PolyGamma Functions of Negative Order

VICTOR S. ADAMCHIK

January 22, 1998

Abstract

Liouville's fractional integration is used to define polygamma functions $\psi^{(n)}(z)$ for negative integer n. It's shown that such $\psi^{(n)}(z)$ can be represented in a closed form by means of the first derivatives of the Hurwitz Zeta function. Relations to the Barnes G-function and generalized Glaisher's constants are also discussed.

1 Introduction

The idea to define the polygamma function $\psi^{(\nu)}(z)$ for every complex ν via Liouville's fractional integration operator is quite natural and was around for a while (see Ross (1974) and Grossman (1976)). However, for arbitrary negative integer ν the closed form of $\psi^{(\nu)}(z)$ was not developed yet - the only two particular cases $\nu = -2$ and $\nu = -3$ have been studied (see Gosper (1997)). It is the purpose of this note is to consider

$$\psi^{(-n)}(z) = \frac{1}{(n-2)!} \int_0^z (z-t)^{n-2} \log , (t)\, dt, \quad \Re(z) > 0 \tag{1}$$

when n is an arbitrary positive integer, and present $\psi^{(-n)}(z)$ in terms of the Bernoulli numbers and polynomials, the harmonic numbers and first derivatives of the Zeta function. Our approach is based on the following series representation of log , $(1+z)$:

$$\log\,,\,(1+z) = (1-\gamma)\,z - \frac{1}{2}\log\Big(\frac{1+z}{1-z}\Big) + \frac{1}{2}\log\Big(\frac{\pi z}{\sin(\pi z)}\Big) + \sum_{k=1}^{\infty}\frac{z^{2k+1}}{2k+1}\Big(1-\zeta(2k+1)\Big) \tag{2}$$

Replacing log , $(1+z)$ in (1) by (2), upon inverting the order of summation and integration, we thus observe that the essential part of this approach depends on whether or not we are able to evaluate series involving the Riemann Zeta function. We will propose here a specific technique (for more details see Adamchik and Srivastava (1998)) dealing with Zeta series and show that generally the latter can be expressed in terms of derivatives of the Hurwitz function $\zeta'(s,a)$ with respect to its first argument. Furthermore, we will show that when s is negative odd and a is rational $a = \frac{1}{6}, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}$ and $\frac{5}{6}$ then $\zeta'(s,a)$ can be always simplified to less transcendental functions, like the polygamma function and the Riemann Zeta function. In case of negative s we will understand the Hurwitz function, usually defined by the series

$$\zeta(s,a) = \sum_{n=0}^{\infty}\frac{1}{(n+a)^s} \qquad \Re(s) > 1;\ \Re(a) > 0 \tag{3}$$

as the analytic continuation, provided by the Fourier expansion (see Magnus *et al* (1966)):

$$\zeta(s,a) = 2\,(2\pi)^{s-1},\,(1-s)\sum_{n=1}^{\infty} n^{s-1}\sin(2n\pi s + \frac{\pi}{2}s) \tag{4}$$

$$\Re(s) < 0;\ 0 < a \le 1$$

2 Series involving the Zeta function

Let us consider the general quantity

$$\mathrm{S} = \sum_{k=1}^{\infty} f(k)\,\zeta(k+1,a) \tag{5}$$

where the function $f(k)$ behaves at infinity like $O(\frac{(-1)^k}{k})$. Replacing the Zeta function in (5) by the integral representation

$$\zeta(s,a) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} e^{-at}}{1-e^{-t}} \, dt, \quad \Re(s) > 1, \Re(a) > 0 \tag{6}$$

and interchanging the order of summation and integration, we obtain

$$\mathrm{S} = \int_0^\infty F(t) \, \frac{e^{-at}}{1-e^{-t}} \, dt, \tag{7}$$

where the function $F(t)$ is a generating function of $f(k)$

$$F(t) = \sum_{k=1}^{\infty} f(k) \, \frac{t^k}{k!}$$

Thus, the problem of summation has been reduced to integration. Though, the integral (7) looks terribly complicated and hopeless for symbolic integration, the point is that we don't want to evaluate the integral (7), but reduce it again to the integral reprezentation (6). It is easy to see that if the generating function $F(t)$ is a combination of the power, exponential, trigonometric or hyperbolic functions then the integral (7) is a combination of Zeta functions and their derivatives, and thus so is the sum (5). In other words, with this approach we are staying in the same class of functions - sums involving the Zeta function are expressible in Zeta functions.

