Chebychev interpolations of the Gamma and Polygamma Functions and their analytical properties

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in memoriam
Cornelius Lanczos[5] 1893-1974[1]

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Contents

1 Introduction 2

2 Chebyshev Interpolations of the Γ Function 3
   2.1 The Γ−1 Function .................................................. 4
   2.2 The LnΓ Function .................................................. 5

3 The Chebyshev Interpolation of the Psi(Digamma) Function 7
   3.1 Summation of the Harmonic Series .............................. 7

4 Interpolating further Polygamma Functions 7
   4.1 Summation of the higher Harmonic Series ................. 8

5 Relations of the Shifted Chebychev Polynomials 8
   5.1 Chebychev approximation of smooth functions ............ 8
       5.1.1 Numerical determination of the \(a_r^*\)-coefficients .... 9

1 http://www.youtube.com/watch?v=avSHHi9QCjA
http://www.youtube.com/watch?v=P06xt8xB5Vg
1 Introduction

The Gamma Function derived by Leonhard Euler (1729) is the generalization of discrete factorials:

\[ z! = \Gamma(z+1) = \int_0^\infty t^{z-1}e^{-t}dt, \quad \Re z > 0 \quad (1) \]

The numerical evaluation is not easy. Whittaker+Watson [9] and Temme [8] give a good discussion of the \( \Gamma \) Function and several basic properties.

In contrast to that Lanczos [4] developed approximations with a restricted precision by using Chebyshev polynomials in the range \([-1..+1]\) (instead of shifted polynomials which will be used exclusively in this paper). Chebychev polynomials were introduced into numerical analysis especially by Lanczos [5] in the US since 1935 and by Clenshaw [2] in GB since 1960.

The next formula is due to James Stirling (1730)

\[ \ln \Gamma(z) \sim \ln \left(\sqrt{2\pi} z^{z-\frac{1}{2}} e^{-z} \right) + \sum_{n=1}^\infty \frac{B_{2n}}{2n (2n-1)}z^{2n-1} \quad (2) \]

The \( B_{2n} \) are the Bernoulli numbers with a poor behaviour:

1, -1/30, 1/42, -1/360, 1/6, 1/5, 1/6, 1/6, 5/2730, 1/6, 1/6, 1/5, 1/6, 1/6, 1/6, 1/510, 1/6, ...

They decrease at the beginning only slowly and then grow with \((2n)!\). The complete terms in the infinite sum eq. (2) depend on \( n \) and \( z \) and grow nevertheless, especially if \( z \) is small:

1, 1/12, 1/360, 1/1260, 1/1260, 1/1188, 1/12492, 1/12492, 1/1156, 1/122400, 1/122400, ...

The summation has to stop before the terms begin to grow unrestricted. There is an optimal position depending on \( z \) where summation has to end. This problem is discussed in some detail in [3].

A further disadvantage is the low convergence of the admitted terms. In fig. 1 the problem is described in some detail depending on \( z \): fig. 1a shows the maximal number of convergent terms, fig. 1b shows the maximal achievable accuracy in decimal digits.

\[ ... \text{page 467} \]
2 Chebyshev Interpolations of the $Γ$ Function

The Chebyshev polynomials were derived by the Russian Mathematician P. L. Chebyshev (1821-1894) [6]. Among all normalized power polynomials of same degree they have the smallest deviation from zero in a predefined intervall. Most of their beautiful properties are described by Snyder [7] and Clenshaw [2] showing many applications to transcendental functions and differential equations.

The approximation of the $Γ$ Function is represented by

$$(z - 1)! \approx Γ(z) = \sqrt{2\pi} \cdot z^{\frac{1}{2}} \cdot e^{-z} \cdot \left[ 0.99999999998 + \frac{0.00029536102066}{z^7} + \frac{0.000052647439438}{z^{10}} \right]$$

the maximal relativ error(Figure 3a) is less than $8 \cdot 10^{-4}$. Using eleven coefficients for the corresponding powerseries

$$(z - 1)! \approx Γ(z) = \sqrt{2\pi} \cdot z^{\frac{1}{2}} \cdot e^{-z} \cdot \left[ 0.999935 + \frac{0.0845506}{z} \right.$$  

$$+ \frac{0.0024711193390}{z^4} + \frac{0.000358599470338}{z^7} + \frac{0.0008333337647}{z^2} + \frac{0.0034720552506}{z^5} - \frac{0.0026788696285}{z^3} + \frac{0.000029536102066}{z^{9}} + \frac{0.000052647439438}{z^{10}} \right]$$

the maximal relativ error(Figure 3b) is less than $2 \cdot 10^{-11}$.  

