A Numerical Exploration of Multiple Zeta Values

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1 Introduction

The Riemann-zeta function has held the attention of mathematicians for centuries. It first arose in 1644, when Pietro Mengoli posed to the mathematical community the problem of finding the sum of the squares of the reciprocals of the natural numbers

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = ? \tag{1}$$

A solution was found by then-28 year old Leonard Euler, launching his mathematical career. His answer, whilst ingenious, relied on an assumption which would not be made rigorous until Hadamard's theory of factorisation of entire functions, however numerical confirmation emboldened him to release his results. Let's start with a simple overview of Euler's proof [2]. Consider the function $\sin(\pi x)$, which has roots at $x = 0, \pm 1, \pm 2, \pm 3, \cdots$. Now define $f(x)$ to be

$$f(x) = \frac{\sin(\pi x)}{\pi x} \tag{2}$$

This removes the root at zero (l'Hopital's rule), and we are left with roots at the non-zero integers. Euler made the leap of presuming that we could treat $f(x)$ as if it were a polynomial with these same roots

$$\begin{aligned} f(x) &= (1-x)(1+x)(1-x/2)(1+x/2)\cdots \\ &= (1-x^2)(1-x^2/4)(1-x^2/9)\cdots \end{aligned} \tag{3}$$

By taking a Taylor series, we have an alternative definition for $f(x)$

$$f(x) = \left(\pi x - \frac{(\pi x)^3}{3!} + \frac{(\pi x)^5}{5!}\cdots\right)/(\pi x) \tag{4}$$

In our polynomial representation for $f(x)$, the coefficient of x^2 is

$$-(1 + \frac{1}{4} + \frac{1}{9} + \cdots) \tag{5}$$

By equating coefficients with the Taylor series for $f(x)$, Euler arrived at his famous result

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{6}$$

Euler continued to explore the sum of the reciprocals of the natural numbers raised to some integer power, s, which was later expanded to the complex plane, and has led to the formal definition of the *Riemann zeta function*

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \;\; \Re(s) > 1 \tag{7}$$

2 Multiple Zeta Function

The *multiple zeta function* is an extension of the Riemann-zeta function to multiple parameters

$$\zeta(s_1, \cdots, s_k) = \sum_{n_{s_1} > n_{s_2} > \cdots > n_{s_k}} \frac{1}{n_{s_1}^{s_1} n_{s_2}^{s_2} \cdots n_{s_k}^{s_k}} \tag{8}$$

In this paper we make reference to *multiple zeta values*, which are defined as the real number $\zeta(s_1, \cdots, s_k)$ for some positive integer arguments $s_1, \cdots, s_k$, with $s_1 > 1$ (i.e an output of the multiple zeta function for some integer arguments). A little terminology: the *length* of a multiple zeta value is the integer $k > 0$, which is the number of parameters supplied, and the *weight* of a multiple zeta value is the sum total of its parameters. For example, $\zeta(3, 1, 2)$ has length 3 and weight 6. The multiple zeta function has some very nice properties. One thing to appreciate is that the space of multiple zeta values is closed under multiplication. That is, the product of any two multiple zeta values is a linear combination of multiple zeta values. Consider the simplest possible case, with two multiple zeta values of length 1

$$\zeta(a)\zeta(b) = \zeta(a, b) + \zeta(a + b) + \zeta(b, a) \tag{9}$$

This may be written more explicitly as

$$\sum_{n_a=1}^{\infty} \frac{1}{n_a^a} \sum_{n_b=1}^{\infty} \frac{1}{n_b^b} = \sum_{n_a > 0, n_b > 0} \frac{1}{n_a^a n_b^b} \tag{10}$$

In each term in the resulting sum, n_a and n_b will obey exactly one of the following relations

$$(n_a > n_b), (n_a = n_b), (n_a < n_b) \tag{11}$$

Thus, the resultant sum may be split as follows:

$$\zeta(a)\zeta(b) = \sum_{n_a > n_b} \frac{1}{n_a^a n_b^b} + \sum_{n_a = n_b} \frac{1}{n_a^a n_b^b} + \sum_{n_a < n_b} \frac{1}{n_a^a n_b^b} \tag{12}$$

And our previous claim becomes clear. For the general case of multiple zeta value multiplication, we have

$$\zeta(s_1, \cdots, s_j)\zeta(t_1, \cdots, t_k) = \sum_{\substack{n_{s1} > \cdots > n_{sj}, \\ n_{t1} > \cdots > n_{tk}}} \frac{1}{n_{s1}^{s1} \cdots n_{sj}^{sj} n_{t1}^{t1} \cdots n_{tk}^{tk}} \tag{13}$$

and we may assume $j \leq k$ without loss of generality. We know from the multiple zeta function definition that the n_s and n_t values will retain their respective ordering, however the ordering *between* n_s and n_t values could be shuffled any number of ways. For example, all of the terms in the resulting product which obey the ordering $(n_{s1} > \cdots > n_{sj} > n_{t1} > \cdots > n_{tk})$ will give rise to the multiple zeta value $\zeta(s_1, \cdots, s_j, t_1, \cdots, t_k)$. In brief, the resulting linear combination of multiple zeta values will correspond to all the ways the s parameters can be shuffled through the t parameters.