Next we will provide a couple of examples demonstrating this technique. Consider

$$\Delta_1(x) = \sum_{k=2}^{\infty} \frac{k^2}{k+1} \Big(\zeta(k) - 1\Big) \, x^k$$

In view of

$$\zeta(s) - 1 = \zeta(s,2) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} e^{-t}}{e^t - 1} \, dt$$

upon inverting the order of summation and integration, which can be justified by the absolute convergence of the series and the integral involved, we find that

$$\Delta_1(x) = \int_0^\infty \frac{e^{-t}}{e^t - 1} \, \frac{dt}{t} \, \sum_{k=2}^{\infty} \frac{k^2 \, (x\,t)^k}{(k+1)\,\Gamma(k)}$$

The inner sum is a combination of power series of the exponential function

$$\sum_{k=2}^{\infty} \frac{k^2\,(x\,t)^k}{(k+1)\,\Gamma\,(k)} = \frac{1}{t\,x} - \frac{t\,x}{2} + e^{t\,x}\Big(t^2x^2 - \frac{1}{t\,x} + 1\Big)$$

Now we need to substitute this into the above integral and integrate the whole expression term by term. Unfortunately, we cannot do that since each integral does not pass the convergency test at $t = 0$. To avoid this obstacle we multiply the whole expression by t^{λ} and then integrate each term. We thus obtain

$$\Delta_1(x) = \lim_{\lambda\to 0}\Bigg(\Gamma\,(\lambda+2)\,\zeta(\lambda+2, 2-x)\,x^2 + \Gamma\,(\lambda)\,\zeta(\lambda, 2-x) -$$
$$\frac{x}{2}\,\Gamma\,(\lambda+1)\,\zeta(\lambda+1, 2) - \frac{\Gamma\,(\lambda-1)\,\zeta(\lambda-1, 2-x)}{x} + \frac{\Gamma\,(\lambda-1)\,\zeta(\lambda-1, 2)}{x}\Bigg)$$

Evaluating the limit, we finally arrive at

$$\Delta_1(x) = \frac{3}{2} - \frac{\gamma\,x}{2} + \zeta(2, 2-x)\,x^2 - \frac{\zeta'(-1)}{x} + \zeta'(0, 2-x) + \frac{\zeta'(-1, 2-x)}{x} \quad (8)$$

where γ is the Euler-Mascheroni constant and ζ' denotes the derivative of $\zeta(s, z)$ with respect to the first parameter. As we will see later, for some rational x the sum $\Delta_1(x)$ can be further simplified. For example, if $x = \frac{1}{4}$, then

$$\Delta_1(\frac{1}{4}) = \frac{25}{18} + \frac{\pi^2}{16} - \frac{\gamma}{8} - (\frac{1}{2} + \frac{1}{\pi})\,G - \frac{9}{2}\,\zeta'(-1) + \log(\frac{27\,\Gamma\,(\frac{7}{4})}{64\,\sqrt{2\pi}})$$

where G is Catalan's constant. If $x = -\frac{1}{3}$, then

$$\Delta_1(-\frac{1}{3}) = \frac{7}{16} + \frac{\pi}{6\sqrt{3}} + \frac{\gamma}{6} + \log(\frac{27\,\sqrt[24]{3}\,\Gamma\,(\frac{1}{3})}{64\,\sqrt{2\pi}}) + \frac{1}{36}(4 - \frac{3\sqrt{3}}{\pi})\,\psi'(\frac{1}{3}) + 4\zeta'(-1)$$

All these bring us to another interesting topic: for what values of x the above expression (8) can be simplified to less transcendental functions? It is well-known that

$$\zeta(2, x) = \psi'(x)$$

$$\zeta'(-1) = \frac{1}{12} - \log A$$

$$\zeta'(0,x) = \log\left(\frac{\Gamma(x)}{\sqrt{2\pi}}\right)$$

where A is Glaisher‘s constant (see Finch (1996)) (also known as the Glaisher-Kinkelin constant). But what is $\zeta'(-1,x)$? Or more general $\zeta'(-2n-1,x), n = 0,1,2...$?

