Fast evaluation for a certain class of lattice sums

Richard E. Crandall
Center for Advanced Computation, Reed College, Portland OR

Abstract. Herein we explain methods for rapid numerical evaluation of certain lattice sums:

$$Z(a,b,c) = \sum_{(m,n)\in Z^2}{}' \frac{m^{2a}n^{2b}}{(m^2+n^2)^c},$$

where a, b are positive integers, while c need not (for at least one evaluation method) be an integer. Two methods are given, the first of which involving incomplete-gamma series and calculating the analytic continuation for general complex c; while the second method is valid for positive integers $c > a+b+1$ yet involves a 1-dimensional convergent sum involving elementary functions alone.

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1. Class of sums

J. Borwein and D. Bailey [Bailey 2000] have indicated an interest in efficient evaluation of sums:

$$Z(a,b,c) = \sum_{m,n \in Z^2}{}' \frac{m^{2a} n^{2b}}{(m^2+n^2)^c},$$

where the $\sum'$ notation means we avoid any singular summands. For computational purposes, we can cast this Z sum in terms of certain Epstein zeta function derivatives, and thereby use different types of acceleration formulae [Crandall 1998, 1999] to achieve high-precision evaluations.

2. Incomplete-gamma series

In what follows, let a, b be positive integers but allow c to be any complex number. A primary observation is that Z is closely related to a certain Epstein zeta function:

$$F(x,y,s) = \sum_{m,n \in Z^2}{}' \frac{1}{(m^2 x + n^2 y)^s}$$

in the sense that direct differentation (assuming absolute convergence of relevant summations) yields:

$$\left.\frac{\partial^{a+b} F}{\partial^a x \partial^b y}\right|_{x=1,\ y=1} = (-1)^{a+b} \frac{\Gamma(s+a+b)}{\Gamma(s)} Z(a,b,s+a+b).$$

Thus

$$Z(a,b,c) = (-1)^{a+b} \frac{\Gamma(c-a-b)}{\Gamma(c)} \left.\frac{\partial^{a+b}}{\partial^a x \partial^b y} F(x,y,c-a-b)\right|_{x=1,\ y=1}.$$

Now we refer to the aforementioned efficient means for evaluating Epstein zeta functions. A key formula is:

$$\frac{\Gamma(s)}{\pi^s} F(x,y,s) = \frac{1}{\sqrt{xy}} \frac{1}{s-1} - \frac{1}{s} + \pi^{-s} \sum_{m,n \in Z^2}{}' \frac{\Gamma(s, \pi(m^2 x + n^2 y))}{(m^2 x + n^2 y)^s} +$$

$$\frac{\pi^{s-1}}{\sqrt{xy}} \sum_{m,n \in Z^2}{}' \frac{\Gamma(1-s, \pi(m^2/x + n^2/y))}{(m^2/x + n^2/y)^{1-s}}.$$

Now to obtain evaluations of Z, one may either take numerical (a,b)-th partial derivatives at $(x,y) = (1,1)$, or proceed symbolically, noting that any derivative after the 0-th of an incomplete gamma function is in fact an elementary function.

One notes there is also the possibility of a functional equation, in the style of that for the Riemann zeta function (and generalizable to Epstein zeta functions), stemming directly from the symbolic-differentiation notion. One thing we can say right off: the previous formula yield a closed-form expression for the analytic continuation for $Z(a,b,a+b)$, which value does not have an absolutely convergent sum, yet said value as an analytic continuation is a computable rational number. Some example analytic continuation values would be $Z(0,0,0) = -1$ and $Z(1,1,2) = -1/4$.

An example of these machinations is afforded by the instance:

$$Z(1,1,4) = \frac{1}{6} F_{,x,y}(1,1,2),$$

where the nomenclature $F_{,x,y}$ denotes the mixed derivative $\partial^2 F/\partial x \partial y$. Taking naive numerical derivatives (with increment $\epsilon = 10^{-30}$ for each of x, y) and each 2-dimensional summation of incomplete-gamma terms over a square of apothem 10 in (m,n) space, we find:

$$Z(1,1,4) \sim 0.3594500046922553231660712813092\ldots,$$

presumably correct to all but the last few displayed digits.

3. Elementary-function series

Though the incomplete-gamma series just discussed is perhaps the series of optimal convergence, being as $\Gamma(a,z)$ generally enjoys Gaussian decay in the z argument, the sums are nevertheless 2-dimensional and of course incomplete-gamma evaluatiosn themselves are problematic. One way to cut down the effort is to store tabulations of $\Gamma(a,z)$ for a strategic set of z values.

