

Multiple Deligne values: a data mine with empirically tamed denominators

David Broadhurst¹, September 26, 2014

Abstract: Multiple Deligne values (MDVs) are iterated integrals on the interval $x \in [0, 1]$ of the differential forms $A = d \log(x)$, $B = -d \log(1 - x)$ and $D = -d \log(1 - \lambda x)$, where λ is a primitive sixth root of unity. MDVs of weight 11 enter the renormalization of the standard model of particle physics at 7 loops, via a counterterm for the self-coupling of the Higgs boson. A recent evaluation by Erik Panzer exhibited the alarming primes 50909 and 121577 in the *denominators* of rational coefficients that reduce this counterterm to a Lyndon basis suggested by ideas from Pierre Deligne. Oliver Schnetz has studied this problem, using a method from Francis Brown. This gave 2111, 14929, 24137, 50909 and 121577 as factors of the denominator of the coefficient of $\pi^{11}/\sqrt{3}$. Here I construct a basis such that no denominator prime greater than 3 appears in the result. This is achieved by building a datamine of 13,369,520 rational coefficients, with tame denominators, for the reductions of 118,097 MDVs with weights up to 11. Then numerical data for merely 53 primitives enables very fast evaluation of all of these MDVs to 20000 digits. In the course of this Aufbau, six conjectures for MDVs are formulated and stringently tested.

1 Introduction

The ever-burning motive² underlying this paper is the pursuit of a better understanding of the number theory of the renormalization of quantum field theory (QFT). Yet the reader need have no acquaintance with QFT. It suffices to know that, in May 2014, Erik Panzer achieved the remarkable feat of evaluating the contribution of a notoriously difficult Feynman diagram [22] to the beta-function for the quartic self-coupling of the Higgs boson.

This beta-function determines the manner in which the coupling changes with the energy-scale of the process. The diagram in question may be obtained from Figure 1 by removing one of the 4-valent vertices, leaving 4 half-edges that correspond to external particles in the Feynman diagram of Figure 2. The resultant contribution to the beta-function does not depend on the renormalization scheme and is given by a positive number that does not depend on external momenta or internal masses. In the census [24] of Oliver Schnetz this number is referred to as the period $P_{7,11}$, since it comes from the 11th in a list of 7-loop diagrams, by which is meant that the first Betti number of these diagrams is 7.

So much for the important physics; now for the mathematics.

$P_{7,11}$ is indeed a period [21], since it may be written as a 13-dimensional integral of a rational function, over a simplex with the rational boundary conditions that the positive

¹ Department of Physical Sciences, Open University, Milton Keynes MK7 6AA, UK; Institut für Mathematik und Institut für Physik, Humboldt-Universität zu Berlin

²Dr Samuel Johnson (1709-1784) remarked that *actions are visible, though motives are secret*. Chapter 4 of [21] offers an account, by Kontsevich, but by not Zagier, of *motives* in mathematics.

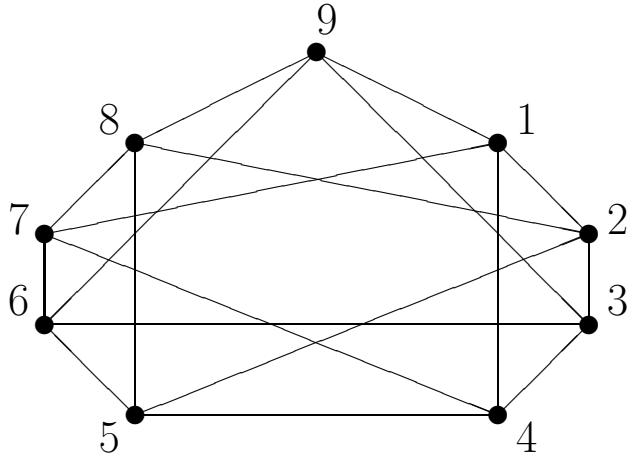


Figure 1: A symmetric graph with 9 indistinguishable 4-valent vertices on a Hamiltonian circuit and chords connecting vertices whose labels are congruent modulo 3.

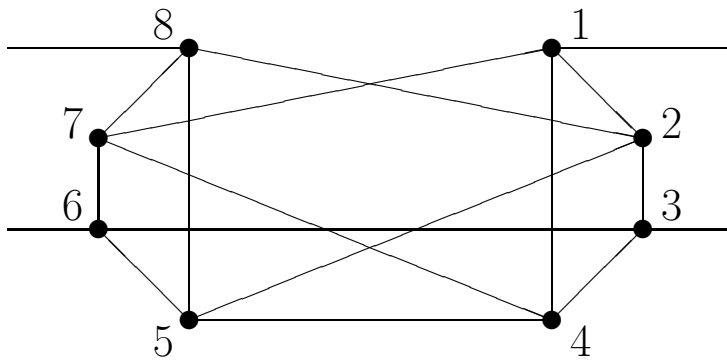


Figure 2: Removal of any vertex from Figure 1 gives a unique 7-loop subdivergence-free Feynman diagram whose counterterm in ϕ^4 theory is given by the MDVs in $P_{7,11}$.

integration variables have a sum no greater than unity, if one uses Feynman parameters. Alternatively, Schwinger parameters give the period as a projective integral. In 1995, using methods radically different from those of Feynman or Schwinger, Dirk Kreimer and I obtained 11 good digits of this period [10]. Since then, my numerical progress has been modest: by 2011, I had obtained 21 good digits of

$$P_{7,11} = 200.357566429275446967\dots \quad (1)$$

For all other 7-loop diagrams in the census, such precision is sufficient [12] to discover an empirical reduction to multiple zeta values (MZVs). Yet no credible fit to MZVs was achieved in the case of $P_{7,11}$.

This was a problem crying out for analytical understanding. Schnetz gave an argument [25], based on counting the zeros of the denominator of Schwinger's integrand in finite fields, that $P_{7,11}$ might evaluate to weight-11 polylogarithms of powers of the sixth root of unity, $\lambda = (1 + i\sqrt{3})/2$. In such a case, there seemed to be little chance that 21 digits of numerical data could be lifted to an exact analytical result. There are $6^{279} = 1,452,729,852$ legal 11-letter words in the 7-letter alphabet for iterated integrals of the differential forms $d\log(x)$ and $-d\log(1 - \lambda^n x)$, with $n = 0, \dots, 5$. The prospects seemed dim that a tiny subset of more than a billion words could be chosen as suitable to fit $P_{7,11}$, at merely 21-digit precision.

Panzer solved this problem, heroically, as part of his larger work on a thesis [22] that implements and extends, by computer algebra, Brown's route map [13, 14] for reducing periods to polylogarithms, when non-linearity of the denominators of integrands may be avoided, in this case with considerable cunning. Moreover, Panzer did this for many other Feynman diagrams. As a notable Christmas present, he sent me in December 2013 almost 1000 good digits of $P_{7,11}$. Yet even this phenomenal precision was insufficient for either of us to obtain an exact result in a basis that might, with good luck, have dimension 144, the 12th Fibonacci number.

Undismayed, Panzer increased the precision of his computations to 5000 digits and, by shrewd use of my generalized parity conjecture [8], obtained an empirical reduction to a basis of size $144/2 = 72$, thereby achieving a result which may be written, with ingenuity, on a single page. But then a remarkable phenomenon was observed. The rational coefficient of $\pi^{11}/\sqrt{3}$ in his result for $P_{7,11}$ was

$$C_{11} = -\frac{964259961464176555529722140887}{2733669078108291387021448260000} \quad (2)$$

whose *denominator* contains 8 primes greater than 11, namely 19, 31, 37, 43, 71, 73, 50909 and 121577. In the normal course of events, this might be attributed to a poor choice of basis. Yet Panzer had chosen what seemed, a priori, to be a rather sensible basis, formed from Lyndon words in much the same manner as I had done for alternating sums [6], with consequent economy in a datamine [2] obtained with Johannes Blümlein and Jos Vermaseren.

To compound the puzzle further, Schnetz used Panzer's 5000 digits of data to obtain an alternative formula [26] that was even more bizarre. His coefficient of $\pi^{11}/\sqrt{3}$ has a

48-digit denominator that contains Panzer's 8 primes, above, and four new ones, namely 47, 2111, 14929 and 24137. Yet Schnetz, like Panzer, had been guided by what appeared to be sensible reasoning.

This paper is devoted to the twin tasks of understanding the origin of such apparently gratuitous primes and of building a datamine that avoids them. It proceeds as follows.

Section 2 defines multiple Deligne values (MDVs), alerts the reader to differing conventions for notating them and gives a useful theorem. Section 3 gives 6 conjectures on MDVs. Three of these are rather general and will be recognized as quite intuitive by a reader familiar with MZVs and alternating sums; the other three are much more specific and concern novel features of MDVs that the author himself did not suspect before undertaking empirical investigation. Section 4 describes some of the large body of recent evidence that supports these 6 conjectures. Section 5 is entitled *the lure of Lyndon* and indicates why the successful use of depth-length Lyndon words for alternating sums is a dubious guide to follow in the case of MDVs. In Section 6, I set about taming denominator primes, by an Aufbau that is relatively straightforward at weights up to 9, becomes more demanding at weight 10 and plain difficult at weight 11. Nonetheless, Section 7 gives a tolerably compact result for the period $P_{7,11}$, in which no coefficient has a denominator divisible by any prime greater than 3. Section 8 explains the structure of a downloadable datamine of 13,369,520 exact data for the 118,097 finite MDVs with weights up to 11, together with high-precision numerical data for merely 53 primitives, thus enabling very fast evaluation of all these MDVs, to 20000-digit precision. Finally, Section 9 offers comments and conclusions.

