods available to compute Padé approximants (Wuytack, 1979). Since many of them are based on continued fractions section 3 provides a basic introduction into the field of continued fractions.

Since celestial mechanics is full of nonlinear problems the reader may find this review helpful and may detect possible applications. The review is tried to be on an elementary level. Examples are provided where possible. In particular, a Padé approximant is used to solve Kepler's equation. Some proves are included to give an idea how they work. The interested reader is also referred to (Cuyt and Wuytack, 1987) from which this paper benefits most.

1.2. Some Historical Remarks on Continued Fractions and Padé Approximants

In 1731, rational fractions [now called Padé approximants after the French mathematician Henri Padé (1863-1953)] are mentioned in a letter of the English mathematician Georges Anderson. They are also given by Leonhard Euler (1707-1783). The first mathematician who was aware of the fundamental property $f(t) - [p/q]_f(t) = O(t^{p+q+1})$ was Joseph Louis Lagrange in a paper (1776) dealing with the solution of differential equations by continued fractions. However continued fractions are already used by Johann Henrich Lambert (1728-1777) in 1756. Padé in his thesis (Padé, 1892) under Charles Hermite (1822-1901) invented the Padé table and studied the so-called block structure. In the 19^{th} century, many contributions to the theory of Padé approximants were made by Carl Gustav Jacobi (1804-1851), Leopold Kronecker (1823-1891), Bernhard Riemann (1826-1866) and Georg

Frobenius (1849-1917). Probably, E.B. van Vleck gave the name Padé approximants to rational fractions (Brezinski, 1983). Since 1965 a growing interest into rational fractions and related topics is observed in pure mathematics, numerical analysis, theoretical physics, chemistry, mechanics and electronics. Nowadays, there is a huge amount of literature available on Padé approximants. (Brezinski, 1991) gives more than 6000 references.

2. Padé Approximations

2.1. An Illustrative Example

A Padé approximant is that rational function whose power series expansion agrees with a prescribed power series to the highest possible order. Consider a given power series

$$f(x) \equiv \sum_{i=0}^{\infty} c_i x^i \tag{1}$$

and a rational function

$$R(x) \equiv \frac{p(x)}{q(x)} \ , \ p(x) = \sum_{i=0}^{m} a_i x^i \ , \ q(x) = \sum_{i=0}^{n} b_i x^i \quad . \tag{2}$$

The rational function $R(x)$ is called Padé approximant to the series $f(x)$ if

$$f(x) - R(x) = O(x^{m+n+1}) \ , \tag{3}$$

i.e., the monom with lowest order in the difference polynom

$$f(x) \cdot q(x) - p(x) = f(x) \cdot \left(\sum_{i=0}^{n} b_i x^i \right) - \sum_{i=0}^{m} a_i x^i \tag{4}$$

is of order $m + n + 1$ or higher. The condition (3) is equivalent to the requirement

$$R(0) = f(0) \ , \ \left. \frac{\mathrm{d}^k}{\mathrm{d}x^k} R(x) \right|_{x=0} = \left. \frac{\mathrm{d}^k}{\mathrm{d}x^k} f(x) \right|_{x=0} \ , \ k = 1, 2, ..., m+n \quad . \tag{5}$$

The required definitions (3) or (5) provide $m + n + 1$ equations for the $m + n + 2$ unknowns $a_0, \ldots, a_m$ and $b_0, b_1, \ldots, b_n$.

$$\begin{array}{rcll} \sum\limits_{j=0}^{n} b_j c_{m-j+k} & = & 0 & , k = 1, ...n \\ \sum\limits_{j=0}^{k} b_j c_{k-j} & = & a_k & , k = 0, ...m \end{array} \quad . \tag{6}$$

Fig. 1. The figure shows the power series based on the first five terms, $f(x)$ is drawn as a solid line, and the Padé approximant $R(x)$ is represented as a dotted curve. Note that within the range $[0, 10]$ the Padé approximant $R(x)$ and the exact expression $f(x) = \left[7 + (1+x)^{(4/3)}\right]^{(1/3)}$ almost agree.

Obviously, this system of equations is underdetermined. Therefore, usually the normalization $b_0 = 1$ is used. However as discussed below some care is necessary with this normalization. In principle, the first n equations may be used to determine the $b's$, from which the $a's$ can be computed using the second set of equations. However considering numerical efficiency, this is not a safe method since the matrix is close to singular. In section 4 different methods are presented to compute the Padé approximant safely.

The following example (Press and Teukolsky, 1992) shows that Padé approximants might be very helpful for extrapolation. The exact function to be analyzed is

$$f(x) = \left[7 + (1+x)^{(4/3)}\right]^{(1/3)} \quad . \tag{7}$$

The first five terms in the power series expansion of that function $f(x)$ are

$$f(x) \approx 2 + \frac{1}{9}x + \frac{1}{81}x^2 - \frac{49}{8748}x^3 + \frac{175}{78732}x^4 + ... \tag{8}$$

The Padé approximants $R(x)$ in the case $m = n = 2$ based on this series is

$$R(x) = \frac{a_0 + a_1 x + a_2 x^2}{1 + b_1 x + b_2 x^2} \tag{9}$$

with the coefficients

$$\begin{array}{ccccc} a_0 & a_1 & a_2 & b_1 & b_2 \\ 2 & 0.92714 & 0.067834 & 0.40801 & 0.0050766 \end{array} . \tag{10}$$

Very often, as shown in this example, Padé approximants maintain accuracy far outside the radius of convergence of the series. The figure shows the power series in the dashed curve, $f(x)$ is the solid line, and the Padé approximant $R(x)$ is represented as a dotted curve. To understand this property, requires some insight in the convergence theory of Padé approximants closely related to analyticity and complex analysis.

2.2. Notations, Definitions, and Formal Foundation of Padé Approximants

In order to present a formal definition and also since they are used in many proofs concerning Padé approximants, the operators ∂ and ω are introduced. If p is a polynomial, ∂p gives the exact degree of a polynomial, i.e., the degree of that nonzero term with highest exponent. $\partial(a_0 + a_1 x + 5x^2) = 2$ may serve as an example. If p is a polynomial or a power series, then ωp returns the order of p, i.e., the degree of the first nonzero term. Let $a_3 \neq 0$, then $\omega\left(\sum_{i=3}^{\infty} a_i x^i\right) = 3$. These operators applied to arbitrary polynomials p and q have the following obvious properties:

$$\partial(pq) = \partial p + \partial q \tag{11}$$

$$\omega(p_+q) = \min\{\omega p, \omega q\} \tag{12}$$

$$c = const \Rightarrow \omega(cp) = \omega(p) \tag{13}$$

$$\omega(x^k p) = k + \omega(p) \tag{14}$$

$$\omega(p) \geq k \Rightarrow \omega(pq) \geq k \tag{15}$$

$$(\partial p \leq n) \wedge (\omega p \geq n+1) \Rightarrow p \equiv 0 \tag{16}$$

which can be easily proven.

The first step towards a concept of Padé approximant is the Padé approximation problem (PAP) of order (m, n). That problem consists in determining polynomials $p(x)$ and $q(x)$ in such a way that

$$\begin{array}{c} \partial p \leq m \\ \partial q \leq n \\ \omega(fq - p) \geq m + n + 1 \end{array} . \tag{17}$$

The last inequality expresses that all coefficients with index $i < m+n+1$ of the power series $fq - p$ vanish. The condition (17) is equivalent to the two

linear systems of equations (6) with $c_i = 0$ for $i < 0$. To solve this system it has already been mentioned that the $b's$ might be determined by the n equations in the $n+1$ unknowns $b_0, ..., b_n$.

The PAP of order $(m, 0)$ is solved by the partial sums of (1) which in most cases is the Taylor series expansion of some function.

Similar to the concept of equivalence classes of rational numbers solving the equation $ax = b$ where a, b are rational numbers, and all rational numbers $\frac{qb}{qa}$ with rational $q \neq 0$ solve $ax = b$, different solutions of the same PAP can exist. However there exists a relation between them according to the following theorem:

THEOREM 1. *If the polynomials p_1, q_1 and p_2, q_2 satisfy (17), then $p_1 q_2 = p_2 q_1$.*

The proof only uses the definition (17) and some properties of the operators ∂ and ω. Since most of the proofs related to Padé approximants have a similar structure it is given in some detail.

Proof.

