Some new uses of the $\eta_m(Z)$ functions

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Abstract

We present a techique and a MATHEMATICA code for the conversion of formulae expressed in terms of the trigonometric functions $\sin(\omega x), \cos(\omega x)$ or hyperbolic functions $\sinh(\lambda x), \cosh(\lambda x)$ to forms expressed in terms of $\eta_m(Z)$ functions. The possibility of such a conversion is important in the evaluation of the coefficients of the approximation rules derived in the frame of the exponential fitting. The converted expressions allow, among others, a full elimination of the 0/0 undeterminacy, uniform accuracy in the computation of the coefficients, and an extended area of validity for the corresponding approximation formulae.

PACS: 02.60.Lj; 02.70.Wz; 03.65.Ge.

Key words: η_m set of functions, exponential fitting, approximation formulae

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PROGRAM SUMMARY

Program Title: formConv
Journal Reference:
Catalogue identifier:
Licensing provisions: none
Programming language: MATHEMATICA
Computer: generic
Operating system: generic
RAM: 15MB

[1] Corresponding author

Keywords: η_m set of functions, exponential fitting, approximation formulae
PACS: 02.60.Lj, 02.70.Wz, 03.65.Ge.
Classification: 5.
Subprograms used: vDeg, etaTransf, ZpowerTransf
Method of solution: analytic algebraic manipulation
Typical tunning time: a few seconds
References:

[1] L. Gr. Ixaru, *Numerical Methods for Differential Equations and Applications*, Reidel, Dordrecht, Boston, Lancaster, 1984.

1 Introduction

The functions $\eta_m(Z)$, $m = -1, 0, 1, \ldots$ have been introduced in [1] to provide a convenient framework when building up CP methods for the Schrödinger equation. However, as observed later on, the area of applications is much larger, including the possibility of a systematic treatment of oscillatory functions or of functions with an exponential behaviour. In particular this set of functions has been used successfully in building up a number of approximation formulae based on the exponential fitting (ef), see [2].
In most applications the argument Z and $\eta_m(Z)$ are real, and in these cases the η_m functions are closely related to the Bessel functions of real/imaginary argument, see property (v) below, but there are also cases when the argument and the function values are complex. Fortran subroutines for these functions are available, e.g., subroutines GEBASE in [3] and CGEBAS in [4] (up to $m = 6$), and GEBASE, GEBASEV, CGEBASE, CGEBASEV in [5]. A matlab version is in [6] and on the web-page http://www.dmi.unisa.it/people/conte/www/codici.html.
In this paper we focus on some new applications when building up formulae in the frame of the exponential fitting procedure. The coefficients in such formulae are functions of the involved frequencies with the property that they tend to the constant values of the coefficients in the associate classical approximation formulae when the frequencies tend to zero.
To fix the ideas we concentrate on the case when only one frequency μ is involved. Its value is real, $\mu = \lambda$, for functions which behave like $\exp(\pm\lambda x)$ or like $\sinh(\lambda x)$ and $\cosh(\lambda x)$, and imaginary $\mu = i\omega$ for oscillatory functions with $\sin(\omega x)$ and $\cos(\omega x)$. In all these cases the coefficients are functions of the product $z = \mu h$ which is either real or purely imaginary. An alternative notation consists in using one and the same real parameter v defined as $v = |z| = |\mu|h$ in both cases but in this situation we have to take care that either hyperbolic or trigonometric functions are involved.
An unpleasant feature with the expressions of the coefficients in the ef-based formulae is that quite often these exhibit an undeterminacy of the form $0/0$ when $z = 0$ or $v = 0$ and therefore additional expressions consisting in power expansions in z or v must be provided for use when $|z|$ or v is smaller than some threshold value. This is how it is done in many papers, to mention only [7], [8], [9], [10], [11], [12].
In this paper we show that the functions $\eta_m(Z)$ where $Z = (\mu h)^2$ (or, with the other

notation, $Z = -v^2$ / $Z = v^2$ in the trigonometric/hyperbolic case) provide a powerful tool for eliminating the 0/0 behaviour entirely, and develop a technique to be used for this aim. The new formulae will then cover all z or v, with no need to invoke series. One and the same expression is then enough irrespective of whether Z is positive or negative, small or big. Even more, the new expression can be used also when Z is complex.

2 Definition and properties of functions $\eta_m(Z)$, $m = -1, 0, 1, \ldots$

These functions have been introduced in [1] as real functions of a real variable, and denoted $\bar{\xi}(Z), \bar{\eta}_0(Z), \bar{\eta}_1(Z), \ldots$. The present notation is that from [2] except for $\eta_{-1}(Z)$ which was there denoted $\xi(Z)$. Later on, [4], these functions have been extended for complex argument Z.

The functions $\eta_{-1}(Z)$ and $\eta_0(Z)$ are defined in terms of some standard functions. When Z is real the familiar trigonometric or hyperbolic functions are used :

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0 \\ \cosh(Z^{1/2}) & \text{if } Z > 0 \end{cases} , \quad \eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \,. \end{cases} \tag{2.1}$$

Notice that when $Z < 0$ function $\eta_0(Z)$ is closely related to the sinc function, $\eta_0(Z) = \mathrm{sinc}(\sqrt{|Z|})$.
When Z is complex the functions sin and cos of a complex argument are involved, as it follows:

$$\eta_{-1}(Z) = \cos(iZ^{1/2}) \,, \quad \eta_0(Z) = \begin{cases} \sin(iZ^{1/2})/iZ^{1/2} & \text{if } Z \neq 0 \\ 1 & \text{if } Z = 0 \,. \end{cases} \tag{2.2}$$