2 Definitions, notations and theorem

A *multiple Deligne value* is the evaluation, $Z(W)$, as an iterated integral, of a word W formed from letters in the alphabet $\{A, B, D\}$ of the differential forms $A = d \log(x)$, $B = -d \log(1 - x)$ and $D = -d \log(1 - \lambda x)$, where $\lambda = (1 + i\sqrt{3})/2$ is a primitive sixth root of unity. Consider, for example, the word $W = DAB$. Then

$$Z(DAB) \equiv \int_0^1 \frac{\lambda dx_1}{1 - \lambda x_1} \int_0^{x_1} \frac{dx_2}{x_2} \int_0^{x_2} \frac{dx_3}{1 - x_3} \quad (3)$$

where it is important to note that I follow the ordering of [5, 8, 2], with the outermost integration associated to the first letter of the word, in this case D . This is sometimes called the *physics convention*. Some mathematicians prefer to write their words the other way round, with the outermost integration corresponding to the last letter of the word.

If a word neither ends with A nor begins with B , it is a *legal* word, else it is a *bad* word, to which Z can assign no value, since the iterated integral diverges. However it is often useful to manipulate bad words at intermediate stages of a calculation, as will be shown.

The *weight* of $Z(W)$ is the length of the word W , in this case $w = 3$, and the *depth* of $Z(W)$ is the number of letters in W that are not equal to A , in this case $d = 2$. The

significance of depth become clearer when one expands

$$-d \log(1 - \lambda^n x) = \frac{dx}{x} \sum_{k>0} (\lambda^n x)^k \quad (4)$$

for $n = 0, 1$, in the case of MDVs, or more generally for $n = 0, \dots, 5$, in the case of words in the 7-letter alphabet $\{A, B, C, D, \bar{D}, E, \bar{E}\}$, where $C = -d \log(1 + x)$, $E = -d \log(1 - \lambda^2 x)$ and bars denote complex conjugation, which gives $\bar{D} = -d \log(1 - \lambda^5 x)$ and $\bar{E} = -d \log(1 - \lambda^4 x)$.

Every legal word of depth d , in the 7-letter alphabet, has an evaluation as a d -fold nested sum of the form

$$S \left(\begin{matrix} z_1, z_2, \dots, z_d \\ a_1, a_2, \dots, a_d \end{matrix} \right) \equiv \sum_{k_1 > k_2 > \dots > k_d > 0} \prod_{j=1}^d \frac{z_j^{k_j}}{k_j^{a_j}} \quad (5)$$

where $z_j^6 = 1$ and a_j is a positive integer. It is important to note that I follow the convention of [11, 9, 3, 4, 5, 8, 2, 20], with the outermost summation associated to the leftmost arguments, z_1 and a_1 , of the symbol S for the nested sum. Thus, for example,

$$Z(DAB) = S \left(\begin{matrix} \lambda, \bar{\lambda} \\ 1, 2 \end{matrix} \right) \equiv \sum_{m=1}^{\infty} \frac{\lambda^m}{m} \sum_{n=1}^{m-1} \frac{\bar{\lambda}^n}{n^2}. \quad (6)$$

Again I remark that some mathematicians write things the other way round, with the parameters of the outermost summation at the end of their lists. As in the case of the Lilliputian little-endians and the Blefuscan big-endians, nothing is gained by arguing about which convention is preferable. All that matters is that authors carefully inform readers of the conventions adopted, so that results are not mangled by mistranslation.

All iterated integrals are endowed with a *shuffle* algebra

$$Z(U)Z(V) = \sum_{W \in \mathcal{S}(U,V)} Z(W) \quad (7)$$

where $\mathcal{S}(U, V)$ is the set of all words W that result from shuffling the words U and V . Shuffles preserve the order of letters in U and the order of letters in V , but are otherwise unconstrained. Thus, for example,

$$\begin{aligned} Z(AB)Z(CD) &= Z(ABCD) + Z(ACBD) + Z(ACDB) & (8) \\ &+ Z(CABD) + Z(CADB) + Z(CDAB). & (9) \end{aligned}$$

The *full* 7-letter alphabet $\{A, B, C, D, \bar{D}, E, \bar{E}\}$ is also endowed with a *stuffle* algebra, resulting from shuffling the arguments of nested sums, taking account of the extra stuff [5] that results from terms when indices of summation coincide. Thus, for example, the stuffle

$$\begin{aligned} Z(AB)Z(D) &= S \left(\begin{matrix} 1 \\ 2 \end{matrix} \right) S \left(\begin{matrix} \lambda \\ 1 \end{matrix} \right) = S \left(\begin{matrix} 1, \lambda \\ 2, 1 \end{matrix} \right) + S \left(\begin{matrix} \lambda, 1 \\ 1, 2 \end{matrix} \right) + S \left(\begin{matrix} \lambda \\ 3 \end{matrix} \right) & (10) \\ &= Z(ABD) + Z(DAD) + Z(AAD) & (11) \end{aligned}$$

may be combined with the shuffle $Z(AB)Z(D) = Z(ABD) + Z(ADB) + Z(DAB)$ to prove that $Z(DAD) + Z(AAD) = Z(ADB) + Z(DAB)$. One may also combine a stuffle

with a shuffle when one of the MDVs in the product is divergent. For example, by equating the stuffle and shuffle for the product $Z(AD)Z(B)$ one obtains the relation $Z(ADD) + Z(AAD) = Z(ADB) + Z(ABD)$, from which the bad term $Z(BAD)$ has been eliminated.

It is important to appreciate that the restricted alphabet $\{A, B, D\}$ of MDVs is *not* endowed with a full stuffle algebra. In most cases, the stuffle of a pair of MDVs does not give a sum of terms each of which is a MDV, even though the shuffle relation ensures that the total is expressible as a sum of MDVs. For example, one may equate the stuffle and shuffle for the product $Z(AD)Z(D)$ to obtain the relation $Z(ADE) + Z(DAE) + Z(AAE) = 2Z(ADD) + Z(DAD)$, which tells us that the left-hand side is an *honorary* MDV, since it is expressible in terms of MDVs. But that stuffle has told us nothing new about relations between MDVs. This is in marked contrast with the alphabet $\{A, B, C\}$ of alternating sums, which is closed under both shuffles *and* stuffles.

To compensate for its lack of closure under stuffles, the alphabet $\{A, B, D\}$ of MDVs has a beautiful feature: the complex conjugate of a MDV is a MDV, as will be shown after a few notational preliminaries.

Notation: The map Z operates on a word W to produce a value $Z(W)$ that is, in general, a complex number. It is notationally convenient to extend Z linearly, so that it may act on sums of words with, in general, complex coefficients. Thus the action on the empty word is $Z(1) = 1$ and for a sum of words $T = \sum_j c_j W_j$ one obtains $Z(T) = \sum_j c_j Z(W_j)$. I define a conjugate map \overline{Z} such that $\overline{Z}(T)$ is the complex conjugate of $Z(T)$. One may abbreviate n successive occurrences of the same letter in a word by raising that letter to the n th power, so that, for example, A^2BD^3 stands for $AABDDDD$. Finally, I define the *dual*, \widetilde{W} , of a word W , to be the word obtained by writing W backwards and then interchanging A and B , so that, for example, the dual of $W = A^2BD^3$ is $\widetilde{W} = D^3AB^2$.

Lemma 1 [complex conjugation of MDVs]:

For any legal word W in the $\{A, B, D\}$ alphabet, $\overline{Z}(W) = (-1)^{n_D} Z(\widetilde{W})$, where n_D is the number of occurrences of D in W .

Proof: Map $x \rightarrow 1 - x$ in the iterated integral and use the easily verified identity $d \log(1 - \overline{\lambda}(1 - x)) = -d \log(1 - \lambda x)$.

Lemma 2 [powers of D]:

Let $P_n \equiv (\pi/3)^n/n!$. Then $Z(D^n) = i^n P_n$.

Proof: $Z(D) = -\log(1 - \lambda) = i\pi/3$. The shuffle algebra gives $Z(D)Z(D^{n-1}) = nZ(D^n)$. Hence $Z(D^n) = i^n P_n$, by induction.

Theorem 1 [sum rule at greatest depth]:

Consider the sum of words $G_w \equiv \sum_{w>n>0} D^n B D^{w-1-n}$. Then $2\Re Z(G_w/i^w) = (w-1)P_w$.

Proof: Equate the shuffle and stuffle for the product $Z(B)Z(D^{w-1})$, to eliminate the divergent term $Z(BD^{w-1})$. This gives $Z(G_w) - Z(\widetilde{G_w}) = (w-1)Z(D^w)$. From Lemma 1, $Z(\widetilde{G_w}) = (-1)^{w-1} \overline{Z}(G_w)$. From Lemma 2, $Z(D^w) = i^w P_w$. Divide by i^w to prove the stated result.

Example: At $w = 3$, Theorem 1 gives $\Im Z(DBD + DDB) = -\pi^3/162$. This will be

needed in Section 4.