Figure 1: restricted summation and limited precision
Figure 2: Chebyshev coefficients $\Gamma$-function 30 digits

2.1 The $\Gamma^{-1}$ Function

Figure 4 contains 53 Chebyshev coefficients of the $\Gamma^{-1}$-function for an accuracy of 30 decimal digits in the whole range $1 \leq z \leq \infty$.

$$
\frac{1}{(z-1)!} \approx \Gamma^{-1}(z) = \frac{1}{\sqrt{2\pi}} z^{\frac{1}{2}-z} e^{z} \ast \sum_{0}^{\infty} b_r T_r^*(\frac{1}{z}), \quad 1 \leq z \leq \infty
$$
With four coefficients the power series expansion is:

\[ \Gamma^{-1}(z) = \frac{1}{\sqrt{2\pi}} z^{\frac{1}{2} - z} e^z \cdot \left( 1.000006 - \frac{0.08354413}{z} + \frac{0.004512425}{z^2} + \frac{0.001168239}{z^3} \right) \] (9)

The maximal relative error (Figure 5) is less than \( 7 \times 10^{-6} \). In contrast to that in the famous Handbook of Mathematical Functions [1], the series expansion for \( \Gamma^{-1} \) is completely wrong.

### 2.2 The \( \ln \Gamma \) Function

The approximation is represented by

\[ \ln[(z - 1)!] \simeq \ln \Gamma(z) = \ln \left( \sqrt{\frac{2\pi}{z}} \cdot z^{\frac{1}{2} - z} \cdot e^{-z} \right) + \sum_{r=0}^{\infty} c_r T_r \left( \frac{1}{z} \right), \quad 1 \leq z \leq \infty \] (10)

Figure 6 contains the Chebyshev coefficients with a precision of 30 decimal digits for the whole range of \( 1 \leq z \leq \infty \). Using only the first two coefficients and building the power series form

\[ \ln \Gamma(z) = \ln \sqrt{\frac{2\pi}{z}} + \left( z - \frac{1}{2} \right) \ln(z) - z + 0.91932 + 0.081160 z \] (11)

the maximum absolute error (Figure 7a) is less than \( 5 \times 10^{-4} \). Using five coefficients

\[ \ln \Gamma(z) = \ln \sqrt{\frac{2\pi}{z}} + \left( z - \frac{1}{2} \right) \ln(z) - z + 0.918935 + \frac{0.0833326}{z} + \frac{0.00037082}{z^2} - \frac{0.00305155}{z^3} + \frac{0.000743418}{z^4} \] (12)

the maximum absolute error (Figure 7b) is less than \( 2 \times 10^{-7} \).
| $r$ | $b_r$                                      | $r$ | $b_r$                                      |
|-----|-------------------------------------------|-----|-------------------------------------------|
| 0   | + 1.92058 34762 54948 20024 18291 34328 | 27  | + 0.00000 00000 00000 00002 45571 98296 |
| 1   | - 0.03896 62376 24892 01214 15331 82954 | 28  | - 1 33445 12573                            |
| 2   | + 0.00078 30980 24559 58872 29636 11440 | 29  | + 46583 60719                              |
| 3   | + 0.00003 65074 79093 94718 63219 85541 | 30  | - 10869 26183                              |
| 4   | - 63995 52363 25099 03462 62930          | 31  | + 689 16332                                |
| 5   | + 2508 67644 41246 12497 57714          | 32  | + 934 45505                                |
| 6   | + 664 29088 71454 74619 02130          | 33  | - 645 45386                                |
| 7   | - 164 72719 66800 61015 61714          | 34  | + 270 90508                                |
| 8   | + 15 22654 03292 35267 51875          | 35  | - 81 55332                                 |
| 9   | + 1 78294 76780 20568 75297          | 36  | + 14 39319                                 |
| 10  | - 1 02239 73513 75719 08376          | 37  | + 2 10256                                  |
| 11  | + 21131 54880 28419 64665          | 38  | - 3 35833                                  |
| 12  | - 1579 76630 19572 63953          | 39  | + 1 87421                                  |
| 13  | - 589 22900 53182 13064          | 40  | - 74017                                   |
| 14  | + 294 26575 02392 08743          | 41  | + 21339                                   |
| 15  | + 71 44837 50686 73310          | 42  | - 3194                                    |
| 16  | + 8 04021 40306 78275          | 43  | - 1095                                    |
| 17  | + 1 79571 80338 19450          | 44  | - 1242                                    |
| 18  | + 1 35094 39033 25037          | 45  | - 684                                     |
| 19  | + 44531 04004 16223          | 46  | + 278                                     |
| 20  | + 9839 21502 24802          | 47  | - 875                                     |
| 21  | + 244 92005 80535          | 48  | + 15                                      |
| 22  | + 681 06936 15141          | 49  | + 4                                       |
| 23  | - 356 97024 27690          | 50  | + 5                                       |
| 24  | + 113 11653 97918          | 51  | + 3                                       |
| 25  | - 22 20176 58614          | 52  | + 1                                       |
| 26  | - 11809 99223          |
3 The Chebyshev Interpolation of the Psi (Digamma) Function