3 Derivatives of the Hurwitz Zeta function

From Lerch's transformation formula (see Bateman *et al.* (1953)):

$$\Phi(z,s,v) = i z^{-v} (2\pi)^{s-1}\, \Gamma(1-s)$$
$$\left(e^{-\frac{1}{2}\pi i s}\Phi\left(e^{-2\pi i v}, 1-s, \frac{\log(z)}{2\pi i}\right) - e^{\pi i\left(\frac{s}{2}+2v\right)}\Phi\left(e^{2\pi i v}, 1-s, 1-\frac{\log(z)}{2\pi i}\right)\right)$$

putting $v = 0$, $s = 1-s$ and $z = e^{2\pi i x}$ it follows, that

$$\zeta(s,1-x) + e^{\pi i s}\zeta(s,x) = \frac{e^{\frac{\pi i s}{2}}(2\pi)^s}{\Gamma(s)}\,\mathrm{Li}_{1-s}(e^{2\pi i x}),$$

where we assume that $0 < x < 1$ and s is real. Differentiating this functional equation with respect to s, setting s to $-n$, where n is a positve integer, we obtain

Proposition 1 *Let n be a positive integer and $0 < x < 1$, then*

$$\zeta'(-n,x) + (-1)^n\zeta'(-n,1-x) = \pi i\,\frac{\mathrm{B}_{n+1}(x)}{n+1} + e^{-\frac{\pi i n}{2}}\frac{n!}{(2\pi)^n}\,\mathrm{Li}_{n+1}(e^{2\pi i x}), \quad (9)$$

where $\mathrm{B}_n(x)$ are Bernoulli polynomials, and $\mathrm{Li}_n(x)$ is the polylogarithm function.

Taking into account the multiplication property of the Zeta function

$$\zeta(s,k\,z) = k^{-s}\sum_{i=0}^{k-1}\zeta\left(s, z+\frac{i}{k}\right)$$

and the proposition 1, we easily derive the following representations

$$\zeta'(-1,\frac{1}{6}) = \frac{\log 12}{144} - \frac{\pi}{12\sqrt{3}} + \frac{\psi'(\frac{1}{3})}{8\sqrt{3}\pi} + \frac{1}{6}\zeta'(-1)$$

$$\zeta'(-3,\frac{1}{6}) = -\frac{13\log 2}{25920} - \frac{7\log 3}{51840} + \frac{\pi}{144\sqrt{3}} - \frac{\psi'''(\frac{1}{3})}{384\sqrt{3}\pi^3} + \frac{91}{216}\zeta'(-3)$$

$$\zeta'(-1,\frac{1}{4}) = \frac{G}{4\pi} - \frac{1}{8}\zeta'(-1)$$

$$\zeta'(-3,\frac{1}{4}) = -\frac{\log 2}{2560} + \frac{\pi}{256} - \frac{\psi'''(\frac{1}{4})}{2048\pi^3} - \frac{7}{128}\zeta'(-3)$$

$$\zeta'(-1,\frac{1}{3}) = -\frac{\log 3}{72} - \frac{\pi}{18\sqrt{3}} + \frac{\psi'(\frac{1}{3})}{12\sqrt{3}\pi} - \frac{1}{3}\zeta'(-1)$$

$$\zeta'(-3,\frac{1}{3}) = \frac{\log 3}{6480} + \frac{\pi}{162\sqrt{3}} - \frac{\psi'''(\frac{1}{3})}{432\sqrt{3}\pi^3} - \frac{13}{27}\zeta'(-3)$$

Similar formulas can be obtained for $\zeta'(-n,x)$ when n is odd and $x = \frac{1}{6}$, $\frac{1}{4}$, $\frac{1}{3}$, $\frac{1}{2}$, $\frac{2}{3}$, $\frac{3}{4}$ and $\frac{5}{6}$. For additional formulas of this kind I refer you to the papers Adamchik (1997), and Miller and Adamchik (1998).