Remarks: Lemma 1 greatly simplifies the problem of reducing MDVs of a given weight w to a basis. In the case of alternating sums [2] the datamine basis at $w = 11$ has dimension 144. For MDVs of weight 11, needed for the Feynman period $P_{7,11}$, I shall construct one basis of dimension 72 for the real parts and another of dimension 72 for the imaginary parts. By halving the size of a basis, one greatly extends the utility of integer-relation searches based on numerical data, using the LLL or PSLQ algorithms that are conveniently provided as options in the `lindep` procedure of `Pari-GP` [23].

3 Conjectures and remarks

Conjecture 1 [Fibonacci enumeration]: Let F_n be the n -th Fibonacci number. Then every \mathbf{Q} -linear combination of MDVs of weight w is reducible to a \mathbf{Q} -linear combination of F_{w+1} basis terms between which there is no \mathbf{Q} -linear relation.

Remarks: A similar enumeration by Fibonacci numbers was conjectured in 1996 for alternating sums [6], constructed from words in the alphabet $\{A, B, C\}$, where $C = -d \log(1 + x)$. Conjecture 1, for the $\{A, B, D\}$ alphabet, was inferred from a helpful letter [18] by Deligne to the author in 1997, as reported in [8].

Conjecture 2 [enumeration of primitives]: The dimension $N_{w,d}$ of the space of primitive MDVs of weight w and depth d is generated by

$$\prod_{w>1} \prod_{d>0} (1 - x^w y^d)^{N_{w,d}} = 1 - \frac{x^2 y}{1 - x}. \quad (12)$$

Remarks: By *primitive*, I mean irreducible to words of lesser depth or their products. The generating function should include $x^2 y$, to record that the Clausen value $\Im Z(AD)$ is primitive. Then I suppose that x stands for $(2\pi i)$ and that all else follows from the combination $(1 - x - x^2 y)$, whose reciprocal, at $y = 1$, generates the Fibonacci numbers of Conjecture 1. In Conjecture 2, I divide by $(1 - x)$, to avoid assigning a depth to $(2\pi i)$. The corresponding generating function for the dimension $E_{w,d}$ of the space of primitives of weight w and depth d in the $\{A, B, C\}$ alphabet was conjectured in [6] to be $(1 - x^2 - xy)/(1 - x^2)$, where xy stands for $Z(C) = -\log(2)$ and x^2 for $(2\pi i)^2$. Closed forms for both dimensions may be obtained by taking a Möbius transformation [6, 2]

$$T(a, b) = \frac{1}{a + b} \sum_{n|a,b} \mu(n) P(a/n, b/n) \quad (13)$$

of the binomial coefficients $P(x, y) \equiv (x + y)! / (x! y!)$ in Pascal's triangle. The sum is over all positive integers n that divide both a and b ; the Möbius function, $\mu(n)$, vanishes if n is divisible by the square of a prime and otherwise is $(-1)^{\omega(n)}$, where $\omega(n)$ is the number of prime divisors of n . Then Conjecture 2 gives $N_{w,d} = T(w - d, d)$, when $w > 2d$. The corresponding conjecture for alternating sums [6, 2] is that $E_{w,d} = T((w - d)/2, d)$, when $w - d$ is even and positive. I shall comment in Section 5 on the relationship of the symmetric array $T(a, b) = T(b, a)$ to the enumeration of Lyndon words.

Conjecture 3 [generalized parity]: The primitives of Conjecture 2 may be taken as real parts of MDVs for which the parities of weight and depth coincide and as imaginary parts of MDVs for which those parities differ.

Remarks: Conjecture 3 is a special case of a wider conjecture of this kind, first made in the context [8] of the 7-letter alphabet formed from $d \log(x)$ and $-d \log(1 - \lambda^n x)$, with $n = 0, \dots, 5$. Here I invoke a generalized parity conjecture only for $n < 2$, where it is far easier to test.

Conjecture 4 [sum rule at odd weight]: At odd weight $w > 1$, there exists a *unique* \mathbf{Z} -linear reducible combination

$$X_w = \sum_{k=1}^{(w-1)/2} C_{w,k} \Im Z(A^{w-2k-1} D A^{2k-1} B), \quad (14)$$

with $C_{w,1} > 0$ and integer coefficients $C_{w,k}$ whose greatest common divisor is unity. Moreover, all of the coefficients are non-zero, X_w is free of products of primitives and hence X_w/π^w reduces to a rational number.

Remarks: Conjecture 4 lies at the heart of the present paper. From Conjecture 2 it follows that there should be $(w-3)/2$ depth-2 primitives, at odd weight $w > 1$, and from Conjecture 3 that one may take these as the imaginary parts of suitable MDVs. Thus there should be at least one combination of the $(w-1)/2$ imaginary parts in X_w that is reducible to π^w and products of depth-1 primitives. Conjecture 4 asserts more than this, namely that there is precisely one such combination, that every coefficient $C_{w,k}$ is non-zero, that products of depth-1 primitives do not occur in the reduction and hence that the result is a rational multiple of π^w . The price of such simplicity is high, since the integers $C_{w,k}$ grow rapidly with w and hence pose a significant obstacle to constructing a sensible set of primitives. By eliminating one of the $(w-1)/2$ imaginary parts in X_w one may end up dividing by a large prime factor of one of the integers $C_{w,k}$. Moreover, this problem may become worse if one chooses depth-2 primitives of odd weight from words in the restricted alphabet $\{A, D\}$, as was done by Panzer [22]. In Section 5, I shall show how this introduced the prime 50909 into denominators at weights 9 and 11 and the prime 121577 into denominators at weight 11.

Conjecture 5 [honorary MZV at even weight]:

At even weight w , the depth-2 real part $\Re Z(A^{w-2} D^2)$ is reducible to MZVs.

Remarks: Conjecture 5 refers to a single depth-2 MDV. So one might suppose, at first sight, that it ought to be fairly easy to prove. In fact, there is a significant obstacle to a proof for all weights: the price that $\Re Z(A^{w-2} D^2)$ pays for being an honorary MZV is that its reduction to MZVs may entail an increase in depth. Thus begins a tussle with the intricacy of the Broadhurst-Kreimer (BK) conjecture for the depth-graded enumeration $D_{w,d}$ of primitive MZVs, via our infamous [17] generating function [11]

$$\prod_{w>2} \prod_{d>0} (1 - x^w y^d)^{D_{w,d}} = 1 - y \frac{x^3}{1-x^2} + y^2 (1-y^2) \frac{x^{12}}{(1-x^4)(1-x^6)} \quad (15)$$

whose final rational function of x also generates the numbers M_w of modular forms of

weight w of the full modular group. The next conjecture circumvents the BK problem of increase of depth, by including an alternating sum for each modular form.

Conjecture 6 [modular forms and alternating sums]: For even weight w , there exists a *unique* \mathbf{Q} -linear combination

$$Y_w = 3^{w-4} \Re Z(A^{w-2} D^2) + \sum_{k=1}^{M_w} Q_{w,k} Z(A^{w-2k-2} C A^{2k} B), \quad (16)$$

with rational coefficients $Q_{w,k}$, such that Y_w reduces to depth-2 MZVs.

Remarks: Conjecture 6 is notable for associating a set of M_w uniquely defined rational numbers to a set of modular forms of the same cardinality. To motivate it, I invoke a phenomenon called *pushdown*, first observed in [6] and later studied in detail using the MZV datamine [2]. Pushdown refers to the fact that some MZVs regarded as irreducible in Don Zagier's MZV alphabet $\{A, B\}$ are reducible to primitives of lesser depth in the alphabet $\{A, B, C\}$ of alternating sums. This occurs at weight 12, where the first modular form appears and a depth-4 MZV has a pushdown to the alternating sum $Z(A^8 C A^2 B) = \sum_{m>n>0} (-1)^{m+n} / (m^9 n^3)$. Then $Q_{12,1} = 2^8$ records this fact rather compactly, since $\Re Z(3^8 A^{10} D^2 + 2^8 A^8 C A^2 B)$ is empirically reducible to depth-2 MZVs. In Section 4, I give all such rational numbers up to weight 36, where 3 modular forms occur.

4 Evidence

The MDV datamine of Section 8 stands as strong witness for Conjectures 1 to 5, which are in perfect accord with the empirical reductions obtained for the 118,097 finite MDVs with weights up to 11. Each of these MDVs was evaluated to 4000-digit precision, using the method in Section 7 of [5], devised with Jonathan Borwein, David Bradley and Petr Lisonek. The datamine of Section 8 now extends the precision to 20000 digits.

This datamine records 13,369,520 non-zero rational coefficients obtained in empirical reductions to putative basis terms whose enumeration accords with the Fibonacci dimensions of Conjecture 1. In no case was it necessary to supply `linddep` with more than 2300 digits, to obtain these results. Thus the probability of a spurious reduction is comfortably less than $1/10^{1700}$. Moreover, `linddep` could discover no credible rational relation between the elements of the putative basis, at 4000-digit precision. I make the obvious, yet sobering, remark that a proof of Conjecture 1 would require, inter alia, a proof that ζ_3^2/ζ_2^3 is not a rational number, which seems to lie beyond the present intellectual capabilities of humankind.