Finally, an equivalent definition is through exponential functions of a complex argument,

$$\eta_{-1}(Z) = \frac{1}{2}[\exp(Z^{1/2}) + \exp(-Z^{1/2})] \,,$$

$$\eta_0(Z) = \begin{cases} \dfrac{1}{2Z^{1/2}}[\exp(Z^{1/2}) - \exp(-Z^{1/2})] & \text{if } Z \neq 0 \\ 1 & \text{if } Z = 0 \,, \end{cases} \tag{2.3}$$

as in [5].
The functions $\eta_m(Z)$ with $m > 0$ are further generated by recurrence

$$\eta_m(Z) = [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z, \ m = \ 1, \ 2, \ 3, \ldots \tag{2.4}$$

if $Z \neq 0$, and by following values at $Z = 0$:

$$\eta_m(0) = 1/(2m+1)!!,\ m = \ 1,\ 2,\ 3, ... \tag{2.5}$$

Some useful properties when Z is real are as follows :
(i) Series expansion :

$$\eta_m(Z) = 2^m \sum_{q=0}^{\infty} \frac{(q+m)!}{q!(2q+2m+1)!} Z^q \,,\ m = \ 0,\ 1,\ 2, \ldots \tag{2.6}$$

(ii) Asymptotic behaviour at large $|Z|$:

$$\eta_m(Z) \approx \begin{cases} \eta_{-1}(Z)/Z^{(m+1)/2} & \text{for odd } m\,, \\ \eta_0(Z)/Z^{m/2} & \text{for even } m\,. \end{cases} \tag{2.7}$$

(iii) Differentiation properties :

$$\eta_m'(Z) = \frac{1}{2}\eta_{m+1}(Z)\,,\ m = -1,\ 0,\ 1,\ 2,\ 3, \ldots \tag{2.8}$$

(iv) Generating differential equation: $\eta_m(Z),\ m = 0,\ 1,\ \ldots$ is the regular solution at $Z = 0$ of

$$Zw'' + \frac{1}{2}(2m+3)w' - \frac{1}{4}w = 0. \tag{2.9}$$

(v) Relation with the spherical Bessel functions :

$$\eta_m(-x^2) = \ x^{-m} j_m(x),\ m = 0,\ 1,\ \ldots \tag{2.10}$$

Most of these, in particular (i) and (iii), remain valid also for complex Z.

The property presented in the following theorem will be crucial for the development of the method described in the next section. It is valid irrespective of whether Z is real or complex.
Theorem. *The functions $\eta_m(Z)$ satisfy the following relations*

$$\eta_m(Z) = \eta_m(0) + ZD_m(Z),\ m = -1, 0, 1, 2, 3\ \ldots \tag{2.11}$$

where

$$D_m(Z) = \eta_m(0)\left[\frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right) - \sum_{i=1}^{m+1}(2i-3)!!\eta_i\,(Z)\right]. \tag{2.12}$$

Proof: We at first observe that, from definition (2.4),

$$\eta_m(Z) = \frac{\eta_{m-1}(Z) - Z\eta_{m+1}(Z)}{2m+1},\ m = \ 0, 1,\ 2, ... \tag{2.13}$$

and proceed by induction on m. For $m=-1$, we have (see book [5])

$$\eta_{-1}(Z) = 1 + \frac{1}{2} Z \eta_0^2 \left(\frac{Z}{4}\right) = \eta_{-1}(0) + Z D_{-1}(Z).$$

Let us suppose $m \geq 0$ and let (2.11)-(2.12) be valid for $m-1$, i.e.

$$\eta_{m-1}(Z) = \eta_{m-1}(0) + Z D_{m-1}(Z) \tag{2.14}$$

with

$$D_{m-1}(Z) = \eta_{m-1}(0) \left[\frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right) - \sum_{i=1}^{m} (2i-3)!!\eta_i(Z)\right]. \tag{2.15}$$

By substituting (2.14) in (2.13), and by using (2.5), which shows that $\eta_{m+1}(0) = \eta_{m-1}(0)/(2m+1)$, we have

$$\begin{aligned}\eta_m(Z) &= \frac{\eta_{m-1}(0) + Z\left(D_{m-1}(Z) - \eta_{m+1}(Z)\right)}{2m+1} \\ &= \eta_{m+1}(0) + Z\frac{D_{m-1}(Z) - \eta_{m+1}(Z)}{2m+1}.\end{aligned}$$

From (2.15) we have

$$\begin{aligned}\frac{D_{m-1}(Z) - \eta_{m+1}(Z)}{2m+1} &= \frac{\eta_{m-1}(0)\left[\frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right) - \sum_{i=1}^{m}(2i-3)!!\eta_i(Z) - (2m-1)!!\eta_{m+1}(Z)\right]}{2m+1} \\ &= D_m(Z),\end{aligned}$$

which concludes the proof.

3 Description of the method and of the program

Let $\phi(v)$ be a linear combination of products of either trigonometric or hyperbolic functions of v (coexistence of these species is not allowed), with the property that $\phi(0)=0$. In this section we develop a method for converting this into a function of the form $v^r Z^k F(Z)$ where r and k are non-negative integers, and $F(Z)$ is a linear combination of products of $\eta(Z)$ functions of the argument $Z=-v^2$ in the trigonometric case and $Z=v^2$ in the hyperbolic case, with the property that $F(0)\neq 0$.
The advantage with such a conversion is that the elements which make the original function $\phi(v)$ vanishing at $v=0$ are now concentrated in the factor $v^r Z^k$. The applicability is straightforward: since the coefficients of the formulae built up in the frame of the exponential fitting procedure are expressed by ratios of two such functions, the use of our procedure analytically eliminates the mentioned unpleasant 0/0 behaviour.