4 Negapolygammas

In the second section dealing with zeta sums we mentioned Glaisher's constant A. First this transcendent was studied by Glaisher (see Glaisher (1877)). He found the following integral representation

$$\log A = -\frac{\log(2^5\pi^6)}{36} + \frac{2}{3}\int_0^{\frac{1}{2}} \log\Gamma(z)\,dz$$

Let us consider a more general integral

$$\int_0^q \log\Gamma(z)\,dz \tag{10}$$

and show that

$$\int_0^q \log\Gamma(z)\,dz = \frac{(1-q)\,q}{2} + \frac{q}{2}\log(2\pi) - \zeta'(-1) + \zeta'(-1,q) \tag{11}$$

The proof is based on the series representation (2). Integrating each term of it with respect to z and taking into account the identity

$$\sum_{k=1}^{\infty} \frac{1-\zeta(2k+1)}{(2k+1)\,(k+1)}\,q^{2k+2} = (\gamma-2)\,q^2 - 2\zeta'(-1) + \zeta'(-1,2-q) + \zeta'(-1,2+q)$$

(that can be easily deduced by using the idea described in the second section), we prove (11). The formula (11) first was obtained in Gosper (1997). The integral (10) can be envisaged from another point of view. It is known that the polygamma function is defined by

$$\psi^{(n)}(z) = \frac{\partial^{n+1}}{\partial z^{n+1}} \log \Gamma(z) \tag{12}$$

for positive integer n. However, using Liouville's fractional integration and differentiation operator we can extend the above definition for negative integer n. Thus, for $n = -1$ and $n = -2$ it follows immediately that

$$\psi^{(-1)}(z) = \log \Gamma(z)$$

and

$$\psi^{(-2)}(z) = \int_0^z \log \Gamma(t)dt$$

respectively. This means that the integral (10) is actually a "negapolygamma" of the second order (the term was proposed by B. Gosper). Generally, if we agree on that the bottom limit of integration is zero, we can define polygammas of the negative order as it follows

$$\psi^{(-n)}(z) = \frac{1}{(n-2)!} \int_0^z (z-t)^{n-2} \log \Gamma(t)\, dt, \quad \Re(z) > 0 \tag{13}$$

As a matter of fact, using the series representation (2) for $\log \Gamma(1+z)$, the integral (13) can be evaluated in a closed form

Proposition 2 *Let n be a positive integer and $\Re(z) > 0$, then*

$$\begin{aligned} n!\, \psi^{(-n)}(z) = {} & \frac{n}{2} \log(2\pi)\, z^{n-1} - \mathrm{B}_n(z)\, \mathrm{H}_{n-1} + n\, \zeta'(1-n, z) - \\ & \sum_{i=1}^{n-1} \binom{n}{i} \zeta'(-i)\, (n-i)\, z^{n-i-1} + \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{2i} \mathrm{B}_{2i}\, \mathrm{H}_{2i-1}\, z^{n-2i} \end{aligned} \tag{14}$$

where B_n and $\mathrm{B}_n(z)$ are Bernoulli numbers and polynomials, and H_n are harmonic numbers.

Here are some particular cases:

$$\psi^{(-2)}(z) = \frac{(1-z)\,z}{2} + \frac{z}{2}\log(2\pi) - \zeta'(-1) + \zeta'(-1,z)$$

$$\psi^{(-3)}(z) = -\frac{z}{24}(6z^2 - 9z + 1) + \frac{z^2}{4}\log(2\pi) - \frac{1}{2}\zeta'(-2) - z\,\zeta'(-1) + \frac{1}{2}\zeta'(-2,z)$$

More formulas:

$$\psi^{(-3)}(1) = \log A + \frac{1}{4}\log(2\pi)$$

$$\psi^{(-3)}(\frac{1}{2}) = \frac{1}{2}\log A + \frac{1}{16}\log(2\pi) - \frac{7}{8}\zeta'(-2)$$

$$\psi^{(-3)}(\frac{1}{3}) + \psi^{(-3)}(\frac{2}{3}) = \log A + \frac{5}{36}\log(2\pi) - \frac{13}{9}\zeta'(-2)$$

If we integrate both sides of the equation (14) with respect to z from 0 to z, we obtain the following recurrence relation for $\zeta'(-n,z)$