By adding and subtracting fq_1q_2, the polynomial $p := p_1q_2 - p_2q_1$ can be written as $p = (fq_2 - p_2)q_1 - (fq_1 - p_1)q_2$. Since p_1, q_1 and p_2, q_2 satisfy (17) the inequalities

$$\begin{aligned} \omega(fq_1 - p_1) &\geq m + n + 1 \\ \omega(fq_2 - p_2) &\geq m + n + 1 \end{aligned}$$

hold. Therefore, if (12) is applied to p, the inequality $\omega(p_1q_2 - p_2q_1) \geq m + n + 1$ is derived. However according to (11) $p_1q_2 - p_2q_1$ is a polynomial of degree at most $m + n$, i.e., $\partial(p_1q_2 - p_2q_1) \leq m + n$. Eventually, applying (16) to p gives $p \equiv 0$ which is equivalent to $p_1q_2 = p_2q_1$.

Similar to rational numbers the rational forms p_1/q_1 and p_2/q_2 are equivalent. If p and q satisfy (17) then

$$[m/n]_f(x) = r_{m,n}(x) = \frac{p_0(x)}{q_0(x)} \tag{18}$$

is called the **Padé approximant** of order (m, n) or irreducible form of p/q normalized in such a way that $q_0(0) = 1$, i.e., $b_0 = 1$. As discussed below, some care is necessary with this normalization. Since in the computation of $p_0(x)$ and $q_0(x)$ a polynomial may be cancelled out, the relation

$$\begin{aligned} m' &:= \partial p_0 \leq m \\ n' &:= \partial q_0 \leq n \end{aligned} \tag{19}$$

needs to be observed. Nevertheless, it is guaranteed that for every non-negative m and n a unique Padé approximant of order (m, n) for f exists.

2.3. Fundamental properties of Padé approximants

The definition given in the section (2.1) shows that some care is necessary when computing the Padé approximant. Consider $f(x) = 1 + x^2$ and $m = n = 1$. That clearly gives $c_0 = c_2 = 1$ and $c_1 = 0$, and the systems of equations

$$\begin{aligned} b_1 c_1 &= -c_2 b_0 \\ a_0 &= c_0 b_0 \\ a_1 &= b_0 c_1 + b_1 c_0 \end{aligned} \tag{20}$$

which, when $b_0 = 1$, cannot be solved because $c_1 = 0$ and $c_2 \neq 0$. The solution $a_0 = b_0 = 0$ and $a_1 = b_1 = 1$, and therefore $p(x) = q(x) = x$, satisfies (17). However $p_0 = q_0 = 1$ which was derived by cancelling out the common factor give a Padé approximant $r_{1,1} = 1$ with $\omega(fq_0 - p_0) = 2 < m + n + 1$ which violates (17).

Fortunately, once p_0 and q_0 are known, it is possible to construct a rational form of order (m, n) as shown in the following theorem (Cuyt and Wuytack, 1987, Theorem 2.3, p.66):

THEOREM 2. *If the Padé approximant of order (m, n) for f is given by $r_{m,n}(x) = \frac{p_0(x)}{q_0(x)}$ then there exists an integer s with $0 \leq s \leq \min\{m - m', n - n'\}$, in such a way that $p(x) = x^s p_0(x)$ and $q(x) = x^s q_0(x)$ satisfy (17).*

In the example discussed above we have $m' = n' = 1$ and therefore again $p(x) = q(x) = x$.

2.4. Padé Table and Normality

In order to establish some relations between Padé approximants $r_{m,n}$ of different order it is helpful to order them in a table

$$\begin{array}{cccc} r_{0,0} & r_{0,1} & r_{0,2} & \cdots \\ r_{1,0} & r_{1,1} & r_{1,2} & \cdots \\ r_{2,0} & r_{2,1} & r_{2,2} & \cdots \\ r_{3,0} & r_{3,1} & \cdots & \\ r_{4,0} & \cdots & & \\ \vdots & & & \end{array}$$

which is called the **Padé table** of f. While the first column consists of the partial sums of f the first row contains the reciprocals of the partial sum of $1/f$. The Padé table, e.g.,

Table 1: Padé table for $f(x) = e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots$

1	$\frac{1}{1-x}$	$\frac{1}{1-x+\frac{1}{2}x^2}$	$\cdots$
$1+x$	$\frac{1+\frac{1}{2}x}{1-\frac{1}{2}x}$	$\frac{1+\frac{1}{3}x}{1-x+\frac{1}{6}x^2}$	$\cdots$
$1+x+\frac{1}{2}x^2$	$\frac{1+\frac{2}{3}x+\frac{1}{6}x^2}{1-\frac{1}{3}x}$	$\frac{1+\frac{1}{2}x+\frac{1}{12}x^2}{1-\frac{1}{2}x+\frac{1}{2}x^2}$	$\cdots$
$1+x+\frac{1}{2}x^2+\frac{1}{6}x^3$	$\frac{1+\frac{3}{4}x+\frac{1}{4}x^2+\frac{1}{24}x^3}{1-\frac{1}{4}x}$	$\vdots$	
$1+x+\frac{1}{2}x^2+\frac{1}{6}x^3+\frac{1}{24}x^4$	$\vdots$		
$\vdots$			

and

Table 2: Padé table for $f(x) = 1 + \sin(x) = 1 + x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots$

1	$\frac{1}{1-x}$	$\frac{1}{1-x+x^2}$	$\frac{1}{1-x+x^2-\frac{5}{6}x^3}$	$\cdots$
$1+x$	$1+x$	$\frac{1+\frac{5}{6}x}{1-\frac{1}{6}x+\frac{1}{6}x^2}$	$\cdots$	
$1+x$	$1+x$	$\frac{1+x+\frac{1}{6}x^2}{1+\frac{1}{6}x^2}$	$\cdots$	
$1+x+\frac{1}{2}x^2-\frac{1}{6}x^3$	$1+x-\frac{1}{6}x^3$	$\vdots$		
$1+x+\frac{1}{2}x^2-\frac{1}{6}x^3$	$1+x-\frac{1}{6}x^3$			
$1+x-\frac{1}{6}x^3+\frac{1}{120}x^5$	$\vdots$			
$\vdots$				

show different structural features which lead to the concept of normality and block structure. The Padé table of $f(x) = 1 + \sin(x)$ has a block structure consisting of square blocks of size 2 containing equal Padé approximants. These block structure is generally characterized by the following theorem:

THEOREM 3. *For a given Padé approximant of order* (m, n)*, i.e.,* $r_{m,n}(x) = \frac{p_0(x)}{q_0(x)}$ *the following relations hold.*

a) $\omega(fq_0 - p_0) = m' + n' + t + 1$ with a non-negative slack variable $t \geq 0$

b) for k and l satisfying $m' \leq k \leq m' + t$ and $n' \leq l \leq n' + t$ the relation $r_{k,l}(x) = \frac{p_0(x)}{q_0(x)}$ holds

c) $m \leq m' + t$ and $n \leq n' + t$

Property b) expresses for $t > 0$ the existance of a block of size $(t+1)\times(t+1)$.

Those Padé approximants which occur only once in the Padé table are called **normal**. As expected from the previous theorem the necessary and sufficient conditions for a Padé approximant to be normal are expressed in the following theorem:

THEOREM 4. *The Padé approximant $r_{m,n} = p_0/q_0$ for f is normal if and only if*

a) $m = m'$ and $n = n'$
b) $\omega(fq_0 - p_0) = m + n + 1$

Since the Padé approximants can be derived from a system of linear equations which might be solved by ratio of determinants it is not a surprise that normality of a Padé approximant can also be guaranteed by the nonvanishing of certain determinants.

In order to express some determinant relation the following notation is introduced:

$$D_{m,n+1} := \begin{vmatrix} c_m & c_{m-1} & \cdots & c_{m-n} \\ c_{m+1} & c_m & \cdots & c_{m+1-n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m+n} & c_{m+n-1} & & c_m \end{vmatrix} \tag{21}$$

with $D_{m,0} = 1$. Using this definition the normality of a Padé approximant $r_{m,n} = p_0/q_0$ can be expressed by the following theorem:

THEOREM 5. *The Padé approximant $r_{m,n} = p_0/q_0$ for f is normal if and only if the following equations hold*

$$\begin{array}{llll} \det & D_{m,n} & \neq 0 & \\ \det & D_{m+1,n} & \neq 0 & \\ \det & D_{m,n+1} & \neq 0 & . \\ \det & D_{m+1,n+1} & \neq 0 & \end{array} \tag{22}$$

3. Continued Fractions

Continued fractions have a very long history in mathematics. In the "Handbook of Mathematical Functions" (Abramowitz and Stegun, 1970) they are listed under elementary analytical methods, and for almost all functions in that book a continued fractions representation is given.

