Fast evaluation of Zucker moment-sums

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1. Zucker moment-sum

J. Zucker has asked for efficient numerical evaluation of certain moment-sums, namely lattice sums appropriate to a regular, bipolar crystal structure

$$K(s,\{a,b,c\}) := \sum_{\vec{r}\in Z^3}{}' \frac{x^a y^b z^c (-1)^{x+y+z}}{r^s},$$

where $\vec{r} := \{x,y,z\}$, $r := \sqrt{x^2+y^2+z^2}$ and $\sum'$ means one avoids an origin singularity during summation. A special instance is the celebrated Madelung constant

$$M = K(1,\{0,0,0\}) = -1.74756459463318219\ldots,$$

calculable via (many) independent methods, and useful for testing the evaluation method herein. One may also test the present method according to formal identities

$$K(s-4,\{0,0,0\}) = 3K(s,4,0,0) + 6K(s,\{2,2,0\}),$$

$$K(s-2,\{0,0,0\}) = 3K(s,\{2,0,0\}),$$

easily obtained by expanding powers of r^2.

Our basic idea for evaluating the Zucker moment-sums K is to start with the Epstein zeta function form:

$$Z(s,\vec{u}) := \sum{}' \frac{e^{2\pi i \vec{u}\cdot\vec{r}}}{r^s},$$

where the relevant 3-vectors are $\vec{u} = \{\alpha, \beta, \gamma\}$ and $\vec{r} = \{x, y, z\}$. Then a formal relation between K and Z is

$$K(s, \vec{u}) = \left(\frac{1}{2\pi i}\right)^{a+b+c} \left(\frac{\partial}{\partial\alpha}\right)^a \left(\frac{\partial}{\partial\beta}\right)^b \left(\frac{\partial}{\partial\gamma}\right)^c Z(s, \vec{u}) \mid_{\vec{u}=\{1/2,1/2,1/2\}}. \tag{1.1}$$

Furthermore, as in [Crandall 1998], one may use Riemann splitting on the Epstein Z for rapid evaluation, in which scheme the cases $\vec{u} := \{\alpha, \beta, \gamma\} \notin Z^3$ involve the form

$$Z(s, \vec{u}) = -\frac{\lambda^{s/2}}{\Gamma(s/2+1)} + {\sum}' \frac{e^{2\pi i \vec{u}\cdot\vec{r}}}{r^s} \frac{\Gamma(s/2, \lambda r^2)}{\Gamma(s/2)} + L(s, \vec{u}, \lambda), \tag{1.2}$$

with

$$L(s, \vec{u}, \lambda) = \pi^{s-3/2} \sum \frac{1}{v^{3-s}} \frac{\Gamma((3-s)/2, \pi^2 v^2/\lambda)}{\Gamma(s/2)}.$$

where λ is a free parameter, and both sums are over the $\vec{r} := \{x, y, z\} \in Z^3$ lattice, but for the second sum we posit $v^2 := (\vec{r} - \vec{u})^2$ (and so by the hypothesis $\vec{u} \notin Z^3$ this second sum need not be "primed").

We note that the above splitting formula for Epstein Z also gives analytic-continuation values: The rapidly-decaying incomplete-gamma function terms have nothing to fear from complex s arguments of arbitrary magnitude. For example, we infer

$$Z(0, \vec{u}) = -1,$$

$$K(0, \{a, b, c\}) = 0,$$

as the analytic-continuation values at $s = 0$, for *any* vector $\vec{u} \notin Z^3$.

From this point onward there are two pathways for arriving at high-precision numerical K values. One method is to differentiate in (1.1) numerically. Note that only L has nontrivial derivatoves. To achieve decimal precision p with $M := a + b + c$, one may choose say $\epsilon = 10^{-p-M}$ and calculate

$$K(s, \vec{u}) \approx {\sum_{\vec{r}\in Z^3}}' \frac{x^a y^b z^c (-1)^{x+y+z}}{r^s} \frac{\Gamma(s/2, \lambda r^2)}{\Gamma(s/2)} \tag{1.3}$$

$$+ \left(\frac{1}{2\pi i \epsilon}\right)^M \sum_{j=0}^{a} \sum_{k=0}^{b} \sum_{l=0}^{c} \binom{a}{j} \binom{b}{k} \binom{c}{l} (-1)^{j+k+l}$$

$$L\left(s, \left\{\frac{1+(a-2j)\epsilon}{2}, \frac{1+(b-2k)\epsilon}{2}, \frac{1+(c-2l)\epsilon}{2}\right\}, \lambda\right)$$

with the L terms themselves each calculated, via (1.2), to a higher precision, say $p \cdot (1 + \max(a, b, c))$ digits. The second pathway to K evaluations is again to employ (1.1) but use *symbolic* differentiation. This is probably a more accurate scheme overall, but rather cumbersome to program.

It is a tremendous experimental advantage of Riemann-splitting schemes that the free parameter λ provides great confidence in the numerics: Whether one is using (1.2) for a Z value such as the Madelung constant, or for K values from (1.1), one simply changes λ and expects the *same* result, up to expected precision. It is highly likely that the computational machinery is functioning correctly if just two distinct λ values yield the same result.

Some values calculated via the numerical-differentiation form (1.3) are:

$$K(1, \{2, 0, 0\}) = -0.127470428758587322...,$$

$$K(2, \{2, 2, 0\}) = 0.150324895970907966...,$$

$$K(8, \{4, 0, 0\}) = -1.583586116167586...$$

References.

Crandall, R. E. 1998, Fast evaluation of Epstein zeta functions, manuscript,

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