Derivatives of the Hurwitz Zeta Function for Rational Arguments

JEFF MILLER AND VICTOR S. ADAMCHIK

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Abstract

The functional equation for the Hurwitz Zeta function $\zeta(s,a)$ is used to obtain formulas for derivatives of $\zeta(s,a)$ at negative odd s and rational a. For several of these rational arguments, closed form expressions are given in terms of simpler transcendental functions, like the logarithm, the polygamma function, and the Riemann Zeta function.

1 Introduction

The Hurwitz Zeta function $\zeta(s,a)$, defined as the analytic continuation of the series

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

is one of several higher transcendental functions that appear in a wide variety of mathematical contexts; see the relevant literature, [1], [2], [3]. Among the most common of these situations is the evaluation of certain class of definite integrals and infinite sums. Recently, V. Adamchik [4] obtained closed form expressions for a class of definite integrals involving cyclotomic polynomials and nested logarithms in terms of derivatives of $\zeta(s, a)$. For example,

$$\frac{1}{4} \int_0^1 \frac{x^4 - 6x^2 + 1}{(1+x^2)^3} \log \log(\frac{1}{x}) dx$$

$$= -\left(\log(4) + \gamma\right) \left(\zeta(-1, \frac{1}{4}) - \zeta(-1, \frac{3}{4})\right) + \zeta'(-1, \frac{1}{4}) - \zeta'(-1, \frac{3}{4})$$

where $\zeta'(s,a)$ denotes the derivative with respect to the first parameter $\frac{\partial}{\partial s}\zeta(s,a)$. By computing $\zeta'(s,a)$ at s=-1, and $a=\frac{1}{4}$ and $\frac{3}{4}$, the above integral can be reduced to just $\frac{G}{2\pi}$, where G is Catalan's constant. He also gave expressions for $\zeta'(-1,p)$ at $p=\frac{1}{2},\frac{1}{3},\frac{1}{6},\frac{2}{3}$ and $\frac{5}{6}$ in terms of other known transcendental functions. These results later were applied to infinite sums involving the Riemann Zeta function (see [5] and [6]), for example

$$4\sum_{k=0}^{\infty} \frac{1-\zeta(2k)}{2k+1} \left(\frac{1}{9}\right)^k = 6\log(2) + \log(3) + 6\zeta'(-1, \frac{1}{3}) - 6\zeta'(-1, \frac{2}{3})$$
$$= \log(192) - \pi \frac{2\sqrt{3}}{9} + \frac{\sqrt{3}}{3\pi} \psi^{(1)}(\frac{1}{3})$$

where $\psi^{(p)}(z)$ is a polygamma function defined by

$$\psi^{(p)}(z) = \frac{d^{p+1}}{dz^{p+1}} \log_{+}(z) \qquad (p = 0, 1, 2, ...),$$

The purpose of this paper is to obtain general representations for $\zeta'(n,p)$ at any negative odd integer n and $p = \frac{1}{6}, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}, \frac{3}{4}, \frac{2}{3}$, and $\frac{5}{6}$. The proof of the general formula will be explicitly shown for $p = \frac{1}{3}$, for others p formulas follow by analogy.

2 Derivatives of the Hurwitz Zeta Function

In this section we develop the closed form expressions for derivatives of $\zeta(s, a)$. First we will need a lemma connecting derivatives of the Riemann Zeta function:

Lemma 1 For any positive integer k,

$$\zeta'(2k) = \frac{(-1)^{k+1} (2\pi)^{2k}}{2(2k)!} \left(2k \zeta'(-2k+1) - (\psi(2k) - \log(2\pi)) B_{2k} \right) \tag{2}$$

This relationship is implied by the functional equation for the Riemann Zeta function:

$$\zeta(1-s) = 2(2\pi)^{-s}, (s) \cos\left(\frac{\pi s}{2}\right)\zeta(s). \tag{3}$$

Differentiating both sides of this equation with respect to s, putting s = 2k, and using Euler's expansion for $\zeta(2k)$,

$$\zeta(2k) = \frac{(-1)^{k+1} (2\pi)^{2k} B_{2k}}{2(2k)!} \qquad (k = 1, 2, 3, \dots)$$
 (4)

we arrive at the desired result.