3.1. Notations and Definitions

A **continued fraction** is an expression of the form

$$C = b_0 + \frac{a_1}{b_1+}\frac{a_2}{b_2+}\frac{a_3}{b_3+}\ldots = b_0 + \sum_{i=1}^{\infty}\frac{a_i}{b_i+} = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + \cdots}}} \tag{23}$$

where the a_i and b_i are real (or complex) numbers or functions and are respectively called **partial numerators** and **partial denominators**. If

the number of terms is finite, C is called a terminating continued fraction. An example for this case is

$$1+\frac{x}{1/2+}\frac{x-1}{2/3+}\frac{x-2}{3/10}=1+\frac{x}{\frac{1}{2}+\frac{x-1}{\frac{2}{3}+\frac{x-2}{3/10}}} \quad . \tag{24}$$

A stepwise evaluation of that expression yields

$$\frac{2}{3}+\frac{x-2}{3/10}=\frac{10x-18}{3} \quad ,$$

$$\frac{1}{2}+\frac{x-1}{\frac{10x-18}{3}}=\frac{4x-6}{5x-9} \quad ,$$

$$1+\frac{x}{\frac{4x-6}{5x-9}}=\frac{4x-6+x(5x-9)}{4x-6}=\frac{5x^2-5x-6}{4x-6} \quad .$$

If the number of terms is infinite, C is called an infinite continued fraction and the terminating fraction

$$C_n=b_0+\sum_{i=1}^{n}\frac{a_i}{b_i+} \tag{25}$$

is called the n^{th} **convergent** of the continued fraction (23). As demonstrated in the above example the n^{th} convergent is the ratio of two polynomials

$$C_n=\frac{P_n}{Q_n}=\frac{P_n(b_0,a_1,b_1,\ldots,a_n,b_n)}{Q_n(b_0,a_1,b_1,\ldots,a_n,b_n)} \tag{26}$$

where P_n and Q_n are polynomials of a certain degree in the $2n+1$ partial numerators and denominators $b_0,a_1,b_1,\ldots,a_n,b_n$. The polynomials P_n and Q_n are respectively called the n^{th} **numerator** and the n^{th} **denominator** of the continued fraction (23). If $\lim_{n\to\infty} C_n$ exists and is finite, then the continued fraction is said to be **convergent** and C is called the value of the continued fraction. A simple case, in which there is always convergence is if $a_i=1$ and the $b's$ are all integers. This case, although it looks very special is significant since by equivalence transformations it is possible to rewrite a continued fraction in that or similars forms which allow simple convergence tests.

3.2. Fundamental Properties of Continued Fractions

3.2.1. Recurrence Relations for P_n and Q_n

As it can be shown by induction, the n^{th} numerator and denominator satisfy the same three-term recurrence relation but with different starting values, i.e., for $n\geq 1$

$$\begin{matrix}P_n=b_nP_{n-1}+a_nP_{n-2}\\ Q_n=b_nQ_{n-1}+a_nQ_{n-2}\end{matrix} \quad , \; P_{-1}=Q_0=1 \; , \; P_0=b_0 \; , \; Q_{-1}=0 \quad . \tag{27}$$

Again by induction, from (27) the relation

$$C_n - C_{n-1} = (-1)^{n+1} \frac{a_1 a_2 \dots a_n}{Q_n Q_{n-1}} \ , \ Q_n Q_{n-1} \neq 0 \tag{28}$$

can be derived which yields for the n^{th} convergent of the continued fraction

$$C_n = b_0 + \sum_{i=1}^{n} (-1)^{n+1} \frac{a_1 a_2 \dots a_n}{Q_n Q_{n-1}} \quad . \tag{29}$$

This sum is the n^{th} partial sum of the **Euler-Minding series**

$$b_0 + \sum_{i=1}^{\infty} (-1)^{n+1} \frac{a_1 a_2 \dots a_n}{Q_n Q_{n-1}} \quad . \tag{30}$$

Note that this establishes a relation between the n^{th} convergent of the continued fraction and the n^{th} partial sum of series. In general, a series $\sum_{i=0}^{\infty} d_i$ and a continued fraction $b_0 + \sum_{i=1}^{\infty} \frac{a_i}{b_i +}$ are called equivalent if for every $n \geq 0$ holds

$$D_n = \sum_{i=0}^{n} d_i = b_0 + \sum_{i=1}^{n} \frac{a_i}{b_i +} = C_n \tag{31}$$

i.e., the n^{th} partial sum D_n equals the n^{th} convergent C_n of the continued fraction . Another relation between successive convergents is

$$a_i, b_i > 0 \Rightarrow C_{2n} < C_{2n+2} \ , \ C_{2n-1} > C_{2n+1} \quad . \tag{32}$$

3.2.2. Equivalence transformations

The purpose of equivalence transformations of continued fractions is to rewrite them in a prescribed form which allows a better analysis, of e.g., convergence properties, of that continued fraction. Let $p_i \neq 0$ for $i \geq 0$. The transformation that alters the continued fraction (23) into

$$b_0 + \frac{p_1 a_1}{p_1 b_1 +} + \sum_{i=2}^{\infty} \frac{p_{i-1} p_i a_i}{p_i b_i +} \tag{33}$$

is called an equivalence transformation. If, for example, $a_i \neq 0, i \geq 1$, then by choosing

$$p_i = \frac{1}{a_i p_{i-1}} \ , \ p_0 = 1 \ , \ i \geq 1 \tag{34}$$

the continued fraction (23) takes the form of a **reduced continued fraction**, i.e.,

$$d_0 + \sum_{i=1}^{\infty} \frac{1}{d_i +} \quad . \tag{35}$$

If all $d's$ are positive then the reduced continued fraction is convergent.

3.2.3. Contraction of a Continued Fraction

The Euler-Minding series showed that there is an interrelation between continued fractions and the partial sums of a series. There is also a relation between the sequence $\{C_n\}_{n\in\mathbf{N}}$ of subsequently different elements and a continued fraction which can be constructed in such a way that C_n is the n^{th} convergent of that continued fraction. In order to do so it is sufficient to define the $a's$ and $b's$ as

$$a_1 = C_1 - C_0, b_0 = C_0, b_1 = 1, a_i = \frac{C_{i-1} - C_i}{C_{i-1} - C_{i-2}}, b_i = \frac{C_i - C_{i-2}}{C_{i-1} - C_{i-2}} \quad .(36)$$

3.3. Methods to construct Continued Fractions

There are many methods to construct continued fractions available. We will cover only a few and refer to other algorithms, e.g., successive substitution, and details to (Cuyt and Wuytack, 1987).

3.3.1. Equivalent continued fractions

A given series $\sum_{i=0}^{\infty} d_i$ can be represented by the continued fraction

$$d_0 + \frac{d_1}{1+}\frac{-d_2}{d_1 + d_2+}\sum_{i=3}^{\infty}\frac{-d_{i-2}d_i}{d_{i-1} + d_i+} \quad . \tag{37}$$

This formula can be derived from (36) with $C_n = \sum_{i=0}^{n} d_i$. In particular, (36) can be applied to the Taylor series expansion of a function, e.g.,

$$f(x) = e^x = \sum_{i=0}^{\infty}\frac{x^i}{i!} \quad . \tag{38}$$

In order to get used to the concepts established above let us consider this example in some detail. Since in the example $d_0 = 1$ (36) reduces to

$$1 + \frac{x}{1+}\sum_{i=2}^{\infty}\frac{-\frac{1}{(i-2)!}\frac{1}{i!}x^{i-2}x^i}{\frac{1}{(i-1)!}x^{i-1} + \frac{1}{i!}x^i+} \quad .$$

Performing the equivalent transformation $p = x^{i-1}$ and applying (33) yields

$$1 + \frac{x}{1+}\sum_{i=2}^{\infty}\frac{-\frac{1}{(i-2)!}\frac{1}{i!}x}{\frac{1}{(i-1)!} + \frac{1}{i!}x+} \quad .$$

Due to

$$\frac{1}{(i-1)!} + \frac{1}{i!}x = \frac{i}{i!} + \frac{1}{i!}x = \frac{i+x}{i!}$$

it is possible to apply another equivalence transformation $p = i!$ and to get the final result

$$e^x = 1 + \frac{x}{1+} \sum_{i=2}^{\infty} \frac{-(i-1)x}{i+x+} \quad . \tag{39}$$

Note that due to equivalence of (38) and (39) and the convergence of e^x in the whole complex plane, the sum $\sum_{i=2}^{\infty} \frac{-(i-1)x}{i+x+}$ is convergent, but by substituting $x \to -x$ and observing that e^{-x} is convergent also the sum $\sum_{i=2}^{\infty} \frac{(i-1)x}{i-x+}$ is convergent.