3 $\mathbb{Q}$-Vector Spaces

Let A_r be defined as the $\mathbb{Q}$-vector space of all multiple zeta values of weight r. In detail, A_r is the vector space spanned by all rational linear combinations of multiple zeta values whose parameters sum to r. For example

$$\begin{aligned} A_2 &= \{\alpha\zeta(2) : \alpha \in \mathbb{Q}\} \\ A_3 &= \{\alpha_1\zeta(3) + \alpha_2\zeta(2,1) : \alpha_1, \alpha_2 \in \mathbb{Q}\} \end{aligned} \tag{14}$$

Notice that when we were multiplying together two multiple zeta values, the weights of the resulting multiple zeta values were the sum of the weights of the operands. In other words, a graded algebra exists over the multiple zeta values

$$A_r A_s \subseteq A_{r+s} \tag{15}$$

This is analogous to spaces spanned by polynomials: a polynomial of degree j multiplied by a polynomial of degree k will yield a polynomial of degree $j + k$.

How many valid multiple zeta values are there in our spanning set for A_r? This turns out to be an integer partitioning problem over r. If we imagine r stars in a line, each star having value 1 towards our total weight, we can partition these into separate parameters by placing bars between them. For example

$$\begin{aligned}\zeta(4) &= \bigstar\bigstar\bigstar\bigstar \\ \zeta(3,1,2) &= \bigstar\bigstar\bigstar|\bigstar|\bigstar\bigstar\end{aligned} \tag{16}$$

There are $r-1$ places we might put a bar, however our requirement that $s_1 > 1$ means there are only $r-2$ valid positions. Since, for each position, we could place a bar or not place a bar, this leads to 2^{r-2} multiple zeta values of weight r.

The next obvious question is: what are the dimensions of the A_r spaces? Hoffman has conjectured that the set of multiple zeta values of weight r, with all parameters either 2 or 3, forms a basis for A_r. Let's call this basis

$$Y_r = \left\{ \zeta(s_1, \cdots, s_k) : \sum_i s_i = r, \text{ each } s_i \in \{2,3\} \right\} \tag{17}$$

This result comes from the study of motivic zeta values, which we will not address here. Zagier has built on this to arrive at the equivalent conjecture that the dimensions of the A_r spaces obey a Fibonnacci-like recurrence

$$d_r = d_{r-2} + d_{r-3}, r \geq 3 \tag{18}$$

where d_r is the dimension of A_r, and with base cases $d_0 = 1, d_1 = 0, d_2 = 1$.

4 $\mathbb{Z}$-Modules

Abandoning the rational numbers, we chose to investigate the $\mathbb{Z}$-modules B_r, where B_r is the integer span of all multiple zeta values of weight r. These modules should satisfy the same conjectured dimensional relationship for our A_r, however it will take more work to find bases. Hoffman's basis vectors will remain linearly independent in B_r, however in general they will no longer be a spanning set. To see why this is, consider $\{5\zeta(2)\}$ which is a basis for A_2, however is not a basis for B_2.

5 Numerical Computation

Numerical calculation of multiple zeta values is complicated by the presence of nested, infinite sums. In order to calculate multiple zeta values rapidly, we employed an algorithm devised by Richard Crandall in his paper *Fast Evaluation of Multiple Zeta Sums* [1]. Crandall makes use of a nested-integral representation of the multiple zeta function. Through several clever manipulations and change of variables, he arrives at a method which treats a multiple zeta value almost as a single sum. After implementing this algorithm, we were able to compute zeta values to over 120 digits of accuracy in a matter of seconds.

To find integer relations among multiple zeta values, and thus construct a basis, we made use of the LLL algorithm - a polynomial-time lattice reduction algorithm invented by Lenstra, Lenstra and Lovasz [4]. In its original form, this algorithm takes as parameters a basis of integer vectors for some lattice in R^n, and outputs a new basis of short, nearly orthogonal vectors. Several problems in mathematics can be converted into lattice reduction problems and thus can be solved with the LLL algorithm. It happens that searching for integer relations amongst real numbers falls into such a category. With the help of a Sage wrapper function, we were able to pass in vectors of multiple zeta values

$$(\zeta_1, \zeta_2, \cdots, \zeta_k) \tag{19}$$

and as output, receive a flag (indicating whether the integer relation search was likely successful) and a vector of integers

$$(\alpha_1, \cdots, \alpha_k) \tag{20}$$

satisfying the following relation:

$$\alpha_1\zeta_1 + \cdots + \alpha_k\zeta_k = 0 \tag{21}$$

Each iteration of this algorithm would find a single integer relation amongst the ζs.