The most general form of $\phi(v)$ to be covered by our procedure is

$$\phi(v) = \sum_{n=1}^{N} \alpha_n(v) \left[\prod_{i=1}^{l_{-1,n}} \psi_{-1}\left(\beta_i^{-1,n} v\right)\right] \left[\prod_{i=1}^{l_{0,n}} \psi_0\left(\beta_i^{0,n} v\right)\right], \tag{3.1}$$

where N, $l_{-1,n}$ and $l_{0,n}$ are known integers, the pair ψ_{-1}, ψ_0 is either $\psi_{-1}(v) = \cos(v)$ and $\psi_0(v) = \sin(v)$ or $\psi_{-1}(v) = \cosh(v)$ and $\psi_0(v) = \sin(v)$, $\alpha_n(v)$ are polynomial coefficients, and $\beta_i^{-1,n}$, $\beta_i^{0,n}$ are nonnegative constants.

Indeed, it can be proved that this function can be brought to the announced form,

$$\phi(v) = v^r Z^k F(Z) \quad \text{where} \quad F(0) \neq 0,$$

in which $F(Z)$ is of the form

$$F(Z) = \sum_{n=1}^{M} a_n(Z) \prod_{j=0}^{k} \left[\prod_{i=1}^{l_{j,n}} \eta_j \left(b_i^{j,n} Z \right) \right], \tag{3.2}$$

where $M \geq N$, $b_i^{j,n} \geq 0$ and $a_n(Z)$ is a polynomial in Z.

The first, introductory stage of the procedure consists in expressing the function $\phi(v)$ as a linear combination of products of the functions $\eta_{-1}(Z)$ and $\eta_0(Z)$, by using the definition of these functions. This means a direct replacement of $\cos(\beta v)$ or $\cosh(\beta v)$ by $\eta_{-1}(\beta^2 Z)$, and of $\sin(\beta v)$ or $\sinh(\beta v)$ by $\beta v \eta_0(\beta^2 Z)$, which leads to

$$\phi(v) = v^r f(Z), \tag{3.3}$$

where $f(Z)$ has the form

$$f(Z) = \sum_{n=1}^{N} a_n(Z) \left[\prod_{i=1}^{l_{-1,n}} \eta_{-1} \left(b_i^{-1,n} Z \right) \right] \left[\prod_{i=1}^{l_{0,n}} \eta_0 \left(b_i^{0,n} Z \right) \right]. \tag{3.4}$$

This introductory step is implemented in the Mathematica module "etaTransf" reported in the Appendix.

Example 3.1 Let us consider

$$\begin{aligned} \phi(v) = &- v\cosh(\theta v)^2 + v\cosh(v/2)\cosh(2\theta v) + 2\cosh(\theta v)\sinh(v/2) + \\ &- 2\cosh(v/2)\cosh(2\theta v)\sinh(v/2) - \cosh(\theta v)\sinh(v) + \cosh(\theta v)^2\sinh(v). \end{aligned}$$

The function $\phi(v)$ is of the form (3.1). Indeed, it contains only one species of functions (hyperbolic), and corresponds to $N = 6$, $\alpha_1(v) = -v = -\alpha_2(v)$, $\alpha_3(v) = -2 = -\alpha_4(v)$, $\alpha_5(v) = -1 = -\alpha_6(v)$, $l_{-1,n} = 2$ for $n = 1, 2, 4, 6$, $l_{-1,n} = 1$ for $n = 3, 5$, $l_{0,n} = 0$ for $n = 1, 2$, $l_{0,n} = 1$ for $n = 3, 4, 5, 6$,

$$\beta_i^{-1,n} = \begin{cases} \theta \;\; n = 1, 6, \quad i = 1, 2 \quad \textit{and} \quad n = 3, 5, \quad i = 1; \\ 2\theta \;\; n = 2, 4, \quad i = 1, 2; \end{cases}$$

and

$$\beta_i^{0,n} = \begin{cases} 1/2 \;\; n = 3, 4, \quad i = 1; \\ 1 \quad\;\; n = 5, 6, \quad i = 1. \end{cases}$$

Then, by replacing $\cosh(\theta v) = \eta_{-1}(\theta^2 Z)$, $\cosh(v/2) = \eta_{-1}(Z/4)$, $\cosh(2\theta v) = \eta_{-1}(4\theta^2 Z)$, $\sinh(v/2) = \frac{v}{2}\eta_0(Z/4)$, $\sinh(v) = v\eta_0(Z)$, we obtain the expression (3.3) with $r = 1$ and

$$f(Z) = \eta_{-1}^2(\theta^2 Z)[\eta_0(Z)-1]+\eta_{-1}(\theta^2 Z)[\eta_0(Z/4)-\eta_0(Z)]+\eta_{-1}(Z/4)\eta_{-1}(4\theta^2 Z)[1-\eta_0(Z/4)]. \tag{3.5}$$