The continued fraction of a function is not unique. (Abramowitz and Stegun, 1970, p.70) give several continued fractions for e^x.

3.3.2. The Method of Viscovatov

The method of Viscovatov (Viscovatov, 1806) is used to develop a continued fraction expansion for functions given as the ratio of two power series

$$f(x) = \frac{d_{10} + d_{11}x + d_{12}x^2 + ...}{d_{00} + d_{01}x + d_{02}x^2 + ...} \tag{40}$$

which leads simply to

$$f(x) = \frac{d_{10}}{d_{00}+} \frac{d_{20}x}{d_{10}+} \frac{d_{30}x}{d_{20} + \cdots} \tag{41}$$

with

$$d_{k,i} = d_{k-1,0} \cdot d_{k-2,i+1} - d_{k-2,0} \cdot d_{k-1,i+1} \ , \ k > 2 \ , \ i \geq 0 \quad . \tag{42}$$

3.3.3. Corresponding and Associated Continued Fractions

Corresponding and associated continued fractions establish a link between Taylor series expansions and continued fractions. A continued fraction $b_0(x)+ \sum_{i=1}^{\infty} \frac{a_i(x)}{b_i(x)+}$ for which the Taylor series expansion of the n^{th} convergent $C_n(x)$ around the origin matches a given power series

$$f(x) = \sum_{i=0}^{\infty} c_i x^i \tag{43}$$

up to and including the term of degree n $(2n)$ is called **corresponding (associated)** to this power series, i.e., for a corresponding continued fraction, if

$$C_n(x) = b_0(x) + \sum_{i=1}^{\infty} \frac{a_i(x)}{b_i(x)+} = \sum_{i=0}^{\infty} d_i x^i \tag{44}$$

then for every n $(2n)$ we have $d_i = c_i$ for $i = 0, \ldots, n$. By applying the algorithm of Viscovatov to $(f(x) - c_0)/x$ with $d_{1i} = c_{1+i}$ for $i \geq 0$ the corresponding continued fraction for $f(x)$ follows as

$$f(x) = \frac{c_1}{1+} \frac{d_{20}x}{c_1+} \frac{d_{30}x}{d_{20} + \cdots} \tag{45}$$

because the Taylor series expansion of the k^{th} convergent matches the power series for $f(x)$ up to and including the term of degree k.

3.4. Convergence of Continued Fraction

A simple case, in which a continued fraction converges was already mentioned in a previous section and was expressed by the condition that $a_i = 1$ and the $b's$ are all integers. Many convergence theorems date to the 19^{th} century, e.g., the theorem by Seidel (Seidel, 1846): If $b_i > 0$ for $i \geq 1$, then the continued fraction $b_0 + \sum_{i=1}^{\infty} \frac{1}{b_i+}$ converges, if and only if the series $\sum_{i=1}^{\infty} b_i$ diverges. Another result is that the continued fraction $\sum_{i=1}^{\infty} \frac{a_i}{b_i+}$ converges if $|b_i| \geq |a_i| + 1$ for $i \geq 2$. For the n^{th} convergent C_n we have $|b_i| \geq |a_i| + 1$ for $i \geq 1$, and for C_n we have $|C_n| < 1$ if $n \geq 1$. While the results or theorems are easy to state, e.g., the continued fraction $\sum_{i=1}^{\infty} \frac{a_i}{1+}$ converges if $|a_i| \leq \frac{1}{4}$ for $i \geq 2$, many convergence properties of continued fractions are related to analyticity and can only be understood on the platform of complex calculus.

4. Methods to compute Padé approximants

There are many methods available to compute Padé approximants: corresponding continued fractions, the qd-algorithm (Cuyt and Wuytack, 1987, pp.79), the algorithm of Gragg (Cuyt and Wuytack, 1987, pp.83), solutions of the system of equations, determinant formulae, the method of Viscovatov (1806), recursive algorithm, and the famous ε-algorithm (Wynn, 1956). Some of them are briefly outlined in the following subsections.

4.1. Corresponding Continued Fractions

With this method it is possible to compute Padé approximants below the main diagonal in the Padé table. In order to do so consider the following sequence

$$T_k = \{r_{k,0}, r_{k+1,0}, r_{k+1,1}, r_{k+2,1}, \ldots\}$$

of elements on a descending staircase in the Padé table and the continued fraction

$$d_0 + d_1 x + \ldots + d_k x^k + \frac{d_{k+1}x^{k+1}}{1+} \frac{d_{k+2}x}{1+} \frac{d_{k+3}x}{1+} + \ldots \quad . \tag{46}$$

If every three consecutive elements in T_k are different, then a continued fraction of the form (46) exists with $d_{k+i} \neq 0$ for $i \geq 1$ and in such a way that the n^{th} convergent equals the $(n+1)^{th}$ element of T_k. If the n^{th} convergent equals the $(n+1)^{th}$ of T_0 $(n \geq 0)$, then (46) is the corresponding continued fraction to the power series (1). Details for the computation of the $d's$ are found in (Cuyt and Wuytack, 1987, pp.77).

4.2. Solution of the linear equations

The formal linear system which defines the Padé approximant has a very special form namely that of a Töplitz matrix. Nevertheless, unfortunately, the equations are frequently close to singular. Therefore, it is not advisable to solve it by specialized Töplitz methods. Rather, it is recommended to solve it by full LU decomposition. Additionally, it is a good idea to refine the solution by iterative improvements. Once the $b's$ are known, the $a's$ can be computed explicitly.

In the case $D = \det D_{m,n} \neq 0$ it is also possible to express the Padé approximant $r_{m,n}(x) = p_0(x)/q_0(x)$ by means of determinant formulae based on the abbreviations

$$F_k(x) := \begin{cases} \sum_{i=0}^{k} c_i x^i & , k \geq 0 \\ 0 & , k < 0 \end{cases} . \tag{47}$$

Then the numerator $p_0(x)$ and denominator $q_0(x)$ have the form

$$p_0(x) = \frac{1}{D} \begin{vmatrix} F_m(x) & xF_{m-1}(x) & \cdots & x^n F_{m-n}(x) \\ c_{m+1} & & & \\ \vdots & & D_{m,n} & \\ c_{m+1} & & & \end{vmatrix} \tag{48}$$

and

$$q_0(x) = \frac{1}{D} \begin{vmatrix} 1 & x & \cdots & x^n \\ c_{m+1} & & & \\ \vdots & & D_{m,n} & \\ c_{m+1} & & & \end{vmatrix} . \tag{49}$$

4.3. Recursive Algorithm to Compute Padé approximants

While corresponding continued fractions provide a mean to compute Padé approximants on descending staircases, the recursive algorithm (Cuyt and

Wuytack, 1987, pp.90) presented and proved in this section allows to calculate Padé approximants on ascending staircases. The recursive scheme is based on the normality of the Padé table and uses the nomenclature

$$r_{m,n} := r_{m,n}(x) = \frac{\sum_{i=0}^{m} a_{m,n}^{(i)} x^i}{\sum_{i=0}^{n} b_{m,n}^{(i)} x^i} \quad . \tag{50}$$

If the Padé approximants $r_{m,n} = \frac{p_3}{q_3}, r_{m,n-1} = \frac{p_2}{q_2}$ and $r_{m+1,n-1} = \frac{p_1}{q_1}$ are normal, then

$$\frac{p_3}{q_3} = \frac{a_{m,n-1}^{(m)} p_1 - a_{m+1,n-1}^{(m+1)} x p_2}{a_{m,n-1}^{(m)} q_1 - a_{m+1,n-1}^{(m+1)} x q_2} \quad . \tag{51}$$

This formula and the scheme behind it can be visualized as

$$\begin{array}{ccc} r_{m,n-1} & \rightarrow & r_{m,n} \\ r_{m+1,n-1} & \nearrow & \end{array} \iff \begin{array}{ccc} 2 & \rightarrow & 3 \\ 1 & \nearrow & \end{array} \quad . \tag{52}$$