By combining Conjectures 2 and 3 one arrives at a divide-and-conquer formula $F_n = F_n^+ + F_n^-$ that splits the n -th Fibonacci number into $F_n^\pm = (F_n \pm \chi_3(n))/2$, where the character $\chi_3(n) = \chi_3(n+3)$ is 0 if n is divisible by 3 and $\chi(\pm 1) = \pm 1$. Then the conjectured dimensions for real and imaginary parts at weight w are $D_R(w) = F_{w+1}^+$ and $D_I(w) = F_{w+1}^-$, respectively. It follows that the generating function for real parts is

$$G(x) \equiv \frac{1}{1 - (x + x^2)^2} = \sum_{w \geq 0} D_R(w) x^w \quad (17)$$

giving sequence A094686 of the OEIS [27]:

1, 0, 1, 2, 2, 4, 7, 10, 17, 28, 44, 72 ...

with an initial entry $D_R(0) = 1$ recording the empty word. For the imaginary parts, the generating function is

$$H(x) \equiv (x + x^2)G(x) = \sum_{w \geq 0} D_I(w)x^w \quad (18)$$

giving sequence A093040 of the OEIS [27]:

0, 1, 1, 1, 3, 4, 6, 11, 17, 27, 45, 72 ...

with an initial entry $D_I(0) = 0$ recording that the empty word evaluates to a real number, $Z(1)=1$. It is rather satisfying that both sequences are generated so simply using only the quadratic $(x + x^2)$ that reminds us that $\Im Z(D)$ is a rational multiple of π and that $\Im Z(AD)$ is not believed to be a rational multiple of π^2 .

Conjectures 1, 2 and 3 are in accord with motivic reasoning [20, 22], which establishes that $N_{w,d} \leq T(w-d, d)$. It seems to me that it would be a waste of time trying to falsify these conjectures at higher weights, $w > 11$. By contrast, Conjectures 4, 5 and 6 seemed to merit close attention at weights greater than 11.

Conjecture 4 concerns the depth-2 imaginary parts

$$I_{a,b} \equiv \Im Z(A^{b-a-1}DA^{2a-1}B) = \sum_{m>n>0} \frac{\sin(\pi(m-n)/3)}{m^{b-a}n^{2a}} \quad (19)$$

with $b > a > 0$ and odd weight $a + b$. At each odd weight $w > 1$, it asserts, inter alia, that there exists a *unique* vector of non-zero integers, $C_{w,k}$ for $k = 1, \dots, (w-1)/2$, with unit content, such that

$$X_w = \sum_{w>2k>0} C_{w,k}I_{k,w-k} = Q_w P_w \quad (20)$$

where $P_w \equiv (\pi/3)^w/w!$ and Q_w is a rational number. I have checked this at 4000-digit precision, up to weight $w = 11$, using `linddep`, which revealed, at each odd weight, the existence of precisely one combination of imaginary parts that is reducible to products of depth-1 primitives and powers of π . To my considerable initial surprise, `linddep` gave 0 for the coefficients of all products, leaving only P_w . This singular circumstance will be pursued in Section 5.

The datamine uses $I_{a,b}$, with $b > a > 1$ and odd weight $a + b$, and the depth-1 primitives

$$R_{2k+1} \equiv Z(A^{2k}B) = \zeta_{2k+1} = \sum_{n>0} \frac{1}{n^{2k+1}}, \quad (21)$$

$$I_{2k} \equiv \Im Z(A^{2k-1}E) = \text{Cl}_{2k}(2\pi/3) = \frac{\sqrt{3}}{2} \sum_{n>0} \frac{\chi_3(n)}{n^{2k}}, \quad (22)$$

with E used for the Clausen values, since $2^n \Im Z(A^n D) = (2^n + 1) \Im Z(A^n E)$ and the use of D may induce unwanted denominator primes such as $43|(2^7+1)$ and $19|(2^9+1)$, at weights 8 and 10. Similarly, B is preferable to D for the real primitives, since $2^{n+1}3^n \Re Z(A^n D) = (2^n - 1)(3^n - 1)Z(A^n B)$ and thus the choice of D may induce the denominator primes 13, 17, 31, 41 and 61, at weights less than 12.

A basis for reductions of imaginary parts of depth-2 MDVs of odd weight $w > 1$ has, according to Conjectures 2 and 3, dimension $(w - 2)$, comprising $(w - 3)/2$ primitives, $(w - 3)/2$ products of primitives and, finally, π^w . There are $N = 3w - 4$ finite imaginary parts, namely those of the words $A^j D A^k D$, $A^j D A^k B$, $A^j B A^k D$, for $j \geq 0$, $k \geq 0$ and $j + k = w - 2$, with the bad w -letter word $B A^{w-2} D$ omitted at $j = 0$, in the last case. Shuffles of products $Z(A^j D)Z(A^k D)$ and $Z(A^j B)Z(A^k D)$ provide us with $(w - 1)/2 + (w - 2)$ relations, since we should avoid the bad shuffle $Z(B)Z(A^{w-2} D)$. As explained in Section 2, stuffles of $Z(A^j D)Z(A^k D)$ are useless, since they take us out of the $\{A, B, D\}$ alphabet. There are $(w - 1)$ useful stuffles of $Z(A^j B)Z(A^k D)$, for which the case with $j = 0$ is now allowed, by subtracting the corresponding shuffle, to eliminate the bad word. The tally of relations is thus $M = (5w - 7)/2$. For a given odd w , it is then a simple exercise in computer algebra to generate the $M \times N$ matrix for these relations and compute its rank deficiency, which was proven to be $(w - 1)/2$ for all odd $w \leq 31$.

Since this rank deficiency exceeds the conjectured number of primitives by unity, *one of our relations is missing*. That is why the reduction X_w of Conjecture 4 is so significant: it is the kernel, at $d = 2$, of the ineluctable deficiency of depth-restricted algebra for MDVs, which suffer from a stuffle algebra that does not close. The remedy is clear: one should use the good features of MDVs, celebrated in the lemmas and theorem of Section 2.

Example: Set $w = 3$. Then Conjecture 4 requires that $X_3 = I_{1,2} = \Im Z(DAB) = Q_3 P_3$, for some rational Q_3 . This is *impossible* to prove using only shuffles and stuffles of products of depth-1 MDVs. But it becomes trivial to prove when one adds the result obtained in Section 2 from Theorem 1, at depth 3, namely that $\Im Z(DBD + DDB) = -\pi^3/162$. Then Lemma 1 converts this to a result that we were lacking at depth 2, namely $\Im Z(DAD + ADD) = \pi^3/162$, and very simple algebra gives the required rational $Q_3 = \frac{7}{2}$.

Now imagine trying to find the rational number Q_{11} by pure algebra. Since Theorem 1 was needed at $w = 3$, one may reasonably suppose that it is also needed at $w = 11$. But Lemma 1 only lowers the depth by unity, to $d = 10$, and we are seeking a rational number at $d = 2$. So it looks as if we may need to do hefty algebra on the 77,708 weight-11 MDVs with depths $d \leq 10$, using the even larger number of relations between them given by shuffles, stuffles and duality. Such a Herculean task might be achievable, using Jos Vermaseren's programme FORM. More economically, `linddep` returns the empirical result

$$Q_{11} = 841838813449645 = 5 \times 11 \times 809 \times 43627 \times 433673 \quad (23)$$

in the twinkling of an eye. It took a good while to obtain and factorize

$$Q_{31} = \frac{5}{7} \times 432650667045719 \times 101610941211668471750779 \times p_{49} \times p_{81} \quad (24)$$

$$p_{49} = 1052453969156963777695781293476878259787114222411 \quad (25)$$

where p_{81} is the following 81-digit prime:

```
5398660771478298532475166018701166835343\  
25958155228637043335803543859216008062953
```

found by GMP-ECM [28], using the parameters `B1=3000000`, `sigma=2086811470`.

I have tested Conjecture 4 up to $w = 31$ and found it to be flawless. The datamine of Section 8 provides a list of integer coefficients, $C_{w,k}$, and the corresponding rationals, Q_w . The largest prime in the denominators of the rationals Q_w , for odd $w \leq 31$, is merely 13, yet the largest prime in the numerators has 137 digits.

An iterative method, devised by Francis Brown [15], is capable of re-deriving this data. The method is superior to brute-force LLL or PSLQ, since it requires only a single rational number to be determined empirically, at each iteration, the rest of the work being achieved by integer arithmetic alone. After I had made the data up to $w = 31$ available in the MDV datamine, Panzer used Brown's method to show that the coefficients $C_{w,k}$ must satisfy the sum rules

$$\sum_{k=1}^j \binom{2j-1}{2k-1} (C_{w,k} - C_{w,k-j+(w-1)/2}) = \frac{1}{2}(1 - 2^{2j+1-w})(1 - 3^{2j+1-w})C_{w,j} \quad (26)$$

for $j = 1, \dots, (w-3)/2$. After requiring that $C_{w,1} > 0$, I showed that for all odd $w \leq 601$ these sum rules require that $C_{w,k} > 0$ for $k = 1, \dots, (w-1)/2$, except for the case $w = 273$, remarked on by Panzer, where $C_{273,k} < 0$ for $k = 52, \dots, 85$, and the case $w = 585$, where $C_{585,k} < 0$ for $k = 41, \dots, 251$. Hans Bethe might have been amused to see that $273 = 2 \times 137 - 1$, in his satire [1] on Eddington, is not unique, in the present context.