Two situations are now possible depending on whether $f(0)$ is vanishing or not. If $f(0) \neq 0$ the procedure is stopped but if $f(0) = 0$ (as is the case also with the function in the above example) it is continued until we can express $f(Z)$ as

$$f(Z) = Z^k F(Z)$$

where $F(0) \neq 0$. The determination in advance of the value of k is important because it helps in conveniently organizing the subsequent steps of the procedure. In fact, the module "etaTransf" has also a section in which this k is evaluated.
Once k is known, an iteration scheme is activated, starting with $f^{(0)}(Z) = f(Z)$ of the form (3.4). Specifically, in a finite number k of steps we determine the functions $f^{(s+1)}(Z)$ such that

$$f^{(s)}(Z) = Zf^{(s+1)}(Z), \quad s = 0, ..., k-1.$$

The final output of this iteration chain is assigned to the desired $F(Z)$, viz.: $F(Z) = f^{(k)}(Z)$. This is of the form (3.3) and $F(0) \neq 0$.
As a matter of fact, the form of $F(Z)$ is not unique, and different iteration procedures may result in different forms. All these forms are equivalent, of course, but it makes sense to give preferrence to the one which produces the shortest form of $F(Z)$. After comparing different conversion versions we decided to present below the one which seems the most advantageous from this point of view.
With this scheme we meet two situations:
If $k = 1$ we simply substitute in $f^{(0)}(Z)$ the expression given by (2.11) for $\eta_j(Z)$, $j = -1, 0$, thus determining $f^{(1)}(Z)$ with $f^{(1)}(0) \neq 0$ and in this way the conversion is completed.
If $k \geq 2$, we care that the last step is slightly different from the previous ones. Thus, at each step $s = 0, ..., k-2$ (we call these regular steps), if $f^{(s)}(0) = 0$, then we define $f^{(s+1)}(Z) = f^{(s)}(Z)/Z$ but, if $f^{(s)}(0) \neq 0$, then we write

$$f^{(s)}(Z) = f_0^{(s)}(Z) + Zf_1^{(s)}(Z) + ... + Z^{M_s} f_{M_s}^{(s)}(Z),$$

where $f_0^{(s)}(Z)$ is a linear combination of products of the functions $\eta_j(Z)$, with $j = -1, 0$ for $s = 0$, and $j = 0, ..., s$ for $s > 0$, and $f_0^{(s)}(0) \neq 0$. Then we substitute in the term $f_0^{(s)}(Z)$ the expression given by (2.11) for $\eta_j(Z)$, thus determining the expression of $f^{(s+1)}(Z)$. In particular, at the second-last step $s = k-2$ we will have determined the expression of

$$f^{(k-1)}(Z) = f_0^{(k-1)}(Z) + Zf_1^{(k-1)}(Z) + ... + Z^{M_{k-1}} f_{M_{k-1}}^{(k-1)}(Z),$$

with $f_0^{(k-1)}(Z)$ being a linear combination of products of the functions η_j for $j = 1, ..., k-1$, η_0^{2j} for $j = 1, ..., k$. If $f_0^{(k-1)}(0) = 0$, then $f^{(k)}(Z) = f^{(k-1)}(Z)/Z$. If $f_0^{(k-1)}(0) \neq 0$, then at the *last step* $s = k-1$ we substitute in $f_0^{(k-1)}(Z)$ the expression given by (2.11) for $\eta_j(Z)$,

$j = 1, ..., k-1$ and the following expression for η_0^{2j}

$$\begin{aligned}\eta_0^{2j}(Z) &= 1 + \left(\eta_0^j(Z) - 1\right)\left(\eta_0^j(Z) + 1\right) \\ &= 1 + (\eta_0(Z) - 1)\left(\eta_0^{j-1}(Z) + ... + 1\right)\left(\eta_0^j(Z) + 1\right) \\ &= 1 + ZD_0(Z)\left(\eta_0^{j-1}(Z) + ... + 1\right)\left(\eta_0^j(Z) + 1\right),\end{aligned}$$

thus determining $f^{(k)}(Z)$ with $f^{(k)}(0) \neq 0$. The desired $F(z)$ therefore is $F(Z) = f^{(k)}(Z)$.

This scheme is implemented in the Mathematica module "ZpowerTransf", reported in the Appendix.

To make the scheme more transparent we come with details on cases when $f(Z)$ is of the form (3.4) where $a_n(Z)$ are simply constants, and $k = 1, 2, 3$.
For further simplicity we also assume that the first I terms of the sum over n represent a linear combination of the values of η_{-1} with different arguments, the subsequent J terms are for a linear combination of the values of η_0, and the last term is simply a constant. Thus we have $N = I + J + 1$, with

$$l^{-1,n} = 1, \quad l^{0,n} = 0 \quad n = 1, \ldots, I,$$

$$l^{-1,n} = 0, \quad l^{0,n} = 1 \quad n = I+1, \ldots, I+J$$

and

$$l^{-1,I+J+1} = 0, \; l^{0,I+J+1} = 0,$$

which can be briefly written as

$$f(Z) = \sum_{i=1}^{I} a_i \eta_{-1}(b_i Z) + \sum_{j=1}^{J} c_j \eta_0(d_j Z) + e, \tag{3.6}$$

where, of course, $\sum_{i=1}^{I} a_i + \sum_{j=1}^{J} c_j + e = 0$ in order to secure that $f(0) = 0$.
This is perhaps the case which is the most frequently met in current evaluations related to the ef approach.