Proposition 1 Let k, p, and q be positive integers such that p < q. Then,

$$\zeta'\left(-2k+1, \frac{p}{q}\right) = \frac{(\psi(2k) - \log(2\pi q))B_{2k}(p/q)}{2k} - \frac{(\psi(2k) - \log(2\pi))B_{2k}}{q^{2k} 2k} + \frac{(-1)^{k+1} \pi}{(2\pi q)^{2k}} \sum_{n=1}^{q-1} \sin\left(\frac{2\pi pn}{q}\right) \psi^{(2k-1)}\left(\frac{n}{q}\right) + \frac{(-1)^{k+1} 2(2k-1)!}{(2\pi q)^{2k}} \sum_{n=1}^{q-1} \cos\left(\frac{2\pi pn}{q}\right) \zeta'\left(2k, \frac{n}{q}\right) + \frac{\zeta'(-2k+1)}{q^{2k}}$$

$$(5)$$

Rademacher's formula states that for all s,

$$\zeta\left(s, \frac{p}{q}\right) = 2, (1-s)(2\pi q)^{s-1} \sum_{n=1}^{q} \sin\left(\frac{\pi s}{2} + \frac{2\pi np}{q}\right) \zeta\left(1-s, \frac{n}{q}\right).$$
 (6)

This is also known as the functional equation for the Hurwitz Zeta function (see Apostol (1976)). By differentiating both sides of the equation with respect to s, letting s = -2k + 1, and then applying identities (see [1], [7])

$$\psi^{(p)}(z) = (-1)^{p+1} p! \zeta(p+1,z) \qquad (p=1,2,3,\ldots), \tag{7}$$

and

$$\zeta(-n,a) = -\frac{B_{n+1}(a)}{n+1} \qquad (n=0,1,2,\ldots).$$
(8)

to the appropriate terms, we get

$$\zeta'\left(-2k+1, \frac{p}{q}\right) = \frac{(\psi(2k) - \log(2\pi q))B_{2k}(p/q)}{2k} + \frac{(-1)^{k+1}\pi}{(2\pi q)^{2k}} \sum_{n=1}^{q} \sin\left(\frac{2\pi pn}{q}\right) \psi^{(2k-1)}\left(\frac{n}{q}\right) + \frac{(-1)^{k+1}2(2k-1)!}{(2\pi q)^{2k}} \sum_{n=1}^{q} \cos\left(\frac{2\pi pn}{q}\right) \zeta'\left(2k, \frac{n}{q}\right)$$
(9)

In the first sum, the n=q term vanishes, and in the second sum, the same term is simply $\zeta'(2k)$. We can pull this term out, but we want to stay within the same class of functions, so Lemma 1 is employed to write $\zeta'(2k)$ in terms of $\zeta'(-2k+1)$, thus completing the proof.

In general, it is not easy to simplify equation (5) for arbitrary p and q. However, for some simple cases, the summed trigonometric terms come out complementary, and relationships can be found among the special functions that yield a nice closed form. As an illustration, consider the p=1, q=3 case:

Proposition 2 For any positive integer k,

$$\zeta'\left(-2k+1,\frac{1}{3}\right) = -\frac{(9^{k}-1)B_{2k}\pi}{\sqrt{3}(3^{2k-1}-1)8k} - \frac{B_{2k}\log(3)}{(3^{2k-1})4k} - \frac{(-1)^{k}\psi^{(2k-1)}(\frac{1}{3})}{2\sqrt{3}(6\pi)^{2k-1}} - \frac{(3^{2k-1}-1)\zeta'(-2k+1)}{2(3^{2k-1})}$$
(10)