These remarkable findings for imaginary parts at odd weights and depth 2, now encapsulated by Conjecture 4, led me to investigate real parts at even weights and depth 2, with results now encapsulated by Conjectures 5 and 6, which have been tested up to weight $w = 36$, which is the first weight for which there are 3 modular forms believed to be relevant to pushdown. Here my intuition suggested that the rational numbers would be under much better control, since real parts in the $\{A, B, D\}$ alphabet include the MZVs of Zagier's $\{A, B\}$ subalphabet, where bizarre primes with more than 100 digits are not expected at depth 2 and weight $w \leq 36$.

I took as my study a single word, $A^{w-2}D^2$, at each even weight w , since $\Re Z(A^{w-2}D^2)$ was readily observed to be an *honorary* MZV for even $w < 12$, as shown here:

$$\Re Z(D^2) = -\frac{1}{3}\zeta_2 \quad (27)$$

$$\Re Z(A^2D^2) = -\frac{23}{216}\zeta_4 \quad (28)$$

$$\Re Z(A^4D^2) = \frac{209}{972}\zeta_6 - \frac{1}{6}\zeta_3^2 \quad (29)$$

$$\Re Z(A^6D^2) = \frac{799331}{1399680}\zeta_8 - \frac{25}{54}\zeta_5\zeta_3 - \frac{7}{270}\zeta_{5,3} \quad (30)$$

$$\Re Z(A^8D^2) = \frac{31013285}{35271936}\zeta_{10} - \frac{535}{2016}\zeta_5^2 - \frac{637}{1296}\zeta_7\zeta_3 - \frac{205}{18144}\zeta_{7,3} \quad (31)$$

where $\zeta_{a,b} \equiv \sum_{m>n>0} 1/(m^a n^b)$.

Had one stopped at this point, there would have been little point in presenting Conjecture 5 as worthy of attention. Surely such reducibility to MZVs will continue? Indeed it

does, but in a very refined manner, which is consistent with Conjecture 5 but also engages the modular forms and alternating sums of Conjecture 6.

A naive empiricist might have expected reducibility of $\Re Z(A^{10}D^2)$ to the basis $\text{MZV}_{12,2} \equiv \{\zeta_{12}, \zeta_9\zeta_3, \zeta_7\zeta_5, \zeta_{9,3}\}$ that is proven [2] to suffice for the reduction of MZVs of weight 12 and depth 2. As an author of [11], I did not expect this and was hence delighted by the absence such of such a reduction. Rather one needs to adjoin to $\text{MZV}_{12,2}$ an alternating sum, such as $Z(A^8CA^2B) = U_{9,3} \equiv \sum_{m>n>0} (-1)^{m+n}/(m^9n^3)$.

The reason is clear: at $w = 12$ there is a depth-4 MZV that is not reducible to MZVs of lesser depth but is pushed down to $U_{9,3}$ in the $\{A, B, C\}$ alphabet. It makes no sense to adjoin a depth-4 MZV to $\text{MZV}_{12,2}$, without also adjoining its miscellaneous entourage of tedious products of primitives, such as $\zeta_5\zeta_4\zeta_3$ in Equation (26) of [6]. It makes perfect sense to adjoin solely $U_{9,3}$, to ensure reducibility of $\Re Z(A^{10}D^2)$.

At $w = 14$, the BK conjecture [11] asserts that there is no such pushdown, and indeed a basis for $\Re Z(A^{12}D^2)$ is provided by a basis $\text{MZV}_{14,2}$ for MZVs of weight 14 and depth 2:

$$6^{10}\Re Z(A^{12}D^2) = \frac{45336887777}{594}\zeta_{14} - 30203052\zeta_{11}\zeta_3 - \frac{292990340}{11}\zeta_9\zeta_5 \quad (32)$$

$$- \frac{400333213}{33}\zeta_7^2 + \frac{19112030}{33}\zeta_{11,3} - \frac{1938020}{9}\zeta_{9,5}. \quad (33)$$

Thereafter one will, by Conjecture 6, always need to adjoin at least one alternating sum. At $w = 24$ two alternating sums are needed, according to Conjecture 6, as is confirmed by `linddep`. At $w = 36$, three alternating sums are predicted to be needed and are indeed found to be present.

The story up to weight 36 is contained in the following delectable list of rational data:

- [12, [256]]
- [16, [19840]]
- [18, [184000]]
- [20, [1630720]]
- [22, [14728000]]
- [24, [165988480, 10183680]]
- [26, [51270856000/43]]
- [28, [13389295360, 808012800]]
- [30, [1573506088000/13, 96652800000/13]]
- [32, [1085492600192, 65740846080]]
- [34, [30030444404360000/307, 182805638400000/307]]
- [36, [95110629053440, 8048874470400, 410097254400]]

where the first entry in each line is the weight w and thereafter I give the unique vector of rational numbers, $Q_{w,k}$, whose existence was asserted in Conjecture 6.

To each set of modular forms of weight $w \leq 36$, I have thus empirically associated a set of eminently printable rational numbers, with the same cardinality as the modular forms. It seems to me that a derivation of this data by *exact* methods ought to be within the reach of our wide community.

5 The lure of Lyndon

Dare, and the world always yields: or, if it beat you sometimes, dare again, and it will succumb, said Barry Lyndon, the eponymous anti-hero of a novel by William Makepeace Thackeray (1811-1863).

In 1954, Roger Lyndon (not to be confused with Thackeray's rogue) defined a subset of words that has remarkable utility in a wide range of problems, including Lie algebras and shuffle algebras. Suppose that we impose on an alphabet an ordering of letters, saying for example that A comes before B , which comes before C , etc, or in the case that we happen to represent letters by positive integers, that 1 comes before 2, which comes before 3, etc. Then we may define a lexicographic ordering of words in that alphabet, saying, for example, that $ABACA$ comes before BCC , as in a dictionary. Then a Lyndon word is a word W such that for every splitting $W = UV$ we have U coming before V . Thus $ABACA$ is not a Lyndon word, because $ABAC$ does not come before A , and BCC is a Lyndon word, because B comes before CC , and BC comes before C . The present significance of this definition is that every shuffle algebra may be solved by taking the Lyndon words as primitive.

In the case of alternating sums, in the alphabet $\{A, B, C\}$, we have two closed algebras, the shuffles of iterated integrals and the stuffles of nested sums, whose stuff may be ignored, for present purposes. Then Lyndon immediately tells us how to solve one of these, say the shuffles, leaving us to tussle with the stuffles, along with, perhaps, further relations, such as the doubling relations and word transformation explained in [2]. Here, Lyndon cannot tell us what to do, since we have already used him once. Yet he may still guide us, if we happen to have a simple conjecture for the enumeration of primitives that remain after all our relations have been satisfied and are able to spot a Lyndon-type prescription with the same enumeration.

That was precisely the situation in which I found myself in the case of alternating sums, after conjecturing [6] the enumeration $E_{w,d} = T((w-d)/2, d)$, mentioned in Section 2. This coincides with the number of Lyndon words in an alphabet of *odd* integers, with the weight corresponding to the sum of the integers and the depth to the length of the word. Then it was easy to guess a set of primitives.

In the present case of MDVs, there is a comparable situation. There is good reason to trust the enumeration $N_{w,d} = T(w-d, d)$ that follows from Conjecture 2. It is easily shown that this coincides with the number of Lyndon words in an alphabet of integers greater than 1, with the weight corresponding to the sum of the integers and the depth to the length of the word. Combining this observation with the generalized parity conjecture [8], one may write down a list of 53 Lyndon *symbols* that act as placeholders for the primitives with weights up to 11. At depth 1, one may write:

$$I_2, R_3, I_4, R_5, I_6, R_7, I_8, R_9, I_{10}, R_{11}, \quad (34)$$

at depth 2:

$$I_{2,3}, R_{2,4}, I_{2,5}, I_{3,4}, R_{2,6}, R_{3,5}, I_{2,7}, I_{3,6}, I_{4,5}, R_{2,8}, R_{3,7}, R_{4,6}, I_{2,9}, I_{3,8}, I_{4,7}, I_{5,6}, \quad (35)$$

at depth 3:

$$R_{2,2,3}, I_{2,2,4}, I_{2,3,3}, R_{2,2,5}, R_{2,3,4}, R_{2,4,3}, I_{2,2,6}, I_{2,3,5}, I_{2,4,4}, \quad (36)$$

$$I_{2,5,3}, I_{3,3,4}, R_{2,2,7}, R_{2,3,6}, R_{2,4,5}, R_{2,5,4}, R_{2,6,3}, R_{3,3,5}, R_{3,4,4}, \quad (37)$$

at depth 4:

$$I_{2,2,2,3}, R_{2,2,2,4}, R_{2,2,3,3}, I_{2,2,2,5}, I_{2,2,3,4}, I_{2,3,2,4}, I_{2,2,4,3}, I_{2,3,3,3}, \quad (38)$$

and, finally, at depth 5,

$$R_{2,2,2,2,3}. \quad (39)$$

Commitments to precise choices for the depth-1 primitives and the imaginary depth-2 primitives were made in Section 4, with sound reasons given there. The remaining 33 choices will be made in Sections 6 and 8. In the rest of this section, I shall discuss an alluring temptation that has been firmly resisted in this paper.