CASE $k = 1$. One step is only involved here and this is treated as a regular step. By substituting the expressions (2.11) for $\eta_{-1}(Z)$ and $\eta_0(Z)$, i.e.

$$\eta_{-1}(Z) = 1 + ZD_{-1}(Z), \quad \eta_0(Z) = 1 + ZD_0(Z), \tag{3.7}$$

with

$$D_{-1}(Z) = \frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right), \quad D_0(Z) = \frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right) - \eta_1(Z),$$

we obtain

$$f(Z) = \sum_{i=1}^{I} a_i + \sum_{j=1}^{J} c_j + e + Z\left(\sum_{i=1}^{I} a_i b_i D_{-1}(b_i Z) + \sum_{j=1}^{J} c_j d_j D_0(d_j Z)\ ,\right).$$

i.e., $f(Z) = Zf^{(1)}(Z)$ with

$$f^{(1)}(Z) = \sum_{i=1}^{I} \frac{a_i b_i}{2} \eta_0^2 \left(\frac{b_i Z}{4} \right) + \sum_{j=1}^{J} \frac{c_j d_j}{2} \eta_0^2 \left(\frac{d_j Z}{4} \right) - \sum_{j=1}^{J} c_j d_j \eta_1 \left(d_j Z \right) . \tag{3.8}$$

We then assign $F(Z) = f^{(1)}(Z)$, and this concludes the conversion procedure.

CASE $k = 2$. Here there are two steps, the regular step $s = 0$ and the final step $s = 1$. The output of the regular step is $f^{(1)}(Z)$ of eq.(3.8) which we write as

$$f^{(1)}(Z) = \sum_{i=1}^{I} a_i \eta_0^2 \left(b_i Z \right) + \sum_{j=1}^{J} c_j \eta_1 \left(d_j Z \right) , \tag{3.9}$$

where, for simplicity of notation, we use the same name for the coefficients a_i, b_i, c_j, d_j. Of course, the coefficients a_i and c_i are related, $\sum_{i=1}^{I} a_i + \sum_{j=1}^{J} c_j = 0$.
The second step is also the last step and therefore, as explained before, we replace in (3.9)

$$\eta_0^2(Z) = 1 + ZD_0(Z) \left(\eta_0(Z) + 1 \right) , \quad \eta_1(Z) = \frac{1}{3} + ZD_1(Z), \tag{3.10}$$

with

$$D_0(Z) = \frac{1}{2} \eta_0^2 \left(\frac{Z}{4} \right) - \eta_1 \left(Z \right) , \quad D_1(Z) = \frac{1}{2} \eta_0^2 \left(\frac{Z}{4} \right) - \eta_1 \left(Z \right) - \eta_2 \left(Z \right) . \tag{3.11}$$

Then we obtain

$$f(Z) = Z^2 f^{(2)}(Z),$$

where

$$f^{(2)}(Z) = \sum_{i=1}^{I} \frac{a_i b_i}{2} \eta_0^2 \left(\frac{b_i Z}{4} \right) \left(\eta_0(b_i Z) + 1 \right) + \sum_{j=1}^{J} c_j d_j \left(\frac{1}{2} \eta_0^2 \left(\frac{d_j Z}{4} \right) - \eta_1 \left(d_j Z \right) - \eta_2 \left(d_j Z \right) \right) , \tag{3.12}$$

and this completes the procedure, with $F(Z) = f^{(2)}(Z)$.

CASE $k = 3$. In this case we have two regular steps, $s = 0, 1$. The output (3.8) of $s = 0$ is just accepted but the output (3.12) of $s = 1$ is inadequate because it has been derived by a technique for the last step. This step must be repeated anew with the technique for a regular step, i.e., we go back to an expression of type (3.9) for $f^{(1)}(Z)$ in which we replace

$$\eta_0(Z) = 1 + ZD_0(Z), \quad \eta_1(Z) = \frac{1}{3} + ZD_1(Z), \tag{3.13}$$

with $D_0(Z)$, $D_1(Z)$ given by (3.11), to obtain

$$f(Z) = Z^2 f^{(2)}(Z),$$

where

$$\begin{aligned} f^{(2)}(Z) &= \sum_{i=1}^{I} a_i \left(1 + b_i Z D_0(b_i Z) \right)^2 + \sum_{j=1}^{J} c_j \left(\frac{1}{3} + d_j Z D_1 \left(d_j Z \right) \right) \\ &= f_0^{(2)}(Z) + Z f_1^{(2)}(Z) \end{aligned} \tag{3.14}$$

with

$$
\begin{aligned}
f_0^{(2)}(Z) &= \sum_{i=1}^{I} 2a_i b_i D_0(b_i Z) + \sum_{j=1}^{J} c_j d_j D_1\left(d_j Z\right), \\
f_1^{(2)}(Z) &= \sum_{i=1}^{I} a_i b_i^2 \left(D_0(b_i Z)\right)^2.
\end{aligned}
$$

The last step follows, with its specific technique. It is applied only on $f_0^{(2)}(Z)$, which satisfies $f_0^{(2)}(0) = 0$ and has the form

$$
f_0^{(2)}(Z) = \sum_{i=1}^{I} a_i \eta_0^2(b_i Z) + \sum_{j=1}^{J} c_j \eta_1\left(d_j Z\right) + \sum_{j=1}^{J} c_j \eta_2\left(d_j Z\right), \tag{3.15}
$$

where, as before, for simplicity of notation, we use the same name for the coefficients a_i, b_i, c_j, d_j. The other term in (3.14) needs no extra treatment because it already contains a factor Z. We replace the expressions (3.10) and

$$
\eta_2(Z) = \frac{1}{15} + Z D_2(Z), \tag{3.16}
$$

$$
D_2(Z) = \frac{1}{2}\eta_0^2\left(\frac{Z}{4}\right) - \eta_1\left(Z\right) - \eta_2\left(Z\right) - 3\eta_3\left(Z\right),
$$

in (3.15) thus obtaining

$$
f(Z) = Z^3 f^{(3)}(Z),
$$

and this concludes the run, with $F(Z) = f^{(3)}(Z) \neq 0$.