The proof of (51) requires to show $\partial p_3 \leq m, \partial q_3 \leq n$ and $\omega(fq_3 - p_3) \geq m + n + 1$. The normality and the uniqueness of the Padé approximants then guarantee $\frac{p_3}{q_3} = r_{m,n}$. The second step ($\partial q_3 \leq n$) is easy. Since $r_{m,n-1}$ and $r_{m+1,n-1}$ are Padé approximants the inequalities $\partial q_1 \leq n - 1$ and $\partial(xq_2) = 1 + \partial q_2 \leq 1 + (n-1) = n$ hold. According to (12) this yields $\partial q_3 \leq n - 1$ as desired. Unfortunately, the same argumentation would only lead to $\partial p_3 \leq m + 1$ in the first case. In order to prove $\partial q_3 \leq m$ it must be shown that the coefficient with highest exponent vanishes. In order to do so define an operator $\hat{P}$ which maps a polynom $p(x)$ onto its term with the highest exponent, e.g., $\hat{P}\left[1 + x + 2x^2\right] = 2x^2, \hat{P}\left[p_1(x)\right] = a_{m+1,n-1}^{(m+1)} x^{m+1}$, or, $\hat{P}\left[p_2(x)\right] = a_{m,n-1}^{(m)} x^m$. Applying this operator onto $p_3(x)$ yields

$$\begin{aligned} \hat{P}\left[p_3(x)\right] &= a_{m,n-1}^{(m)} P\left[p_1\right] - a_{m+1,n-1}^{(m+1)} x P\left[p_2\right] \\ &= a_{m,n-1}^{(m)} a_{m+1,n-1}^{(m+1)} x^{m+1} - a_{m+1,n-1}^{(m+1)} x a_{m,n-1}^{(m)} x^m = 0 \end{aligned}$$

as wanted. Eventually, to prove the third property, consider $fq_3 - p_3$ in more details:

$$fq_3 - p_3 = a_{m,n-1}^{(m)}(fq_1 - p_1) - a_{m+1,n-1}^{(m+1)} x(fq_2 - p_2) \quad . \tag{53}$$

Then, again with (12) it follows

$$\begin{aligned} \omega(fq_3 - p_3) &= \min\{\omega(fq_3 - p_3), \omega(fq_3 - p_3)\} \\ &\geq \min\{(m+1) + (n+1), 1 + (m) + (n-1) + 1\} \\ &\geq m + n + 1 \end{aligned}$$

as desired.

As an example, we compute the Padé approximant $r_{0,2}$ of $f(x) = e^x = 1 + x + \frac{x^2}{2!} + \ldots$ (see Table 1), i.e.,

$$\begin{array}{lll} r_{0,1} = \frac{1}{1-x} & \rightarrow & r_{0,2} \\ r_{1,1} = \frac{1+\frac{1}{2}x}{1-\frac{1}{2}x} & \nearrow & \end{array} \quad .$$

Applying (51) yields

$$r_{0,2} = \frac{1 \cdot (1 + \frac{1}{2}x) - \frac{1}{2}x \cdot 1}{1 \cdot (1 - \frac{1}{2}x) - \frac{1}{2}x \cdot (1 - x)} \quad .$$

A similar formula as (51) provides a recursive scheme

$$\begin{array}{lll} & r_{m-1,n} & \\ \nearrow & \uparrow & \\ r_{m,n-1} & r_{m,n} & \end{array} \quad \Longleftrightarrow \quad \begin{array}{ll} & 3 \\ \nearrow & \uparrow \\ 1 & 2 \end{array} \quad . \tag{54}$$

As another application of (51) the Padé approximant $r_{1,1}$ of a second-order Taylor series expansion of a function

$$f(x) = f_0 + f_0' \cdot x + \frac{1}{2} f_0'' \cdot x^2 \tag{55}$$

is computed. In order to make things easier, put $c_0 = f_0 = f(0), c_1 = f_0' = f'(0)$, and $c_2 = f_0'' = \frac{1}{2} f''(0)$. The Padé table of that problem is

	0	1
0	c_0	
1	$c_0 + c_1 x$	?
2	$c_0 + c_1 x + c_2 x^2$	

.

Then, it is easy to derive the following results

$$\begin{aligned} r_{1,1} &= \frac{c_1(c_0 + c_1 x + c_2 x^2) - c_2(c_0 + c_1 x)}{c_1 \cdot 1 - c_2 \cdot 1} \\ &= \frac{c_0 c_1 + (c_1^2 - c_0 c_2)x}{c_1 - c_2} = c_1^2 \frac{c_0/c_1 + (1 - c_0 c_1 / c_1^2)x}{c_1 - c_2} \end{aligned}$$

or in the original notation

$$r_{1,1} = \frac{f_0'^2}{f_0' - \frac{1}{2} f_0''} \cdot \left[\frac{f_0}{f_0'} + \left(1 - \frac{1}{2} \frac{f_0 f_0''}{f_0'^2} \right) x \right] \quad . \tag{56}$$

This result is used later to derive a formula based on Padé approximants for solving nonlinear equations.

5. Rational Interpolants

Rational interpolants (Stoer, 1989, 2.2 Interpolation mit rationalen Funktionen) are defined in such a way that they reproduce a given data set of real or complex points $\{x_i, f_i\}_{i\in\mathbf{N}}$. These points may, or may not, represent a function f. This concept was first investigated by Cauchy (Cauchy, 1821). It generalizes that of Lagrangian interpolation based on polynomial interpolation. The rational interpolation problem of order (m, n) for f consists in finding a rational function $p(x)/q(x)$ or polynomials $p(x)$ and $q(x)$ defined in (2) with $p(x)/q(x)$ irreducible and in such a way that

$$f(x_i) = \frac{p(x_i)}{q(x_i)} \ , \ i = 0, \ldots, m+n \tag{57}$$

leading to the homogeneous system of $m + n + 1$ linear equations in the $m + n + 2$ unknown coefficients a_i and b_i of p and q

$$f(x_i)q(x_i) = p(x_i) \ , \ i = 0, \ldots, m+n \quad . \tag{58}$$

Similar as in the Padé approximation problem, an equivalence class is associated with this problem and the rational interpolant $r_{m,n}(x)$ is chosen to be the irreducible representative of this class. If the normalization $q_0(x_0) = 1$ leads to a rational function not fulfilling (57) anymore, then, the polynomials $p(x)$ and $q(x)$ may be multiplied by $\prod_{i=1}^{s}(x - y_i)$ where the s points y_i are elements of the set $\{x_0, , x_{m+n}\}$. Analogue to the Padé table, it is possible to construct the table of rational interpolants, which in its first column has the polynomial interpolant for f and in the first row the inverses of the polynomial interpolants for $1/f$. The table has features which are comparable with the block structure of the Padé table, and it has an analogue definition of normality.

5.1. Interpolating Data

The methods to compute rational interpolants are similar to those of Padé approximants. Most of them are based on continued fractions.

5.1.1. Interpolating continued fractions

This method is similar to the computation of Padé approximants by corresponding continued fractions. For a staircase of rational interpolants

$$T_k = \{r_{k,0}, r_{k+1,0}, r_{k+1,1}, r_{k+2,1}, \ldots \ , \ k \geq 0\} \tag{59}$$

coefficients d_i can be computed in such a way that the convergents $C_n(x_i)$ of the continued fraction

$$d_0 + d_1(x - x_0) + \ldots + d_k(x - x_0) \cdot \ldots \cdot (x - x_{k-1}) \tag{60}$$

$$+\frac{d_{k+1}d_k(x - x_0)\ldots(x - x_{k-1})}{1+}\frac{d_{k+2}(x - x_{k+1})}{1+}\frac{d_{k+3}(x - x_{k+2})}{1+} + \tag{61}$$

are precisely the subsequent elements of T_k. In order to have the property $C_n(x_i) = f(x_i)$ the $d's$ are chosen as $d_i = \varphi_i[x_0, \ldots, x_i]$, where $\varphi_k[x_0, \ldots, x_k]$ is called the k^{th} **inverse difference** of f in the points $x_0, \ldots, x_k$.