The temptation is to model a basis for MDVs on the basis that I successfully devised for alternating sums. In the $\{A, B, C\}$ alphabet, I discovered that the primitives may be taken to be words in the subalphabet $\{A, C\}$, where they are hence words of the form $A^{n_1-1}CA^{n_2-1}C \dots A^{n_d-1}C$ at depth d and weight $w = \sum_j n_j$. If one demands that the n_j are *odd* integers and form a vector whose reverse is a Lyndon word, then a viable basis results, as I informed Deligne, Ihara and Zagier, in May 1997 [7], providing what Deligne has described as *une évidence numérique écrasante* [20].

So it seemed natural, both to Panzer and to Schnetz, that a sound basis for MDVs would be achieved by using the words $A^{n_1-1}DA^{n_2-1}D \dots A^{n_d-1}D$ with integers $n_j > 1$ whose reversed vector is a Lyndon word in the alphabet whose letters are the integers *greater than unity* [20]. Then by taking the real parts when the depth and weight have the same parity, and the imaginary parts when those parities differ, one has a perfect fit to the enumerations of Conjectures 1, 2 and 3. I shall refer to this as the *Deligne basis* for MDVs, since in response to my study of the $\{A, B, C\}$ alphabet Pierre wrote: “If $\lambda = \frac{1}{2}(1 + \sqrt{-3})$ (sixth root of 1), one could hope for having a similar story...” as I gratefully recorded in Section 5.4 of [8].

It was by choosing this Deligne basis that Panzer and Schnetz obtained the disturbing primes 50909 and 121577 in the *denominators* of their rational coefficients of reduction.

First, let’s see how 50909 infected the Feynman period. At weight 9 and depth 2,

$$X_9 = 2592I_{1,8} + 2538I_{2,7} + 2607I_{3,6} + 1318I_{4,5} = \frac{1357169441}{5}P_9 \quad (40)$$

is the sole relation between imaginary parts that is not obtainable by trivial algebra restricted to depth 2. Note well that X_9 causes no inconvenience whatsoever to the datamine of Section 8, which is already committed to eliminating $I_{1,8}$, whose coefficient $2592 = 2^53^4$ is quite harmless, as a divisor.

Now suppose that one elects to use the Deligne basis. Consider the imaginary parts $J_{a,b} \equiv \Im Z(A^{b-1}DA^{a-1}D)$, with $b > a > 0$ and odd weight $a + b$. The Deligne basis regards these as primitive when $a > 1$, but not when $a = 1$. It is very easy to transform

the set $\{I_{1,8}, I_{2,7}, I_{3,6}, I_{4,5}\}$ in X_9 to the corresponding set in the J -language. Of course that will introduce products of depth-1 primitives, from which X_9 is notably free, but these are not at issue at present; what we care about here are the integer coefficients in the reducible combination of J 's. So let us abandon equality, pro tempore, and content ourselves with using the symbol \sim to indicate that we are working modulo products and powers of π . Then simple shuffles and stuffles at depth 2 tell us how to record, in J -language, the inescapable fact that X_9 is reducible. Here is the result

$$50909J_{1,8} + 25020J_{2,7} + 10083J_{3,6} + 2538J_{4,5} \sim 0 \quad (41)$$

whence came the infection by the denominator prime 50909 in the work of both Panzer and Schnetz, who had adopted the Deligne basis, in which one has pledged, in advance, to eliminate $J_{1,8}$.

Similarly, at weight 11, the reducibility of X_{11} translates, in their J -language, to

$$6239210063J_{1,10} + 3133054680J_{2,9} + 1337436381J_{3,8} \quad (42)$$

$$+ 443069676J_{4,7} + 87845202J_{5,6} \sim 0 \quad (43)$$

and hence they were, albeit unwittingly, committed to dividing by $6239210063 = 19 \times 37 \times 73 \times 121577$, which circumstance explains the large prime 121577 noted in the abstract. At $w = 13$, the elimination of $J_{1,12}$ produces two large denominator primes: 10137187 and 216364363. Moreover the destructive effect of such denominator primes is cumulative: at weight 11, the denominator of the coefficient of π^{11} of a reduction of the imaginary part of a depth-4 MDV to the Deligne basis will, generically, contain the primes 19, 37, 73, 50909, and 121577. For the imaginary parts of depth-6 MDVs of weight 13, those primes will, in general, be joined by 10137187 and 216364363. In consequence, one must be prepared to encounter huge numerators of the coefficients of reduction to the Deligne basis. This is disastrous when attempting to fit a numerical result using the LLL or PSLQ algorithms, which will require much greater precision than would have been needed had one forsaken the Deligne basis for a more practical one.

In retrospect, it is now clear why Panzer needed to increase his numerical precision from 1000 to 5000 digits before finding a fit to the Feynman period: the Deligne basis is extremely unfriendly to empiricists.

6 Taming the basis

My Aufbau for the basis of the datamine of Section 8 is unashamedly empirical. I was determined to explore *all* of the relations between MDVs up to weight 11, starting at low weight and working my way up, by weight. Moreover, at each weight, I started at low depth and worked my way up, by depth.

There is no more to say here about weights $w < 6$, since the die is already cast for the depth-1 primitives and the imaginary primitives of depth 2. At weights 6 and 7, no harm is done by setting $R_{2,4} = \Re Z(ADA^3D)$ and $R_{2,2,3} = \Re Z(ADADA^2D)$. At weight 8,

the depth-3 choices $I_{2,2,4} = \mathfrak{S}Z(ADADA^3D)$ and $I_{2,3,3} = \mathfrak{S}Z(ADA^2DA^2D)$ are likewise unobjectionable. An attentive reader may have noticed that my powers of A , thus far, were precisely the *reverse* of those for the Deligne basis. Life becomes more interesting at $w = 8$ and $d = 2$, where we meet an irreducible MZV. Here I chose $R_{2,6} = \mathfrak{R}Z(A^5DAD)$ and $R_{3,5} = Z(A^5BAB)$, the latter being a MZV. I remind the reader that the indices of primitives are purely formal: they imply no prior commitment to specific powers of A or to the presence or absence of B .

Weight 9 was a little trickier. There was no objection to $I_{2,2,2,3} = \mathfrak{S}Z(ADADADA^2D)$ but effort was needed to determine that

$$R_{2,2,5} = \mathfrak{R}Z(A^2DA^4D^2), \quad R_{2,3,4} = \mathfrak{R}Z(ADA^2DA^3D), \quad R_{2,4,3} = \mathfrak{R}Z(A^5D^2AD) \quad (44)$$

avoid unwanted denominator primes. Here the strategy was empirical: choose 3 words of weight 9 and depth 3, more or less at random; if `linddep` reveals that a combination of them is reducible, then go back and choose another triple, else take this triple as a part of a *temporary* basis to which all such words of this weight and depth may be reduced; perform those reductions and throw away all products and powers of π ; look for unwanted denominator primes; if some are found remove them, where possible, by studying the determinants of 3×3 matrices relating alternative triples to those of the temporary basis. This may give a *refined* basis at the current depth. But we are still not done. Study reductions of MDVs of the same weight, but greater depth, to the refined basis and determine whether new primes appear. If they do, go back and try a different refinement.

I shall refer to such a strategy as *trial and error*. Conjecture 4 indicates that this is bound to fail, eventually. Then I resort to a method of *modular rectification* illustrated below at weights 10 and 11.

At weight 10, trial and error took a good deal of effort, which was rewarded by the successful choices

$$I_{2,2,6} = \mathfrak{S}Z(A^7D^3), \quad I_{2,3,5} = \mathfrak{S}Z(DBA^7D), \quad I_{2,4,4} = \mathfrak{S}Z(ADA^2DA^4B), \quad (45)$$

$$I_{2,5,3} = \mathfrak{S}Z(A^2DA^2DA^3D), \quad I_{3,3,4} = \mathfrak{S}Z(A^2DA^2DA^3B) \quad (46)$$

at depth 3, where I left the $\{A, D\}$ subalphabet to achieve refinement. At depth 4, the simplistic choices $R_{2,2,2,4} = \mathfrak{R}Z(ADADADA^3D)$ and $R_{2,2,3,3} = \mathfrak{R}Z(ADADA^2DA^2D)$ proved harmless. At depth 2, the choices

$$R_{2,8} = \mathfrak{R}Z(ADA^7D), \quad R_{3,7} = \mathfrak{R}Z(A^5DA^3D), \quad R_{4,6} = Z(A^7BAB) \quad (47)$$

are a good refinement, but then reductions from greater depths produce the denominator prime 43, which I did not succeed in removing by a new refinement. However that is not a problem. I computed the reductions of *all* of the 26,244 finite MDVs of weight 10, multiplied by 43 and then took residues modulo 43. This showed that a *single* transformation

$$R_{2,8} = 43T_{2,8} + 2R_{3,7} - 9R_{4,6} - 5R_3R_7 - 6I_4I_6 + (\pi/3)^{10}/11! \quad (48)$$

removes the unwanted prime 43 at weight 10. So the MDV datamine uses $T_{2,8}$ instead of $R_{2,8}$. Note that, in contrast with trial and error, modular rectification requires one to

retain products and powers of π in the reductions to the unrefined basis. Moreover it is not known in advance whether a single transformation will be effective in removing all the poles at a given prime. When several primes must be removed, a transformation may (but need not necessarily) be required for each.