Example 3.2 Let us consider the function

$$
f(Z) = 2\eta_{-1}\left(\theta^2 Z\right) - 2\eta_{-1}\left(4\theta^2 Z\right),
$$

with $f^{(0)}(0) = 0$, which is in the form (3.6). By substituting the expression (3.7) for $\eta_{-1}(Z)$ we obtain

$$
f^{(1)}(Z) = \theta^2\left(\eta_0^2\left(\frac{\theta^2 Z}{4}\right) - 4\eta_0^2\left(\theta^2 Z\right)\right),
$$

with $f^{(1)}(0) = -3\theta^2 \neq 0$.

Example 3.3 We consider the function of *Example 3.1*.

In this case $f(Z)$ is not of the form (3.6), then we have to apply the generical procedure. We have $k = 2$ and we start with $f^{(0)}(Z) = f(Z)$ given in (3.5).

For $s = 0$ we have

$$
f_0^{(0)}(Z) = f^{(0)}(Z),
$$

and, by substituting the expression (2.11) with $\eta_j(Z)$, $j=-1,0$ we obtain:

$$
\begin{aligned}
&f^{(1)}(Z) = -\tfrac{Z}{64}\left[\eta_0^4\left(\tfrac{Z}{16}\right)(1+2Z\theta^2\eta_0^2(Z\theta^2))+\right.\\
&-2\eta_0^2\left(\tfrac{Z}{16}\right)\left(\eta_1\left(\tfrac{Z}{4}\right)+2\theta^2\left(\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)+\eta_0^2(Z\theta^2)\left(-4+Z\eta_1\left(\tfrac{Z}{4}\right)\right)\right)\right)+\\
&+8\theta^2\left(-\eta_0^2\left(\tfrac{Z}{4}\right)\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)\left(2+Z\theta^2\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)\right)-4\eta_0^2(Z\theta^2)\,\eta_1\left(\tfrac{Z}{4}\right)+2Z\theta^2\eta_0^4\left(\tfrac{Z\theta^2}{4}\right)\eta_1(Z)+\right.\\
&\left.\left.+\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)\left(\eta_1\left(\tfrac{Z}{4}\right)+4\eta_1(Z)\right)\right)\right].
\end{aligned}
$$

For $s=1=k-1$ we have $f^{(1)}(0)=0$ and $f^{(2)}(Z)$ is defined by

$$f^{(2)}(Z) = f^{(1)}(Z)/Z. \tag{3.17}$$

4 Applications

The coefficients and the error factor of any ef-based approximation formula are typically expressed by ratios of two functions of the form (3.1) and therefore they exhibit a 0/0 behaviour at $v=0$. To eliminate this we apply the conversion procedure described in the previous Section separately on the numerator and denominator. Finally, when evaluating the ratio Den/Num the factor $v^r Z^k$ disappears, and this eliminates the undeterminacy. In the following we report on results obtained with this technique on some coefficients derived in the papers [9], [10], [11]. All these are of the mentioned form, see eqs.(4.1-4.3) below. In particular, the case considered in Examples 3.1 and 3.3 is just the numerator of α_3 in (4.1) after the mentioned expression of γ_1 has been introduced.

- In the paper [9] some sixth order symmetric and symplectic exponentially fitted modified Runge-Kutta methods of Gauss type were derived. The authors give the formulae of the coefficients in terms of hyperbolic functions. We consider three of them, chosen at random. These are

$$
\begin{aligned}
b_1 &= \tfrac{v-2\sinh(v/2)}{2v(1-\cosh(\theta v))},\\
\gamma_1 &= \tfrac{2\sinh(v/2)-v\cosh(2\theta v)}{2\sinh(v/2)-\sinh(v)+(\sinh(v)-v)\cosh(\theta v)},\\
\alpha_3 &= \tfrac{\gamma_1\cosh(v/2)-\cosh(\theta v)}{v\sinh(\theta v)},
\end{aligned}
\tag{4.1}
$$

whose series expansions in powers of v are also listed in that paper for $\theta=\sqrt{15}/10$:

$$
\begin{aligned}
b_1 &= \tfrac{5}{18}+\tfrac{v^4}{302400}-\tfrac{v^6}{62208000}+\tfrac{17v^8}{212889600000}-\tfrac{15641v^{10}}{41845579776000000}+\ldots,\\
\gamma_1 &= 1-\tfrac{3v^6}{56000}+\tfrac{649v^8}{44800000}-\tfrac{983177v^{10}}{275968000000}+\tfrac{2248000621v^{12}}{2583060480000000}+\ldots.,\\
\alpha_3 &= \tfrac{\sqrt{15}}{30}+\tfrac{\sqrt{15}v^2}{3600}-\tfrac{71\sqrt{15}v^4}{1890000}+\tfrac{1849\sqrt{15}v^6}{302400000}-\tfrac{47169209\sqrt{15}v^8}{33530112000000}+\tfrac{178746672227\sqrt{15}v^{10}}{523069747200000000}+\ldots
\end{aligned}
$$