Corollary 1 *Let n be a positive integer and $\Re(z) > 0$, then*

$$n\int_0^z \zeta'(1-n,x)\,dx = \frac{\mathrm{B_{n+1}} - \mathrm{B_{n+1}}(z)}{n\,(n+1)} - \zeta'(-n) + \zeta'(-n,z) \qquad (15)$$

4.1 Integrals with Polygamma Functions

From the definition (12), using simple integration by parts, we can express the integral

$$\int_0^z x^n\,\psi(x)\,dx$$

in terms of negapolygammas. We have

$$\psi^{(-2)}(z) = z\,\psi^{(-1)}(z) - \int_0^z x\,\psi(x)\,dx$$

$$\psi^{(-3)}(z) = z\,\psi^{(-2)}(z) - \frac{z^2}{2}\,\psi^{(-1)}(z) + \frac{1}{2}\int_0^z x^2\,\psi(x)\,dx$$

and more generally,

$$\int_0^z x^n\,\psi(x)\,dx = (-1)^n\,n!\,\sum_{k=0}^{n}(-1)^k\,\psi^{(k-n-1)}(z)\,\frac{z^k}{k!} \qquad (16)$$

Thus, taking into account the representation (14) of negapolygammas, we obtain

Proposition 3 *Let n be a nonnegative integer and $\Re(z) > 0$, then*

$$\int_0^z x^n\,\psi(x)\,dx = (-1)^{n-1}\zeta'(-n) + \frac{(-1)^n}{n+1}\,\mathrm{B}_{n+1}\,\mathrm{H}_n - \sum_{k=0}^{n}(-1)^k\binom{n}{k}\frac{z^{n-k}}{k+1}\,\mathrm{B}_{k+1}(z)\,\mathrm{H}_k + \sum_{k=0}^{n}(-1)^k\binom{n}{k}z^{n-k}\zeta'(-k,z) \tag{17}$$

4.2 Barnes G-functon

Choi *et al.* (1995) considered a class of series involving the Zeta function that can be evaluated by means of the double Gamma function G (see Barnes (1899)) and their integrals. If we apply our technique described in the second section to those sums we get results in terms of the Hurwitz functions. To compare both approaches we need to establish a connection between the Barnes G-function and the derivatives of the Hurwitz function. The G-function and ζ' are related to each other by

$$\log \mathrm{G}(z+1) - z\,\log\Gamma(z) = \zeta'(-1) - \zeta'(-1,z) \tag{18}$$

The identity pops up immediately from Alexeiewsky's theorem (see Barnes (1899)) and the formula (11). Integrating both sides of (18) with respect to z, in view of formulas (14) and (15), we obtain the following (presumably new) representation

$$\int_0^z \log \mathrm{G}(x+1)\,dx = \frac{z\,(1-2z^2)}{12} + \frac{z^2}{4}\log(2\pi) + z\left(\zeta'(-1)+\zeta'(-1,z)\right) + \zeta'(-2) - \zeta'(-2,z) \tag{19}$$

5 Generalized Glaisher's constants

In 1933 L. Bendersky (see Bendersky (1933) or Finch (1996)) considered the limit

$$\log \mathrm{A_k} = \lim_{n\to\infty}\left(\sum_{m=1}^{n} m^k\,\log m - p(n,k)\right), \tag{20}$$

where

$$p(n,k) = \frac{n^k}{2} \log n + \frac{n^{k+1}}{k+1} \left(\log n - \frac{1}{k+1} \right) +$$

$$k! \sum_{j=1}^{k} \frac{n^{k-j} \, \mathrm{B_{j+1}}}{(j+1)! \, (k-j)!} \left[\log n + (1 - \delta_{k-j}) \sum_{i=1}^{k} \frac{1}{k-i+1} \right]$$

and δ_k is the Kronecker symbol. He found that

$$\log \mathrm{A}_0 = \frac{1}{2} \log(2\pi)$$

and

$$\log \mathrm{A}_1 = \frac{1}{12} - \zeta'(-1) = \log \mathrm{A}$$

and for the next three values he gave their numerical approximations. However, it turns out that all $\mathrm{A_k}$ can be expressed in terms of derivatives of the Zeta function, by using the asymptotic expansion of the Hurwitz Zeta function (see Magnus *et al* (1966)):