5.1.2. Inverse differences

The inverse differences are defined as

$$\varphi_0[x] = f(x) \ , \forall x \in G \subset \mathbf{C} \tag{62}$$

$$\varphi_1[x_0, x_1] = \frac{x_1 - x_0}{\varphi_0[x_1] - \varphi_0[x_0]} \ , \forall x_0, x_1 \in G \subset \mathbf{C} \tag{63}$$

$$= \frac{\varphi_k[x_0, x_1, \ldots, x_{k-2}, x_{k-1}, x_k]}{\varphi_{k-1}[x_0, x_1, \ldots, x_{k-2}, x_k] - \varphi_{k-1}[x_0, x_1, \ldots, x_{k-2}, x_{k-1}]} \quad . \tag{64}$$

The continued fraction

$$\varphi_0[x] + \frac{x - x_0}{\varphi_1[x_0, x_1] +} \frac{x - x_1}{\varphi_2[x_0, x_1, x_2] +} \tag{65}$$

is called **Thiele interpolating continued fraction**. As an example for a rational interpolant consider the four data points $\{(0,1),(1,3),(2,2),(3,4)\}$ which lead to the table

$$\begin{array}{llll} 1 & & & \\ 3 & 1/2 & & \\ 2 & 2 & 2/3 & \\ 4 & 1 & 4 & 3/10 \end{array} \quad .$$

The rational interpolant $r(x)$ interpolating these data points is the continued fraction (24)

$$1 + \frac{x}{1/2 +} \frac{x-1}{2/3 +} \frac{x-2}{3/10} = \frac{5x^2 - 5x - 6}{4x - 6} \quad .$$

For other algorithms to compute rational interpolants the reader is referred to (Cuyt and Wuytack, 1987, pp.143). In particular, a generalized ε-algorithm [(Wynn, 1956); (Cuyt and Wuytack, 1987, pp.151)] is available.

5.1.3. Stoer's recursive method

Particularly interesting is Stoer's recursive method since it is embedded in the Bulirsch-Stoer integrator for initial value problems (Bulirsch and Stoer, 1966). This method computes the value of an interpolant and not the interpolant itself. The polynomials

$$p_{m,n}^{(j)}(x) = \sum_{i=0}^{m} a_i x^i \ , \ q_{m,n}^{(j)}(x) = \sum_{i=0}^{n} a_i x^i \tag{66}$$

fulfill the interpolating conditions

$$f q_{m,n}^{(j)}(x) - p_{m,n}^{(j)}(x) = 0 \ , \ i = j, \ldots, j+m+n \quad .$$

Note that the interpolating problem starts at the point x_j. To express some relations between successive rational interpolants lying on the main descending staircase

$$\left\{ \frac{p_{0,0}^{(j)}}{q_{0,0}^{(j)}}, \frac{p_{1,0}^{(j)}}{q_{1,0}^{(j)}}, \frac{p_{1,1}^{(j)}}{q_{1,1}^{(j)}}, \frac{p_{2,1}^{(j)}}{q_{2,1}^{(j)}}, \ldots \right\} \tag{67}$$

let $a_{m,n}^{(j)}$ and $b_{m,n}^{(j)}$ indicate the coefficients of degree m and n in the polynomial $p_{m,n}^{(j)}$ and $q_{m,n}^{(j)}$ respectively:

$$\begin{aligned} p_{n,n}^{(j)} &= (x - x_j) a_{n,n-1}^{(j)} p_{n,n-1}^{(j+1)}(x) - (x - x_{j+2n}) a_{n,n-1}^{(j)} p_{n,n-1}^{(j+1)}(x) \\ q_{n,n}^{(j)} &= (x - x_j) a_{n,n-1}^{(j)} q_{n,n-1}^{(j+1)}(x) - (x - x_{j+2n}) a_{n,n-1}^{(j)} q_{n,n-1}^{(j+1)}(x) \end{aligned} \tag{68}$$

and

$$\begin{aligned} p_{n+1,n}^{(j)} &= (x - x_j) b_{n,n}^{(j)} p_{n,n}^{(j+1)}(x) - (x - x_{j+2n+1}) b_{n,n}^{(j+1)} p_{n,n}^{(j)}(x) \\ q_{n+1,n}^{(j)} &= (x - x_j) b_{n,n}^{(j)} q_{n,n}^{(j+1)}(x) - (x - x_{j+2n+1}) b_{n,n}^{(j+1)} q_{n,n}^{(j)}(x) \end{aligned} \tag{69}$$

with

$$p_{0,0}^{(j)} = f_j \ , \ q_{0,0}^{(j)} = 1 \quad . \tag{70}$$

Based on this fundamental relations it is possible to derive rational interpolants on the descending staircase

$$\left\{ \frac{p_{k,0}^{(j)}}{q_{k,0}^{(j)}}, \frac{p_{k+1,0}^{(j)}}{q_{k+1,0}^{(j)}}, \frac{p_{k+1,1}^{(j)}}{q_{k+1,1}^{(j)}}, \ldots \right\} \tag{71}$$

with

$$p_{k,0}^{(j)} = c_0 + \sum_{i=1}^{k} c_i \cdot (x - x_j) \cdot \ldots \cdot (x - x_{j+i-1}) \ , \ p_{k,0}^{(j)} = 1 \tag{72}$$

where the c_i are divided divergences of f.

5.2. Rational Hermite Interpolation

A more general interpolation problem is the rational Hermite interpolation problem of order (m, n) for f which consists in computing polynomials $p(x)$ and $q(x)$ with p/q irreducible and satisfying

$$\begin{aligned} f^{(l)}(x_i) &= \left(\frac{p}{q}\right)^{(l)}(x_i) \ \forall l = 0, \ldots, s_i - 1 \ ; \ i = 0, \ldots, j \\ f^{(l)}(x_{j+1}) &= \left(\frac{p}{q}\right)^{(l)}(x_{j+1}) \ \forall l = 0, \ldots, k - 1 \end{aligned} \tag{73}$$

where (l) denotes the l^{th} derivative, and s_i interpolation points coincidence with x_i, i.e., s_i interpolation conditions must be fulfilled in x_i, and

$$1 \leq k \leq s_{j+1} \ , \ m + n + 1 = \sum_{i=0}^{j} s_i + k \quad . \tag{74}$$

There are two special cases: $s_i = 1$ for all $i \geq 0$ reproduces the rational interpolation problem, and $j = 0$, i.e., all conditions must be fulfilled in one single point, which is identical to the Padé approximation problem. A related problem is the **Newton-Padé approximation problem** (Cuyt and Wuytack, 1987, pp.157) which is solved by the **Newton-Padé approximant**. As the other problems presented in this paper, determinant representation, continued fraction representation, or Thiele's continued fraction expansion may be applied to derive the Newton-Padé approximant.

5.3. Fitting Rational Functions to Data

Similar to the generalized concept between polynomial interpolation and fitting polynomials to given data sets, it is possible to fit rational functions to a set of data points adjusting the parameters a_i and b_i. However different from polynomial least squares problems, rational function least squares problems are nonlinear least squares problem (Eichhorn, 1993). They are much more difficult to solve and therefore fitting rational functions is a only rarely discussed topic. They may be formulated as a special case of unconstrained minimization with an objective function of the form

$$f(\mathbf{y}) = \sum_{\nu=1}^{N} [r_\nu(\mathbf{y})]^2 = \mathbf{r}^t\mathbf{r} \quad . \tag{75}$$

in such a way a structure may arise either from a nonlinear over-determined systems of equations

$$r_\nu(\mathbf{y}) = 0 \ , \ \nu = 1, ..., N \ , \ N > M \quad , \tag{76}$$

or from a data fitting problem with N given data points (x_ν, d_ν) and variances σ_ν, a model function $\Phi(x, \mathbf{y})$, possibly a rational function, and M adjustable parameters $\mathbf{x}$:

$$r_\nu := r_\nu(\mathbf{y}) = \frac{1}{\sqrt{\sigma_\nu}} \left[\Phi(x_\nu, \mathbf{y}) - d_\nu\right] \quad . \tag{77}$$

The weights w_ν may be derived from the variances σ_ν and chosen as

$$w_\nu := \frac{1}{\sigma_\nu^2} \quad . \tag{78}$$

If the model function $\Phi(x, \mathbf{y})$ is chosen as a rational function $R(x) = p(x)/q(x)$ then the vector $\mathbf{y}$ represents the coefficients of the polynomials, i.e., $\mathbf{y} = [a_0, a_1, \ldots, a_m, b_1, \ldots, b_n]^t$ and $M = m + n + 1$. The special case $N = M$ is again the rational interpolation problem.