This function is the first derivative of the LnΓ Function:

$$\psi(0)(z) = \psi(z) = \ln' \Gamma(z) = \frac{\Gamma'(z)}{\Gamma(z)} = \ln z - \frac{1}{2z} + \sum_{0}^{\infty} c_r^* T_r^* \left(\frac{1}{z}\right), \quad 1 \leq z \leq \infty$$  \hspace{1cm} (13)

After differentiating the sum using eq. (23) and eq. (24), \(-\frac{1}{2z}=\frac{1}{4} \left( T_0^* \left(\frac{1}{z}\right) + T_1^* \left(\frac{1}{z}\right) \right)\) has to be added. The final result is

$$\psi(0)(z) = \psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} = \ln z + \sum_{0}^{\infty} \alpha_{(0)r}^* T_r^* \left(\frac{1}{z}\right), \quad 1 \leq z \leq \infty$$  \hspace{1cm} (14)

3.1 Summation of the Harmonic Series

\(-\psi(0)(1) = \gamma = 0.57721 \ 56649 \ 01532 \ 86061\) is Euler’s constant.

$$\psi(0)(n + 1) - \psi(0)(1) = H_n = 1 + \frac{1}{2} + \frac{1}{3} + ... + \frac{1}{n}, \quad n \in N$$

defines and computes the n-th harmonic number \(H_n\).

4 Interpolating further Polygamma Functions

Differentiating the result of eq. (14) as before one gets

$$\psi(1)(z) = \psi'(z) = \frac{1}{z} + \sum_{0}^{\infty} \alpha_{(0)r}^* T_r^* \left(\frac{1}{z}\right), \quad 1 \leq z \leq \infty$$  \hspace{1cm} (15)
Finally \( \frac{1}{z} = \frac{1}{2} \ast (T^*_0(z) + T^*_1(z)) \) has to be added yielding

\[
\psi^{(1)}(z) = \sum_{0}^{\infty} \alpha_{(1)r} T^*_r(z), \quad 1 \leq z \leq \infty \tag{16}
\]

The higher Polygamma Functions can be approximated applying the two step differentiation repeatedly without additional correction. Each next generated function looses about two decimal digits in precision.

### 4.1 Summation of the higher Harmonic Series

The general relation is:

\[
\frac{(-1)^{m+1}}{m!} \psi^{(m)}(z) = \sum_{k=0}^{\infty} \frac{1}{(z+k)^{m+1}} = \frac{1}{z^{m+1}} + \frac{1}{(z+1)^{m+1}} + \frac{1}{(z+2)^{m+1}} + ... \tag{17}
\]

and especially for \( z=n \) integer

\[
\frac{(-1)^{m+1}}{m!} [\psi^{(m)}(1) - \psi^{(m)}(n)] = \frac{1}{1^{m+1}} + \frac{1}{2^{m+1}} + \frac{1}{3^{m+1}} + ... + \frac{1}{(n-1)^{m+1}} \tag{18}
\]

and further specialized with \( m=1 \)

\[
\psi^{(1)}(1) - \psi^{(1)}(n) = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + ... + \frac{1}{(n-1)^2} \tag{19}
\]

### 5 Relations of the Shifted Chebychev Polynomials

The Shifted Chebyshev polynomials are defined by

\[
T^*_r(z) = \cos(r\theta) \quad \begin{array}{l}
-1 \leq \cos \theta \leq +1 \\
-1 \leq T^*_r \leq +1
\end{array} \quad \begin{array}{l}
2z - 1 = \cos \theta \\
0 \leq z \leq +1
\end{array}
\]

They are power polynomials in \( z \). Their highest coefficient \( 2^{r-1} \) is used for normalization.