By applying the procedure described in the previous section we obtain the expressions

$$
\begin{aligned}
b_1 &= \frac{\eta_0^2\left(\frac{Z}{16}\right)-2\eta_1\left(\frac{Z}{4}\right)}{8\theta^2\eta_0^2\left(\frac{Z\theta^2}{4}\right)},\\
\gamma_1 &= \frac{\left(1+2Z\theta^2\eta_0^2\left(Z\theta^2\right)\right)\left(\eta_0^2\left(\frac{Z}{16}\right)-2\eta_1\left(\frac{Z}{4}\right)\right)}{\eta_0^2\left(\frac{Z}{16}\right)-2\eta_1\left(\frac{Z}{4}\right)+2Z\theta^2\eta_0^2\left(\frac{Z\theta^2}{4}\right)\left[\eta_0^2\left(\frac{Z}{4}\right)-2\eta_1(Z)\right]},\\
\alpha_3 &= \frac{Num(Z)}{Den(Z)}
\end{aligned}
$$

where $Num(Z)$ is given by (3.17), and

$$
\begin{aligned}
Den(Z) = 4\theta &\left(\eta_0^2\left(\tfrac{Z}{16}\right)-2\eta_1\left(\tfrac{Z}{4}\right)+2Z\theta^2\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)\left(\eta_0^2\left(\tfrac{Z}{4}\right)-2\eta_1\left(Z\right)\right)\right)\cdot\\
\cdot&\left(2+Z\theta^2\left(\eta_0^2\left(\tfrac{Z\theta^2}{4}\right)-2\eta_1\left(Z\theta^2\right)\right)\right).
\end{aligned}
$$

Of course, the argument Z associated to v from eq.(4.1) is positive, $Z = v^2$. However the new formulae automatically cover also the analog of (4.1) for oscillatory functions, that is when the hyperbolic functions are replaced by trigonometric functions; in this case Z will be negative, $Z = -v^2$. We also mention that the new formulae are valid for *any* value of θ. Finally, the new formulae allow computing the coefficients with *uniform accuracy* for any Z.

- In paper [10] some sixth order symmetric and symplectic exponentially fitted Runge-Kutta methods of Gauss type were derived. We consider for example the coefficient

$$b_1 = \frac{\sinh(v)-2\sinh(v/2)}{2v(\cosh(\theta v)-\cosh(2\theta v))}, \tag{4.2}$$

for which the authors report the Taylor expansion when $\theta = \sqrt{15}/10$

$$b_1 = \frac{5}{18} + \frac{v^4}{14400} - \frac{191v^6}{87091200} + \frac{623v^8}{8294400000} - \frac{78713v^{10}}{30656102400000} + \ldots$$

The new formula for this coefficient, obtained by applying our procedure, is

$$b_1 = \frac{\left[\eta_0^2\left(\frac{Z}{16}\right)-2\eta_1\left(\frac{Z}{4}\right)\right]}{8\theta^2\eta_0^2\left(\frac{Z\theta^2}{4}\right)}.$$

It has the same practical advantages as in the previous case.

- In [11] a family of four-step trigonometrically fitted methods has been derived. We focus on one of the coefficients reported there, viz.:

$$b_0 = \frac{\sin(2v)-4v\cos(v)+4\sin(v)-2v}{-3v^2\sin(2v)+4v^3\cos(v)+2v^3}, \tag{4.3}$$

whose Taylor expansion is

$$
\begin{aligned}
b_0 = &\frac{1}{15} + \frac{17v^2}{1575} + \frac{163v^4}{94500} + \frac{60607v^6}{218295000} + \frac{1697747v^8}{37837800000} + \frac{519335027v^{10}}{71513442000000} +\\
&+ \frac{12254045443v^{12}}{10420530120000000} + \frac{609739626367891v^{14}}{3201499468767600000000} + \ldots
\end{aligned}
$$

The expression of this coefficient in terms of $\eta_m(Z)$ functions is:

$$b_0 = \frac{-\eta_0^2\left(\frac{Z}{4}\right)(2+3\eta_0(Z))+8\eta_0^2(Z)+4\eta_1(Z)+6\eta_0(Z)\eta_1(Z)-16\eta_1(4Z)-2\eta_2(Z)-16\eta_2(4Z)}{3\left(\eta_0^2\left(\frac{Z}{4}\right)-6\eta_0^2(Z)+12\eta_1(4Z)\right)}.$$

The latter covers not only the trigonometric case, as in the original derivation, but also the hyperbolic case. Also the series expansion is no more needed.

5 Test Program

The main program which follows applies the conversion procedure to the coefficient b_1 in (4.1).

(* PROGRAM formConv : converts a rational formula, containing oscillatory or hyperbolic functions, in terms of $\eta_m(Z)$ functions and allows a full elimination of the 0/0 undeterminacy *)

Num $=v - 2\sinh(v/2)$;

Den $= 2v(1-\cosh(\theta v))$;

type = 2 ;

Off[General::spell]

degNum = vDeg[Num]; {NumEta, kNum, rNum} = etaTransf[Num, degNum];

NumNew = ZpowerTransf[NumEta, kNum];

degDen = vDeg[Den]; {DenEta, kDen, rDen} = etaTransf[Den, degDen];

DenNew = ZpowerTransf[DenEta, kDen];

Print["Transformed coefficient:", FullSimplify[$\frac{NumNew}{DenNew}$]]

6 Conclusions

We have presented a method for the conversion of formulae obtained in the frame of the exponential fitting for various approximation schemes, to forms expressed in terms of functions $\eta_m(Z)$. The new forms secure automatic elimination of 0/0 behaviour, enable a uniform accuracy in the evaluation and allow an extended area of applicability. We also presented a code for this conversion. Another possible application, mentioned but not detailed in the text, consists in obtaining converted expressions for the corresponding factor in the error formula, thus making possible an evaluation of the accuracy.