Due to the limited space, for the case $N > M$, it is only possible to give a brief scetch on how $f(\mathbf{y})$ is minimized with respect to $\mathbf{y}$. With the definition

$$A_{\nu j} := \frac{\partial r_\nu}{\partial y_j} \Longleftrightarrow A(\mathbf{y}) := [\bigtriangledown r_1, \bigtriangledown r_2, ..., \bigtriangledown r_N.] \tag{79}$$

the first and second derivatives, i.e, the Jacobian J and the Hessian H of $f(\mathbf{y})$ follows as

$$J = 2A\mathbf{r} \ , \ H = 2AA^t + 2 \cdot \sum_{\nu=1}^{N} \left[r_\nu \bigtriangledown^2 r_\nu\right] \quad . \tag{80}$$

If the second derivatives $\bigtriangledown^2 r_\nu$ are at hand then (80) can be used in the quasi-Newton method. However in most practical cases it is possible to utilize a typical property of least squares problems. The components r_ν are expected to be small, and H might be sufficiently well approximated by

$$H \approx 2AA^t \quad . \tag{81}$$

This approximation of the Hessian matrix is also achieved if the residuals r_ν are taken up to linear order. Note, that by this approximation the second derivative method only requires first derivative information. This is typical for least squares problems and this special variant of Newton's method is called *Gauss-Newton method* (or generalized least squares method). The damped Gauss-Newton method including a line search iterates the solution of $\mathbf{y}_k$ of the k^{th} iteration to $\mathbf{y}_{k+1}$ according to the following scheme:

- determination of a search direction $\mathbf{s}_k$ by solving $A_k A_k^t \mathbf{s}_k = -A_k \mathbf{r}_k$ which is analagous to the normal equation of linear least squares
- solving the *line search subproblem*, i.e, finding $\alpha_k = \arg\min\{\ f(\mathbf{y}_k + \alpha \mathbf{s}_k) \mid 0 < \alpha \leq 1\}$

– defining $\mathbf{y}_{k+1} = \mathbf{y}_k + \alpha_k \mathbf{s}_k$

Note, that the Gauss-Newton method and its convergence properties depend strongly and the approximation of the Hessian matrix. In large residual problems the term $\sum_{\nu=1}^{N} \left[r_\nu \bigtriangledown^2 r_\nu \right]$ in (80) becomes substantial, and the rate of convergence becomes poor.

6. Applications of Padé approximants in Applied Mathematics

There is a wide variety of problems occurring in applied mathematics which benefit from Padé approximants. Some examples like nonlinear equation solving or integration of initial value problems are briefly discussed while for applications of Padé approximants or rational interpolants to partial differential equations or integral equations the reader is referred to (Cuyt and Wuytack, 1987). Another application is the Laplace transform inversion (Brezinski, 1983).

6.1. Solving nonlinear equations $f(x) = 0$

Let x_i be an approximate solution of the equation $f(x) = 0$. Most numerical procedures iterate as

$$x_{i+1} = x_i + \Delta x_i \quad . \tag{82}$$

They differ in the way Δx_i is computed. For abbreviation let us define

$$f = f(x_i) \ , \ f' = f'(x_i) \ , \ f'' = f''(x_i) \quad .$$

While Newton's method ($m = 1, n = 0$) is based on the linearization

$$f(x) \approx f(x_i) + f'(x_i)(x - x_i) \tag{83}$$

yielding

$$\Delta x_i = -\frac{f}{f'} \tag{84}$$

the 2^{nd} order Taylor expansion ($m = 2, n = 0$)

$$f(x) \approx f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(x_i)(x - x_i)^2 \tag{85}$$

gives

$$\Delta x_i = -\frac{1}{f''} \cdot \left[f' \mp \sqrt{(f')^2 - 2ff''} \right] \tag{86}$$

with a much smaller convergence region and the problem of choosing the right sign. With the knowledge of f, f', and f'' the Padé approximant corresponding to the expansion (85) follows according to (56) as

$$r_{11}(x) = \frac{f'(x_i)^2}{f'(x_i) - \frac{1}{2}f''(x_i)} \cdot \left[\frac{f(x_i)}{f'(x_i)} + \left(1 - \frac{1}{2} \frac{f(x_i)f'(x_i)}{f'(x_i)^2} \right) (x - x_i) \right] \quad .(87)$$

Putting $r_{11}(x) = 0$, yields

$$\Delta x_i = -\frac{f/f'}{1 - \frac{1}{2}\frac{f''f}{f'^2}} = -\frac{ff'}{f'^2 - \frac{1}{2}ff''} \tag{88}$$

which is known as Halley's method. Note the similarities between the Newton algorithm and the result based on $r_{11}(x)$. Both contain the term $-f/f'$. In general, if instead of $r_{11}(x)$ the Padé approximant $r_{m,n}(x)$ of order (m, n) is used to determine Δx_i, the order of convergence is at least $m+n+1$, i.e.,

$$\lim_{i \to \infty} \frac{|x_{i+1} - x^*|}{|x_i - x^*|^{m+n+1}} = C^* < \infty \quad .$$

This is in agreement with the known convergence properties of Newton's method (2^{nd} order). Both, the iteration based on the second order Taylor series, and Halley's method have at least an order of convergence which is 3. However iterative methods resulting from the use of (m, n) Padé approximants with $n > 0$ can be interesting because the asymptotic error constant C^* may be smaller than in the case of $n = 0$ (Merz, 1968).

Similar to Newton's method, it is also possible to generalize Halley's method for the solution of a system of nonlinear equations (Cuyt and Wuytack, 1987, pp.222).

6.1.1. Solving Kepler's equation using Padé approximants

In order to demonstrate the application of the Padé approximants to a problem relevant to Astronomy consider Kepler's equation

$$E - e \sin E = M \ , \ M \in [0, 2\pi) \ , \ e \in [0, 1] \tag{89}$$

which yields

$$f(x) = x - e \sin x - M \tag{90}$$

and

$$f'(x) = 1 - e \cos x \ , \ f''(x) = e \sin x \quad . \tag{91}$$

The correction Δx_i derived from the Padé approximant of order (m, n) is

$$\begin{aligned} \Delta x_i &= -\frac{f/f'}{1-\frac{1}{2}\frac{f''f}{f'^2}} = -\frac{ff'}{f'^2-\frac{1}{2}ff''} \\ &= -\frac{(x-e\sin x-M)\cdot(1-e\cos x)}{(1-e\cos x)^2-\frac{1}{2}(x-e\sin x-M)\cdot e\sin x} \quad . \end{aligned} \tag{92}$$

Table 3 contains the iterations for solving (89) for $M = 0.6$ and $e = 0.9$ with the initial approximation $x_0 = 0.08$ and the result $x = 1.497589413390409$. Note that this result is achieved first by the iteration based on the Padé approximant $r_{11}(x)$. The second order Taylor series ansatz also beats the Newton procedure. However this ansatz cannot be used with the initial value $x_0 = 0$. Even more drastically is the result achieved with the initial value $x_0 = 0.07$. In that case, Newton's method diverges while the other methods perform as for $x_0 = 0.08$.

Table 3: Different approaches to solve of Kepler's equation

i	Newton's method	2^{nd} order Taylor series	Halley's method (Padé)
0	0.08	0.08	0.08
1	5.83361644869743	2.951454104137709	1.990737759621929
2	-23.8595077579223	1.725646756896568	1.515004434940171
3	10.53662172774097	1.497774911860013	1.497590554024128
4	2.855615982488301	1.497589413390334	1.497589413390409
5	1.78140789166866	1.497589413390408	1.497589413390409
6	1.527825081877051	1.497589413390409	1.497589413390409
7	1.498016733395694	1.497589413390409	1.497589413390409
8	1.497589501081973	1.497589413390409	1.497589413390409
9	1.497589413390412	1.497589413390409	1.497589413390409
10	1.497589413390408	1.497589413390409	1.497589413390409

6.2. Integrating Differential Equations - Initial Value Problems

Numerically, a first order differential equation initial value problem

$$y' = \frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y) \ , \ x \in [a, b] \ , \ y(a) = y_0 \tag{93}$$

is solved by discretizing the interval $[a, b]$ in, say k points

$$x_i = a + ih \ , \ i = 0, \ldots, k \tag{94}$$

with

$$h = \frac{b-a}{k} \ , \ k > 0 \quad .$$

In general, methods which calculate approximations y_{i+1} for $y(x_{i+1})$ by constructing local approximations for the solution $y(x)$ of (93) at the point x_i of the form

$$y_{i+1} = y_i + hg(x_i, y_i, h) \ , \ i = 0, \ldots, k-1 \tag{95}$$

are called **explicit one-step methods**. Usually, the function $g(x_i, y_i, h)$ is related to the power series

$$y_i + (x - x_i)f(x_i, y_i) + f'(x_i, y_i) + \ldots \tag{96}$$

which approximates the Taylor series expansion

$$y(x_i) + (x - x_i)f(x_i, y(x_i)) + f'(x_i, y(x_i) + \ldots \quad .$$

Now it is possible to construct the Padé approximant $r_i(x)$ of order (m, n) for the power series (96). Putting $x = x_{i+1}$ and replacing $x - x_i = h$ leads to $y_{i+1} = r_i(x_{i+1})$. The method is of order p if the Taylor series expansion for $g(x, y, h)$ satisfies

$$y(x_{i+1}) - y(x_i) - hg(x_i, y(x_i), h) = O\left(h^{p+1}\right) \quad . \tag{97}$$