At weight 11, the choice $I_{2,2,3,4} = \Im Z(A^5 DA^2 D^3)$ was useful. Then trial and error yielded

$$I_{2,2,2,5} = \Im Z(A^5 D^2 ADAD), \quad I_{2,3,2,4} = \Im Z(A^3 DADADA^2 D), \quad (49)$$

$$I_{2,2,4,3} = \Im Z(A^3 DADA^3 D^2), \quad I_{2,3,3,3} = \Im Z(A^2 DA^2 DA^2 DAD) \quad (50)$$

as a successful refinement for depth 4. Thus we are almost done, as far as the Feynman period is concerned, since that does not involve the real parts at weight 11, which are postponed to Section 8.

It remains to address the ineluctable difficulty posed by the success of Conjecture 4, whose faithful witness, X_{11} , at weight 11 is

$$79816752I_{1,10} + 84001536I_{2,9} + 87845202I_{3,8} \quad (51)$$

$$+ 80697891I_{4,7} + 40070327I_{5,6} = 841838813449645P_{11}. \quad (52)$$

Here the problem is less severe than in the Deligne basis, since my commitment to eliminate $I_{1,10}$ introduces only a 4-digit prime, namely $2281 = 79816752/(2^4 3^7)$. As in the case of weight 10, the prime 43 also creeps down from depths $d > 2$.

So now the method is clear: compute the reductions of the imaginary parts of the 78,732 MDVs of weight 11 and determine from the residues of their poles, modulo 43 and modulo 2281, whether two transformations suffice to remove both primes from the datamine. Happily, this modular rectification

$$I_{2,9} = 91(11T_{2,9}) - 898T_{3,8} + 11I_{4,7} - 292P_{11} \quad (53)$$

$$I_{3,8} = 24(11T_{2,9}) + 841T_{3,8} - 190I_{4,7} - 255P_{11} \quad (54)$$

suffices, with a determinant $91 \times 841 + 24 \times 898 = 43 \times 2281$ that neatly solves the problem of 43 and 2281. As a bonus, inclusion of 11 in the multiples of $T_{2,9}$ renders reductions of the imaginary parts of weight-11 MDVs in the $\{A, D\}$ alphabet free of the denominator prime 11, up to depth 4. So now we are ready for the Feynman period.

7 The Feynman period $P_{7,11}$

All imaginary parts of MDVs with weight 11 and depth $d \leq 4$ are reducible to a sub-basis of dimension of 57; the additional 15 terms in the full basis appear only in MDVs with $d > 4$. If one gives 1050 digits of $\sqrt{3}P_{7,11}$ to `linddep` and asks for a reduction to the 57-dimensional sub-basis of the datamine, a valid answer is returned, agreeing with Panzer's 5000-digit result. The MDV datamine then enables one to investigate whether the terms of depth 4 have any distinctive pattern. They do indeed.

In the datamine basis, the depth-4 contribution is a linear combination of $\Im Z(A^5 DA^2 D^3)$ and 6 products terms, *all* of which contain ζ_3 . Then a beautiful thing happens if one uses

the datamine to transform to $\Im Z(A^7 D^4)$. Now one simply obtains the depth-4 term as an integer multiple of $\Im Z(W_{7,4})$ with a word-combination

$$W_{7,4} \equiv A^7 D^4 + \zeta_3 A^5 D^3 + \frac{1}{2} \zeta_3^2 A^3 D^2 + \frac{1}{6} \zeta_3^3 A D \quad (55)$$

having the formal appearance of a Taylor expansion in ζ_3 in which taking a derivative corresponds to removing the sub-word AAD . For $m \geq 2(n-1)$, we may adopt this general definition:

$$W_{m,n} \equiv \sum_{k=0}^{n-1} \frac{\zeta_3^k}{k!} A^{m-2k} D^{n-k}. \quad (56)$$

Then, wonderful to relate, the depth-3 terms involve only $\pi^2 \Im Z(W_{7,2})$ and MZVs multiplied by π , as shown here:

$$\sqrt{3} P_{7,11} = -10080 \Im Z(W_{7,4} + W_{7,2} P_2) + 50400 \zeta_3 \zeta_5 P_3 \quad (57)$$

$$+ \left(35280 \Re Z(W_{8,2}) + \frac{46130}{9} \zeta_3 \zeta_7 + 17640 \zeta_5^2 \right) P_1 \quad (58)$$

$$- 13277952 T_{2,9} - 7799049 T_{3,8} + \frac{6765337}{2} I_{4,7} - \frac{583765}{6} I_{5,6} \quad (59)$$

$$- \frac{121905}{4} \zeta_3 I_8 - 93555 \zeta_5 I_6 - 102060 \zeta_7 I_4 - 141120 \zeta_9 I_2 \quad (60)$$

$$+ \frac{42452687872649}{6} P_{11} \quad (61)$$

where, as usual, $P_n \equiv (\pi/3)^n/n!$.

Remarks: On the first line we see that $W_{7,2} \equiv A^7 D^2 + \zeta_3 A^5 D$ combines with $W_{7,4}$ in the simplest manner imaginable. On the second line, $W_{8,2} \equiv A^8 D^2 + \zeta_3 A^6 D$ gives MZVs, since $\Re Z(A^8 D^2)$ is an honorary MZV of depth 2, in accord with Conjecture 6, and $\Re Z(A^6 D)$ is a rational multiple of ζ_7 . Thanks to the use of the datamine transforms $T_{2,9}$ and $T_{3,8}$ on the third line, no prime greater than 3 appears in any denominator. On the final line we see that the numerator of the coefficient of π^{11} is $42452687872649 = 31 \times 1369441544279$, with 14 digits. Panzer had a 30-digit numerator and Schnetz obtained a 50-digit numerator in the course of investigating a very interesting coaction conjecture for Feynman periods [26].

8 Structure of the MDV datamine

For the real parts at weight 11, I began with the Deligne basis: $R_{2,2,7} = \Re Z(A^6 DADAD)$, $R_{2,3,6} = \Re Z(A^5 DA^2 DAD)$, $R_{2,4,5} = \Re Z(A^4 DA^3 DAD)$, $R_{2,5,4} = \Re Z(A^3 DA^4 DAD)$, $R_{2,6,3} = \Re Z(A^2 DA^5 DAD)$, $R_{3,3,5} = \Re Z(A^4 DA^2 DA^2 D)$, $R_{3,4,4} = \Re Z(A^3 DA^3 DA^2 D)$ and $R_{2,2,2,2,3} = \Re Z(A^2 DADADADAD)$. This is, of course, very inefficient. I found that it introduces the denominator primes 47, 71 and 19766363. By computing the residues of poles at these primes, I found a pair of transformations, from $\{R_{2,6,3}, R_{3,4,4}\}$ to rectified datamine primitives $\{T_{2,6,3}, T_{3,4,4}\}$ that remove those primes from the denominators.

The datamine <http://physics.open.ac.uk/~dbroadhu/cert/MDV.tar.gz> contains 24 files, which have been tarred and zipped for downloading as a single 84-megabyte file. After opening this, a user should consult `readme.txt`, which lists the 24 files.

`MDVdef.txt` defines 53 primitives, to which 5 transformations, recorded in `MDVtra.txt`, are applied, to determine the symbols used in the basis file `MDVbas.txt`, which also uses the symbol `p3` for $\pi/3 = \Im Z(D)$. Rational data for the MDVs are contained in 10 files, organized by weight, and in the case of weight 11 also by depth. Each of the 118,097 lines in these files gives a word and a pair of vectors of rational coefficients. Thus, for example, the entries

```
[[A, B, D, B], [[-9/8, 201/20], [-27/8, 0, 33/4]]]
[[I2^2, 1/24*p3^4], [I4, R3*p3, 1/2*I2*p3^2]]
```

in `MDVw7.txt` and `MDVbas.txt` record the reduction

$$Z(ABDB) = -\frac{9}{8}I_2^2 + \frac{201}{20}\frac{(\pi/3)^4}{4!} - \frac{27i}{8}I_4 + \frac{33i}{4}I_2\frac{(\pi/3)^2}{2!} \quad (62)$$

and one may use evaluations of primitives in `MDVpri.txt` to obtain up to 20000 digits of this MDV. This has been conveniently automated, for unix users of `Pari-GP`, by a utility file `MDVgrep.gp`. Here is a very simple example of its use

```
? \r MDVgrep.gp
? default(realprecision, 25);
? print(grep(ABDB))
-0.01147228319232732872517521 + 0.3132313899574234502633605*I
```

which works by issuing an `extern` command to find the relevant line of rational data. Hence it is not necessary to load the full datamine into memory; only a single megabyte of numerical data for the primitives is needed. Yet that megabyte provides speedy access to about 5 gigabytes of numerical values for all MDVs up to weight 11.

`MDVconj4.txt` has data on Conjecture 4, up to $w = 31$, and `MDVconj6.txt` has data on Conjecture 6, up to $w = 36$. `MDVprime.txt` provides a list of primes sufficient to factorize the large integers in `MDVconj4.txt`, as is done by `MDVfact.gp`, with results in `MDVfact.out`.

`MDVtest.gp` tests the definition file and `MDVfeyn.gp` tests the formula for the Feynman period $P_{7,11}$ against the 20000-digit value stored in `P7_11.txt`. Unix users are advised to run these two tests, to check that the datamine is being correctly accessed on their operating system. Windows users are left high and dry by the inability of their system to respond to the `extern` command that greps the relevant line for a given word.