Chebyshev proved [6] that among all normalized power polynomials of same degree (or less) they have the smallest deviation from zero in the range \( 0 \leq z \leq +1 \). That makes them unique for optimal interpolation in the declared region. The ranges may be adapted by linear or even nonlinear transformations.

The polynomials for the interval \( 0 \leq z \leq +1 \) are called the shifted polynomials. They are used here exclusively. Explicit expressions for the first few shifted Chebyshev polynomials are:

\[
T^*_0(z) = 1, \quad T^*_1(z) = 2z - 1, \quad T^*_2(z) = 8z^2 - 8z + 1, \quad T^*_3(z) = 32z^3 - 48z^2 + 18z - 1, ...
\]

Inversion gives:

\[
1 = T^*_0(z), \quad 2z = T^*_0(z) + T^*_1(z), \quad 8z^2 = 3T^*_0(z) + 4T^*_1(z) + T^*_2(z), \quad 32z^3 = 10T^*_0(z) + 15T^*_1(z) + 6T^*_2(z) + T^*_3(z), ...
\]

### 5.1 Chebychev approximation of smooth functions

\[
f(z) = \sum_{0}^{\infty} a_r T^*_r(z) = \frac{1}{2} a_0 + a_1 T^*_1(z) + a_2 T^*_2(z) + a_3 T^*_3(z) + ...
\]
5.1.1 Numerical determination of the $a^*_r$-coefficients

For the given function $f(z)$ the $a^*_r$ can be determined by

$$a^*_r = \sum_{j=0}^{m} f(\cos^2(\frac{j\pi}{2m})) \cos(\frac{rj\pi}{m})$$

\(^\_\_\_\_\_\_\_\_ \) means: terms with $j=0$ and $j=m$ must be halved and $m$ should be chosen sufficiently large for a good approximation.

5.1.2 Summation

1. substituting the $T^*$-polynomials by their powerseries representations and thereafter applying the Horner Scheme or

2. it is better to use the coefficients directly: starting with a sufficiently large index $n$ and applying recursion:

$$b^*_r = (2 * z - 1) * b^*_{r+1} - b^*_{r+2} + a^*_r, \quad b^*_{n+1} = b^*_{n+2} = 0, \quad r = n, n-1, ..., 0 \quad (22)$$

$$f(z) = \frac{1}{2}(b^*_0 - b^*_2)$$

5.1.3 Differentiation

1. In order to get $f'(z) = \sum_{0}^{n-1} a^*_r T^*_r(z)$ from eq. (20) one starts with a sufficiently large index $n$ and applies the recursion:

$$a^*_r = a^*_{r+1} + 4 r a^*_r, \quad a^*_n = 0, \quad a^*_n+1 = 0 \quad (23)$$

and applies the recursion till $r=1$.

2. Differentiation (chainrule) of

$$f(x) = \sum_{0}^{n} a^*_r T^*_r(x) \text{ with } x = \frac{1}{2}$$

results in

$$f'(z) = -\frac{1}{z^2} \sum_{0}^{n-1} a^*_r T^*_r\left(\frac{1}{2}\right)$$

In addition to the former derivation step each coefficient of the derived form has to be multiplied by

$$-\frac{1}{z^2} = -(\frac{3}{8}T^*_0(\frac{1}{2}) + \frac{1}{2}T^*_1(\frac{1}{2}) + \frac{1}{8}T^*_2(\frac{1}{2})) \quad (24)$$

applying the multiplication rule of the next subsection.

5.1.4 Multiplication of two Chebyshev approximations

The relation

$$T^*_m(z) * T^*_n(z) = \frac{1}{2} [T^*_{m+n}(z) + T^*_{m-n}(z)] \quad (25)$$
is used for multiplying two polynomials eq. (20). The resulting polynomial has $m+n+1$ coefficients and may be further reduced in length with a minor loss in accuracy.