But a very different approach leads to 1-dimensional, efficient series involving only elementary functions. Restrict the c parameter to be an integer, and assuming $c > a+b+1$ (so that the defining sum for Z enjoys absolute convergence), we start from a symbolic realization about a non-singular sum $\sum{}'$:

$$\sum_{(m,n)\in Z^2}{}' = \sum_{m=0,\ n\neq 0} + 2\sum_{m=1}^{\infty}\sum_{n\in Z}$$

so that

$$Z(a,b,c) = 2\delta_{0a}\zeta(2c-2b) + 2\sum_{m=1}^{\infty} m^{2a} \sum_{n\in Z} n^{2b}/(m^2+n^2)^c.$$

Now one reduces one of the sums via the identity:

$$\sum_{n\in Z} \frac{1}{(m^2+n^2y+z)} = \frac{\pi}{\sqrt{y}\sqrt{m^2+z}} \coth(\pi\sqrt{(m^2+z)/y}),$$

which identity may be derived via Poisson summation. Noting that the coth function is asymptotic to 1, we may subtract off such a 1 to arrive at the following general formula:

$$Z(a,b,c) = 2\delta_{0a}\zeta(2c-2b) + \frac{2\pi(2b-1)!!(2c-2b-3)!!}{2^{c-1}(c-1)!}\zeta(2c-2a-2b-1) +$$

$$2\frac{(-1)^{c-1}}{(c-1)!}\sum_{m=1}^{\infty} m^{2a}\frac{\partial^{c-1}}{\partial^b y \partial^{c-1-b} z}\frac{\pi}{\sqrt{y}\sqrt{m^2+z}}\left(\coth(\pi\sqrt{(m^2+z)/y})-1\right)\Big|_{z=0,\ y=1}.$$

(Note that we are defining (-1)!! = 1.) Speaking qualitatively, we have cast $Z(a,b,c)$ in a form:

$$Z = (\zeta \text{ term}) + (\zeta \text{ term}) + (\text{rapidly convergent series}).$$

The indicated series, in other words, is comprised always of elementary functions with each summand enjoying exponential decay.

It is of interest that such a "one-sided" summation technique (after all, we use the coth identity on the n sum but not the m sum) achieved a certain vogue in the study of crystallographic lattice sums. Celebrated crystal expansions due to Hautot, Glasser, and Zucker have exploited the coth expedient to yield extremely efficient and practical series [Crandall 1999].

As an example of the present elementary-function series, one has the specific example:

$$Z(1,1,4) = \frac{\pi}{8}\zeta(3) + \frac{\pi}{24}\sum_{m=1}^{\infty}\frac{1}{m^3}[-3+3\coth(m\pi)+$$

$$3m\pi\operatorname{csch}^2(m\pi) - 2m^3\pi^3(2+\cosh(2m\pi))\operatorname{csch}^4(m\pi)].$$

4. Further analyses

We have indicated that the former, incomplete-gamma series can conceivably be used to develop analytic relations amongst Z instances. But there is another interesting analytic avenue, namely the use of known Z evaluations. For example, one has:

$$Z(0,0,c) = \sum_{(m,n)\in Z^2}{}' \frac{1}{(m^2+n^2)^c} = 4\zeta(c)\beta(c),$$

where the new L-series appearing here is $\beta(s) = 1^{-s} - 3^{-s} + 5^{-s} - \ldots$. For example, $\beta(2) = G$ is the celebrated Catalan constant, and we have from the elementary-series formalism applied to $Z(0,0,2)$ the result:

$$G = \frac{\pi^2}{30} + \frac{3}{2\pi}\zeta(3) - \frac{3}{\pi}\sum_{m=1}^{\infty}\frac{1-e^{2\pi m}(1+2\pi m)}{m^3(e^{2\pi m}-1)^2}$$

for the Catalan constant. In this example for G the exponential summand decay is particularly manifest. Clearly such a scheme can also be used for other β-function evaluations.

One may also use the elementary-series approach on $Z(0,0,3) = 4\zeta(3)\pi^3/27$ to arrive at a rapidly converging series for a certain linear combination of $\zeta(3),\ \zeta(5)$. It should be possible in this way to obtain exponentially-convergent expansions for general $\zeta(\text{odd})$. If one desires an inductive chain involving linear combinations of $\zeta(\text{odd}),\ \zeta(\text{odd}\ +2)$, it is possible to "ignite" such a chain by exploiting the inherent asymmetry in the elementary-series scheme. For example, the mere observation that $Z(1,0,3) = Z(0,1,3)$ immediately yields, upon comparison of the two resulting Z expansions, an exponential series for $\zeta(3)$ alone. Though the resulting exponential series may be previously known, it remains unclear how wide is the class of coth-series identities attendant on the symmetry properties of the original $Z(a,b,c)$ function. Likewise it is not yet clear how simple Z-symmetries, for example:

$$Z(4,0,6) + Z(1,1,6) = \frac{1}{2}Z(0,0,4) = 2\zeta(4)\beta(4)$$

yield new coth identities; or conversely, how coth manipulations might uncover new Z interrelations.

5. References

Bailey D 2000, private communication.

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