9 Comments and conclusions

Adapting a remark by Pliny the Elder, I observe *ex QFT semper aliquid novi*. It was a 3-loop radiative correction, to the relation between the Weinberg angle and the masses

of the W and Z bosons of the standard model, that led me to intensive investigation of weight-4 polylogs of the sixth root of unity in [8], which resulted in Conjectures 1, 2 and 3. Now weight-11 polylogs from the restricted alphabet $\{A, B, D\}$ of MDVs have emerged as contributors to the renormalization of QFT at 7 loops. The standard model includes a ϕ^4 term, as the quartic self-coupling of the Higgs boson, for which at 7 loops we now know all the counterterms from subdivergence-free diagrams and hence may be confident that the period $P_{7,11}$ of Figure 2, given in tolerably compact form by expressions (57-61), contributes to the beta-function, in a scheme-independent manner, since the other subdivergence-free 7-loop diagrams evaluate to MZVs [12].

In the course of obtaining a formula for $P_{7,11}$ that is free of any denominator prime greater than 3, I was led to the rather specific Conjectures 4, 5 and 6 and to an Aufbau that provides a datamine of 13,369,520 rational coefficients, free of denominator primes greater than 11, from which one may now speedily obtain 20000 good digits of the real and imaginary parts of all of the 118,097 MDVs with weights up to 11, using a handy utility `MDVgrep.gp` provided with the MDV datamine.

I have formulated all but one of Conjectures 1 to 6 in a form strong enough to make proof within my lifetime improbable. The exception is Conjecture 5, which may be accessible to a method that Claire Glanois has developed to determine classes of alternating sums that yield honorary MZVs.

In conclusion, I offer the following observations.

1. MDVs are radically different from alternating sums in the $\{A, B, C\}$ alphabet, since the $\{A, B, D\}$ alphabet of MDVs is not closed under stuffles.
2. Conjecture 4 asserts the existence of reducible combinations of depth-2 imaginary parts that cannot be reduced by algebra restricted to depths $d \leq 2$.
3. To compensate for the paucity of useful stuffles, MDVs are endowed with the powerful relation of Lemma 1, whereby the complex conjugate of a MDV is, up to a sign, a MDV of different depth, in general.
4. This latter feature permits a divide-and-conquer splitting of the Fibonacci numbers, by the real and imaginary generating functions (17,18), thereby extending the reach of integer-relation searches by the LLL and PSLQ methods.
5. This advantage was negated in the work of Panzer and Schnetz by their adoption of a Deligne basis that generates gratuitously large primes in denominators.
6. Such denominator primes are avoided in the MDV datamine of Section 8, whose construction at weights 10 and 11 took a combination of trial and error with a method of modular rectification, exemplified in Section 6.
7. My simplification in Section 7 of Panzer's result for the counterterm for the Feynman diagram in Figure 2 depended crucially on the new datamine, which revealed a notable Taylor-like expansion (55) at depth 4. This was generalized in (56) to clean up, in similar fashion, the depth-3 contributions in expressions (57-61).

8. In the spirit of Grothendieck, Deligne [19, 20] and Brown [16, 17], it is motivically possible to prove a weakened version of Conjecture 2, obtaining upper bounds for the numbers of primitive MDVs, graded by both weight and depth. Here, one would dearly like to have an explanation of why my simple-minded route to the generating function (12) does *not* work for MZVs of the subalphabet $\{A, B\}$, where the BK conjecture (15) insists on an extra term, which also enumerates modular forms at even weights $w = 12$ and $w > 14$.
9. Conjecture 6 asserts that a single MDV assigns a unique set of rational numbers to a set of modular forms with the same cardinality. This seems to me to be worthy of further investigation.

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References

- [1] G. Beck, H. Bethe, W. Riezler, *Bemerkung zur Quantentheorie der Nullpunktstemperatur*, *Naturwissenschaften* **19** (1931) 39; translation in *Selected Works of Hans A. Bethe*, World Scientific Series in 20th Century Physics, Volume 18 (1997) p. 186, <http://books.google.com/books?id=5baAG1WqgYQC&q=273+perfect> .
- [2] J. Blümlein, D.J. Broadhurst, J.A.M. Vermaseren, *The multiple zeta value data mine*, *Comput. Phys. Commun.* **181** (2010) 582-625, [arXiv:0907.2557].
- [3] J.M. Borwein, D.M. Bradley, D.J. Broadhurst, *Evaluations of k -fold Euler/Zagier sums: a compendium of results for arbitrary k* , *Electron. J. Combin.* **4** (1997) R5, [arXiv:hep-th/9611004].
- [4] J.M. Borwein, D.M. Bradley, D.J. Broadhurst, P. Lisonek, *Combinatorial aspects of multiple zeta values*, *Electron. J. Combin.* **5** (1998) R38, [arXiv:math/9812020].
- [5] J.M. Borwein, D.M. Bradley, D.J. Broadhurst, P. Lisonek, *Special values of multiple polylogarithms*, *Trans. Amer. Math. Soc.* **353** (2001) 907-941, [arXiv:math/9910045].

- [6] D.J. Broadhurst, *On the enumeration of irreducible k -fold Euler sums and their roles in knot theory and field theory*, [arXiv:hep-th/9604128].
- [7] David Broadhurst, *Tests of the enumeration $E_{n,k}$* , letter to Deligne, Ihara, Zagier, et al, May 1997.
- [8] D.J. Broadhurst, *Massive 3-loop Feynman diagrams reducible to SC^* primitives of algebras of the sixth root of unity*, Eur. Phys. J. **C8** (1999) 311-333, [arXiv:hep-th/9803091].
- [9] D.J. Broadhurst, J.A. Gracey, D. Kreimer, *Beyond the triangle and uniqueness relations: non-zeta counterterms at large N from positive knots*, Z. Phys. **C75** (1997) 559-574, [arXiv:hep-th/9607174].
- [10] D.J. Broadhurst, D. Kreimer, *Knots and numbers in ϕ^4 theory to 7 loops and beyond*, Int. J. Mod. Phys. **C6** (1995) 519-524, [arXiv:hep-ph/9504352].
- [11] D.J. Broadhurst, D. Kreimer, *Association of multiple zeta values with positive knots via Feynman diagrams up to 9 loops*, Phys. Lett. **B393** (1997) 403-412, [arXiv:hep-th/9609128].
- [12] David Broadhurst, Oliver Schnetz, *Algebraic geometry informs perturbative quantum field theory*, Proc. Sci. **211** (2014) 078, [arXiv:1409.5570].
- [13] F.C.S. Brown, *The massless higher-loop two-point function*, Commun. Math. Phys. **287** (2009) 925-958, [arXiv:0804.1660].
- [14] F.C.S. Brown, *On the periods of some Feynman integrals*, [arXiv:0910.0114].
- [15] Francis Brown, *On the decomposition of motivic multiple zeta values*, [arXiv:1102.1310].
- [16] Francis Brown, *Mixed Tate motives over \mathbf{Z}* , Ann. Math. **175** (2012) 949-976, [arXiv:1102.1312].
- [17] Francis Brown, *Depth-graded motivic multiple zeta values*, [arXiv:1301.3053].
- [18] Pierre Deligne, *About your "Conjectured enumeration of irreducible Multiple Zeta values..."*, letter to the author, May 1997.
- [19] Pierre Deligne, *Multizêtas, d'après Francis Brown*, Séminaire Bourbaki, Jan. 2012, Exposé 1048; Astérisque **352** (2013) 161-185, <http://www.math.ias.edu/files/deligne/012312MultiZetas.pdf> .
- [20] Pierre Deligne, *Le groupe fondamental de $\mathbf{G}_m - \mu_N$ pour $N = 2, 3, 4, 6$ ou 8* , <http://www.math.ias.edu/files/deligne/121108Fondamental.pdf> .
- [21] M. Kontsevich, D. Zagier, *Periods*, in Mathematics Unlimited, 2001 and Beyond (B. Engquist and W. Schmid, eds.), Springer, Berlin (2001) 771-808, <http://people.mpim-bonn.mpg.de/zagier/files/periods/fulltext.pdf> .

- [22] Erik Panzer, *Feynman integrals via hyperlogarithms*, Proc. Sci. **211** (2014) 049, [arXiv:1407.0074] and thesis recently submitted.
- [23] PARI Group, *PARI/GP version 2.5.0*, Bordeaux, 2014, <http://pari.math.u-bordeaux.fr/> .
- [24] Oliver Schnetz, *Quantum periods: a census of ϕ^4 -transcendentals*, Commun. Number Theory Phys. **4** (2010) 1-48, [arXiv:0801.2856].
- [25] Oliver Schnetz, *Quantum field theory over \mathbf{F}_q* , Electron. J. Combin. **18** (2011) 102, [arXiv:0909.0905].
- [26] Oliver Schnetz, *$P_{7,11}$ identified*, letter to Bloch, Broadhurst, Brown, Kreimer, Panzer, et al, May 2014.
- [27] Neil Sloane, *On-Line Encyclopedia of Integer Sequences*, <http://oeis.org> .
- [28] Paul Zimmermann, Bruce Dodson, *20 years of ECM*, <http://www.loria.fr/~zimmerma/papers/40760525.pdf> .