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| \( r \) | \( c_r^* \) | \( r \) | \( c_r^* \) |
|---|---|---|---|
| 0 | + 0.08185 98159 04678 13286 79379 08794 | 27 | - 0.00000 00000 00000 00002 52444 70512 |
| 1 | + 0.04057 97417 47366 64225 70346 89356 | 28 | + 1 32814 92164 |
| 2 | - 0.00040 49079 31144 69879 91516 29808 | 29 | - 15497 24058 |
| 3 | - 0.00094 88972 89378 19193 19687 07281 | 30 | + 1 0336 96592 |
| 4 | + 5.0879 53853 61925 40892 36122 | 31 | - 512 94655 |
| 5 | - 12.63 98282 71842 96931 39424 | 32 | - 973 13164 |
| 6 | - 734 49134 70322 01656 85808 | 33 | + 646 80725 |
| 7 | + 153 71553 54944 52438 97676 | 34 | - 666 93664 |
| 8 | - 12 30594 52195 28798 08799 | 35 | + 78 99455 |
| 9 | - 2 14161 16407 73544 01689 | 36 | - 13 34338 |
| 10 | + 1 01696 97689 38973 88713 | 37 | - 2 41499 |
| 11 | - 19745 33328 72290 64398 | 38 | + 3 41305 |
| 12 | + 215 14210 52726 46241 | 39 | - 1 86412 |
| 13 | + 637 30023 89944 34722 | 40 | + 723 |
| 14 | - 291 75788 31163 52078 | 41 | - 20440 |
| 15 | + 67 97660 47992 56588 | 42 | + 2907 |
| 16 | - 6 92586 21512 51366 | 43 | + 1180 |
| 17 | + 2 00266 46187 92255 | 44 | - 1256 |
| 18 | + 1 57756 74519 07662 | 45 | + 681 |
| 19 | - 4 3329 38804 96534 | 46 | - 274 |
| 20 | + 8271 25257 24804 | 47 | + 82 |
| 21 | - 87 83512 79129 | 48 | - 14 |
| 22 | + 705 72119 91064 | 49 | - 4 |
| 23 | + 354 89122 49033 | 50 | + 5 |
| 24 | - 109 85798 10742 | 51 | - 3 |
| 25 | + 20 73348 40963 | 52 | + 1 |
| 26 | + 52755 41308 | | |
Figure 7: overall convergence

(a) absolute error using only 2 coefficients
(b) absolute error using 5 coefficients

Chebyshev coefficients

| r  | $a_{(0)}^r$ | $a_{(0)}^r$ |
|----|-------------|-------------|
| 0  | 0.44099     | 98884      |
| 1  | 0.21108     | 63054      |
| 2  | 0.00912     | 29231      |
| 3  | 0.0031      | 64394      |
| 4  | 0.0001      | 53324      |
| 5  |             | 36953      |
| 6  |             | 34872      |
| 7  |             | 37346      |
| 8  |             | 15161      |
| 9  |             | 19235      |
| 10 |             | 59626      |
| 11 |             | 19625      |
| 12 |             | 48530      |
| 13 |             | 17755      |
| 14 |             | 18059      |

ψ(0)-function 20 digits

| r  | $a_{(0)}^r$ | $a_{(0)}^r$ |
|----|-------------|-------------|
| 15 | 0.00000     | 00000      |
| 16 | 0.00000     | 00227      |
| 17 |             | 98195      |
| 18 |             | 60526      |
| 19 |             | 54435      |
| 20 |             | 62634      |
| 21 |             | 24377      |
| 22 |             | 5992       |
| 23 |             | 650       |
| 24 |             | 2388      |
| 25 |             | 199       |
| 26 |             | 718       |
| 27 |             | 20       |
| 28 |             | 3       |
| 29 |             | 1       |

Figure 8: The $\psi(0)$-approximation 20 digits
Chebyshev coefficients $\psi^{(1)}$-function 20 digits

| $r$ | $\alpha^{(1)}_r$ | $r$ | $\alpha^{(1)}_r$ |
|-----|----------------|-----|----------------|
| 0   | 0.65708        | 16  | 0.00000        |
| 1   | 0.43109        | 17  | 78 98169       |
| 2   | 0.09873        | 18  | 53 57073       |
| 3   | 0.00356        | 19  | 17 10043       |
| 4   | 0.00025        | 20  | 3 26492        |
| 5   | 0.911   691249 | 21  | 2479           |
| 6   | 3108 83744     | 22  | 27852          |
| 7   | 6189 17377     | 23  | 14009          |
| 8   | 468 49899      | 24  | 4337           |
| 9   | 87 01963       | 25  | 820            |
| 10  | 40 20193       | 26  | 21             |
| 11  | 7 75739        | 27  | 100            |
| 12  | 47235 75596    | 28  | 52             |
| 13  | 25200 70766    | 29  | 18             |
| 14  | 11306 14546    | 30  | 4              |
| 15  | 2679 83664     |     |                |

Figure 9: The $\psi^{(1)}$-function 20 digits