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Appendix

Below are listed the MATHEMATICA main program formConv.nb and modules *vDeg, etaTransf* and *ZpowerTransf.*

Main program: formConv.nb

(* PROGRAM formConv : converts a rational formula, containing oscillatory or hyperbolic functions, in terms of $\eta_m(Z)$ functions and allows a full elimination of the 0/0 undeterminacy *)

Num = (* Please insert here your numerator *) ;

Den =(* Please insert here your denominator *) ;

type = (* Please insert 1 for oscillatory case and 2 for hyperbolic case*) ;

Off[General::spell]

degNum = vDeg[Num]; {NumEta, kNum, rNum} = etaTransf[Num, degNum];

NumNew = ZpowerTransf[NumEta, kNum];

degDen = vDeg[Den]; {DenEta, kDen, rDen} = etaTransf[Den, degDen];

DenNew = ZpowerTransf[DenEta, kDen];

Print["Transformed coefficient:", FullSimplify[$\frac{NumNew}{DenNew}$]]

Module vDeg

(* Function that computes the powers of v to highlight *)

vDeg[funz_] := Module[{Nmax, tmp, deg}, Nmax = 100; tmp = 0;

    For[deg = 1, (deg < Nmax && tmp == 0),

        tmp = SeriesCoefficient[Series[funz, {v, 0, Nmax}], deg]; deg++];

    deg = deg - 1; deg]

Module etaTransf

(* Function that reveals the full power of v and changes in the eta functions*)

etaTransf[funzSt_, deg_] := Module[{degNew, deg1, tmp, Nmax, r, k, funz},

    funz = funzSt; tmp = 0;

    For[deg1 = 1, (deg1 < Nmax && tmp == 0),

        tmp = Coefficient[Denominator[Together[funz/(v^deg1)]], v]; deg1++;];

    deg1 = deg1 - 2;

    If[deg1 > 0, funz = Together[funz/(v^deg1)]; degNew = deg - deg1,

        degNew = deg;];

    k = IntegerPart[degNew/2]; r = Mod[degNew, 2];

    funz=Together[$\frac{1}{v^r}$ (funz /. {HoldPattern[Cos[a : __]] :> η_{-1}[-a^2],

                HoldPattern[Cosh[a : __]] :>η_{-1}[-a^2], HoldPattern[Sin[a : __]] :> a*η_0[-a^2],

HoldPattern[Sinh[a : __]] :> a*η_0[-a^2]})

/. {v^2 -> ((-1)^type))*Z})];

If[(Mod[(deg1 + r)/2, 2] == 1) && type == 1, funzMod = -funzMod;];

If[deg1 > 0, r = r + deg1;]; {funz, k, r}]

Module ZpowerTransf

ZpowerTransf[funzSt_,kSt_]:=Module[{funz,Nmax,tmp,deg,k,deg1,s},

Nmax=100; funz=funzSt; k=kSt; $\eta_{-1}[0] = 1$;

$\eta_{m\_}[0] = \frac{1}{Factorial2[2*m+1]}$;

$D_{m\_}[Z\_] = \eta_m[0] * \left(\frac{1}{2} * \eta_0 \left[\frac{Z}{4}\right] * \eta_0 \left[\frac{Z}{4}\right] - \sum_{i=1}^{m+1} \left(Factorial2[2 * i - 3] * \eta_i[Z]\right) \right)$;

$\bar{\eta}_{m\_}[Z\_] := \eta_m[0] + Z * D_m[Z]$;

s=0; st=-1;

If[k $\geq$ 0,funz=Together[$\frac{funz/.Table[\eta_i->\bar{\eta}_i,\{j,st,s\}]}{Z}$];];

funz=Simplify[funz]/.Table[$v^{2*j} -> (((-1)\hat{~}type) * Z)^j, \{j, 1, s+1\}$];

tmp=0;

For[deg1=1,($deg1 < Nmax$&&tmp==0),

tmp=Coefficient[Denominator[Together[funz/(Z^deg1)]],Z]; deg1++];

deg1=deg1-2;

If[deg1>0,funz=Together[funz/(Z^deg1)];k=k-deg1;];

st=0;

For[s=1,s¡k-1,s++,

funzCoeff=CoefficientList[funz,Z]; funzTNot=funzCoeff[[1]];

funzTNot=funzTNot/.Table[$\eta_i -> \bar{\eta}_i, \{j, st, s\}$];

M=Length[funzCoeff];

funz=Together$\left[\left(\sum_{k=2}^{M} \left(funzCoeff[[k]] * Z^{k-1}\right) + funzTNot \right) /Z \right]$;];

If[s==k-1,

funzCoeff=CoefficientList[funz,Z]; funzTNot=funzCoeff[[1]];

funzTNot=funzTNot/.Flatten[Table[$\left\{a:((\eta_0)\,[\_\_])^{2j}:->1+Factor[a-1]\right\}$,

$\{j,1,s+1\}]]$;

funzTNot=funzTNot/.Flatten[$\{a:(-1+(\eta_0)\,[\_\_]):->$

$ReplaceAll[a,\eta_0->\bar{\eta}_0],Table\,[\eta_i->\bar{\eta}_i,\{j,st,s\}]\}]$;

M=Length[funzCoeff];

funz=Together$\left[\left(\sum_{k=2}^{M}\left(funzCoeff[[k]]*Z^{k-1}\right)+funzTNot\right)/Z\right]$;]; funz]

TEST RUN OUTPUT

Transformed coefficient: $\frac{\eta_0^2\left(\frac{Z}{16}\right)-2\eta_1\left(\frac{Z}{4}\right)}{8\theta^2\eta_0^2\left(\frac{Z\theta^2}{4}\right)}$