By taking equation (5) with p = 1 and q = 3, we immediately obtain

$$\zeta'\left(-2k+1, \frac{1}{3}\right) = \frac{(\psi(2k) - \log(6\pi))B_{2k}(\frac{1}{3})}{2k} - \frac{(\psi(2k) - \log(2\pi))B_{2k}}{9^k 2k} + \frac{(-1)^{k+1}}{4\sqrt{3}(6\pi)^{2k-1}} \left(\psi^{(2k-1)}\left(\frac{1}{3}\right) - \psi^{(2k-1)}\left(\frac{2}{3}\right)\right) - \frac{(-1)^{k+1}(2k-1)!}{(6\pi)^{2k}} \left(\zeta'\left(2k, \frac{1}{3}\right) + \zeta'\left(2k, \frac{2}{3}\right)\right) + \frac{\zeta'(-2k+1)}{9^k}$$

$$(11)$$

Now we will apply three easily derivable identities to simplify this result. Consider the multiplication formula for the Hurwitz Zeta function:

$$\zeta(s,kz) = k^{-s} \sum_{n=0}^{k-1} \zeta(s,z + \frac{n}{k}) \qquad (k = 1, 2, 3, \ldots).$$
 (12)

Putting z = 1/k and using equation (7) yields

$$\psi^{(n)}\left(\frac{2}{3}\right) = (-1)^{n+1} n! \left(3^{n+1} - 1\right) \zeta(n+1) - \psi^{(n)}\left(\frac{1}{3}\right) \qquad (n = 1, 2, 3, \ldots). \tag{13}$$

By differentiating the multiplication formula, we obtain a similar identity,

$$\sum_{n=1}^{k-1} \zeta'\left(s, \frac{n}{k}\right) = (k^s - 1)\zeta'(s) + k^s \log(k)\zeta(s) \qquad (k = 1, 2, 3, \ldots), \tag{14}$$

which implies

$$\zeta'\left(2k, \frac{1}{3}\right) + \zeta'\left(2k, \frac{2}{3}\right) = (9^k - 1)\zeta'(2k) + 9^k \log(3)\zeta(2k). \tag{15}$$

Finally, through some simple identities of the Bernoulli polynomials, one can see that

$$B_{2k}\left(\frac{1}{3}\right) = \frac{(3^{1-2k} - 1)B_{2k}}{2} \qquad (k = 1, 2, 3, \ldots). \tag{16}$$

Substituting (13), (15), and (16) into (11) leaves an equation that is solely in terms of the transcendentals π , $\log(3)$, $\psi^{(2k-1)}(\frac{1}{3})$, and $\zeta'(-2k+1)$. Grouping according to these terms yields the desired result.

By following the method just demonstrated, additional cases for $\zeta'(-2k+1,p)$ with $p=\frac{1}{2},\,\frac{2}{3},\,\frac{1}{4},\,\frac{3}{4},\,\frac{1}{6}$ and $\frac{5}{6}$ can be derived. Though some different simplifications regarding Bernoulli polynomials and the polygamma function are required, they are simple analogs of the identities already stated.

Proposition 3 For any positive integer k,

$$\zeta'\left(-2k+1,\frac{1}{2}\right) = -\frac{B_{2k}\log(2)}{4^kk} - \frac{(2^{2k-1}-1)\zeta'(-2k+1)}{2^{2k-1}}$$
(17)

$$\left. \begin{array}{l} \zeta'\left(-2k+1,\frac{1}{3}\right) \\ \zeta'\left(-2k+1,\frac{2}{3}\right) \end{array} \right\} = \mp \frac{(9^{k}-1)B_{2k}\pi}{\sqrt{3}(3^{2k-1}-1)8k} - \frac{B_{2k}\log(3)}{(3^{2k-1})4k} + \\ \mp \frac{(-1)^{k}\psi^{(2k-1)}(\frac{1}{3})}{2\sqrt{3}(6\pi)^{2k-1}} - \frac{(3^{2k-1}-1)\zeta'(-2k+1)}{2(3^{2k-1})} \end{array} \right. \tag{18}$$

$$\left. \begin{cases} \zeta'\left(-2k+1,\frac{1}{4}\right) \\ \zeta'\left(-2k+1,\frac{3}{4}\right) \end{cases} \right\} = \mp \frac{(4^{k}-1)B_{2k}\pi}{4^{k+1}k} + \frac{(4^{k-1}-1)B_{2k}\log(2)}{2^{4k-1}k} - \frac{(19)}{4(8\pi)^{2k-1}} + \frac{(-1)^{k}\psi^{(2k-1)}(\frac{1}{4})}{4(8\pi)^{2k-1}} - \frac{(2^{2k-1}-1)\zeta'(-2k+1)}{2^{4k-1}} \right)$$