Therefore, the method is of order $(m + n)$ if $r_i(x)$ is a normal Padé approximant. The Padé approximant of order $(1, 0)$ reproduces Euler's method

$$y_{i+1} = y_i + hf(x_i, y_i) \tag{98}$$

and the Padé approximant of order $(1, 1)$ has the form

$$y_{i+1} = y_i + h\left[\frac{2f^2(x_i, y_i)}{2f(x_i, y_i) - hf'(x_i, y_i)}\right] \quad . \tag{99}$$

Padé approximants can be very interesting when integrating stiff differential equations which have the property that $\frac{\partial f(x,y)}{\partial y}$ has a large real negative part, e.g., $y' = \lambda y$ with $\mathrm{Re}(\lambda)$ large and negative, and the solution $y(x) = e^{\lambda x}$, and therefore $\lim y(x) = \lim e^{\lambda x} = 0$. Methods are called **A-stable** (Dahlquist, 1963) if they yield a numerical solution of $y' = \lambda y$ with $\mathrm{Re}(\lambda) < 0$ which tends to zero as $i \to \infty$ for any fixed positive h. If a Padé approximant of order $(m, m), (m, m + 1)$, or $(m, m + 2)$ is used to construct $g(x_i, y(x_i), h)$ then the resulting scheme is A-stable (Ehle, 1973).

6.3. Numerical Integration

Consider $I = \int_a^b f(x)dx$. Many methods for computing an approximate value to this integral replace f by an interpolating polynomial and hence compute I as a linear combination of function values. Popular quadrature rules are the Newton-Cotes formulas (Trapez-rule, Simpson-rule). Polynomial Hermite interpolation also considers derivative information. Naturally, after what has been said in the previous section, rational interpolants are an appropriate mean to compute I. Alternatively, Padé approximants may be used as for integrating initial value problems, realizing that

$$I = y(b) \ , \ y'(x) = f(x) \ , \ y(a) = 0 \tag{100}$$

leads

$$\int_{x_i}^{x_{i+1}} f(t)\mathrm{d}t \simeq h\frac{2f^2(x_i)}{2f(x_i) - hf'(x_i)} \quad . \tag{101}$$

7. Applications of Padé approximants in Applied Sciences

Padé approximants are used in statistical physics of phase transitions and critical phenomena (Hunter and Baker, 1973), scattering physics, e.g., non-relativistic, quantum mechanical scattering by a fixed potential source, electric circuits (passive, linear, lumped, reciprocal networks), dynamic dipole polarizability for an atomic or molecular system. They are very helpful on problems where the solution is obtained as a (divergent or convergent) power series whose coefficients can be hardly computed.

8. Remarks and Conclusions

8.1. Multivariate Cases

The problems and the methods to deal with them presented in this paper were explained for the univariate case, i.e., for functions

$$f : \Re \to \Re, x \to f(x) \quad . \tag{102}$$

In some places it has been stressed that the formalism works also for complex functions with complex arguments. Furthermore, it is possible to generalize the concepts to the multivariate case

$$f : \Re^n \to \Re^m, \mathbf{x} \to f(\mathbf{x}) \tag{103}$$

for which the reader is referred to (Cuyt and Wuytack, 1987).

8.2. Convergence of Rational interpolants and Padé approximants

At several places throughout this paper it has been mentioned that the convergence properties of rational interpolants and Padé approximants are connected analyticity and need to be investigated on the background of complex calculus. It was beyond the scope of this contribution to cover those aspects. The reader is referred to (Baker, 1975) for convergence theory. There are fascinating results which relate convergence properties of Padé approximants to the distribution of poles and zeros of the underlying function f, e.g., the Baker-Gammel-Wills conjecture.

8.3. Topics not covered

It was not possible either to illuminate the connection of Padé approximants and the theory of formal orthogonal polynomials (Brezinski, 1983) which plays a fundamental role in the algebraic theory of Padé approximants. They provide a natural basis to derive recursive methods for computing any sequence of Padé approximants. Furthermore, Padé approximants are closely related to Gaussian quadrature methods.

A generalization of Padé approximants themselves is a relaxation of the requirements with respect to the denominator (choice of the poles), leads to the concept of Padé-type approximants [(Brezinski, 1979);(Brezinski, 1980)].

8.4. Linear methods and nonlinear analogues

As a conclusion it can be said that every linear method has its nonlinear analogue. In case, the linear methods are inaccurate or divergent it is recommended to use a similar nonlinear technique. Padé approximants and rational techniques (rational interpolants, continued fractions, etc.) are useful for that purpose. The price to be paid for the ability of the nonlinear method to cope with the singularities is the programming difficulty of avoiding divisions by small numbers within actual programs. Closing the circle, the latter, is a well-known problem within perturbations methods in celestial mechanics.

References

Abramowitz, M. and Stegun, I.: 1970, *Handbook of Mathematical Functions*, Dover Publications, New York - Oxford, ninth edition

Baker, G.: 1975, *Essentials of Padé Approximants*, Academic Press, New York - San Francisco - London

Brezinski, C.: 1979, Rational approximations to formal power series, *J. Approx. Theory* **25**, 295–317

Brezinski, C.: 1980, *Padé-type approximation and general orthogonal polynomials*, Vol. 50 of *ISNM*, Birkhäuser, Basel

Brezinski, C.: 1983, *Padé Approximants: Old and New*, pp 37–63, Bibliographisches Institut, Mannheim

Brezinski, C.: 1991, *A Bibliography on Continued Fractions, Padé Approximations, Extrapolation and Related Subjects*, Technical report, Prensas Universitarias de Zaragosa, Zaragoza

Bulirsch, R. and Stoer, J.: 1966, Numerical treatment of ordinary differential equations by extrapolation methods, *Numerische Mathematik* **8**, 1–13

Cauchy, M.-L.: 1821, *Cours d'Analyse de L'École Royale Polytechnique. I.^{re} Partie: Analyse Algébrique*, Límprimerie Royal, Paris

Contopoulos, G. and Seimenis, J.: 1975, Application of the Prendergast method to a logarithmic potential, *Astronomy and Astropyhsics* **227**, 49–53

Cuyt, A. and Wuytack, L.: 1987, *Nonlinear Methods in Numerical Analysis*, North Holland Publishing Company, Amsterdam - New York - Oxford - Tokyo

Dahlquist, G.: 1963, A special stability problem for linear multistep methods, *BIT* **3**, 27–43

Ehle, B.: 1973, A-stable methods and Padé approximants to the exponential, *SIAM J.Math.Anal.* **4**, 671–680

Eichhorn, H.: 1993, Generalized least squares adjustment, a timely but much neglected tool, *Celestial Mechanics and Dynamical Astronomy* **56**, 337–351

Hunter, D. and Baker, G.: 1973, Methods of series analysis I. comparison of current methods used in the theory of critical phenomena, *Phys.Rev. B* **7**, 3346

Merz, G.: 1968, Padésche Näherungsbrüche und Iterationsverfahren höherer Ordnung, *Computing* **3**, 165–183

Padé, H.: 1892, Sur la représentation approchée d'une fonction pour des fractions rationelles, *Ann.Sci.École Norm.Sup.Suppl.* **9**, 1–93

Prendergast, K.: 1982, Rational approximation for nonlinear ordinary nonlinear least squares problems, in D. Chudnovsky and G. Chudnovsky (eds.), *The Riemann Problem*, No. 925 in Springer Lecture Notes in Mathematics, Springer

Press, W. and Teukolsky, S.: 1992, Padé Approximants, *Computers in Physics* **6**, 82–83

Seidel, L.: 1846, Habilschrift, München

Stoer, J.: 1989, *Numerische Mathematik 1*, Springer, Berlin Heidelberg New York, 5th edition edition

Viscovatov, B.: 1803-1806, *De la méthode génerale pour reduire toutes sortes de quantités en fractions continues*, Technical Report 1, Mém. Acad. Impériale Sci., St. Petersburg, Russia

Wuytack, L.: 1979, *Padé approximation and its application*, Vol. 765 of *Lectures Notes in Mathematics*, Springer, Berlin

Wynn, P.: 1956, On a device for computing the $e_m(s_n)$ transformation, *Math. Tables Aids Comput.* **10**, 91–96