6 Finding a Basis

We know, whilst not generally a basis for B_r, Hoffman's conjectured Y basis will still remain a linearly independent set of vectors within B_r (after all, the integers are a subset of the rational numbers). Our method for constructing bases is as outlined. For each $r \geq 3$, we found the set of multiple zeta values, Z, which span B_r

$$Z = \left\{ \zeta(s_1, \cdots, s_k) : \sum_i s_i = r \right\} \tag{22}$$

Z can be split into two subsets, Y and X, where:

$$\begin{aligned} Y &= \{z \in Z : \text{ each of } z\text{'s parameters } \in \{2,3\}\} \\ X &= Z \backslash Y \end{aligned} \tag{23}$$

We know that each of the elements in X will be expressible in terms of elements in Y, and thus it is possible to construct a matrix M, such that

$$M \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{pmatrix} = \text{ a basis for } B_r \tag{24}$$

To find M, we cycle through each $z \in Z$, and run our integer relation algorithm on the vector

$$(y_1, \cdots, y_d, z_i) \tag{25}$$

which outputs an integer vector of the form

$$(\alpha_1, \cdots, \alpha_{d+1}) \tag{26}$$

This satisfies the relation

$$\alpha_1 y_1 + \cdots + \alpha_d y_d + \alpha_{d+1} z_i = 0 \tag{27}$$

The lowest common denominator of all the α_{d+1} values is calculated, let's call this number L, and each vector $(\alpha_1, \cdots, \alpha_d)$ is scaled up by L/α_{d+1}. These $(\beta_1, \cdots, \beta_d)$ vectors (we've truncated the last entry) now form the rows of a preliminary matrix, H, and are coefficient vectors for each z_i in terms of elements in Y, scaled up by common factor L.

$$H = \begin{pmatrix} L & 0 & \cdots & 0 \\ 0 & L & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & L \\ \beta_{1,1} & \beta_{1,2} & \cdots & \beta_{1,d} \\ \vdots & & \ddots & \\ \beta_{e,1} & \beta_{e,2} & \cdots & \beta_{e,d} \end{pmatrix} \tag{28}$$

H now satisfies the following

$$H \begin{pmatrix} y_1 \\ \vdots \\ y_d \end{pmatrix} = -L \begin{pmatrix} z_1 \\ \vdots \\ z_{d+e} \end{pmatrix} \tag{29}$$

Note that the scaled identity matrix forming the upper dxd portion of H arises from when z_i comes from within the subset Y. H now describes each multiple zeta value $z \in Z$, in terms of elements of Y. It remains for H to be reduced somehow to M (with only d non-zero rows), which will give us our d basis vectors for B_r. There is a slight complication; since we are dealing with finding integer spans of multiple zeta values, we are not allowed to scale up any row (negation is still allowed). This is due to integers not having multiplicative inverses. We can switch rows, and add multiples of one row to another. This type of reduction (for which we utilised a builtin Sage function) produces the *Hermite Normal Form* of a matrix, which is an analogue of row-reduced Echelon form when one is dealing with integers rather than real or rational numbers. Finding M is now just a matter of reducing H to its Hermite Normal Form, then multiplying it by $-1/L$. Finally,

$$M \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{pmatrix} \tag{30}$$

gives our basis vectors. Our program was able to calculate bases for B_r for r up to 9, after which computation time grew infeasible. Further optimisation should find bases for larger r. We have not yet found a pattern amongst the bases.

7 Results

$$
\begin{aligned}
&r = 2\colon \zeta(2)\\
&r = 3\colon \zeta(3)\\
&r = 4\colon \frac{1}{3}\zeta(2,2)\\
&r = 5\colon \frac{1}{5}\zeta(3,2) + \frac{4}{5}\zeta(2,3), \zeta(2,3)\\
&r = 6\colon \zeta(3,3), \frac{1}{9}\zeta(2,2,2)\\
&r = 7\colon \frac{1}{151}\zeta(3,2,2) + \frac{98}{151}\zeta(2,3,2) + \frac{80}{453}\zeta(2,2,3),\\
&\qquad \zeta(2,3,2), \frac{1}{3}\zeta(2,2,3)\\
&r = 8\colon \frac{1}{275}\zeta(3,3,2) + \frac{194}{275}\zeta(3,2,3) + \frac{236}{275}\zeta(2,3,3)+\\
&\qquad \frac{169}{4125}\zeta(2,2,2,2), \zeta(3,2,3), \zeta(2,3,3), \frac{1}{15}\zeta(2,2,2,2)\\
&r = 9\colon \zeta(3,3,3), \frac{1}{43785}\zeta(3,2,2,2)+\\
&\qquad \frac{1566}{4865}\zeta(2,3,2,2) + \frac{4237}{14595}\zeta(2,2,3,2) + \frac{811}{4865}\zeta(2,2,2,3),\\
&\qquad \frac{1}{3}\zeta(2,3,2,2) + \frac{1}{9}\zeta(2,2,2,3), \frac{1}{3}\zeta(2,2,3,2),\\
&\qquad \frac{1}{3}\zeta(2,2,2,3)
\end{aligned}
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8 References

[1] R. Crandall, 1998, *Fast Evaluation of Multiple Zeta Sums*, Mathematics of Computation, vol. 67, no. 223, pp. 1163-1172.

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[4] P. Nguyen, B. Vallee, 1998, *The LLL Algorithm: Survey and Applications*, Springer, pp 265-282.