$$\left. \begin{array}{l} \zeta'\left(-2k+1,\frac{1}{6}\right) \\ \zeta'\left(-2k+1,\frac{5}{6}\right) \end{array} \right\} = \mp \frac{(9^{k}-1)(2^{2k-1}+1)B_{2k}\pi}{\sqrt{3}(6^{2k-1})8k} + \frac{B_{2k}(3^{2k-1}-1)\log(2)}{(6^{2k-1})4k} + \\ \frac{B_{2k}(2^{2k-1}-1)\log(3)}{(6^{2k-1})4k} \mp \frac{(-1)^{k}(2^{2k-1}+1)\psi^{(2k-1)}(\frac{1}{3})}{2\sqrt{3}(12\pi)^{2k-1}} + \\ \frac{(2^{2k-1}-1)(3^{2k-1}-1)\zeta'(-2k+1)}{2(6^{2k-1})} \end{array} \right. \tag{20}$$

3 Discussion

Some values of $\zeta'(s,a)$ are conspicuously missing from the analysis presented. For one, s was restricted to be a negative odd integer. Considering negative even integers turns out not to be fruitful: the change in parity leads to terms with differences of Hurwitz Zeta derivatives instead of sums of them. This is also why closed form expressions for other rational arguments, such as $p = \frac{1}{5}$, could not be possibly obtained. Summed trigonometric terms give rise to sums of Hurwitz Zeta derivatives with alternating signs that can't be removed with the multiplication formula or other known identities. This fundamental problem is embodied in the following equation from [4]:

$$\zeta'(-n,x) + (-1)^n \zeta'(-n,1-x) = \pi i \frac{B_{n+1}(x)}{n+1} + e^{-\frac{\pi i n}{2}} \frac{n!}{(2\pi)^n} \operatorname{Li}_{n+1}(e^{2\pi i x}). \tag{21}$$

The presence of the $(-1)^n$ term on the left suggests that evaluating differences of Hurwitz Zeta derivatives at negative even integers is inherently more difficult than evaluating them for negative odd integers.

Odd-even issues like this have deep roots in the study of Zeta functions. For example, it has been known since Euler that the Riemann Zeta function at positive even integers can be evaluated as a rational function of π (see equation (4)). However, for positive odd integers, a formula is still nonexistent. There is also an odd-even problem with the polygamma function $\psi^{(p)}(z)$, as demonstrated in the work of Kolbig [8], in which he gives closed-form expressions for both sums and differences of the polygamma function at several rational arguments. For polygammas of even order, the difference was expressible in terms of simple constants, but the sum was not, and vice-versa for polygammas of the negative order. The problematic term in both cases was an infinite series with no known formula. A related example is found in the Clausen functions, which are also replete with symmetry mismatches in the even and odd orders. These problems are all exact parallels of the difficulties encountered in this paper with derivatives of the Hurwitz Zeta function.

References

[1] W. Magnus, F. Oberhettinger, R. P. Soni, Formulas and Theorems for

- the Special Functions of Mathematical Physics, (Springer-Verlag, 1966).
- [2] T. M. Apostol, Introduction to Analytic Number Theory, Vol.1, (Springer-Verlag, 1976).
- [3] E. Elizalde, at al., Zeta Regularization Techniques with Applications, (World Scientific, 1994).
- [4] V.S. Adamchik, A Class of Logarithmic Integrals, *Proc. of ISSAC'97*, 1997 1-8.
- [5] V.S. Adamchik, PolyGamma Functions of Negative Order. J. Comp. and Appl. Math., to appear.
- [6] V.S. Adamchik, H.M. Srivastava, Some Series of the Zeta and Related Functions. Analysis, 31 (1998) 131-144.
- [7] H. Bateman, A. Erdelyi, *Higher Transcendental Functions*, Vol.1, (McGraw-Hill, 1953).
- [8] V. Kolbig, The Polygamma Function $\psi^{(k)}(x)$ for $x = \frac{1}{4}$ and $x = \frac{3}{4}$. J. Comp. and Appl. Math., 75 (1996) 43-46.