$$\zeta(z,\alpha) = \frac{\alpha^{1-z}}{z-1} + \frac{\alpha^{-z}}{2} + \sum_{j=1}^{m-1} \frac{\mathrm{B_{2j}}}{(2j)!} \frac{\Gamma(z+2j-1)}{\Gamma(z)} \, \alpha^{-2j-z+1} + \mathrm{O}(\alpha^{-2m-z-1}) \tag{21}$$

when $|\alpha| \to \infty$ and $|\arg \alpha| < \pi$. Differentiating (21) with respect to z and setting z to -1 and -2, for example, we have

$$\zeta'(-1,\alpha) = \frac{1}{12} - \frac{\alpha^2}{4} + \log \alpha \, \left(\frac{1}{12} - \frac{\alpha}{2} + \frac{\alpha^2}{2} \right) + \mathrm{O}(\frac{1}{\alpha^2}) \tag{22}$$

and

$$\zeta'(-2,\alpha) = \frac{\alpha}{12} - \frac{\alpha^3}{9} + \log \alpha \, \left(\frac{\alpha}{6} - \frac{\alpha^2}{2} + \frac{\alpha^3}{3} \right) + \mathrm{O}(\frac{1}{\alpha}) \tag{23}$$

Now, taking into account the analytical property of the Hurwitz function, the sum in (20) is

$$\sum_{m=1}^{n} m^k \, \log m = \zeta'(-k, n+1) - \zeta'(-k)$$

Therefore, applying asymptotic expansions of the derivatives of the Hurwitz functions to (20), we find that

$$\log \mathrm{A}_2 = -\zeta'(-2)$$

$$\log \mathrm{A}_3 = -\frac{11}{720} - \zeta'(-3)$$

$$\log \mathrm{A}_4 = -\zeta'(-4)$$

Generally,

Proposition 4 *Let k be a nonnegative integer, then the generalized Glaisher constants* A_k *are of the form*

$$\log \mathrm{A}_\mathrm{k} = \frac{\mathrm{B}_{\mathrm{k}+1}\,\mathrm{H}_\mathrm{k}}{k+1} - \zeta'(-k) \tag{24}$$

where B_n *are Bernoulli numbers and* H_n *are harmonic numbers.*

References

[1] Adamchik,V. S. , Srivastava,H. M. (1998) *Some Series of the Zeta and Related Functions. Analysis* (accepted for publication).

[2] Adamchik V. S.,(1997), A Class of Logarithmic Integrals, *Proc. of ISSAC'97* , 1–8.

[3] Adamchik, V.S., Srivastava, H.M. (1998),Some Series of the Zeta and Related Functions. *Analysis*, accepted for publication.

[4] Barnes,E. W. (1899), The Theory of G-function, *Quart. J. Math*, **31**, 264-314.

[5] Bateman,H. , Erdelyi,A. (1953) *Higher Transcendental Functions*, Vol.1, McGraw-Hill.

[6] Bendersky, L. (1933), Sur la function gamma généralisée, *Acta Math*, **61**, 263-322.

[7] Choi,J., Srivastava,H. M , Quine,J. R. (1995), Some Series Involving the Zeta Function, *Bull. Austral. Math. Soc.*, **51**, 383-393.

[8] Finch, S. (1996), Glaisher-Kinkelin Constant, In *HTML essay at URL*, www.mathsoft.com/asolve/ constant/glshkn/glshkn.html.

[9] Glaisher,J. W. L. (1877), On a Numerical Continued Product, *Messenger of Math.*, **6**, 71-76.

[10] Gosper,R. W. (1997), $\int_{\frac{n}{4}}^{\frac{m}{6}} \log , (z)dz$, In *Special Functions, q-series and related topics*, Amer. Math. Soc. Vol. 14.

[11] Magnus,W. , Oberhettinger,F. , Soni,R. P. (1966), *Formulas and Theorems for the Special Functions of Mathematical Physics*, Springer-Verlag.

[12] Miller,J., Adamchik, V.S. (1998), Derivatives of the Hurwitz Zeta Function for Rational Arguments, J. Symb. Comput., to appear.

[13] Ross, B.. (1974), Problem 6002, Amer. Math. Monthly, **81**, 1121.

[14] Grossman, N.. (1976), Polygamma Functions of Arbitrary Order, SIAM J. Math. Anal., **7**, 366-372.